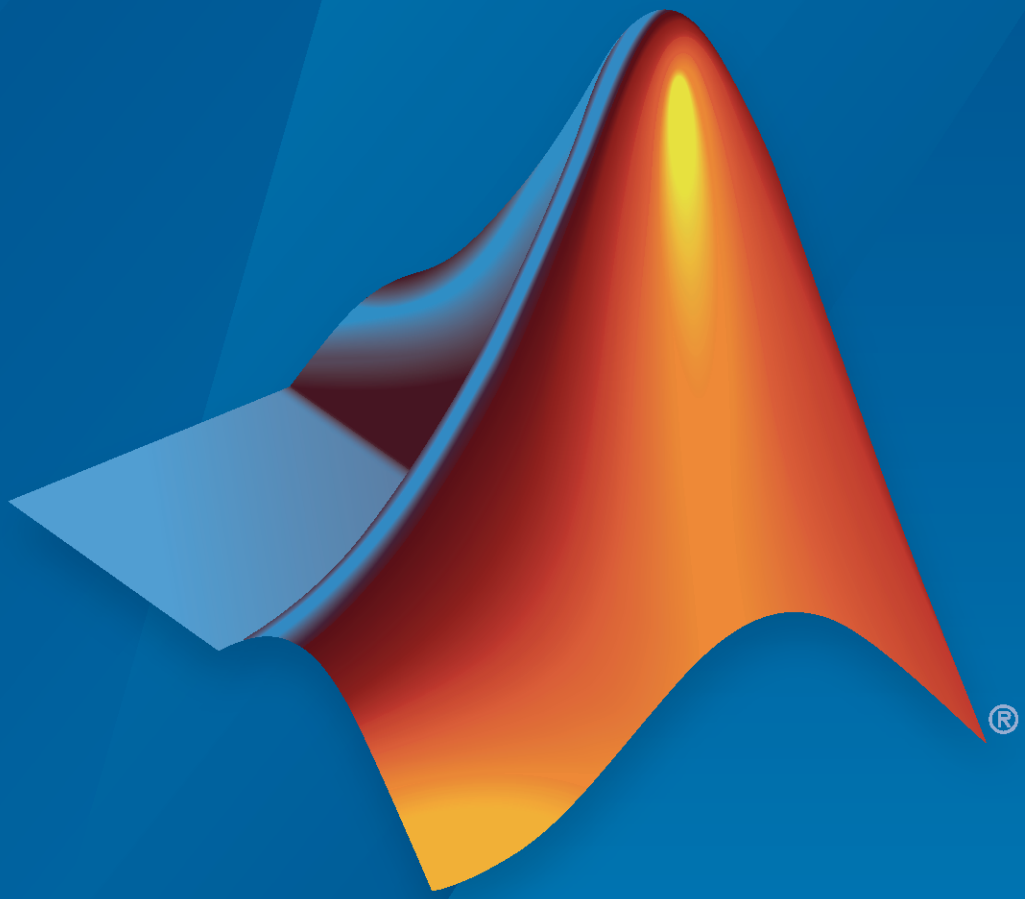
SimBiology®

Reference



MATLAB®

R2023a

MathWorks®

How to Contact MathWorks

Latest news: `www.mathworks.com`

Sales and services: `www.mathworks.com/sales_and_services`

User community: `www.mathworks.com/matlabcentral`

Technical support: `www.mathworks.com/support/contact_us`

Phone: 508-647-7000

The MathWorks, Inc.
1 Apple Hill Drive
Natick, MA 01760-2098

SimBiology® Reference

Revision History

September 2005	Online only	New for Version 1.0 (Release 14SP3+)
March 2006	Online only	Updated for Version 1.0.1 (Release 2006a)
May 2006	Online only	Updated for Version 2.0 (Release 2006a+)
September 2006	Online only	Updated for Version 2.0.1 (Release 2006b)
March 2007	Online only	Rereleased for Version 2.1.1 (Release 2007a)
September 2007	Online only	Rereleased for Version 2.1.2 (Release 2007b)
October 2007	Online only	Updated for Version 2.2 (Release 2007b+)
March 2008	Online only	Updated for Version 2.3 (Release 2008a)
October 2008	Online only	Updated for Version 2.4 (Release 2008b)
March 2009	Online only	Updated for Version 3.0 (Release 2009a)
September 2009	Online only	Updated for Version 3.1 (Release 2009b)
March 2010	Online only	Updated for Version 3.2 (Release 2010a)
September 2010	Online only	Updated for Version 3.3 (Release 2010b)
April 2011	Online only	Updated for Version 3.4 (Release 2011a)
September 2011	Online only	Updated for Version 4.0 (Release 2011b)
March 2012	Online only	Updated for Version 4.1 (Release 2012a)
September 2012	Online only	Updated for Version 4.2 (Release 2012b)
March 2013	Online only	Updated for Version 4.3 (Release 2013a)
September 2013	Online only	Updated for Version 4.3.1 (Release 2013b)
March 2014	Online only	Updated for Version 5.0 (Release 2014a)
October 2014	Online only	Updated for Version 5.1 (Release 2014b)
March 2015	Online only	Updated for Version 5.2 (Release 2015a)
September 2015	Online only	Updated for Version 5.3 (Release 2015b)
March 2016	Online only	Updated for Version 5.4 (Release 2016a)
September 2016	Online only	Updated for Version 5.5 (Release 2016b)
March 2017	Online only	Updated for Version 5.6 (Release 2017a)
September 2017	Online only	Updated for Version 5.7 (Release 2017b)
March 2018	Online only	Updated for Version 5.8 (Release 2018a)
September 2018	Online only	Updated for Version 5.8.1 (Release 2018b)
March 2019	Online only	Updated for Version 5.8.2 (Release 2019a)
September 2019	Online only	Updated for Version 5.9 (Release 2019b)
March 2020	Online only	Updated for Version 5.10 (Release 2020a)
September 2020	Online only	Updated for Version 6.0 (Release 2020b)
March 2021	Online only	Updated for Version 6.1 (Release 2021a)
September 2021	Online only	Updated for Version 6.2 (Release 2021b)
March 2022	Online only	Updated for Version 6.3 (Release 2022a)
September 2022	Online only	Updated for Version 6.4 (Release 2022b)
March 2023	Online only	Updated for Version 6.4.1 (Release 2023a)

Contents

Functions

sbioabstractkineticlaw

Create kinetic law definition

Syntax

```
abstkineticlawObj = sbioabstractkineticlaw('Name')
abstkineticlawObj = sbioabstractkineticlaw('Name','Expression')

abstkineticlawObj = sbioabstractkineticlaw(...'PropertyName',
PropertyValue...)
```

Arguments

Name	Enter a name for the kinetic law definition. `Name` can be a character vector or string. It must be unique in the user-defined kinetic law library. `Name` is referenced by *`kineticlawObj`*.
Expression	The mathematical expression that defines the kinetic law.

Description

`abstkineticlawObj` `= sbioabstractkineticlaw('`*`Name`*`')` creates an abstract kinetic law object, with the name *`Name`* and returns it to *`abstkineticlawObj`*. Use the abstract kinetic law object to specify a *kinetic law definition*.

The *kinetic law definition* provides a mechanism for applying a specific rate law to multiple reactions. It acts as a mapping template for the reaction rate. The kinetic law definition defines a reaction rate expression, which is shown in the property `Expression`, and the species and parameter variables used in the expression. The species variables are defined in the `SpeciesVariables` on page 3-138 property, and the parameter variables are defined in the `ParameterVariables` on page 3-105 property of the abstract kinetic law object.

To use the kinetic law definition, you must add it to the user-defined library with the `sbioaddtolibrary` function. To retrieve the kinetic law definitions from the user-defined library, first create a root object using `sbioroot`, then use the command `get(rootObj.UserDefinedLibrary, 'KineticLaws')`.

`abstkineticlawObj` `= sbioabstractkineticlaw('`*`Name`*`','`*`Expression`*`')` constructs a SimBiology abstract kinetic law object, *`abstkineticlawObj`* with the name `'`*`Name`*`'` and with the expression `'`*`Expression`*`'` and returns it to *`abstkineticlawObj`*.

`abstkineticlawObj` `= sbioabstractkineticlaw(...'`*`PropertyName`*`',` *`PropertyValue`*`...)` defines optional properties. The name-value pairs can be in any format supported by the function `set`.

Additional *`abstkineticlawObj`* properties can be viewed with the `get` command. *`abstkineticlawObj`* properties can be modified with the `set` command.

Note If you use the `sbioabstractkineticlaw` constructor function to create an object containing a reaction rate expression that is not continuous and differentiable, see "Using Events to Address Discontinuities in Rule and Reaction Rate Expressions" before simulating your model.

Method Summary

delete	Delete SimBiology object
display	Display summary of SimBiology object
findUsages	Find out how an `AbstractKineticLaw` object is used
get	Get SimBiology object properties
rename	Rename object and update expressions
set	Set SimBiology object properties

Property Summary

Expression	Expression to determine reaction rate equation or expression of observable object
Name	Specify name of object
Notes	HTML text describing SimBiology object
ParameterVariables	Parameters in kinetic law definition
Parent	Indicate parent object
SpeciesVariables	Species in abstract kinetic law
Tag	Specify label for SimBiology object
Type	Display SimBiology object type
UserData	Specify data to associate with object

Examples

1. Create a kinetic law definition.

```
abstkineticlawObj = sbioabstractkineticlaw('ex_mylaw1', '(k1*s)/(k2+k1+s)');
```

2. Assign the parameter and species variables in the expression.

```
set (abstkineticlawObj, 'SpeciesVariables', {'s'});
set (abstkineticlawObj, 'ParameterVariables', {'k1', 'k2'});
```

3. Add the new kinetic law definition to the user-defined library.

```
sbioaddtolibrary(abstkineticlawObj);
```

`sbioaddtolibrary` adds the kinetic law definition to the user-defined library. You can verify this using `sbiowhos`.

```
sbiowhos -kineticlaw -userdefined

SimBiology Abstract Kinetic Law Array

   Index:    Library:       Name:        Expression:
   1         UserDefined    ex_mylaw1    (k1*s)/(k2+k1+s)
```

4 Use the new kinetic law definition when defining a reaction's kinetic law.

```
modelObj = sbiomodel('cell');
reactionObj = addreaction(modelObj, 'A + B <-> B + C');
kineticlawObj = addkineticlaw(reactionObj, 'ex_mylaw1');
```

Note Remember to specify the `SpeciesVariableNames` and the `ParameterVariableNames` in `kineticlawObj` to fully define the `ReactionRate` of the reaction.

Version History

Introduced in R2006a

See Also

`addkineticlaw` | `addparameter` | `addreaction` | `sbiomodel`

sbioaccelerate

Prepare model object for accelerated simulations

Syntax

```
sbioaccelerate(modelObj)
sbioaccelerate(modelObj,csObj)
sbioaccelerate(modelObj,dvObj)

sbioaccelerate(modelObj,csObj,dvObj)

sbioaccelerate(modelObj,csObj,variantObj,doseObj)
```

Description

`sbioaccelerate(modelObj)` prepares a model object for an accelerated simulation using its active configuration set (configset), any active variants and active doses. A SimBiology model can contain multiple configsets with only one being active at any given time. The active configset contains the settings to use in model preparation for acceleration.

For accelerated simulations, use `sbioaccelerate` before running `sbiosimulate`. You must use the same model and configset for both functions.

Rerun `sbioaccelerate`, before calling `sbiosimulate`, if you modify this model, such as changing reactions or adding events. However, there are exceptions. For details, see “When to Rerun Acceleration”.

Note If you are using a `SimFunction object` for simulations, it automatically accelerates the model on its first function evaluation. Hence it is not necessary to run `sbioaccelerate` beforehand.

Prerequisites To prepare your models for accelerated simulations, install and set up a supported compiler. For details, see “Prerequisites for Accelerating Simulations and Analyses”.

`sbioaccelerate(modelObj,csObj)` uses the specified configset object `csObj` and any active variants and active doses. Any other configsets are ignored. If you set `csObj` to empty `[]`, the function uses the active configset.

`sbioaccelerate(modelObj,dvObj)` uses doses or variants specified by `dvObj` and the active configset. `dvObj` can be one of the following:

- `Variant object`
- `ScheduleDose object`
- `RepeatDose object`
- array of doses or variants

If you set `dvObj` to empty `[]`, the function uses the active configset, active variants, and active doses.

If you specify `dvObj` as variants, the function uses the specified variants and active doses. Any other variants are ignored.

If you specify `dvObj` as doses, the function uses the specified doses and active variants. Any other doses are ignored.

Currently, a particular dose object can only be accelerated with a single model. You cannot use the same dose object for multiple models to be accelerated. You must create a new copy of the dose for each model.

`sbioaccelerate(modelObj,csObj,dvObj)` uses a configset object `csObj` and doses or variants specified by `dvObj`.

If you set `csObj` to `[]`, then the function uses the active configset object.

If you set `dvObj` to `[]`, then the function uses no variants, but uses active doses.

If you set `dvObj` to variants, the function uses the specified variants and active doses. Any other variants are ignored.

If you set `dvObj` to doses, the function uses the specified doses and active variants. Any other doses are ignored.

`sbioaccelerate(modelObj,csObj,variantObj,doseObj)` uses a configset object `csObj`, variant object or variant array specified by `variantObj` and dose object or dose array specified by `doseObj`. Any other configset, doses, and variants are ignored.

If you set `csObj` to `[]`, then the function uses the active configset object.

If you set `variantObj` to `[]`, then the function uses no variants.

If you set `doseObj` to `[]`, then the function uses no doses.

Examples

Prepare a Model for Accelerated Simulation

Load a SimBiology project, named `lotka`, that contains a model `m1`.

```
sbioloadproject('lotka','m1')
```

Prepare the model for accelerated simulation.

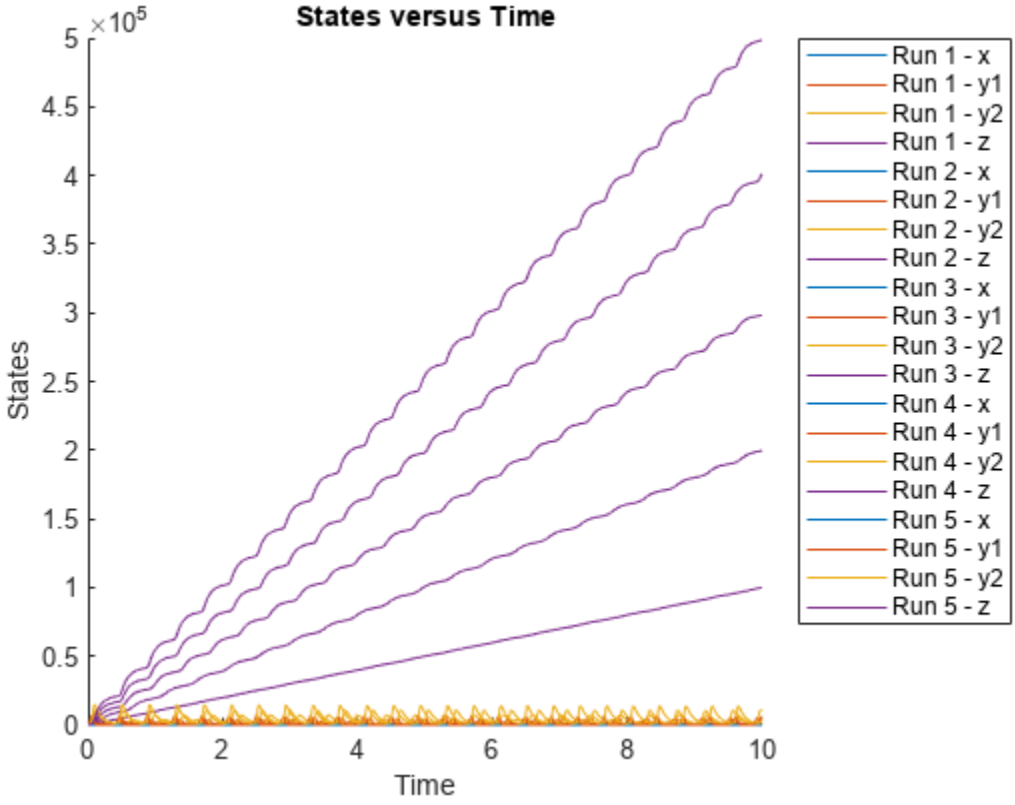
```
sbioaccelerate(m1);
```

Simulate the model using different initial amounts of species `x`.

```
x = sbioselect(m1,'type','species','name','x');
for i=1:5
    x.initialAmount = i;
    sd(i) = sbiosimulate(m1);
end
```

Plot the results.

```
sbioplot(sd);
```



Accelerate Simulation Using a User-Defined Configset Object

Load a sample SimBiology project.

```
sbioloadproject radiodecay.sbproj
```

Add a new configuration set using a different stop time of 15 seconds.

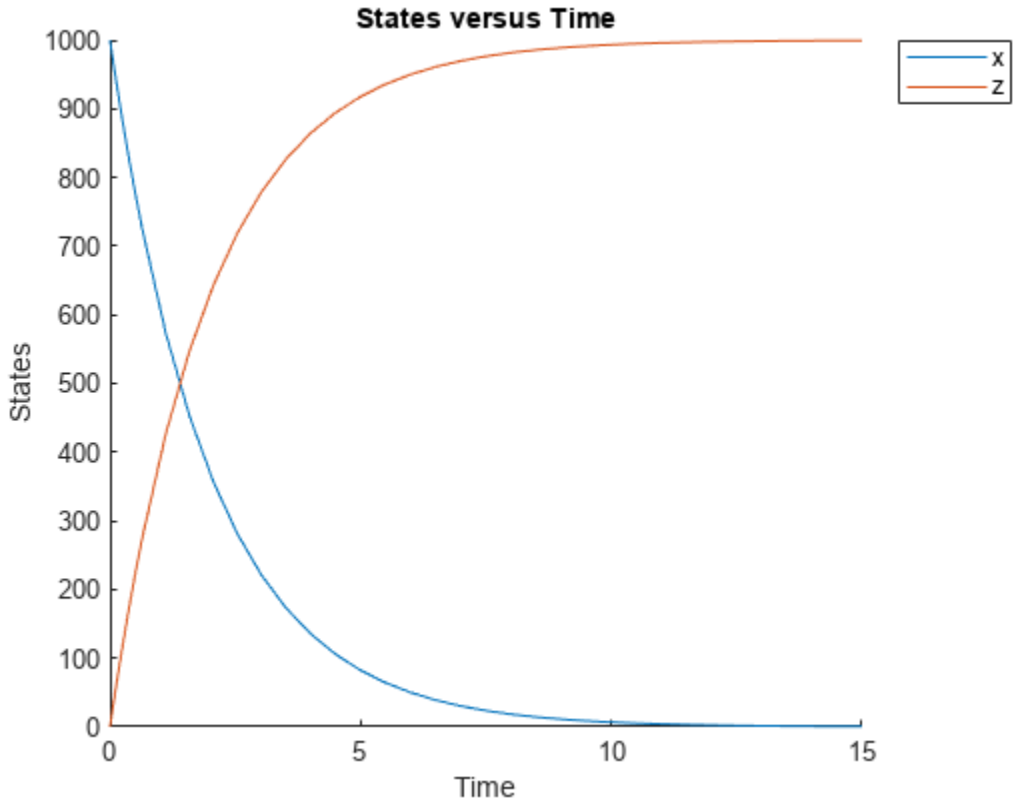
```
csObj = addconfigset(m1,'newStopTimeConfigSet');
csObj.StopTime = 15;
```

Prepare the model for accelerated simulation using the new configset object.

```
sbioaccelerate(m1,csObj);
```

Simulate the model using the same configset object.

```
sim = sbiosimulate(m1,csObj);
sbioplot(sim);
```



Accelerate Simulation With Array of Doses

Load a sample SimBiology project.

```
sbioloadproject radiodecay.sbproj
```

Increase the amount of species x by 100 molecules at 2 and 4 seconds by adding a schedule dose.

```
dObj1 = adddose(m1,'d1','schedule');
dObj1.Amount = 100;
dObj1.AmountUnits = 'molecule';
dObj1.TimeUnits = 'second';
dObj1.Time = 2;
dObj1.TargetName = 'unnamed.x';

dObj2 = adddose(m1,'d2','schedule');
dObj2.Amount = 100;
dObj2.AmountUnits = 'molecule';
dObj2.TimeUnits = 'second';
dObj2.Time = 4;
dObj2.TargetName = 'unnamed.x';
```

Prepare the model for accelerated simulation using the array of both doses.

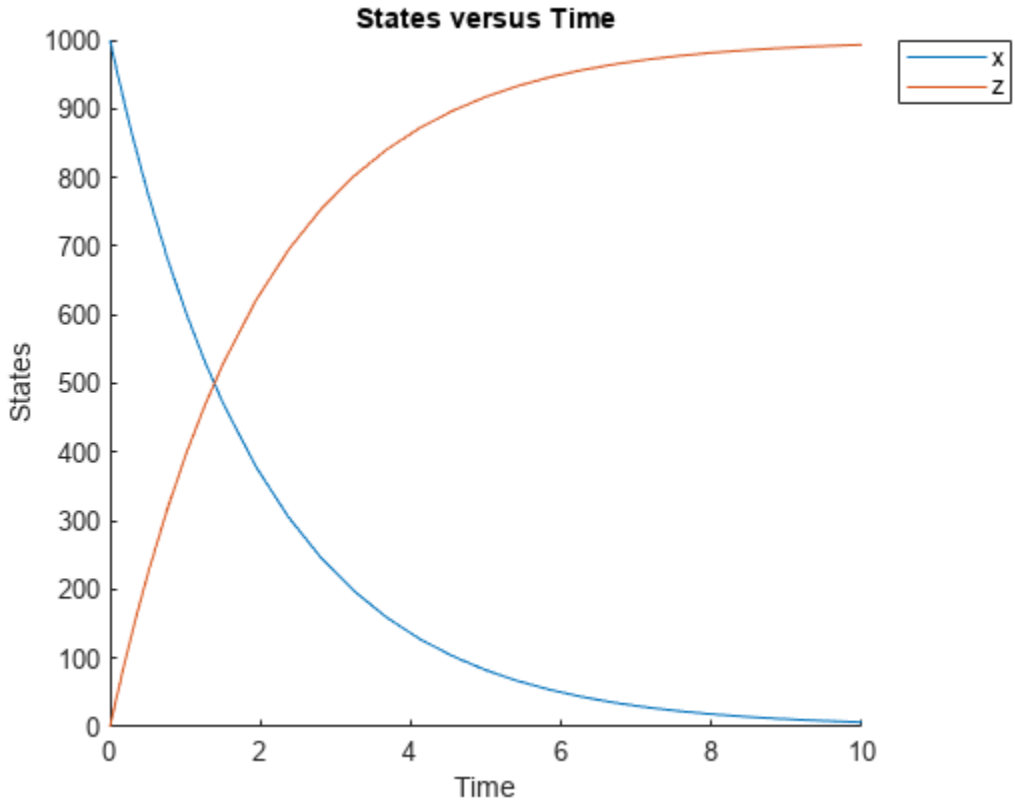
```
sbioaccelerate(m1,[dObj1,dObj2]);
```

Simulate the model using no dose or any subset of the dose array without having to rerun `sbioaccelerate`.

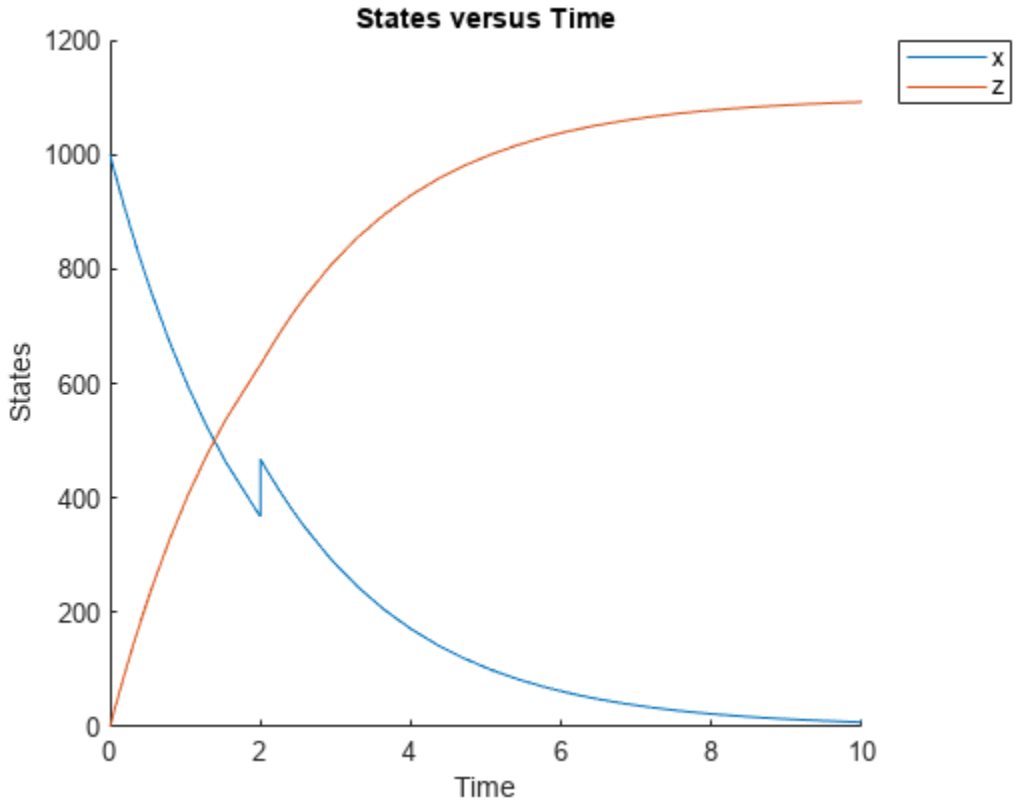
```
sim1 = sbiosimulate(m1);
sim2 = sbiosimulate(m1,dObj1);
sim3 = sbiosimulate(m1,dObj2);
sim4 = sbiosimulate(m1,[dObj1,dObj2]);
```

Plot the results.

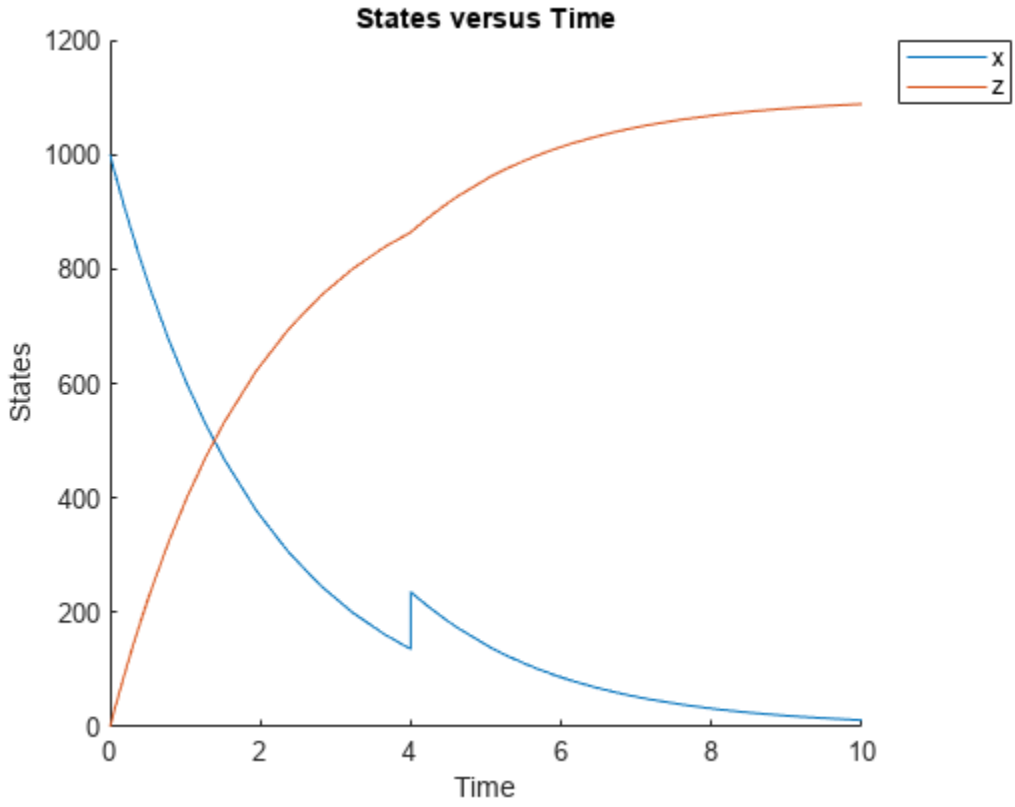
```
sbioplot(sim1);
```



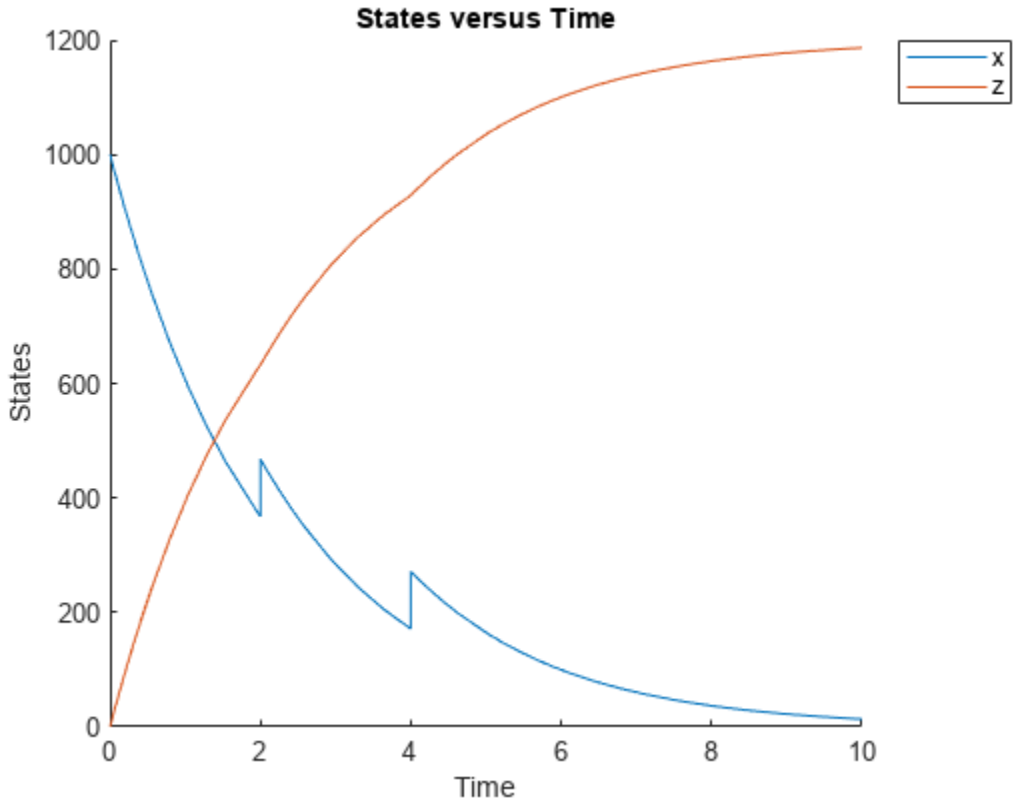

```
sbioplot(sim2);
```




```
sbioplot(sim3);
```




```
sbioplot(sim4);
```



Accelerate Simulation Using Configset and Dose Objects

Load a sample SimBiology project.

```
sbioloadproject radiodecay.sbproj
```

Get the default configuration set from the model.

```
defaultConfigSet = getconfigset(m1,'default');
```

Increase the amount of species x by 100 molecules at 2 seconds by adding a schedule dose.

```
dObj = adddose(m1,'d1','schedule');
dObj.Amount = 100;
dObj.AmountUnits = 'molecule';
dObj.TimeUnits = 'second';
dObj.Time = 2;
dObj.TargetName = 'unnamed.x';
```

Prepare the model for accelerated simulation using the default configset object and added dose object.

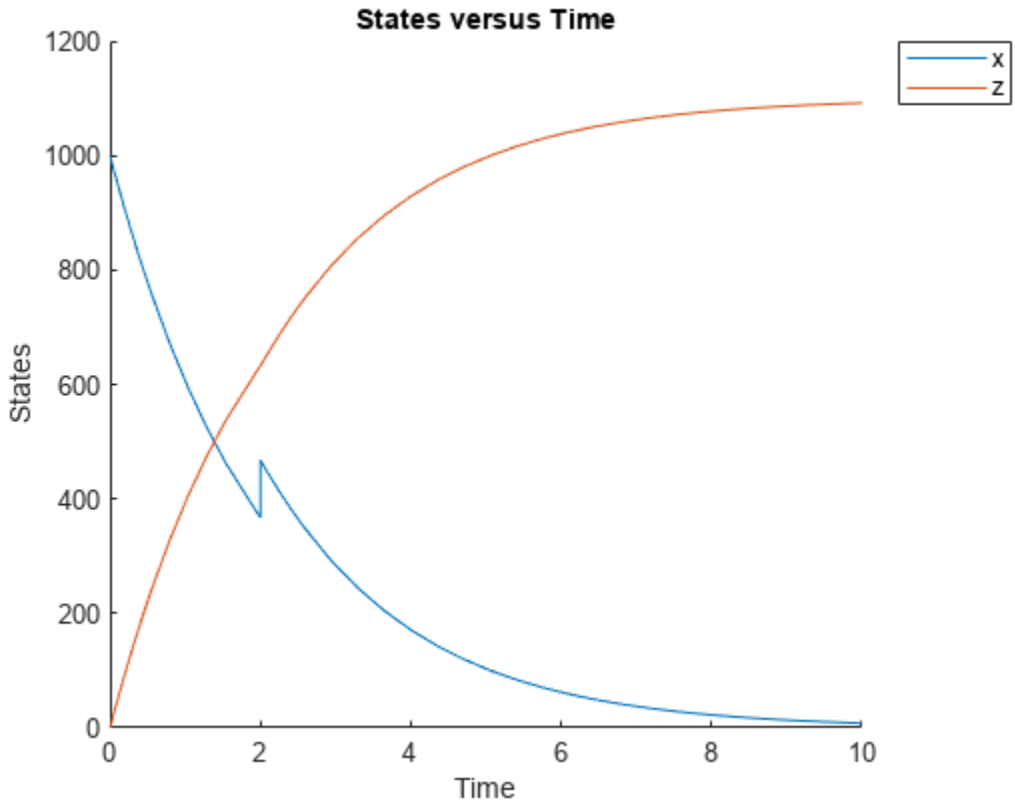
```
sbioaccelerate(m1,defaultConfigSet,dObj);
```

Simulate the model using the same configset and dose objects.

```
sim = sbiosimulate(m1,defaultConfigSet,dObj);
```

Plot the result.

```
sbioplot(sim);
```



Accelerate Simulation Using Configset, Dose, and Variant Objects

Load a sample SimBiology project.

```
sbioloadproject radiodecay.sbproj
```

Add a new configuration set using a different stop time of 15 seconds.

```
csObj = m1.addconfigset('newStopTimeConfigSet');
csObj.StopTime = 15;
```

Increase the amount of species x by 100 molecules at 2 seconds by adding a schedule dose.

```
dObj = adddose(m1,'d1','schedule');
dObj.Amount = 100;
dObj.AmountUnits = 'molecule';
dObj.TimeUnits = 'second';
dObj.Time = 2;
dObj.TargetName = 'unnamed.x';
```

Add a variant of species x using a different initial amount of 500 molecules.

```
vObj = addvariant(m1,'v1');
addcontent(vObj,{'species','x','InitialAmount',500});
```

Prepare the model for accelerated simulation using the configset, dose, and variant objects. In this case, the third argument of `sbioaccelerate` must be the variant object.

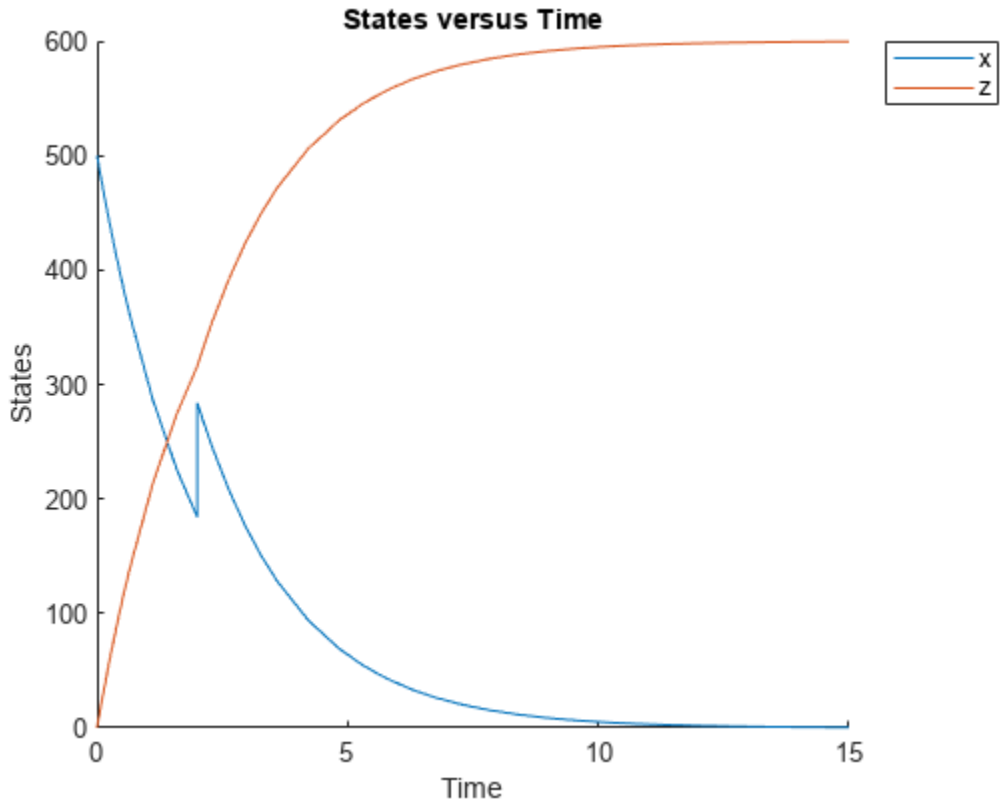
```
sbioaccelerate(m1,csObj,vObj,dObj);
```

Simulate the model using the same configset, variant, and dose objects.

```
sim = sbiosimulate(m1,csObj,vObj,dObj);
```

Plot the result.

```
sbioplot(sim);
```



Input Arguments

`modelObj` — SimBiology model

SimBiology model object

SimBiology model, specified as a SimBiology model object. The model minimally needs one reaction or rate rule to be accelerated for simulations.

`csObj` — Configuration set object
configset object | `[]`

Configuration set object, specified as a `configset object` that stores simulation-specific information. When you specify `csObj` as`[]`, `sbioaccelerate` uses the currently active configset.

`dvObj` — Dose or variant object
dose object or array of dose objects | variant object or array of variant objects | `[]`

Dose or variant object, specified as one of the following: `ScheduleDose object`, `RepeatDose object`, array of dose objects, `Variant object`, or array of variant objects.

- Use `[]` when you want to explicitly exclude any variant objects from the `sbioaccelerate` function.
- When `dvObj` is a dose object, `sbioaccelerate` uses the specified dose object as well as any active variant objects if available. When you accelerate the model using an array of dose objects, you can simulate the model using any subset of the dose objects from the array.
- When `dvObj` is a variant object, `sbioaccelerate` uses the specified variant object as well as any active dose objects if available. You can use any or no variant input arguments when running `sbioaccelerate`.

`variantObj` — Variant object
variant object or array of variant objects | `[]`

Variant object, specified as a `Variant object` or array of variant objects. Use `[]` when you want to explicitly exclude any variant object from `sbioaccelerate`.

`doseObj` — Dose object
dose object or array of dose objects | `[]`

Dose object, specified as a `ScheduleDose object`, `RepeatDose object`, or array of dose objects. A dose object defines additions that are made to species amounts or parameter values. Use `[]` when you want to explicitly exclude any dose objects from `sbioaccelerate`.

Note If you pass in an array of doses to `sbioaccelerate`, you can simulate the model using any subset of doses and do not need to run acceleration again.

Version History

Introduced in R2010a

See Also

`sbiosimulate` | `SimFunction object`

Topics
“Accelerating Model Simulations and Analyses”

sbioaddtolibrary

Add to user-defined library

Syntax

```
sbioaddtolibrary (abstkineticlawObj)
sbioaddtolibrary (unitObj)
sbioaddtolibrary (unitprefixObj)
```

Arguments

abstkineticlawObj	Specify the abstract kinetic law object that holds the kinetic law definition. The `Name` of the kinetic law must be unique in the user-defined kinetic law library. `Name` is referenced by *`kineticlawObj`*. For more information about creating *`kineticlawObj`*, see `sbioabstractkineticlaw`.
unitObj	Specify the user-defined unit to add to the library. For more information about creating *`unitObj`*, see `sbiounit`.
unitprefixObj	Specify the user-defined unit prefix to add to the library. For more information about creating *`unitprefixObj`*, see `sbiounitprefix`.

Description

The function `sbioaddtolibrary` adds kinetic law definitions, units, and unit prefixes to the user-defined library.

`sbioaddtolibrary (`*`abstkineticlawObj`*`)` adds the abstract kinetic law object (`abstkineticlawObj`) to the user-defined library.

`sbioaddtolibrary (`*`unitObj`*`)` adds the user-defined unit (`unitObj`) to the user-defined library.

`sbioaddtolibrary (`*`unitprefixObj`*`)` adds the user-defined unit prefix (`unitprefixObj`) to the user-defined library.

The `sbioaddtolibrary` function adds any kinetic law definition, unit, or unit prefix to the root object's `UserDefinedLibrary` property. These library components become available automatically in future MATLAB® sessions.

Use the kinetic law definitions in the built-in and user-defined library to construct a kinetic law object with the method `addkineticlaw`.

To get a component of the built-in and user-defined libraries, use the commands `get(sbioroot, 'BuiltInLibrary')` and `(get(sbioroot, 'UserDefinedLibrary'))`.

To remove the library component from the user-defined library, use the function `sbioremovefromlibrary`. You cannot remove a kinetic law definition being used by a reaction.

Examples

This example shows how to create a kinetic law definition and add it to the user-defined library.

1. Create a kinetic law definition.

```
abstkineticlawObj = sbioabstractkineticlaw('ex_mylaw1', '(k1*s)/(k2+k1+s)');
```

2. Assign the parameter and species variables in the expression.

```
set (abstkineticlawObj, 'SpeciesVariables', {'s'});
set (abstkineticlawObj, 'ParameterVariables', {'k1', 'k2'});
```

3. Add the new kinetic law definition to the user-defined library.

```
sbioaddtolibrary(abstkineticlawObj);
```

The function adds the kinetic law definition to the user-defined library. You can verify this using `sbiowhos`.

```
sbiowhos -kineticlaw -userdefined

SimBiology Abstract Kinetic Law Array

Index:    Library:       Name:     Expression:
1         UserDefined    mylaw1    (k1*s)/(k2+k1+s)
```

4. Use the new kinetic law definition when defining a reaction's kinetic law.

```
modelObj = sbiomodel('cell');
reactionObj = addreaction(modelObj, 'A + B <-> B + C');
kineticlawObj = addkineticlaw(reactionObj, 'ex_mylaw1');
```

Note Remember to specify the `SpeciesVariableNames` and the `ParameterVariableNames` in `kineticlawObj` to fully define the `ReactionRate` of the reaction.

Version History

Introduced in R2006a

See Also

`addkineticlaw` | `sbioabstractkineticlaw` | `sbioremovefromlibrary` | `sbioroot` | `sbiounit` | `sbiounitprefix`

sbioconsmoiety

Find conserved moieties in SimBiology model

Syntax

```
[G, Sp] = sbioconsmoiety(modelObj)
[G, Sp] = sbioconsmoiety(modelObj, alg)
H = sbioconsmoiety(modelObj, alg,'p')
H = sbioconsmoiety(modelObj, alg,'p', FormatArg)
[SI, SD, L0, NR, ND] = sbioconsmoiety(modelObj,'link')
```

Arguments

G	An `m-by-n` matrix, where `m` is the number of conserved quantities found and `n` is the number of species in the model. Each row of *G* specifies a linear combination of species whose rate of change over time is zero.
Sp	Cell array of species names that labels the columns of *G*. If the species are in multiple compartments, species names are qualified with the compartment name in the form `compartmentName.speciesName`. For example, `nucleus.DNA`, `cytoplasm.mRNA`.
modelObj	Model object to be evaluated for conserved moieties.
alg	Specify algorithm to use during evaluation of conserved moieties. Valid values are `'qr'`, `'rreduce'`, or `'semipos'`.
H	Cell array of character vectors containing the conserved moieties.
`p`	Prints the output according to the format defined by *FormatArg*.
FormatArg	Specifies formatting for the output *H*. *FormatArg* must either be a character vector or string specifying a `C-style` format, or a positive integer specifying the maximum number of digits of precision used.
SI	Cell array containing the names of independent species in the model.
SD	Cell array containing the names of dependent species in the model.
L0	Link matrix relating `SI` and `SD`. The link matrix *L0* satisfies `ND = L0*NR`. For the `'link'` functionality, species with their BoundaryCondition or ConstantAmount properties set to true are treated as having stoichiometry of zero in all reactions. *L0* is a sparse matrix. To convert it to a full matrix, use the `full` function.
NR	Reduced stoichiometry matrices containing one row for each independent species. The concatenated matrix `[NR;ND]` is a row-permuted version of the full stoichiometry matrix of *modelObj*. *NR* is a sparse matrix. To convert it to a full matrix, use the `full` function.

ND	Reduced stoichiometry matrices containing one row for each dependent species. The concatenated matrix [*NR*;*ND*] is a row-permuted version of the full stoichiometry matrix of *modelObj*. *ND* is a sparse matrix. To convert it to a full matrix, use the `full` function.

Description

[*G*, *Sp*] = sbioconsmoiety(*modelObj*) calculates a complete set of linear conservation relations for the species in the SimBiology model object *modelObj*.

`sbioconsmoiety` computes conservation relations by analyzing the structure of the model object's stoichiometry matrix. Thus, `sbioconsmoiety` does not include species that are governed by algebraic or rate rules.

[*G*, *Sp*] = sbioconsmoiety(*modelObj*, *alg*) provides an algorithm specification. For *alg*, specify `'qr'` , `'rreduce'` , or `'semipos'`.

- When you specify `'qr'`, `sbioconsmoiety` uses an algorithm based on QR factorization. From a numerical standpoint, this is the most efficient and reliable approach.
- When you specify `'rreduce'`, `sbioconsmoiety` uses an algorithm based on row reduction, which yields better numbers for smaller models. This is the default.
- When you specify `'semipos'`, `sbioconsmoiety` returns conservation relations in which all the coefficients are greater than or equal to 0, permitting a more transparent interpretation in terms of physical quantities.

For larger models, the QR-based method is recommended. For smaller models, row reduction or the semipositive algorithm may be preferable. For row reduction and QR factorization, the number of conservation relations returned equals the row rank degeneracy of the model object's stoichiometry matrix. The semipositive algorithm may return a different number of relations. Mathematically speaking, this algorithm returns a generating set of vectors for the space of semipositive conservation relations.

H = sbioconsmoiety(*modelObj*, *alg*,'p') returns a cell array of character vectors *H* containing the conserved quantities in *modelObj*.

H = sbioconsmoiety(*modelObj*, *alg*,'p', *FormatArg*) specifies formatting for the output H. *FormatArg* should either be a C-style format string, or a positive integer specifying the maximum number of digits of precision used.

[*SI*, *SD*, *L0*, *NR*, *ND*] = sbioconsmoiety(*modelObj*,'link') uses a QR-based algorithm to compute information relevant to the dimensional reduction, via conservation relations, of the reaction network in *modelObj*.

Examples

Example 1

This example shows conserved moieties in a cycle.

1 Create a model with a cycle. For convenience use arbitrary reaction rates, as this will not affect the result.

```
modelObj = sbiomodel('cycle');
modelObj.addreaction('a -> b','ReactionRate','1');
modelObj.addreaction('b -> c','ReactionRate','b');
modelObj.addreaction('c -> a','ReactionRate','2*c');
```

2 Look for conserved moieties.

```
 [g sp] = sbioconsmoiety(modelObj)

g =

     1     1     1


sp =

    'a'
    'b'
    'c'
```

Example 2

Explore semipositive conservation relations in the `oscillator` model.

```
modelObj = sbmlimport('oscillator');
 sbioconsmoiety(modelObj,'semipos','p')

 ans =

    'pol + pol_OpA + pol_OpB + pol_OpC'
    'OpB + pol_OpB + pA_OpB1 + pA_OpB_pA + pA_OpB2'
    'OpA + pol_OpA + pC_OpA1 + pC_OpA2 + pC_OpA_pC'
    'OpC + pol_OpC + pB_OpC1 + pB_OpC2 + pB_OpC_pB'
```

Version History

Introduced in R2006a

See Also

`getstoichmatrix`

Topics

“Conserved Moiety Determination”

sbioconvertunits

Convert unit and unit value to new unit

Syntax

`sbioconvertunits(`*`Obj`*`, '`*`unit`*`')`

Description

`sbioconvertunits(`*`Obj`*`, '`*`unit`*`')` converts the current *`Units` property on SimBiology object, *`Obj`* to the unit, *`unit`*. This function configures the *`Units` property to *`unit`* and updates the corresponding value property. For example, `sbioconverunits` on a `speciesObj` updates the `InitialAmount` property value and the `InitialAmountUnits` property value.

`Obj` can be an array of SimBiology objects. *`Obj`* must be a SimBiology object that contains a unit property. The SimBiology objects that contain a unit property are compartment, parameter, and species objects. For example, if *`Obj`* is a species object with `InitialAmount` configured to `1` and `InitialAmountUnits` configured to `mole`, after the call to `sbioconvertunits` with *`unit`* specified as `molecule`, `speciesObj` `InitialAmount` is `6.0221e23` and `InitialAmountUnits` is `molecule`.

Examples

Convert the units of the initial amount of glucose from `molecule` to `mole`.

1 Create the species `'glucose'` and assign an initial amount of `23 molecule`.

At the command prompt, type:

```
modelObj = sbiomodel('cell');
compObj = addcompartment(modelObj, 'C');
speciesObj = addspecies (compObj, 'glucose', 23, 'InitialAmountUnits', 'molecule')


SimBiology Species Array

   Index:    Compartment:    Name:      InitialAmount:    InitialAmountUnits:
   1         C               glucose    23                molecule
```

2 Convert the `InitialAmountUnits` of glucose from `molecule` to `mole`.

```
sbioconvertunits (speciesObj, 'mole')
```

3 Verify the conversion of units and `InitialAmount` value.

Units are converted from molecule to mole.

```
get (speciesObj, 'InitialAmountUnits')


ans =

mole
```

The `InitialAmount` value is changed.

```
get (speciesObj, 'InitialAmount')

ans =

  3.8192e-023
```

Version History

Introduced in R2006a

See Also

sbioshowunits

Topics

sbioshowunits

sbiocopylibrary

Copy library to disk

Syntax

```
sbiocopylibrary ('kineticlaw','LibraryFileName')
sbiocopylibrary ('unit','LibraryFileName')
```

Description

`sbiocopylibrary ('kineticlaw','LibraryFileName')` copies all user-defined kinetic law definitions to the file `LibraryFileName.sbklib` and places the copied file in the current directory.

`sbiocopylibrary ('unit','LibraryFileName')` copies all user-defined units and unit prefixes to the file `LibraryFileName.sbulib`.

To get the kinetic law definitions that are in the built-in or user-defined libraries, first create a root object using `sbioroot`, then use the commands `get(rootObj.BuiltInLibrary, 'KineticLaws')` or `get(rootObj.UserDefinedLibrary, 'KineticLaws')`.

To add a kinetic law definition to the user-defined library, use `sbioaddtolibrary`.

To add a unit to the user-defined library, use `sbiounit` followed by `sbioaddtolibrary`. To add a unit prefix to the user-defined library, use `sbiounitprefix` followed by `sbioaddtolibrary`.

Examples

Create a kinetic law definition, add it to the user-defined library, and then copy the user-defined kinetic law library to a `.sbklib` file.

1. Create a kinetic law definition.

   ```
   abstkineticlawObj = sbioabstractkineticlaw('mylaw1', '(k1*s)/(k2+k1+s)');
   ```

2. Add the new a kinetic law definition to the user-defined library.

   ```
   sbioaddtolibrary(abstkineticlawObj);
   ```

   `sbioaddtolibrary` adds the kinetic law definition to the user-defined library. You can verify this using `sbiowhos`.

   ```
   sbiowhos -kineticlaw -userdefined

   SimBiology Abstract Kinetic Law Array

   Index:    Library:       Name:        Expression:
     1       UserDefined    mylaw1    (k1*s)/(k2+k1+s)
   ```

3. Copy the user-defined kinetic law library.

   ```
   sbiocopylibrary ('kineticlaw','myLibFile')
   ```

4. Verify with `sbiowhos`.

```
sbiowhos -kineticlaw myLibFile
```

Version History

Introduced in R2006a

See Also

`sbioaddtolibrary` | `sbioabstractkineticlaw` | `sbioremovefromlibrary` | `sbiounit` | `sbiounitprefix`

sbiodose

Construct dose object

Syntax

```
dose = sbiodose(DoseName)
dose = sbiodose(DoseName,DoseType)
dose = sbiodose(DoseName,Name,Value)
```

Description

`dose = sbiodose(DoseName)` creates a `RepeatDose object` and sets its Name property to `DoseName`.

`dose = sbiodose(DoseName,DoseType)` creates either a `RepeatDose object` or `ScheduleDose object` based on `DoseType`.

`dose = sbiodose(DoseName,Name,Value)` uses name-value pair arguments to define the properties of the dose object. You can enter the name-value pairs in the same format supported by the function `set`. Use the `get` function to view all the properties of the object.

Examples

Increase Drug Concentration in a One-Compartment Model via First-Order Dosing

This example shows how to set up a dosing regimen that follows the first-order absorption kinetics.

Background

Suppose you have a one-compartment model with a species named `drug` that represents the total amount of drug in the body. The drug is added to the body via the first-order dosing represented by the reaction `dose -> drug`, with the absorption rate constant `ka`. It is removed from the body via the first-order elimination represented by the reaction `drug -> null`, with the elimination rate constant `ke`. This example shows how to set up such a one-compartment model, the first-order absorption and elimination.

Create a One-Compartment Model

Create a SimBiology model named `onecomp`.

```
m1 = sbiomodel('onecomp');
```

Define the drug elimination by adding a reaction `drug -> null` to the model. The `drug` species represents the total amount of drug in the compartment.

```
r1 = addreaction(m1,'drug -> null');
```

Note that a compartment and the species `drug` are automatically created, and `drug` is added to the compartment. The `null` species is a reserved species that acts as a sink in this reaction.

Add a mass action kinetic law to the reaction. This kinetic law defines the drug elimination to follow the first-order kinetics.

```
k1 = addkineticlaw(r1,'MassAction');
```

Define the elimination rate parameter `ke` and add it to the kinetic law.

```
p1 = addparameter(k1,'ke','Value',1.0,'ValueUnits','1/hour');
```

Specify the rate parameter `ke` as the forward rate parameter of the reaction by setting the `ParameterVariableNames` property of kinetic law object `k2`. This allows SimBiology to determine the reaction rate for `drug -> null` reaction.

```
k1.ParameterVariableNames = 'ke';
```

Set Up the First-Order Dosing

Add a reaction that represents the drug absorption using the second species `dose`. It represents an intermediate species that will be dosed directly and is required to set up the first-order absorption kinetics.

```
r2 = addreaction(m1,'dose -> drug');
```

Add a mass action kinetic law to the reaction. This kinetic law defines the drug absorption to follow the first-order kinetics.

```
k2 = addkineticlaw(r2,'MassAction');
```

Define the absorption rate parameter `ka` and add it to the kinetic law.

```
p2 = addparameter(k2,'ka','Value',0.1,'ValueUnits','1/hour');
```

Specify the rate parameter `ka` as the forward rate parameter of the reaction by setting the `ParameterVariableNames` property of kinetic law object `k1`. This allows SimBiology to determine the reaction rate for `dose -> drug` reaction.

```
k2.ParameterVariableNames = 'ka';
```

Suppose you want to increase the drug concentration in the system by administering a series of doses: 250 mg three times a day (t.i.d) for two days. Specify the amount of the dose (`Amount`), the time interval between each dose (`Interval`), and the total number of doses (`RepeatCount`). You also need to set the `Active` property of the dose object to `true` so that the dose will be applied to the model during simulation. `RepeatCount` was set to 5, instead of 6 since it represents the number of doses *after* the first dose at the default dose start time (`d1.StartTime` = 0).

```
d1 = sbiodose('d1','repeat');
d1.Amount = 250;
d1.AmountUnits = 'milligram';
d1.Interval = 8;
d1.TimeUnits = 'hour';
d1.RepeatCount = 5;
d1.Active = true;
```

Specify the target species of the dose object. The target must be the `dose` species, not the `drug` species, so that the drug absorption follows the first-order kinetics.

```
d1.TargetName = 'dose';
```

Simulate the Model

Change the simulation stop time to 48 hours to match the dosing schedule.

```
cs = getconfigset(m1);
cs.StopTime = 48;
cs.TimeUnits = 'hour';
```

In addition, do not log the dose species data as you are mainly interested in monitoring the drug species which is the drug concentration in the system. This makes visualizing the species in a plot more convenient. To accomplish this, set the `StatesToLog` property to include the species `drug` only.

```
cs.RuntimeOptions.StatesToLog = {'drug'};
```

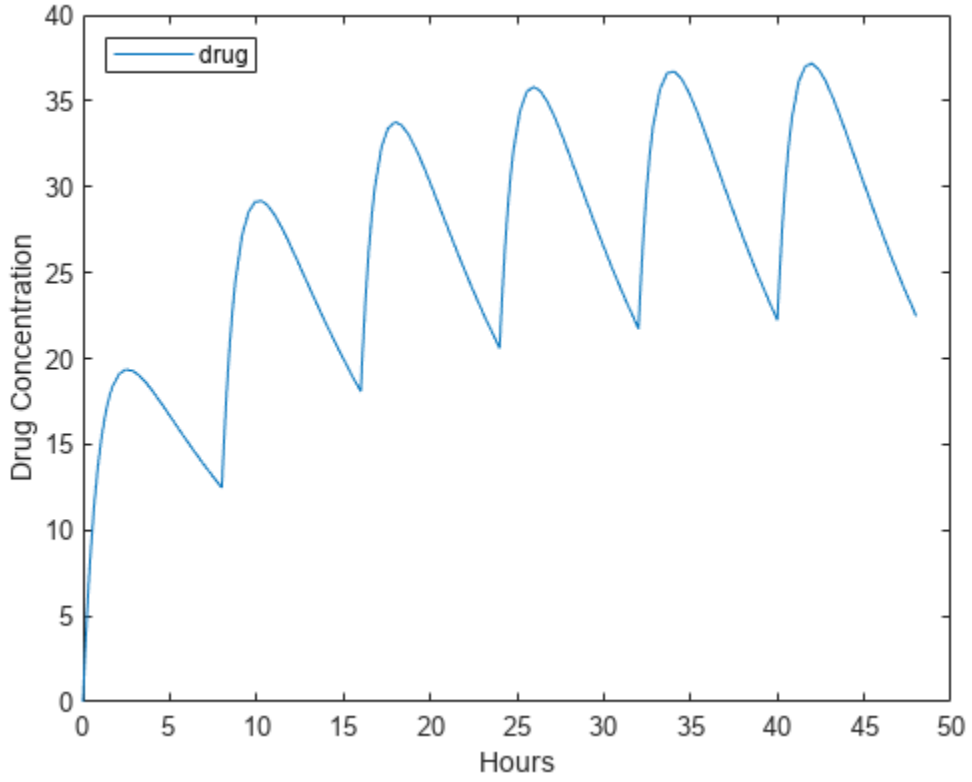
Simulate the model using the dosing schedule defined by the |d1 |dose object.

```
[t,sd,species] = sbiosimulate(m1,d1);
```

Plot Results

Plot the concentration versus the time profile of the drug in the compartment.

```
plot(t,sd);
legend(species,'Location','NorthWest');
xlabel('Hours');
ylabel('Drug Concentration');
```



Add a Series of Bolus Doses to a One-Compartment Model

This example shows how to add a series of bolus doses to one-compartment model.

Background

Suppose you have a one-compartment model with a species named `drug` that represents the total amount of drug in the body. The drug is removed from the body via the first-order elimination represented by the reaction `drug -> null`, with the elimination rate constant `ke`. In other words, the drug concentration versus the time profile follows the monoexponential decline $C_t = C_0 e^{-k_e t}$, where C_t is the drug concentration at time t, C_0 is the initial concentration, and `ke` is the elimination rate constant. This example shows how to set up such a one-compartment model and administer a series of bolus doses, namely 250 mg three times a day (tid) for two days.

Create a One-Compartment Model

First create a SimBiology model named `onecomp`.

```
m1 = sbiomodel('onecomp');
```

Define the elimination of the drug from the system by adding a reaction `drug -> null` to the model.

```
r1 = addreaction(m1,'drug -> null');
```

The species `drug` is automatically created and the reaction is added to the compartment. The `null` species is a reserved species that acts as a sink in this reaction.

Add a mass action kinetic law to the reaction. This kinetic law defines the drug elimination to follow the first-order kinetics.

```
k1 = addkineticlaw(r1,'MassAction');
```

Define the elimination rate parameter `ke` and add it to the kinetic law.

```
p1 = addparameter(k1,'ke','Value',1.0,'ValueUnits','1/hour');
```

Specify the rate parameter `ke` as the forward rate parameter of the reaction by setting the `ParameterVariableNames` property of kinetic law object `k1`. This allows SimBiology to determine the reaction rate for `drug -> null` reaction.

```
k1.ParameterVariableNames = 'ke';
```

Set Up a Series of Bolus Doses

Suppose you want to increase the drug concentration in the system by administering a series of bolus doses: 250 mg three times a day (tid) for two days. Create a repeat dose object. Specify the amount of the dose (`Amount`), the dose target, the time interval between each dose (`Interval`), and the total number of doses (`RepeatCount`). You also need to set the `Active` property of the dose object to `true` so that the dose is applied to the model during simulation.

```
d1 = sbiodose('d1','repeat');
d1.Amount = 250;
d1.AmountUnits = 'milligram';
d1.TargetName = 'drug';
d1.Interval = 8;
d1.TimeUnits = 'hour';
```

```
d1.RepeatCount = 5;
d1.Active = true;
```

`RepeatCount` was set to 5, instead of 6 since it represents the number of doses *after* the first dose at the default dose start time (`d1.StartTime` = 0).

Simulate the Model

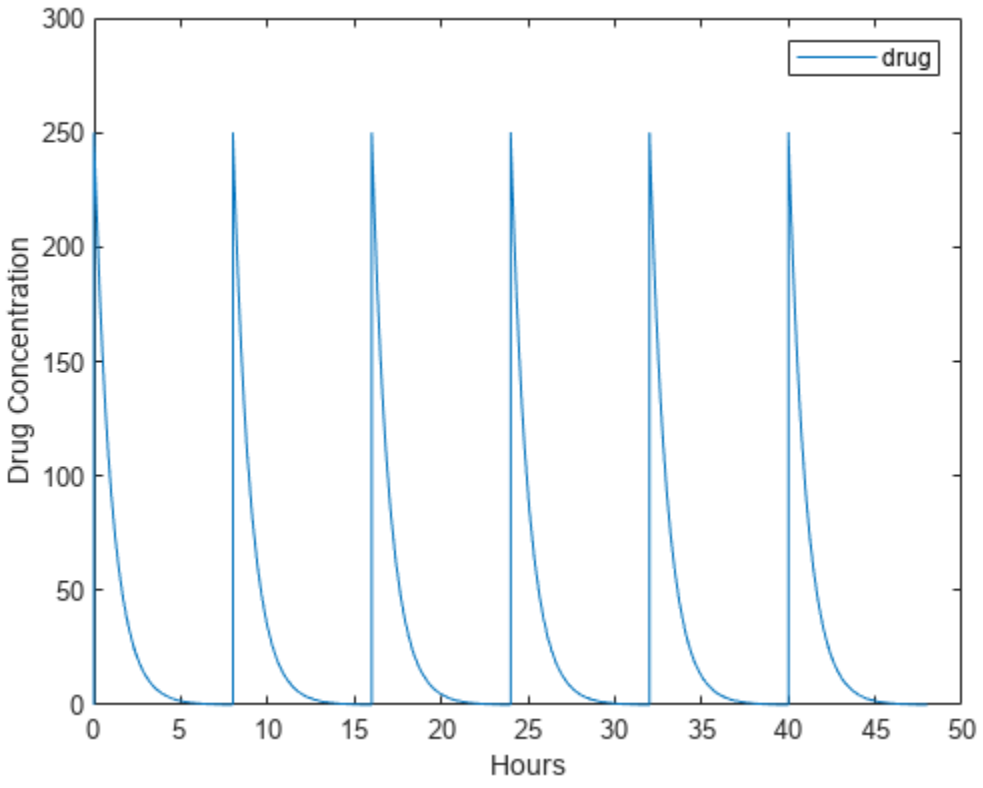
Change the simulation stop time to 48 hours to match the dosing schedule defined by the `d1` dose object.

```
cs = getconfigset(m1);
cs.StopTime = 48;
cs.TimeUnits = 'hour';
[t,sd,species] = sbiosimulate(m1,d1);
```

Plot Results

Plot the concentration versus the time profile of the drug in the system.

```
plot(t,sd);
legend(species);
xlabel('Hours');
ylabel('Drug Concentration');
```



Increase Drug Concentration in a One-Compartment Model via Zero-Order Dosing

This example shows how to set up a dosing regimen that follows the zero-order absorption kinetics.

Background

Suppose you have a one-compartment model with a species named `drug` that represents the total amount of drug in the body. The drug is removed from the body via the first-order elimination represented by the reaction `drug -> null`, with the elimination rate constant `ke`. In other words, the drug concentration versus the time profile follows the monoexponential decline $C_t = C_0 e^{-k_e t}$, where C_t is the drug concentration at time t, C_0 is the initial concentration, and `ke` is the elimination rate constant. This example shows how to set up such a one-compartment model and increase the drug concentration in the compartment via the zero-order absorption that takes 25 hours to administer the total dose amount of 250 mg.

Create a One-Compartment Model

Create a SimBiology model named `onecomp`.

```
m1 = sbiomodel('onecomp');
```

Define the elimination of the drug from the system by adding a reaction `drug -> null` to the model.

```
r1 = addreaction(m1,'drug -> null');
```

The species `drug` is automatically created and added to the compartment. The `null` species is a reserved species that acts as a sink in this reaction.

Add a mass action kinetic law to the reaction. This kinetic law defines the drug elimination to follow the first-order kinetics.

```
k1 = addkineticlaw(r1,'MassAction');
```

Define the elimination rate parameter `ke` and add it to the kinetic law.

```
p1 = addparameter(k1,'ke','Value',1.0,'ValueUnits','1/hour');
```

Specify the rate parameter `ke` as the forward rate parameter of the reaction by setting the `ParameterVariableNames` property of kinetic law object `k1`. This allows SimBiology to determine the reaction rate for `drug -> null` reaction.

```
k1.ParameterVariableNames = 'ke';
```

Set Up Zero-Order Dosing

To set up zero-order dosing, first create a zero-order duration parameter `p2` that represents the time it takes to administer a dose. Next, specify the amount of the dose (`Amount`), the dose target (`TargetName`), and the name of the zero-order duration parameter (`DurationParameterName`). You also need to set the `Active` property of the dose object to `true` so that the dose is applied to the model during simulation.

```
p2 = addparameter(m1,'duration','Value',25,'ValueUnits','hour');
d1 = sbiodose('d1');
d1.Amount = 250;
d1.AmountUnits = 'milligram';
d1.TargetName = 'drug';
```

```
d1.DurationParameterName = 'duration'; %Name of the duration parameter |p2|
d1.Active = true;
```

Simulate the Model

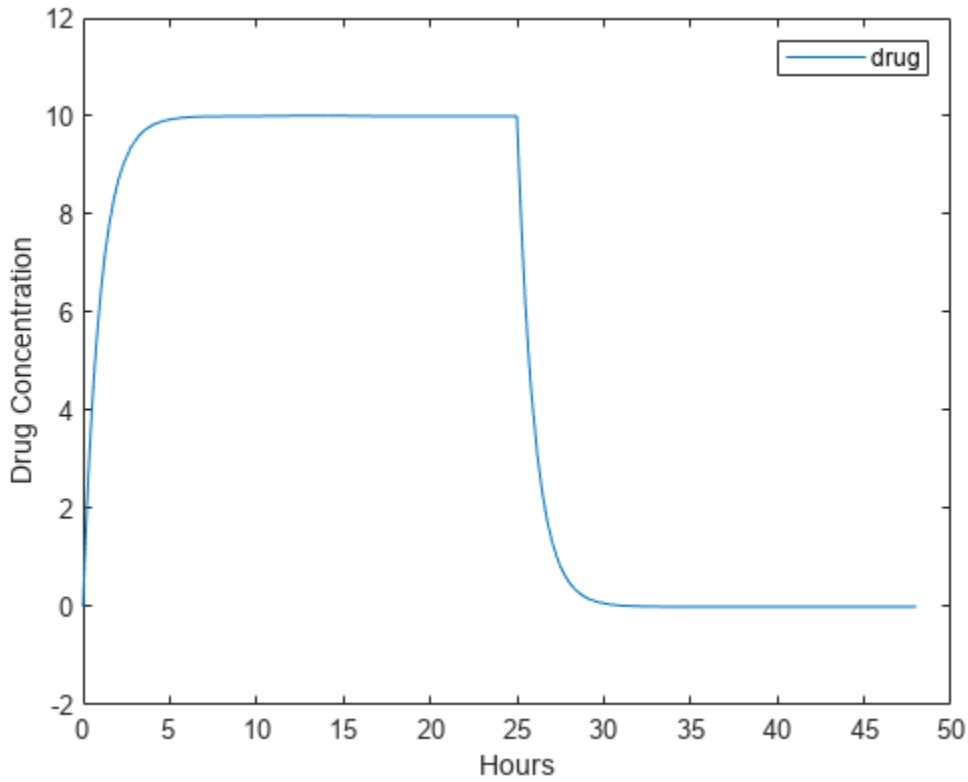
Change the simulation stop time to 48 hours to see the complete time profile. Apply the dosing schedule defined by `d1` to the model during simulation.

```
cs = getconfigset(m1);
cs.StopTime = 48;
cs.TimeUnits = 'hour';
[t,sd,species] = sbiosimulate(m1,d1);
```

Plot Results

Plot the concentration versus the time profile of the drug in the compartment.

```
plot(t,sd);
legend(species);
xlabel('Hours');
ylabel('Drug Concentration');
```



Add an Infusion Dose to a One-Compartment Model

This example shows how to add a constant-rate infusion dose to one-compartment model.

Background

Suppose you have a one-compartment model with a species named `drug` that represents the total amount of drug in the body. The drug is removed from the body via the first-order elimination represented by the reaction `drug -> null`, with the elimination rate constant `ke`. In other words, the drug concentration versus the time profile follows the monoexponential decline $C_t = C_0 e^{-k_e t}$, where C_t is the drug concentration at time t, C_0 is the initial concentration, and `ke` is the elimination rate constant. This example shows how to set up such a one-compartment model and add an infusion dose at a constant rate of 10 mg/hour for the total dose amount of 250 mg.

Create a One-Compartment Model

Create a SimBiology model named `onecomp`.

```
m1 = sbiomodel('onecomp');
```

Define the elimination of the drug from the system by adding a reaction `drug -> null` to the model.

```
r1 = addreaction(m1,'drug -> null');
```

The species `drug` is automatically created and added to the compartment. The `null` species is a reserved species that acts as a sink in this reaction.

Add a mass action kinetic law to the reaction. This kinetic law defines the drug elimination to follow the first-order kinetics.

```
k1 = addkineticlaw(r1,'MassAction');
```

Define the elimination rate parameter `ke` and add it to the kinetic law.

```
p1 = addparameter(k1,'ke','Value',1.0,'ValueUnits','1/hour');
```

Specify the rate parameter `ke` as the forward rate parameter of the reaction by setting the `ParameterVariableNames` property of kinetic law object `k1`. This allows SimBiology to determine the reaction rate for `drug -> null` reaction.

```
k1.ParameterVariableNames = 'ke';
```

Set Up an Infusion Dose

Specify the amount of the dose (`Amount`), the dose target (`TargetName`), and the infusion rate (`Rate`). You also need to set the `Active` property of the dose object to `true` so that the dose is applied to the model during simulation.

```
d1 = sbiodose('d1');
d1.Amount = 250;
d1.TargetName = 'drug';
d1.Rate = 10;
d1.RateUnits = 'milligram/hour';
d1.Active = true;
```

Simulate the Model

Change the simulation stop time to 48 hours to see the complete time course. Apply the dosing schedule defined by `d1` to the model during simulation.

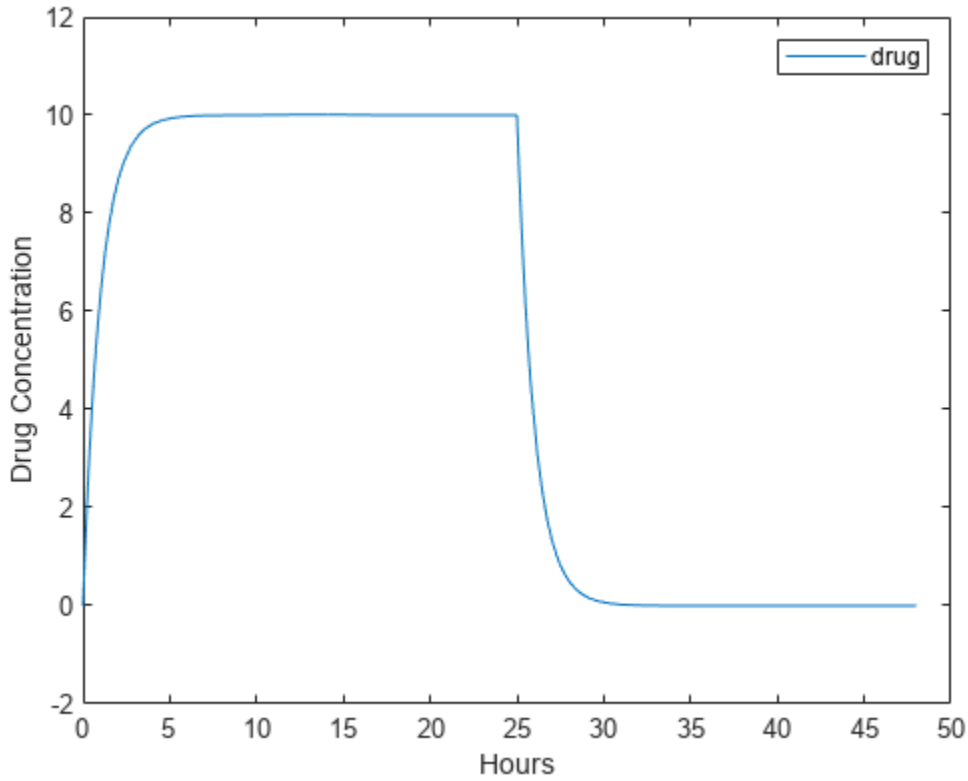
```
cs = getconfigset(m1);
cs.StopTime = 48;
```

```
cs.TimeUnits = 'hour';
[t,sd,species] = sbiosimulate(m1,d1);
```

Plot Results

Plot the concentration versus the time profile of the drug in the system.

```
plot(t,sd);
legend(species);
xlabel('Hours');
ylabel('Drug Concentration');
```



Input Arguments

`DoseName` — Name of the dose object
character vector | string

Name of the dose object, specified as a character vector or string.

Example: `'250mg_tid'`

Data Types: `char`

`DoseType` — Type of the dose object
`'schedule'` | `'repeat'`

Type of the dose object, specified as `'schedule'` for a `ScheduleDose object` and `'repeat'` for a `RepeatDose object`.

Example: `'schedule'`

Data Types: `char`

Output Arguments

dose — Dose object
`RepeatDose object` | `ScheduleDose object`

Dose object, returned as a `RepeatDose object` or `ScheduleDose object`.

Version History

Introduced in R2010a

See Also

`adddose` | `getdose` | `removedose` | `copyobj` | `get` | `set` | `ScheduleDose object` | `RepeatDose object`

Topics
`Model`
“Doses in SimBiology Models”

sbiodiff

Compare SimBiology models and diagram information

Syntax

```
diffResults = sbiodiff(source,target)
diffResults = sbiodiff(projectFile)
diffResults = sbiodiff( ___ ,Name=Value)
```

Description

`diffResults = sbiodiff(source,target)` compares two SimBiology models or SBPROJ files `source` and `target` and returns the comparison results as the `SimBiology.DiffResults` object `diffResults`. If `source` and `target` are SBPROJ files that contain more than one model, specify which model to compare using the name-value arguments `SourceModelName` and `TargetModelName`. For details on how SimBiology compares and matches model components, see "SimBiology Model Matching Policy".

`diffResults = sbiodiff(projectFile)` compares two SimBiology models contained in the `SBPROJ` file `projectFile`. If the project file contains more than two models, specify which models to compare using the name-value arguments `SourceModelName` and `TargetModelName`.

`diffResults = sbiodiff( ___ ,Name=Value)` specifies additional options using one or more name-value arguments in addition to any of the input argument combinations in the previous syntaxes.

Examples

Compare SimBiology Models

Load a source model.

```
model1      = sbmlimport("lotka");
y1          = sbioselect(model1, "Type", "species", "Name", "y1");
y1.Value    = 880;
```

Load a target model to compare against the source model.

```
model2      = sbmlimport("lotka");
y1          = sbioselect(model2, "Type", "species", "Name", "y1");
y1.Value    = 920;
```

Compare the models using `sbiodiff` and display the comparison table.

```
diffResults = sbiodiff(model1,model2);
diffTable   = diffResults.Comparisons
```

```
diffTable=1×6 table
           Class      Source    Target    Property    SourceValue    TargetValue
          _________    ______    ______    ________    ___________    ___________
```

```
    1    "Species"     "y1"      "y1"     "Value"       {[880]}        {[920]}
```

You can also view the comparison results graphically in the Comparison tool.

```
visdiff(diffResults);
```

Get a table of model components associated with the changes reported in the comparison table.

```
tbl = getComponents(diffResults)
```

```
tbl=1×2 table
                  Source                          Target
        ____________________________    ____________________________

    1    {1x1 SimBiology.Species}    {1x1 SimBiology.Species}
```

Input Arguments

`source` — Source model or SBPROJ file name

`model` object | character vector | string scalar

Source model to compare against the target model, specified as a SimBiology `Model` object or SBPROJ file name. Specify the file name as a character vector or string scalar.

If the SBPROJ file contains more than one model, specify which model to compare using the name-value argument `SourceModelName`.

`target` — Target model or SBPROJ file name

`model` object | character vector | string scalar

Target model to compare against the source model, specified as a SimBiology `Model` object or SBPROJ file name. Specify the file name as a character vector or string scalar.

The SBPROJ file contains more than one model, specify which model to compare using the name-value argument `TargetModelName`.

`projectFile` — SBPROJ file name

character vector | string scalar

SBPROJ file name, specified as a character vector or string scalar. The SBPROJ file must contain at least 2 models. If the file contains more than two models, specify which two models to compare using the name-value arguments `SourceModelName` and `TargetModelName`.

Data Types: `char` | `string`

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Example: `diffResults = sbiodiff("myproj.sbproj",SourceModelName="m1",TargetModelName="m2")` compares two SimBiology models `m1` and `m2` from `myproj.sbproj`.

`SourceModelName` — Name of source model
character vector | string scalar

Name of the source model from the input SBPROJ file to compare, specified as a character vector or string scalar.

Data Types: `char` | `string`

`TargetModelName` — Name of target model
character vector | string scalar

Name of the target model from the input SBPROJ file to compare, specified as a character vector or string scalar.

Data Types: `char` | `string`

Output Arguments

`diffResults` — Results of comparison between two models
`SimBiology.DiffResults`

Results of comparison between two models, returned as a `SimBiology.DiffResults` object. The comparison results are the snapshot of the model state when you ran `sbiodiff`.

The results include differences of the diagrams if the input SBPROJ file contains diagram information or if the specified models are open in the **SimBiology Model Builder** app when you run the function.

Version History

Introduced in R2022a

See Also

`Model` | `sbioloadproject` | **SimBiology Model Builder** | `SimBiology.DiffResults` | `getComponents` | `visdiff`

Topics
“Compare SimBiology Models”
“SimBiology Model Matching Policy”
“What is a SimBiology Model?”

sbioelementaryeffects

Perform global sensitivity analysis (GSA) by computing elementary effects (requires Statistics and Machine Learning Toolbox)

Syntax

```
elementaryEffectsResults = sbioelementaryeffects(modelObj,params,observables)
elementaryEffectsResults = sbioelementaryeffects(modelObj,params,observables,
Name=Value)
```

Description

`elementaryEffectsResults = sbioelementaryeffects(modelObj,params,observables)` performs a global sensitivity analysis of a SimBiology model `modelObj` by computing elementary effects of `observables` with respect to individual model quantities or parameters specified in `params`.

`elementaryEffectsResults = sbioelementaryeffects(modelObj,params,observables, Name=Value)` uses additional options specified by one or more name-value arguments.

Examples

Perform GSA by Computing Elementary Effects

Load the “Tumor Growth Model”.

```
sbioloadproject tumor_growth_vpop_sa.sbproj
```

Get a variant with estimated parameters and the dose to apply to the model.

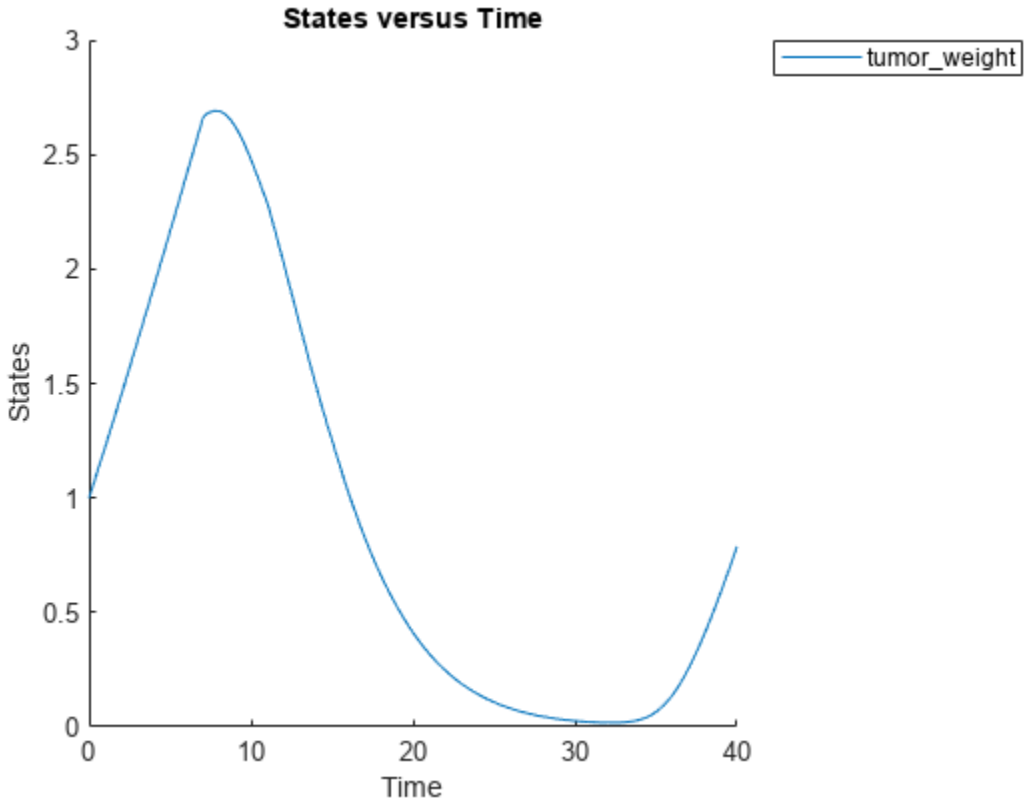
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

Get the active configset and set the tumor weight as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'tumor_weight';
```

Simulate the model and plot the tumor growth profile.

```
sbioplot(sbiosimulate(m1,cs,v,d));
```



Perform global sensitivity analysis (GSA) on the model to find the model parameters that the tumor growth is sensitive to.

First, define model parameters of interest, which are involved in the pharmacodynamics of the tumor growth. Define the model response as the tumor weight.

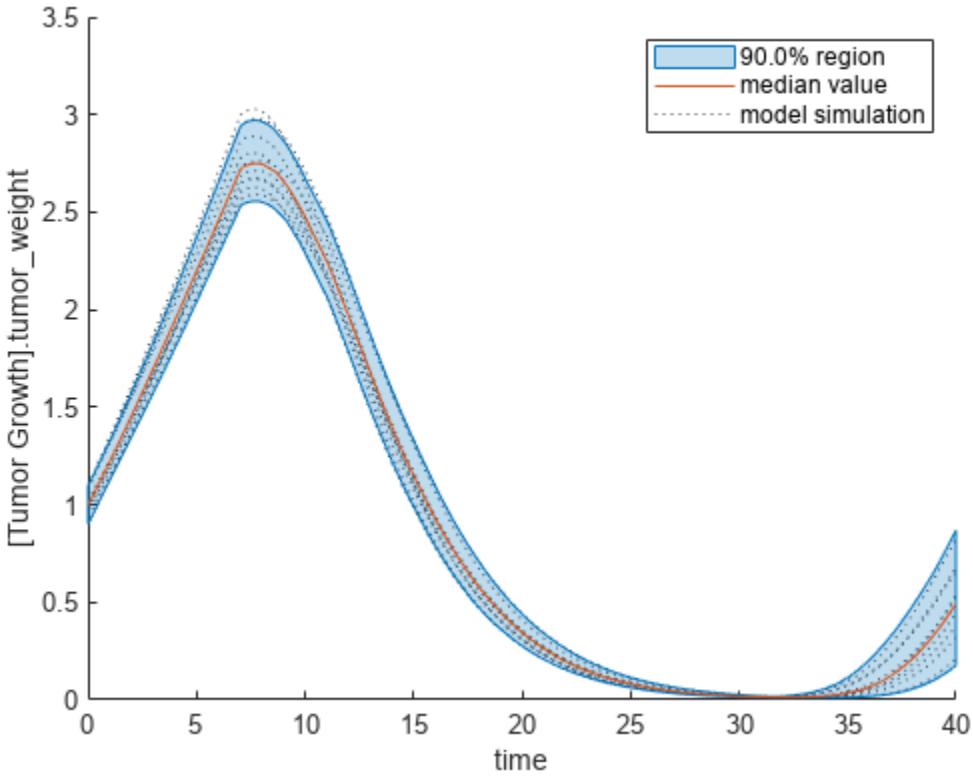
```
modelParamNames = {'L0','L1','w0','k1'};
outputName = 'tumor_weight';
```

Then perform GSA by computing the elementary effects using `sbioelementaryeffects`. Use `100` as the number of samples and set `ShowWaitBar` to `true` to show the simulation progress.

```
rng('default');
eeResults = sbioelementaryeffects(m1,modelParamNames,outputName,Variants=v,Doses=d,NumberSamples=
```

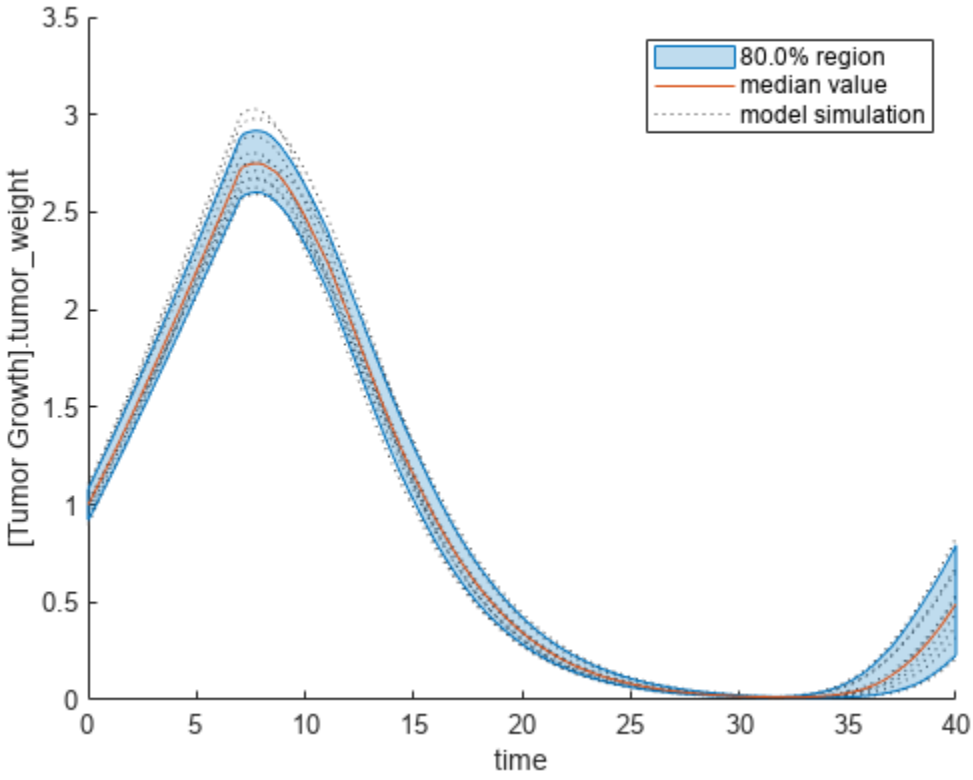
Show the median model response, the simulation results, and a shaded region covering 90% of the simulation results.

```
plotData(eeResults,ShowMedian=true,ShowMean=false);
```



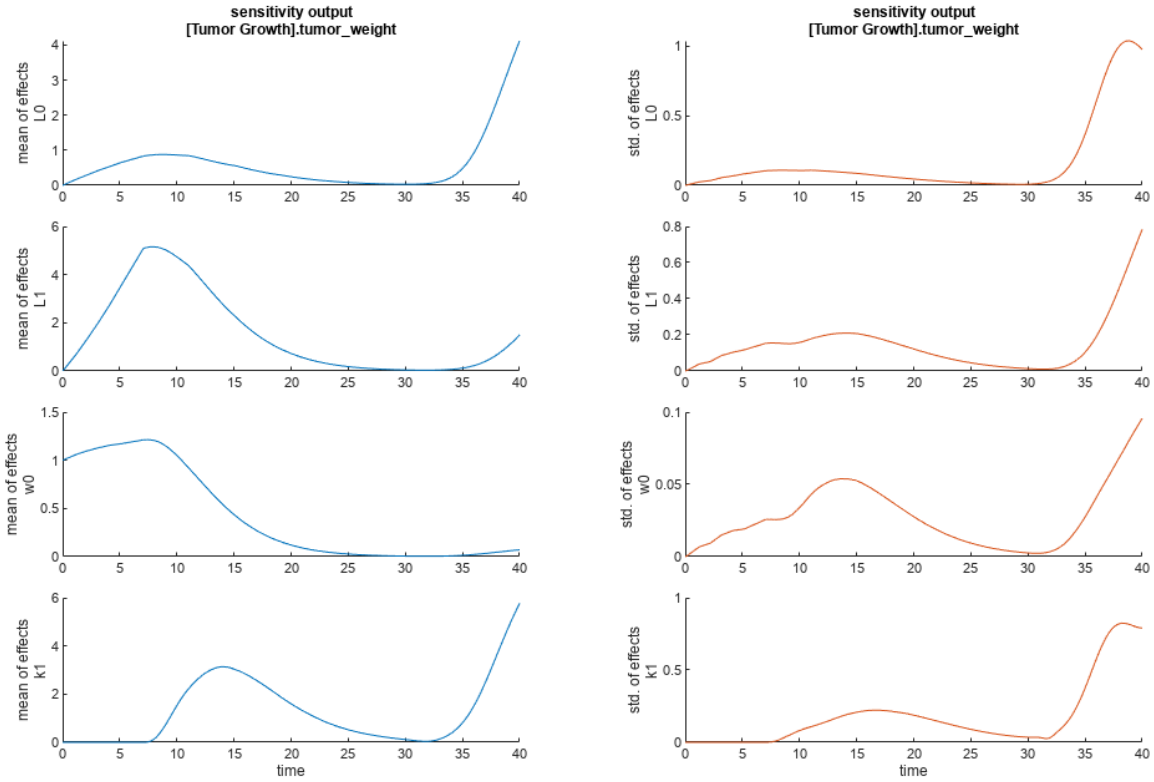
You can adjust the quantile region to a different percentage by specifying `Alphas` for the lower and upper quantiles of all model responses. For instance, an `alpha` value of 0.1 plots a shaded region between the `100*alpha` and `100*(1-alpha)` quantiles of all simulated model responses.

```
plotData(eeResults,Alphas=0.1,ShowMedian=true,ShowMean=false);
```



Plot the time course of the means and standard deviations of the elementary effects.

```
h = plot(eeResults);
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```

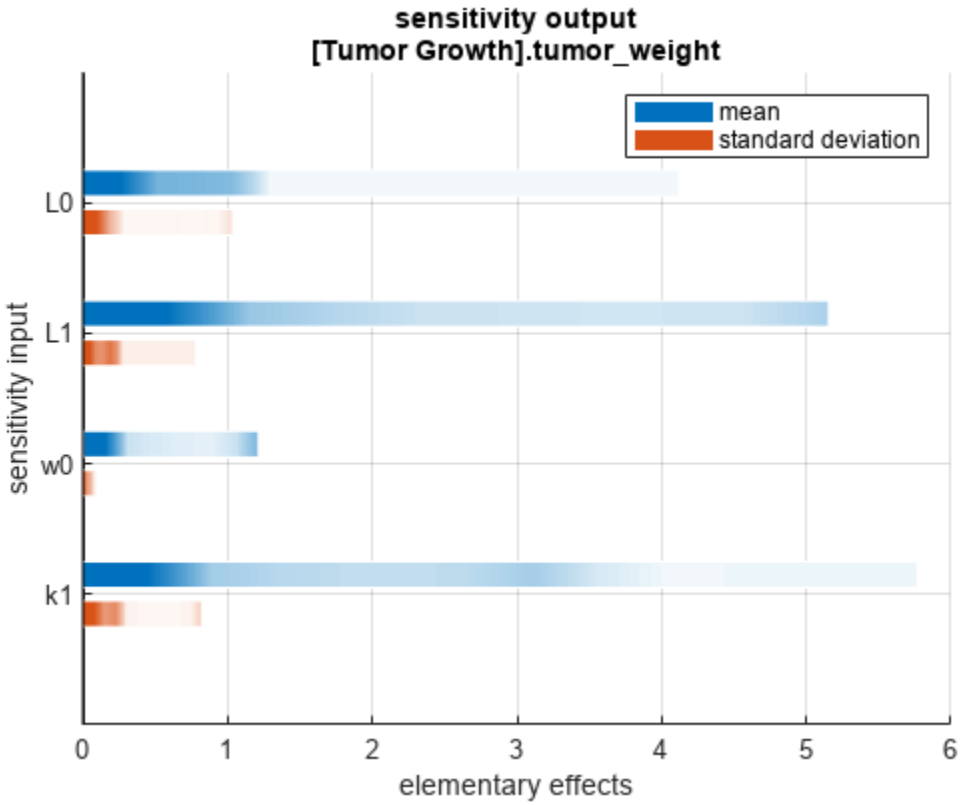


The mean of effects explains whether variations in input parameter values have any effect on the tumor weight response. The standard deviation of effects explains whether the sensitivity change is dependent on the location in the parameter domain.

From the mean of effects plots, parameters `L1` and `w0` seem to be the most sensitive parameters to the tumor weight before the dose is applied at t = 7. But, after the dose is applied, `k1` and `L0` become more sensitive parameters and contribute most to the after-dosing stage of the tumor weight. The plots of standard deviation of effects show more deviations for the larger parameter values in the later stage (t > 35) than for the before-dose stage of the tumor growth.

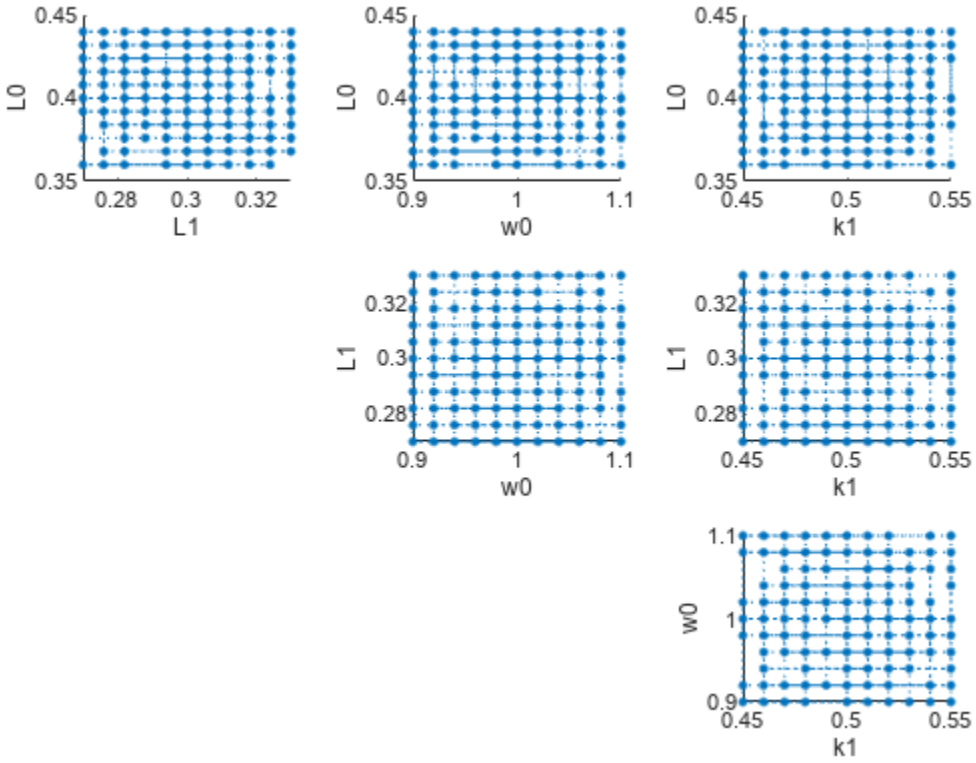
You can also display the magnitudes of the sensitivities in a bar plot. Each color shading represents a histogram representing values at different times. Darker colors mean that those values occur more often over the whole time course.

```
bar(eeResults);
```



You can also plot the parameter grids and samples used to compute the elementary effects.

```
plotGrid(eeResults)
```



You can specify more samples to increase the accuracy of the elementary effects, but the simulation can take longer to finish. Use `addsamples` to add more samples.

```
eeResults2 = addsamples(eeResults,200);
```

The `SimulationInfo` property of the result object contains various information for computing the elementary effects. For instance, the model simulation data (SimData) for each simulation using a set of parameter samples is stored in the `SimData` field of the property. This field is an array of `SimData` objects.

```
eeResults2.SimulationInfo.SimData
```

```
SimBiology SimData Array : 1500-by-1

Index:    Name:         ModelName:         DataCount:
1           -           Tumor Growth Model 1
2           -           Tumor Growth Model 1
3           -           Tumor Growth Model 1
...
1500        -           Tumor Growth Model 1
```

You can find out if any model simulation failed during the computation by checking the `ValidSample` field of `SimulationInfo`. In this example, the field shows no failed simulation runs.

```
all(eeResults2.SimulationInfo.ValidSample)
```

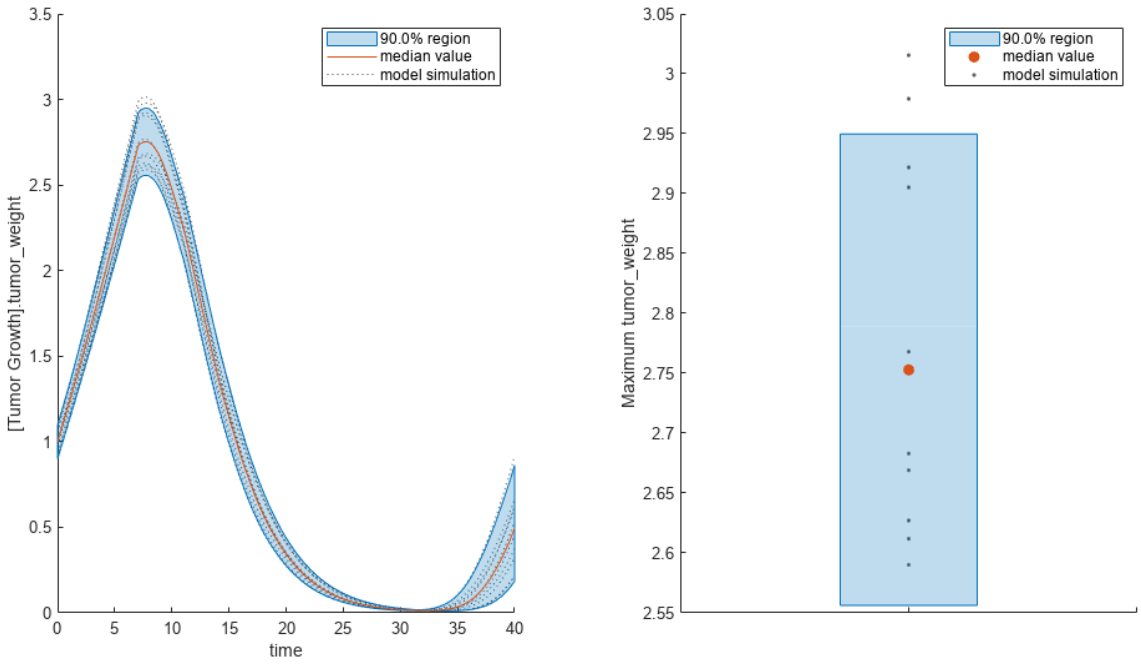
```
ans = logical
   1
```

You can add custom expressions as observables and compute the elementary effects of the added observables. For example, you can compute the effects for the maximum tumor weight by defining a custom expression as follows.

```
% Suppress an information warning that is issued.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
% Add the observable expression.
eeObs = addobservable(eeResults2,'Maximum tumor_weight','max(tumor_weight)','Units','gram');
```

Plot the computed simulation results showing the 90% quantile region.

```
h2 = plotData(eeObs,ShowMedian=true,ShowMean=false);
h2.Position(:) = [100 100 1500 800];
```



You can also remove the observable by specifying its name.

```
eeNoObs = removeobservable(eeObs,'Maximum tumor_weight');
```

Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

`modelObj` — SimBiology model

SimBiology model object

SimBiology model, specified as a SimBiology `model object`.

`params` — Names of model parameters, species, or compartments
character vector | string | string vector | cell array of character vectors

Names of model parameters, species, or compartments, specified as a character vector, string, string vector, or cell array of character vectors.

Example: `["k1","k2"]`

Data Types: `char` | `string` | `cell`

`observables` — Model responses
character vector | string | string vector | cell array of character vectors

Model responses, specified as a character vector, string, string vector, or cell array of character vectors. Specify the names of species, parameters, compartments, or `observables`.

Example: `"tumor_growth"`

Data Types: `char` | `string` | `cell`

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Example: `eeResults = sbioelementaryeffects(modelObj,params,observables,StopTime=10)` specifies to use a stop time of 10.

`Bounds` — Parameter bounds
numeric matrix

Parameter bounds, specified as a numeric matrix with two columns. The first column contains the lower bounds and the second column contains the upper bounds. The number of rows must be equal to the number of parameters in `params`.

If a parameter has a nonzero value, the default bounds are ±10% of the value. If the parameter value is zero, the default bounds are `[0 1]`.

Example: `[0.5 5]`

Data Types: `double`

`Doses` — Doses to use during simulations
`ScheduleDose` object | `RepeatDose` object | vector of dose objects

Doses to use during model simulations, specified as a `ScheduleDose` or `RepeatDose` object or a vector of dose objects.

`Variants` — Variants to apply before simulations
variant object | vector of variant objects

Variants to apply before model simulations, specified as a variant object or vector of variant objects.

When you specify multiple variants with duplicate specifications for a property's value, the last occurrence for the property value in the array of variants is used during simulation.

`NumberSamples` — Number of samples to compute elementary effects
`1000` (default) | positive integer

Number of samples to compute elementary effects, specified as a positive integer. The function requires `(number of input params + 1) * NumberSamples` model simulations to compute the elementary effects.

Data Types: `double`

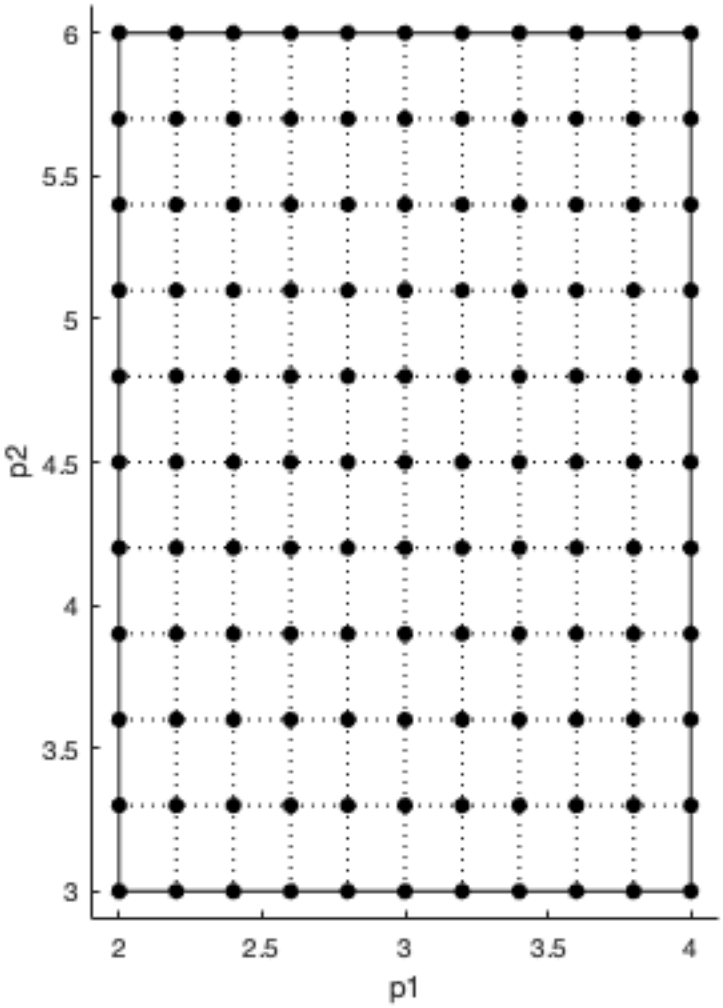
`PointSelection` — Method to select sample points to compute elementary effects
`"chain"` (default) | `"radial"`

Method to select sample points to compute elementary effects, specified as `"chain"` or `"radial"`. The `"chain"` point selection uses the Morris method [1]. The `"radial"` point selection uses the Sohier method [2]. For details, see “Elementary Effects for Global Sensitivity Analysis” on page 1-51.

Data Types: `char` | `string`

`GridLevel` — Discretization level of parameter domain
`10` (default) | positive even integer

Discretization level of the parameter domain, specified as a positive even integer. This parameter defines a grid of equidistant points in the parameter domain, where each dimension is discretized using `Gridlevel+1` points. The following figure shows an example of a grid for parameters *p1* and *p2* within given parameter bounds.

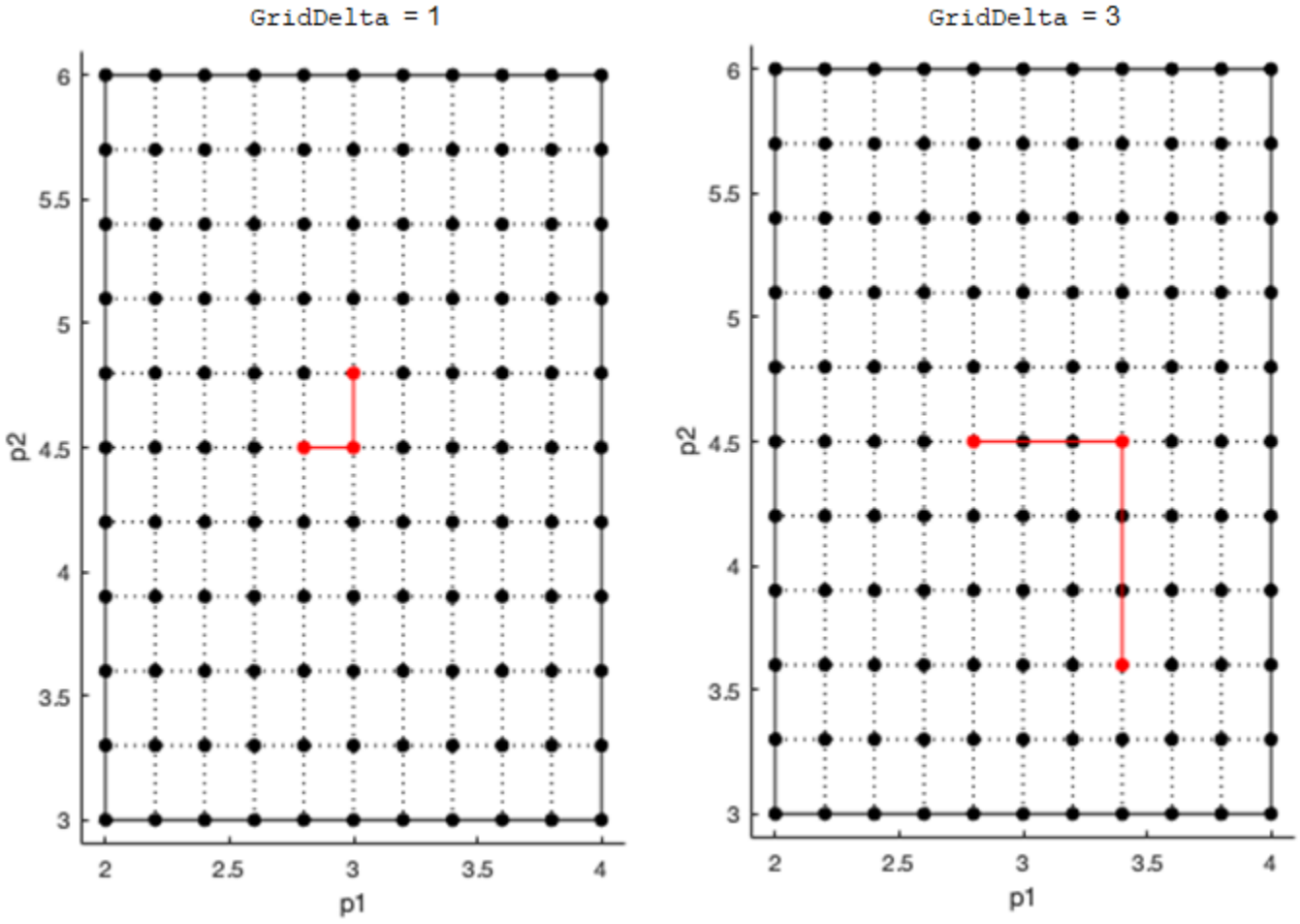


For details, see “Elementary Effects for Global Sensitivity Analysis” on page 1-51.

Data Types: `double`

`GridDelta` — Step size to compute elementary effects
`GridLevel/2` (default) | positive integer

Step size for computing elementary effects, specified as a positive integer between 1 and `GridLevel`. The step size is measured in terms of grid points between neighboring points. The following figure shows examples of different grid delta values.



For details, see “Elementary Effects for Global Sensitivity Analysis” on page 1-51.

Data Types: `double`

`AbsoluteEffects` — Flag to use absolute values of elementary effects
`true` (default) | `false`

Flag to use the absolute values of elementary effects, specified as `true` or `false`. By default, the function uses the absolute values of elementary effects. Using nonabsolute values can average out when calculating the mean. For details, see “Elementary Effects for Global Sensitivity Analysis” on page 1-51.

Data Types: `logical`

`SamplingMethod` — Method to generate parameter samples
`"lhs"` (default) | `"random"`

Method to generate parameter samples, specified as one of the following:

- `"lhs"` — Use low-discrepancy Latin hypercube samples.
- `"random"` — Use uniformly distributed random samples.

The function selects generated parameter samples by sampling the grid points.

`StopTime` — Simulation stop time
nonnegative scalar

Simulation stop time, specified as a nonnegative scalar. If you specify neither `StopTime` nor `OutputTimes`, the function uses the stop time from the active configuration set of the model. You cannot specify both `StopTime` and `OutputTimes`.

Data Types: `double`

`OutputTimes` — Simulation output times
numeric vector

Simulation output times, specified as a numeric vector. The function computes the elementary effects at these output time points. You cannot specify both `StopTime` and `OutputTimes`. By default, the function uses the reported time points of the first model simulation.

Example: `[0 1 2 3.5 4 5 5.5]`

Data Types: `double`

`UseParallel` — Flag to run model simulations in parallel
`false` (default) | `true`

Flag to run model simulations in parallel, specified as `true` or `false`. When the value is `true` and Parallel Computing Toolbox™ is available, the function runs simulations in parallel.

Data Types: `logical`

`Accelerate` — Flag to turn on model acceleration
`true` (default) | `false`

Flag to turn on model acceleration, specified as `true` or `false`.

Data Types: `logical`

`InterpolationMethod` — Method for interpolation of model simulations
`"interp1q"` (default) | character vector | string

Method for interpolation of model responses to a common set of output times, specified as a character vector or string. The valid options follow.

- `"interp1q"` — Use the `interp1q` function.
- Use the `interp1` function by specifying one of the following methods:
  - `"nearest"`
  - `"linear"`
  - `"spline"`
  - `"pchip"`
  - `"v5cubic"`
- `"zoh"` — Specify zero-order hold.

Data Types: `char` | `string`

`ShowWaitbar` — Flag to show progress of model simulations
`false` (default) | `true`

Flag to show the progress of model simulations by displaying a wait bar, specified as `true` or `false`. By default, no wait bar is displayed.

Data Types: `logical`

Output Arguments

`elementaryEffectsResults` — Results containing means and standard deviations of elementary effects

`SimBiology.gsa.ElementaryEffects` object

Results containing means and standard deviations of elementary effects, returned as a `SimBiology.gsa.ElementaryEffects` object. The object includes information such as the mean and standard deviation of elementary effects as well as parameter samples and model simulations used to compute the elementary effects.

More About

Elementary Effects for Global Sensitivity Analysis

`sbioelementaryeffects` lets you assess global sensitivity of a model response with respect to variations in model parameters.

Consider a simple case with one sensitivity input parameter P. The elementary effect EE of P with respect to a model response R is defined as follows.

$$EE_P(x) = \frac{R(x) - R(x + delta)}{delta}$$

Here, $EE_P(x)$ is the elementary effect of P . $R(x)$ and $R(x+delta)$ are model responses at a specific time or the values of observables, evaluated for parameter values x and $x+delta$.

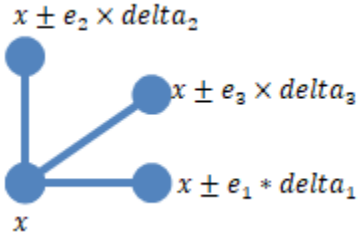
In the general case of k sensitivity input parameters, x is a vector of different parameter values, $x = [v_1, v_2, v_3, \ldots, v_k]$. The elementary effect of the ith parameter is computed as follows.

$$\begin{aligned} EE_{Pi}(x) &= \frac{R(v_1, v_2, v_3, \ldots, v_i, \ldots, v_k) - R(v_1, v_2, v_3, \ldots, v_i + delta_i, \ldots, v_k)}{delta_i} \\ &= \frac{R(x) - R(x + e_i \times delta_i)}{delta_i} \end{aligned}$$

Here, e_i is the ith canonical unit vector. Thus, calculating the elementary effects of all parameters $P_1, P_2, P_3, \ldots, P_k$ requires $k+1$ model simulations.

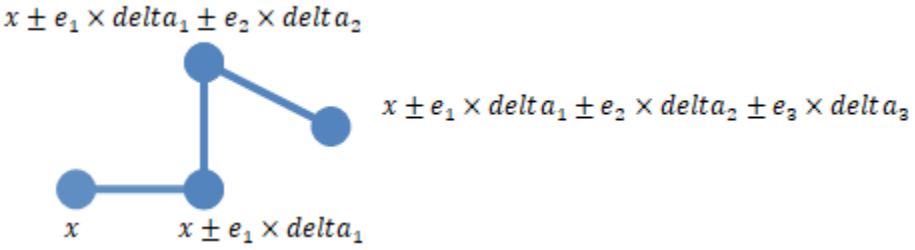
The function provides two methods (`'PointSelection'`) to select a set of $k+1$ points required to compute these elementary effects.

- `radial` — This method [2] uses k points, $x \pm e_1 \times delta_1, x \pm e_2 \times delta_2, \ldots, x \pm e_k \times delta_k$, that are arranged around one center point x to compute elementary effects for each of k parameters.



- `chain` — This method [1] uses chains of points, instead of radially-arranged points around a center points:

  $x + \sum_{i=1}^{n} e_i \times delta_i$, where $n = 0, 1, \ldots, k$



To get the mean and standard deviation of elementary effects, the function computes N (`'NumberSamples'`) elementary effects per parameter, which requires $N*(k+1)$ simulations. By default, the function reports the mean and standard deviation of *absolute* elementary effects of each parameter $P_1, P_2, P_3, \ldots, P_k$.

Mean of EE_{Pi} = mean($|EE_{Pi}|$)

Standard deviation of EE_{Pi} = std($|EE_{Pi}|$)

- The mean of elementary effects explains whether variations in parameter P have any effect on response R on average.
- The standard deviation explains whether the sensitivity change is dependent on the location in the parameter domain.

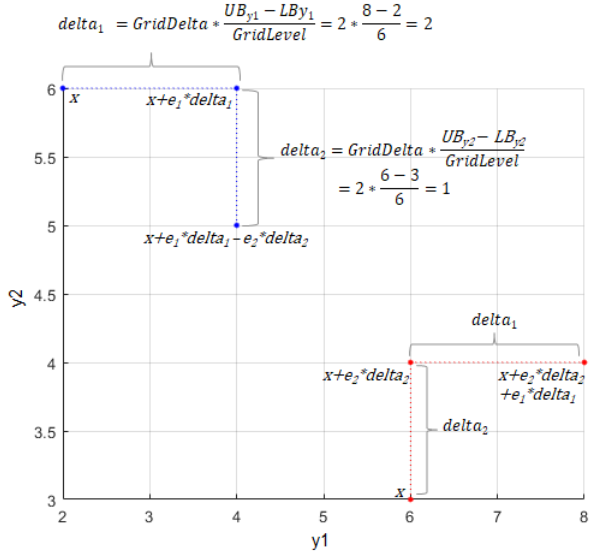
The function uses the *absolute* elementary effects by default because the elementary effects can average out when calculating the mean otherwise. Optionally, you can set the `'AbsoluteEffects'` name-value argument to `false` to get the means and standard deviations of *nonabsolute* elementary effects.

The function reports the points used to compute elementary effects in the `ParameterSamples` property of the returned results object. Each block of $k+1$ rows in the table of `ParameterSamples` corresponds to the k+1 radial or chained points used to compute the elementary effects. The `SimulationInfo.SimData` property of the results object contains the corresponding model simulations. The function samples the points from the parameter grid defined by `'GridLevel'` and `'GridDelta'`. The following figure illustrates a simple case with two sensitivity inputs (*y1* and *y2*) with `'NumberSamples'` = 2 using the `chain` `'PointSelection'` method.

Example: k (# of sensitivity inputs) = 2, `NumberSamples` = 2, `GridLevel` = 6, `GridDelta` = 2

y1 Upper Bound (UBy_1) = 8
y1 Lower Bound (LBy_1) = 2

y2 Upper Bound (UBy_2) = 6
y2 Lower Bound (LBy_2) = 3



`ParameterSamples` table

y1	y2	
4	5	1st block of *k+1* rows
4	6	
2	6	
6	3	2nd block of *k+1* rows
6	4	
8	4	

Total number of *k+1* blocks = `NumberSamples` = 2

Version History

Introduced in R2021b

References

[1] Morris, Max D. “Factorial Sampling Plans for Preliminary Computational Experiments.” *Technometrics* 33, no. 2 (May 1991): 161–74.

[2] Sohier, Henri, Jean-Loup Farges, and Helene Piet-Lahanier. “Improvement of the Representativity of the Morris Method for Air-Launch-to-Orbit Separation.” *IFAC Proceedings Volumes* 47, no. 3 (2014): 7954–59.

See Also

`SimBiology.gsa.ElementaryEffects` | `sbiosobol` | `sbiompgsa` | `Observable`

Topics

“Sensitivity Analysis in SimBiology”

sbioensembleplot

Show results of ensemble run using 2-D or 3-D plots

Syntax

```
sbioensembleplot(simdataObj)
sbioensembleplot(simdataObj, Names)
sbioensembleplot(simdataObj, Names, Time)

FH = sbioensembleplot(simdataObj, Names)
FH = sbioensembleplot(simdataObj, Names, Time)
```

Arguments

simdataObj	An object that contains simulation data. You can generate a *simdataObj* object using the function `sbioensemblerun`. All elements of *simdataObj* must contain data for the same states in the same model.
Names	Character vector, string, string vector, string array, or cell array of character vectors. *Names* may include qualified names such as *'CompartmentName.SpeciesName'* or *'ReactionName.ParameterName'* to resolve ambiguities. Specifying `{}` or empty string array (`string.empty`) for *Names* plots data for all states contained in *simdataObj*.
Time	A numeric scalar value. If the specified *Time* is not an element of the time vectors in *simdataObj*, then the function resamples *simdataObj* as necessary using linear interpolation.
FH	Array of handles to figure windows.

Description

`sbioensembleplot(simdataObj)` shows a 3-D shaded plot of time-varying distribution of all logged states in the SimData array *simdataObj*. The `sbioensemblerun` function plots an approximate distribution created by fitting a normal distribution to the data at every time step.

`sbioensembleplot(simdataObj, Names)` plots the distribution for the data specified by *Names*.

`sbioensembleplot(simdataObj, Names, Time)` plots a 2-D histogram of the actual data of the ensemble distribution of the states specified by *Names* at the particular time point *Time*.

FH = `sbioensembleplot(simdataObj, Names)` returns an array of handles *FH*, to the figure window for the 3-D distribution plot.

FH = `sbioensembleplot(simdataObj, Names, Time)` returns an array of handles *FH*, to the figure window for the 2-D histograms.

Examples

This example shows how to plot data from an ensemble run without interpolation.

1. The project file, `radiodecay.sbproj`, contains a model stored in a variable called `m1`. Load `m1` into the MATLAB workspace.

   ```
   sbioloadproject('radiodecay.sbproj','m1');
   ```

2. Change the solver of the active configuration set to be `ssa`. Also, adjust the `LogDecimation` property on the `SolverOptions` property of the configuration set to reduce the size of the data generated.

   ```
   cs = getconfigset(m1, 'active');
   set(cs, 'SolverType', 'ssa');
   so = get(cs, 'SolverOptions');
   set(so, 'LogDecimation', 10);
   ```

3. Perform an ensemble of 20 runs with no interpolation.

   ```
   simdataObj = sbioensemblerun(m1, 20);
   ```

4. Create a 2-D distribution plot of the species `'z'` at time = 1.0.

   ```
   FH1 = sbioensembleplot(simdataObj, 'z', 1.0);
   ```

5. Create a 3-D shaded plot of both species.

   ```
   FH2 = sbioensembleplot(simdataObj, {'x','z'});
   ```

Version History

Introduced in R2006a

See Also

`sbioensemblerun` | `sbioensemblestats` | `sbiomodel`

sbioensemblerun

Multiple stochastic ensemble runs of SimBiology model

Syntax

```
simdataObj = sbioensemblerun(modelObj, Numruns)
simdataObj = sbioensemblerun(modelObj, Numruns, Interpolation)
simdataObj = sbioensemblerun(modelObj, Numruns, configsetObj)
simdataObj = sbioensemblerun(modelObj, Numruns, configsetObj, Interpolation)
simdataObj = sbioensemblerun(modelObj, Numruns, variantObj)
simdataObj = sbioensemblerun(modelObj, Numruns, variantObj, Interpolation)
simdataObj = sbioensemblerun(modelObj, Numruns, configsetObj, variantObj)
simdataObj = sbioensemblerun(modelObj, Numruns, configsetObj, variantObj,
Interpolation)
```

Arguments

simdataObj	An array of `SimData objects` containing simulation data generated by `sbioensemblerun`. All elements of *simdataObj* contain data for the same states in the same model.
modelObj	Model object to be simulated.
Numruns	Integer scalar representing the number of stochastic runs to make.
Interpolation	Character vector or string denoting the interpolation scheme to be used if data should be interpolated to get a consistent time vector. Valid values are `'linear'` (linear interpolation), `'zoh'` (zero-order hold), or `'off'` (no interpolation). Default is `'off'`. If interpolation is on, the data is interpolated to match the time vector with the smallest simulation stop time.
configsetObj	Specify the configuration set object to use in the ensemble simulation. For more information about configuration sets, see `Configset object`.
variantObj	Specify the variant object to apply to the model during the ensemble simulation. For more information about variant objects, see `Variant object`.

Description

simdataObj = `sbioensemblerun(`*modelObj, Numruns*`)` performs a stochastic ensemble run of the SimBiology model object (*modelObj*), and returns the results in *simdataObj*, an array of `SimData objects`. The active configset and the active variants are used during simulation and are saved in the output, SimData object (*simdataObj*).

`sbioensemblerun` uses the settings in the active configset on the model object (*modelObj*) to perform the repeated simulation runs. The `SolverType` property of the active configset must be set to one of the stochastic solvers: `'ssa'`, `'expltau'`, or `'impltau'`. `sbioensemblerun` generates an error if the `SolverType` property is set to any of the deterministic (ODE) solvers.

`simdataObj = sbioensemblerun(modelObj, Numruns, Interpolation)` performs a stochastic ensemble run of a model object (*`modelObj`*), and interpolates the results of the ensemble run onto a common time vector using the interpolation scheme (*`Interpolation`*).

`simdataObj = sbioensemblerun(modelObj, Numruns, configsetObj)` performs an ensemble run of a model object (*`modelObj`*), using the specified configuration set (*`configsetObj`*).

`simdataObj = sbioensemblerun(modelObj, Numruns, configsetObj, Interpolation)` performs an ensemble run of a model object (*`modelObj`*), using the specified configuration set (*`configsetObj`*), and interpolates the results of the ensemble run onto a common time vector using the interpolation scheme (*`Interpolation`*).

`simdataObj = sbioensemblerun(modelObj, Numruns, variantObj)` performs an ensemble run of a model object (*`modelObj`*), using the variant object or array of variant objects (*`variantObj`*).

`simdataObj = sbioensemblerun(modelObj, Numruns, variantObj, Interpolation)` performs an ensemble run of a model object (*`modelObj`*), using the variant object or array of variant objects (*`variantObj`*), and interpolates the results of the ensemble run onto a common time vector using the interpolation scheme (*`Interpolation`*).

`simdataObj = sbioensemblerun(modelObj, Numruns, configsetObj, variantObj)` performs an ensemble run of a model object (*`modelObj`*), using the configuration set (*`configsetObj`*), and the variant object or array of variant objects (*`variantObj`*). If the configuration set object (*`configsetObj`*) is empty, the active configset on the model is used for simulation. If the variant object (*`variantObj`*) is empty, then no variant (not even the active variants in the model) is used for the simulation.

`simdataObj = sbioensemblerun(modelObj, Numruns, configsetObj, variantObj, Interpolation)` performs an ensemble run of a model object (*`modelObj`*), using the configuration set (*`configsetObj`*), and the variant object or array of variant objects (*`variantObj`*), and interpolates the results of the ensemble run onto a common time vector using the interpolation scheme (*`Interpolation`*).

Examples

This example shows how to perform an ensemble run and generate a 2-D distribution plot.

1 The project file, `radiodecay.sbproj`, contains a model stored in a variable called `m1`. Load `m1` into the MATLAB workspace.

```
sbioloadproject('radiodecay.sbproj','m1');
```

2 Change the solver of the active configset to be `ssa`. Also, adjust the `LogDecimation` property on the `SolverOptions` property of the configuration set.

```
cs = getconfigset(m1, 'active');
set(cs, 'SolverType', 'ssa');
so = get(cs, 'SolverOptions');
set(so, 'LogDecimation', 10);
```

Tip The `LogDecimation` property lets you define how often the simulation data is recorded as output. If your model has high concentrations or amounts of species, or a long simulation time (for example, `600s`), you can record simulation data less often to manage the amount of data

generated. Be aware that by doing so you might miss some transitions if your model is very dynamic. Try setting `LogDecimation` to 10 or more.

3 Perform an ensemble of 20 runs with linear interpolation to get a consistent time vector.

```
simdata = sbioensemblerun(m1, 20, 'linear');
```

4 Create a 2-D distribution plot of the species `'z'` at a time = 1.0.

```
FH = sbioensembleplot(simdata, 'z', 1.0);
```

Version History

Introduced in R2006a

See Also

`addconfigset` | `getconfigset` | `sbioensemblestats` | `sbioensembleplot` | `setactiveconfigset` | `SimData object`

sbioensemblestats

Get statistics from ensemble run data

Syntax

```
[t,m] = sbioensemblestats(simDataObj)
[t,m,v] = sbioensemblestats(simDataObj)
[t,m,v,n] = sbioensemblestats(simDataObj)
[t,m,v,n] = sbioensemblestats(simDataObj,names)
[t,m,v,n] = sbioensemblestats(simDataObj,names,interpolation)
```

Arguments

t	Column vector of time points
m	Matrix of mean values from the ensemble data. The number of rows in *m* is the length of the time vector *t* and the number of columns is equal to the number of species.
simDataObj	A cell array of SimData objects, where each SimData object holds data for a separate simulation run. All elements of *simDataObj* must contain data for the same states in the same model. When the time vectors of the elements of *simDataObj* are not identical, *simDataObj* is first resampled onto a common time vector (see *interpolation* below).
v	Matrix of variance obtained from the ensemble data. *v* has the same dimensions as *m*.
n	Cell array of character vectors for the quantity names whose mean and variance are returned in *m* and *v*, respectively. The number of elements in *n* is the same as the number of columns of *m* and *v*. The order of names in *n* corresponds to the order of columns of *m* and *v*.
names	Character vector, string, string vector, string array, or cell array of character vectors. *names* may include qualified names such as *'CompartmentName.SpeciesName'* or *'ReactionName.ParameterName'* to resolve ambiguities. If you specify empty `{}` or empty string array (`string.empty`) for *names*, `sbioensemblestats` returns statistics on all time courses contained in *simDataObj*.
interpolation	Character vector or string denoting the interpolation method to use for resampling of the data onto a common time vector with the smallest simulation stop time. See `resample` for a list of interpolation methods. Default is `'linear'`.

Description

`[t,m] = sbioensemblestats(simDataObj)` computes the time-dependent ensemble mean *m* of the ensemble data *simDataObj*. If the time vectors of the ensemble data are not identical, by default, the function uses the `'linear'` interpolation method to resample the data onto the common time vector. See `resample` for a list of interpolation methods.

`[t,m,v] = sbioensemblestats(simDataObj)` also returns the variance `v` for the ensemble run data `simDataObj`.

`[t,m,v,n] = sbioensemblestats(simDataObj)` also returns the names of quantities `n` corresponding to the mean `m` and variance `v` columns. Each column of `m` or `v` describes the ensemble mean or variance of a quantity (or state) as a function of time.

`[t,m,v,n] = sbioensemblestats(simDataObj,names)` computes statistics only for the quantities specified by `names`.

`[t,m,v,n] = sbioensemblestats(simDataObj,names,interpolation)` uses the interpolation method `interpolation` to resample the simulation data to have a consistent time vector. If the time vectors of the ensemble data are not identical and if you do not specify any interpolation method, the function uses the `'linear'` interpolation method by default.

Examples

The project file, `radiodecay.sbproj`, contains a model stored in a variable called `m1`. Load `m1` into the MATLAB workspace.

1. Load a SimBiology model `m1` from a SimBiology project file.

   ```
   sbioloadproject('radiodecay.sbproj','m1');
   ```

2. Change the solver of the active configuration set to be `ssa`. Also, adjust the `LogDecimation` property on the `SolverOptions` property of the configuration set.

   ```
   cs = getconfigset(m1, 'active');
   set(cs, 'SolverType', 'ssa');
   so = get(cs, 'SolverOptions');
   set(so, 'LogDecimation', 10);
   ```

3. Perform an ensemble of 20 runs with no interpolation.

   ```
   simDataObj = sbioensemblerun(m1, 20);
   ```

4. Get ensemble statistics for all species using the default interpolation method.

   ```
   [T,M,V] = sbioensemblestats(simDataObj);
   ```

5. Get ensemble statistics for a specific species using the default interpolation scheme.

   ```
   [T2,M2,V2] = sbioensemblestats(simDataObj, {'z'});
   ```

Version History

Introduced in R2006a

See Also

`sbioensemblerun` | `sbioensembleplot` | `sbiomodel`

sbiofit

Perform nonlinear least-squares regression

Note Statistics and Machine Learning Toolbox™, Optimization Toolbox™, and Global Optimization Toolbox are recommended for this function.

Syntax

```
fitResults = sbiofit(sm,grpData,ResponseMap,estiminfo)
fitResults = sbiofit(sm,grpData,ResponseMap,estiminfo,dosing)
fitResults = sbiofit(sm,grpData,ResponseMap,estiminfo,dosing,functionName)
fitResults = sbiofit(sm,grpData,ResponseMap,estiminfo,dosing,functionName,
options)
fitResults = sbiofit(sm,grpData,ResponseMap,estiminfo,dosing,functionName,
options,variants)
fitResults = sbiofit(_,Name,Value)

[fitResults,simdata] = sbiofit(_)
```

Description

`fitResults = sbiofit(sm,grpData,ResponseMap,estiminfo)` estimates parameters of a SimBiology model `sm` using nonlinear least-squares regression.

`grpData` is a `groupedData object` specifying the data to fit. `ResponseMap` defines the mapping between the model components and response data in `grpData`. `estimatedInfo` is an `EstimatedInfo object` that defines the estimated parameters in the model `sm`. `fitResults` is a `OptimResults object` or `NLINResults object` or a vector of these objects.

`sbiofit` uses the first available estimation function among the following: `lsqnonlin`, `nlinfit`, or `fminsearch`.

By default, each group in `grpData` is fit separately, resulting in group-specific parameter estimates. If the model contains active doses and variants, they are applied before the simulation.

`fitResults = sbiofit(sm,grpData,ResponseMap,estiminfo,dosing)` uses the dosing information specified by a matrix of SimBiology dose objects `dosing` instead of using the active doses of the model `sm` if there is any.

`fitResults = sbiofit(sm,grpData,ResponseMap,estiminfo,dosing,functionName)` uses the estimation function specified by `functionName`. If the specified function is unavailable, a warning is issued and the first available default function is used.

`fitResults = sbiofit(sm,grpData,ResponseMap,estiminfo,dosing,functionName, options)` uses the additional options specified by `options` for the function `functionName`.

`fitResults = sbiofit(sm,grpData,ResponseMap,estiminfo,dosing,functionName, options,variants)` applies variant objects specified as `variants` instead of using any active variants of the model.

`fitResults = sbiofit(_,Name,Value)` uses additional options specified by one or more `Name,Value` pair arguments.

`[fitResults,simdata] = sbiofit(_)` also returns a vector of SimData objects `simdata` using any of the input arguments in the previous syntaxes.

Note

- `sbiofit` unifies `sbionlinfit` and `sbioparamestim` estimation functions. Use `sbiofit` to perform nonlinear least-squares regression.
- `sbiofit` simulates the model using a `SimFunction object`, which automatically accelerates simulations by default. Hence it is not necessary to run `sbioaccelerate` before you call `sbiofit`.

Examples

Fit One-Compartment Model to Individual PK Profile

Background

This example shows how to fit an individual's PK profile data to one-compartment model and estimate pharmacokinetic parameters.

Suppose you have drug plasma concentration data from an individual and want to estimate the volume of the central compartment and the clearance. Assume the drug concentration versus the time profile follows the monoexponential decline $C_t = C_0 e^{-k_e t}$, where C_t is the drug concentration at time t, C_0 is the initial concentration, and k_e is the elimination rate constant that depends on the clearance and volume of the central compartment $k_e = Cl/V$.

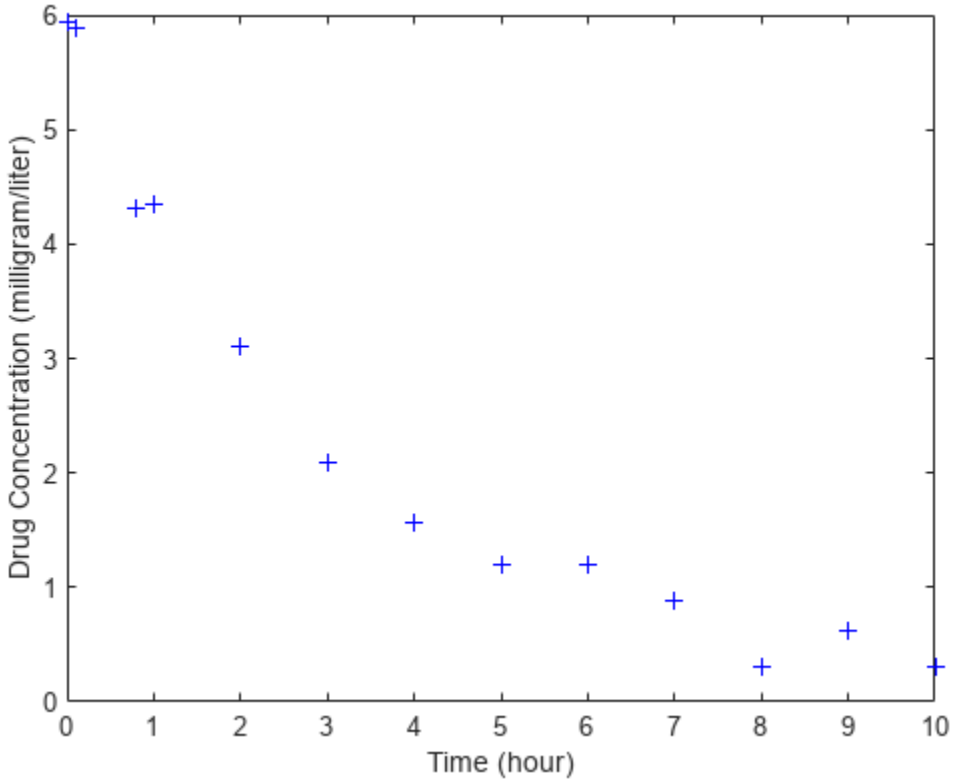
The synthetic data in this example was generated using the following model, parameters, and dose:

- One-compartment model with bolus dosing and first-order elimination
- Volume of the central compartment (`Central`) = 1.70 liter
- Clearance parameter (`Cl_Central`) = 0.55 liter/hour
- Constant error model
- Bolus dose of 10 mg

Load Data and Visualize

The data is stored as a table with variables `Time` and `Conc` that represent the time course of the plasma concentration of an individual after an intravenous bolus administration measured at 13 different time points. The variable units for `Time` and `Conc` are hour and milligram/liter, respectively.

```
load('data15.mat')
plot(data.Time,data.Conc,'b+')
xlabel('Time (hour)');
ylabel('Drug Concentration (milligram/liter)');
```



Convert to groupedData Format

Convert the data set to a `groupedData` object, which is the required data format for the fitting function `sbiofit` for later use. A `groupedData` object also lets you set independent variable and group variable names (if they exist). Set the units of the `Time` and `Conc` variables. The units are optional and only required for the `UnitConversion` feature, which automatically converts matching physical quantities to one consistent unit system.

```
gData = groupedData(data);
gData.Properties.VariableUnits = {'hour','milligram/liter'};
gData.Properties
```

```
ans = struct with fields:
                Description: ''
                   UserData: []
             DimensionNames: {'Row'  'Variables'}
              VariableNames: {'Time'  'Conc'}
       VariableDescriptions: {}
              VariableUnits: {'hour'  'milligram/liter'}
         VariableContinuity: []
                   RowNames: {}
           CustomProperties: [1x1 matlab.tabular.CustomProperties]
          GroupVariableName: ''
    IndependentVariableName: 'Time'
```

`groupedData` automatically set the name of the `IndependentVariableName` property to the `Time` variable of the data.

Construct a One-Compartment Model

Use the built-in PK library to construct a one-compartment model with bolus dosing and first-order elimination where the elimination rate depends on the clearance and volume of the central compartment. Use the `configset` object to turn on unit conversion.

```
pkmd                    = PKModelDesign;
pkc1                    = addCompartment(pkmd,'Central');
pkc1.DosingType         = 'Bolus';
pkc1.EliminationType    = 'linear-clearance';
pkc1.HasResponseVariable = true;
model                   = construct(pkmd);
configset               = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
```

For details on creating compartmental PK models using the SimBiology® built-in library, see “Create Pharmacokinetic Models”.

Define Dosing

Define a single bolus dose of 10 milligram given at time = 0. For details on setting up different dosing schedules, see “Doses in SimBiology Models”.

```
dose                = sbiodose('dose');
dose.TargetName     = 'Drug_Central';
dose.StartTime      = 0;
dose.Amount         = 10;
dose.AmountUnits    = 'milligram';
dose.TimeUnits      = 'hour';
```

Map Response Data to the Corresponding Model Component

The data contains drug concentration data stored in the `Conc` variable. This data corresponds to the `Drug_Central` species in the model. Therefore, map the data to `Drug_Central` as follows.

```
responseMap = {'Drug_Central = Conc'};
```

Specify Parameters to Estimate

The parameters to fit in this model are the volume of the central compartment (Central) and the clearance rate (Cl_Central). In this case, specify log-transformation for these biological parameters since they are constrained to be positive. The `estimatedInfo` object lets you specify parameter transforms, initial values, and parameter bounds if needed.

```
paramsToEstimate    = {'log(Central)','log(Cl_Central)'};
estimatedParams     = estimatedInfo(paramsToEstimate,'InitialValue',[1 1],'Bounds',[1 5;0.5 2]);
```

Estimate Parameters

Now that you have defined one-compartment model, data to fit, mapped response data, parameters to estimate, and dosing, use `sbiofit` to estimate parameters. The default estimation function that `sbiofit` uses will change depending on which toolboxes are available. To see which function was used during fitting, check the `EstimationFunction` property of the corresponding results object.

```
fitConst = sbiofit(model,gData,responseMap,estimatedParams,dose);
```

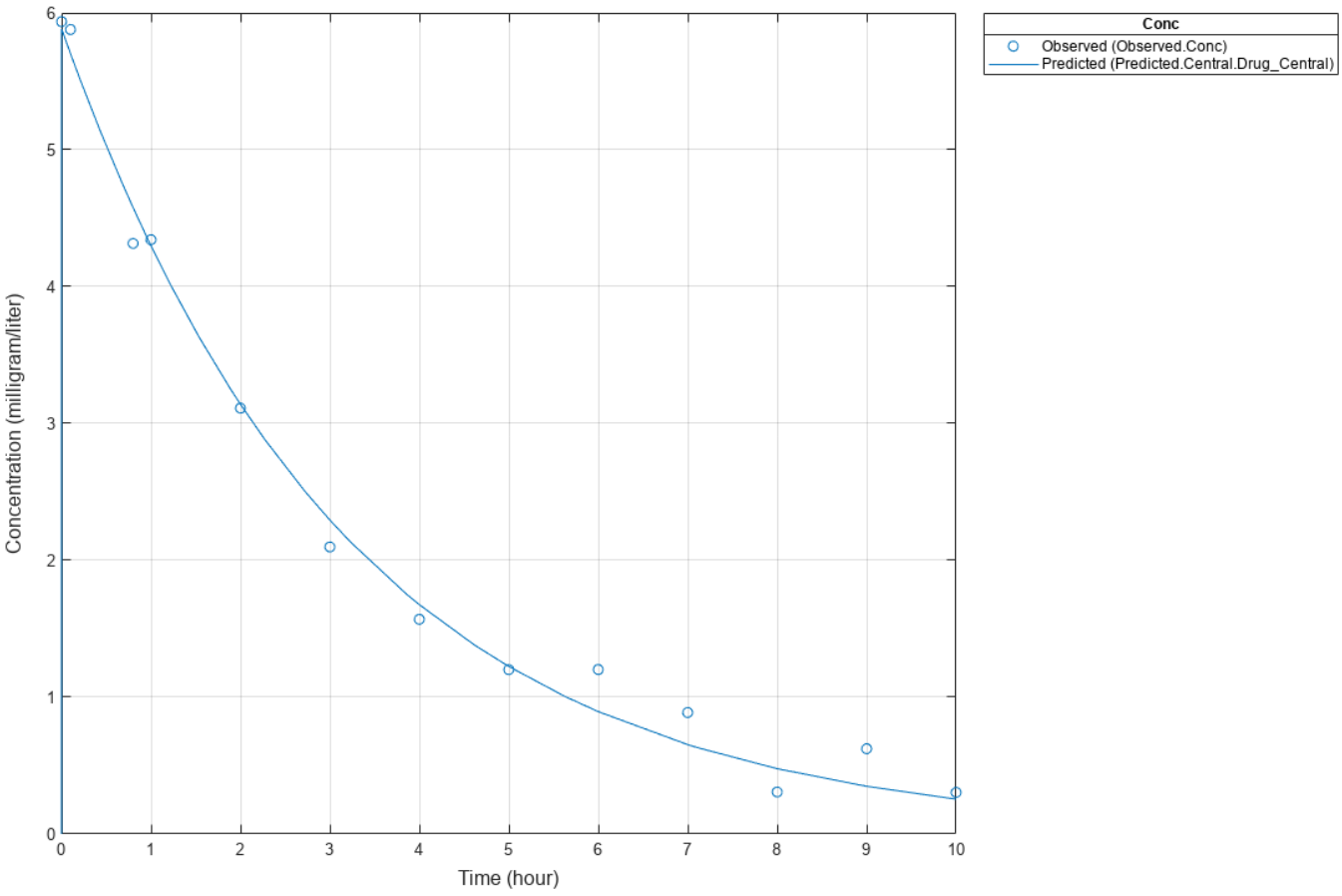
Display Estimated Parameters and Plot Results

Notice the parameter estimates were not far off from the true values (1.70 and 0.55) that were used to generate the data. You may also try different error models to see if they could further improve the parameter estimates.

```
fitConst.ParameterEstimates
```

```
ans=2×4 table
        Name          Estimate    StandardError      Bounds
    ______________    ________    _____________    __________

    {'Central'   }     1.6993       0.034821          1      5
    {'Cl_Central'}    0.53358        0.01968        0.5      2
```

```
s.Labels.XLabel     = 'Time (hour)';
s.Labels.YLabel     = 'Concentration (milligram/liter)';
plot(fitConst,'AxesStyle',s);
```



Use Different Error Models

Try three other supported error models (proportional, combination of constant and proportional error models, and exponential).

```
fitProp = sbiofit(model,gData,responseMap,estimatedParams,dose,...
                        'ErrorModel','proportional');
fitExp  = sbiofit(model,gData,responseMap,estimatedParams,dose,...
                        'ErrorModel','exponential');
fitComb = sbiofit(model,gData,responseMap,estimatedParams,dose,...
                        'ErrorModel','combined');
```

Use Weights Instead of an Error Model

You can specify weights as a numeric matrix, where the number of columns corresponds to the number of responses. Setting all weights to 1 is equivalent to the constant error model.

```
weightsNumeric = ones(size(gData.Conc));
fitWeightsNumeric = sbiofit(model,gData,responseMap,estimatedParams,dose,'Weights',weightsNumeric
```

Alternatively, you can use a function handle that accepts a vector of predicted response values and returns a vector of weights. In this example, use a function handle that is equivalent to the proportional error model.

```
weightsFunction = @(y) 1./y.^2;
fitWeightsFunction = sbiofit(model,gData,responseMap,estimatedParams,dose,'Weights',weightsFunct
```

Compare Information Criteria for Model Selection

Compare the loglikelihood, AIC, and BIC values of each model to see which error model best fits the data. A larger likelihood value indicates the corresponding model fits the model better. For AIC and BIC, the smaller values are better.

```
allResults = [fitConst,fitWeightsNumeric,fitWeightsFunction,fitProp,fitExp,fitComb];
errorModelNames = {'constant error model','equal weights','proportional weights', ...
                   'proportional error model','exponential error model',...
                   'combined error model'};
LogLikelihood = [allResults.LogLikelihood]';
AIC = [allResults.AIC]';
BIC = [allResults.BIC]';
t = table(LogLikelihood,AIC,BIC);
t.Properties.RowNames = errorModelNames;
t
```

```
t=6×3 table
                               LogLikelihood      AIC        BIC
                               _____________    _______    _______

    constant error model           3.9866       -3.9732    -2.8433
    equal weights                  3.9866       -3.9732    -2.8433
    proportional weights          -3.8472        11.694     12.824
    proportional error model      -3.8257        11.651     12.781
    exponential error model        1.1984        1.6032     2.7331
    combined error model           3.9163       -3.8326    -2.7027
```

Based on the information criteria, the constant error model (or equal weights) fits the data best since it has the largest loglikelihood value and the smallest AIC and BIC.

Display Estimated Parameter Values

Show the estimated parameter values of each model.

```
Estimated_Central       = zeros(6,1);
Estimated_Cl_Central    = zeros(6,1);
t2 = table(Estimated_Central,Estimated_Cl_Central);
t2.Properties.RowNames = errorModelNames;
for i = 1:height(t2)
    t2{i,1} = allResults(i).ParameterEstimates.Estimate(1);
    t2{i,2} = allResults(i).ParameterEstimates.Estimate(2);
end
t2
```

```
t2=6×2 table
                                Estimated_Central    Estimated_Cl_Central
                                _________________    ____________________

    constant error model             1.6993                0.53358
    equal weights                     1.6993                0.53358
    proportional weights              1.9045                0.51734
    proportional error model          1.8777                0.51147
    exponential error model           1.7872                0.51701
    combined error model              1.7008                0.53271
```

Conclusion

This example showed how to estimate PK parameters, namely the volume of the central compartment and clearance parameter of an individual, by fitting the PK profile data to one-compartment model. You compared the information criteria of each model and estimated parameter values of different error models to see which model best explained the data. Final fitted results suggested both the constant and combined error models provided the closest estimates to the parameter values used to generate the data. However, the constant error model is a better model as indicated by the loglikelihood, AIC, and BIC information criteria.

Fit Two-Compartment Model to PK Profiles of Multiple Individuals

Suppose you have drug plasma concentration data from three individuals that you want to use to estimate corresponding pharmacokinetic parameters, namely the volume of central and peripheral compartment (`Central`, `Peripheral`), the clearance rate (`Cl_Central`), and intercompartmental clearance (`Q12`). Assume the drug concentration versus the time profile follows the biexponential decline $C_t = Ae^{-at} + Be^{-bt}$, where C_t is the drug concentration at time t, and a and b are slopes for corresponding exponential declines.

The synthetic data set contains drug plasma concentration data measured in both central and peripheral compartments. The data was generated using a two-compartment model with an infusion dose and first-order elimination. These parameters were used for each individual.

	`Central`	`Peripheral`	`Q12`	`Cl_Central`
Individual 1	1.90	0.68	0.24	0.57
Individual 2	2.10	6.05	0.36	0.95
Individual 3	1.70	4.21	0.46	0.95

The data is stored as a table with variables `ID`, `Time`, `CentralConc`, and `PeripheralConc`. It represents the time course of plasma concentrations measured at eight different time points for both central and peripheral compartments after an infusion dose.

```
load('data10_32R.mat')
```

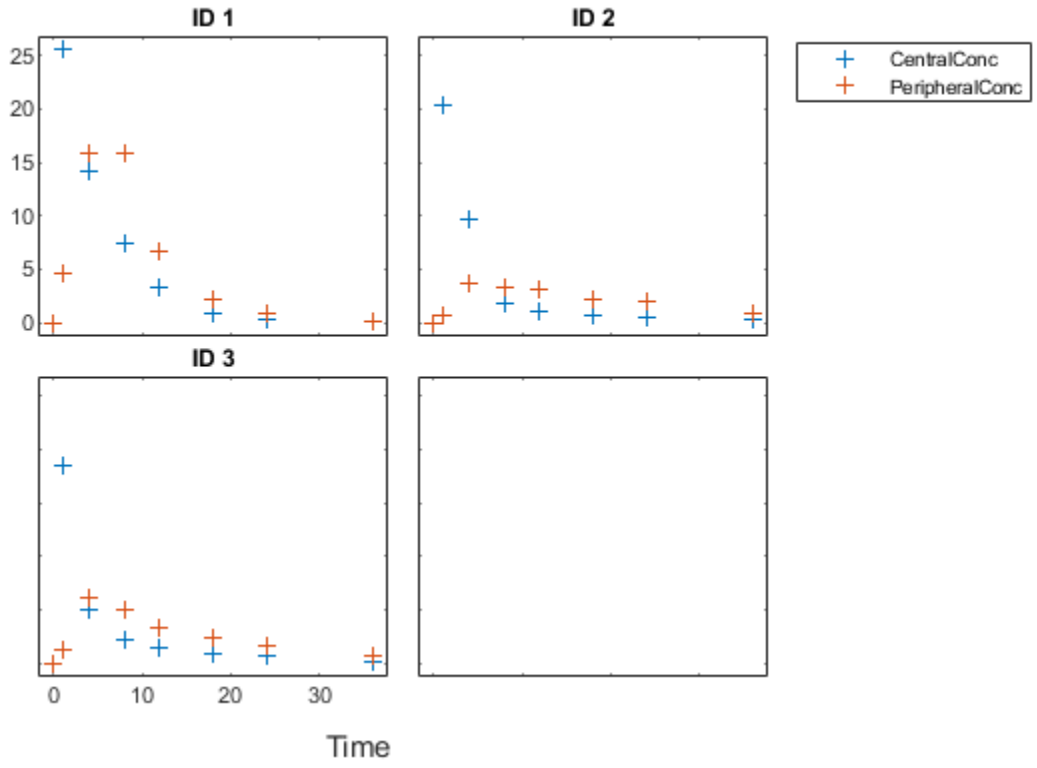
Convert the data set to a `groupedData` object which is the required data format for the fitting function `sbiofit` for later use. A `groupedData` object also lets you set independent variable and group variable names (if they exist). Set the units of the `ID`, `Time`, `CentralConc`, and `PeripheralConc` variables. The units are optional and only required for the `UnitConversion` feature, which automatically converts matching physical quantities to one consistent unit system.

```
gData = groupedData(data);
gData.Properties.VariableUnits = {'','hour','milligram/liter','milligram/liter'};
gData.Properties
```

```
ans =

  struct with fields:

                Description: ''
                   UserData: []
             DimensionNames: {'Row'  'Variables'}
              VariableNames: {'ID'  'Time'  'CentralConc'  'PeripheralConc'}
        VariableDescriptions: {}
               VariableUnits: {1x4 cell}
          VariableContinuity: []
                     RowNames: {}
           CustomProperties: [1x1 matlab.tabular.CustomProperties]
          GroupVariableName: 'ID'
    IndependentVariableName: 'Time'
```

Create a trellis plot that shows the PK profiles of three individuals.

```
sbiotrellis(gData,'ID','Time',{'CentralConc','PeripheralConc'},...
            'Marker','+','LineStyle','none');
```



Use the built-in PK library to construct a two-compartment model with infusion dosing and first-order elimination where the elimination rate depends on the clearance and volume of the central compartment. Use the configset object to turn on unit conversion.

```
pkmd                 = PKModelDesign;
pkc1                 = addCompartment(pkmd,'Central');
pkc1.DosingType      = 'Infusion';
pkc1.EliminationType = 'linear-clearance';
pkc1.HasResponseVariable = true;
pkc2                 = addCompartment(pkmd,'Peripheral');
model                = construct(pkmd);
configset            = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
```

Assume every individual receives an infusion dose at time = 0, with a total infusion amount of 100 mg at a rate of 50 mg/hour. For details on setting up different dosing strategies, see “Doses in SimBiology Models”.

```
dose             = sbiodose('dose','TargetName','Drug_Central');
dose.StartTime   = 0;
dose.Amount      = 100;
dose.Rate        = 50;
dose.AmountUnits = 'milligram';
dose.TimeUnits   = 'hour';
dose.RateUnits   = 'milligram/hour';
```

The data contains measured plasma concentrations in the central and peripheral compartments. Map these variables to the appropriate model species, which are `Drug_Central` and `Drug_Peripheral`.

```
responseMap = {'Drug_Central = CentralConc','Drug_Peripheral = PeripheralConc'};
```

The parameters to estimate in this model are the volumes of central and peripheral compartments (`Central` and `Peripheral`), intercompartmental clearance `Q12`, and clearance rate `Cl_Central`. In this case, specify log-transform for `Central` and `Peripheral` since they are constrained to be positive. The `estimatedInfo` object lets you specify parameter transforms, initial values, and parameter bounds (optional).

```
paramsToEstimate   = {'log(Central)','log(Peripheral)','Q12','Cl_Central'};
estimatedParam     = estimatedInfo(paramsToEstimate,'InitialValue',[1 1 1 1]);
```

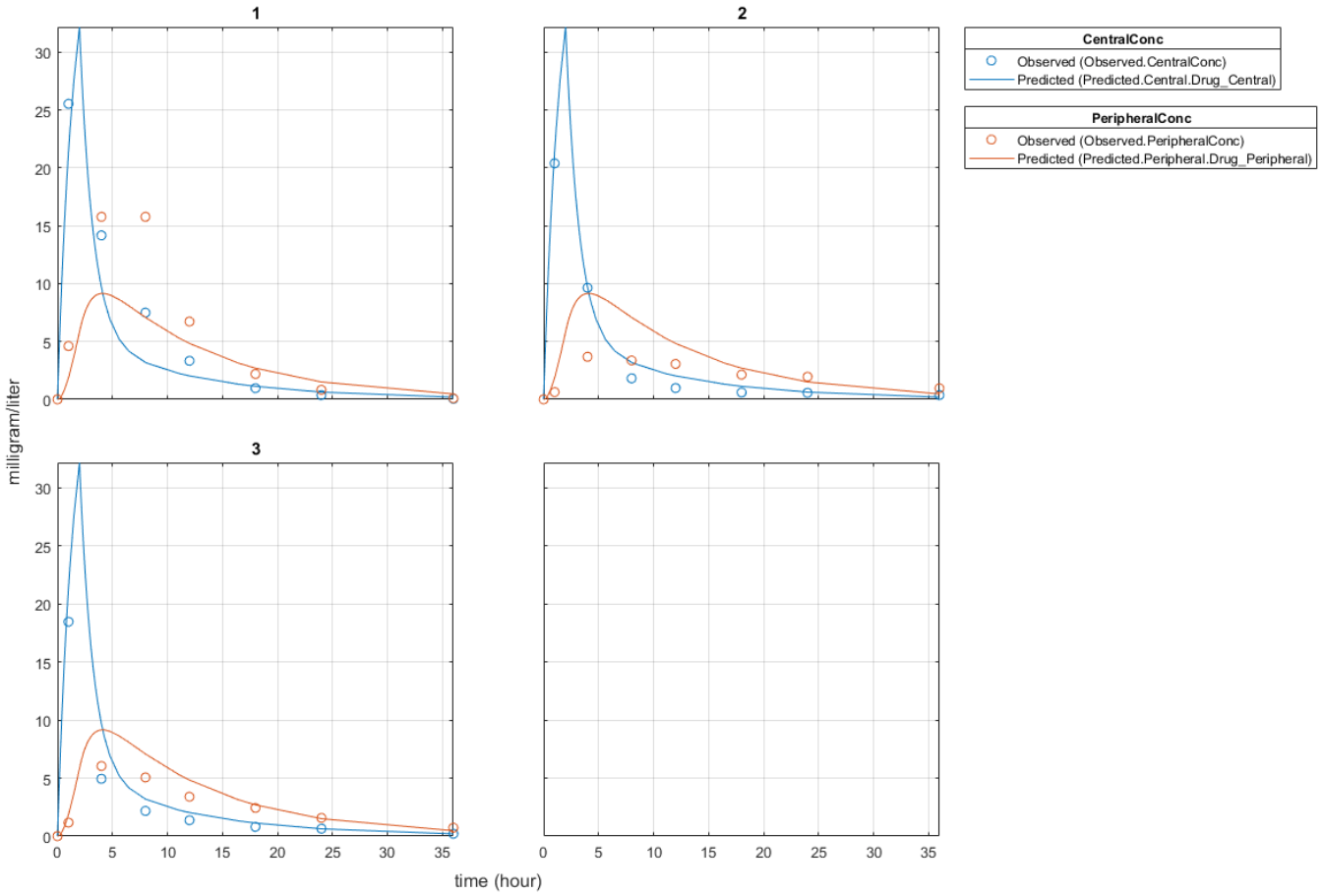
Fit the model to all of the data pooled together, that is, estimate one set of parameters for all individuals. The default estimation method that `sbiofit` uses will change depending on which toolboxes are available. To see which estimation function `sbiofit` used for the fitting, check the `EstimationFunction` property of the corresponding results object.

```
pooledFit = sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',true)
```

```
pooledFit =

  OptimResults with properties:

                  ExitFlag: 3
                    Output: [1x1 struct]
                 GroupName: []
                      Beta: [4x3 table]
        ParameterEstimates: [4x3 table]
                         J: [24x4x2 double]
                      COVB: [4x4 double]
          CovarianceMatrix: [4x4 double]
                         R: [24x2 double]
                       MSE: 6.6220
                       SSE: 291.3688
                   Weights: []
              LogLikelihood: -111.3904
                       AIC: 230.7808
                       BIC: 238.2656
                       DFE: 44
            DependentFiles: {1x3 cell}
                      Data: [24x4 groupedData]
   EstimatedParameterNames: {'Central'  'Peripheral'  'Q12'  'Cl_Central'}
            ErrorModelInfo: [1x3 table]
        EstimationFunction: 'lsqnonlin'
```

Plot the fitted results versus the original data. Although three separate plots were generated, the data was fitted using the same set of parameters (that is, all three individuals had the same fitted line).

```
plot(pooledFit);
```

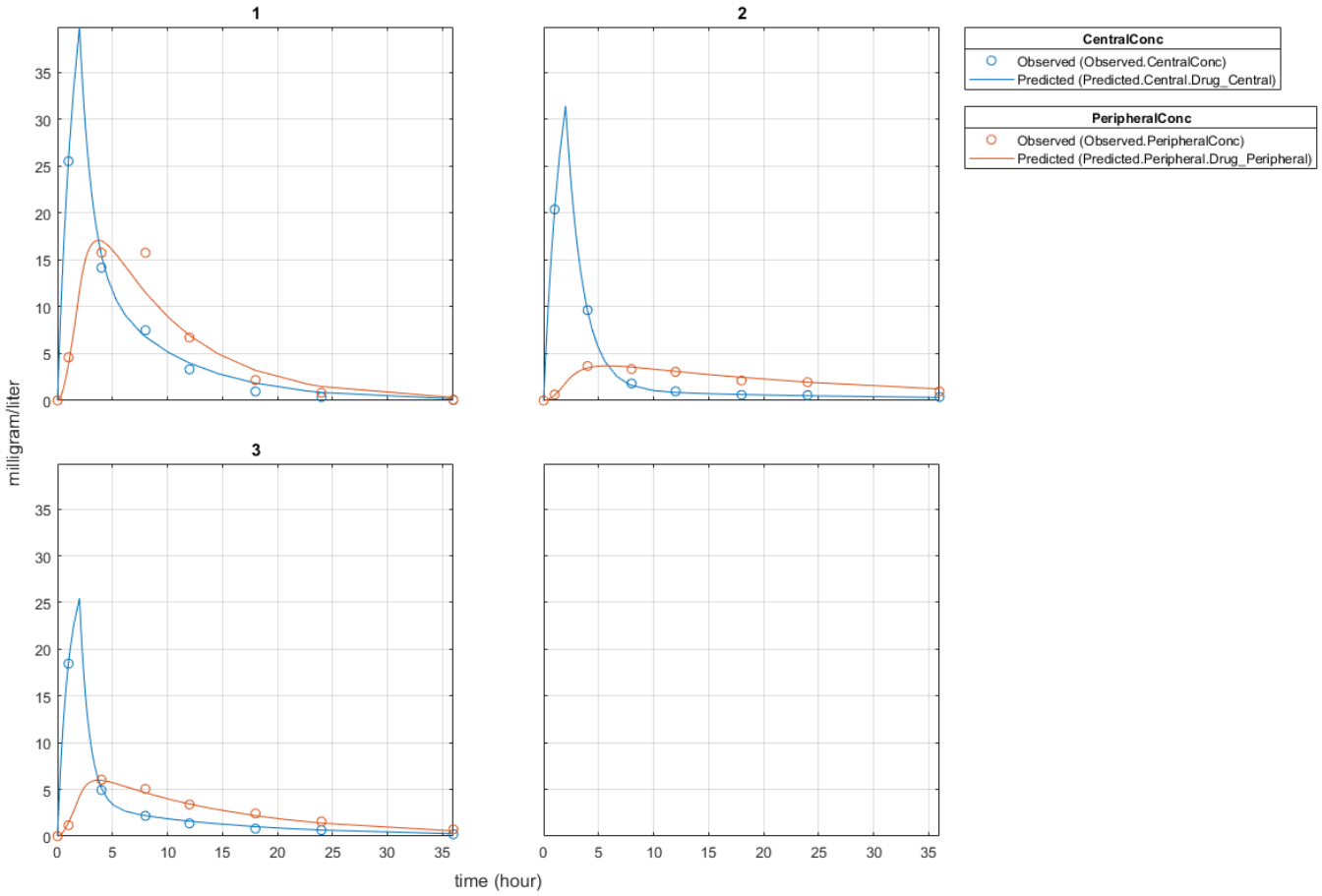


Estimate one set of parameters for each individual and see if there is any improvement in the parameter estimates. In this example, since there are three individuals, three sets of parameters are estimated.

```
unpooledFit =  sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',false);
```

Plot the fitted results versus the original data. Each individual was fitted differently (that is, each fitted line is unique to each individual) and each line appeared to fit well to individual data.

```
plot(unpooledFit);
```



Display the fitted results of the first individual. The MSE was lower than that of the pooled fit. This is also true for the other two individuals.

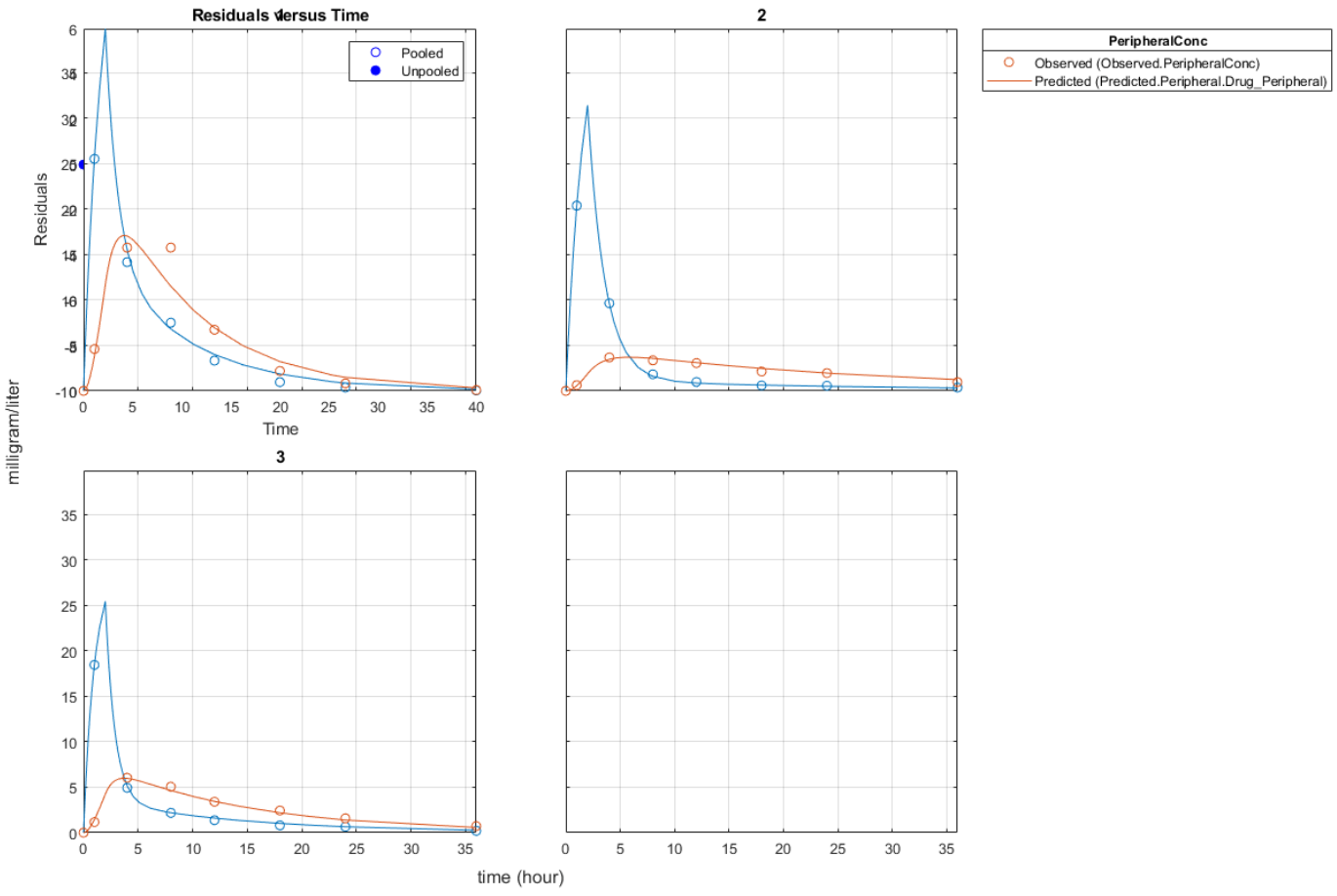
```
unpooledFit(1)
```

```
ans =

  OptimResults with properties:

                 ExitFlag: 3
                   Output: [1x1 struct]
                GroupName: 1
                     Beta: [4x3 table]
       ParameterEstimates: [4x3 table]
                        J: [8x4x2 double]
                     COVB: [4x4 double]
         CovarianceMatrix: [4x4 double]
                        R: [8x2 double]
                      MSE: 2.1380
                      SSE: 25.6559
                  Weights: []
            LogLikelihood: -26.4805
                      AIC: 60.9610
                      BIC: 64.0514
```

```
                    DFE: 12
          DependentFiles: {1x3 cell}
                    Data: [8x4 groupedData]
EstimatedParameterNames: {'Central'  'Peripheral'  'Q12'  'Cl_Central'}
          ErrorModelInfo: [1x3 table]
      EstimationFunction: 'lsqnonlin'
```

Generate a plot of the residuals over time to compare the pooled and unpooled fit results. The figure indicates unpooled fit residuals are smaller than those of pooled fit as expected. In addition to comparing residuals, other rigorous criteria can be used to compare the fitted results.

```
t = [gData.Time;gData.Time];
res_pooled = vertcat(pooledFit.R);
res_pooled = res_pooled(:);
res_unpooled = vertcat(unpooledFit.R);
res_unpooled = res_unpooled(:);
plot(t,res_pooled,'o','MarkerFaceColor','w','markerEdgeColor','b')
hold on
plot(t,res_unpooled,'o','MarkerFaceColor','b','markerEdgeColor','b')
refl = refline(0,0); % A reference line representing a zero residual
title('Residuals versus Time');
xlabel('Time');
ylabel('Residuals');
legend({'Pooled','Unpooled'});
```



This example showed how to perform pooled and unpooled estimations using `sbiofit`. As illustrated, the unpooled fit accounts for variations due to the specific subjects in the study, and, in this case, the model fits better to the data. However, the pooled fit returns population-wide parameters. If you want to estimate population-wide parameters while considering individual variations, use `sbiofitmixed`.

Estimate Category-Specific PK Parameters for Multiple Individuals

This example shows how to estimate category-specific (such as young versus old, male versus female), individual-specific, and population-wide parameters using PK profile data from multiple individuals.

Background

Suppose you have drug plasma concentration data from 30 individuals and want to estimate pharmacokinetic parameters, namely the volumes of central and peripheral compartment, the clearance, and intercompartmental clearance. Assume the drug concentration versus the time profile follows the biexponential decline $C_t = Ae^{-at} + Be^{-bt}$, where C_t is the drug concentration at time t, and a and b are slopes for corresponding exponential declines.

Load Data

This synthetic data contains the time course of plasma concentrations of 30 individuals after a bolus dose (100 mg) measured at different times for both central and peripheral compartments. It also contains categorical variables, namely `Sex` and `Age`.

```
clear
load('sd5_302RAgeSex.mat')
```

Convert to groupedData Format

Convert the data set to a `groupedData` object, which is the required data format for the fitting function `sbiofit`. A `groupedData` object also allows you set independent variable and group variable names (if they exist). Set the units of the `ID`, `Time`, `CentralConc`, `PeripheralConc`, `Age`, and `Sex` variables. The units are optional and only required for the `UnitConversion` feature, which automatically converts matching physical quantities to one consistent unit system.

```
gData = groupedData(data);
gData.Properties.VariableUnits = {'','hour','milligram/liter','milligram/liter','',''};
gData.Properties
```

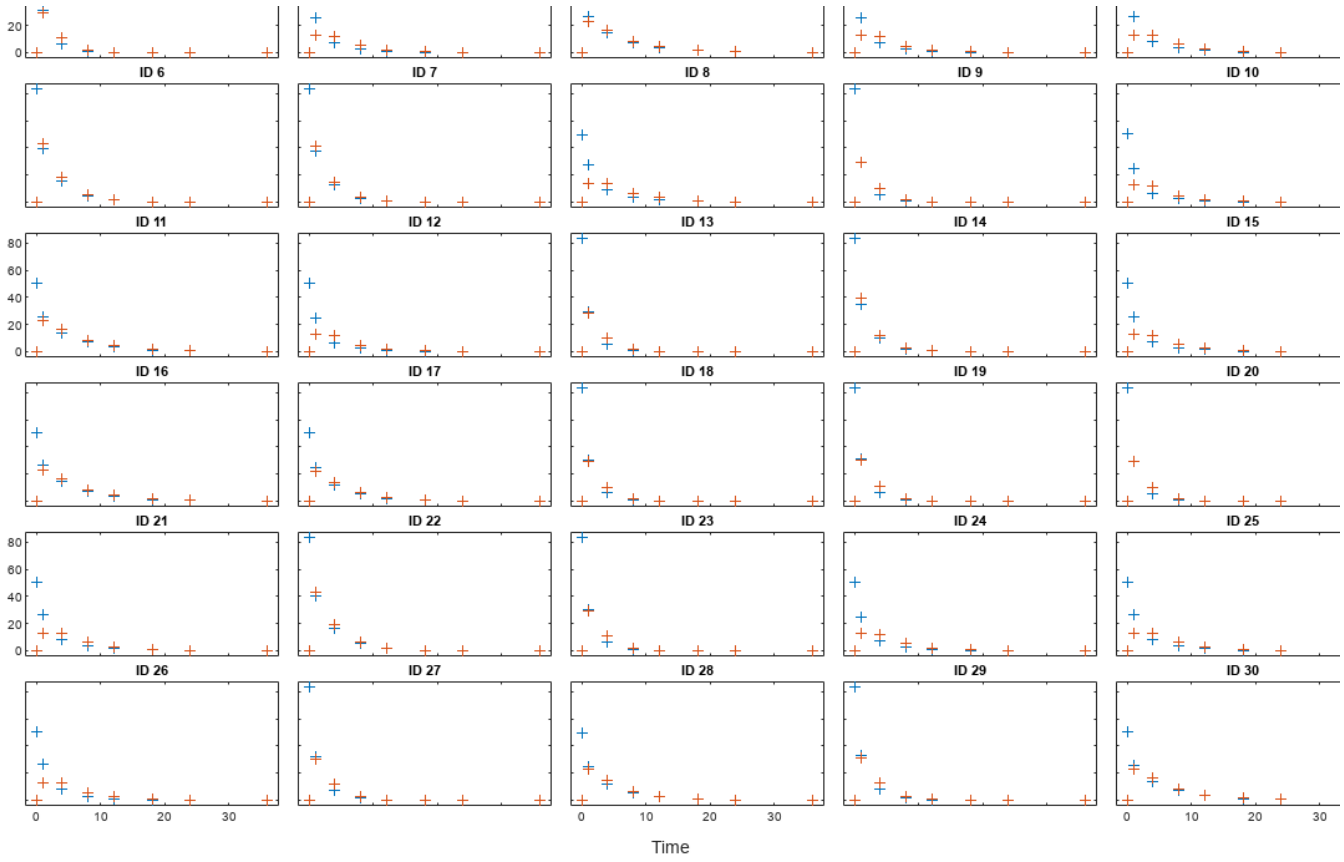
```
ans = struct with fields:
                Description: ''
                   UserData: []
              DimensionNames: {'Row'  'Variables'}
               VariableNames: {'ID'  'Time'  'CentralConc'  'PeripheralConc'  'Sex'  'Age'}
       VariableDescriptions: {}
              VariableUnits: {''  'hour'  'milligram/liter'  'milligram/liter'  ''  ''}
         VariableContinuity: []
                   RowNames: {}
           CustomProperties: [1x1 matlab.tabular.CustomProperties]
          GroupVariableName: 'ID'
    IndependentVariableName: 'Time'
```

The `IndependentVariableName` and `GroupVariableName` properties have been automatically set to the `Time` and `ID` variables of the data.

Visualize Data

Display the response data for each individual.

```
t = sbiotrellis(gData,'ID','Time',{'CentralConc','PeripheralConc'},...
                'Marker','+','LineStyle','none');
% Resize the figure.
t.hFig.Position(:) = [100 100 1280 800];
```



Set Up a Two-Compartment Model

Use the built-in PK library to construct a two-compartment model with infusion dosing and first-order elimination where the elimination rate depends on the clearance and volume of the central compartment. Use the `configset` object to turn on unit conversion.

```
pkmd                                    = PKModelDesign;
pkc1                                    = addCompartment(pkmd,'Central');
pkc1.DosingType                         = 'Bolus';
pkc1.EliminationType                    = 'linear-clearance';
pkc1.HasResponseVariable                = true;
pkc2                                    = addCompartment(pkmd,'Peripheral');
model                                   = construct(pkmd);
configset                               = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
```

For details on creating compartmental PK models using the SimBiology® built-in library, see “Create Pharmacokinetic Models”.

Define Dosing

Assume every individual receives a bolus dose of 100 mg at time = 0. For details on setting up different dosing strategies, see “Doses in SimBiology Models”.

```
dose             = sbiodose('dose','TargetName','Drug_Central');
dose.StartTime   = 0;
dose.Amount      = 100;
dose.AmountUnits = 'milligram';
dose.TimeUnits   = 'hour';
```

Map the Response Data to Corresponding Model Components

The data contains measured plasma concentration in the central and peripheral compartments. Map these variables to the appropriate model components, which are `Drug_Central` and `Drug_Peripheral`.

```
responseMap = {'Drug_Central = CentralConc','Drug_Peripheral = PeripheralConc'};
```

Specify Parameters to Estimate

Specify the volumes of central and peripheral compartments `Central` and `Peripheral`, intercompartmental clearance `Q12`, and clearance `Cl_Central` as parameters to estimate. The `estimatedInfo` object lets you optionally specify parameter transforms, initial values, and parameter bounds. Since both `Central` and `Peripheral` are constrained to be positive, specify a log-transform for each parameter.

```
paramsToEstimate    = {'log(Central)', 'log(Peripheral)', 'Q12', 'Cl_Central'};
estimatedParam      = estimatedInfo(paramsToEstimate,'InitialValue',[1 1 1 1]);
```

Estimate Individual-Specific Parameters

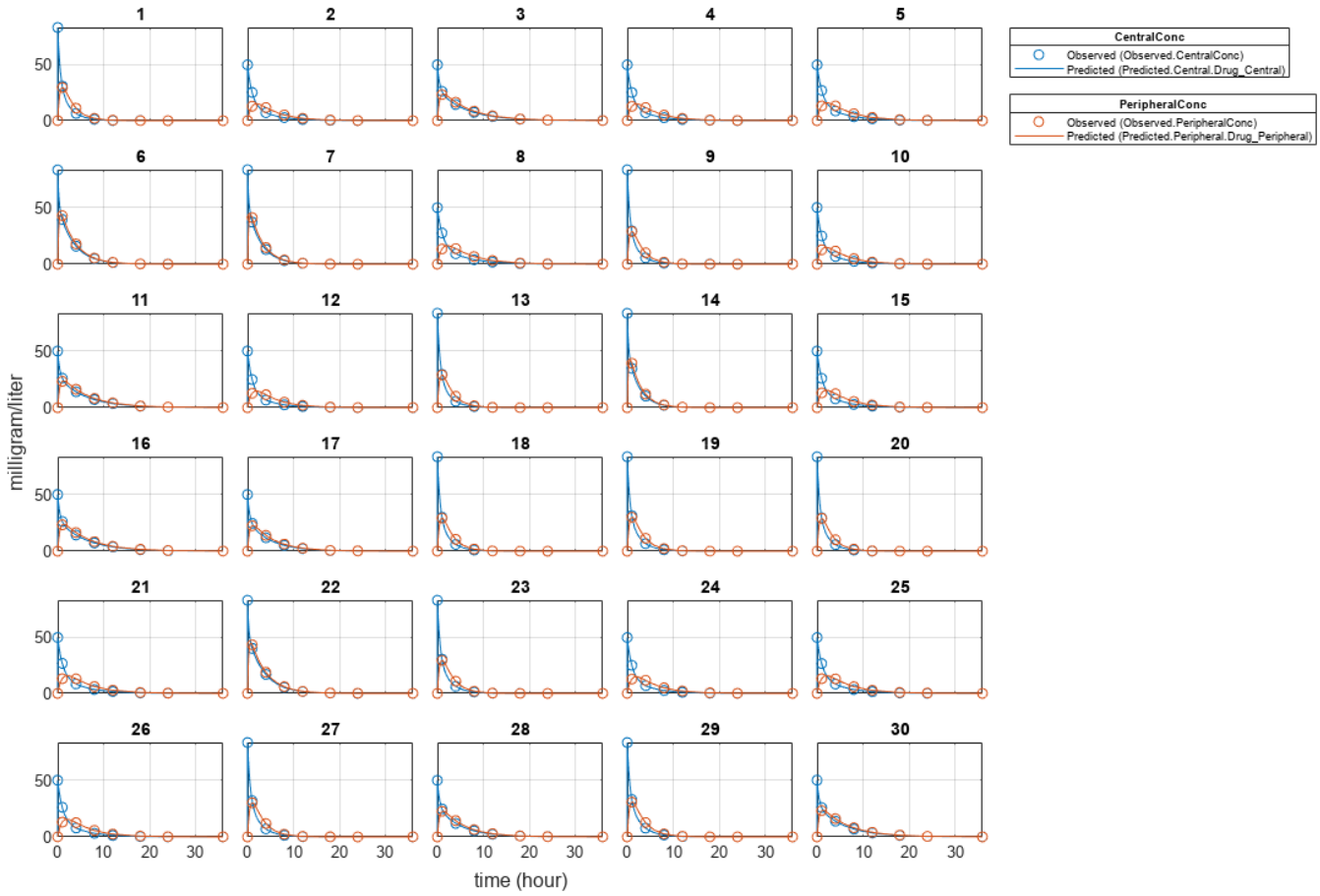
Estimate one set of parameters for each individual by setting the `'Pooled'` name-value pair argument to `false`.

```
unpooledFit =  sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',false);
```

Display Results

Plot the fitted results versus the original data for each individual (group).

```
plot(unpooledFit);
```



For an unpooled fit, `sbiofit` always returns one results object for each individual.

Examine Parameter Estimates for Category Dependencies

Explore the unpooled estimates to see if there is any category-specific parameters, that is, if some parameters are related to one or more categories. If there are any category dependencies, it might be possible to reduce the number of degrees of freedom by estimating just category-specific values for those parameters.

First extract the ID and category values for each ID

```
catParamValues = unique(gData(:,{'ID','Sex','Age'}));
```

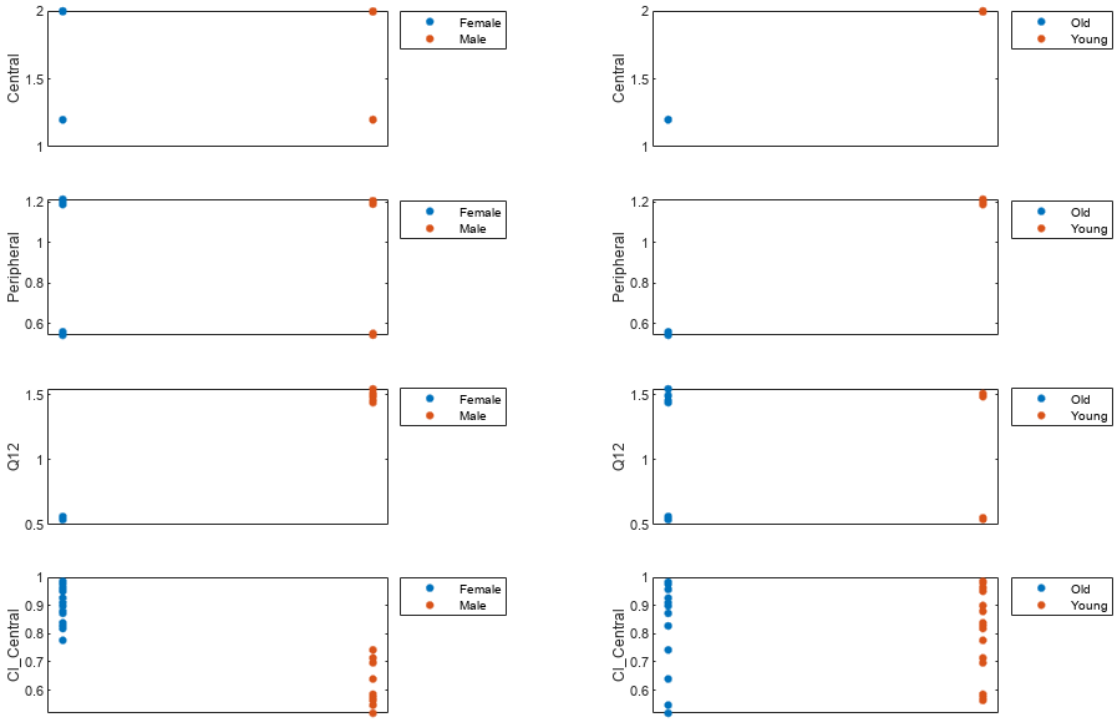
Add variables to the table containing each parameter's estimate.

```
allParamValues            = vertcat(unpooledFit.ParameterEstimates);
catParamValues.Central    = allParamValues.Estimate(strcmp(allParamValues.Name, 'Central'));
catParamValues.Peripheral = allParamValues.Estimate(strcmp(allParamValues.Name, 'Peripheral'));
catParamValues.Q12        = allParamValues.Estimate(strcmp(allParamValues.Name, 'Q12'));
catParamValues.Cl_Central = allParamValues.Estimate(strcmp(allParamValues.Name, 'Cl_Central'));
```

Plot estimates of each parameter for each category. `gscatter` requires Statistics and Machine Learning Toolbox™. If you do not have it, use other alternative plotting functions such as `plot`.

```
h           = figure;
ylabels     = ["Central","Peripheral","Q12","Cl\_Central"];
```

```
plotNumber  = 1;
for i = 1:4
    thisParam = estimatedParam(i).Name;

    % Plot for Sex category
    subplot(4,2,plotNumber);
    plotNumber  = plotNumber + 1;
    gscatter(double(catParamValues.Sex), catParamValues.(thisParam), catParamValues.Sex);
    ax          = gca;
    ax.XTick    = [];
    ylabel(ylabels(i));
    legend('Location','bestoutside')
    % Plot for Age category
    subplot(4,2,plotNumber);
    plotNumber  = plotNumber + 1;
    gscatter(double(catParamValues.Age), catParamValues.(thisParam), catParamValues.Age);
    ax          = gca;
    ax.XTick    = [];
    ylabel(ylabels(i));
    legend('Location','bestoutside')
end
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```



Based on the plot, it seems that young individuals tend to have higher volumes of central and peripheral compartments (`Central`, `Peripheral`) than old individuals (that is, the volumes seem to

be age-specific). In addition, males tend to have lower clearance rates (`Cl_Central`) than females but the opposite for the Q12 parameter (that is, the clearance and Q12 seem to be sex-specific).

Estimate Category-Specific Parameters

Use the `'CategoryVariableName'` property of the `estimatedInfo` object to specify which category to use during fitting. Use `'Sex'` as the group to fit for the clearance `Cl_Central` and `Q12` parameters. Use `'Age'` as the group to fit for the `Central` and `Peripheral` parameters.

```
estimatedParam(1).CategoryVariableName = 'Age';
estimatedParam(2).CategoryVariableName = 'Age';
estimatedParam(3).CategoryVariableName = 'Sex';
estimatedParam(4).CategoryVariableName = 'Sex';
categoryFit = sbiofit(model,gData,responseMap,estimatedParam,dose)
```

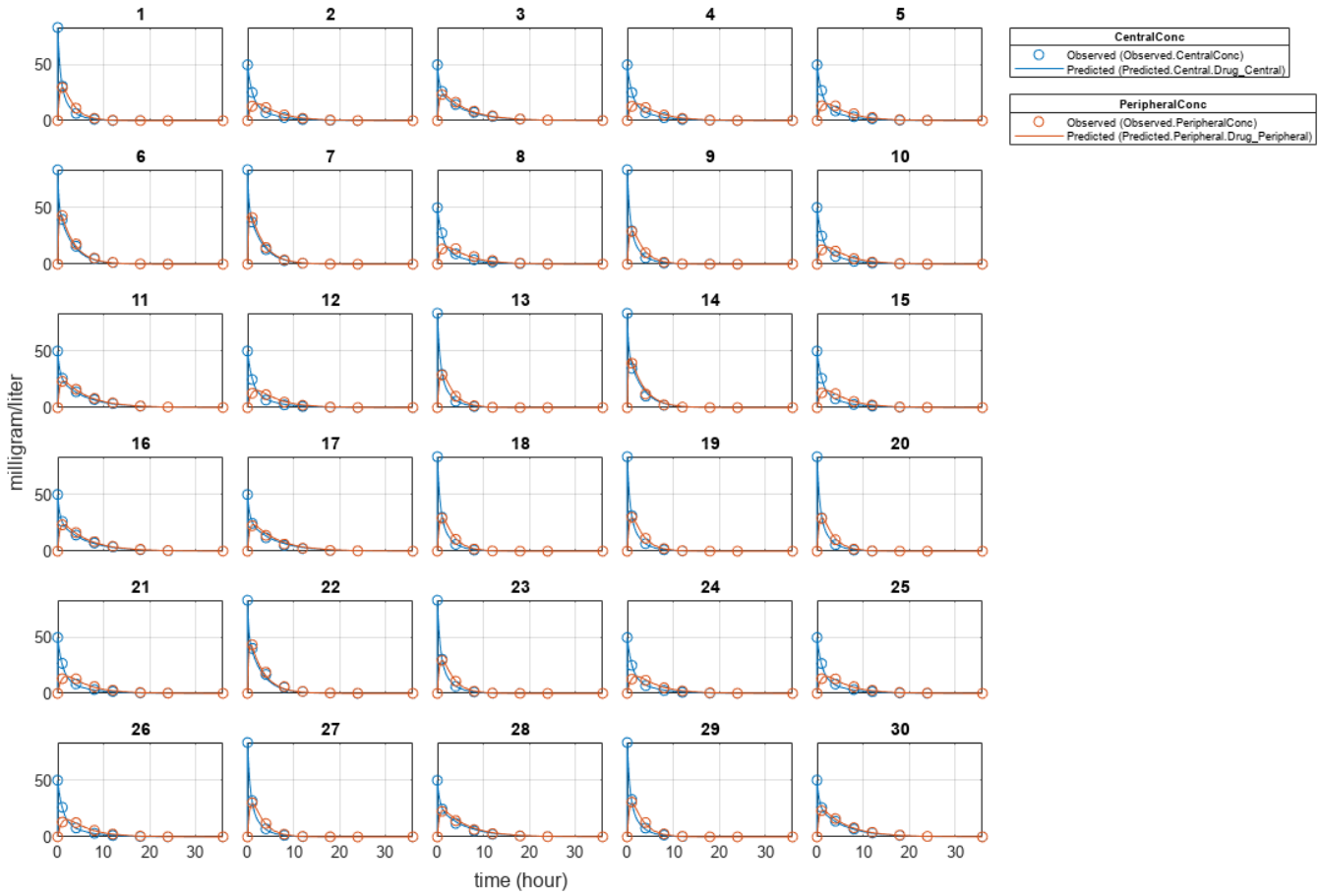
```
categoryFit =
  OptimResults with properties:

                  ExitFlag: 3
                    Output: [1x1 struct]
                 GroupName: []
                      Beta: [8x5 table]
        ParameterEstimates: [120x6 table]
                         J: [240x8x2 double]
                      COVB: [8x8 double]
          CovarianceMatrix: [8x8 double]
                         R: [240x2 double]
                       MSE: 0.4362
                       SSE: 205.8690
                   Weights: []
              LogLikelihood: -477.9195
                       AIC: 971.8390
                       BIC: 1.0052e+03
                       DFE: 472
            DependentFiles: {1x3 cell}
                      Data: [240x6 groupedData]
   EstimatedParameterNames: {'Central'  'Peripheral'  'Q12'  'Cl_Central'}
            ErrorModelInfo: [1x3 table]
        EstimationFunction: 'lsqnonlin'
```

When fitting by category (or group), `sbiofit` always returns one results object, not one for each category level. This is because both male and female individuals are considered to be part of the same optimization using the same error model and error parameters, similarly for the young and old individuals.

Plot Results

Plot the category-specific estimated results.

```
plot(categoryFit);
```



For the `Cl_Central` and `Q12` parameters, all males had the same estimates, and similarly for the females. For the `Central` and `Peripheral` parameters, all young individuals had the same estimates, and similarly for the old individuals.

Estimate Population-Wide Parameters

To better compare the results, fit the model to all of the data pooled together, that is, estimate one set of parameters for all individuals by setting the `'Pooled'` name-value pair argument to `true`. The warning message tells you that this option will ignore any category-specific information (if they exist).

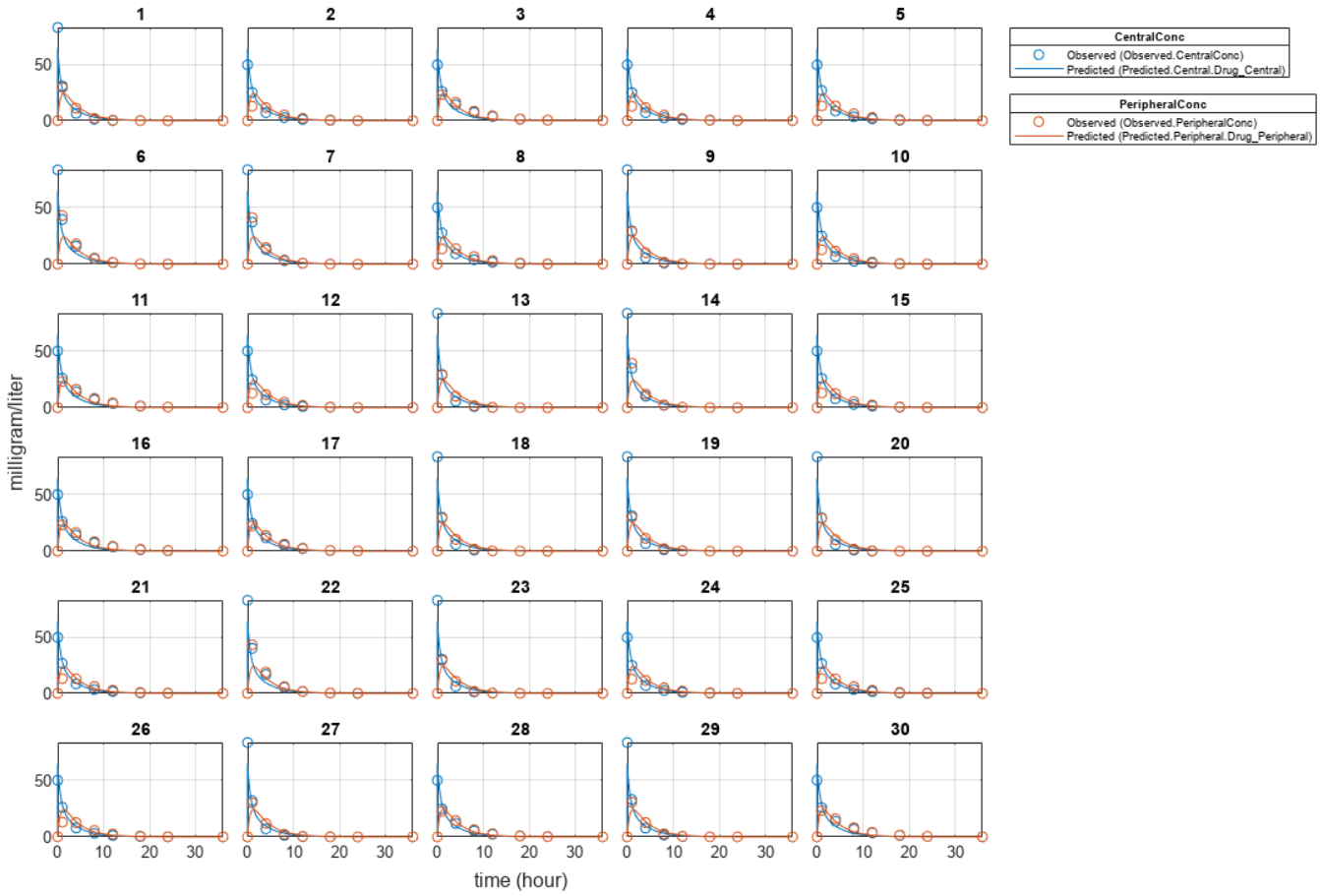
```
pooledFit = sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',true);
```

```
Warning: CategoryVariableName property of the estimatedInfo object is ignored when using the 'Poo
```

Plot Results

Plot the fitted results versus the original data. Although a separate plot was generated for each individual, the data was fitted using the same set of parameters (that is, all individuals had the same fitted line).

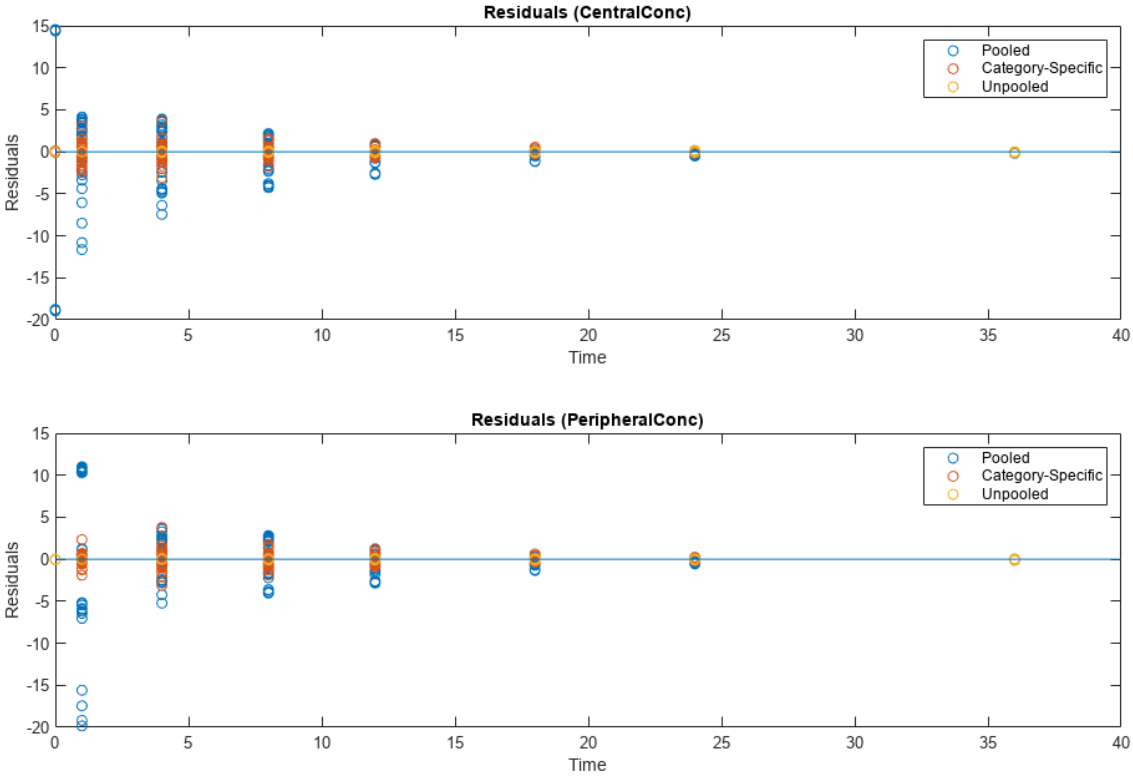
```
plot(pooledFit);
```



Compare Residuals

Compare residuals of `CentralConc` and `PeripheralConc` responses for each fit.

```
t = gData.Time;
allResid(:,:,1) = pooledFit.R;
allResid(:,:,2) = categoryFit.R;
allResid(:,:,3) = vertcat(unpooledFit.R);

h = figure;
responseList = {'CentralConc', 'PeripheralConc'};
for i = 1:2
    subplot(2,1,i);
    oneResid = squeeze(allResid(:,i,:));
    plot(t,oneResid,'o');
    refline(0,0); % A reference line representing a zero residual
    title(sprintf('Residuals (%s)', responseList{i}));
    xlabel('Time');
    ylabel('Residuals');
    legend({'Pooled','Category-Specific','Unpooled'});
end
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```



As shown in the plot, the unpooled fit produced the best fit to the data as it fit the data to each individual. This was expected since it used the most number of degrees of freedom. The category-fit reduced the number of degrees of freedom by fitting the data to two categories (sex and age). As a result, the residuals were larger than the unpooled fit, but still smaller than the population-fit, which estimated just one set of parameters for all individuals. The category-fit might be a good compromise between the unpooled and pooled fitting provided that any hierarchical model exists within your data.

Estimate Yeast G Protein Model Parameter

This example uses the yeast heterotrimeric G protein model and experimental data reported by [1]. For details about the model, see the **Background** section in “Parameter Scanning, Parameter Estimation, and Sensitivity Analysis in the Yeast Heterotrimeric G Protein Cycle”.

Load the G protein model.

```
sbioloadproject gprotein
```

Store the experimental data containing the time course for the fraction of active G protein.

```
time = [0 10 30 60 110 210 300 450 600]';
GaFracExpt = [0 0.35 0.4 0.36 0.39 0.33 0.24 0.17 0.2]';
```

Create a `groupedData` object based on the experimental data.

```
tbl = table(time,GaFracExpt);
grpData = groupedData(tbl);
```

Map the appropriate model component to the experimental data. In other words, indicate which species in the model corresponds to which response variable in the data. In this example, map the model parameter `GaFrac` to the experimental data variable `GaFracExpt` from `grpData`.

```
responseMap = 'GaFrac = GaFracExpt';
```

Use an `estimatedInfo` object to define the model parameter `kGd` as a parameter to be estimated.

```
estimatedParam = estimatedInfo('kGd');
```

Perform the parameter estimation.

```
fitResult = sbiofit(m1,grpData,responseMap,estimatedParam);
```

View the estimated parameter value of `kGd`.

```
fitResult.ParameterEstimates
```

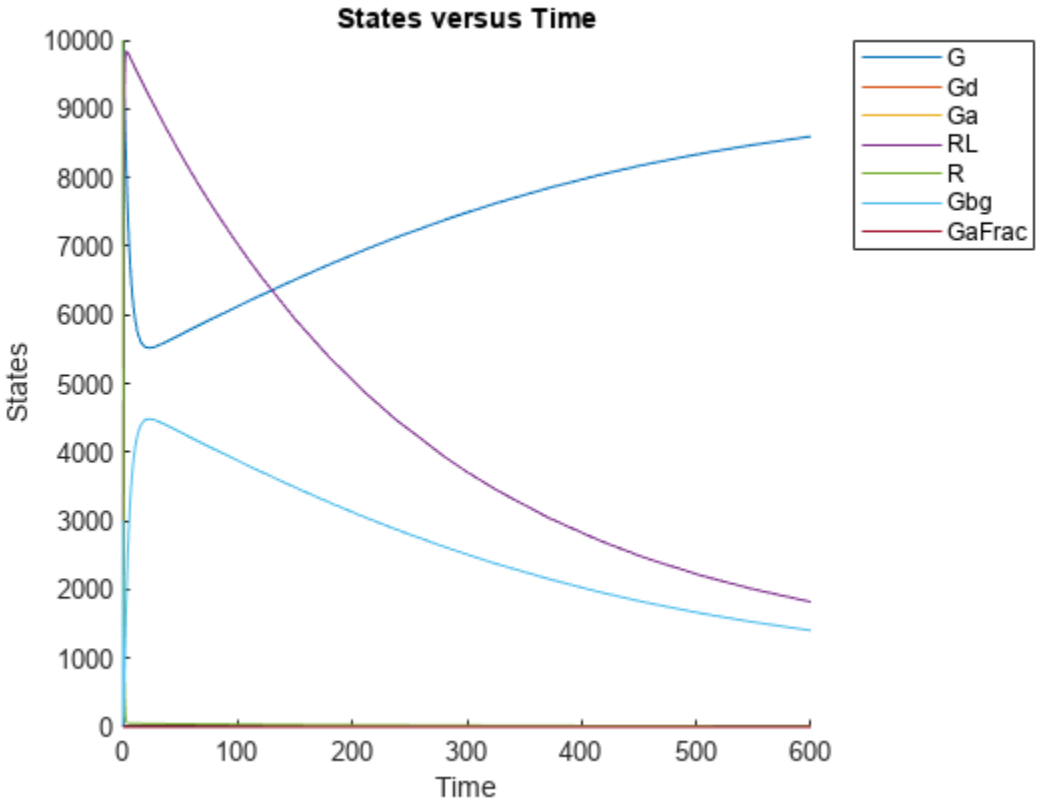
```
ans=1×3 table
     Name      Estimate    StandardError
    _______    ________    _____________

    {'kGd'}    0.11307      3.4439e-05
```

Suppose you want to plot the model simulation results using the estimated parameter value. You can either rerun the `sbiofit` function and specify to return the optional second output argument, which contains simulation results, or use the `fitted` method to retrieve the results without rerunning `sbiofit`.

```
[yfit,paramEstim] = fitted(fitResult);
```

Plot the simulation results.

```
sbioplot(yfit);
```



Estimate Time Lag and Duration of a Dose

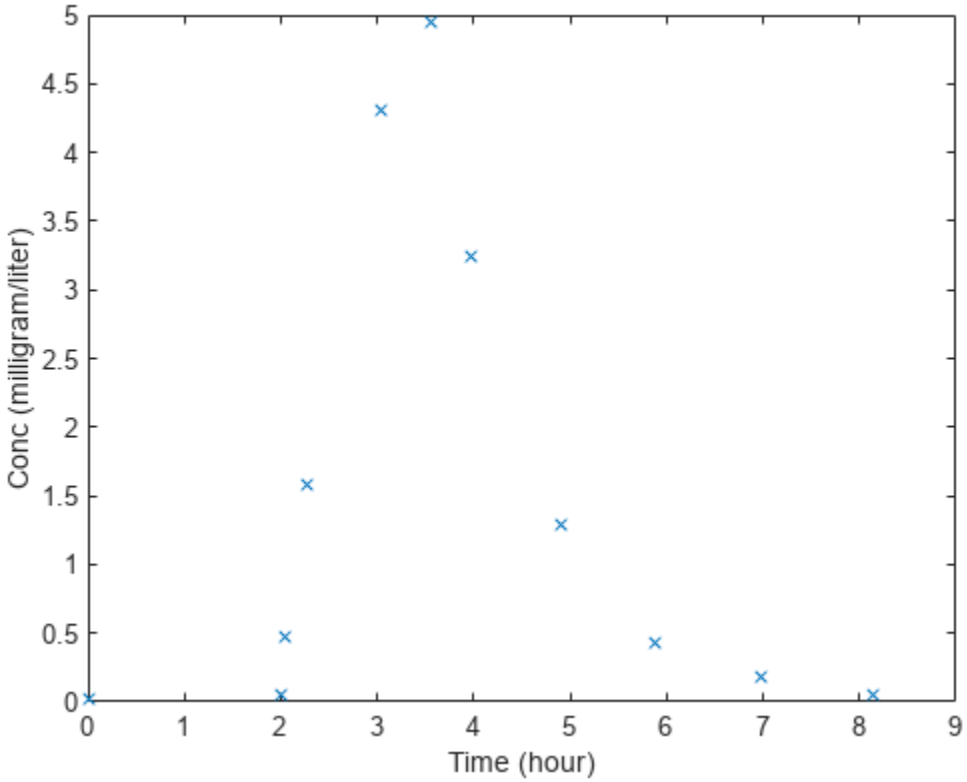
This example shows how to estimate the time lag before a bolus dose was administered and the duration of the dose using a one-compartment model.

Load a sample data set.

```
load lagDurationData.mat
```

Plot the data.

```
plot(data.Time,data.Conc,'x')
xlabel('Time (hour)')
ylabel('Conc (milligram/liter)')
```



Convert to groupedData.

```
gData = groupedData(data);
gData.Properties.VariableUnits = {'hour','milligram/liter'};
```

Create a one-compartment model.

```
pkmd                    = PKModelDesign;
pkc1                    = addCompartment(pkmd,'Central');
pkc1.DosingType         = 'Bolus';
pkc1.EliminationType    = 'linear-clearance';
pkc1.HasResponseVariable = true;
model                   = construct(pkmd);
configset               = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
```

Add two parameters that represent the time lag and duration of a dose. The lag parameter specifies the time lag before the dose is administered. The duration parameter specifies the length of time it takes to administer a dose.

```
lagP = addparameter(model,'lagP');
lagP.ValueUnits = 'hour';
durP = addparameter(model,'durP');
durP.ValueUnits = 'hour';
```

Create a dose object. Set the `LagParameterName` and `DurationParameterName` properties of the dose to the names of the lag and duration parameters, respectively. Set the dose amount to 10 milligram which was the amount used to generate the data.

```
dose                = sbiodose('dose');
dose.TargetName     = 'Drug_Central';
dose.StartTime      = 0;
dose.Amount         = 10;
dose.AmountUnits    = 'milligram';
dose.TimeUnits      = 'hour';
dose.LagParameterName = 'lagP';
dose.DurationParameterName = 'durP';
```

Map the model species to the corresponding data.

```
responseMap = {'Drug_Central = Conc'};
```

Specify the lag and duration parameters as parameters to estimate. Log-transform the parameters. Initialize them to 2 and set the upper bound and lower bound.

```
paramsToEstimate    = {'log(lagP)','log(durP)'};
estimatedParams     = estimatedInfo(paramsToEstimate,'InitialValue',2,'Bounds',[1 5]);
```

Perform parameter estimation.

```
fitResults = sbiofit(model,gData,responseMap,estimatedParams,dose,'fminsearch')
```

```
fitResults =
  OptimResults with properties:

                  ExitFlag: 1
                    Output: [1x1 struct]
                 GroupName: One group
                      Beta: [2x4 table]
        ParameterEstimates: [2x4 table]
                         J: [11x2 double]
                      COVB: [2x2 double]
          CovarianceMatrix: [2x2 double]
                         R: [11x1 double]
                       MSE: 0.0024
                       SSE: 0.0213
                   Weights: []
              LogLikelihood: 18.7511
                       AIC: -33.5023
                       BIC: -32.7065
                       DFE: 9
            DependentFiles: {1x2 cell}
                      Data: [11x2 groupedData]
    EstimatedParameterNames: {'lagP'  'durP'}
             ErrorModelInfo: [1x3 table]
         EstimationFunction: 'fminsearch'
```

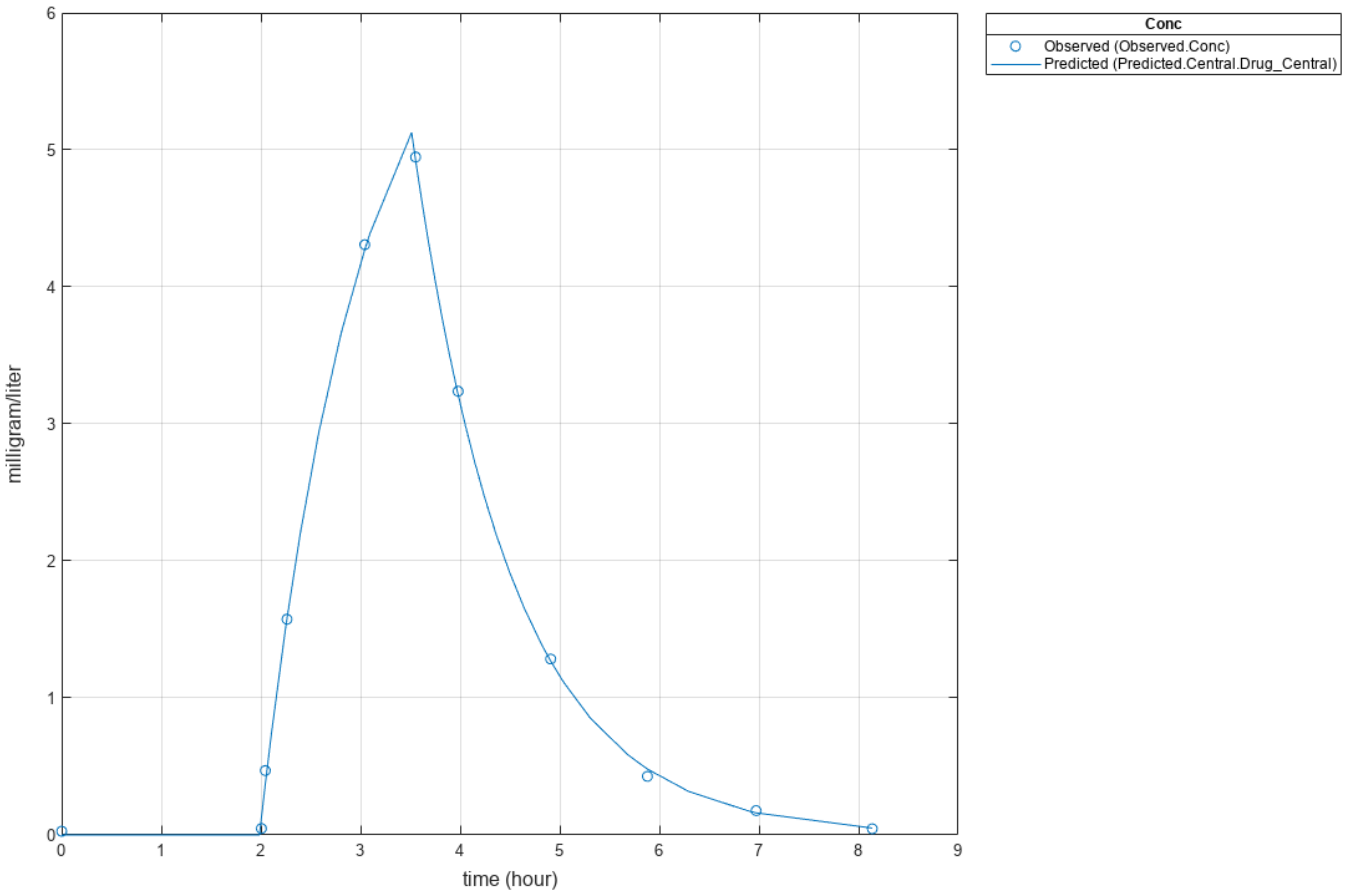
Display the result.

```
fitResults.ParameterEstimates
```

```
ans=2×4 table
      Name      Estimate    StandardError    Bounds
    ________    ________    _____________    ______

    {'lagP'}     1.986        0.0051568      1    5
```

```
    {'durP'}     1.527         0.012956      1    5
```

```
plot(fitResults)
```



Input Arguments

`sm` — SimBiology model

SimBiology model object

SimBiology model, specified as a SimBiology `model object`. The active `configset object` of the model contains solver settings for simulation. Any active doses and variants are applied to the model during simulation unless specified otherwise using the `dosing` and `variants` input arguments, respectively.

`grpData` — Data to fit

groupedData object

Data to fit, specified as a `groupedData object`.

The name of the time variable must be defined in the `IndependentVariableName` property of `grpData`. For instance, if the time variable name is `'TIME'`, then specify it as follows.

```
grpData.Properties.IndependentVariableName = 'TIME';
```

If the data contains more than one group of measurements, the grouping variable name must be defined in the `GroupVariableName` property of `grpData`. For example, if the grouping variable name is `'GROUP'`, then specify it as follows.

```
grpData.Properties.GroupVariableName = 'GROUP';
```

A group usually refers to a set of measurements that represent a single time course, often corresponding to a particular individual, or experimental condition.

Note `sbiofit` uses the `categorical` function to identify groups. If any group values are converted to the same value by `categorical`, then those observations are treated as belonging to the same group. For instance, if some observations have no group information (that is, an empty character vector `''`), then `categorical` converts empty character vectors to `<undefined>`, and these observations are treated as one group.

ResponseMap — Mapping information of model components to grpData

character vector | string | string vector | cell array of character vectors

Mapping information of model components to `grpData`, specified as a character vector, string, string vector, or cell array of character vectors.

Each character vector or string is an equation-like expression, similar to assignment rules in SimBiology. It contains the name (or qualified name) of a quantity (species, compartment, or parameter) or an `observable` object in the model `sm`, followed by the character `'='` and the name of a variable in `grpData`. For clarity, white spaces are allowed between names and `'='`.

For example, if you have the concentration data `'CONC'` in `grpData` for a species `'Drug_Central'`, you can specify it as follows.

```
ResponseMap = 'Drug_Central = CONC';
```

To name a species unambiguously, use the qualified name, which includes the name of the compartment. To name a reaction-scoped parameter, use the reaction name to qualify the parameter.

If the model component name or `grpData` variable name is not a valid MATLAB variable name, surround it by square brackets, such as:

```
ResponseMap = '[Central 1].Drug = [Central 1 Conc]';
```

If a variable name itself contains square brackets, you cannot use it in the expression to define the mapping information.

An error is issued if any (qualified) name matches two components of the same type. However, you can use a (qualified) name that matches two components of different types, and the function first finds the species with the given name, followed by compartments and then parameters.

estiminfo — Estimated parameters

`estimatedInfo` object | vector of `estimatedInfo` objects

Estimated parameters, specified as an `EstimatedInfo object` or vector of `estimatedInfo` objects that defines the estimated parameters in the model `sm`, and other optional information such

as their initial estimates, transformations, bound constraints, and categories. Supported transforms are `log`, `logit`, and `probit`. For details, see “Parameter Transformations”.

You can specify bounds for all estimation methods. The lower bound must be less than the upper bound. For details, see “Bounds” on page 2-0 .

When using `scattersearch`, you must specify finite transformed bounds for each estimated parameter.

When using `fminsearch`, `nlinfit`, or `fminunc` with bounds, the objective function returns `Inf` if bounds are exceeded. When you turn on options such as `FunValCheck`, the optimization might error if bounds are exceeded during estimation. If using `nlinfit`, it might report warnings about the Jacobian being ill-conditioned or not being able to estimate if the final result is too close to the bounds.

If you do not specify `Pooled` name-value pair argument, `sbiofit` uses `CategoryVariableName` property of `estiminfo` to decide if parameters must be estimated for each individual, group, category, or all individuals as a whole. Use the `Pooled` option to override any `CategoryVariableName` values. For details about `CategoryVariableName` property, see `EstimatedInfo object`.

Note `sbiofit` uses the `categorical` function to identify groups or categories. If any group values are converted to the same value by `categorical`, then those observations are treated as belonging to the same group. For instance, if some observations have no group information (that is, an empty character vector `''` as a group value), then `categorical` converts empty character vectors to `<undefined>`, and these observations are treated as one group.

`dosing` — Dosing information

`[]` | `{}` | 2-D matrix of dose objects | cell vector of dose objects

Dosing information, specified as an empty array (`[]` or `{}`), 2-D matrix or cell vector of dose objects (`ScheduleDose object` or `RepeatDose object`).

If you omit the `dosing` input, the function applies the active doses of the model if there are any.

If you specify the input as empty `[]` or `{}`, no doses are applied during simulation, even if the model has active doses.

For a matrix of dose objects, it must have a single row or one row per group in the input data. If it has a single row, the same doses are applied to all groups during simulation. If it has multiple rows, each row is applied to a separate group, in the same order as the groups appear in the input data. Multiple columns are allowed so that you can apply multiple dose objects to each group.

Note As of R2021b, doses in the columns are no longer required to have the same configuration. If you previously created default (dummy) doses to fill in the columns, these default doses have no effect and indicate no dosing.

For a cell vector of doses, it must have one element or one element per group in the input data. Each element must be `[]` or a vector of doses. Each element of the cell is applied to a separate group, in the same order as the groups appear in the input data.

In addition to manually constructing dose objects using `sbiodose`, if the input `groupedData` object has dosing information, you can use the `createDoses` method to construct doses.

`functionName` — Estimation function name
character vector | string

Estimation function name, specified as a character vector or string. Choices are as follows.

- `"fminsearch"`
- `"nlinfit"` (Statistics and Machine Learning Toolbox is required.)
- `"fminunc"` (Optimization Toolbox is required.)
- `"fmincon"` (Optimization Toolbox is required.)
- `"lsqcurvefit"` (Optimization Toolbox is required.)
- `"lsqnonlin"` (Optimization Toolbox is required.)
- `"patternsearch"` (Global Optimization Toolbox is required.)
- `"ga"` (Global Optimization Toolbox is required.)
- `"particleswarm"` (Global Optimization Toolbox is required.)
- `"scattersearch"` on page 1-98

By default, `sbiofit` uses the first available estimation function among the following: `lsqnonlin`, `nlinfit`, or `fminsearch`. The same priority applies to the default local solver choice for `scattersearch`.

For the summary of supported methods and fitting options, see “Supported Methods for Parameter Estimation in SimBiology”.

`options` — Options specific to estimation function
struct | `optimoptions` object

Options specific to the estimation function, specified as a struct or `optimoptions` object.

- `statset` struct for `nlinfit`
- `optimset` struct for `fminsearch`
- `optimoptions` object for `lsqcurvefit`, `lsqnonlin`, `fmincon`, `fminunc`, `particleswarm`, `ga`, and `patternsearch`
- `struct` for `scattersearch`

See “Default Options for Estimation Algorithms” on page 1-96 for more details and default options associated with each estimation function.

`variants` — Variants
`[]` | `{}` | vector of variant objects

Variants, specified as an empty array (`[]` or `{}`) or vector of variant objects.

If you

- Omit this input argument, the function applies the active variants of the model if there are any.
- Specify this input as empty, no variants are used even if the model has active variants.

- Specify this input as a vector of variants, the function applies the specified variants to all simulations, and the model active variants are not used.
- Specify this input as a vector of variants and also specify the `Variants` name-value argument, the function applies the variants specified in this input argument before applying the ones specified in the name-value argument.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `'ErrorModel','constant','UseParallel',true` specifies a constant error model and to run simulations in parallel during parameter estimation.

`ErrorModel` — Error model

`'constant'` (default) | character vector | string | string vector | cell array of character vector | categorical vector | table

Error models used for estimation, specified as a character vector, string, string vector, cell array of character vectors, categorical vector, or table.

If it is a table, it must contain a single variable that is a column vector of error model names. The names can be a cell array of character vectors, string vector, or a vector of categorical variables. If the table has more than one row, then the `RowNames` property must match the response variable names specified in the right hand side of `ResponseMap`. If the table does not use the `RowNames` property, the nth error is associated with the nth response.

If you specify only one error model, then `sbiofit` estimates one set of error parameters for all responses.

If you specify multiple error models using a categorical vector, string vector, or cell array of character vectors, the length of the vector or cell array must match the number of responses in `ResponseMap`.

You can specify multiple error models only if you are using these methods: `lsqnonlin`, `lsqcurvefit`, `fmincon`, `fminunc`, `fminsearch`, `patternsearch`, `ga`, and `particleswarm`.

Four built-in error models are available. Each model defines the error using a standard mean-zero and unit-variance (Gaussian) variable e, simulation results f, and one or two parameters a and b.

- `"constant"`: $y = f + ae$
- `"proportional"`: $y = f + b|f|e$
- `"combined"`: $y = f + (a + b|f|)e$
- `"exponential"`: $y = f * \exp(ae)$

Note

- If you specify an error model, you cannot specify weights except for the constant error model.
- If you use a proportional or combined error model during data fitting, avoid specifying data points at times where the solution (simulation result) is zero or the steady state is zero. Otherwise, you

can run into division-by-zero problems. It is recommended that you remove those data points from the data set. For details on the error parameter estimation functions, see “Maximum Likelihood Estimation” on page 1-94.

`Weights` — Weights used for fitting
`[]` (default) | matrix | function handle

Weights used for fitting, specified as an empty array `[]`, matrix of real positive weights where the number of columns corresponds to the number of responses, or a function handle that accepts a vector of predicted response values and returns a vector of real positive weights.

If you specify an error model, you cannot use weights except for the constant error model. If neither the `ErrorModel` or `Weights` is specified, by default, the software uses the constant error model with equal weights.

`Variants` — Group-specific variants
`[]` | `{}` | 2-D matrix of variants | cell vector of variants

Group-specific variants, specified as an empty array (`[]` or `{}`), 2-D matrix or cell vector of variant objects. These variants let you specify parameter values for specific groups during fitting. The software applies these group-specific variants after active variants or the `variants` input argument. If the value is empty (`[]` or `{}`), no group-specific variants are applied.

For a matrix of variant objects, the number of rows must be one or must match the number of groups in the input data. The *i*th row of variant objects is applied to the simulation of the *i*th group. The variants are applied in order from the first column to the last. If this matrix has only one row of variants, they are applied to all simulations.

For a cell vector of variant objects, the number of cells must be one or must match the number of groups in the input data. Each element must be `[]` or a vector of variants. If this cell vector has a single cell containing a vector of variants, they are applied to all simulations. If the cell vector has multiple cells, the variants in the *i*th cell are applied to the simulation of the *i*th group.

In addition to manually constructing variant objects using `sbiovariant`, if the input `groupedData` object has variant information, you can use `createVariants` to construct variants.

`Pooled` — Fit option flag
`false` or `0` (default) | `true` or `1`

Fit option flag to fit each individual or pool all individual data, specified as a numeric or logical `1` (`true`) or `0` (`false`).

When `true`, the software performs fitting for all individuals or groups simultaneously using the same parameter estimates, and `fitResults` is a scalar results object.

When `false`, the software fits each group or individual separately using group- or individual-specific parameters, and `fitResults` is a vector of results objects with one result for each group.

Note Use this option to override any `CategoryVariableName` values of `estiminfo`.

`UseParallel` — Flag for parallel simulations
`false` or `0` (default) | `true` or `1`

Flag to enable parallelization, specified as a numeric or logical `1` (`true`) or `0` (`false`). If `true` and Parallel Computing Toolbox is available, `sbiofit` supports several levels of parallelization, but only one level is used at a time.

For an unpooled fit (`Pooled = false`) for multiple groups, each fit is run in parallel.

For a pooled fit (`Pooled = true`), parallelization happens at the solver level. In other words, solver computations, such as objective function evaluations, are run in parallel.

For details, see “Multiple Parameter Estimations in Parallel” on page 1-102.

`SensitivityAnalysis` — Flag to use parameter sensitivities to determine gradients of the objective function
`false` or `0` (default) | `true` or `1`

Flag to use parameter sensitivities to determine gradients of the objective function, specified as a numeric or logical `1` (`true`) or `0` (`false`). By default, it is `true` for `fmincon`, `fminunc`, `lsqnonlin`, `lsqcurvefit`, and `scattersearch` methods. Otherwise, it is `false`.

If it is `true`, the software always uses the `sundials` solver, regardless of what you have selected as the SolverType property in the `Configset` object.

The software uses the complex-step approximation method to calculate parameter sensitivities. Such calculated sensitivities can be used to determine gradients of the objective function during parameter estimation to improve fitting. The default behavior of `sbiofit` is to use such sensitivities to determine gradients whenever the algorithm is gradient-based and if the SimBiology model supports sensitivity analysis. For details about the model requirements and sensitivity analysis, see “Sensitivity Analysis in SimBiology”.

`ProgressPlot` — Flag to show the progress of parameter estimation
`false` or `0` (default) | `true` or `1`

Flag to show the progress of parameter estimation, specified as a numeric or logical `1` (`true`) or `0` (`false`). If `true`, a new figure opens containing plots.

Plots show the log-likelihood, termination criteria, and estimated parameters for each iteration. This option is not supported for `nlinfit`.

If you are using the Optimization Toolbox functions (`fminunc`, `fmincon`, `lsqcurvefit`, `lsqnonlin`), the figure also shows the First Order Optimality (Optimization Toolbox) plot.

For an unpooled fit, each line on the plots represents an individual. For a pooled fit, a single line represents all individuals. The line becomes faded when the fit is complete. The plots also keep track of the progress when you run `sbiofit` (for both pooled and unpooled fits) in parallel using remote clusters. For details, see “Progress Plot”.

Output Arguments

`fitResults` — Estimation results
`OptimResults` object | `NLINResults` object | vector of results objects

Estimation results, returned as a `OptimResults object` or `NLINResults object` or a vector of these objects. Both results objects are subclasses of the `LeastSquaresResults object`.

If the function uses `nlinfit`, then `fitResults` is a `NLINResults object`. Otherwise, `fitResults` is an `OptimResults object`.

For an unpooled fit, the function fits each group separately using group-specific parameters, and `fitResults` is a vector of results objects with one results object for each group.

For a pooled fit, the function performs fitting for all individuals or groups simultaneously using the same parameter estimates, and `fitResults` is a scalar results object.

When the pooled option is not specified, and `CategoryVariableName` values of `estimatedInfo` objects are all `<none>`, `fitResults` is a single results object. This is the same behavior as a pooled fit.

When the pooled option is not specified, and `CategoryVariableName` values of `estimatedInfo` objects are all `<GroupVariableName>`, `fitResults` is a vector of results objects. This is the same behavior as an unpooled fit.

In all other cases, `fitResults` is a scalar object containing estimated parameter values for different groups or categories specified by `CategoryVariableName`.

`simdata` — Simulation results
vector of `SimData` objects

Simulation results, returned as a vector of `SimData` objects representing simulation results for each group or individual.

If the `'Pooled'` option is `false`, then each simulation uses group-specific parameter values. If `true`, then all simulations use the same (population-wide) parameter values.

The states reported in `simdata` are the states that were included in the `ResponseMap` input argument and any other states listed in the `StatesToLog` property of the runtime options (`RuntimeOptions`) of the SimBiology model `sm`.

More About

Maximum Likelihood Estimation

SimBiology estimates parameters by the method of maximum likelihood. Rather than directly maximizing the likelihood function, SimBiology constructs an equivalent minimization problem. Whenever possible, the estimation is formulated as a weighted least squares (**WLS**) optimization that minimizes the sum of the squares of weighted residuals. Otherwise, the estimation is formulated as the minimization of the negative of the logarithm of the likelihood (**NLL**). The **WLS** formulation often converges better than the **NLL** formulation, and SimBiology can take advantage of specialized **WLS** algorithms, such as the Levenberg-Marquardt algorithm implemented in `lsqnonlin` and `lsqcurvefit`. SimBiology uses **WLS** when there is a single error model that is constant, proportional, or exponential. SimBiology uses **NLL** if you have a combined error model or a multiple-error model, that is, a model having an error model for each response.

`sbiofit` supports different optimization methods, and passes in the formulated **WLS** or **NLL** expression to the optimization method that minimizes it. For simplicity, each expression shown below assumes only one error model and one response. If there are multiple responses, SimBiology takes the sum of the expressions that correspond to error models of given responses.

	Expression that is being minimized
Weighted Least Squares (**WLS**)	For the constant error model, $\sum_i^N (y_i - f_i)^2$
	For the proportional error model, $\sum_i^N \frac{(y_i - f_i)^2}{f_i^2 / f_{gm}^2}$
	For the exponential error model, $\sum_i^N (\ln y_i - \ln f_i)^2$
	For numeric weights, $\sum_i^N \frac{(y_i - f_i)^2}{w_{gm}/w_i}$
Negative Log-likelihood (**NLL**)	For the combined error model and multiple-error model, $\sum_i^N \frac{(y_i - f_i)^2}{2\sigma_i^2} + \sum_i^N \ln\sqrt{2\pi\sigma_i^2}$

The variables are defined as follows.

N	Number of experimental observations
y_i	The ith experimental observation
f_i	Predicted value of the ith observation
σ_i	Standard deviation of the ith observation. • For the constant error model, $\sigma_i = a$ • For the proportional error model, $\sigma_i = b\lvert f_i\rvert$ • For the combined error model, $\sigma_i = a + b\lvert f_i\rvert$
f_{gm}	$f_{gm} = \left(\prod_i^N \lvert f_i\rvert\right)^{1/N}$
w_i	The weight of the ith predicted value
w_{gm}	$w_{gm} = \left(\prod_i^N w_i\right)^{1/N}$

When you use numeric weights or the weight function, the weights are assumed to be inversely proportional to the variance of the error, that is, $\sigma_i^2 = \frac{a^2}{w_i}$ where a is the constant error parameter. If you use weights, you cannot specify an error model except the constant error model.

Various optimization methods have different requirements on the function that is being minimized. For some methods, the estimation of model parameters is performed independently of the estimation of the error model parameters. The following table summarizes the error models and any separate formulas used for the estimation of error model parameters, where a and b are error model parameters and e is the standard mean-zero and unit-variance (Gaussian) variable.

Error Model	Error Parameter Estimation Function
`'constant'`: $y_i = f_i + ae$	$a^2 = \frac{1}{N}\sum_i^N (y_i - f_i)^2$
`'exponential'`: $y_i = f_i \exp(ae)$	$a^2 = \frac{1}{N}\sum_i^N (\ln y_i - \ln f_i)^2$
`'proportional'`: $y_i = f_i + b\lvert f_i\rvert e$	$b^2 = \frac{1}{N}\sum_i^N \left(\frac{y_i - f_i}{f_i}\right)^2$
`'combined'`: $y_i = f_i + (a + b\lvert f_i\rvert)e$	Error parameters are included in the minimization.
Weights	$a^2 = \frac{1}{N}\sum_i^N (y_i - f_i)^2 w_i$

Note `nlinfit` only support single error models, not multiple-error models, that is, response-specific error models. For a combined error model, it uses an iterative **WLS** algorithm. For other error models, it uses the **WLS** algorithm as described previously. For details, see `nlinfit`.

Default Options for Estimation Algorithms

The following table summarizes the default options for various estimation functions.

Function	Default Options
`nlinfit`	`sbiofit` uses the default options structure associated with `nlinfit`, except for: `FunValCheck = 'off'` `DerivStep = max(eps^(1/3), min(1e-4,SolverOptions.RelativeTolerance))`, where the `SolverOptions` property corresponds to the model's active `configset object`.

Function	Default Options
`fmincon`	`sbiofit` uses the default options structure associated with `fmincon`, except for: `Display = 'off'` `FunctionTolerance = 1e-6*abs(f0)`, where `f0` is the initial value of the objective function. `OptimalityTolerance = 1e-6*abs(f0)`, where `f0` is the initial value of the objective function. `Algorithm = 'trust-region-reflective'` when `'SensitivityAnalysis'` is true, or `'interior-point'` when `'SensitivityAnalysis'` is false. `FiniteDifferenceStepSize = max(eps^(1/3),min(1e-4,SolverOptions.RelativeTolerance))`, where the `SolverOptions` property corresponds to the model active `configset object`. `TypicalX = 1e-6*x0`, where `x0` is an array of transformed initial estimates.
`fminunc`	`sbiofit` uses the default options structure associated with `fminunc`, except for: `Display = 'off'` `FunctionTolerance = 1e-6*abs(f0)`, where `f0` is the initial value of the objective function. `OptimalityTolerance = 1e-6*abs(f0)`, where `f0` is the initial value of the objective function. `Algorithm = 'trust-region'` when `'SensitivityAnalysis'` is true, or `'quasi-newton'` when `'SensitivityAnalysis'` is false. `FiniteDifferenceStepSize = max(eps^(1/3),min(1e-4,SolverOptions.RelativeTolerance))`, where the `SolverOptions` property corresponds to the model active `configset object`. `TypicalX = 1e-6*x0`, where `x0` is an array of transformed initial estimates.
`fminsearch`	`sbiofit` uses the default options structure associated with `fminsearch`, except for: `Display = 'off'` `TolFun = 1e-6*abs(f0)`, where `f0` is the initial value of the objective function.

Function	Default Options
`lsqcurvefit`, `lsqnonlin`	Requires Optimization Toolbox. `sbiofit` uses the default options structure associated with `lsqcurvefit` and `lsqnonlin`, except for: `Display = 'off'` `FunctionTolerance = 1e-6*norm(f0)`, where `f0` is the initial value of the objective function. `OptimalityTolerance = 1e-6*norm(f0)`, where `f0` is the initial value of the objective function. `FiniteDifferenceStepSize = max(eps^(1/3),min(1e-4,SolverOptions.RelativeTolerance))`, where the `SolverOptions` property corresponds to the model active `configset object`. `TypicalX = 1e-6*x0`, where `x0` is an array of transformed initial estimates.

`patternsearch`	Requires Global Optimization Toolbox.
	
	`sbiofit` uses the default options object (`optimoptions`) associated with `patternsearch`, except for:
	`Display = 'off'`
	`FunctionTolerance = 1e-6*abs(f0)`, where `f0` is the initial value of the objective function.
	`MeshTolerance = 1.0e-3`
	`AccelerateMesh = true`

`ga`	Requires Global Optimization Toolbox.
	
	`sbiofit` uses the default options object (`optimoptions`) associated with `ga`, except for:
	`Display = 'off'`
	`FunctionTolerance = 1e-6*abs(f0)`, where `f0` is the initial value of the objective function.
	`MutationFcn = @mutationadaptfeasible`

`particleswarm`	Requires Global Optimization Toolbox. `sbiofit` uses the following default options for the `particleswarm` algorithm, except for: `Display = 'off'` `FunctionTolerance = 1e-6*abs(f0)`, where `f0` is the initial value of the objective function. `InitialSwarmSpan = 2000 or 8`; `2000` for estimated parameters with no transform; `8` for estimated parameters with `log`, `logit`, or `probit` transforms.
`scattersearch`	See “Scatter Search Algorithm” on page 1-98.

Scatter Search Algorithm

The `scattersearch` method implements a global optimization algorithm [2] that addresses some challenges of parameter estimation in dynamic models, such as convergence to local minima.

Algorithm Overview

The algorithm selects a subset of points from an initial pool of points. In that subset, some points are the best in quality (that is, lowest function value) and some are randomly selected. The algorithm iteratively evaluates the points and explores different directions around various solutions to find better solutions. During this iteration step, the algorithm replaces any old solution with a new one of better quality. Iterations proceed until any stopping criteria are met. It then runs a local solver on the best point.

Initialization

To start the scatter search, the algorithm first decides the total number of points needed (`NumInitialPoints`). By default, the total is `10*`N, where N is the number of estimated parameters. It selects `NumInitialPoints` points (rows) from `InitialPointMatrix`. If `InitialPointMatrix` does not have enough points, the algorithm calls the function defined in `CreationFcn` to generate the additional points needed. By default, Latin hypercube sampling is used to generate these additional points. The algorithm then selects a subset of `NumTrialPoints` points from `NumInitialPoints` points. A fraction (`FractionInitialBest`) of the subset contains the best points in terms of quality. The remaining points in the subset are randomly selected.

Iteration Steps

The algorithm iterates on the points in the subset as follows:

1. Define hyper-rectangles around each pair of points by using the relative qualities (that is, function values) of these points as a measure of bias to create these rectangles.
2. Evaluate a new solution inside each rectangle. If the new solution outperforms the original solution, replace the original with the new one.
3. Apply the go-beyond strategy to the improved solutions and exploit promising directions to find better solutions.
4. Run a local search at every `LocalSearchInterval` iteration. Use the `LocalSelectBestProbability` probability to select the best point as the starting point for a local search. By default, the decision is random, giving an equal chance to select the best point or a random point from the trial points. If the new solution outperforms the old solution, replace the old one with the new one.
5. Replace any stalled point that does not produce any new outperforming solution after `MaxStallTime` seconds with another point from the initial set.
6. Evaluate stopping criteria. Stop iterating if any criteria are met.

The algorithm then runs a local solver on the best point seen.

Stopping Criteria

The algorithm iterates until it reaches a stopping criterion.

Stopping Option	Stopping Test
`FunctionTolerance` and `MaxStallIterations`	Relative change in best objective function value over the last `MaxStallIterations` is less than `FunctionTolerance`.
`MaxIterations`	Number of iterations reaches `MaxIterations`.
`OutputFcn`	`OutputFcn` can halt the iterations.

Stopping Option	Stopping Test
`ObjectiveLimit`	Best objective function value at an iteration is less than or equal to `ObjectiveLimit`.
`MaxStallTime`	Best objective function value did not change in the last `MaxStallTime` seconds.
`MaxTime`	Function run time exceeds `MaxTime` seconds.

Algorithm Options

You create the options for the algorithm using a `struct`.

Option	Description
`CreationFcn`	Handle to the function that creates additional points needed for the algorithm. Default is the character vector `'auto'`, which uses Latin hypercube sampling. The function signature is: `points = CreationFcn(s,N,lb,ub)`, where *s* is the total number of sampled points, *N* is the number of estimated parameters, *lb* is the lower bound, and *ub* is the upper bound. If any output from the function exceeds bounds, these results are truncated to the bounds.
`Display`	Level of display returned to the command line. • `'off'` or `'none'` (default) displays no output. • `'iter'` gives iterative display. • `'final'` displays just the final output.
`FractionInitialBest`	Numeric scalar from `0` through `1`. Default is `0.5`. This number is the fraction of the `NumTrialPoints` that are selected as the best points from the `NumInitialPoints` points.
`FunctionTolerance`	Numeric scalar from `0` through `1`. Default is `1e-6`. The solver stops if the relative change in best objective function value over the last `MaxStallIterations` is less than `FunctionTolerance`. This option is also used to remove duplicate local solutions. See `XTolerance` for details.
`InitialPointMatrix`	Initial (or partial) set of points. *M*-by-*N* real finite matrix, where *M* is the number of points and *N* is the number of estimated parameters. If *M* < `NumInitialPoints`, then `scattersearch` creates more points so that the total number of rows is `NumInitialPoints`. If *M* > `NumInitialPoints`, then `scattersearch` uses the first `NumInitialPoints` rows. Default is the initial transformed values of estimated parameters stored in the `InitialTransformedValue` property of the `EstimatedInfo object`, that is, `[estiminfo.InitialTransformedValue]`.

Option	Description
`LocalOptions`	Options for the local solver. It can be a `struct` (created with `optimset` or `statset`) or an `optimoptions` object, depending on the local solver. Default is the character vector `'auto'`, which uses the default options of the selected solver with some exceptions on page 1-96. In addition to these exceptions, the following options limit the time spent in the local solver because it is called repeatedly: • `MaxFunEvals` (maximum number of function evaluations allowed) = `300` • `MaxIter` (maximum number of iterations allowed) = `200`
`LocalSearchInterval`	Positive integer. Default is `10`. The `scattersearch` algorithm applies the local solver to one of the trial points after the first iteration and again every `LocalSearchInterval` iteration.
`LocalSelectBestProbability`	Numeric scalar from `0` through `1`. Default is `0.5`. It is the probability of selecting the best point as the starting point for a local search. In other cases, one of the trial points is selected at random.
`LocalSolver`	Character vector or string specifying the name of a local solver. Supported methods are `'fminsearch'`, `'lsqnonlin'`, `'lsqcurvefit'`, `'fmincon'`, `'fminunc'`, `'nlinfit'`. Default local solver is selected with the following priority: • If Optimization Toolbox is available, the solver is `lsqnonlin`. • If Statistics and Machine Learning Toolbox is available, the solver is `nlinfit`. • Otherwise, the solver is `fminsearch`.
`MaxIterations`	Positive integer. Default is the character vector `'auto'` representing `20*`N, where N is the number of estimated parameters.
`MaxStallIterations`	Positive integer. Default is `50`. The solver stops if the relative change in the best objective function value over the last `MaxStallIterations` iterations is less than `FunctionTolerance`.
`MaxStallTime`	Positive scalar. Default is `Inf`. The solver stops if `MaxStallTime` seconds have passed since the last improvement in the best-seen objective function value. Here, the time is the wall clock time as opposed to processor cycles.
`MaxTime`	Positive scalar. Default is `Inf`. The solver stops if `MaxTime` seconds have passed since the beginning of the search. The time here means the wall clock time as opposed to processor cycles.
`NumInitialPoints`	Positive integer that is `>= NumTrialPoints`. The solver generates `NumInitialPoints` points before selecting a subset of trial points (`NumTrialPoints`) for subsequent steps. Default is the character vector `'auto'`, which represents `10*`N, where N is the number of estimated parameters.
`NumTrialPoints`	Positive integer that is `>= 2` and `<= NumInitialPoints`. The solver generates `NumInitialPoints` initial points before selecting a subset of trial points (`NumTrialPoints`) for subsequent steps. Default is the character vector `'auto'`, which represents the first even number n for which $n^2 - n \geq 10*N$, where N is the number of estimated parameters.
`ObjectiveLimit`	Scalar. Default is `-Inf`. The solver stops if the best objective function value at an iteration is less than or equal to `ObjectiveLimit`.

Option	Description

`OutputFcn`	Function handle or cell array of function handles. Output functions can read iterative data and stop the solver. Default is `[]`.
	
	Output function signature is `stop = myfun(optimValues,state)`, where:
	
	• `stop` is a logical scalar. Set to `true` to stop the solver.
	• `optimValues` is a structure containing information about the trial points with fields.
	
	  • `bestx` is the best solution point found, corresponding to the function value `bestfval`.
	  • `bestfval` is the best (lowest) objective function value found.
	  • `iteration` is the iteration number.
	  • `medianfval` is the mean objective function value among all the current trial points.
	  • `stalliterations` is the number of iterations since the last change in `bestfval`.
	  • `trialx` is a matrix of the current trial points. Each row represents one point, and the number of rows is equal to `NumTrialPoints`.
	  • `trialfvals` is a vector of objective function values for trial points. It is a matrix for `lsqcurvefit` and `lsqnonlin` methods.
	• `state` is a character vector giving the status of the current iteration.
	
	  • `'init'` – The solver has not begun to iterate. Your output function can use this state to open files, or set up data structures or plots for subsequent iterations.
	  • `'iter'` – The solver is proceeding with its iterations. Typically, this state is where your output function performs its work.
	  • `'done'` – The solver reaches a stopping criterion. Your output function can use this state to clean up, such as closing any files it opened.

`TrialStallLimit`	Positive integer, with default value of `22`. If a particular trial point does not improve after `TrialStallLimit` iterations, it is replaced with another point.
`UseParallel`	Logical flag to compute objective function in parallel. Default is `false`.
`XTolerance`	Numeric scalar from `0` through `1`. Default is `1e-6`. This option defines how close two points must be to consider them identical for creating the vector of local solutions. The solver calculates the distance between a pair of points with `norm`, the Euclidean distance. If two solutions are within `XTolerance` distance of each other and have objective function values within `FunctionTolerance` of each other, the solver considers them identical. If both conditions are not met, the solver reports the solutions as distinct. To get a report of every potential local minimum, set `XTolerance` to `0`. To get a report of fewer results, set `XTolerance` to a larger value.

Multiple Parameter Estimations in Parallel

There are two ways to use parallel computing for parameter estimation.

Set 'UseParallel' to true

To enable parallelization for `sbiofit`, set the name-value pair `'UseParallel'` to `true`. The function supports several levels of parallelization, but only one level is used at a time.

- For an unpooled fit for multiple groups (or individuals), each group runs in parallel.
- For a pooled fit with multiple groups using a solver that has the parallel option, parallelization happens at the solver level. That is, `sbiofit` sets the parallel option of the corresponding estimation method (solver) to `true`, and the objective function evaluations are performed in parallel. For instance, for a gradient-based method (such as `lsqnonlin`), the gradients might be computed in parallel. If the solver is not already executing in parallel, then simulations (of different groups) are run in parallel.

  If you have a single group and are using a solver that does not have the parallel option, setting `UseParallel=true` will run nothing in parallel but still run simulations serially on workers. Thus, It might not be beneficial to enable parallelization because of the overhead time needed by the workers. It might be faster to run without parallelization instead.

Use parfeval or parfor

You can also call `sbiofit` inside a `parfor` loop or use a `parfeval` inside a `for`-loop to perform multiple parameter estimations in parallel. It is recommended that you use `parfeval` because these parallel estimations run asynchronously. If one fit produces an error, it does not affect the other fits.

If you are trying to find a global minimum, you can use global solvers, such as `particleswarm` or `ga` (Global Optimization Toolbox is required). However, if you want to define the initial conditions and run the fits in parallel, see the following example that shows how to use both `parfor` and `parfeval`.

Model and Data Setup

Load the G protein model.

```
sbioloadproject gprotein
```

Store the experimental data containing the time course for the fraction of active G protein [1].

```
time = [0 10 30 60 110 210 300 450 600]';
GaFracExpt = [0 0.35 0.4 0.36 0.39 0.33 0.24 0.17 0.2]';
```

Create a `groupedData object` based on the experimental data.

```
tbl = table(time,GaFracExpt);
grpData = groupedData(tbl);
```

Map the appropriate model element to the experimental data.

```
responseMap = 'GaFrac = GaFracExpt';
```

Specify the parameter to estimate.

```
paramToEstimate    = {'kGd'};
```

Generate initial parameter values for `kGd`.

```
rng('default');
iniVal = abs(normrnd(0.01,1,10,1));
fitResultPar = [];
```

Parallel Pool Setup

Start a parallel pool using the local profile.

```
poolObj = parpool('local');
```

```
Starting parallel pool (parpool) using the 'local' profile ...
Connected to the parallel pool (number of workers: 6).
```

Using `parfeval` (Recommended)

First, define a function handle that uses the local function `sbiofitpar` for estimation. Make sure the function `sbiofitpar` is defined at the end of the script.

```
optimfun = @(x) sbiofitpar(m1,grpData,responseMap,x);
```

Perform multiple parameter estimations in parallel via `parfeval` using different initial parameter values.

```
for i=1:length(iniVal)
    f(i) = parfeval(optimfun,1,iniVal(i));
end
fitResultPar = fetchOutputs(f);
```

Summarize the results for each run.

```
allParValues = vertcat(fitResultPar.ParameterEstimates);
allParValues.LogLikelihood = [fitResultPar.LogLikelihood]';
allParValues.RunNumber = (1:length(iniVal))';
allParValues.Name = categorical(allParValues.Name);
allParValues.InitialValue = iniVal;
% Rearrange the columns.
allParValues = allParValues(:,[5 1 6 2 3 4]);
% Sort rows by LogLikelihood.
sortrows(allParValues,'LogLikelihood')
```

```
ans=10×6 table
    RunNumber    Name    InitialValue    Estimate    StandardError    LogLikelihood
    _________    ____    ____________    ________    _____________    _____________

        9        kGd        3.5884         3.022          0.127          -1.2843
       10        kGd        2.7794         2.779        0.029701         -1.2319
        3        kGd        2.2488        2.2488        0.096013         -1.0786
        2        kGd        1.8439         1.844         0.28825         -0.90104
        6        kGd        1.2977        1.2977        0.011344         -0.48209
        4        kGd       0.87217       0.65951        0.003583           0.9279
        1        kGd       0.54767       0.54776       0.0020424           1.5323
        7        kGd       0.42359       0.42363       0.0024555           2.6097
        8        kGd       0.35262       0.35291      0.00065289           3.6098
        5        kGd       0.32877       0.32877      0.00042474           4.0604
```

Define the local function `sbiofitpar` that performs parameter estimation using `sbiofit`.

```
function fitresult = sbiofitpar(model,grpData,responseMap,initialValue)
estimatedParam = estimatedInfo('kGd');
estimatedParam.InitialValue = initialValue;
fitresult = sbiofit(model,grpData,responseMap,estimatedParam);
end
```

Using parfor

Alternatively, you can perform multiple parameter estimations in parallel via the `parfor` loop.

```
parfor i=1:length(iniVal)
    estimatedParam = estimatedInfo(paramToEstimate,'InitialValue',iniVal(i));
    fitResultTemp = sbiofit(m1,grpData,responseMap,estimatedParam);
    fitResultPar = [fitResultPar;fitResultTemp];
end
```

Close the parallel pool.

```
delete(poolObj);
```

Parameter Estimation with Hybrid Solvers

`sbiofit` supports global optimization methods, namely `ga` and `particleswarm` (Global Optimization Toolbox required). To improve optimization results, these methods lets you run a hybrid function after the global solver stops. The hybrid function uses the final point returned by the global solver as its initial point. Supported hybrid functions are:

- `fminunc`
- `fmincon`
- `patternsearch`
- `fminsearch`

Make sure that your hybrid function accepts your problem constraints. That is, if your parameters are bounded, use an appropriate function (such as `fmincon` or `patternsearch`) for a constrained optimization. If not bounded, use `fminunc`, `fminsearch`, or `patternsearch`. Otherwise, `sbiofit` throws an error.

For an illustrated example, see Perform Hybrid Optimization Using sbiofit.

Version History

Introduced in R2014a

References

[1] Yi, T-M., Kitano, H., and Simon, M. (2003). A quantitative characterization of the yeast heterotrimeric G protein cycle. PNAS. 100, 10764–10769.

[2] Gábor, A., and Banga, J.R. (2015). Robust and efficient parameter estimation in dynamic models of biological systems. BMC Systems Biology. 9:74.

Extended Capabilities

Automatic Parallel Support

Accelerate code by automatically running computation in parallel using Parallel Computing Toolbox™.

To run in parallel, set `'UseParallel'` to `true`.

For more information, see the `'UseParallel'` name-value pair argument.

See Also

`EstimatedInfo object` | `groupedData object` | `LeastSquaresResults object` | `NLINResults object` | `OptimResults object` | `sbiofitmixed` | `nlinfit` | `fmincon` | `fminunc` | `fminsearch` | `lsqcurvefit` | `lsqnonlin` | `patternsearch` | `ga` | `particleswarm`

Topics

“Parameter Scanning, Parameter Estimation, and Sensitivity Analysis in the Yeast Heterotrimeric G Protein Cycle”
“What is Nonlinear Regression?”
“Fitting Options in SimBiology”
“Parameter Transformations”
“Maximum Likelihood Estimation”
“Fitting Workflow”
“Supported Methods for Parameter Estimation in SimBiology”
“Sensitivity Analysis in SimBiology”
“Progress Plot”
“Supported Files and Data Types”
“Create Data File with SimBiology Definitions”

sbiofitmixed

Fit nonlinear mixed-effects model (requires Statistics and Machine Learning Toolbox software)

Syntax

```
fitResults = sbiofitmixed(sm,grpData,ResponseMap,covEstiminfo)
fitResults = sbiofitmixed(sm,grpData,ResponseMap,covEstiminfo,dosing)
fitResults = sbiofitmixed(sm,grpData,ResponseMap,covEstiminfo,dosing,
functionName)
fitResults = sbiofitmixed(sm,grpData,ResponseMap,covEstiminfo,dosing,
functionName,opt)
fitResults = sbiofitmixed(sm,grpData,ResponseMap,covEstiminfo,dosing,
functionName,opt,variants)
fitResults = sbiofitmixed(___,Name,Value)

[fitResults,simDataI,simDataP] = sbiofitmixed(_)
```

Description

`fitResults = sbiofitmixed(sm,grpData,ResponseMap,covEstiminfo)` performs nonlinear mixed-effects estimation using the SimBiology model `sm` and returns a `NLMEResults` object `fitResults`.

`grpData` is a `groupedData object` specifying the data to fit. `ResponseMap` defines the mapping between the model components and response data in `grpData`. `covEstiminfo` is a `CovariateModel` object or an array of `estimatedInfo` objects that defines the parameters to be estimated.

If the model contains active doses and variants, they are applied during the simulation.

`fitResults = sbiofitmixed(sm,grpData,ResponseMap,covEstiminfo,dosing)` uses the dosing information specified by a matrix of SimBiology dose objects `dosing` instead of using the active doses of the model `sm` if there are any.

`fitResults = sbiofitmixed(sm,grpData,ResponseMap,covEstiminfo,dosing, functionName)` uses the estimation function specified by `functionName` that must be either `'nlmefit'` or `'nlmefitsa'`.

`fitResults = sbiofitmixed(sm,grpData,ResponseMap,covEstiminfo,dosing, functionName,opt)` uses the additional options specified by `opt` for the estimation function `functionName`.

`fitResults = sbiofitmixed(sm,grpData,ResponseMap,covEstiminfo,dosing, functionName,opt,variants)` applies variant objects specified as `variants` instead of using any active variants of the model.

`fitResults = sbiofitmixed(___,Name,Value)` uses additional options specified by one or more name-value arguments.

`[fitResults,simDataI,simDataP] = sbiofitmixed(_)` returns a vector of results objects `fitResults`, vector of simulation results `simDataI` using individual-specific parameter estimates, and vector of simulation results `simDataP` using population parameter estimates.

Note

- `sbiofitmixed` unifies `sbionlmefit` and `sbionlmefitsa` estimation functions. Use `sbiofitmixed` to perform nonlinear mixed-effects modeling and estimation.
- `sbiofitmixed` simulates the model using a `SimFunction object`, which automatically accelerates simulations by default. Hence it is not necessary to run `sbioaccelerate` before you call `sbiofitmixed`.

Examples

Fit a One-Compartment PK Model to the Phenobarbital Data

This example uses data collected on 59 preterm infants given phenobarbital during the first 16 days after birth [1]. Each infant received an initial dose followed by one or more sustaining doses by intravenous bolus administration. A total of between 1 and 6 concentration measurements were obtained from each infant at times other than dose times, for a total of 155 measurements. Infant weights and APGAR scores (a measure of newborn health) were also recorded.

Load the data.

```
load pheno.mat ds
```

Convert the dataset to a `groupedData object`, a container for holding tabular data that is divided into groups. It can automatically identify commonly used variable names as the grouping variable or independent (time) variable. Display the properties of the data and confirm that `GroupVariableName` and `IndependentVariableName` are correctly identified as `'ID'` and `'TIME'`, respectively.

```
data = groupedData(ds);
data.Properties
```

```
ans = struct with fields:
                 Description: ''
                    UserData: []
              DimensionNames: {'Observations'  'Variables'}
               VariableNames: {'ID'  'TIME'  'DOSE'  'WEIGHT'  'APGAR'  'CONC'}
       VariableDescriptions: {}
              VariableUnits: {}
         VariableContinuity: []
                   RowNames: {}
           CustomProperties: [1×1 matlab.tabular.CustomProperties]
          GroupVariableName: 'ID'
    IndependentVariableName: 'TIME'
```

Create a simple one-compartment PK model with bolus dosing and linear clearance to fit such data. Use the `PKModelDesign` object to construct the model. Each compartment is defined by a name, dosing type, a clearance type, and whether or not the dosing requires a lag parameter. After

constructing the model, you can also get a `PKModelMap` object `map` that lists the names of species and parameters in the model that are most relevant for fitting.

```
pkmd = PKModelDesign;
addCompartment(pkmd,'Central','DosingType','Bolus',...
                    'EliminationType','linear-clearance',...
                    'HasResponseVariable',true,'HasLag',false);
[onecomp, map] = pkmd.construct;
```

Describe the experimentally measured response by mapping the appropriate model component to the response variable. In other words, indicate which species in the model corresponds to which response variable in the data. The `PKModelMap` property `Observed` indicates that the relevant species in the model is `Drug_Central`, which represents the drug concentration in the system. The relevant data variable is `CONC`, which you visualized previously.

```
map.Observed
```

```
ans = 1×1 cell array
    {'Drug_Central'}
```

Map the `Drug_Central` species to the `CONC` variable.

```
responseMap = 'Drug_Central = CONC';
```

The parameters to estimate in this model are the volume of the central compartment `Central` and the clearance rate `Cl_Central`. The `PKModelMap` property `Estimated` lists these relevant parameters. The underlying algorithm of `sbiofit` assumes parameters are normally distributed, but this assumption may not be true for biological parameters that are constrained to be positive, such as volume and clearance. Specify a log transform for the estimated parameters so that the transformed parameters follow a normal distribution. Use an `estimatedInfo` object to define such transforms and initial values (optional).

```
map.Estimated
```

```
ans = 2×1 cell
    {'Central'   }
    {'Cl_Central'}
```

Define such estimated parameters, appropriate transformations, and initial values.

```
estimatedParams = estimatedInfo({'log(Central)','log(Cl_Central)'},'InitialValue',[1 1]);
```

Each infant received a different schedule of dosing. The amount of drug is listed in the data variable `DOSE`. To specify these dosing during fitting, create dose objects from the data. These objects use the property `TargetName` to specify which species in the model receives the dose. In this example, the target species is `Drug_Central`, as listed by the `PKModelMap` property `Dosed`.

```
map.Dosed
```

```
ans = 1×1 cell array
    {'Drug_Central'}
```

Create a sample dose with this target name and then use the `createDoses` method of `groupedData` object `data` to generate doses for each infant based on the dosing data `DOSE`.

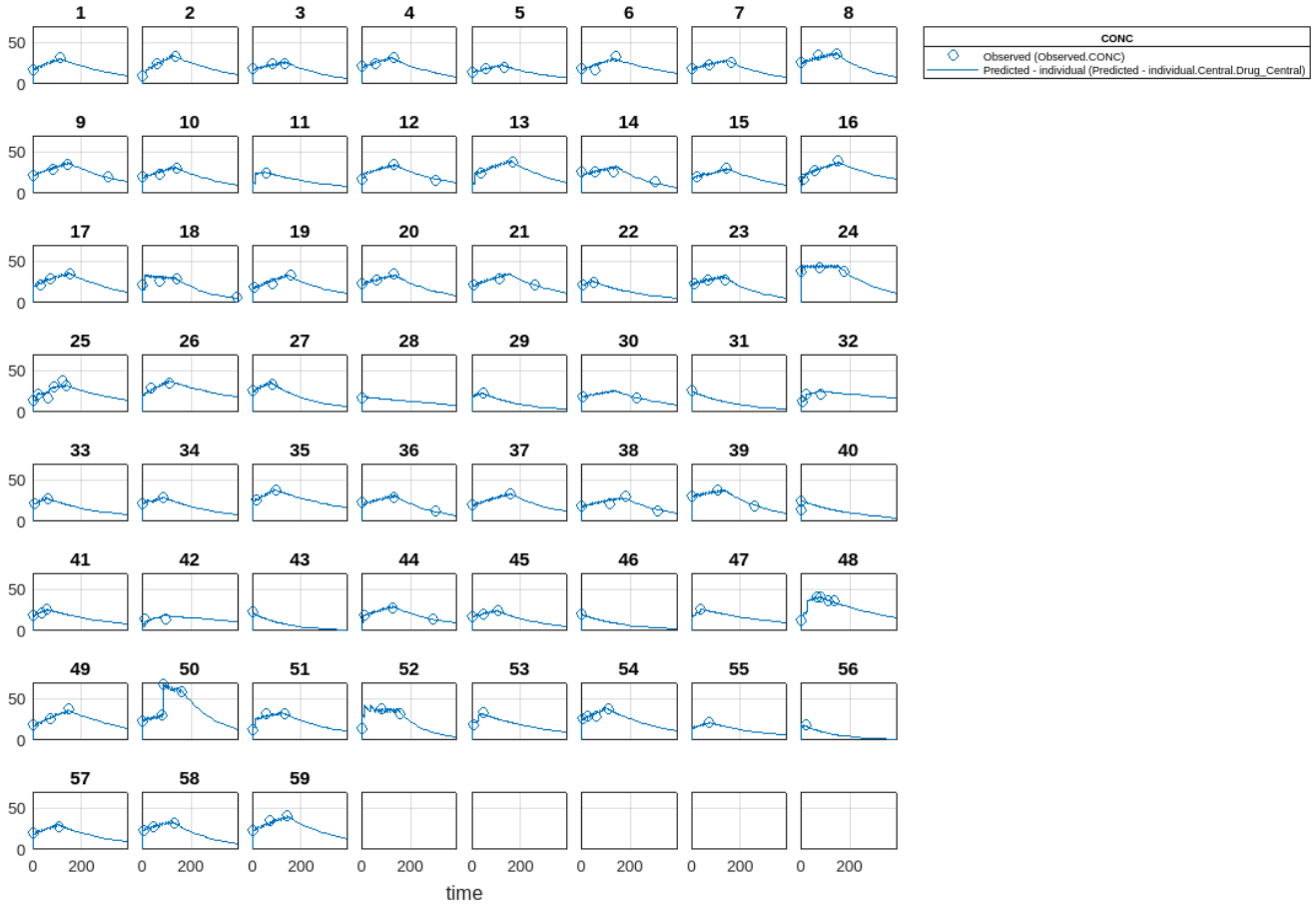
```
sampleDose = sbiodose('sample','TargetName','Drug_Central');
doses = createDoses(data,'DOSE','',sampleDose);
```

Fit the model.

```
[nlmeResults,simI,simP] = sbiofitmixed(onecomp,data,responseMap,estimatedParams,doses,'nlmefit')
```

Visualize the fitted results using individual-specific parameter estimates.

```
plot(nlmeResults,'ParameterType','individual');
```

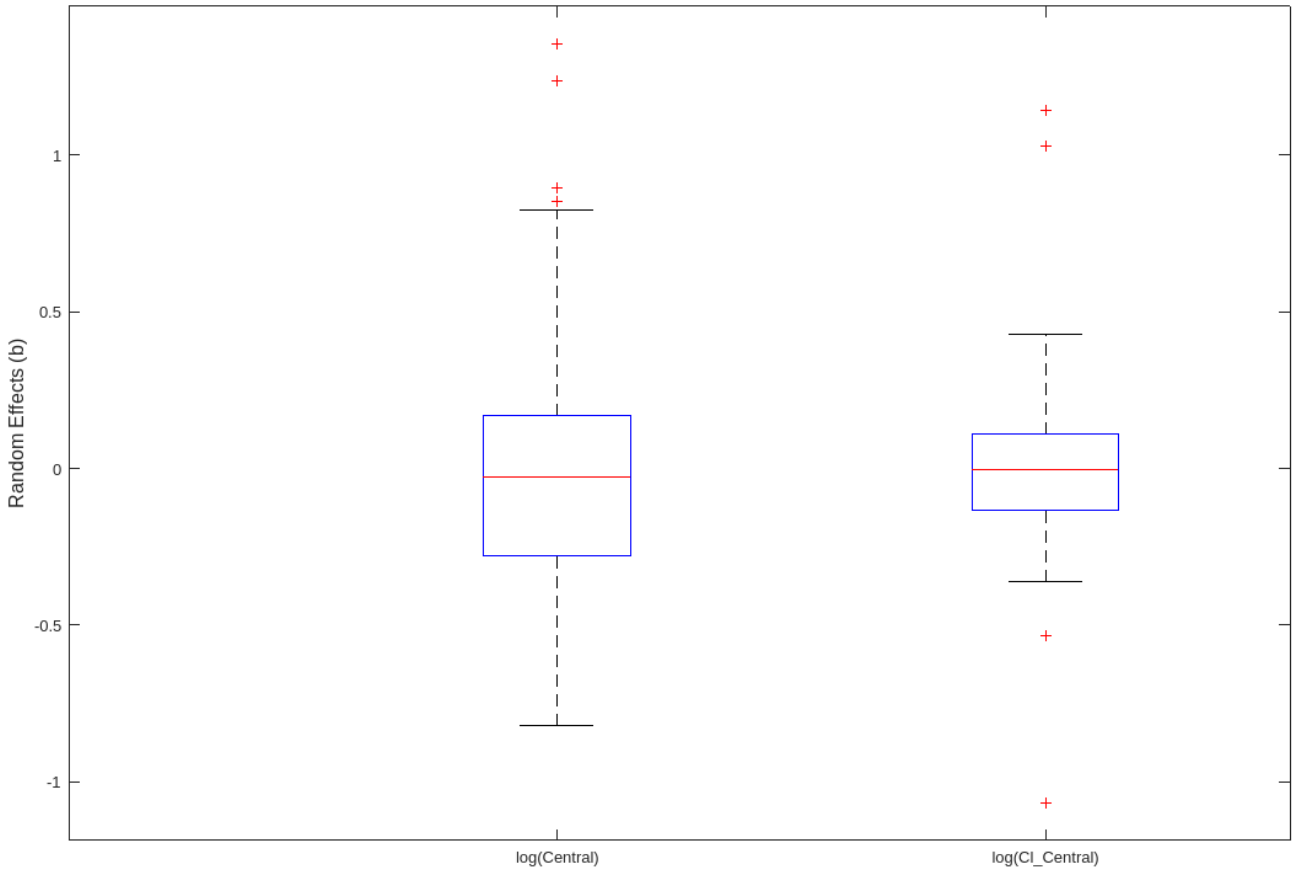


Visualize the fitted results using population parameter estimates.

```
plot(nlmeResults,'ParameterType','population');
```

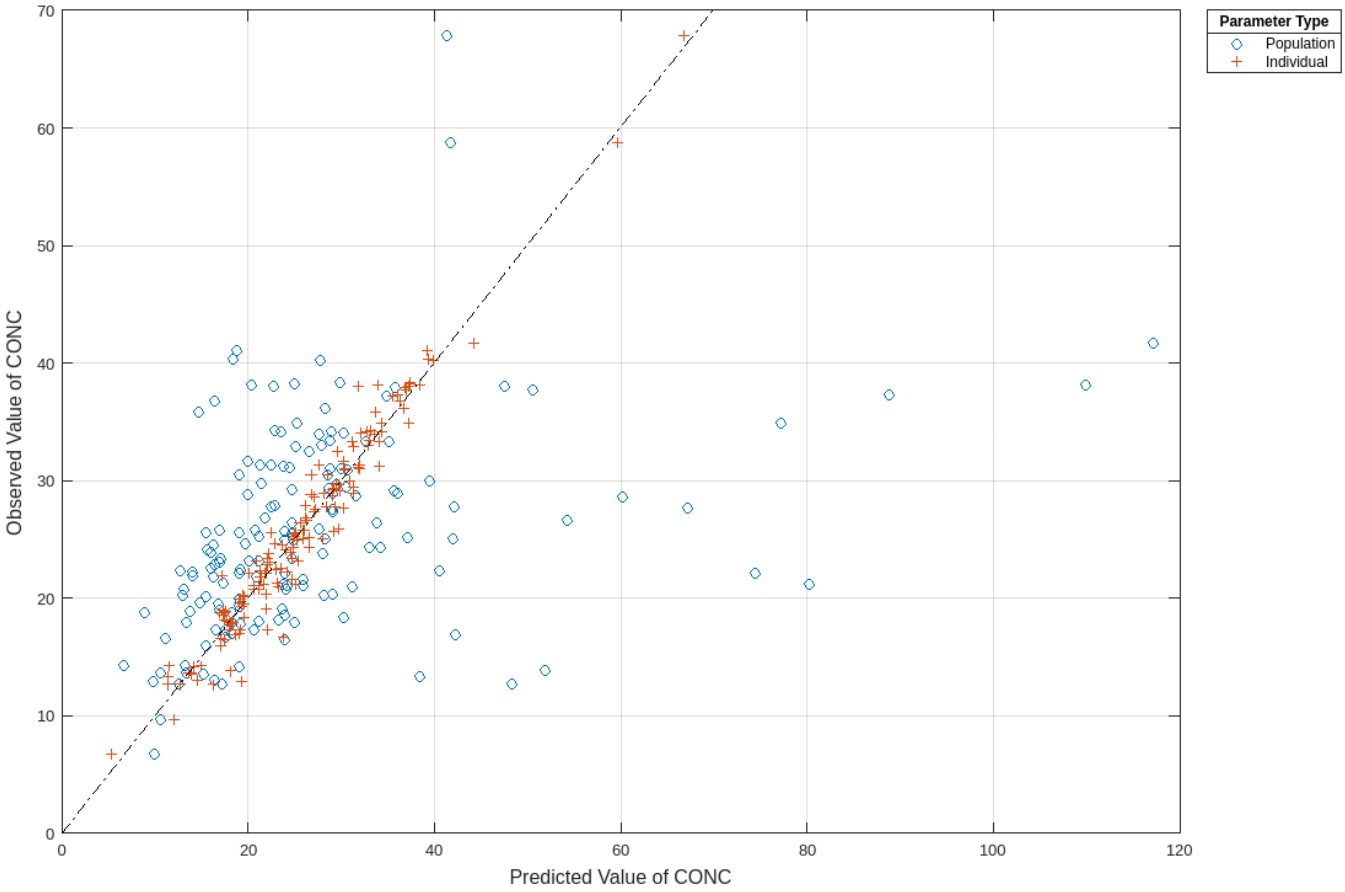
Display the variation of estimated parameters using boxplot.

```
boxplot(nlmeResults)
```



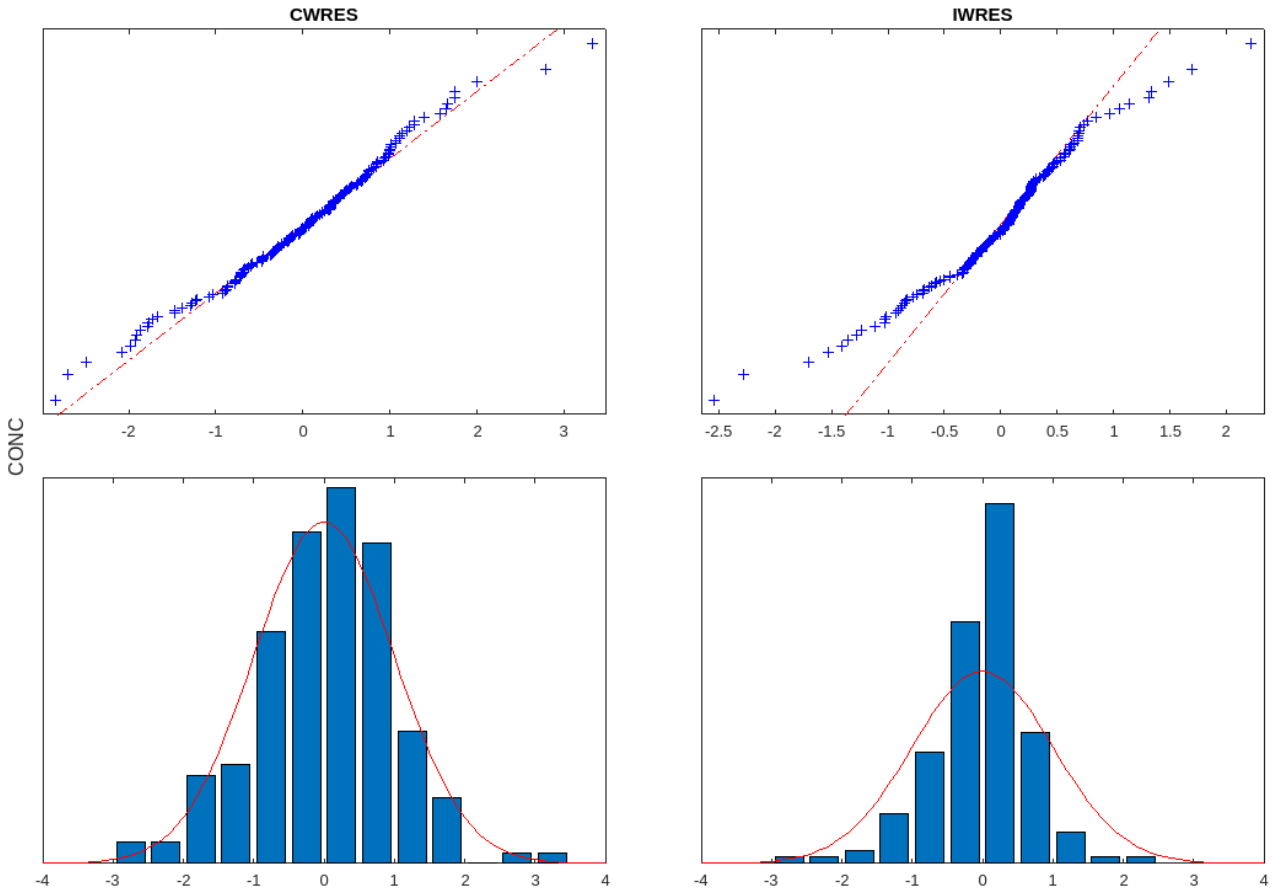
Compare the model predictions to the actual data.

```
plotActualVersusPredicted(nlmeResults)
```



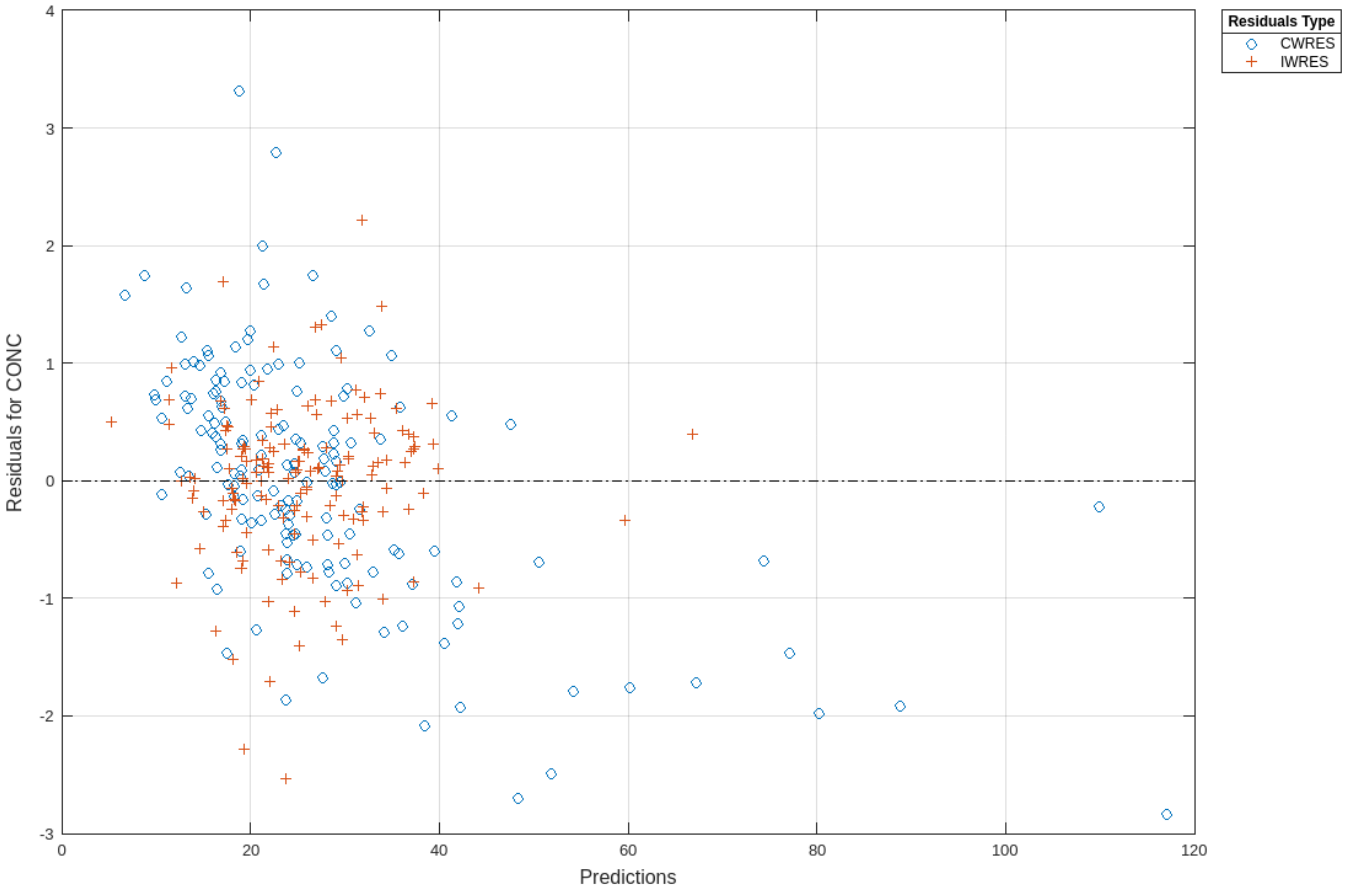
Plot the distribution of residuals.

```
plotResidualDistribution(nlmeResults)
```



Plot residuals for each response using the model predictions on *x*-axis.

```
plotResiduals(nlmeResults,'Predictions')
```



Input Arguments

`sm` — SimBiology model

model object

SimBiology model, specified as a SimBiology `model object`. The active `configset object` of the model contains solver settings for simulation. Any active doses and variants are applied to the model during simulation unless specified otherwise using the `dosing` and `variants` input arguments, respectively.

`grpData` — Data to fit

`groupedData` object

Data to fit, specified as a `groupedData object`.

The name of the time variable must be defined in the `IndependentVariableName` property of `grpData`. For instance, if the time variable name is `'TIME'`, then specify it as follows.

```
grpData.Properties.IndependentVariableName = 'TIME';
```

`grpData` must have at least two groups, and the name of grouping variable name must be defined in the `GroupVariableName` property of `grpData`. For example, if the grouping variable name is `'GROUP'`, then specify it as follows.

```
grpData.Properties.GroupVariableName = 'GROUP';
```

A group usually refers to a set of measurements that represent a single time course, often corresponding to a particular individual or experimental condition.

Note `sbiofitmixed` uses the `categorical` function to identify groups. If any group values are converted to the same value by `categorical`, then those observations are treated as belonging to the same group. For instance, if some observations have no group information (that is, empty character vector), then `categorical` converts empty character vectors to `<undefined>`, and these observations are treated as one group.

ResponseMap — Mapping information of model components to response data

character vector | string | string vector | cell array of character vectors

Mapping information of model components to `grpData`, specified as a character vector, string, string vector, or cell array of character vectors.

Each character vector or string is an equation-like expression, similar to assignment rules in SimBiology. It contains the name (or qualified name) of a quantity (species, compartment, or parameter) or an `observable` object in the model `sm`, followed by the character `'='` and the name of a variable in `grpData`. For clarity, white spaces are allowed between names and `'='`.

For example, if you have the concentration data `'CONC'` in `grpData` for a species `'Drug_Central'`, you can specify it as follows.

```
ResponseMap = 'Drug_Central = CONC';
```

To name a species unambiguously, use the qualified name, which includes the name of the compartment. To name a reaction-scoped parameter, use the reaction name to qualify the parameter.

If the model component name or `grpData` variable name is not a valid MATLAB variable name, surround it by square brackets, such as:

```
ResponseMap = '[Central 1].Drug = [Central 1 Conc]';
```

If a variable name itself contains square brackets, you cannot use it in the expression to define the mapping information.

An error is issued if any (qualified) name matches two components of the same type. However, you can use a (qualified) name that matches two components of different types, and the function first finds the species with the given name, followed by compartments and then parameters.

covEstiminfo — Estimated parameters

vector of `estimatedInfo` objects | `CovariateModel`

Estimated parameters, specified as a vector of `estimatedInfo` objects or a `CovariateModel` object that defines the estimated parameters in the model `sm`, their initial estimates (optional), and their relationship to group-specific covariates included in `grpData` (optional). If this is a vector of `estimatedInfo` objects, then no covariates are used, and all parameters are estimated with group-specific random effects.

You can also specify parameter transformations if necessary. Supported transforms are `log`, `logit`, and `probit`. For details, see `EstimatedInfo object` and `CovariateModel` object.

If `covEstiminfo` is a vector of `estimatedInfo` objects, the `CategoryVariableName` property of each of these objects is ignored.

`dosing` — Dosing information
`[]` | `{}` | 2-D matrix of dose objects | cell vector of dose objects

Dosing information, specified as an empty array (`[]` or `{}`), 2-D matrix or cell vector of dose objects (`ScheduleDose object` or `RepeatDose object`).

If you omit the `dosing` input, the function applies the active doses of the model if there are any.

If you specify the input as empty `[]` or `{}`, no doses are applied during simulation, even if the model has active doses.

For a matrix of dose objects, it must have a single row or one row per group in the input data. If it has a single row, the same doses are applied to all groups during simulation. If it has multiple rows, each row is applied to a separate group, in the same order as the groups appear in the input data. Multiple columns are allowed so that you can apply multiple dose objects to each group.

Note As of R2021b, doses in the columns are no longer required to have the same configuration. If you previously created default (dummy) doses to fill in the columns, these default doses have no effect and indicate no dosing.

For a cell vector of doses, it must have one element or one element per group in the input data. Each element must be `[]` or a vector of doses. Each element of the cell is applied to a separate group, in the same order as the groups appear in the input data.

In addition to manually constructing dose objects using `sbiodose`, if the input `groupedData` object has dosing information, you can use the `createDoses` method to construct doses.

`functionName` — Estimation function name
character vector | string

Estimation function name, specified as a character vector or string. Choices are `'nlmefit'` or `'nlmefitsa'`. For the summary supported methods and fitting options, see “Supported Methods for Parameter Estimation in SimBiology”.

`opt` — Options specific to estimation function
struct

Options specific to the estimation function, specified as a structure.

The structure can contain fields and default values that are the name-value arguments accepted by `nlmefit` and `nlmefitsa`, except the following that are not supported.

- `'FEConstDesign'`
- `'FEGroupDesign’`
- `'FEObsDesign'`
- `'FEParamsSelect'`
- `'ParamTransform'`
- `'REConstDesign'`

- 'REGroupDesign'
- 'REObsDesign'
- 'Vectorization'

'REParamsSelect' is only supported when you provide a vector of estimatedInfo objects when specifying the estimated parameters.

Use the statset function only to set the 'Options' field of the structure (opt), as follows.

```
opt.Options = statset('Display','iter','TolX',1e-3,'TolFun',1e-3);
```

For other supported name-value arguments (see nlmefit and nlmefitsa), set them as follows.

```
opt.ErrorModel = 'proportional';
opt.ApproximationType = 'LME';
```

variants — Variants
[] | {} | vector of variant objects

Variants, specified as an empty array ([] or {}) or vector of variant objects.

If you

- Omit this input argument, the function applies the active variants of the model if there are any.
- Specify this input as empty, no variants are used even if the model has active variants.
- Specify this input as a vector of variants, the function applies the specified variants to all simulations, and the model active variants are not used.
- Specify this input as a vector of variants and also specify the Variants name-value argument, the function applies the variants specified in this input argument before applying the ones specified in the name-value argument.

Name-Value Pair Arguments

Specify optional pairs of arguments as Name1=Value1,...,NameN=ValueN, where Name is the argument name and Value is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose Name *in quotes.*

Example: 'UseParallel',true,'ProgressPlot',true specifies to run the simulations in parallel and show the progress of parameter estimation.

UseParallel — Flag for parallel simulations
false or 0 (default) | true or 1

Flag to enable parallelization, specified as a numeric or logical 1 (true) or 0 (false). If true and Parallel Computing Toolbox is available, the function performs parameter estimation in parallel.

ProgressPlot — Flag to show the progress of parameter estimation
false or 0 (default) | true or 1

Flag to show the progress of parameter estimation, specified as a numeric or logical 1 (true) or 0 (false). If true, a new figure opens containing plots.

Plots show the values of fixed effects parameters (`theta`), the estimates of the variance parameters, that is, the diagonal elements of the covariance matrix of the random effects (Ψ), and the log-likelihood. For details, see “Progress Plot”.

`Variants` — Group-specific variants
`[]` | `{}` | 2-D matrix of variants | cell vector of variants

Group-specific variants, specified as an empty array (`[]` or `{}`), 2-D matrix or cell vector of variant objects. These variants let you specify parameter values for specific groups during fitting. The software applies these group-specific variants after active variants or the `variants` input argument. If the value is empty (`[]` or `{}`), no group-specific variants are applied.

For a matrix of variant objects, the number of rows must be one or must match the number of groups in the input data. The *i*th row of variant objects is applied to the simulation of the *i*th group. The variants are applied in order from the first column to the last. If this matrix has only one row of variants, they are applied to all simulations.

For a cell vector of variant objects, the number of cells must be one or must match the number of groups in the input data. Each element must be `[]` or a vector of variants. If this cell vector has a single cell containing a vector of variants, they are applied to all simulations. If the cell vector has multiple cells, the variants in the *i*th cell are applied to the simulation of the *i*th group.

In addition to manually constructing variant objects using `sbiovariant`, if the input `groupedData` object has variant information, you can use `createVariants` to construct variants.

Output Arguments

`fitResults` — Estimation results
`NLMEResults` object

Estimation results, returned as an `NLMEResults object`.

`simDataI` — Simulation results
vector of `SimData` objects

Simulation results, returned as a vector of `SimData` objects representing simulation results for each group (or individual) using fixed-effect and random-effect estimates (individual-specific parameter estimates).

The states reported in `simDataI` are the states that were included in the `ResponseMap` input argument as well as any other states listed in the `StatesToLog` property of the runtime options (`RuntimeOptions`) of the SimBiology model `sm`.

`simDataP` — Simulation results
vector of `SimData` objects

Simulation results, returned as a vector of `SimData` objects representing simulation results for each group (or individual) using only fixed-effect estimates (population parameter estimates).

The states reported in `simDataP` are the states that were included in the `ResponseMap` input argument as well as any other states listed in the `StatesToLog` property of the runtime options (`RuntimeOptions`) of the SimBiology model `sm`.

Version History

Introduced in R2014a

References

[1] Grasela Jr, T.H., Donn, S.M. (1985) Neonatal population pharmacokinetics of phenobarbital derived from routine clinical data. Dev Pharmacol Ther. 8(6), 374–83.

Extended Capabilities

Automatic Parallel Support

Accelerate code by automatically running computation in parallel using Parallel Computing Toolbox™.

To run in parallel, set `'UseParallel'` to `true`.

For more information, see the `'UseParallel'` name-value pair argument.

See Also

`sbiofit` | `nlmefit` | `nlmefitsa` | `groupedData` | `EstimatedInfo object` | `NLMEResults object` | `sbiofitstatusplot` | `CovariateModel`

Topics

“Model the Population Pharmacokinetics of Phenobarbital in Neonates”
“What Is a Nonlinear Mixed-Effects Model?”
“Nonlinear Mixed-Effects Modeling Workflow”
“Specify a Covariate Model”
“Specify an Error Model”
“Maximum Likelihood Estimation”
“Obtain the Fitting Status”
“Supported Methods for Parameter Estimation in SimBiology”
“Progress Plot”
“Supported Files and Data Types”
“Create Data File with SimBiology Definitions”

sbiofitstatusplot

Plot status of nonlinear mixed-effects estimation

Syntax

```
stop = sbiofitstatusplot(beta, status, state)
stop = sbiofitstatusplot(beta, status, state, fenames)
```

Description

`stop = sbiofitstatusplot(beta, status, state)` initializes or updates a plot with the fixed effects, *`beta`*, the log likelihood *`status`*`.fval`, and the variance of the random effects, `diag(`*`status`*`.Psi)`.

The function returns an output (`stop`) to satisfy requirements for the `'OutputFcn'` option of `nlmefit` or `nlmefitsa`. For `sbiofitstatusplot`, the value of `stop` is always `false`.

`stop = sbiofitstatusplot(`*`beta`*`, `*`status`*`, `*`state`*`, `*`fenames`*`)` specifies the names for the fixed-effects *`fenames`*.

Use `sbiofitstatusplot` to obtain status information about NLME fitting when using the `sbiofitmixed` function. Specify `@sbiofitstatusplot` for the `'OutputFcn'` field of a `statset` option structure and then pass in the structure as an input argument to `sbiofitmixed`.

Alternatively, you can set the `'ProgressPlot'` name-value pair argument to `true` when you run `sbiofitmixed`. The function `sbiofitmixed` then calls `sbiofitstatusplot` at each function iteration. For details, see “Progress Plot”.

Input Arguments

`beta`

Current fixed effects

`status`

Structure containing several fields

Field	Value

`inner`	Structure describing the current status of the inner iterations within the ALT and LAP procedures, with the fields:
	• `procedure`
	  • `'PNLS'`, `'LME'`, or `'none'` when the procedure is `'ALT'`
	  • `'PNLS'`, `'PLM'`, or `'none'` when the procedure is `'LAP'`
	• `state` — `'init'`, `'iter'`, `'done'`, or `'none'`
	• `iteration` — Integer starting from 0, or NaN

Field	Value
`procedure`	`'ALT'` or `'LAP'`
`iteration`	Integer starting from 0
`fval`	Current log-likelihood
`Psi`	Current random-effects covariance matrix
`theta`	Current parameterization of `Psi`
`mse`	Current error variance

`state`

Either `'init'`, `'iter'`, or `'done'`.

`fenames`

Character vector, string, string vector, or cell array of character vectors specifying the names of fixed effects

Examples

Obtain status information for NLME fitting:

```
% Create a statset option with 'OutputFcn'.
fitOptions.Options = statset('OutputFcn',@sbiofitstatusplot);
% Pass the structure to sbiofitmixed function.
results = sbiofitmixed(..., fitOptions);
```

More About

Alt

Alternating algorithm for the optimization of the LME or RELME approximations

FO

First-order estimate

FOCE

First-order conditional estimate

LAP

Optimization of the Laplacian approximation for FO or FOCE

LME

Linear mixed-effects estimation

NLME

Nonlinear mixed effects

PLM

Profiled likelihood maximization

PNLS

Penalized nonlinear least squares

RELME

Restricted likelihood for the linear mixed-effects model

Version History

Introduced in R2009b

See Also

`sbiofitmixed` | `nlmefit` | `sbionlinfit` | `sbionlmefit` | `sbionlmefitsa`

Topics

“Progress Plot”

sbiofittool

(To be removed) Open SimBiology Model Builder

Note `sbiofittool` will be removed in a future release. Use `simBiologyModelBuilder` or `simbiology` to open the **SimBiology Model Builder** app. Use `simBiologyModelAnalyzer` to open the **SimBiology Model Analyzer** app.

Syntax

```
sbiofittool
```

Description

`sbiofittool` opens the **SimBiology Model Builder** app.

Version History

Introduced in R2011a

R2013b: To be removed

Warns starting in R2013b

`sbiofittool` issues a warning that it will be removed in a future release. Use `simBiologyModelBuilder` or `simbiology` to open the **SimBiology Model Builder** app. Use `simBiologyModelAnalyzer` to open the **SimBiology Model Analyzer** app.

See Also

SimBiology Model Builder | SimBiology Model Analyzer

sbiogetmodel

Get model object that generated simulation data

Syntax

`modelObj = sbiogetmodel(simDataObj)`

Arguments

simDataObj	SimData object returned by the function `sbiosimulate` or by `sbioensemblerun`.
modelObj	Model object associated with the SimData object.

Description

`modelObj = sbiogetmodel(simDataObj)` returns the SimBiology model (*modelObj*) associated with the results from a simulation run (*simDataObj*). You can use this function to find the model object associated with the specified SimData object when you load a project with several model objects and SimData objects.

If the SimBiology model used to generate the SimData object (*simDataObj*) is not currently loaded, *modelObj* is empty.

Examples

Retrieve the model object that generated the SimData object.

1. Create a model object, simulate, and then return the results as a SimData object.

```
modelObj = sbmlimport('oscillator');
simDataObj = sbiosimulate(modelObj);
```

2. Get the model that generated the simulation results.

```
modelObj2 = sbiogetmodel(simDataObj)
SimBiology Model - Oscillator

Model Components:
  Models:            0
  Parameters:        0
  Reactions:         42
  Rules:             0
  Species:           23
```

3. Check that the two models are the same.

```
modelObj == modelObj2
ans =
       1
```

Version History

Introduced before R2006a

See Also

`sbiosimulate`

sbiolasterror

SimBiology last error message

Syntax

```
sbiolasterror
diagstruct = sbiolasterror
sbiolasterror([])
sbiolasterror(diagstruct)
```

Arguments

diagstruct	The diagnostic structure holding `Type`, `Message ID`, and `Message` for the errors.

Description

`sbiolasterror` or *`diagstruct`* `= sbiolasterror` return a SimBiology diagnostic structure array containing the last error(s) generated by the software. The fields of the diagnostic structure are:

Type	`'error'`
MessageID	The message ID for the error (for example, `'SimBiology:ConfigSetNameClash'`)
Message	The error message

`sbiolasterror([])` resets the SimBiology last error so that it will return an empty array until the next SimBiology error is encountered.

`sbiolasterror(`*`diagstruct`*`)` will set the SimBiology last error(s) to those specified in the diagnostic structure (*`diagstruct`*).

Examples

This example shows how to use `verify` and `sbiolasterror`.

1 Import a model.

```
a = sbmlimport('radiodecay.xml')
```

```
a =

  SimBiology Model - RadioactiveDecay

  Model Components:
    Compartments:      1
    Events:            0
    Parameters:        1
    Reactions:         1
    Rules:             0
```

```
    Species:           2
    Observables:       0
```

2 Change the `ReactionRate` of a reaction to make the model invalid.

```
a.reactions(1).reactionrate = 'x*y'
```

```
a =

   SimBiology Model - RadioactiveDecay

   Model Components:
     Compartments:      1
     Events:            0
     Parameters:        1
     Reactions:         1
     Rules:             0
     Species:           2
     Observables:       0
```

3 Use the function `verify` to validate the model.

```
a.verify
```

```
Error using SimBiology.Model/verify
--> Error reported from Expression Validation:
Name 'y' in reaction 'Reaction1' does not uniquely refer to any species, parameters, or
compartments according to SimBiology precedence rules.
```

4 Retrieve the error diagnostic `struct`.

```
p = sbiolasterror
```

```
p =

  struct with fields:

        Type: 'Error'
   MessageID: 'SimBiology:ReactionObjectDoesNotResolve'
     Message: 'Name 'y' in reaction 'Reaction1' does not uniquely refer to any species, para
```

5 Reset `sbiolasterror`.

```
sbiolasterror([]);
```

6 Set `sbiolasterror` to the diagnostic structure *p*.

```
sbiolasterror(p);
```

Version History

Introduced in R2006a

See Also

`sbiolastwarning` | `verify`

Topics

sbioroot on page 1-226

sbiolastwarning

SimBiology last warning message

Syntax

```
sbiolastwarning
diagstruct = sbiolastwarning
sbiolastwarning([])
sbiolastwarning(diagstruct)
```

Arguments

diagstruct	The diagnostic structure holding `Type`, `Message ID`, and `Message` for the warnings.

Description

`sbiolastwarning` or *`diagstruct`* `= sbiolastwarning` return a SimBiology diagnostic structure array containing the last warnings generated by the software. The fields of the diagnostic structure are:

Type	`'warning'`
MessageID	The message ID for the warning (for example, `'SimBiology:DANotPerformedReactionRate'`)
Message	The warning message

`sbiolastwarning([])` resets the SimBiology last warning so that it will return an empty array until the next SimBiology warning is encountered.

`sbiolastwarning(`*`diagstruct`*`)` will set the SimBiology last warnings to those specified in the diagnostic structure (*`diagstruct`*).

Version History

Introduced in R2006a

See Also

`sbiolasterror` | `verify`

Topics

sbioroot on page 1-226

sbioloadproject

Load project from file

Syntax

```
sbioloadproject('projFilename')
sbioloadproject ('projFilename','variableName')
sbioloadproject projFilename variableName1 variableName2...
s = sbioloadproject (...)
```

Description

`sbioloadproject('projFilename')` loads a SimBiology project from a project file (*`projFilename`*). If no extension is specified, `sbioloadproject` assumes a default extension of `.sbproj`. Alternatively, the command syntax is `sbioloadproject projFilename`.

`sbioloadproject ('projFilename','variableName')` loads only the variable *`variableName`* from the project file.

`sbioloadproject projFilename variableName1 variableName2...` loads the specified variables from the project.

`s = sbioloadproject (...)` returns the contents of *`projFilename`* in a variable `s`. `s` is a `struct` containing fields matching the variables retrieved from the SimBiology project.

You can display the contents of the project file using the `sbiowhos` command.

Version History

Introduced in R2006a

See Also

`sbioaddtolibrary` | `sbioremovefromlibrary` | `sbiosaveproject` | `sbiowhos`

Topics

sbiosaveproject on page 1-243
sbiowhos on page 1-311
sbioaddtolibrary on page 1-16
sbioremovefromlibrary on page 1-222

sbiomodel

Construct model object

Syntax

```
modelObj = sbiomodel('NameValue')

modelObj = sbiomodel(...'PropertyName', PropertyValue...)
```

Arguments

NameValue	Required property to specify a unique name for a `model` object. Enter a character vector or string.
PropertyName	Property name for a `Model` object from “Property Summary” on page 1-133.
PropertyValue	Property value. Valid value for the specified property.

Description

modelObj = `sbiomodel(`*NameValue*`)` creates and returns a SimBiology `model object` (*modelObj*). In the model object, this method assigns a value (*NameValue*) to the property `Name`.

`modelObj = sbiomodel(...'`*PropertyName*`', `*PropertyValue*`...)` defines optional properties. The name-value pairs can be in any format supported by the function `set`.

Simulate *modelObj* with the function `sbiosimulate`.

Add objects to a model object using the methods `addkineticlaw on page 2-43`, `addparameter` on page 2-75, `addreaction` on page 2-84, `addrule` on page 2-89, and `addspecies` on page 2-108.

All SimBiology model objects can be retrieved from the SimBiology root object. A SimBiology model object has its `Parent` property set to the SimBiology root object.

Method Summary

addcompartment (model, compartment)	Create compartment object
addconfigset (model)	Create configuration set object and add to model object
adddose (model)	Add dose object to model
addevent (model)	Add event object to model object
addobservable	Add observable object to SimBiology model
addparameter (model, kineticlaw)	Create parameter object and add to model or kinetic law object
addreaction (model)	Create reaction object and add to model object
addrule (model)	Create rule object and add to model object
addspecies (model, compartment)	Create species object and add to compartment object within model object
addvariant (model)	Add variant to model
copyobj	Copy SimBiology object and its children
createSimFunction (model)	Create SimFunction object
delete	Delete SimBiology object
display	Display summary of SimBiology object
export (model)	Export SimBiology models for deployment and standalone applications
findUnusedComponents (model)	Find unused species, parameters, and compartments in a model
get	Get SimBiology object properties
getadjacencymatrix (model)	Get adjacency matrix from model object
getconfigset (model)	Get configuration set object from model object
getdose (model)	Return SimBiology dose object
getequations	Return system of equations for model object
getstoichmatrix (model)	Get stoichiometry matrix from model object
getvariant (model)	Get variant from model
removeconfigset (model)	Remove configuration set from model
removedose (model)	Remove dose object from model
removevariant (model)	Remove variant from model
rename	Rename object and update expressions
reorder (model, compartment, kinetic law)	Reorder component lists
set	Set SimBiology object properties
setactiveconfigset (model)	Set active configuration set for model object
verify (model, variant)	Validate and verify SimBiology model

Property Summary

Compartments	Array of compartments in model or compartment
Events	Contain all event objects
Name	Specify name of object
Notes	HTML text describing SimBiology object
Observables	Array of observable objects
Parameters	Array of parameter objects
Parent	Indicate parent object
Reactions	Array of reaction objects
Rules	Array of rules in model object
Tag	Specify label for SimBiology object
Type	Display SimBiology object type
UserData	Specify data to associate with object

Examples

1 Create a SimBiology model object.

```
modelObj = sbiomodel('cell', 'Tag', 'mymodel');
```

2 List all `modelObj` properties and the current values.

```
get(modelObj)
```

MATLAB returns:

```
    Annotation: ''
        Models: [0x1 double]
          Name: 'cell'
         Notes: ''
    Parameters: [0x1 double]
        Parent: [1x1 SimBiology.Root]
       Species: [0x1 double]
     Reactions: [0x1 double]
         Rules: [0x1 double]
           Tag: 'mymodel'
          Type: 'sbiomodel'
      UserData: []
```

3 Display a summary of `modelObj` contents.

```
modelObj
```

```
  SimBiology Model - cell

   Model Components:
     Models:            0
     Parameters:        0
     Reactions:         0
     Rules:             0
     Species:           0
```

Version History

Introduced in R2006a

See Also

`model object` | `addcompartment` | `addconfigset` | `addevent` | `addkineticlaw` | `addparameter` | `addreaction` | `addrule` | `addspecies` | `copyobj` | `get` | `sbioroot` | `sbiosimulate` | `set`

sbiompgsa

Perform multiparametric global sensitivity analysis (requires Statistics and Machine Learning Toolbox)

Syntax

```
mpgsaResults = sbiompgsa(modelObj,params,classifiers)
mpgsaResults = sbiompgsa(modelObj,samples,classifiers)
mpgsaResults = sbiompgsa(modelObj,scenarios,classifiers)
mpgsaResults = sbiompgsa(simdata,samples,classifiers)
mpgsaResults = sbiompgsa(simdata,scenarios,classifiers)
mpgsaResults = sbiompgsa( ___ ,Name,Value)
```

Description

`mpgsaResults = sbiompgsa(modelObj,params,classifiers)` performs a multiparametric global sensitivity analysis (MPGSA on page 1-145) [1] of `classifiers` with respect to model parameters `params` on a SimBiology model `modelObj`. `params` are model quantities (sensitivity inputs) and `classifiers` define the expressions of model responses (model outputs).

`mpgsaResults = sbiompgsa(modelObj,samples,classifiers)` uses parameter `samples` to perform a multiparametric global sensitivity analysis of `classifiers`.

`mpgsaResults = sbiompgsa(modelObj,scenarios,classifiers)` draws samples from `scanarios`, a `SimBiology.Scenarios` object, to perform the analysis.

`mpgsaResults = sbiompgsa(simdata,samples,classifiers)` uses model simulation data `simdata` to perform a multiparametric global sensitivity analysis of `classifiers`.

`mpgsaResults = sbiompgsa(simdata,scenarios,classifiers)` uses samples specified in `scenarios`, a `SimBiology.Scenarios` object.

`mpgsaResults = sbiompgsa( ___ ,Name,Value)` uses additional options specified by one or more name-value pair arguments. Available name-value arguments differ depending on which syntax you are using.

Examples

Perform Multiparametric Global Sensitivity Analysis (MPGSA)

Load the “Target-Mediated Drug Disposition (TMDD) Model”.

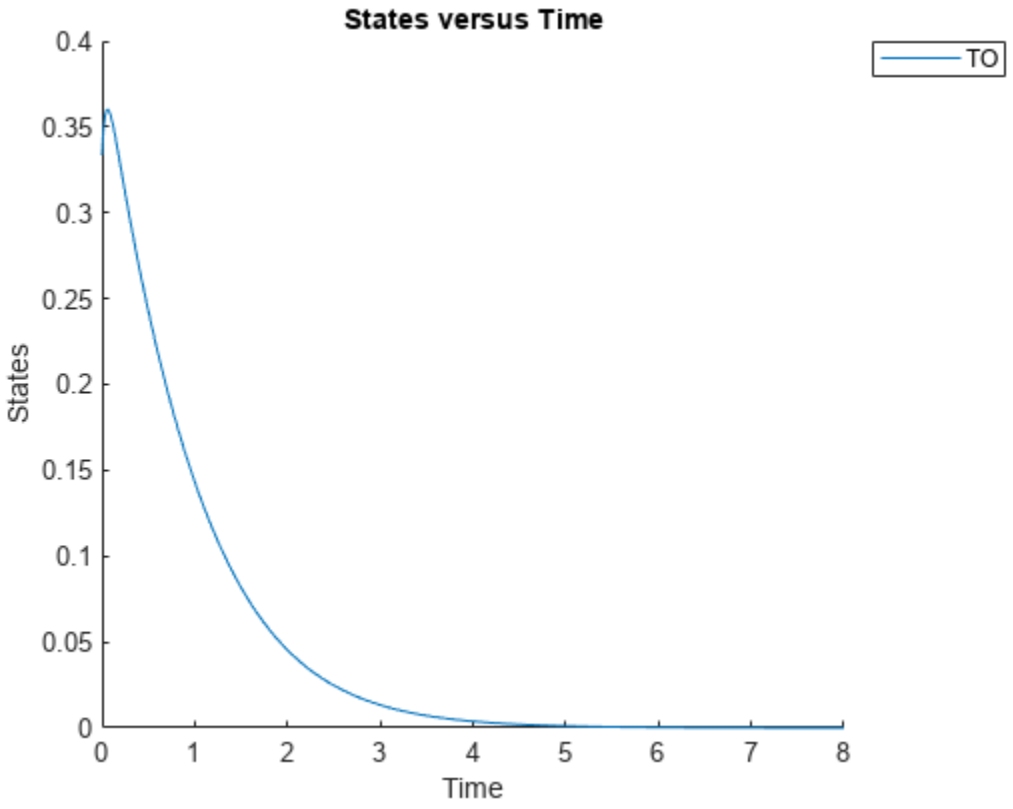
```
sbioloadproject tmdd_with_T0.sbproj
```

Get the active configset and set the target occupancy (`T0`) as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'T0';
```

Simulate the model and plot the `T0` profile.

```
sbioplot(sbiosimulate(m1,cs));
```



Define an exposure (area under the curve of the TO profile) threshold for the target occupancy.

```
classifier = 'trapz(time,TO) <= 0.1';
```

Perform MPGSA to find sensitive parameters with respect to the TO. Vary the parameter values between predefined bounds to generate 10,000 parameter samples.

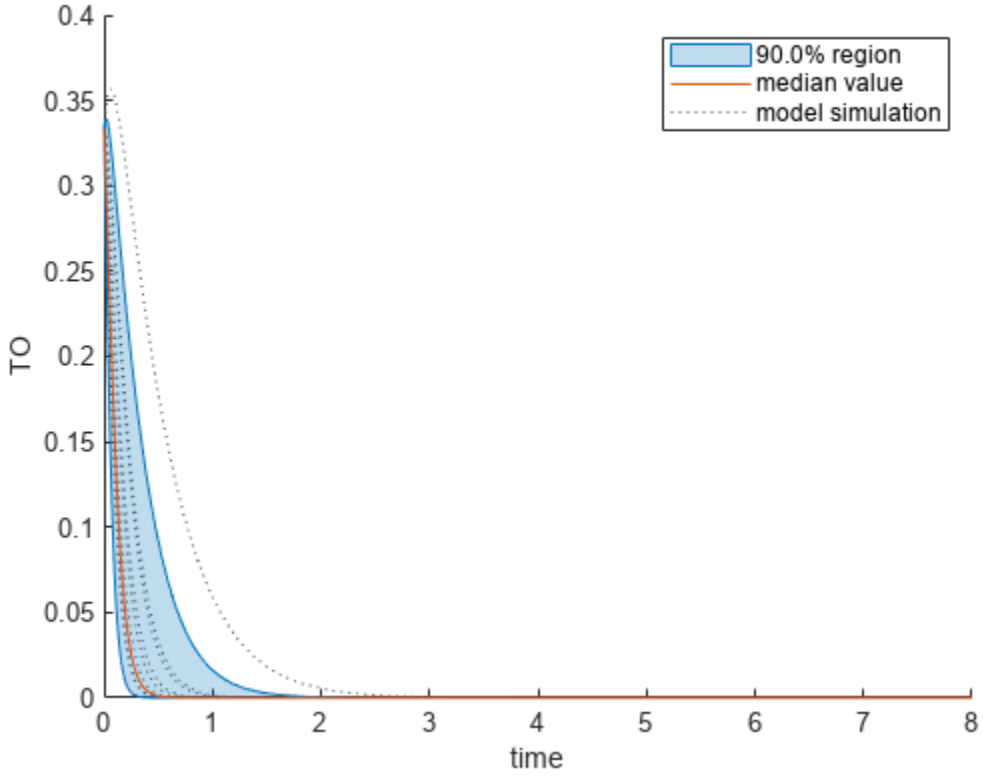
```
% Suppress an information warning that is issued during simulation.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
rng(0,'twister'); % For reproducibility
params = {'kel','ksyn','kdeg','km'};
bounds = [0.1, 1;
          0.1, 1;
          0.1, 1;
          0.1, 1];
mpgsaResults = sbiompgsa(m1,params,classifier,Bounds=bounds,NumberSamples=10000)
```

```
mpgsaResults =
  MPGSA with properties:

                   Classifiers: {'trapz(time,TO) <= 0.1'}
    KolmogorovSmirnovStatistics: [4x1 table]
                      ECDFData: {4x4 cell}
            SignificanceLevel: 0.0500
                       PValues: [4x1 table]
            SupportHypothesis: [10000x1 table]
```

```
    ParameterSamples: [10000x4 table]
        Observables: {'TO'}
      SimulationInfo: [1x1 struct]
```

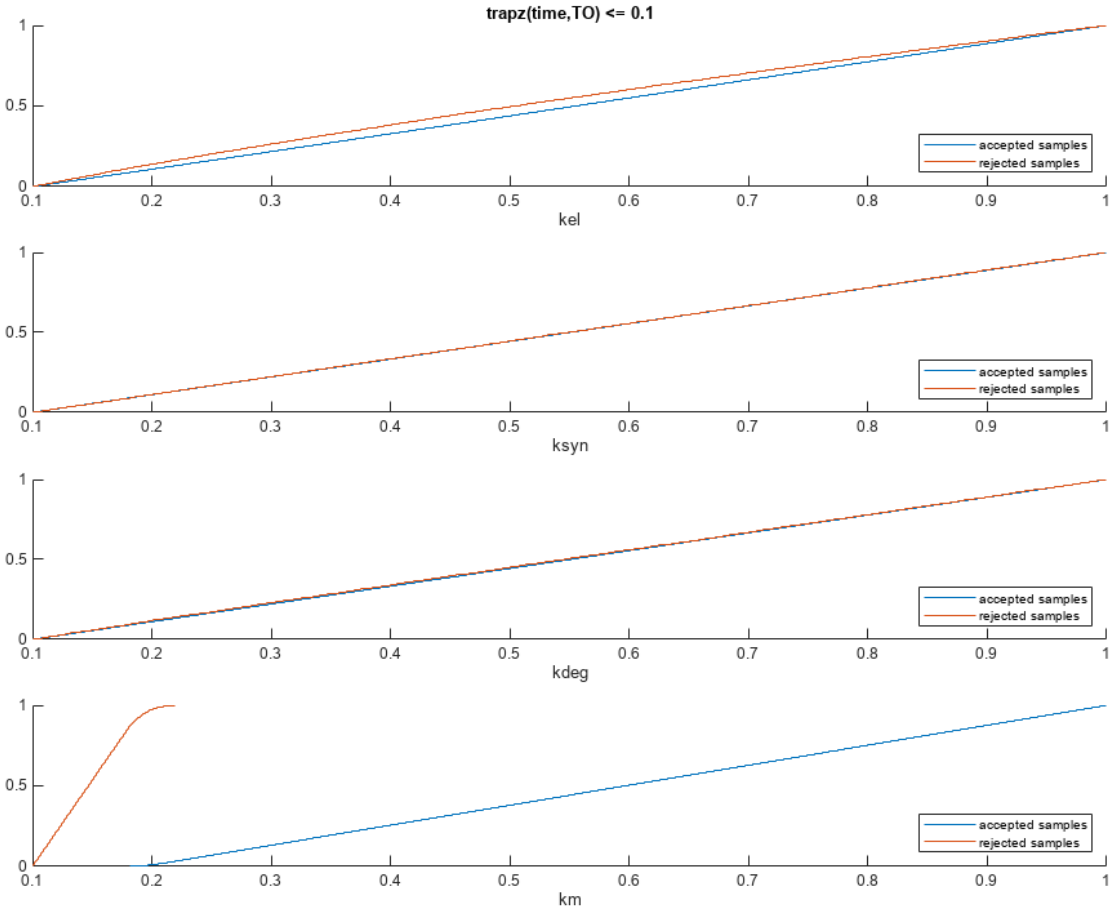
Plot the quantiles of the simulated model response.

```
plotData(mpgsaResults,ShowMedian=true,ShowMean=false);
```



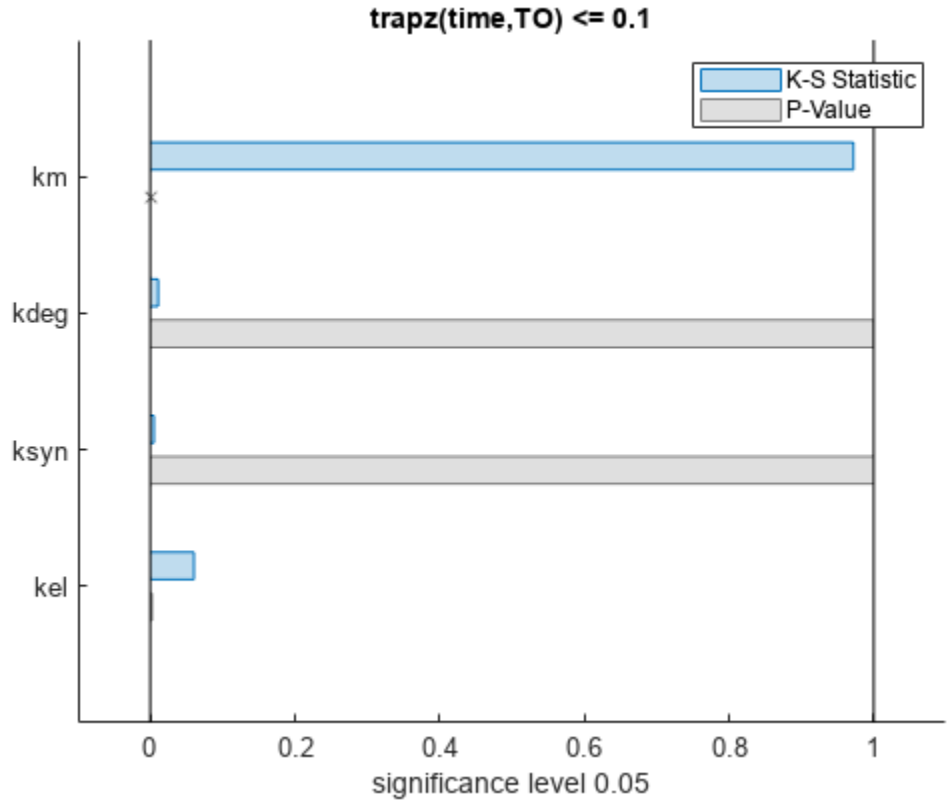
Plot the empirical cumulative distribution functions (eCDFs) of the accepted and rejected samples. Except for `km`, none of the parameters shows a significant difference in the eCDFs for the accepted and rejected samples. The `km` plot shows a large Kolmogorov-Smirnov (K-S) distance between the eCDFs of the accepted and rejected samples. The K-S distance is the maximum absolute distance between two eCDFs curves.

```
h = plot(mpgsaResults);
% Resize the figure.
pos = h.Position(:);
h.Position(:) = [pos(1) pos(2) pos(3)*2 pos(4)*2];
```



To compute the K-S distance between the two eCDFs, SimBiology uses a two-sided test based on the null hypothesis that the two distributions of accepted and rejected samples are equal. See `kstest2` (Statistics and Machine Learning Toolbox) for details. If the K-S distance is large, then the two distributions are different, meaning that the classification of the samples is sensitive to variations in the input parameter. On the other hand, if the K-S distance is small, then variations in the input parameter do not affect the classification of samples. The results suggest that the classification is insensitive to the input parameter. To assess the significance of the K-S statistic rejecting the null-hypothesis, you can examine the p-values.

```
bar(mpgsaResults)
```



The bar plot shows two bars for each parameter: one for the K-S distance (K-S statistic) and another for the corresponding p-value. You reject the null hypothesis if the p-value is less than the significance level. A cross (`x`) is shown for any p-value that is almost 0. You can see the exact p-value corresponding to each parameter.

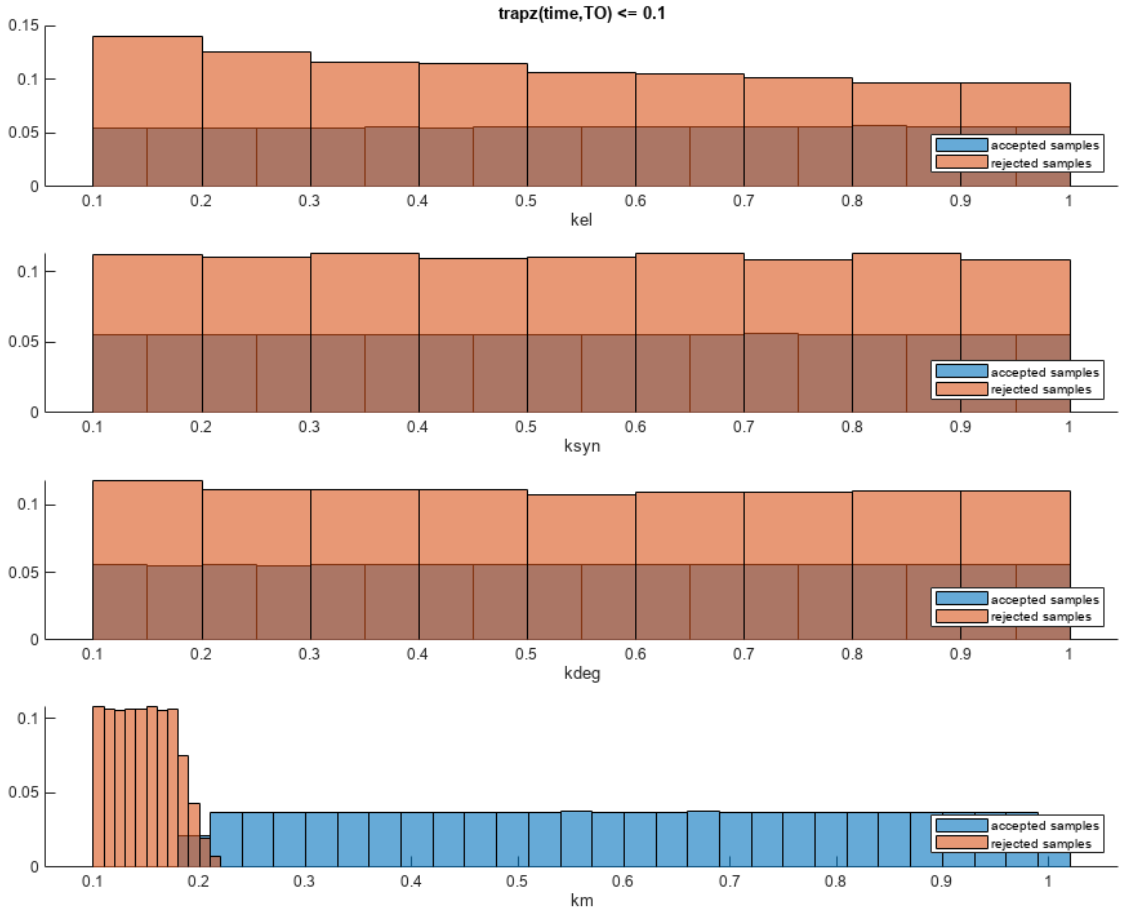
```
[mpgsaResults.ParameterSamples.Properties.VariableNames',mpgsaResults.PValues]
```

```
ans=4×2 table
      Var1      trapz(time,TO) <= 0.1
    ________    _____________________

    {'kel' }          0.0021877
    {'ksyn'}                  1
    {'kdeg'}            0.99983
    {'km'  }                  0
```

The p-values of `km` and `kel` are less than the significance level (0.05), supporting the alternative hypothesis that the accepted and rejected samples come from different distributions. In other words, the classification of the samples is sensitive to `km` and `kel` but not to other parameters (`kdeg` and `ksyn`).

You can also plot the histograms of accepted and rejected samples. The historgrams let you see trends in the accepted and rejected samples. In this example, the histogram of `km` shows that there are more accepted samples for larger `km` values, while the `kel` histogram shows that there are fewer rejected samples as `kel` increases.

```
h2 = histogram(mpgsaResults);
% Resize the figure.
pos = h2.Position(:);
h2.Position(:) = [pos(1) pos(2) pos(3)*2 pos(4)*2];
```



Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

`modelObj` — SimBiology model

SimBiology model object

SimBiology model, specified as a SimBiology `model object`.

`params` — Names of model parameters, species, or compartments

character vector | string | string vector | cell array of character vectors

Names of model parameters, species, or compartments, specified as a character vector, string, string vector, or cell array of character vectors.

Example: `["k1","k2"]`

Data Types: `char` | `string` | `cell`

`simdata` — Model simulation data
vector of `SimData` objects

Model simulation data, specified as a vector of `SimData` objects.

`scenarios` — Source for drawing samples
`SimBiology.Scenarios` object

Source for drawing samples, specified as a `SimBiology.Scenarios` object.

Note The object must not contain doses or variants as its entries.

`classifiers` — Expressions of model responses
character vector | string | string vector | cell array of character vectors

Expressions of model responses, specified as a character vector, string, string vector, or cell array of character vectors. Specify expressions referencing simulated model quantities, observables, time, or MATLAB functions that are on the path.

Each classifier must evaluate to a logical vector of the same length as the number of parameter samples. Entities, such as model quantities or observables, referenced in a classifier expression are evaluated as a matrix with columns containing time courses of the simulated quantity values. Each column represents one sample. Each row represents one output time. For details, see “Multiparametric Global Sensitivity Analysis (MPGSA)” on page 1-145.

If you specify a `SimData` object as the first input, each quantity or `observable` referenced by the classifier must resolve to a logged component in the `SimData` object.

You can formulate a classifier as a modeling question such as whether a model parameter have an effect on the model response exceeding or falling below a target threshold. For example, the following classifier defines an exposure (area under the curve) threshold for the target occupancy `TO`: `trapz(time,TO) <= 0.1`. Another classifier, used by the authors in [1], measures the deviation of the averaged model response from the mean model response over the parameter domain: `mean(TO,1) < mean(TO,'all')`. Here `mean(TO,1)` computes the averaged model response across time for each sample of the sensitivity inputs, and `mean(TO,'all')` computes the mean value of the `TO` response across all output times and all samples.

Example: `"max(Central.Drug(time > 1,:),[],1) <= 7"`

Data Types: `char` | `string` | `cell`

`samples` — Sampled values of model quantities
table

Sampled values of model quantities, specified as a table. The variable names of the table indicate the quantity names.

Data Types: `table`

Name-Value Pair Arguments

Specify one or more comma-separated pairs of `Name,Value` arguments. `Name` is the argument name and `Value` is the corresponding value. `Name` must appear inside quotes. You can specify several name and value pair arguments in any order as `Name1,Value1,...,NameN,ValueN`.

Note Depending on which syntax you use, available name-value pairs differ.

Example: `mpgsaResults = sbiompgsa(m1,{'k1','k2'},classifier,'Bounds',[0.5 5;0.1 1])` specifies parameter bounds for *k1* and *k2*.

For the First Syntax

`Bounds` — Parameter bounds

numeric matrix

Parameter bounds, specified as a numeric matrix with two columns. The first column contains the lower bounds and the second column contains the upper bounds. The number of rows must be equal to the number of parameters in `params`.

If a parameter has a nonzero value, the default bounds are ±10% of the value. If the parameter value is zero, the default bounds are `[0 1]`.

Example: `[0.5 5]`

Data Types: `double`

`NumberSamples` — Number of samples drawn to perform multiparametric global sensitivity analysis

`1000` (default) | positive integer

Number of samples drawn to perform multiparametric global sensitivity analysis, specified as the comma-separated pair consisting of `'NumberSamples'` and a positive integer.

Data Types: `double`

`SamplingMethod` — Method to generate parameter samples

`'Sobol'` (default) | character vector | string

Method to generate parameter samples, specified as a character vector or string. Valid options are:

- `'Sobol'` — Use the low-discrepancy Sobol sequence to generate samples.
- `'Halton'` — Use the low-discrepancy Halton sequence to generate samples.
- `'lhs'` — Use the low-discrepancy Latin hypercube samples.
- `'random'` — Use uniformly distributed random samples.

Data Types: `char` | `string`

`SamplingOptions` — Options for sampling method

struct

Options for the sampling method, specified as a scalar struct. The options differ depending on the sampling method: `sobol`, `halton`, or `lhs`.

For `sobol` and `halton`, specify each field name and value of the structure according to each name-value argument of the `sobolset` or `haltonset` function. SimBiology uses the default value of `1` for the `Skip` argument for both methods. For all other name-value arguments, the software uses the same default values of `sobolset` or `haltonset`. For instance, set up a structure for the `Leap` and `Skip` options with nondefault values as follows.

```
s1.Leap = 50;
s1.Skip = 0;
```

For `lhs`, there are three samplers that support different sampling options.

- If you specify a covariance matrix, SimBiology uses `lhsnorm` for sampling. `SamplingOptions` argument is not allowed.
- Otherwise, use the field name `UseLhsdesign` to select a sampler.
  - If the value is `true`, SimBiology uses `lhsdesign`. You can use the name-value arguments of `lhsdesign` to specify the field names and values.
  - If the value is `false` (default), SimBiology uses a nonconfigurable Latin hypercube sampler that is different from `lhsdesign`. This sampler does not require Statistics and Machine Learning Toolbox. `SamplingOptions` cannot contain any other options, except `UseLhsdesign`.

For instance, set up a structure to use `lhsdesign` with the `Criterion` and `Iterations` options.

```
s2.UseLhsdesign  = true;
s2.Criterion     = "correlation";
s2.Iterations    = 10;
```

You cannot specify this argument when a `SimBiology.Scenarios` object is an input.

`sbiompgsa` ignores this argument if you are also specifying a table of samples as the second input.

`Distributions` — Probability distributions
`prob.UniformDistribution` (default) | `prob.ProbabilityDistribution` object | vector of `prob.ProbabilityDistribution` objects

Probability distributions used to draw samples, specified as a `prob.ProbabilityDistribution` object or vector of these objects. Specify a scalar `prob.ProbabilityDistribution` or vector of length N, where N is the number of input parameters. You can create distribution objects to sample from various distributions, such as uniform, normal, or lognormal distributions, using `makedist`.

If you specify a scalar `prob.ProbabilityDistribution` object, and there are multiple input parameters, `sbiompgsa` uses the same distribution object to draw samples for each parameter.

You cannot specify this argument together with “Bounds” on page 1-0 .

You cannot specify this argument when a `SimBiology.Scenarios` object is an input.

`sbiompgsa` ignores this argument when a table of samples is an input.

For the First and Second Syntaxes

`Doses` — Doses to use during simulations
`ScheduleDose` object | `RepeatDose` object | vector of dose objects

Doses to use during model simulations, specified as a `ScheduleDose` or `RepeatDose` object or a vector of dose objects.

`Variants` — Variants to apply before simulations
variant object | vector of variant objects

Variants to apply before model simulations, specified as a variant object or vector of variant objects.

When you specify multiple variants with duplicate specifications for a property's value, the last occurrence for the property value in the array of variants is used during simulation.

`StopTime` — Simulation stop time
nonnegative scalar

Simulation stop time, specified as a nonnegative scalar. If you specify neither `StopTime` nor `OutputTimes`, the function uses the stop time from the active configuration set of the model. You cannot specify both `StopTime` and `OutputTimes`.

Data Types: `double`

`UseParallel` — Flag to run model simulations in parallel
`false` (default) | `true`

Flag to run model simulations in parallel, specified as `true` or `false`. When the value is `true` and Parallel Computing Toolbox is available, the function runs simulations in parallel.

Data Types: `logical`

`Accelerate` — Flag to turn on model acceleration
`true` (default) | `false`

Flag to turn on model acceleration, specified as `true` or `false`.

Data Types: `logical`

For All Syntaxes

`OutputTimes` — Simulation output times
numeric vector

Simulation output times, specified as the comma-separated pair consisting of `'OutputTimes'` and a numeric vector. The function computes model responses at these output time points. You cannot specify both `StopTime` and `OutputTimes`. By default, the function uses the output times of the first model simulation.

Example: `[0 1 2 3.5 4 5 5.5]`

Data Types: `double`

`SignificanceLevel` — Significance level for Kolmogorov-Smirnov test
`0.05` (default) | numeric scalar between 0 and 1

Significance level for Kolmogorov-Smirnov test, specified as the comma-separated pair consisting of `'SignificanceLevel'` and a numeric scalar between 0 and 1. For details, see “Two-Sample Kolmogorov-Smirnov Test” (Statistics and Machine Learning Toolbox).

Example: `0.1`

Data Types: `double`

`InterpolationMethod` — Method for interpolation of model simulations
`"interp1q"` (default) | character vector | string

Method for interpolation of model responses to a common set of output times, specified as a character vector or string. The valid options follow.

- `"interp1q"` — Use the `interp1q` function.
- Use the `interp1` function by specifying one of the following methods:
  - `"nearest"`
  - `"linear"`
  - `"spline"`
  - `"pchip"`
  - `"v5cubic"`
- `"zoh"` — Specify zero-order hold.

Data Types: `char` | `string`

Output Arguments

`mpgsaResults` — Multiparametric global sensitivity analysis results
`SimBiology.gsa.MPGSA` object

Multiparametric global sensitivity analysis results, returned as a `SimBiology.gsa.MPGSA` object. The object also contains model simulation data used to perform MPGSA.

More About

Multiparametric Global Sensitivity Analysis (MPGSA)

Multiparametric global sensitivity analysis lets you study the relative importance of parameters with respect to a classifier defined by model responses. A classifier is an expression of model responses that evaluates to a logical vector. `sbiompgsa` implements the MPSA method described by Tiemann et. al. (see supporting information text S2) [1].

`sbiompgsa` performs the following steps.

1. Generate *N* parameter samples using a sampling method. `sbiompgsa` stores these samples as a table in a property, `mpgsaResults.ParameterSamples`, of the returned object. The number of rows is equal to the number of samples and the number of columns is equal to the number of input parameters.

   Tip You can specify *N* and the sampling method using the `'NumberSamples'` and `'SamplingMethod'` name-value pair arguments, respectively, when you call `sbiompgsa`.

2. Calculate the model response by simulating the model for each parameter set, which is a single realization of the model parameter values. In this case, a parameter set is equal to a row in the `ParameterSamples` table.

3. Evaluate the classifier. A classifier is an expression that evaluates to a logical vector. For instance, if your model response is the AUC of plasma drug concentration, you can define a classifier with a toxicity threshold of 0.8 where the AUC of the drug concentration above that threshold is considered toxic.
4. Parameter sets are then separated into two different groups, such as accepted (nontoxic) and rejected (toxic) groups.
5. For each input parameter, compute the empirical cumulative distribution functions (`ecdf`) of accepted and rejected sample values.
6. Compare the two eCDFs of accepted and rejected groups using the "Two-Sample Kolmogorov-Smirnov Test" (Statistics and Machine Learning Toolbox) to compute the Kolmogorov-Smirnov distance. The default significance level of the Kolmogorov-Smirnov test is `0.05`. If two eCDFs are similar, the distance is small, meaning the model response is not sensitive with respect to the input parameter. If two eCDFs are different, the distance is large, meaning the model response is sensitive to the parameter.

Note The Kolmogorov-Smirnov test assumes that the samples follow a continuous distribution. Make sure that the eCDF plots are continuous as you increase the number of samples. If eCDFs are not continuous but step-like in the limit of infinite samples, then the results might not reflect the true sensitivities.

Version History

Introduced in R2020a

References

[1] Tiemann, Christian A., Joep Vanlier, Maaike H. Oosterveer, Albert K. Groen, Peter A. J. Hilbers, and Natal A. W. van Riel. "Parameter Trajectory Analysis to Identify Treatment Effects of Pharmacological Interventions." Edited by Scott Markel. *PLoS Computational Biology* 9, no. 8 (August 1, 2013): e1003166. https://doi.org/10.1371/journal.pcbi.1003166.

See Also

`SimBiology.gsa.MPGSA` | `sbiosobol` | `sbioelementaryeffects` | `ecdf` | `kstest2` | `Observable`

Topics

"Sensitivity Analysis in SimBiology"

sbionca

Compute noncompartmental analysis (NCA) parameters (requires Statistics and Machine Learning Toolbox)

Syntax

```
ncaparameters = sbionca(data,opt)
```

Description

`ncaparameters = sbionca(data,opt)` computes NCA parameters from the concentration-time `data`. The options object `opt` defines the data columns and other calculation options. `ncaparameters` is a table of calculated NCA parameter values for each group.

Examples

Compute NCA Parameters from Concentration-Time Data

Load a synthetic data set that contains the drug concentration measurements of four individuals after an IV bolus dose.

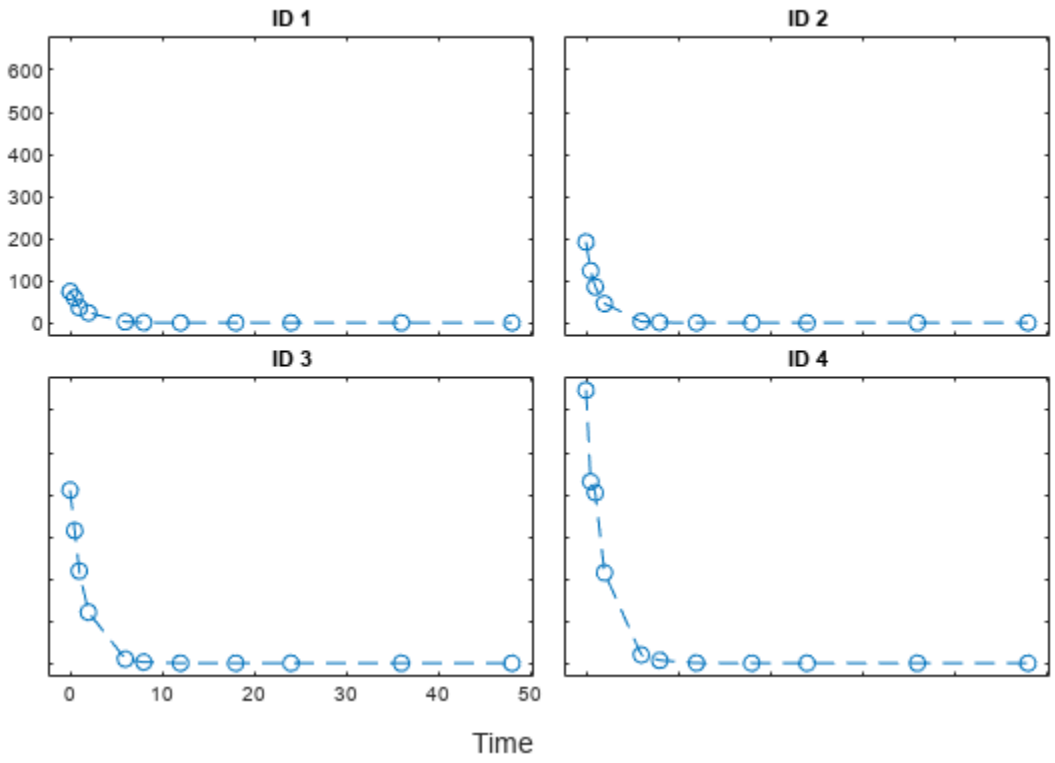
```
load data1.mat
```

Set the dose amounts to NaN at time points when no dose was administered.

```
data1.Dose(data1.Dose(:) == 0) = NaN;
```

Display the data.

```
sbiotrellis(data1,'ID','Time','DrugConc','Marker','o','LineStyle','--');
```



Categorize the data columns using an NCA options object.

```
opt = sbioncaoptions;
opt.groupColumnName         = 'ID';
opt.concentrationColumnName = 'DrugConc';
opt.timeColumnName          = 'Time';
opt.IVDoseColumnName        = 'Dose';
```

Compute NCA parameters for each individual.

```
ncaparameters = sbionca(data1,opt);
```

Display the first few columns of the table. Each row of `ncaparameters` table represents an individual (or group), and each column lists the corresponding NCA parameter value.

```
ncaparameters(:,1:15)
```

```
ans=4×15 table
    ID    doseSchedule    administrationRoute    Lambda_Z      R2       adjusted_R2    Num_points
    __    ____________    ___________________    ________    _______    ___________    __________

    1      {'Single'}         {'IVBolus'}        0.57893     0.99991      0.9999           11
    2      {'Single'}         {'IVBolus'}        0.66798     0.99998     0.99998           11
    3      {'Single'}         {'IVBolus'}        0.62124     0.99999     0.99999           11
    4      {'Single'}         {'IVBolus'}        0.58011     0.99995     0.99995           11
```

You can also specify a custom time range to compute `T_max` and `C_max` within that time range, say from time = 0 to 20. You can do so by setting the `C_max_ranges` property as a cell array of two-element row vector.

```
opt.C_max_ranges    = {[5.5 20]};
ncaparameters2       = sbionca(data1,opt);
```

The function reports the T_max and C_max values within the range by adding two new columns: T_max_5_5__20 and C_max_5_5__20. Note that in the names of these two columns, the last time point is preceded by two consecutive underscores (__).

```
ncaparameters2.T_max_5_5__20(:)
```

```
ans = 4×1

     6
     6
     6
     6
```

```
ncaparameters2.C_max_5_5__20(:)
```

```
ans = 4×1

    2.2719
    3.0213
   10.0233
   19.9006
```

Similarly, you can specify a custom time range to compute the partial AUC value for each group.

```
opt.PartialAreas    = {[0 20]};
ncaparameters3      = sbionca(data1,opt);
ncaparameters3.AUC_0__20(:)
```

```
ans = 4×1
10^3 ×

    0.1436
    0.2994
    0.7665
    1.3017
```

You can also specify multiple time ranges for `C_max_ranges` and `PartialAreas`.

```
opt.C_max_ranges    = {[0 20],[0 10],[0 15]};
opt.PartialAreas    = {[0 12],[0 30]};
ncaparameters4      = sbionca(data1,opt);
```

Input Arguments

data — Concentration-time data

table | dataset

Concentration-time data for NCA parameter computation, specified as a table or dataset.

Example: `concData`

`opt` — Options object to define data columns and calculation options
options object

Options object to define data columns and calculation options, specified as an NCA options object. Use `sbioncaoptions` to create this object and set the options.

Example: `ncaopt`

Output Arguments

`ncaparameters` — Calculated NCA parameters
table

Calculated NCA parameters, returned as a table. For details on how the parameters are computed, see “Noncompartmental Analysis”.

Version History

Introduced in R2017b

See Also

`sbioncaoptions`

Topics
“Noncompartmental Analysis”
“Supported Files and Data Types”
“Create Data File with SimBiology Definitions”

sbioncaoptions

Specify options to calculate noncompartmental analysis (NCA) parameters

Syntax

```
opt = sbioncaoptions
```

Description

`opt = sbioncaoptions` returns an NCA options object. Use dot notation to set the object properties for the options.

Examples

Compute NCA Parameters from Concentration-Time Data

Load a synthetic data set that contains the drug concentration measurements of four individuals after an IV bolus dose.

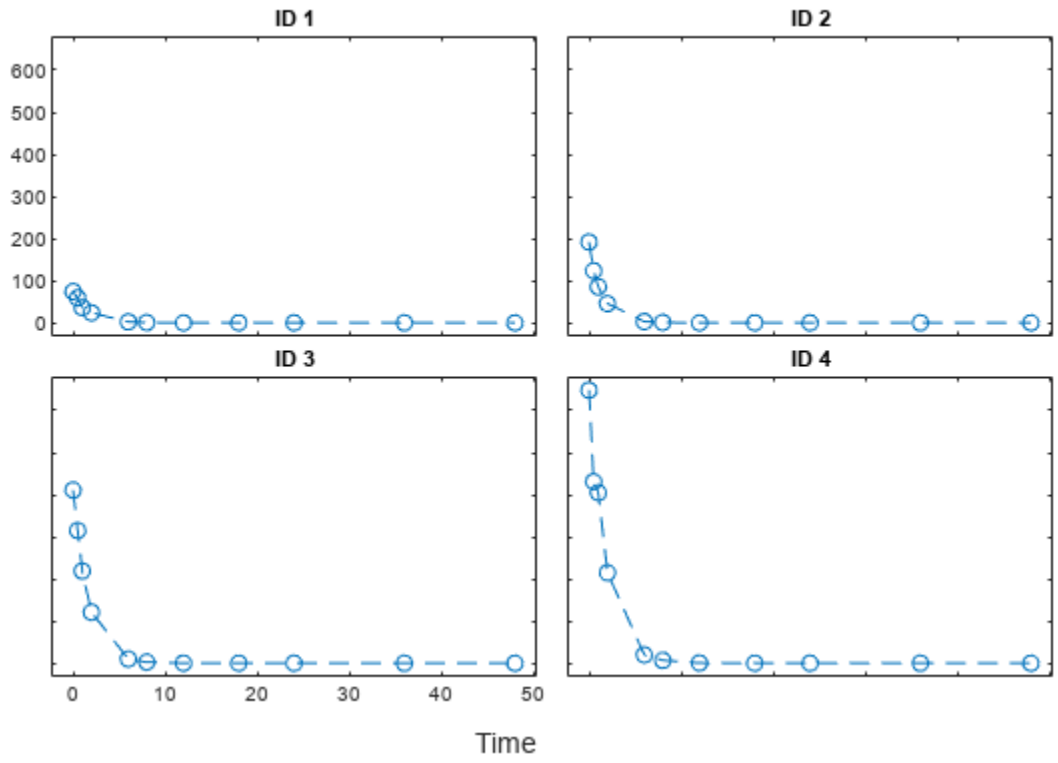
```
load data1.mat
```

Set the dose amounts to NaN at time points when no dose was administered.

```
data1.Dose(data1.Dose(:) == 0) = NaN;
```

Display the data.

```
sbiotrellis(data1,'ID','Time','DrugConc','Marker','o','LineStyle','--');
```



Categorize the data columns using an NCA options object.

```
opt = sbioncaoptions;
opt.groupColumnName         = 'ID';
opt.concentrationColumnName = 'DrugConc';
opt.timeColumnName          = 'Time';
opt.IVDoseColumnName        = 'Dose';
```

Compute NCA parameters for each individual.

```
ncaparameters = sbionca(data1,opt);
```

Display the first few columns of the table. Each row of `ncaparameters` table represents an individual (or group), and each column lists the corresponding NCA parameter value.

```
ncaparameters(:,1:15)
```

```
ans=4×15 table
    ID    doseSchedule    administrationRoute    Lambda_Z      R2       adjusted_R2    Num_points
    __    ____________    ___________________    ________    _______    ___________    __________

    1      {'Single'}         {'IVBolus'}        0.57893     0.99991      0.9999           11
    2      {'Single'}         {'IVBolus'}        0.66798     0.99998     0.99998           11
    3      {'Single'}         {'IVBolus'}        0.62124     0.99999     0.99999           11
    4      {'Single'}         {'IVBolus'}        0.58011     0.99995     0.99995           11
```

You can also specify a custom time range to compute `T_max` and `C_max` within that time range, say from time = 0 to 20. You can do so by setting the `C_max_ranges` property as a cell array of two-element row vector.

```
opt.C_max_ranges    = {[5.5 20]};
ncaparameters2       = sbionca(data1,opt);
```

The function reports the T_max and C_max values within the range by adding two new columns: T_max_5_5__20 and C_max_5_5__20. Note that in the names of these two columns, the last time point is preceded by two consecutive underscores (__).

```
ncaparameters2.T_max_5_5__20(:)
```

```
ans = 4×1

     6
     6
     6
     6
```

```
ncaparameters2.C_max_5_5__20(:)
```

```
ans = 4×1

    2.2719
    3.0213
   10.0233
   19.9006
```

Similarly, you can specify a custom time range to compute the partial AUC value for each group.

```
opt.PartialAreas    = {[0 20]};
ncaparameters3      = sbionca(data1,opt);
ncaparameters3.AUC_0__20(:)
```

```
ans = 4×1
10^3 ×

    0.1436
    0.2994
    0.7665
    1.3017
```

You can also specify multiple time ranges for `C_max_ranges` and `PartialAreas`.

```
opt.C_max_ranges    = {[0 20],[0 10],[0 15]};
opt.PartialAreas    = {[0 12],[0 30]};
ncaparameters4      = sbionca(data1,opt);
```

Output Arguments

opt — Options to calculate NCA parameters

`SimBiology.nca.Options` object

Options to calculate NCA parameters, returned as a `SimBiology.nca.Options` object. The properties of the object are classified into two groups, data classification options and parameter calculation options.

Data Classification Options

Property	Description
`IVDoseColumnName`	Name of the data column that contains the IV dose amount.
`EVDoseColumnName`	Name of the data column that contains the extravascular (EV) dose amount.
`concentrationColumnName`	Name of the data column that contains the measured concentrations.
`timeColumnName`	Name of the data column that contains the time points.
`groupColumnName`	Name of the data column that contains the grouping information. You can specify grouping using two levels of hierarchy. Specify the outer level of grouping in this column. Specify the inner level of grouping (subgroups) in `idColumnName`. If you specify `idColumnName`, then you must also specify `groupColumnName`. For example, consider data that contains three groups, where each group contains four patients. The group column labels the three groups, and the ID column labels each patient.
`idColumnName`	Name of the data column that contains the grouping information. You can specify grouping using two levels of hierarchy. Specify the inner level of grouping (subgroups) in this column. Specify the outer level of grouping in `groupColumnName`. If you specify `idColumnName`, then you must also specify `groupColumnName`.
`infusionRateColumnName`	Name of the data column that contains the infusion rates.

Parameter Calculation Options

Property	Description
`LOQ`	Lower limit of quantization, a threshold below which the values of dependent variable are truncated to zero.
`AdministrationRoute`	Drug administration route. Three types of administration are supported: `IVBolus`, `IVInfusion`, and `ExtraVascular`.
`TAU`	Dosing interval for multiple-dosing data.
`SparseData`	Boolean that indicates whether or not the values of dependent variable are averaged between subgroups to further populate a profile for a group. Time values for each measurement across subgroups (IDs) within a group must be identical.
`Lambda_Z_Time_Min_Max`	Two-element row vector that specifies a custom time range to compute the terminal rate constant (Lambda_z). The time range applies to all groups; you cannot specify a different time range for each group. For details, see “Noncompartmental Analysis”.
`PartialAreas`	Cell array of one or more two-element row vectors that specify one or more time ranges used to compute the partial AUC values. You can specify multiple rows for group-specific ranges, where the number of rows equal the number of groups. If there is only one row, the same time ranges are used for all groups.
`C_max_ranges`	Cell array of one or more two-element row vectors that specify one or more time ranges used to report the `T_max,C_max` pairs within the specified ranges. You can specify multiple rows for group-specific ranges, where the number of rows equal the number of groups. If there is only one row, the same time ranges are used for all groups.

Version History

Introduced in R2017b

See Also

`sbionca`

Topics

“Noncompartmental Analysis”
“Supported Files and Data Types”
“Create Data File with SimBiology Definitions”

sbionlinfit

Perform nonlinear least-squares regression using SimBiology models (requires Statistics and Machine Learning Toolbox software)

Note `sbionlinfit` will be removed in a future release. Use `sbiofit` instead.

Syntax

```
results = sbionlinfit(modelObj, pkModelMapObject, pkDataObj, InitEstimates)
results = sbionlinfit(modelObj, pkModelMapObject, pkDataObj, InitEstimates,
Name,Value)
results = sbionlinfit(modelObj, pkModelMapObject, pkDataObj, InitEstimates,
optionStruct)
[results, SimDataI] = sbionlinfit(...)
```

Description

`results = sbionlinfit(modelObj, pkModelMapObject, pkDataObj, InitEstimates)` performs least-squares regression using the SimBiology model, *`modelObj`*, and returns estimated results in the *`results`* structure.

`results = sbionlinfit(modelObj, pkModelMapObject, pkDataObj, InitEstimates, Name,Value)` performs least-squares regression, with additional options specified by one or more *`Name,Value`* pair arguments.

Following is an alternative to the previous syntax:

`results = sbionlinfit(modelObj, pkModelMapObject, pkDataObj, InitEstimates, optionStruct)` specifies *`optionStruct`*, a structure containing fields and values used by the `options` input structure to the `nlinfit` function.

`[results, SimDataI] = sbionlinfit(...)` returns simulations of the SimBiology model, *`modelObj`*, using the estimated values of the parameters.

Input Arguments

modelObj

SimBiology model object used to fit observed data.

Note If using a model object containing active doses (that is, containing dose objects created using the `adddose` method, and specified as active using the `Active` property of the dose object), be aware that these active doses are ignored by the `sbionlinfit` function.

`pkModelMapObject`

`PKModelMap` object that defines the roles of the model components in the estimation. For details, see `PKModelMap object`.

Note If using a `PKModelMap` object that specifies multiple doses, ensure each element in the `Dosed` property is unique.

`pkDataObj`

`PKData` object that defines the data to use in fitting, and the roles of the data columns used for estimation. For details, see `PKData object`.

Note For each subset of data belonging to a single group (as defined in the data column specified by the `GroupLabel` property), the software allows multiple observations made at the same time. If this is true for your data, be aware that:

- These data points are not averaged, but fitted individually.
- Different numbers of observations at different times cause some time points to be weighted more.

`InitEstimates`

Vector of initial parameter estimates for each parameter estimated in *`pkModelMapObject`*`.Estimated`. The length of *`InitEstimates`* must equal at least the length of *`pkmodelMapObject`*`.Estimated`. The elements of *`InitEstimates`* are transformed as specified by the `ParamTransform` name-value pair argument.

`optionStruct`

Structure containing fields and values used by the `options` input structure to the `nlinfit` function. The structure can also use the name-value pairs listed below as fields and values. Defaults for *`optionStruct`* are the same as for the `options` input structure to `nlinfit`, except for:

- `DerivStep` — Default is the lesser of `1e-4`, or the value of the `SolverOptions.RelativeTolerance` property of the configuration set associated with *`modelObj`*, with a minimum of `eps^(1/3)`.
- `FunValCheck` — Default is `off`.

If you have Parallel Computing Toolbox, you can enable parallel computing for faster data fitting by setting the name-value pair argument `'UseParallel'` to `true` in the `statset` options structure as follows:

```
parpool; % Open a parpool for parallel computing
opt = statset(...,'UseParallel',true); % Enable parallel computing
results = sbionlinfit(...,opt); % Perform data fitting
```

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

The `Name,Value` arguments are the same as the fields and values in the `options` structure accepted by `nlinfit`. For a complete list, see the `options` input argument in the `nlinfit` reference page in the Statistics and Machine Learning Toolbox documentation. The defaults for `Name,Value` arguments are the same as for the `options` structure accepted by `nlinfit`, except for:

- `DerivStep` — Default is the lesser of `1e-4`, or the value of the `SolverOptions.RelativeTolerance` property of the configuration set associated with *`modelObj`*, with a minimum of `eps^(1/3)`.
- `FunValCheck` — Default is `off`.

Following are additional `Name,Value` arguments that you can use with `sbionlinfit`.

`ParamTransform`

Vector of integers specifying a transformation function for each estimated parameter. The transformation function, `f`, takes `estimate` as an input and returns `beta`:

```
beta = f(estimate)
```

Each element in the vector must be one of these integers specifying the transformation for the corresponding value of `estimate`:

- `0` – `beta = estimate`
- `1` – `beta = log(estimate)` (default)
- `2` – `beta = probit(estimate)`
- `3` – `beta = logit(estimate)`

`ErrorModel`

Character vector specifying the form of the error term. Default is `'constant'`. Each model defines the error using a standard normal (Gaussian) variable e, the function value f, and one or two parameters a and b. Choices are:

- `'constant'`: $y = f + a*e$
- `'proportional'`: $y = f + b*\text{abs}(f)*e$
- `'combined'`: $y = f + (a+b*\text{abs}(f))*e$
- `'exponential'`: $y = f*\exp(a*e)$, or equivalently $\log(y) = \log(f) + a*e$

If you specify an error model, the `results` output argument includes an `errorparam` property, which has the value:

- a for `'constant'` and `'exponential'`
- b for `'proportional'`
- [a b] for `'combined'`

Note If you specify an error model, you cannot specify weights.

`Weights`

Either of the following:

- A matrix of real positive weights, where the number of columns corresponds to the number of responses. That is, the number of columns must equal the number of entries in the `DependentVarLabel` property of *`pkDataObj`*. The number of rows in the matrix must equal the number of rows in the data set.
- A function handle that accepts a vector of predicted response values and returns a vector of real positive weights.

> **Note** If using a function handle, the weights must be a function of the response (dependent variable).

Default is no weights. If you specify weights, you cannot specify an error model.

`Pooled`

Logical specifying whether `sbionlinfit` does fitting for each individual (`false`) or if it pools all individual data and does one fit (`true`). If set to `true`, `sbionlinfit` uses the same model parameters for each dose level.

Default: `false`

Output Arguments

`results`

1-by-*N* array of objects, where *N* is the number of groups in *`pkDataObj`*. There is one object per group, and each object contains these properties:

- `ParameterEstimates` — A `dataset (Statistics and Machine Learning Toolbox)` array containing fitted coefficients and their standard errors.
- `CovarianceMatrix` — Estimated covariance matrix for the fitted coefficients.
- `beta` — Vector of scalars specifying the fitted coefficients in transformed space.
- `R` — Vector of scalars specifying the residual values, where $R(i,j)$ is the residual for the ith time point and the jth response in the group of data. If your model incudes:
  - A single response, then `R` is a column vector of residual values associated with time points in the group of data.
  - Multiple responses, then `R` is a matrix of residual values associated with time points in the group of data, for each response.
- `J` — Matrix specifying the Jacobian of the model, with respect to an estimated parameter, that is

  $$J(i,j,k) = \left.\frac{\partial y_k}{\partial \beta_j}\right|_{t_i}$$

  where t_i is the ith time point, β_j is the jth estimated parameter in the transformed space, and y_k is the kth response in the group of data.

  If your model incudes:

  - A single response, then `J` is a matrix of Jacobian values associated with time points in the group of data.
  - Multiple responses, then `J` is a 3-D array of Jacobian values associated with time points in the group of data, for each response.
- `COVB` — Estimated covariance matrix for the transformed coefficients.
- `mse` — Scalar specifying the estimate of the error of the variance term.
- `errorparam` — Estimated parameters of the error model. This property is a scalar if you specify `'constant'`, `'exponential'`, or `'proportional'` for the error model. This property is a two-element vector if you specify `'combined'` for the error model. This property is an empty array if you specify weights using the `'Weights'` name-value pair argument.

`SimDataI`

`SimData object` containing data from simulating the model using estimated parameter values for individuals. This object includes observed states and logged states.

Version History

Introduced in R2009a

See Also

`PKData object` | `PKModelDesign object` | `PKModelDesign object` | `PKModelMap object` | `Model object` | `sbionlmefit` | `nlinfit` | `sbionlmefitsa`

sbionlmefit

Estimate nonlinear mixed effects using SimBiology models (requires Statistics and Machine Learning Toolbox software)

Note `sbionlmefit` will be removed in a future release. Use `sbiofitmixed` instead.

Syntax

```
results = sbionlmefit(modelObj, pkModelMapObject, pkDataObject,
InitEstimates)
results = sbionlmefit(modelObj, pkModelMapObject, pkDataObject, CovModelObj)
results = sbionlmefit(..., Name,Value)
results = sbionlmefit(..., optionStruct)
[results, SimDataI, SimDataP] = sbionlmefit(...)
```

Description

`results = sbionlmefit(modelObj, pkModelMapObject, pkDataObject, InitEstimates)` performs nonlinear mixed-effects estimation using the SimBiology model, `modelObj`, and returns estimated results in the `results` structure.

`results = sbionlmefit(modelObj, pkModelMapObject, pkDataObject, CovModelObj)` specifies the relationship between parameters and covariates using `CovModelObj`, a `CovariateModel` object. The `CovariateModel` object also provides the parameter transformation.

`results = sbionlmefit(..., Name,Value)` performs nonlinear mixed-effects estimation, with additional options specified by one or more `Name,Value` pair arguments.

Following is an alternative to the previous syntax:

`results = sbionlmefit(..., optionStruct)` specifies `optionStruct`, a structure containing fields and values, that are the name-value pair arguments accepted by `nlmefit`. The defaults for `optionStruct` are the same as the defaults for the arguments used by `nlmefit`, with the exceptions explained in “Input Arguments” on page 1-161.

`[results, SimDataI, SimDataP] = sbionlmefit(...)` returns simulation data of the SimBiology model, `modelObj`, using the estimated values of the parameters.

Input Arguments

modelObject

SimBiology model object used to fit observed data.

Note If using a model object containing active doses (that is, containing dose objects created using the `adddose` method, and specified as active using the `Active` property of the dose object), be aware that these active doses are ignored by the `sbionlmefit` function.

pkModelMapObject

PKModelMap object that defines the roles of the model components used for estimation. For details, see PKModelMap on page 2-494 object.

Note If using a PKModelMap object that specifies multiple doses, ensure each element in the Dosed property is unique.

pkDataObject

PKData object that defines the data to use in fitting, and the roles of the columns used for estimation. *pkDataObject* must define target data for at least two groups. For details, see PKData object.

Note For each subset of data belonging to a single group (as defined in the data column specified by the GroupLabel property), the software allows multiple observations made at the same time. If this is true for your data, be aware that:

- These data points are not averaged, but fitted individually.
- Different numbers of observations at different times cause some time points to be weighted more.

InitEstimates

Vector of initial estimates for the fixed effects. The first P elements of *InitEstimates* correspond to the fixed effects for each P element of *pkModelMapObject*.Estimated. Additional elements correspond to the fixed effects for covariate factors. The first P elements of *InitEstimates* are transformed as specified by the ParamTransform name-value pairs (log transformed by default).

CovModelObj

CovariateModel object that defines the relationship between parameters and covariates. For details, see CovariateModel.

Tip To simultaneously fit data from multiple dose levels, omit the random effect (eta) from the expressions in the CovariateModel object.

optionStruct

Structure containing fields and values that are the name-value pairs accepted by the nlmefit function. The defaults for *optionStruct* are the same as the defaults for the arguments used by nlmefit, with the exceptions noted in “Name-Value Pair Arguments” on page 1-163.

If you have Parallel Computing Toolbox, you can enable parallel computing for faster data fitting by setting the name-value pair argument 'UseParallel' to true in the statset options structure as follows:

```
parpool; % Open a parpool for parallel computing
opt = statset(...,'UseParallel',true); % Enable parallel computing
results = sbionlmefit(...,'Options',opt); % Perform data fitting
```

Tip SimBiology software includes the `sbiofitstatusplot` function, which you can specify in the `OutputFcn` field of the `Options` field. This function lets you monitor the status of fitting.

Tip To simultaneously fit data from multiple dose levels, use the `InitEstimates` input argument and set the value of the `REParamsSelect` field to a 1-by-*n* logical vector, with all entries set to `false`, where *n* equals the number of fixed effects.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

The `sbionlmefit` function uses the name-value pair arguments supported by the `nlmefit` function.

These `nlmefit` name-value pairs are hard-coded in `sbionlmefit`, and therefore, you cannot set them:

- `FEParamsSelect`
- `FEConstDesign`
- `FEGroupDesign`
- `FEObsDesign`
- `REConstDesign`
- `REGroupDesign`
- `REObsDesign`
- `Vectorization`

If you provide a `CovariateModel` object as input to `sbionlmefit`, then these `nlmefit` name-value pairs are computed from the covariate model, and therefore, you cannot set them:

- `FEGroupDesign`
- `ParamTransform`
- `REParamsSelect`

You can set all other `nlmefit` name-value pairs. For details, see the `nlmefit` reference page.

Be aware that the defaults for these `nlmefit` name-value pairs differ when used by `sbionlmefit`:

`FEGroupDesign`

Numeric array specifying the design matrix for each group.

Default: `repmat(eye(P),[1 1 nGroups])`, where `P` = the number of estimated parameters, and `nGroups` = the number of groups in the observed data.

`ParamTransform`

Vector of integers specifying how the parameters are distributed.

Note Do not use the `ParamTransform` option to specify parameter transformations when providing a `CovariateModel` object to a fitting function. The `CovariateModel` object provides the parameter transformation.

Default: Vector of ones, which specifies all parameters are log transformed.

`OptimFun`

Character vector specifying the optimization function used in maximizing the likelihood.

Default: `fminunc`, if you have Optimization Toolbox installed. Otherwise, the default is `fminsearch`.

`Options`

Structure containing multiple fields, including `DerivStep`, a scalar or vector specifying the relative difference used in the finite difference gradient calculation, and `FunValCheck`, a logical specifying whether to check for invalid values, such as `NaN` or `Inf`, from `modelfun`.

Default: The default for `DerivStep` is the lesser of `1e-4`, or the value of the `SolverOptions.RelativeTolerance` property of the configuration set associated with *`modelObj`*, with a minimum of `eps^(1/3)`. The default for `FunValCheck` is `off`.

Tip SimBiology software includes the `sbiofitstatusplot` function, which you can specify in the `OutputFcn` field of the `Options` name-value pair input argument. This function lets you monitor the status of fitting.

Tip To simultaneously fit data from multiple dose levels, use the `InitEstimates` input argument and set the `REParamsSelect` name-value pair input argument to a 1-by-*n* logical vector, with all entries set to `false`, where *n* equals the number of fixed effects.

Output Arguments

`results`

Structure containing these fields:

- `FixedEffects` — A `dataset (Statistics and Machine Learning Toolbox)` array containing estimated fixed effects, including standard errors.
- `RandomEffects` — A `dataset` array containing sampled random effects for each group in the observed data in *`pkDataObject`*.
- `IndividualParametereEstimates` — A `dataset` array containing estimated parameter values for individuals, including random effects.
- `PopulationParameterEstimates` — A `dataset` array containing estimated parameter values for the population, without random effects.
- `RandomEffectCovarianceMatrix` — A `dataset` array containing the estimated covariance matrix of the random effects.
- `EstimatedParameterNames` — Cell array of character vectors specifying names of the estimated parameters.

- `CovariateNames` — Cell array of character vectors specifying names of the covariates in *`CovModelObj`*.
- `FixedEffectsStruct` — Structure containing the values of the estimated fixed effects.
- `stats` — Structure containing information such as `AIC`, `BIC`, and weighted residuals. For details on the fields in this structure, see the `stats` structure in `nlmefit` in the Statistics and Machine Learning Toolbox documentation. However, the fields in the `stats` structure returned by `sbionlmefit` vary slightly from those returned by `nlmefit`, namely:
  - `ires`, `pres`, `iwres`, `pwres`, and `cwres` each contain a matrix of raw or weighted residuals, with the number of columns equal to the number of responses in the model.
  - The `stats` structure returned by `sbionlmefit` includes an additional field, `Observed`. This field contains a character vector or cell array of character vectors specifying the measured responses that correspond to the columns in the matrices of the `ires`, `pres`, `iwres`, `pwres`, and `cwres` fields. The `Observed` field is the same as the `Observed` property of the `PKModelMap` input argument.

`SimDataI`

`SimData object` containing data from simulating the model using the estimated parameter values for individuals. This object includes observed states and logged states.

`SimDataP`

`SimData object` containing data from simulating the model using the estimated parameter values for the population. This object includes observed states and logged states.

Version History

Introduced in R2009a

See Also

`Model object` | `nlmefit` | `PKData object` | `SimData object` | `PKModelDesign object` | `PKModelMap object` | `sbiofitstatusplot` | `sbionlinfit` | `sbionlmefitsa`

sbionlmefitsa

Estimate nonlinear mixed effects with stochastic EM algorithm (requires Statistics and Machine Learning Toolbox software)

Note `sbionlmefitsa` will be removed in a future release. Use `sbiofitmixed` instead.

Syntax

```
results = sbionlmefitsa(modelObj, pkModelMapObject, pkDataObject,
InitEstimates)
results = sbionlmefitsa(modelObj, pkModelMapObject, pkDataObject,
CovModelObj)
results = sbionlmefitsa(..., Name,Value)
results = sbionlmefitsa(..., optionStruct)
[results, SimDataI, SimDataP] = sbionlmefitsa(...)
```

Description

`results = sbionlmefitsa(modelObj, pkModelMapObject, pkDataObject, InitEstimates)` performs estimations using the Stochastic Approximation Expectation-Maximization (SAEM) algorithm for fitting population data with the SimBiology model, *`modelObj`*, and returns the estimated results in the *`results`* structure.

`results = sbionlmefitsa(modelObj, pkModelMapObject, pkDataObject, CovModelObj)` specifies the relationship between parameters and covariates using *`CovModelObj`*, a `CovariateModel` object. The `CovariateModel` object also provides the parameter transformation.

`results = sbionlmefitsa(..., Name,Value)` performs estimations using the SAEM algorithm, with additional options specified by one or more *`Name,Value`* pair arguments.

Following is an alternative to the previous syntax:

`results = sbionlmefitsa(..., optionStruct)` specifies *`optionStruct`*, a structure containing fields and values, that are the name-value pair arguments accepted by `nlmefitsa`. The defaults for *`optionStruct`* are the same as the defaults for the name-value pair arguments used by `nlmefitsa`, with the exceptions explained in “Input Arguments” on page 1-166.

`[results, SimDataI, SimDataP] = sbionlmefitsa(...)` returns simulation data of the SimBiology model, *`modelObj`*, using the estimated values of the parameters.

Input Arguments

`modelObject`

SimBiology model object used to fit observed data.

Note If using a model object containing active doses (that is, containing dose objects created using the `adddose` method, and specified as active using the `Active` property of the dose object), be aware that these active doses are ignored by the `sbionlmefitsa` function.

`pkModelMapObject`

`PKModelMap` object that defines the roles of the model components used for estimation. For details, see `PKModelMap object`.

Note If using a `PKModelMap` object that specifies multiple doses, ensure each element in the `Dosed` property is unique.

`pkDataObject`

`PKData` object that defines the data to use in fitting and the roles of the columns used for estimation. *`pkDataObject`* must define target data for at least two groups. For details, see `PKData object`.

Note For each subset of data belonging to a single group (as defined in the data column specified by the `GroupLabel` property), the software allows multiple observations made at the same time. If this is true for your data, be aware that:

- These data points are not averaged, but fitted individually.
- Different numbers of observations at different times cause some time points to be weighted more.

`InitEstimates`

Vector of initial estimates for the fixed effects. The first `P` elements of *`InitEstimates`* correspond to the fixed effects for each `P` element of *`pkModelMapObject`*.`Estimated`. Additional elements correspond to the fixed effects for covariate factors. The first `P` elements of *`InitEstimates`* are transformed as specified by the `ParamTransform` name-value pair argument (log transformed by default).

`CovModelObj`

`CovariateModel` object that defines the relationship between parameters and covariates. For details, see `CovariateModel`.

`optionStruct`

Structure containing fields and values that are name-value pair arguments accepted by the `nlmefitsa` function. The defaults for *`optionStruct`* are the same as the defaults for the arguments used by `nlmefitsa`, with the exceptions noted in “Name-Value Pair Arguments” on page 1-168.

If you have Parallel Computing Toolbox, you can enable parallel computing for faster data fitting by setting the name-value pair argument `'UseParallel'` to `true` in the `statset` options structure as follows:

```
parpool; % Open a parpool for parallel computing
opt = statset(...,'UseParallel',true); % Enable parallel computing
results = sbionlmefitsa(...,'Options',opt); % Perform data fitting
```

Tip SimBiology software includes the `sbiofitstatusplot` function, which you can specify in the `OutputFcn` field of the `Options` field. This function lets you monitor the status of fitting.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

The `sbionlmefitsa` function uses the name-value pair arguments supported by the `nlmefitsa` function.

These `nlmefitsa` name-value pair arguments are hard-coded in `sbionlmefitsa`, and therefore, you cannot set them:

- `FEParamsSelect`
- `FEConstDesign`
- `FEGroupDesign`
- `FEObsDesign`
- `REConstDesign`
- `REGroupDesign`
- `REObsDesign`
- `Vectorization`

If you provide a `CovariateModel` object as input to `sbionlmefitsa`, then these `nlmefitsa` name-value pairs are computed from the covariate model, and therefore, you cannot set them:

- `FEGroupDesign`
- `ParamTransform`
- `REParamsSelect`

You can set all other `nlmefitsa` name-value pair arguments. For details on these arguments, see the `nlmefitsa` reference page.

Be aware that the defaults for these `nlmefitsa` name-value pair arguments differ when used by `sbionlmefitsa`:

`FEGroupDesign`

Numeric array specifying the design matrix for each group.

Default: `repmat(eye(P),[1 1 nGroups])`, where `P` = the number of estimated parameters, and `nGroups` = the number of groups in the observed data.

`ParamTransform`

Vector of integers specifying how the parameters are distributed.

Note Do not use the `ParamTransform` option to specify parameter transformations when providing a `CovariateModel` object to a fitting function. The `CovariateModel` object provides the parameter transformation.

Default: Vector of ones, which specifies all parameters are log transformed.

`OptimFun`

Character vector specifying the optimization function used in maximizing the likelihood.

Default: `fminunc`, if you have Optimization Toolbox installed. Otherwise, the default is `fminsearch`.

`Options`

Structure containing multiple fields, including `DerivStep`, a scalar or vector specifying the relative difference used in the finite difference gradient calculation, and `FunValCheck`, a logical specifying whether to check for invalid values, such as `NaN` or `Inf`, from `modelfun`.

Default: The default for `DerivStep` is the lesser of `1e-4`, or the value of the `SolverOptions.RelativeTolerance` property of the configuration set associated with *`modelObj`*, with a minimum of `eps^(1/3)`. The default for `FunValCheck` is `off`.

Tip SimBiology software includes the `sbiofitstatusplot` function, which you can specify in the `OutputFcn` field of the `Options` name-value pair input argument. This function lets you monitor the status of fitting.

Output Arguments

`results`

Structure containing these fields:

- `FixedEffects` — A `dataset (Statistics and Machine Learning Toolbox)` array containing estimated fixed effects, including standard errors.
- `RandomEffects` — A `dataset` array containing sampled random effects for each group in the observed data in *`pkDataObject`*.
- `IndividualParametereEstimates` — A `dataset` array containing estimated parameter values for individuals, including random effects.
- `PopulationParameterEstimates` — A `dataset` array containing estimated parameter values for the population, without random effects.
- `RandomEffectCovarianceMatrix` — A `dataset` array containing the estimated covariance matrix of the random effects.
- `EstimatedParameterNames` — Cell array of character vectors specifying names of the estimated parameters.
- `CovariateNames` — Cell array of character vectors specifying names of the covariates in *`CovModelObj`*.
- `FixedEffectsStruct` — Structure containing the values of the estimated fixed effects.
- `stats` — Structure containing information such as `AIC`, `BIC`, and weighted residuals. For details on the fields in this structure, see the `stats` structure in `nlmefitsa` in the Statistics and

Machine Learning Toolbox documentation. However, the fields in the `stats` structure returned by `sbionlmefitsa` vary slightly from those returned by `nlmefitsa`, namely:

- `ires`, `pres`, `iwres`, `pwres`, and `cwres` each contain a matrix of raw or weighted residuals, with the number of columns equal to the number of responses in the model.
- The `stats` structure returned by `sbionlmefit` includes an additional field, `Observed`. This field contains a character vector or cell array of character vectors specifying the measured responses that correspond to the columns in the matrices of the `ires`, `pres`, `iwres`, `pwres`, and `cwres` fields. The `Observed` field is the same as the `Observed` property of the `PKModelMap` input argument.

`SimDataI`

`SimData object` containing data from simulating the model using the estimated parameter values for individuals. This object includes observed states and logged states.

`SimDataP`

`SimData object` containing data from simulating the model using the estimated parameter values for the population. This object includes observed states and logged states.

Version History

Introduced in R2010a

See Also

`Model object` | `nlmefitsa` | `PKData object` | `SimData object` | `PKModelDesign object` | `PKModelMap object` | `sbiofitstatusplot` | `sbionlinfit` | `sbionlmefit`

sbionmfiledef

NONMEM file definition object for sbionmimport

Syntax

```
nmdefObj = sbionmfiledef
nmdefObj = sbionmfiledef('PropertyName', PropertyValue)
```

Description

`nmdefObj = sbionmfiledef` creates an NONMEM® file definition object. The NONMEM file definition object contains properties for specifying the NONMEM data items such as group, time, and dependent variable. The NONMEM file definition object lets you configure the properties to the column heading or the index of the column. Use the NONMEM file definition object in conjunction with the `sbionmimport` function to import NONMEM formatted files for use in fitting.

`nmdefObj = sbionmfiledef('PropertyName', PropertyValue)` accepts one or more comma-separated property name/value pairs. Specify *`PropertyName`* inside single quotes. To see the default interpretations for NONMEM formatted files see “Support for Importing NONMEM Formatted Files”.

Input Arguments

`Filename`

If *`Filename`* extension is `.xls` or `.xlsx` it is assumed to be an Excel® file, otherwise it is assumed to be a text file. `sbionmfiledef` file reads the file using the `dataset` constructor.

Property Name/Value Pairs

`CompartmentLabel`

Identifies the column in the NONMEM formatted file that contains the compartment. Specify the header name as a character vector or specify the index number of the header. During import the `sbionmimport` function uses the information in the column to interpret which compartment receives a dose or measured an observation. The `EventIDLabel` property specifies whether the value is a dose or an observation.

Default: `''`

`ContinuousCovariateLabels`

Identifies the column in the NONMEM formatted file that contains continuous covariates. Specify the header name as a character vector or specify the index number of the header.

Default: `{}`

`DateLabel`

Identifies the column in the NONMEM formatted file that contains the date. Specify the header name as a character vector or specify the index number of the header. During import the `sbionmimport`

function uses the information in the column to interpret time information for each dose, response and covariate measurement.

Default: `''`

`DependentVariableLabel`

Identifies the column in the NONMEM formatted file that contains observations. Specify the header name as a character vector or specify the index number of the header.

Default: `''`

`DoseLabel`

Identifies the column in the NONMEM formatted file that contains the dosing information. Specify the header name as a character vector or specify the index number of the header.

Default: `''`

`DoseIntervalLabel`

Identifies the column in the NONMEM formatted file that contains the time between doses. Specify the header name as a character vector or specify the index number of the header.

Default: `''`

`DoseRepeatLabel`

Identifies the column in the NONMEM formatted file that contains the number of times (excluding the initial dose) that the dose is repeated. Specify the header name as a character vector or specify the index number of the header.

Default: `''`

`EventIDLabel`

Identifies the column in the NONMEM formatted file that contains the event identification specifying whether the value is a dose, observation, or covariate. Specify the header name as a character vector or specify the index number of the header.

Default: `''`

`GroupLabel`

Identifies the column in the NONMEM formatted file that contains the Group ID. Specify the header name as a character vector or specify the index number of the header.

Default: `''`

`MissingDependentVariableLabel`

Identifies the column in the NONMEM formatted file that contains information about whether a row contains an observation event (`0`), or not (`1`). Specify the header name as a character vector or specify the index number of the header.

Default: `''`

`RateLabel`

Identifies the column in the NONMEM formatted file that contains the rate of infusion. Specify the header name as a character vector or specify the index number of the header.

Default: `''`

`TimeLabel`

Identifies the column in the NONMEM formatted file that contains the time or date of observation. During import the `sbionmimport` function uses this information to interpret when a dose was given, an observation or covariate measurement recorded. Specify the header name as a character vector or specify the index number of the header.

Default: `''`

`Type`

Identifies the object as `'NMFileDef'`, (Read-only).

Output Arguments

`nmdefObj`

Defines the meanings of the file column headings. It contains properties for specifying data items such as group, time and date. `TimeLabel` and `DependentVariableLabel` must be specified.

Examples

Configure a NONMEM file definition object and import data from a NONMEM formatted file.

```
% Configure a NMFileDef object.
       def = sbionmfiledef;
       def.CompartmentLabel       = 'CPT';
       def.DoseLabel              = 'AMT';
       def.DoseIntervalLabel      = 'II';
       def.DoseRepeatLabel        = 'ADDL';
       def.GroupLabel             = 'ID';
       def.TimeLabel              = 'TIME';
       def.DependentVariableLabel = 'DV';
       def.EventIDLabel           = 'EVID';

       filename = 'C:\work\datafiles\dose.xls';
       ds = sbionmimport(filename, def);
```

Tips

- Use `sbionmfiledef` with `sbionmimport` if you want to apply NONMEM interpretation of headers, and the data file has column header labels different from the table shown in “Support for Importing NONMEM Formatted Files”.
- Use `sbionmimport` if the data file has column header labels identical to the table shown in “Support for Importing NONMEM Formatted Files”.

Version History

Introduced in R2010a

See Also

`sbionmimport`

Topics

“Import Tabular Data from Files”
“Support for Importing NONMEM Formatted Files”

sbionmimport

Import NONMEM-formatted data

Syntax

```
data = sbionmimport('Filename')
data = sbionmimport (nmds)
data = sbionmimport('Filename', nmdefObj)
data = sbionmimport(_,'ParameterName',ParameterValue)
data = sbionmimport(nmds,nmdefObj)
[data, PKDataObj] = sbionmimport(_)
```

Description

`data = sbionmimport('Filename')` or `data = sbionmimport (nmds)` converts a NONMEM formatted file, and assumes that the file is configured to use the following default values for column headers: `ADDL`, `AMT`, `CMT`, `DATE` , `DV`, `EVID`, `ID`, `II`, `MDV`, `RATE`, `TIME`. See “Support for Importing NONMEM Formatted Files” for more information on each of the headers.

`data = sbionmimport('Filename', nmdefObj)` imports a NONMEM formatted file named *`Filename`*, into a SimBiology formatted dataset *`data`* using the meanings of the file column headings defined in the NONMEM file definition object *`nmdefObj`*.

`data = sbionmimport(_,'ParameterName',ParameterValue)` accepts one or more comma-separated name-value pairs that are accepted by the `readtable` method. If additional information is required to read the file such as the delimiter, specify required name-value pairs. See `readtable` for a list of supported name-value pairs.

`data = sbionmimport(nmds,nmdefObj)` reads a NONMEM formatted dataset *`nmds`* and returns a `groupedData object` *`data`*. Each variable in `nmds` must be a column vector.

`[data, PKDataObj] = sbionmimport(_)` returns a `PKData object`, *`PKDataObj`* containing the dataset *`data`*. The *`PKDataObj`* properties show the labels specified in *`data`*.

Input Arguments

`Filename`

If extension of *`Filename`* is `.xls` or `.xlsx`, `sbionmimport` assumes it to be an Excel file. Otherwise `sbionmimport` assumes *`Filename`* is a text file. `sbionmimport` reads the file using `dataset` or `readtable`.

`nmds`

NONMEM-formatted data, specified as a `dataset`, `table`, or `groupedData object`. Each variable in `nmds` must be a column vector.

`nmdefObj`

`nmdefObj` defines the meanings of the file column headings. *`nmdefObj`* is a NONMEM file definition object created using the `sbionmfiledef` function. It contains properties for specifying data items

such as group, time, and date. You must specify the `TimeLabel` and the `DependentVariableLabel` properties.

When this argument is omitted or empty `[]`, the default NONMEM interpretation is used.

Output Arguments

`data`

`groupedData object`. It contains a separate column for each dose and observation. The `Description` property of *`data`* contains a list of warnings, if any, that occurred while constructing *`data`*. To view the warnings, enter the following in the command line.

```
data.Properties.Description
```

`PkDataObj`

The `PKData` object defines the data to use in fitting and the roles of the columns used for estimation. For more information, see `PKData object`.

Examples

Import a Dataset

Load a sample dataset.

```
load pheno ds;
```

The dataset contains 6 variables (columns). Display the names of these variables.

```
ds.Properties.VariableNames
```

```
ans = 1x6 cell
    {'ID'}    {'TIME'}    {'DOSE'}    {'WEIGHT'}    {'APGAR'}    {'CONC'}
```

Define what these variables mean according to the NONMEM definition.

```
def = sbionmfiledef;
def.GroupLabel = 'ID';
def.TimeLabel = 'TIME';
def.DependentVariableLabel = 'CONC';
def.DoseLabel = 'DOSE'
```

```
def =
  NMFileDef with properties:

                CompartmentLabel: ''
       ContinuousCovariateLabels: {}
                       DateLabel: ''
          DependentVariableLabel: 'CONC'
                       DoseLabel: 'DOSE'
            DoseIntervalLabel: ''
              DoseRepeatLabel: ''
                 EventIDLabel: ''
```

```
                     GroupLabel: 'ID'
    MissingDependentVariableLabel: ''
                      RateLabel: ''
                      TimeLabel: 'TIME'
                           Type: 'NMFileDef'
```

```
def.ContinuousCovariateLabels = {'WEIGHT', 'APGAR'};
```

Import the dataset.

```
data = sbionmimport(ds,def);
```

Import Data from a GroupedData Object

Load a sample dataset.

```
load pheno ds
```

Create a `groupedData` object.

```
grpData = groupedData(ds);
```

Use the `groupedData` object variable names and define what column headings or variables mean according to the NONMEM definition.

```
def = sbionmfiledef;
def.GroupLabel = grpData.Properties.GroupVariableName;
def.TimeLabel = grpData.Properties.IndependentVariableName;
def.DependentVariableLabel = 'CONC';
def.DoseLabel = 'DOSE';
def.ContinuousCovariateLabels = {'WEIGHT', 'APGAR'};
```

Import the dataset.

```
data = sbionmimport(grpData,def);
```

Version History

Introduced in R2010a

See Also

`sbionmfiledef`

Topics

“Import Tabular Data from Files”
“Support for Importing NONMEM Formatted Files”

sbioparameterci

Compute confidence intervals for estimated parameters (requires Statistics and Machine Learning Toolbox)

Syntax

```
ci = sbioparameterci(fitResults)
ci = sbioparameterci(fitResults,Name,Value)
```

Description

`ci = sbioparameterci(fitResults)` computes 95% confidence intervals for the estimated parameters from `fitResults`, an `NLINResults` or `OptimResults` returned by the `sbiofit` function. `ci` is a `ParameterConfidenceInterval` object that contains the computed confidence intervals.

`ci = sbioparameterci(fitResults,Name,Value)` uses additional options specified by one or more `Name,Value` pair arguments.

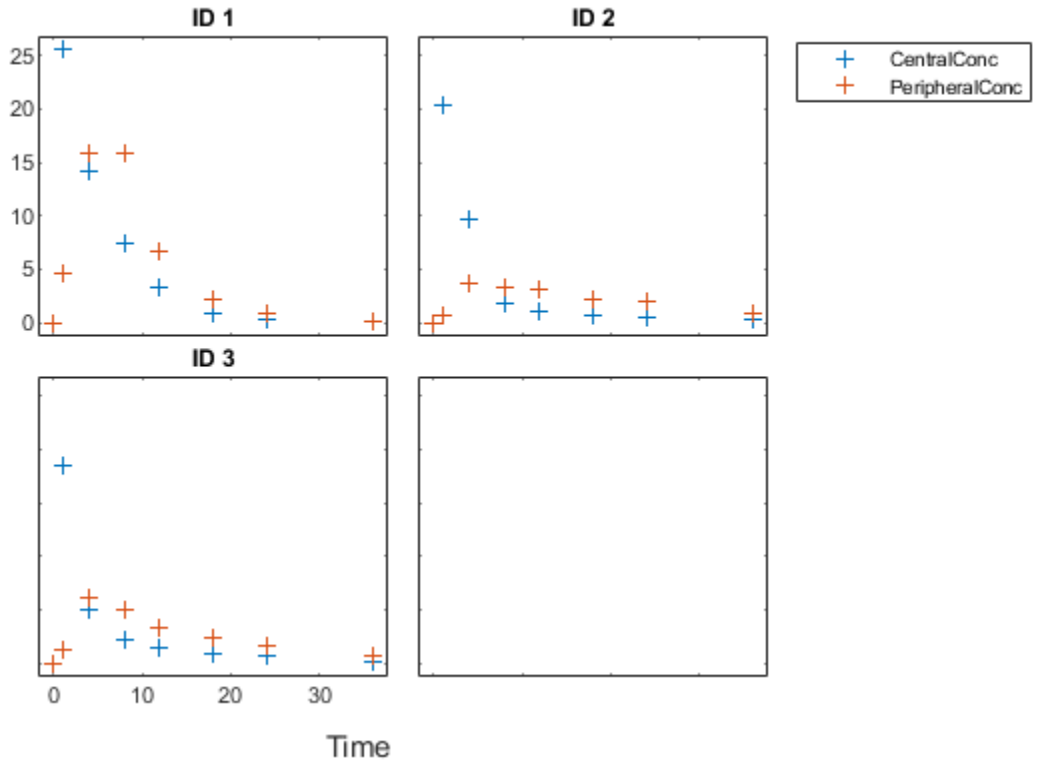
Examples

Compute Confidence Intervals for Estimated PK Parameters and Model Predictions

Load Data

Load the sample data to fit. The data is stored as a table with variables *ID* , *Time* , *CentralConc* , and *PeripheralConc*. This synthetic data represents the time course of plasma concentrations measured at eight different time points for both central and peripheral compartments after an infusion dose for three individuals.

```
load data10_32R.mat
gData = groupedData(data);
gData.Properties.VariableUnits = {'','hour','milligram/liter','milligram/liter'};
sbiotrellis(gData,'ID','Time',{'CentralConc','PeripheralConc'},'Marker','+',...
            'LineStyle','none');
```



Create Model

Create a two-compartment model.

```
pkmd                 = PKModelDesign;
pkc1                 = addCompartment(pkmd,'Central');
pkc1.DosingType      = 'Infusion';
pkc1.EliminationType = 'linear-clearance';
pkc1.HasResponseVariable = true;
pkc2                 = addCompartment(pkmd,'Peripheral');
model                = construct(pkmd);
configset            = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
```

Define Dosing

Define the infusion dose.

```
dose             = sbiodose('dose','TargetName','Drug_Central');
dose.StartTime   = 0;
dose.Amount      = 100;
dose.Rate        = 50;
dose.AmountUnits = 'milligram';
dose.TimeUnits   = 'hour';
dose.RateUnits   = 'milligram/hour';
```

Define Parameters

Define the parameters to estimate. Set the parameter bounds for each parameter. In addition to these explicit bounds, the parameter transformations (such as log, logit, or probit) impose implicit bounds.

```
responseMap = {'Drug_Central = CentralConc','Drug_Peripheral = PeripheralConc'};
paramsToEstimate   = {'log(Central)','log(Peripheral)','Q12','Cl_Central'};
estimatedParam     = estimatedInfo(paramsToEstimate,...
                                   'InitialValue',[1 1 1 1],...
                                   'Bounds',[0.1 3;0.1 10;0 10;0.1 2]);
```

Fit Model

Perform an unpooled fit, that is, one set of estimated parameters for each patient.

```
unpooledFit = sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',false);
```

Perform a pooled fit, that is, one set of estimated parameters for all patients.

```
pooledFit = sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',true);
```

Compute Confidence Intervals for Estimated Parameters

Compute 95% confidence intervals for each estimated parameter in the unpooled fit.

```
ciParamUnpooled = sbioparameterci(unpooledFit);
```

Display Results

Display the confidence intervals in a table format. For details about the meaning of each estimation status, see “Parameter Confidence Interval Estimation Status” on page 2-666.

```
ci2table(ciParamUnpooled)
```

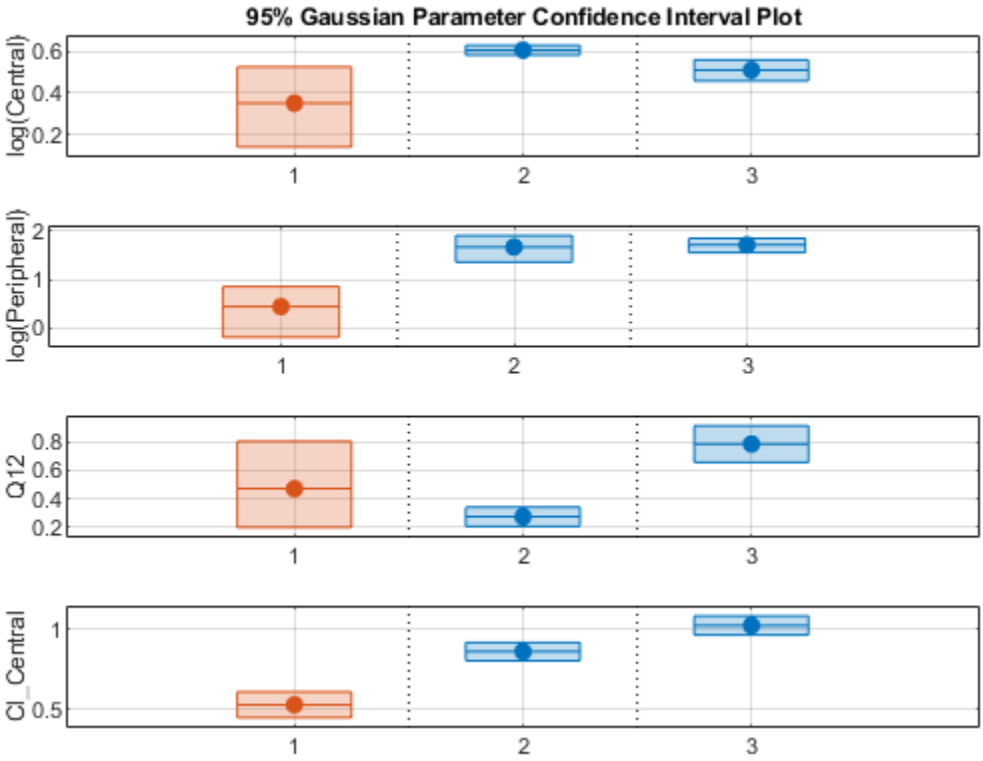
```
ans =

  12x7 table

    Group         Name         Estimate    ConfidenceInterval      Type      Alpha      Status
    _____    _____________    ________    __________________    ________    _____    __________

      1      {'Central'   }      1.422      1.1533     1.6906    Gaussian    0.05     estimable
      1      {'Peripheral'}     1.5629     0.83143     2.3551    Gaussian    0.05     constrained
      1      {'Q12'       }    0.47159     0.20093    0.80247    Gaussian    0.05     constrained
      1      {'Cl_Central'}    0.52898     0.44842    0.60955    Gaussian    0.05     estimable
      2      {'Central'   }     1.8322      1.7893     1.8751    Gaussian    0.05     success
      2      {'Peripheral'}     5.3368      3.9133     6.7602    Gaussian    0.05     success
      2      {'Q12'       }    0.27641      0.2093    0.34351    Gaussian    0.05     success
      2      {'Cl_Central'}    0.86034     0.80313    0.91755    Gaussian    0.05     success
      3      {'Central'   }     1.6657      1.5818     1.7497    Gaussian    0.05     success
      3      {'Peripheral'}     5.5632      4.7557     6.3708    Gaussian    0.05     success
      3      {'Q12'       }    0.78361     0.65581    0.91142    Gaussian    0.05     success
      3      {'Cl_Central'}     1.0233     0.96375     1.0828    Gaussian    0.05     success
```

Plot the confidence intervals. If the estimation status of a confidence interval is `success`, it is plotted in blue (the first default color). Otherwise, it is plotted in red (the second default color), which

indicates that further investigation into the fitted parameters may be required. If the confidence interval is `not estimable`, then the function plots a red line with a centered cross. If there are any transformed parameters with estimated values 0 (for the log transform) and 1 or 0 (for the probit or logit transform), then no confidence intervals are plotted for those parameter estimates. To see the color order, type `get(groot,'defaultAxesColorOrder')`.

Groups are displayed from left to right in the same order that they appear in the `GroupNames` property of the object, which is used to label the x-axis. The y-labels are the transformed parameter names.

```
plot(ciParamUnpooled)
```



Compute the confidence intervals for the pooled fit.

```
ciParamPooled = sbioparameterci(pooledFit);
```

Display the confidence intervals.

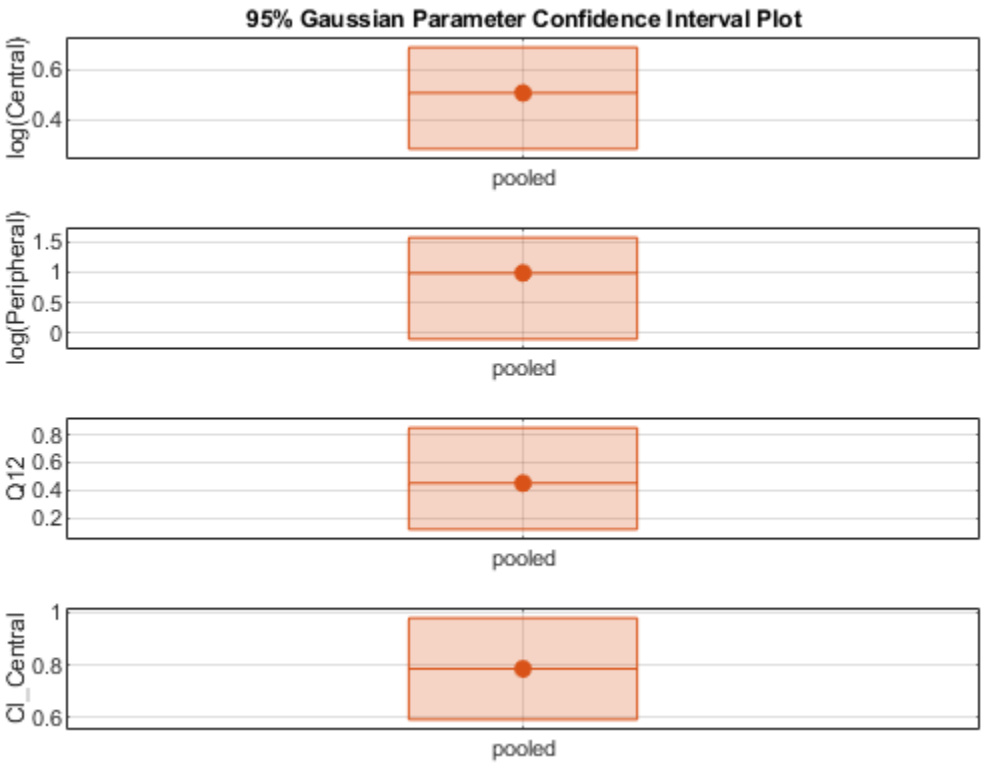
```
ci2table(ciParamPooled)
```

```
ans =

  4x7 table

    Group          Name          Estimate    ConfidenceInterval      Type       Alpha      Status
    _____    _______________    ________    __________________    ________    _____    _________
```

```
pooled    {'Central'   }     1.6626      1.3287      1.9965    Gaussian    0.05     estimable
pooled    {'Peripheral'}      2.687     0.89848      4.8323    Gaussian    0.05     constraine
pooled    {'Q12'       }    0.44956     0.11445     0.85152    Gaussian    0.05     constraine
pooled    {'Cl_Central'}    0.78493     0.59222     0.97764    Gaussian    0.05     estimable
```

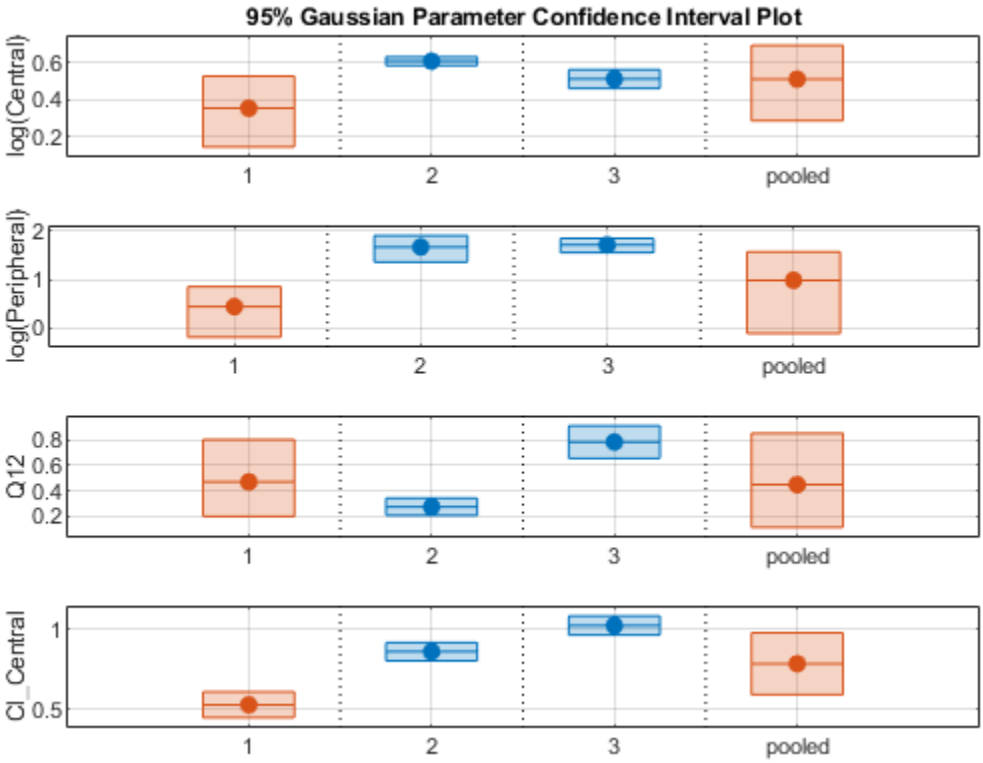
Plot the confidence intervals. The group name is labeled as "pooled" to indicate such fit.

```
plot(ciParamPooled)
```



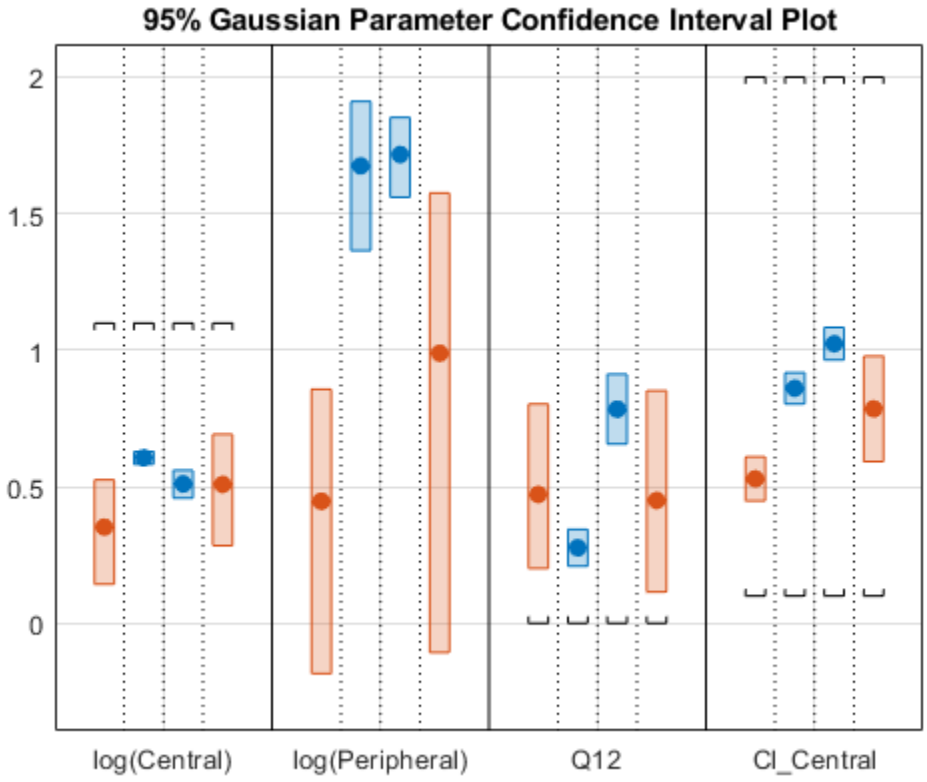
Plot all the confidence interval results together. By default, the confidence interval for each parameter estimate is plotted on a separate axes. Vertical lines group confidence intervals of parameter estimates that were computed in a common fit.

```
ciAll = [ciParamUnpooled;ciParamPooled];
plot(ciAll)
```



You can also plot all confidence intervals in one axes grouped by parameter estimates using the 'Grouped' layout.

```
plot(ciAll,'Layout','Grouped')
```



In this layout, you can point to the center marker of each confidence interval to see the group name. Each estimated parameter is separated by a vertical black line. Vertical dotted lines group confidence intervals of parameter estimates that were computed in a common fit. Parameter bounds defined in the original fit are marked by square brackets. Note the different scales on the y-axis due to parameter transformations. For instance, the y-axis of `Q12` is in the linear scale, but that of `Central` is in the log scale due to its log transform.

Compute Confidence Intervals for Model Predictions

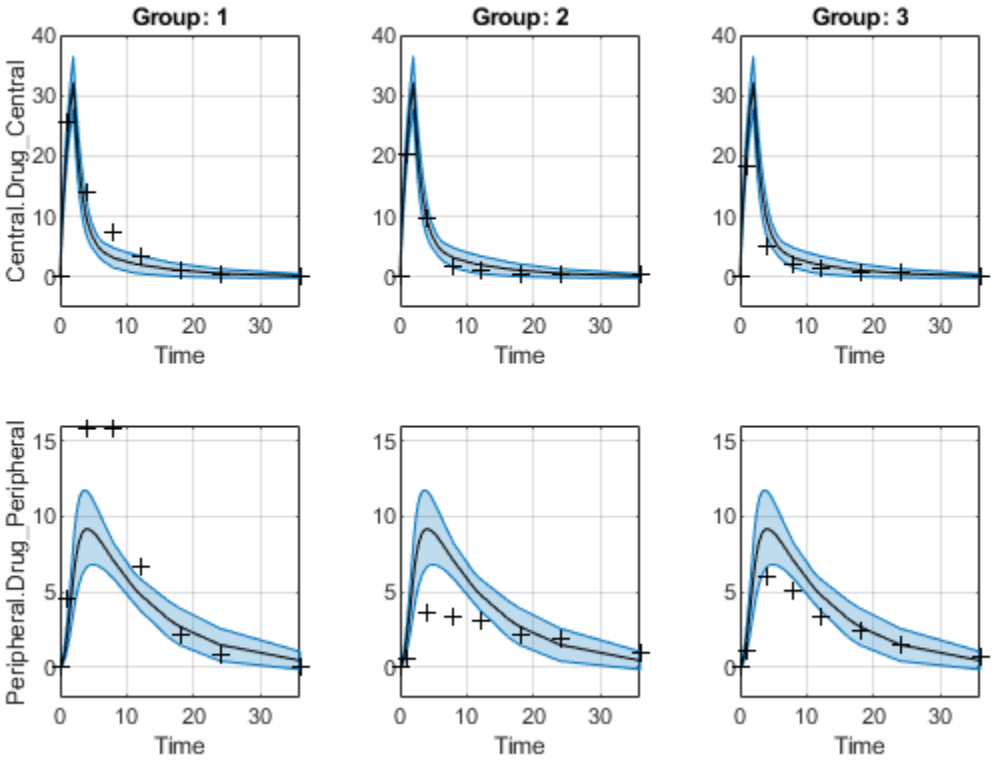
Calculate 95% confidence intervals for the model predictions, that is, simulation results using the estimated parameters.

```
% For the pooled fit
ciPredPooled = sbiopredictionci(pooledFit);
% For the unpooled fit
ciPredUnpooled = sbiopredictionci(unpooledFit);
```

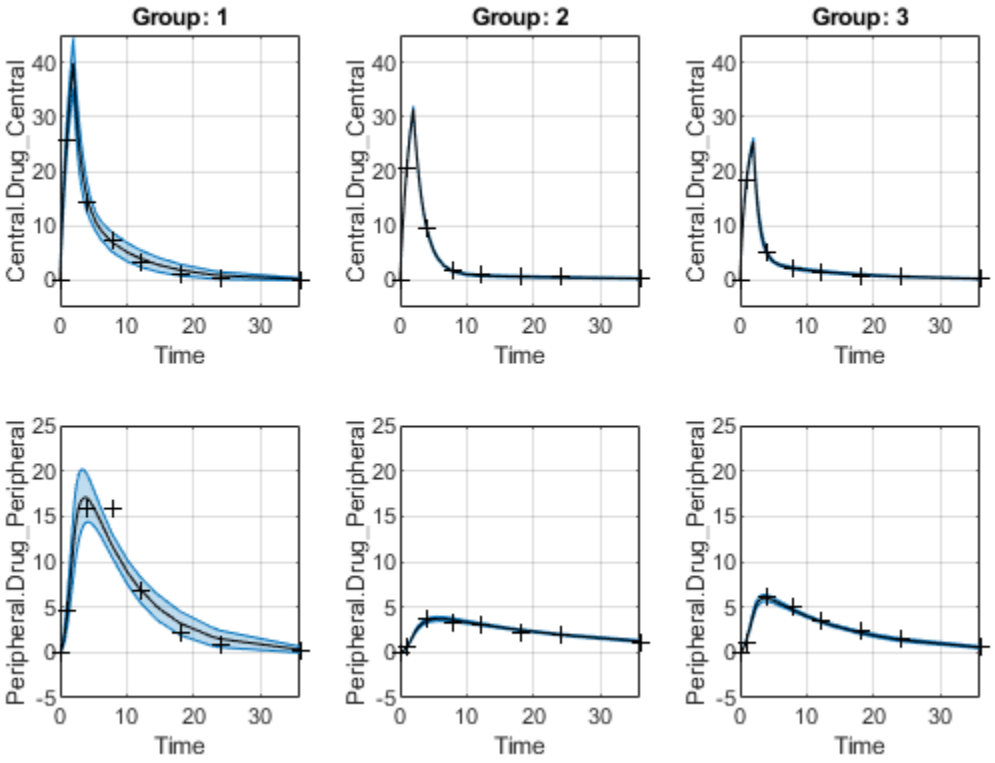
Plot Confidence Intervals for Model Predictions

The confidence interval for each group is plotted in a separate column, and each response is plotted in a separate row. Confidence intervals limited by the bounds are plotted in red. Confidence intervals not limited by the bounds are plotted in blue.

```
plot(ciPredPooled)
```




```
plot(ciPredUnpooled)
```



Input Arguments

`fitResults` — Parameter estimation results from `sbiofit`

`NLINResults` object | `OptimResults` object | vector

Parameter estimation results from `sbiofit`, specified as an `NLINResults`, `OptimResults`, or a vector of objects for unpooled fits that were returned from the same `sbiofit` call.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `'Alpha',0.01,'Type','profileLikelihood'` specifies to compute a 99% confidence interval using the profile likelihood approach.

Depending on the type of confidence interval, the compatible name-value arguments differ. The table below lists all the name-value arguments and their corresponding confidence interval types. A check mark (✔) indicates that the name-value argument is applicable for that type.

Name-Value Argument	Gaussian (default)	Optimization-based profile likelihood	Integration-based profile likelihood	Bootstrap
“Alpha” on page 1-0	✔	✔	✔	✔
“Type” on page 1-0	✔	✔	✔	✔
“Display” on page 1-0	✔	✔	✔	✔
“UseParallel” on page 1-0	✔	✔	✔	✔
“NumSamples” on page 1-0				✔
“Tolerance” on page 1-0		✔	✔	✔
“Parameters” on page 1-0		✔	✔	
“MaxStepSize” on page 1-0		✔	✔	
“UseIntegration” on page 1-0		✔	✔	
“IntegrationOptions” on page 1-0			✔	

`Alpha` — Confidence level
0.05 (default) | positive scalar

Confidence level, `(1-Alpha) * 100`%, specified as the comma-separated pair consisting of `'Alpha'` and a positive scalar between 0 and 1. The default value is `0.05`, meaning a 95% confidence interval is computed.

Example: `'Alpha',0.01`

Type — Confidence interval type
`'gaussian'` (default) | `'profileLikelihood'` | `'bootstrap'`

Confidence interval type, specified as the comma-separated pair consisting of `'Type'` and a character vector. The valid choices are:

- `'gaussian'` — Use the Gaussian approximation on page 1-191 of the distribution of parameter estimates.
- `'profileLikelihood'` — Compute the profile likelihood intervals. The function has two methods to compute profile likelihood curves. By default, the function uses the optimization-based method. To use the integration-based method, you must also set `'UseIntegration'` to `true`.

  The optimization-based method fixes one parameter value at a time and reruns an optimization to compute the maximum likelihood. This optimization is done for every parameter and every point

on the curve of the profile likelihood. The integration-based method is based on integrating the differential equations derived from the Lagrange equations of the optimization-based method. For details about these two methods, see “Profile Likelihood Confidence Interval Calculation” on page 1-191.

Note This type is not supported for parameter estimates from hierarchical models, that is, estimated results from fitting different categories on page 1-74 (such as age or sex). In other words, if you set the `CategoryVariableName` property of the `estimatedInfo` in your original fit, then the fit results are hierarchical and you cannot compute the `profileLikelihood` confidence intervals on the results.

- `'bootstrap'` — Compute confidence intervals using the bootstrap method on page 1-193.

Example: `'Type','bootstrap'`

`Display` — Level of display returned to the command line
`'off'` (default) | `'none'` | `'final'` | `'iter'`

Level of display returned to the command line, specified as the comma-separated pair consisting of `'Display'` and a character vector. `'off'` (default) or `'none'` displays no output. `'final'` displays a message when a computation finishes. `'iter'` displays output at each iteration.

Example: `'Display','final'`

`UseParallel` — Logical flag to compute confidence intervals in parallel
`true` | `false`

Logical flag to compute confidence intervals in parallel, specified as the comma-separated pair consisting of `'UseParallel'` and `true` or `false`. By default, the parallel options in the original fit are used. If this argument is set to `true` and Parallel Computing Toolbox is available, the parallel options in the original fit are ignored, and confidence intervals are computed in parallel.

For the Gaussian confidence intervals:

- If the input `fitResults` is a vector of results objects, then the computation of confidence intervals for each object is performed in parallel. The Gaussian confidence intervals are quick to compute. So, it might be more beneficial to parallelize the original fit (`sbiofit`) and not set `UseParallel` to true for `sbioparameterci`.

For the Profile Likelihood confidence intervals:

- If the number of results objects in the input `fitResults` vector is greater than the number of estimated parameters, then the computation of confidence intervals for each object is performed in parallel.
- Otherwise, the confidence intervals for all estimated parameters within one results object are computed in parallel before the function moves on to the next results object.

For the Bootstrap confidence intervals:

- The function forwards the `UseParallel` flag to `bootci`. There is no parallelization over the input vector of results objects.

Note If you have a global stream for random number generation with several substreams to compute in parallel in a reproducible fashion, `sbioparameterci` first checks to see if the number of workers

is same as the number of substreams. If so, `sbioparameterci` sets `UseSubstreams` to `true` in the `statset` option and passes it to `bootci`. Otherwise, the substreams are ignored by default.

Example: `'UseParallel',true`

`NumSamples` — Number of samples for bootstrapping
1000 (default) | positive integer

Number of samples for bootstrapping, specified as the comma-separated pair consisting of `'NumSamples'` and a positive integer. This number defines the number of fits that are performed during the confidence interval computation to generate bootstrap samples. The smaller the number is, the faster the computation of the confidence intervals becomes, at the cost of decreased accuracy.

Example: `'NumSamples',500`

`Tolerance` — Tolerance for profile likelihood and bootstrap confidence interval computations
`1e-5` (default) | positive scalar

Tolerance for the profile likelihood and bootstrap confidence interval computations, specified as the comma-separated pair consisting of `'Tolerance'` and a positive scalar.

The profile likelihood method uses this value as a termination tolerance. For details, see “Profile Likelihood Confidence Interval Calculation” on page 1-191.

The bootstrap method uses this value to determine whether a confidence interval is constrained by bounds specified in the original fit. For details, see “Bootstrap Confidence Interval Calculation” on page 1-193.

Example: `'Tolerance',1e-6`

`Parameters` — Names of parameters for which profile likelihood curves are calculated
character vector | string | string vector | cell array of character vectors

Names of parameters for which the profile likelihood curves are calculated, specified as a character vector, string, string vector, or cell array of character vectors. By default, the function computes the confidence intervals for all parameters listed in the EstimatedParameterNames property of the `fitResults` object. You can also specify a subset of those parameters if needed.

Note This name-value argument is applicable only when you specify `Type` as `'profileLikelihood'`.

Example: `'Parameters',{'ka'}`

`MaxStepSize` — Maximum step size used for computing profile likelihood curves
positive scalar | `[]` | cell array

Maximum step size used for computing profile likelihood curves, specified as the comma-separated pair consisting of `'MaxStepSize'` and a positive scalar, `[]`, or cell array.

- For the optimization-based method, the default value is `0.1`. If you set `'MaxStepSize'` to `[]`, then the maximum step size is set to 10% of the width of the Gaussian approximation of the

confidence interval, if it exists. You can specify a maximum step size (or `[]`) for each estimated parameter using a cell array.

- For the integration-based method, the default value is `Inf`. Internally, the function uses the `ode15s` solver.

Example: `'MaxStepSize',0.5`

`UseIntegration` — Flag to use integration-based profile likelihood confidence interval method
`false` (default) | `true`

Flag to use the integration-based profile likelihood confidence interval method, specified as `true` or `false`. The integration-based method integrates differential equations derived from the Lagrange equations. By default, the function uses the optimization-based method. For details about these two methods, see “Profile Likelihood Confidence Interval Calculation” on page 1-191.

Example: `'UseIntegration',true`

`IntegrationOptions` — Options for integration-based profile likelihood confidence interval method
structure

Options for the integration-based profile likelihood confidence interval method, specified as a structure. Specify options as fields of the structure as follows.

Field Name	Field Value Description
`Hessian`	`'finiteDifference'` — Use the finite difference approximation of the Hessian matrix. This is the default value. `'identity'` — Use the identity matrix as the Hessian matrix approximation. You must also specify a positive `CorrectionFactor` value.
`CorrectionFactor`	Nonnegative scalar. The default value is 0.
`AbsoluteTolerance`	Positive scalar for the step size control in `ode15s`. The default value is `1e-2`.
`RelativeTolerance`	Positive scalar less than 1 for the step size control in `ode15s`. The default value is `1e-2`.
`InitialStepSize`	Positive scalar as the initial step size for solving the differential equations. If a parameter is bounded, the function uses the default initial step size of `ode15s`. If not, it uses `1e-4`.

Output Arguments

`ci` — Confidence interval results
`ParameterConfidenceInterval` object

Confidence interval results, returned as a `ParameterConfidenceInterval` object. For an unpooled fit, `ci` can be a vector of `ParameterConfidenceInterval` objects.

More About

Note All confidence interval computations are based on the untransformed parameters. Only when plotted, the confidence intervals are mapped to the transformed space using the parameter transformations defined in the original fit.

Gaussian Confidence Interval Calculation

The function uses the Wald test statistic [1] to compute the confidence intervals. Assuming that there are enough data, the parameter estimates, P_{est}, are approximately Student's t-distributed with the covariance matrix S (the `CovarianceMatrix` property of the results object) returned by `sbiofit`.

The confidence interval for the ith parameter estimate $P_{est,i}$ is computed as follows:

$Pest,i \pm \sqrt{Si,i} * Tinv\left(1 - \frac{Alpha}{2}\right)$, where T_{inv} is the Student's t inverse cumulative distribution function (`tinv`) with the probability `1-(Alpha/2)`, and $S_{i,i}$ is the diagonal element (variance) of the covariance matrix S.

In cases where the confidence interval is constrained by the parameter bounds defined in the original fit, the confidence interval bounds are adjusted according to the approach described by Wu, H. and Neale, M. [2].

Setting Estimation Status

- For each parameter estimate, the function first decides whether the confidence interval of the parameter estimate is unbounded. If so, the function sets the estimation status of the corresponding parameter estimate to `not estimable`.
- Otherwise, if the confidence interval for a parameter estimate is constrained by a parameter bound defined in the original fit, the function sets the estimation status to `constrained`. Parameter transformations (such as `log`, `probit`, or `logit`) impose implicit bounds on the estimated parameters, for example, positivity constraints. Such bounds can lead to the overestimation of confidence, that is, the confidence interval can be smaller than expected.
- If no confidence interval has the estimation status `not estimable` or `constrained`, then the function sets the estimation statuses of all parameter estimates to `success`. Otherwise, the estimation statuses of remaining parameter estimates are set to `estimable`.

Profile Likelihood Confidence Interval Calculation

Define L to be the likelihood, LH, of the parameter estimates (stored in the `ParameterEstimates` property of the results object) returned by `sbiofit`, $L = LH(Pest)$, where P_{est} is a vector of parameter estimates, $P_{est,1}$, $P_{est,2}$, ..., $P_{est,n}$.

The profile likelihood function PL for a parameter P_i is defined as $PL(Pi) = \max_{Pj,\, j \neq i} LH(P1, ..., Pi, .., Pn)$, where n is the total number of parameters.

Per Wilks's Theorem [3], the likelihood ratio test statistic, $-2\log\left(\frac{PL(Pi)}{L}\right)$, is chi-square distributed with 1 degree of freedom.

Therefore, find all P_i so that: $\log(L) - \log(PL(P_i)) \leq \frac{chiinv(1, 1 - alpha)}{2}$.

Equivalently, $\log(PL(P_i)) \geq \log(L) - \frac{chiinv(1, 1 - alpha)}{2}$, where $\log(L) - \frac{chiinv(1, 1 - alpha)}{2}$ is the target value used in computing the log profile likelihood curve. The function provides two methods to compute such curve.

Optimization-based Method to Compute Log Profile Likelihood Curve

1. Start at $P_{est,i}$ and evaluate the likelihood L.
2. Compute the log profile likelihood at $P_{est,i}$ `+ k * MaxStepSize` for each side (or direction) of the confidence interval, that is, `k = 1, 2, 3,…` and `k = -1, -2, -3,….`
3. Stop if one of these stopping criteria is met on each side.

   - The log profile likelihood falls below the target value. In this case, start bisecting between P_{below} and P_{above}, where P_{below} is the parameter value with the largest log profile likelihood value below the target value, and P_{above} the parameter value with the smallest log profile likelihood value greater than the target value. Stop the bisection if one of the following is true:

     - Either neighboring log profile likelihood values are less than Tolerance on page 1-0 apart. Set the status for the corresponding side of the confidence interval to `success`.
     - The bisection interval becomes smaller than `max(Tolerance,2*eps('double'))` and the profile likelihood curve computed so far is above the target value. Set the status of the corresponding side to `not estimable`.
     - The linear gradient approximation of the profile likelihood curve (finite difference between two neighboring parameter values) is larger than -Tolerance on page 1-0 (the negative value of the tolerance). Set the status of the corresponding side to `not estimable`.
   - The step is limited by a bound defined in the original fit. Evaluate at the bound and set the status of the corresponding side to `constrained`.

Integration-Based Method to Compute Log Profile Likelihood Curve

This method [4] solves the constrained optimization problem $PL(Pi) = \max_{Pj,\, j \neq i} LH(P1, ..., Pi, .., Pn)$ by integrating the differential equations derived from the Lagrange equations

$$-\nabla_{\vec{p}} L(\vec{p}(c)) + \lambda(c)\vec{e}_i = 0$$

$$\vec{p}(_c = c$$

Here, $\vec{e}_i$ is the i^{th} canonical unit vector, the Lagrange multiplier is $\lambda(c)$, and $c = P_i$.

In other words, instead of optimizing point by point, this method solves differential equations that define the profile likelihood curve as follows.

$$\begin{pmatrix} -\nabla^2_{\vec{p}} L(\vec{p}(c)) & \vec{e}_i \\ \pm\vec{e}_i^{\,T} & 0 \end{pmatrix} \begin{pmatrix} \dot{\vec{p}}(c) \\ \dot{\lambda}(c) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Here, $\dot{\vec{p}}(c) = \frac{\partial \vec{p}(c)}{\partial c}, \dot{\lambda}(c) = \frac{\partial \lambda(c)}{\partial c}, and - \nabla^2_{\vec{p}} L(\vec{p}(c))$ is the Hessian of the log likelihood function.

Using the finite-difference approximation of the Hessian matrix is recommended. However, the numerical computation of the Hessian matrix using finite differencing can be computationally

expensive. To reduce the computational costs, Chen and Jennrich [4] proposed an approximate version based on the assumption that the second-order sufficient Karush-Kuhn-Tucker conditions must hold with strict inequality at every point in the domain of the profile likelihood curve as outlined in Assumption 2 in the Appendix of [4]. In other words, at every point on the profile likelihood curve, the remaining parameters must be estimable.

If this assumption holds, then the Hessian can be replaced with the identity matrix I as follows:

$$\begin{pmatrix} -I & \vec{e}_i \\ \pm\vec{e}_i^T & 0 \end{pmatrix}\begin{pmatrix} \dot{\vec{p}}(c) \\ \dot{\lambda}(c) \end{pmatrix} = \begin{pmatrix} -\gamma\nabla_{\vec{p}}L(\vec{p}(c)) \\ 1 \end{pmatrix}$$

Here, $\nabla_{\vec{p}}L(\vec{p}(c))$ is the gradient of the log likelihood and γ is a correction factor to ensure the solution of the differential equation stays on the path of the profile likelihood curve.

If γ is too small, the approximation of the profile likelihood curve may become inaccurate, resulting in an underestimation of the profile likelihood confidence intervals. Setting γ to a large value ensures accurate results, but might require `ode15s` to take smaller steps, which increases the computational cost.

Tip You can specify the Hessian approximation and correction factor using the "IntegrationOptions" on page 1-0 name-value argument.

The stopping criterion of the algorithm is when one of the following conditions becomes true:

- The gradient approximation of the profile likelihood curve is larger than -Tolerance on page 1-0 .
- The profile likelihood falls below the target value.
- A parameter bound is reached.

Setting Estimation Status

- If both sides of the confidence interval are unsuccessful, that is, have the status `not estimable`, the function sets the estimation status (`ci`.Results.Status on page 2-0) to `not estimable`.
- If no side has the status `not estimable` and one side has the status `constrained`, the function sets the estimation status (`ci`.Results.Status on page 2-0) to `constrained`.
- If the computation for all parameters on both sides of the confidence intervals is successful, set the estimation status (`ci`.Results.Status on page 2-0) to `success`.
- Otherwise, the function sets the estimation statuses of the remaining parameter estimates to `estimable`.

Bootstrap Confidence Interval Calculation

The `bootci` function from Statistics and Machine Learning Toolbox is used to compute the bootstrap confidence intervals. The first input *nboot* is the number of samples (`NumSamples`), and the second input *bootfun* is a function that performs these actions:

- Resample the data (independently within each group, if multiple groups are available).
- Run a parameter fit with the resampled data.
- Return the estimated parameters.

Setting Estimation Status

If a confidence interval is closer than `Tolerance` to a parameter bound, as defined in the original fit, the function sets the estimation status to `constrained`. If all confidence intervals are further away from the parameter bounds than `Tolerance`, the function sets the status to `success`. Otherwise, it is set to `estimable`.

Version History

Introduced in R2017b

References

[1] Wald, A. "Tests of Statistical Hypotheses Concerning Several Parameters when the Number of Observations is Large." *Transactions of the American Mathematical Society*. 54 (3), 1943, pp. 426-482.

[2] Wu, H., and M.C. Neale. "Adjusted Confidence Intervals for a Bounded Parameter." *Behavior Genetics*. 42 (6), 2012, pp. 886-898.

[3] Wilks, S.S. "The Large-Sample Distribution of the Likelihood Ratio for Testing Composite Hypotheses." *The Annals of Mathematical Statistics*. 9 (1), 1938, pp. 60–62.

[4] Chen, Jian-Shen, and Robert I. Jennrich. “Simple Accurate Approximation of Likelihood Profiles.” *Journal of Computational and Graphical Statistics* 11, no. 3 (September 2002): 714–32.

Extended Capabilities

Automatic Parallel Support

Accelerate code by automatically running computation in parallel using Parallel Computing Toolbox™.

To run in parallel, set `'UseParallel'` to `true`.

For more information, see the `'UseParallel'` name-value pair argument.

See Also

`sbiopredictionci` | `sbiofit` | `ConfidenceInterval` | `ParameterConfidenceInterval`

sbioparamestim

Perform parameter estimation

Note `sbioparamestim` will be removed in a future release. Use `sbiofit` instead.

Note Statistics and Machine Learning Toolbox™, Optimization Toolbox™, and Global Optimization Toolbox are recommended for this function.

Syntax

```
[k, result]= sbioparamestim(modelObj, tspan, xtarget, observed_array,
estimated_array)
[ ___ ]= sbioparamestim( ___ , observed_array, estimated_array, k0)
[ ___ ]= sbioparamestim( ___ , observed_array, estimated_array, k0, method)
```

Arguments

`k`	Vector of estimated parameter values. For all optimization methods except `'fminsearch'`, the parameters are constrained to be greater than or equal to 0.
`result`	Structure with fields that provide information about the progress of optimization.
`modelObj`	SimBiology model object.
`tspan`	*n*-by-1 vector representing the time span of the target data `xtarget`.
`xtarget`	*n*-by-*m* matrix, where *n* is the number of time samples and *m* is the number of states to match during the simulation. The number of rows in `xtarget` must equal the number of rows in `tspan`.

`observed_array`	Either of the following: • Array of objects (species, compartment, or nonconstant parameter) in `modelObj`, whose values should be matched during the estimation process • Cell array of character vectors or string vector containing the names of objects (species, compartment, or nonconstant parameter) in `modelObj`, whose values should be matched during the estimation process **Note** If duplicate names exist for any species or parameters, ensure there are no ambiguities by specifying either an array of objects or a cell array of qualified names, such as *`compartmentName.speciesName`* or *`reactionName.parameterName`*. For example, for a species named `sp1` that is in a compartment named `comp2`, the qualified name is `comp2.sp1`. The length of `observed_array` must equal the number of columns in `xtarget`. `sbioparamestim` assumes that the order of elements in `observed_array` is the same as the order of columns in `xtarget`.
`estimated_array`	Either of the following: • Array of objects (compartment, species, or parameter) in `modelObj` whose initial values should be estimated • Cell array of character vectors or string vector containing the names of objects (compartment, species, or parameter) in `modelObj` whose initial values should be estimated **Note** If duplicate names exist for any compartments, species, or parameters, ensure there are no ambiguities by specifying either an array of objects or a cell array of qualified names, such as *`compartmentName.speciesName`* or *`reactionName.parameterName`*. For example, for a parameter named `param1` scoped to a reaction named `reaction1`, the qualified name is `reaction1.param1`.
`k0`	Numeric vector containing the initial values of compartments, species, or parameters to be estimated. The length of `k0` must equal that of `estimated_array`. If you do not specify `k0`, or specify an empty vector for `k0`, then `sbioparamestim` takes initial values for compartments, species, or parameters from `modelObj`, or, if there are active variants, `sbioparamestim` uses any initial values specified in the active variants. For details about variants, see `Variant object`.

`method`

Optimization algorithm to use during the estimation process, specified by either of the following:

- Character vector (or string) specifying one of the following functions:
  - `'fminsearch'`
  - `'lsqcurvefit'`
  - `'lsqnonlin'`
  - `'fmincon'`
  - `'patternsearch'`
  - `'patternsearch_hybrid'`
  - `'ga'`
  - `'ga_hybrid'`
  - `'particleswarm'`
  - `'particleswarm_hybrid'`

  For descriptions of how `sbioparamestim` uses the previous functions, see the Function Descriptions table.
- Two-element cell array, with the first element being one of the previous functions, and the second element being an options structure or object. Use an appropriate options structure or object for each method listed next.

Method	Options Structure or Object
`'fminsearch'`	`optimset`

`'fmincon'`
`'lsqcurvefit'`
`'lsqnonlin'`
`'particleswarm'`
`'particleswarm_hybrid'`
`'patternsearch'`
`'patternsearch_hybrid'`
`'ga'`
`'ga_hybrid'`
	`optimoptions`

Tip Use a two-element cell array to provide your own options structure for the optimization algorithm.

If you have Parallel Computing Toolbox, you can enable parallel computing for faster data fitting by:

1 Opening a MATLAB worker pool:

	`parpool` **2** Setting the name-value pair argument `'UseParallel'` to `true` in an options structure or object.

Function Descriptions

Function	Description
`fminsearch`	`sbioparamestim` uses the default options structure associated with `fminsearch`, except for: `Display = 'off'` `TolFun = 1e-6*` (Initial value of objective function) **Note** `'fminsearch'` is an unconstrained optimization method, which can result in negative values for parameters.

`lsqcurvefit`	Requires Optimization Toolbox.
	
	`sbioparamestim` uses the default options structure associated with `lsqcurvefit`, except for:
	`Display = 'off'`
	`FiniteDifferenceStepSize` = value of the `SolverOptions.RelativeTolerance` property of the configuration set associated with `modelObj`, with a minimum of `eps^(1/3)`
	`FunctionTolerance = 1e-6*` (Initial value of objective function)
	`TypicalX = 1e-6*` (Initial values of components to be estimated)

`lsqnonlin`	Requires Optimization Toolbox.
	
	`sbioparamestim` uses the default options structure associated with `lsqnonlin`, except for:
	`Display = 'off'`
	`FiniteDifferenceStepSize` = value of the `SolverOptions.RelativeTolerance` property of the configuration set associated with *`modelObj`*, with a minimum of `eps^(1/3)`
	`FunctionTolerance = 1e-6*` (Initial value of objective function)
	`TypicalX = 1e-6*` (Initial values of components to be estimated)

`fmincon`	Requires Optimization Toolbox.
	
	`sbioparamestim` uses the default options structure associated with `fmincon`, except for:
	`Algorithm = 'interior-point'`
	`Display = 'off'`
	`FiniteDifferenceStepSize` = value of the `SolverOptions.RelativeTolerance` property of the configuration set associated with *`modelObj`*, with a minimum of `eps^(1/3)`
	`FunctionTolerance = 1e-6*` (Initial value of objective function)
	`TypicalX = 1e-6*` (Initial values of components to be estimated)

`patternsearch`	Requires Global Optimization Toolbox.
	
	`sbioparamestim` uses the default options structure associated with `patternsearch`, except for:
	`Display = 'off'`
	`FunctionTolerance = 1e-6*` (Initial value of objective function)
	`MeshTolerance = 1.0e-3`
	`AccelerateMesh = true`

Function	Description

`patternsearch_hybrid`	Requires Global Optimization Toolbox.
	
	`sbioparamestim` calls the `patternsearch` function with the additional option `SearchMethod = {@searchlhs,10,15}`. This option adds an additional search step that uses Latin hypercube sampling.
	
	The `sbioparamestim` function uses the default options structure associated with `patternsearch`, except for:
	`Display = 'off'`
	`FunctionTolerance = 1e-6*` (Initial value of objective function)
	`MeshTolerance = 1.0e-3`
	`AccelerateMesh = true`
	`SearchMethod = {@searchlhs,10,15}`

`ga`	Requires Global Optimization Toolbox.
	
	`sbioparamestim` uses the default options structure associated with `ga`, except for:
	`Display = 'off'`
	`FunctionTolerance = 1e-6*` (Initial value of objective function)
	`PopulationSize = 10`
	`Generations = 30`
	`MutationFcn = @mutationadaptfeasible`

`ga_hybrid`	Requires Global Optimization Toolbox.
	
	`sbioparamestim` calls the `ga` function with the additional option `HybridFcn = {@fmincon, fminopt}`, where `fminopt` is the same set of default options `sbioparamestim` uses for `fmincon`. This option causes an additional gradient-based minimization after the genetic algorithm step ends.
	
	The `sbioparamestim` function uses the default options structure associated with `ga`, except for:
	`Display = 'off'`
	`FunctionTolerance = 1e-6*` (Initial value of objective function)
	`PopulationSize = 10`
	`Generations = 30`
	`MutationFcn = @mutationadaptfeasible`
	`HybridFcn = {@fmincon,` *`structure of name/value pairs for fmincon`*`}`

`particleswarm`	Requires Global Optimization Toolbox.
	`sbioparamestim` uses the following default options for `particleswarm`, except for:
	
	`Display = 'off';`
	`FunctionTolerance = 1e-6*[Initial objective function value]`
	`SwarmSize = 10;`
	`MaxIter = 30;`

Function	Description
particleswarm_hybrid	Requires Global Optimization Toolbox. sbioparamestim calls the particleswarm function with the additional option HybridFcn = {@objFcn, options}. The objective function, objFcn, is one of these supported functions: patternsearch, fminsearch, fminunc, or fmincon. options is a structure of options for these functions and their values. Display = 'off'; FunctionTolerance = 1e-6*[Initial objective function value] SwarmSize = 10; MaxIter = 30; HybridFcn = {@fmincon, [Fmincon Options, described above]}

Note sbioparamestim does not support setting the Vectorized option to 'on' in algorithms that support this option.

Description

[k, result]= sbioparamestim(modelObj, tspan, xtarget, observed_array, estimated_array) estimates the initial values of compartments, species, and parameters of modelObj, a SimBiology model object, specified in estimated_array, so as to match the values of species and nonconstant parameters given by observed_array with the target state, xtarget, whose time variation is given by the time span tspan. If you have Optimization Toolbox installed, sbioparamestim uses the lsqnonlin function as the default method for the parameter estimation. If you do not have Optimization Toolbox installed, sbioparamestim uses the MATLAB function fminsearch as the default method for the parameter estimation.

[___]= sbioparamestim(___ , observed_array, estimated_array, k0) specifies the initial values of compartments, species, and parameters listed in estimated_array.

[___]= sbioparamestim(___ , observed_array, estimated_array, k0, method) specifies the optimization method to use.

Examples

Given a model and some target data, estimate all of its parameters without explicitly specifying any initial values:

1. Load a model from the project, gprotein_norules.sbproj. The project contains two models, one for the wild-type strain (stored in variable m1), and one for the mutant strain (stored in variable m2). Load the G protein model for the wild-type strain.

   ```
   sbioloadproject gprotein_norules m1;
   ```

2. Store the target data in a variable:

   ```
   Gt = 10000;
   tspan  = [0 10 30 60 110 210 300 450 600]';
   Ga_frac = [0 0.35 0.4 0.36 0.39 0.33 0.24 0.17 0.2]';
   xtarget = Ga_frac * Gt;
   ```

3 Store all model parameters in an array:

```
p_array = sbioselect(m1,'Type','parameter');
```

4 Store the species that should match target:

```
Ga = sbioselect(m1,'Type','species','Name','Ga');
% In this example only one species is selected.
% To match more than one targeted species data
% replace with selected species array.
```

5 Estimate the parameters:

```
[k, result] = sbioparamestim(m1, tspan, xtarget, Ga, p_array)
```

```
k =

    0.0100
    0.0000
    0.0004
    4.0000
    0.0040
    1.0000
    0.0000
    0.1100


result =

          fval: 1.4193e+06
      residual: [9x1 double]
      exitflag: 2
    iterations: 2
     funccount: 27
     algorithm: 'trust-region-reflective'
       message: [1x413 char]
```

Estimate parameters specified in `p_array` for species `Ga` using different algorithms.

```
[k1,r1] = sbioparamestim(m1,tspan,xtarget,Ga,p_array, ...
          {},'fmincon');
[k2,r2] = sbioparamestim(m1,tspan,xtarget,Ga,p_array, ...
          {},'patternsearch');
[k3,r3] = sbioparamestim(m1,tspan,xtarget,Ga,p_array, ...
          {},'ga');
[k4,r4] = sbioparamestim(m1,tspan,xtarget,Ga,p_array, ...
      {},'particleswarm');
```

Estimate parameters specified in `p_array` for species `Ga`, and change default optimization options to use user-specified options.

```
myopt1 = optimoptions('Display','iter');
[k1,r1] = sbioparamestim(m1,tspan,xtarget, ...
          Ga,p_array,{},{'fmincon',myopt1});

myopt2 = optimoptions('MeshTolerance',1.0e-4);
[k2,r2] = sbioparamestim(m1,tspan,xtarget, ...
          Ga,p_array,{},{'patternsearch',myopt2});

myopt3 = optimoptions('PopulationSize',25, 'Generations', 10);
```

```
[k3,r3] = sbioparamestim(m1,tspan,xtarget, ...
          Ga,p_array,{},{'ga',myopt3});

myopt4 = optimoptions('particleswarm','Display','iter');
[k4,r4] = sbioparamestim(m1,tspan,xtarget,Ga,p_array,{},{'particleswarm',myopt4});
```

Algorithms

`sbioparamestim` estimates parameters by attempting to minimize the discrepancy between simulation results and the data to fit. The minimization uses one of these optimization algorithms: `fminsearch` (from MATLAB); `lsqcurvefit`, `lsqnonlinfit`, or `fmincon` (from Optimization Toolbox); or `patternsearch` or `ga` (from Global Optimization Toolbox). All optimization methods require an objective function as an input. This objective function takes as input a vector of parameter values and returns an estimate of the discrepancy between simulation and data. When using `lsqcurvefit` or `lsqnonlinfit` as the optimization method, this objective function returns a vector of the residuals. For other optimization methods, the objective function returns the 2-norm of the residuals.

Version History

Introduced in R2006a

References

[1] Yi, T-M., Kitano, H., and Simon, M.I. (2003) A quantitative characterization of the yeast heterotrimeric G protein cycle. PNAS *100*, 10764–10769.

See Also

`sbiomodel` | `optimset`

sbiopredictionci

Compute confidence intervals for model predictions (requires Statistics and Machine Learning Toolbox)

Syntax

```
ci = sbiopredictionci(fitResults)
ci = sbiopredictionci(fitResults,Name,Value)
```

Description

`ci = sbiopredictionci(fitResults)` computes 95% confidence intervals for the model simulation results from `fitResults`, an `NLINResults` or `OptimResults` returned by `sbiofit`. `ci` is a `PredictionConfidenceInterval` object that contains the computed confidence interval data.

`ci = sbiopredictionci(fitResults,Name,Value)` uses additional options specified by one or more `Name,Value` pair arguments.

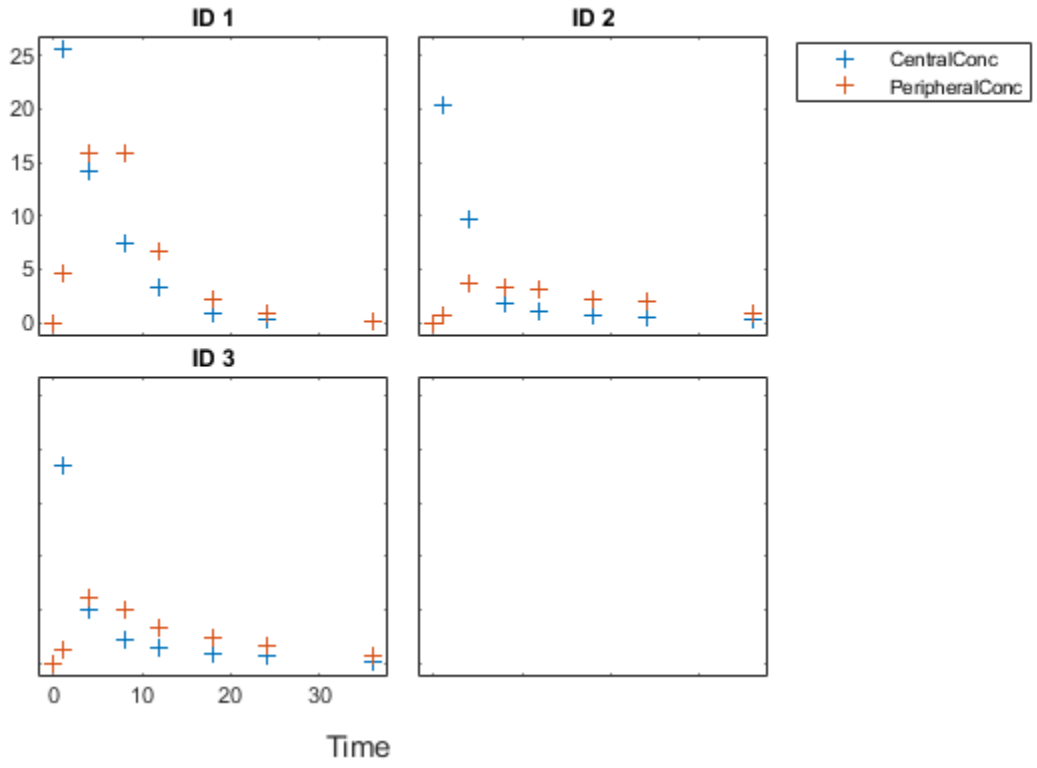
Examples

Compute Confidence Intervals for Estimated PK Parameters and Model Predictions

Load Data

Load the sample data to fit. The data is stored as a table with variables *ID* , *Time* , *CentralConc* , and *PeripheralConc*. This synthetic data represents the time course of plasma concentrations measured at eight different time points for both central and peripheral compartments after an infusion dose for three individuals.

```
load data10_32R.mat
gData = groupedData(data);
gData.Properties.VariableUnits = {'','hour','milligram/liter','milligram/liter'};
sbiotrellis(gData,'ID','Time',{'CentralConc','PeripheralConc'},'Marker','+',...
            'LineStyle','none');
```



Create Model

Create a two-compartment model.

```
pkmd                 = PKModelDesign;
pkc1                 = addCompartment(pkmd,'Central');
pkc1.DosingType      = 'Infusion';
pkc1.EliminationType = 'linear-clearance';
pkc1.HasResponseVariable = true;
pkc2                 = addCompartment(pkmd,'Peripheral');
model                = construct(pkmd);
configset            = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
```

Define Dosing

Define the infusion dose.

```
dose             = sbiodose('dose','TargetName','Drug_Central');
dose.StartTime   = 0;
dose.Amount      = 100;
dose.Rate        = 50;
dose.AmountUnits = 'milligram';
dose.TimeUnits   = 'hour';
dose.RateUnits   = 'milligram/hour';
```

Define Parameters

Define the parameters to estimate. Set the parameter bounds for each parameter. In addition to these explicit bounds, the parameter transformations (such as log, logit, or probit) impose implicit bounds.

```
responseMap = {'Drug_Central = CentralConc','Drug_Peripheral = PeripheralConc'};
paramsToEstimate   = {'log(Central)','log(Peripheral)','Q12','Cl_Central'};
estimatedParam     = estimatedInfo(paramsToEstimate,...
                                   'InitialValue',[1 1 1 1],...
                                   'Bounds',[0.1 3;0.1 10;0 10;0.1 2]);
```

Fit Model

Perform an unpooled fit, that is, one set of estimated parameters for each patient.

```
unpooledFit = sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',false);
```

Perform a pooled fit, that is, one set of estimated parameters for all patients.

```
pooledFit = sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',true);
```

Compute Confidence Intervals for Estimated Parameters

Compute 95% confidence intervals for each estimated parameter in the unpooled fit.

```
ciParamUnpooled = sbioparameterci(unpooledFit);
```

Display Results

Display the confidence intervals in a table format. For details about the meaning of each estimation status, see “Parameter Confidence Interval Estimation Status” on page 2-666.

```
ci2table(ciParamUnpooled)
```

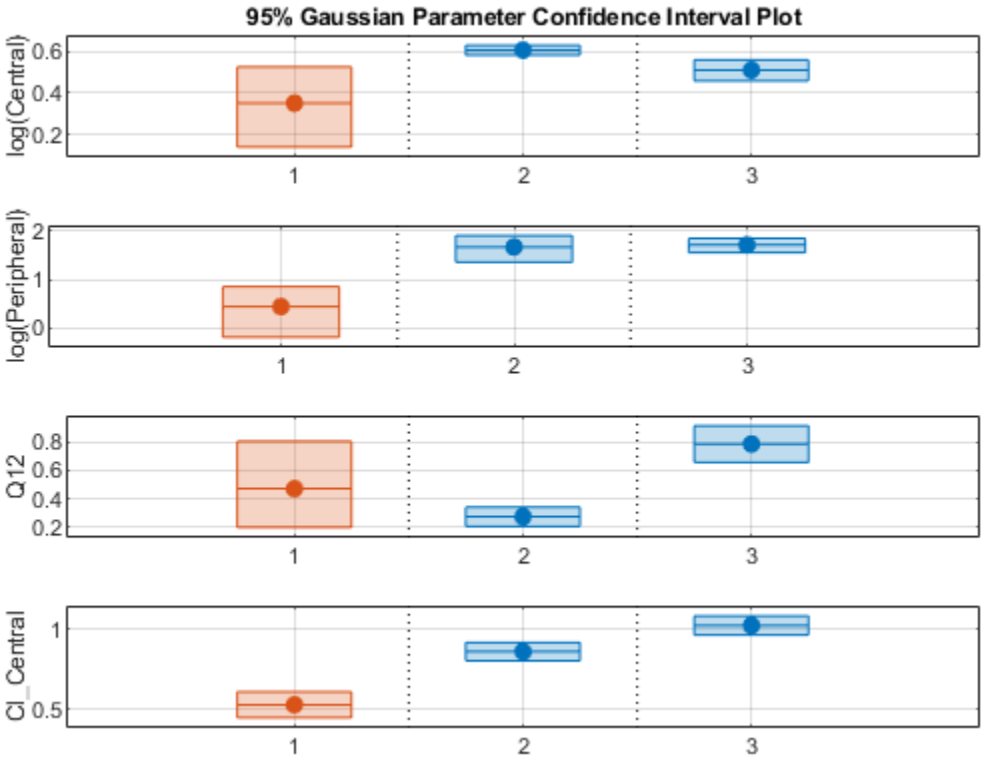
```
ans =

  12x7 table

    Group         Name         Estimate    ConfidenceInterval      Type      Alpha      Status
    _____    _____________    ________    __________________    ________    _____    __________

      1      {'Central'   }      1.422      1.1533     1.6906    Gaussian    0.05     estimable
      1      {'Peripheral'}     1.5629     0.83143     2.3551    Gaussian    0.05     constrained
      1      {'Q12'       }    0.47159     0.20093    0.80247    Gaussian    0.05     constrained
      1      {'Cl_Central'}    0.52898     0.44842    0.60955    Gaussian    0.05     estimable
      2      {'Central'   }     1.8322      1.7893     1.8751    Gaussian    0.05     success
      2      {'Peripheral'}     5.3368      3.9133     6.7602    Gaussian    0.05     success
      2      {'Q12'       }    0.27641      0.2093    0.34351    Gaussian    0.05     success
      2      {'Cl_Central'}    0.86034     0.80313    0.91755    Gaussian    0.05     success
      3      {'Central'   }     1.6657      1.5818     1.7497    Gaussian    0.05     success
      3      {'Peripheral'}     5.5632      4.7557     6.3708    Gaussian    0.05     success
      3      {'Q12'       }    0.78361     0.65581    0.91142    Gaussian    0.05     success
      3      {'Cl_Central'}     1.0233     0.96375     1.0828    Gaussian    0.05     success
```

Plot the confidence intervals. If the estimation status of a confidence interval is `success`, it is plotted in blue (the first default color). Otherwise, it is plotted in red (the second default color), which

indicates that further investigation into the fitted parameters may be required. If the confidence interval is `not estimable`, then the function plots a red line with a centered cross. If there are any transformed parameters with estimated values 0 (for the log transform) and 1 or 0 (for the probit or logit transform), then no confidence intervals are plotted for those parameter estimates. To see the color order, type `get(groot,'defaultAxesColorOrder')`.

Groups are displayed from left to right in the same order that they appear in the `GroupNames` property of the object, which is used to label the x-axis. The y-labels are the transformed parameter names.

```
plot(ciParamUnpooled)
```



Compute the confidence intervals for the pooled fit.

```
ciParamPooled = sbioparameterci(pooledFit);
```

Display the confidence intervals.

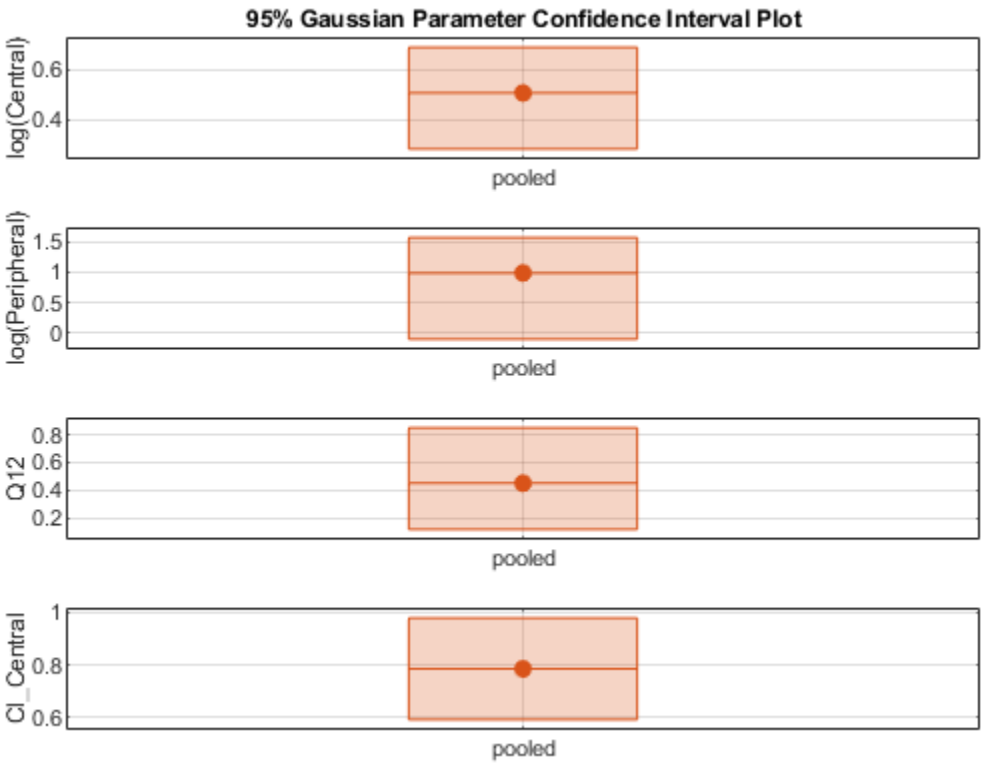
```
ci2table(ciParamPooled)
```

```
ans =

  4x7 table

    Group          Name          Estimate    ConfidenceInterval      Type       Alpha      Status
    _____    _______________    ________    __________________    ________    _____    __________
```

```
pooled    {'Central'   }     1.6626      1.3287      1.9965    Gaussian    0.05     estimable
pooled    {'Peripheral'}      2.687     0.89848      4.8323    Gaussian    0.05     constraine
pooled    {'Q12'       }    0.44956     0.11445     0.85152    Gaussian    0.05     constraine
pooled    {'Cl_Central'}    0.78493     0.59222     0.97764    Gaussian    0.05     estimable
```

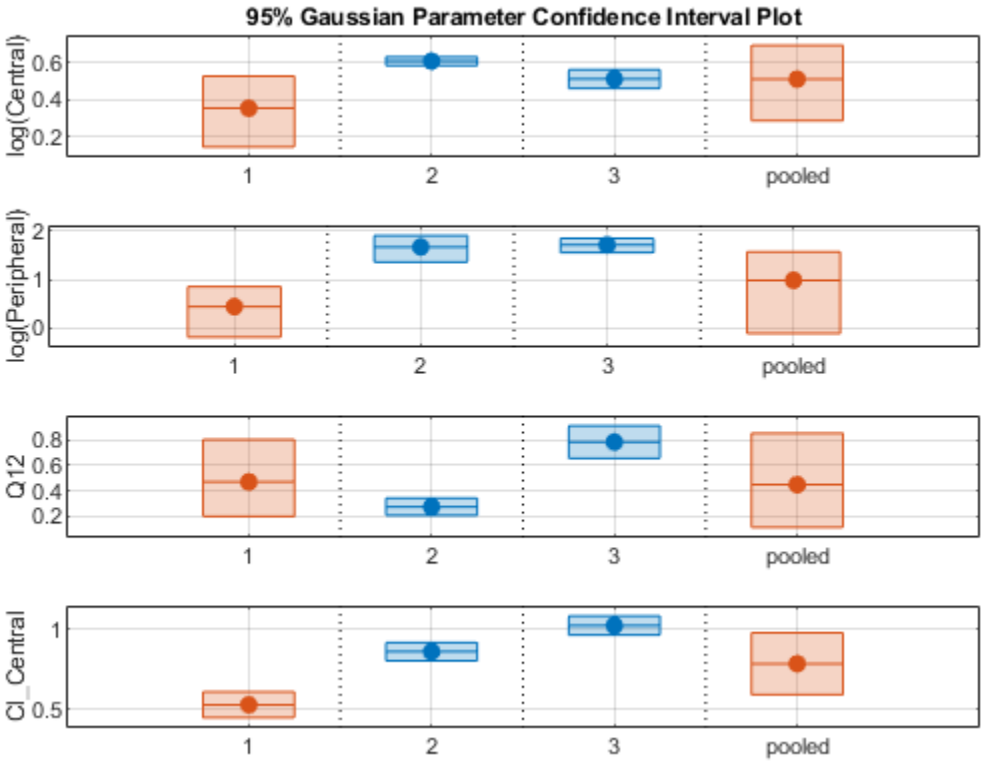
Plot the confidence intervals. The group name is labeled as "pooled" to indicate such fit.

```
plot(ciParamPooled)
```



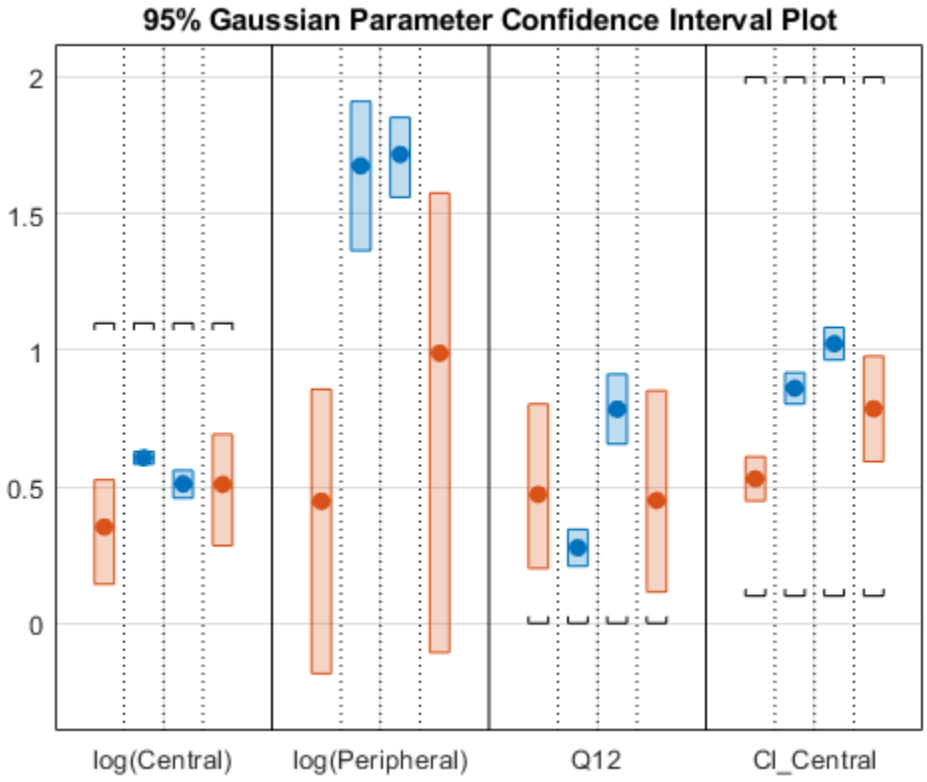
Plot all the confidence interval results together. By default, the confidence interval for each parameter estimate is plotted on a separate axes. Vertical lines group confidence intervals of parameter estimates that were computed in a common fit.

```
ciAll = [ciParamUnpooled;ciParamPooled];
plot(ciAll)
```



You can also plot all confidence intervals in one axes grouped by parameter estimates using the 'Grouped' layout.

```
plot(ciAll,'Layout','Grouped')
```



In this layout, you can point to the center marker of each confidence interval to see the group name. Each estimated parameter is separated by a vertical black line. Vertical dotted lines group confidence intervals of parameter estimates that were computed in a common fit. Parameter bounds defined in the original fit are marked by square brackets. Note the different scales on the y-axis due to parameter transformations. For instance, the y-axis of `Q12` is in the linear scale, but that of `Central` is in the log scale due to its log transform.

Compute Confidence Intervals for Model Predictions

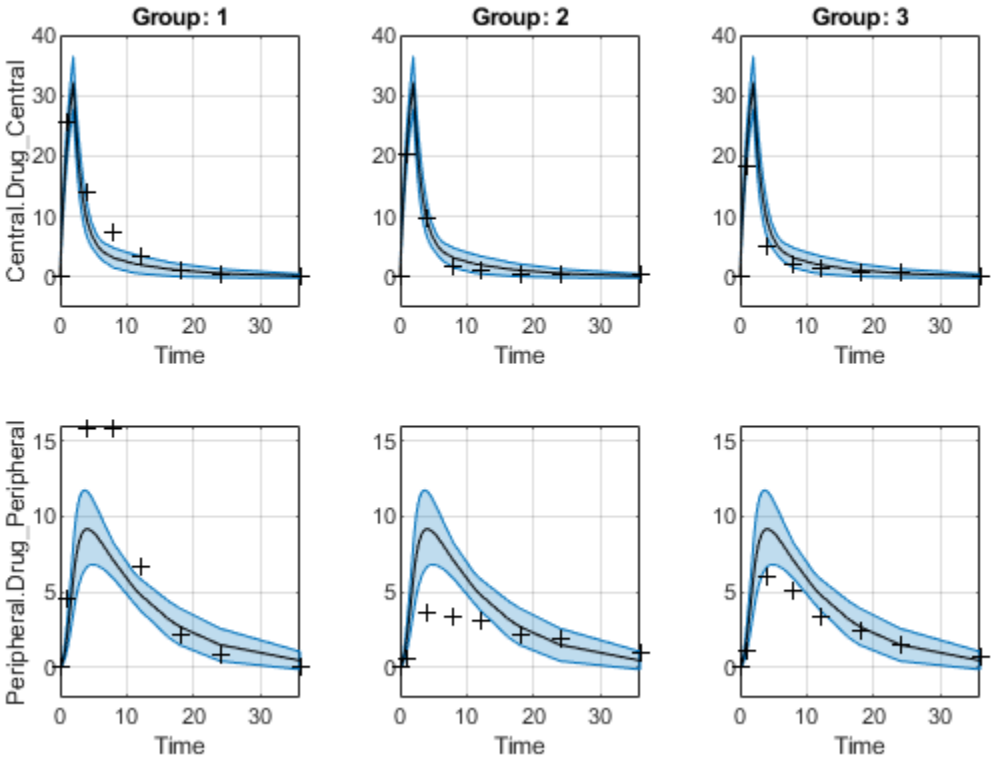
Calculate 95% confidence intervals for the model predictions, that is, simulation results using the estimated parameters.

```
% For the pooled fit
ciPredPooled = sbiopredictionci(pooledFit);
% For the unpooled fit
ciPredUnpooled = sbiopredictionci(unpooledFit);
```

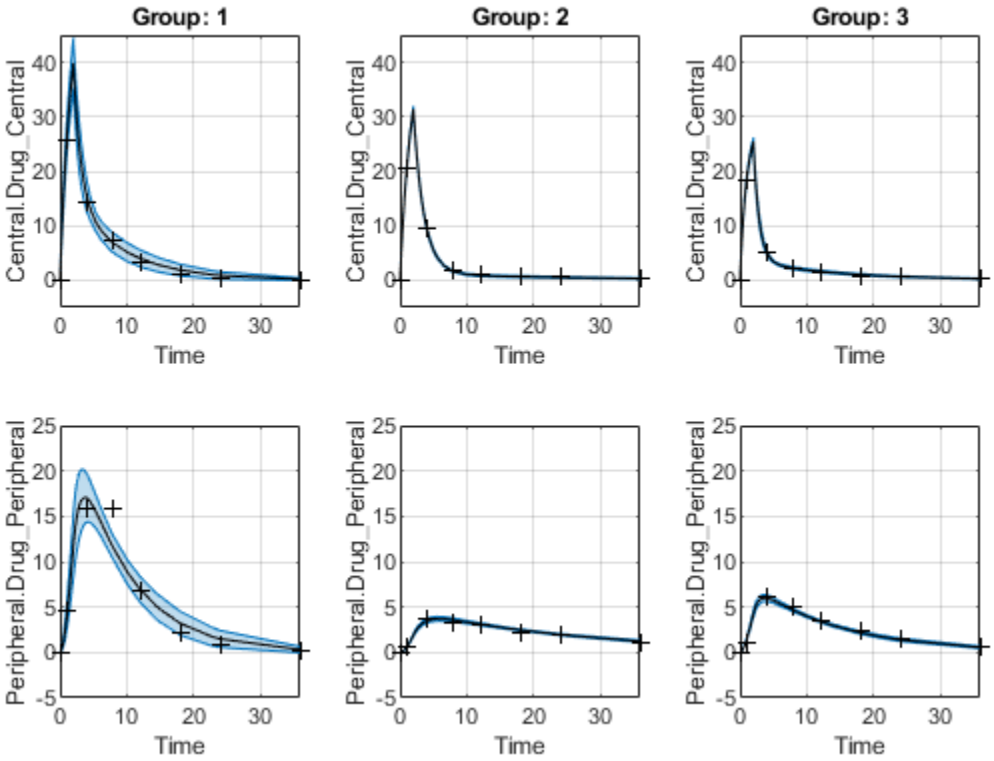
Plot Confidence Intervals for Model Predictions

The confidence interval for each group is plotted in a separate column, and each response is plotted in a separate row. Confidence intervals limited by the bounds are plotted in red. Confidence intervals not limited by the bounds are plotted in blue.

```
plot(ciPredPooled)
```




```
plot(ciPredUnpooled)
```



Input Arguments

`fitResults` — Parameter estimation results from `sbiofit`

`NLINResults` object | `OptimResults` object | vector

Parameter estimation results from `sbiofit`, specified as an `NLINResults`, `OptimResults`, or a vector of objects for unpooled fits that were returned from the same `sbiofit` call.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `'Alpha',0.01,'Type','bootstrap'` specifies to compute a 99% confidence interval using the bootstrap method.

`Alpha` — Confidence level

0.05 (default) | positive scalar

Confidence level, `(1-`*`Alpha`*`) * 100`%, specified as the comma-separated pair consisting of `'Alpha'` and a positive scalar between 0 and 1. The default value is `0.05`, meaning a 95% confidence interval is computed.

Example: `'Alpha',0.01`

Type — Confidence interval type
`'gaussian'` (default) | `'bootstrap'`

Confidence interval type, specified as the comma-separated pair consisting of `'Type'` and a character vector. The valid choices are:

- `'gaussian'`– Use the Gaussian approximation on page 1-214 of the distribution of the linearized model responses around the parameter estimates.
- `'bootstrap'`– Compute confidence intervals using the bootstrap method on page 1-215.

Example: `'Type','bootstrap'`

NumSamples — Number of samples for bootstrapping
1000 (default) | positive integer

Number of samples for bootstrapping, specified as the comma-separated pair consisting of `'NumSamples'` and a positive integer. This number defines the number of fits that are performed during the confidence interval computation to generate bootstrap samples. The smaller the number is, the faster the computation of the confidence intervals becomes, at the cost of decreased accuracy.

Example: `'NumSamples',500`

Display — Level of display returned to the command line
`'off'` (default) | `'none'` | `'final'`

Level of display returned to the command line, specified as the comma-separated pair consisting of `'Display'` and a character vector. `'off'` (default) or `'none'` displays no output. `'final'` displays a message when the computation finishes.

Example: `'Display','final'`

UseParallel — Logical flag to compute confidence intervals in parallel
`true` | `false`

Logical flag to compute confidence intervals in parallel, specified as the comma-separated pair consisting of `'UseParallel'` and `true` or `false`. By default, the parallel options in the original fit are used. If this argument is set to `true` and Parallel Computing Toolbox is available, the parallel options in the original fit are ignored, and confidence intervals are computed in parallel.

For the Gaussian confidence intervals:

- If the input `fitResults` is a vector of results objects, then the computation of confidence intervals for each object is performed in parallel. The Gaussian confidence intervals are quick to compute. So, it might be more beneficial to parallelize the original fit (`sbiofit`) and not set `UseParallel` to true for `sbiopredictionci`.

For the Bootstrap confidence intervals:

- The function forwards the `UseParallel` flag to `bootci`. There is no parallelization over the input vector of results objects.

Note If you have a global stream for random number generation with a number of substreams to compute in parallel in a reproducible fashion, `sbiopredictionci` first checks to see if the number

of workers is same as the number of substreams. If so, the function sets `UseSubstreams` to `true` in the `statset` option and passes to `bootci`. Otherwise, the substreams are ignored by default.

Example: `'UseParallel',true`

Output Arguments

`ci` — Confidence interval results

`PredictionConfidenceInterval` object

Confidence interval results, returned as a `PredictionConfidenceInterval` object. For an unpooled fit, `ci` can be a vector of `PredictionConfidenceInterval` objects.

More About

Gaussian Confidence Interval Calculation for Model Predictions

The model is linearized around the parameter estimates P_{est} that are obtained from the fit results returned by `sbiofit`. The `CovarianceMatrix` is transformed using the linearized model. In addition, implicit parameter bounds (`log`, `probit`, or `logit` parameter transforms specified in the original fit) and explicit parameter bounds (if specified in the original fit) are also mapped through the linearized model.

To linearize the model, `sbiopredictionci` first checks to see if the sensitivity analysis feature is turned on in the original fit. If the feature is on, the function uses the Jacobian computed via the complex step differentiation. If the feature is off, the Jacobian is computed using finite differencing. Finite differencing can be inaccurate, and consider turning on the sensitivity analysis on page 1-0 feature when you run `sbiofit`.

The function uses the transformed `CovarianceMatrix` and computes the Gaussian confidence intervals for each estimated model response at every time step.

In cases where the confidence interval is constrained by the parameter bounds defined in the original fit, the confidence interval bounds are adjusted according to the approach described by Wu, H. and Neale, M. [1].

Setting Estimation Status

- For each model response, the function first decides whether the confidence interval is unbounded. If so, the estimation status of the corresponding model response is set to `not estimable`.
- Otherwise, if the confidence interval for a response is constrained by a parameter bound defined in the original fit, the function sets its status to `constrained`. Parameter transformations (such as `log`, `probit`, or `logit`) impose implicit bounds on the estimated parameters, for example, positivity constraints. Such bounds can lead to the overestimation of confidence, that is, the confidence interval can be smaller than expected.
- If no confidence interval has the estimation status `not estimable` or `constrained`, then the function sets the estimation statuses of all model responses to `success`. Otherwise, the estimation statuses of remaining model responses are set to `estimable`.

Bootstrap Confidence Interval Calculation

The `bootci` function from Statistics and Machine Learning Toolbox is used to compute the bootstrap confidence intervals. The first input *nboot* is the number of samples (`NumSamples`), and the second input *bootfun* is a function that performs these actions.

- Resample the data (independently within each group, if multiple groups are available).
- Run a parameter fit with the resampled data.
- Simulate the model using the estimated parameters to get model responses.
- Return model responses.

Setting Estimation Status

The estimation status is always set to `estimable` since the function cannot determine if the confidence intervals are constrained by the bounds on the parameter estimates.

Version History

Introduced in R2017b

References

[1] Wu, H., and M.C. Neale. "Adjusted Confidence Intervals for a Bounded Parameter." *Behavior Genetics*. 42 (6), 2012, pp. 886-898.

Extended Capabilities

Automatic Parallel Support

Accelerate code by automatically running computation in parallel using Parallel Computing Toolbox™.

To run in parallel, set `'UseParallel'` to `true`.

For more information, see the `'UseParallel'` name-value pair argument.

See Also

`PredictionConfidenceInterval` | `sbioparameterci` | `sbiofit` | `ParameterConfidenceInterval`

sbioplot

Plot simulation results in one figure

Syntax

```
sbioplot(sd)
sbioplot(sd,fcnHandle,xArgs,yArgs,Name,Value)
```

Description

`sbioplot(sd)` plots each simulation run from `sd`, a `SimData` object or array of objects, in the same figure. The plot is a time plot of each state in `sd`. The figure also shows a hierarchical display of all the runs as different nodes in a tree, and you can select which run to display.

`sbioplot(sd,fcnHandle,xArgs,yArgs,Name,Value)` plots simulation results by calling the function handle `fcnHandle` with inputs `sd`, `xArgs`, and `yArgs`, and uses additional options specified by one or more name-value pair arguments. For example, you can specify the x-label and y-label of the plot. `xArgs` and `yArgs` must be cell arrays or string vectors of the names of the states to plot.

Examples

Plot Selected States from Simulation Data

Plot the prey versus predator data from the stochastically simulated lotka model by using a custom function (`plotXY`).

Load the model. Set the solver type to SSA to perform stochastic simulations, and set the stop time to 3.

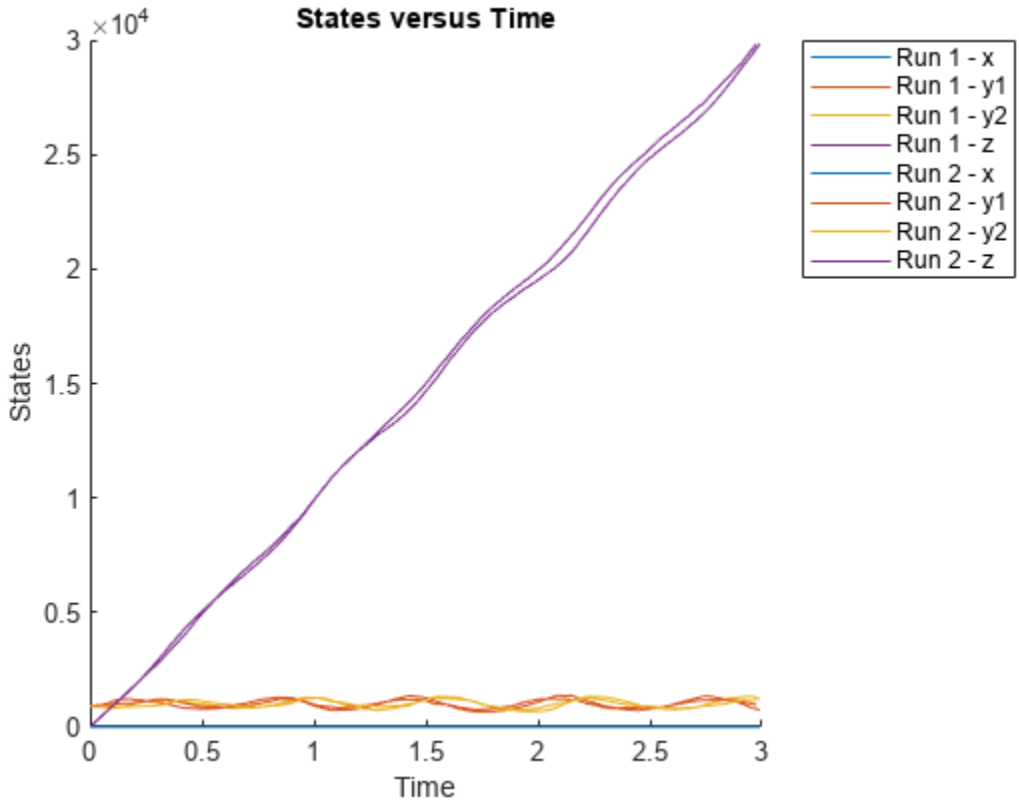
```
sbioloadproject lotka;
cs              = getconfigset(m1);
cs.SolverType   = 'SSA';
cs.StopTime     = 3;
rng('default') % For reproducibility
```

Set the number of runs and use `sbioensemblerun` for simulation.

```
numRuns = 2;
sd      = sbioensemblerun(m1,numRuns);
```

Plot the simulation data. By default, `sbioplot` shows the time plot of each species for each run.

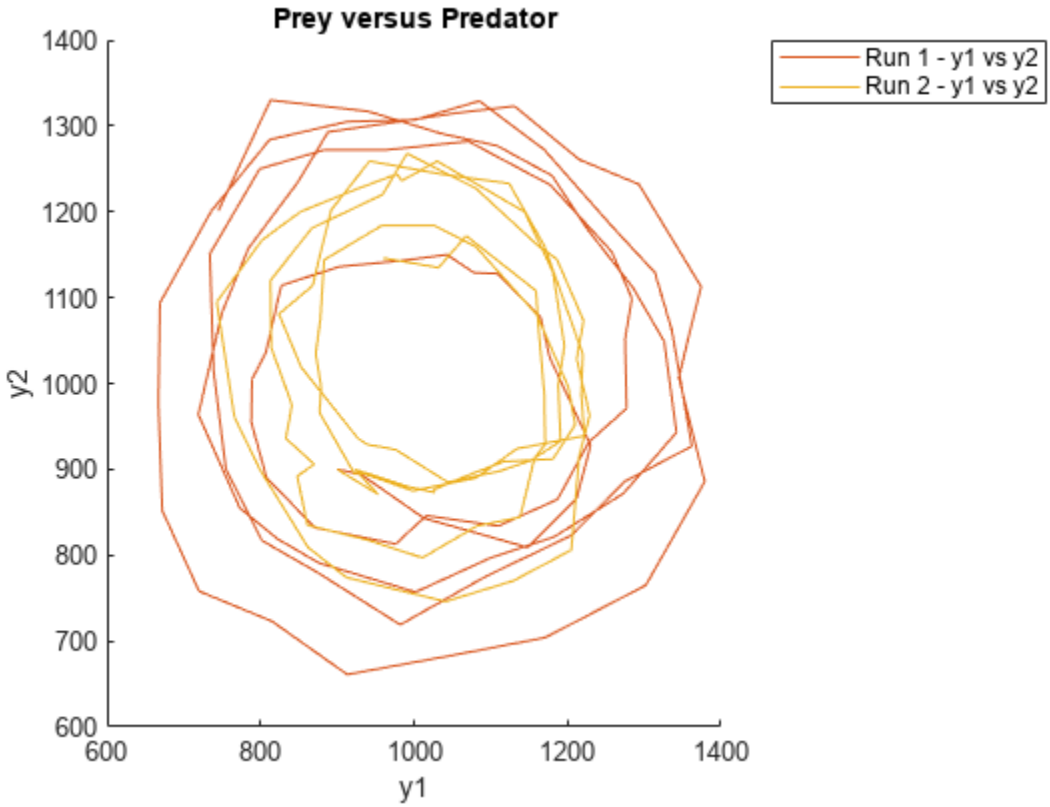
```
sbioplot(sd);
```



Plot selected states against each other; in this case, plot the prey population versus the predator population. Use the function `plotXY` (shown at the end of this example) to plot the simulated y1 (prey) data versus the y2 (predator) data. Specify the function as a function handle.

If you use the live script file for this example, the `plotXY` function is already included at the end of the file. Otherwise, you must define the `plotXY` function at the end of your .m or .mlx file or add it as a file on the MATLAB path.

```
sbioplot(sd,@plotXY,{'y1'},{'y2'},'xlabel','y1','ylabel','y2','title','Prey versus Predator');
```



Define plotXY Function

sbioplot accepts a function handle for a function with the signature:

`function [handles,names] = functionName(sd,xArgs,yArgs).`

The `plotXY` function plots two selected states against each other. The first input `sd` is the simulation data (SimBiology `SimData` object or vector of objects). In this particular example, xArgs is a cell array containing the name of the species to be plotted on the x-axis, and yArgs is a cell array containing the name of the second species to be plotted on the y-axis. However, you can use the inputs xArgs and yArgs in any way in *your* custom plotting function. The function returns `handles`, an array of function handles to the line plots, and `names`, a cell array of character vectors shown on the nodes that are children of a **Run** node in a hierarchical display.

```
function [handles,names] = plotXY(sd,xArgs,yArgs)

% Select simulation data for each state from each run.
xData1 = selectbyname(sd(1),xArgs);
xData2 = selectbyname(sd(2),xArgs);
yData1 = selectbyname(sd(1),yArgs);
yData2 = selectbyname(sd(2),yArgs);

% Plot the species against each other.
fH1 = plot(xData1.Data,yData1.Data);
fH2 = plot(xData2.Data,yData2.Data);

% The first output, handles, is a two-dimensional array of handles of the line plots. It must be
```

```
% where M is the number of line plots for each run and N is the number of runs.
handles = [fH1,fH2];

% The second output, names, must be a one-dimensional cell array of character vectors.
% Its length must be equal to the number of rows in handles, and the texts are displayed on the
% nodes that are children of a Run node.
names = {'y1 vs y2'};

end
```

Input Arguments

`sd` — Simulation results

`SimData` object

Simulation results, specified as a `SimData` object or vector of `SimData` objects.

This argument corresponds to the first input of the function referenced by `fcnHandle`.

Example: `simdata`

`fcnHandle` — Function to generate line plots

function handle

Function to generate line plots, specified as a function handle. For an example of a custom function to plot selected species from simulation data, see Plot Selected States from Simulation Data on page 1-216.

The function must have the signature:

`function [handles,names] = functionName(sd,xArgs,yArgs)`.

The inputs `sd`, `xArgs`, and `yArgs` are the same inputs that you pass in when you call `sbioplot`.

The first output `handles` is a two-dimensional array of handles of the line plots generated by the function. Its size must be *P*-by-*R*, where *P* is the number of line plots, and *R* is the number of runs.

The second output `names` is a one-dimensional cell array of character vectors containing the names to be displayed on the nodes that are children of a **Run** node in a hierarchical display. The length of `names` must be equal to the number of rows in `handles`.

Example: `@plotXY`

Data Types: `function_handle`

`xArgs` — State names

string vector | cell array of character vectors

State names to plot, specified as a string vector or cell array of character vectors. For instance, you can use `xArgs` to represent the states to be plotted on the *x*-axis of your custom plot.

This argument corresponds to the second input of the function referenced by `fcnHandle`.

Example: `{'y1'}`

Data Types: `cell`

yArgs — State names
string vector | cell array of character vectors

State names to plot, specified as a string vector or cell array of character vectors. For instance, you can use `yArgs` to represent the states to be plotted on the *y*-axis of your custom plot.

This argument corresponds to the third input of the function referenced by `fcnHandle`.

Example: `{'y2','z'}`

Data Types: `cell`

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `'title','Species X versus Species Y'` specifies the axes title of the plot.

title — Axes title
character vector | string

Axes title, specified as the comma-separated pair consisting of `'title'` and character vector or string.

Example: `'title','Prey versus Predator'`

Data Types: `char` | `string`

xlabel — Label for *x*-axis
character vector | string

Label for the *x*-axis of the plot, specified as the comma-separated pair consisting of `'xlabel'` and a character vector or string.

Example: `'xlabel','y1'`

Data Types: `char` | `string`

ylabel — Label for *y*-axis
character vector | string

Label for the *y*-axis of the plot, specified as the comma-separated pair consisting of `'ylabel'` and a character vector or string.

Example: `'ylabel','y2'`

Data Types: `char` | `string`

Version History

Introduced in R2008a

R2020a: Legends are statically displayed
Behavior changed in R2020a

Starting in R2020a, the figure legends are statistically displayed. The **All Runs** checkbox has been removed.

See Also

`sbiosubplot` | `SimData`

sbioremovefromlibrary

Remove kinetic law, unit, or unit prefix from library

Syntax

```
sbioremovefromlibrary (Obj)
sbioremovefromlibrary ('Type', 'Name')
```

Description

`sbioremovefromlibrary (Obj)` removes the kinetic law definition, unit, or unit prefix object (`Obj`) from the user-defined library. The removed component will no longer be available automatically in future MATLAB sessions.

`sbioremovefromlibrary` does not remove a kinetic law definition that is being used in a model.

You can use a built-in or user-defined kinetic law definition when you construct a kinetic law object with the method `addkineticlaw`.

`sbioremovefromlibrary ('Type', 'Name')` removes the object of type `'Type'` with name `'Name'` from the corresponding user-defined library. `Type` can be `'kineticlaw'`, `'unit'` or `'unitprefix'`.

To get a component of the built-in and user-defined libraries, use the commands `get(sbioroot, 'BuiltInLibrary')` and `get(sbioroot, 'UserDefinedLibrary')`.

To create a kinetic law definition, unit, or unit prefix, use `sbioabstractkineticlaw`, `sbiounit`, or `sbiounitprefix` respectively.

To add a kinetic law definition, unit, or unit prefix to the user-defined library, use the function `sbioaddtolibrary`.

Examples

This example shows how to remove a kinetic law definition from the user-defined library.

1. Create a kinetic law definition.

   ```
   abstkineticlawObj = sbioabstractkineticlaw('mylaw1', '(k1*s)/(k2+k1+s)');
   ```

2. Add the new kinetic law definition to the user-defined library.

   ```
   sbioaddtolibrary(abstkineticlawObj);
   ```

   `sbioaddtolibrary` adds the kinetic law definition to the user-defined library. You can verify this using `sbiowhos`.

   ```
   sbiowhos -kineticlaw -userdefined

   SimBiology Abstract Kinetic Law Array

   Index:    Library:       Name:     Expression:
   1         UserDefined    mylaw1    (k1*s)/(k2+k1+s)
   ```

3 Remove the kinetic law definition.

```
sbioremovefromlibrary('kineticlaw', 'mylaw1');
```

Version History

Introduced in R2006a

See Also

`sbioaddtolibrary` | `sbioabstractkineticlaw` | `sbiounit` | `sbiounitprefix`

sbioreset

Delete all model objects

Syntax

```
sbioreset
```

Description

`sbioreset` deletes all SimBiology model objects at the root level. You cannot use a SimBiology model object after it is deleted.

Tip To remove a SimBiology model object from the MATLAB workspace, without deleting it from the root level, use the `clear` function.

Note If the SimBiology desktop is open, calling `sbioreset` at the command line deletes all model objects that are open in the desktop.

The SimBiology root object contains a list of SimBiology model objects, available units, unit prefixes, and kinetic law objects. A SimBiology model object has its `Parent` property set to the SimBiology root object.

To add a kinetic law definition to the SimBiology root user-defined library, use the `sbioaddtolibrary` function. To add a unit to the SimBiology user-defined library on the root, use `sbiounit` followed by `sbioaddtolibrary`. To add a unit prefix to the SimBiology user-defined library on the root, use `sbiounitprefix` followed by `sbioaddtolibrary`.

Examples

This example shows the difference between `sbioreset` and `clear all`.

1. Import a model into the workspace.

   ```
   modelObj = sbmlimport('oscillator');
   ```

   Note that the workspace contains `modelObj` and if you query the SimBiology root, there is one model on the root object.

   ```
   rootObj = sbioroot

   SimBiology Root Contains:

    Models:                          1
    Builtin Abstract Kinetic Laws:   3
    User Abstract Kinetic Laws:      0
    Builtin Units:                   54
    User Units:                      0
    Builtin Unit Prefixes:           13
    User Unit Prefixes:              0
   ```

2 Use `clear all` to clear the workspace. The `modelObj` still exists on the `rootObj`.

```
clear all

rootObj


SimBiology Root Contains:

 Models:                           1
 Builtin Abstract Kinetic Laws:    3
 User Abstract Kinetic Laws:       0
 Builtin Units:                    54
 User Units:                       0
 Builtin Unit Prefixes:            13
 User Unit Prefixes:               0
```

3 Use`sbioreset` to delete the `modelObj` from the root.

```
sbioreset
rootObj


SimBiology Root Contains:

 Models:                           0
 Builtin Abstract Kinetic Laws:    3
 User Abstract Kinetic Laws:       0
 Builtin Units:                    54
 User Units:                       0
 Builtin Unit Prefixes:            13
 User Unit Prefixes:               0
```

Version History

Introduced before R2006a

See Also

`sbioaddtolibrary` | `sbioroot` | `sbiounit` | `sbiounitprefix`

Topics

sbioroot on page 1-226

sbioroot

Return SimBiology root object

Syntax

```
rootObj = sbioroot
```

Arguments

rootObj	Return `sbioroot` to this object.

Description

rootObj `= sbioroot` returns the SimBiology root object to `root`. The SimBiology root object contains a list of the SimBiology model objects, available units, unit prefixes, and available kinetic laws.

The units define the set of built-in units and user-defined units. See `Unit object` for more information.

The unit prefixes define the set of built-in prefixes and user-defined prefixes. See `Unit Prefix object` for more information.

The kinetic laws define the built-in kinetic laws and user-defined kinetic laws. See `AbstractKineticLaw object` for more information.

To add a unit, prefix or kinetic law to the root (in the user-defined library), use the `sbioaddtolibrary` function. To remove, use `sbioremovefromlibrary`.

The models opened in the SimBiology desktop are stored in the root object.

Method Summary

copyobj	Copy SimBiology object and its children
delete	Delete SimBiology object
display	Display summary of SimBiology object
get	Get SimBiology object properties
reset (root)	Delete all model objects from root object
set	Set SimBiology object properties

Property Summary

BuiltInLibrary	Library of built-in components
Models	Contain all model objects
Type	Display SimBiology object type
UserDefinedLibrary	Library of user-defined components

Version History

Introduced in R2006a

See Also

`addkineticlaw` | `sbiomodel` | `sbioreset` | `Unit object` | `UnitPrefix object`

Topics

sbiomodel on page 1-131
addkineticlaw on page 2-43
sbioreset on page 1-224

sbiosampleparameters

Generate parameters by sampling covariate model (requires Statistics and Machine Learning Toolbox software)

Syntax

```
phi = sbiosampleparameters(covexpr,thetas,omega,ds)
phi = sbiosampleparameters(covexpr,thetas,omega,n)
[phi,covmodel] = sbiosampleparameters(_)
```

Description

`phi = sbiosampleparameters(covexpr,thetas,omega,ds)` generates a matrix `phi` containing sampled parameter values using the covariate model specified by the covariate expression `covexpr`, fixed effects `thetas`, covariance matrix `omega`, and covariate data `ds`.

`phi = sbiosampleparameters(covexpr,thetas,omega,n)` uses a scalar `n` that specifies the number of rows in `phi` when the parameters are not dependent on any covariate.

`[phi,covmodel] = sbiosampleparameters(_)` returns a matrix `phi` and a covariate model object `covmodel` using any of the input arguments from previous syntaxes.

Examples

Sample Parameter Values from a Covariate Model

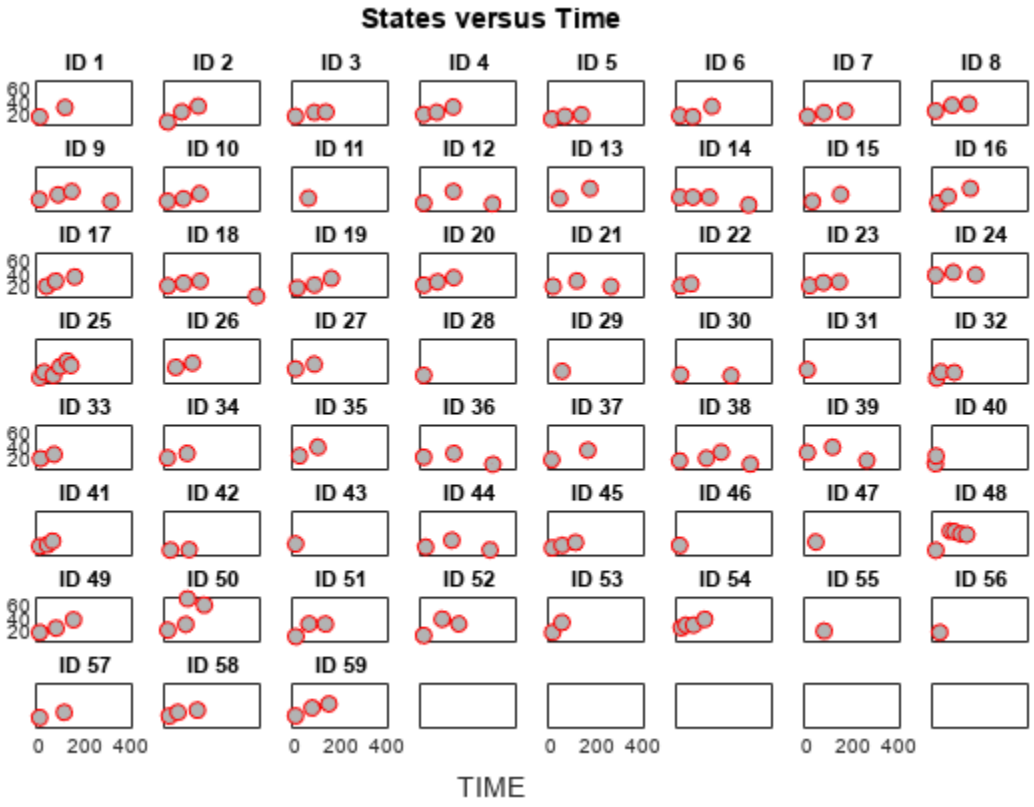
This example uses data collected on 59 preterm infants given phenobarbital during the first 16 days after birth. Each infant received an initial dose followed by one or more sustaining doses by intravenous bolus administration. A total of between 1 and 6 concentration measurements were obtained from each infant at times other than dose times, for a total of 155 measurements. Infant weights and APGAR scores (a measure of newborn health) were also recorded. Data was described in [1], a study funded by the NIH/NIBIB grant P41-EB01975.

Load the data.

```
load pheno.mat ds
```

Visualize the data.

```
t = sbiotrellis(ds,'ID','TIME','CONC','marker','o','markerfacecolor',[.7 .7 .7],'markeredgecolor
t.plottitle = 'States versus Time';
```



Create a one-compartment PK model with bolus dosing and linear clearance to model such data.

```
pkmd = PKModelDesign;
pkmd.addCompartment('Central','DosingType','Bolus','EliminationType','linear-clearance',...
                    'HasResponseVariable',true,'HasLag',false);
onecomp = pkmd.construct;
```

Suppose there is a correlation between the volume of the central compartment (`Central`) and the weight of infants. You can define this parameter-covariate relationship using a covariate model that can be described as

$$\log(V_i) = \theta_V + \theta V_{/WEIGHT} * WEIGHT_i + \eta_{V,i},$$

where, for each ith infant, V is the volume, θs (thetas) are fixed effects, η (eta) represents random effects, and `WEIGHT` is the covariate.

```
covM = CovariateModel;
covM.Expression = {'Central = exp(theta1+theta2*WEIGHT+eta1)'};
```

Define the fixed and random effects. The column names of each table must have the names of fixed effects and random effects, respectively.

```
thetas = table(1.4,0.05,'VariableNames',{'theta1','theta2'});
eta1 = table(0.2,'VariableNames',{'eta1'});
```

Change the group label ID to GROUP as required by the `sbiosampleparameters` function.

```
ds.Properties.VariableNames{'ID'} = 'GROUP';
```

Generate parameter values for the volumes of central compartments Central based on the covariate model for all infants in the data set.

```
phi = sbiosampleparameters(covM.Expression,thetas,eta1,ds);
```

You can then simulate the model using the sampled parameter values. For convenience, use the function-like interface provided by a SimFunction object.

First, construct a SimFunction object using the createSimFunction method, specifying the volume (Central) as the parameter, and the drug concentration in the compartment (Drug_Central) as the output of the SimFunction object, and the dosed species.

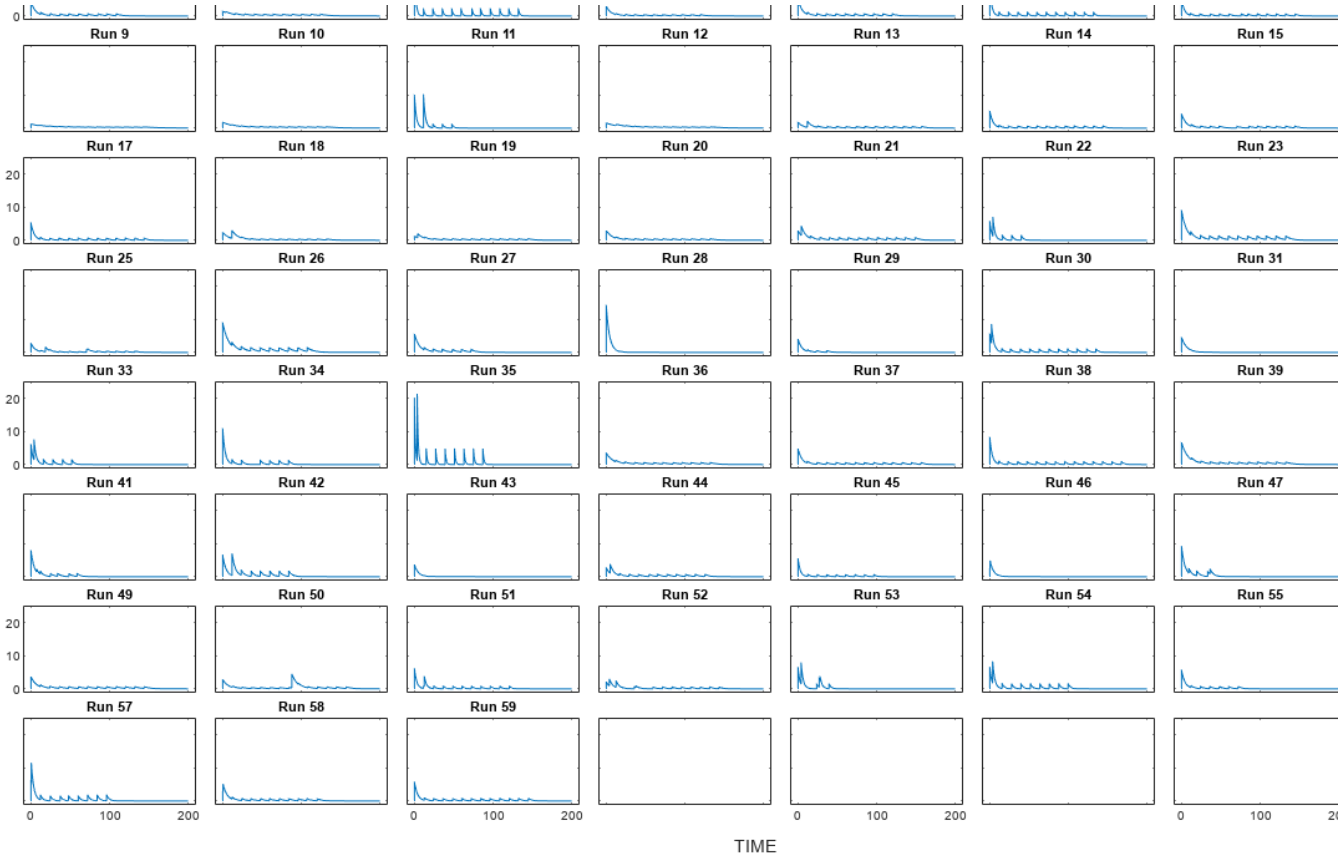
```
f = createSimFunction(onecomp,covM.ParameterNames,'Drug_Central','Drug_Central');
```

The data set ds contains dosing information for each infant, and the groupedData object provides a convenient way to extract such dosing information. Convert ds to a groupedData object and extract dosing information.

```
grpData = groupedData(ds);
doses = createDoses(grpData,'DOSE');
```

Simulate the model using the sampled parameter values from phi and the extracted dosing information of each infant, and plot the results. The ith run uses the ith parameter value in phi and dosing information of the ith infant.

```
t = sbiotrellis(f(phi,200,doses.getTable),[],'TIME','Drug_Central');
% Resize the figure.
t.hFig.Position(:) = [100 100 1280 800];
```



Input Arguments

`covexpr` — Covariate expressions

cell array of character vectors | string vector

Covariate expressions, specified as a cell array of character vectors or string vector that defines the parameter-covariate relationships.

If a model component name or covariate name is not a valid MATLAB variable name, surround it by square brackets when referring to it in the expression. For example, if the name of a species is *DNA polymerase+*, write `[DNA polymerase+]`. If a covariate name itself contains square brackets, you cannot use it in the expression.

See `CovariateModel` to learn more about covariate expressions.

`thetas` — Fixed effects

table | `groupedData` | dataset | numeric vector

Fixed effects, specified as a table, `groupedData`, dataset, or numeric vector containing values for fixed effect parameters defined in the covariate expressions `covexpr`. Fixed effect parameter names must start with `'theta'`.

- If `thetas` is a table, `thetas.Properties.VariableNames` must match the names of the fixed effects.

For example, suppose that you have three *thetas*: `thetaOne = 0.1`, `theta2 = 0.2`, and `theta3 = 0.3`. You can create the corresponding table.

```
thetas = table(0.1,0.2,0.3);
thetas.Properties.VariableNames = {'thetaOne','theta2','theta3'}
```

```
thetas =

  1×3 table

    thetaOne    theta2    theta3
    ________    ______    ______

      0.1         0.2       0.3
```

- If `thetas` is a dataset, `thetas.Properties.VarNames` must match the names of the fixed effects.
- If `thetas` is a numeric vector, the order of the values in the vector must be the same ascending ASCII dictionary order as the fixed effect names.

  Use the `sort` function to sort a cell array of character vectors to see the order.

  ```
  sort({'thetaOne','theta2','theta3'})
  ```

  ```
  ans =

    1×3 cell array

      {'theta2'}    {'theta3'}    {'thetaOne'}
  ```

  Then specify the value of each *theta* in the same order.

  ```
  thetas = [0.2 0.3 0.1];
  ```

`omega` — Covariance matrix of random effects
table | `groupedData` | dataset | matrix

Covariance matrix of random effects, specified as a table, `groupedData`, dataset, or matrix. Random effect parameter names must start with `'eta'`.

- If `omega` is a table, `omega.Properties.VariableNames` must match the names of the random effects. Specifying the row names (`RowNames`) is optional, but if you do, they must also match the names of random effects.

  Suppose that you want to define a diagonal covariance matrix with three random effect parameters *`eta1`*, *`eta2`*, and *`eta3`* with the values `0.1`, `0.2`, and `0.3`, respectively.

  $$\begin{bmatrix} Cov(\eta_1,\eta_1) & Cov(\eta_1,\eta_2) & Cov(\eta_1,\eta_3) \\ Cov(\eta_2,\eta_1) & Cov(\eta_2,\eta_2) & Cov(\eta_2,\eta_3) \\ Cov(\eta_3,\eta_1) & Cov(\eta_3,\eta_2) & Cov(\eta_3,\eta_3) \end{bmatrix} = \begin{bmatrix} eta1 & 0 & 0 \\ 0 & eta2 & 0 \\ 0 & 0 & eta3 \end{bmatrix}$$

  You can construct the corresponding table.

  ```
  eta1 = [0.1;0;0];
  eta2 = [0;0.2;0];
  eta3 = [0;0;0.3];
  omega = table(eta1,eta2,eta3,'VariableNames',{'eta1','eta2','eta3'})
  ```

```
omega =

  3×3 table

    eta1    eta2    eta3
    ____    ____    ____

    0.1       0       0
      0     0.2       0
      0       0     0.3
```

- If `omega` is a dataset, `omega.Properties.VarNames` must match the names of the random effects. Specifying the row names (`ObsNames`) is optional, but if you do, they must also match the names of random effects.
- If `omega` is a matrix, the rows and columns must have the same ascending ASCII dictionary order as the random effect names.

  Use the `sort` function to sort a cell array of character vectors to see the order.

```
sort({'eta1','eta2','eta3'})

ans =

  1×3 cell array

    {'eta1'}    {'eta2'}    {'eta3'}
```

`ds` — Covariate data
dataset | table | `groupedData`

Covariate data, specified as a dataset, table, or `groupedData` containing the covariate data for all groups.

`ds` must have a column for each covariate used in the covariate model. The column names must match the names of the corresponding covariates used in the covariate expressions.

`n` — Number of rows in `phi`
scalar

Number of rows in `phi`, specified as a scalar.

Output Arguments

`phi` — Sampled parameter values
matrix

Sampled parameter values, returned as a matrix of size S-by-P, where `S` is the number of groups specified in `ds` or specified by `n` and `P` is the number of parameters which is equal to the number of elements in `covexpr`.

`covmodel` — Covariate model
`CovariateModel` object

Covariate model, returned as a `CovariateModel` object which represents the model defined by `covexpr`.

Version History

Introduced in R2014a

R2022b: Covariate data no longer requires group column

The covariate data (the `ds` input argument) no longer requires a group column that specifies the group labels.

R2018b: Support for numeric vector and matrix inputs for fixed and random effects will be removed
Warns starting in R2018b

Support for specifying a numeric vector for the fixed effects (`thetas`) or a matrix for the covariance matrix of random effects (`omega`) will be removed in a future release. Use a table instead.

References

[1] Grasela Jr, T.H., Donn, S.M. (1985) Neonatal population pharmacokinetics of phenobarbital derived from routine clinical data. Dev Pharmacol Ther. 8(6), 374–83.

See Also

`sbiosampleerror` | `createSimFunction` | `SimFunction object` | `CovariateModel`

sbiosampleerror

Sample error based on error model and add noise to input data

Syntax

```
noisydata = sbiosampleerror(inputdata,errormodel,errorparam)
```

Description

`noisydata = sbiosampleerror(inputdata,errormodel,errorparam)` adds noise to the input data using one or more error models and error parameters.

Examples

Add Noise to Simulation Data

This example adds noise (or error) to the simulation data from a radioactive decay model with the first-order reaction: $\frac{dz}{dt} = c \cdot x$, where `x` and `z` are species and `c` is the forward rate constant.

Load the sample project containing the radiodecay model `m1`.

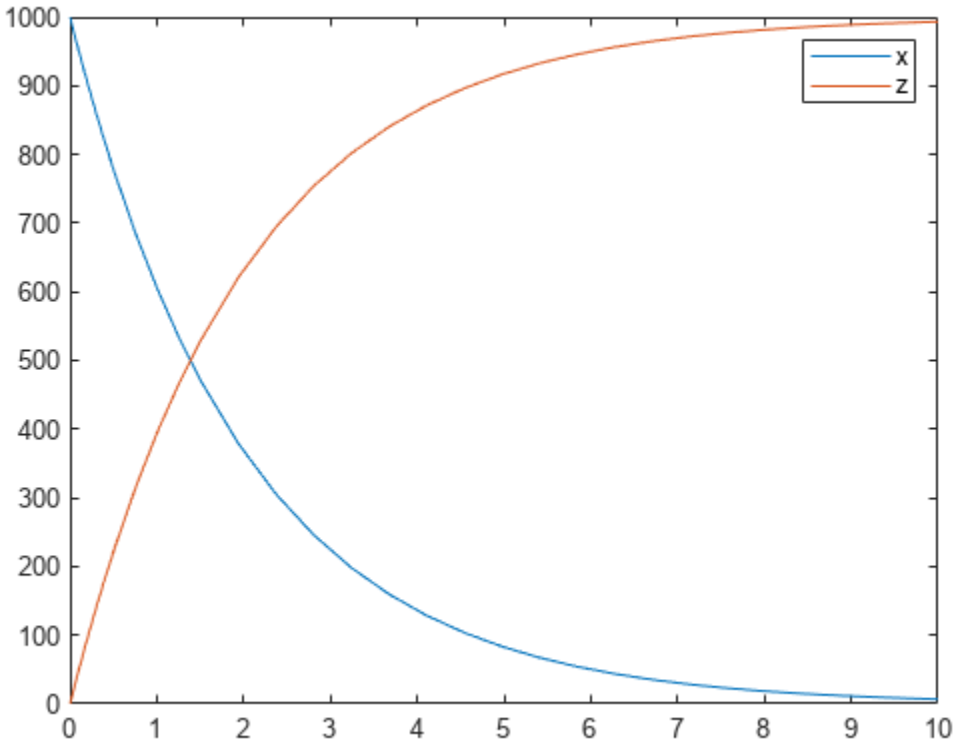
```
sbioloadproject radiodecay;
```

Simulate the model.

```
[t,sd,names] = sbiosimulate(m1);
```

Plot the simulation results.

```
plot(t,sd);
legend(names,'AutoUpdate','off');
hold on
```

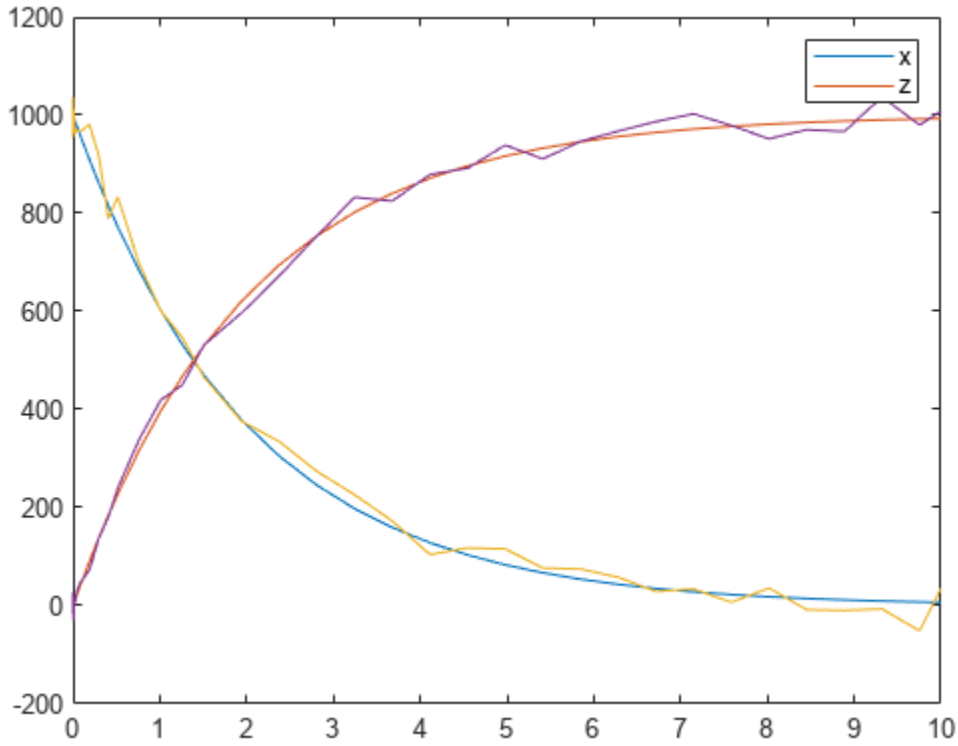


Add noise to the simulation results using the constant error model with the error parameter set to 20.

```
noisydata = sbiosampleerror(sd,'constant',20);
```

Plot the noisy simulation data.

```
plot(t,noisydata);
```



Define a Custom Error Model Using a Function Handle

This example defines a custom error model using a function handle and adds noise to simulation data of a radioactive decay model with the first-order reaction $\frac{dz}{dt} = c \cdot x$, where `x` and `z` are species, and `c` is the forward rate constant.

Load the sample project containing the radiodecay model `m1`.

```
sbioloadproject radiodecay;
```

Suppose you have a simple custom error model with a standard mean-zero and unit-variance (Gaussian) normal variable `e`, simulation results `f`, and two parameters `p1` and `p2`:
$y = f + p1 + p2 * e$

Define a function handle that represents the error model.

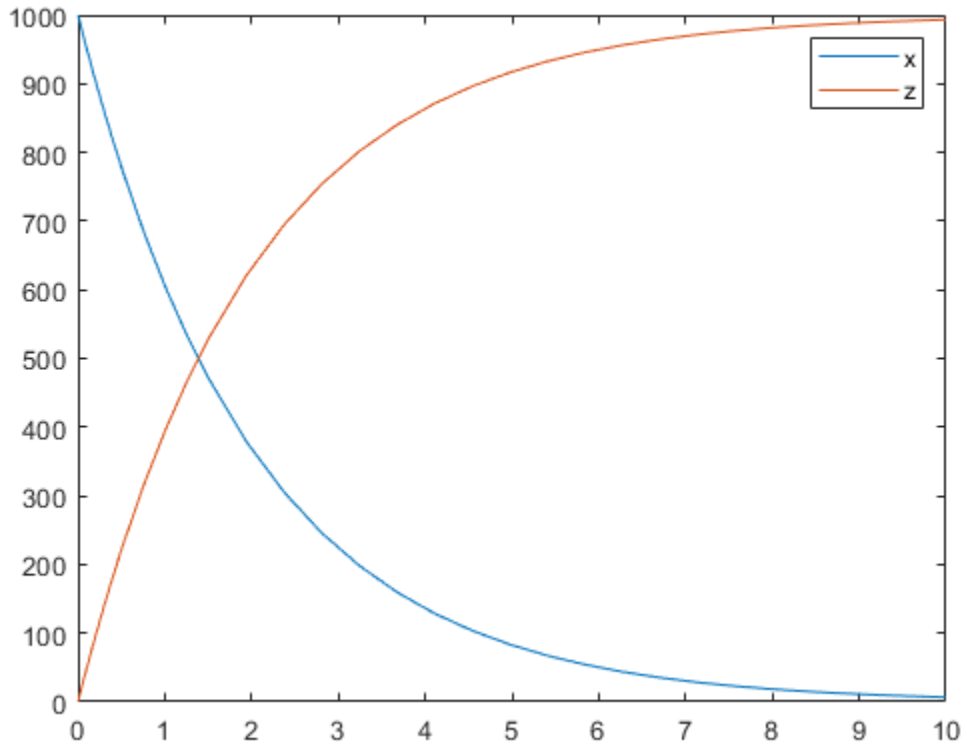
```
em = @(y,p1,p2) y+p1+p2*randn(size(y));
```

Simulate the model.

```
[t,sd,names] = sbiosimulate(m1);
```

Plot the simulation results and hold the plot.

```
plot(t,sd);
legend(names,'AutoUpdate','off');
hold on
```

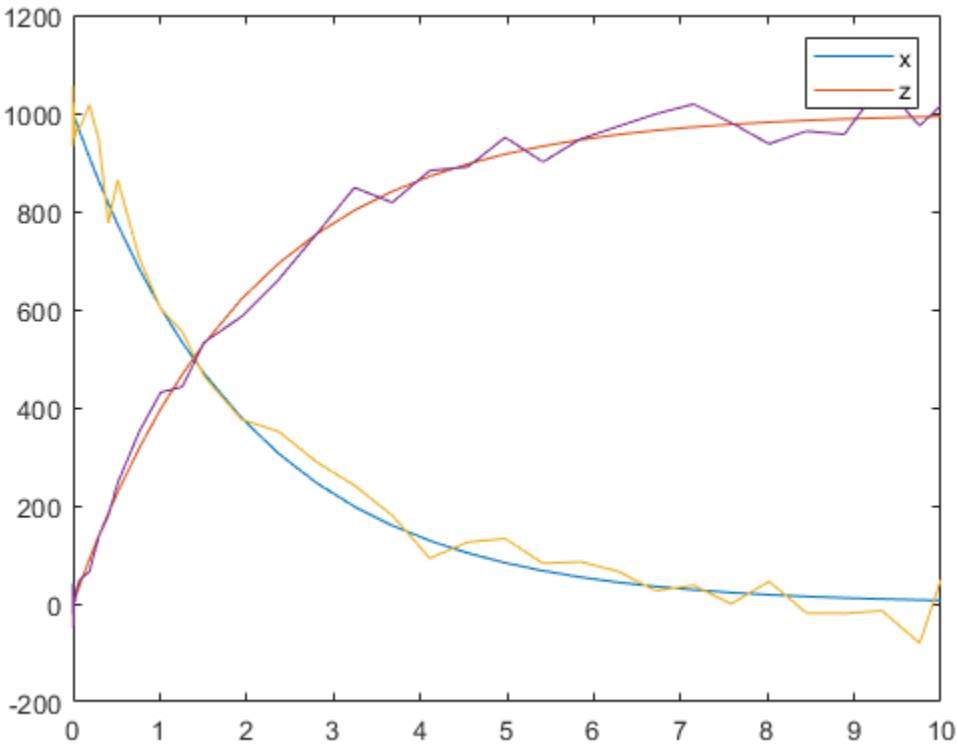


Sample the error using the previously defined custom function with two parameters set to 0.5 and 30, respectively.

```
noisydata = sbiosampleerror(sd,em,{0.5,30});
```

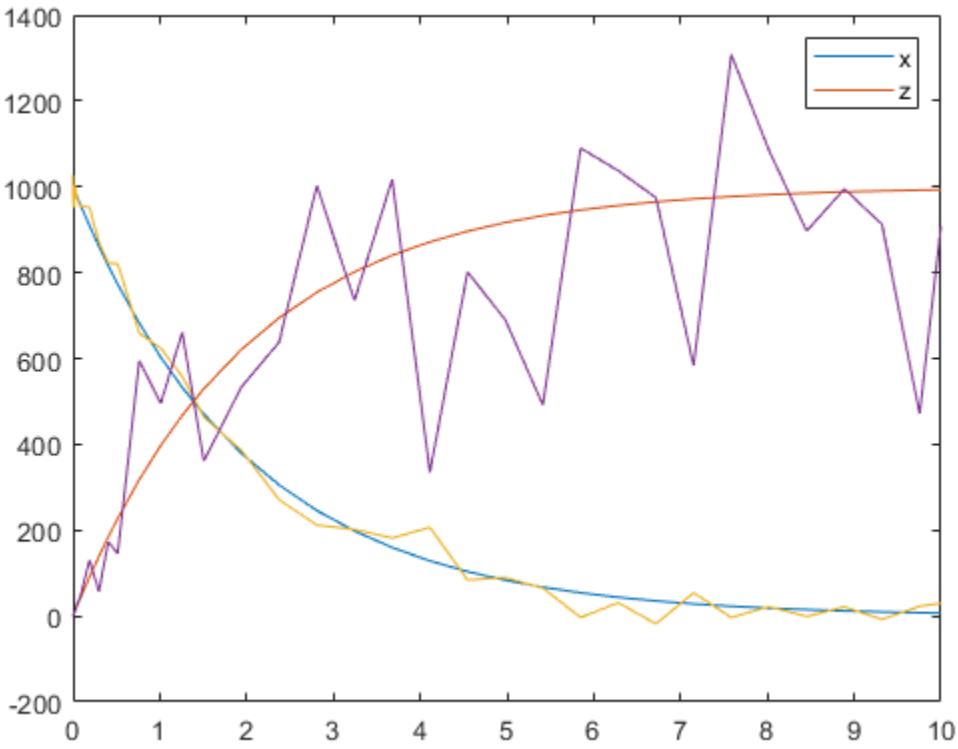
Plot the noisy simulation data.

```
plot(t,noisydata);
```



You can also apply a different error model to each state, which is a column in `sd`. Suppose you want to apply the custom error model (`em`) to the first column (species `x` data) and the proportional error model to the second column (species `z` data).

```
hold off
noisydata = sbiosampleerror(sd,{em,'proportional'},{{0.5,30},0.3});
plot(t,sd);
legend(names,'AutoUpdate','off');
hold on
plot(t,noisydata);
```



Input Arguments

`inputdata` — Input data

`SimData` object | vector of `SimData` objects | numeric matrix

Input data, specified as a `SimData object`, vector of `SimData` objects, or numeric matrix. If it is a vector of `SimData` objects, the error is added to each of the columns in the Data property. If it is a numeric matrix, the error is added to each column in the matrix.

`errormodel` — Error model

character vector | string | function handle | string vector | cell array of character vectors

Error model(s), specified as a character vector, string, function handle, string vector, cell array of character vectors, or cell array containing a mixture of character vectors and function handles.

If it is a string vector or cell array, its length must match the number of columns (responses) in `inputdata`, and each error model is applied to the corresponding column in `inputdata`. If it is a single character vector, string, or function handle, the same error model is applied to all columns in `inputdata`.

The first argument of a function handle must be a matrix of simulation results. The subsequent arguments are the parameters of the error model supplied in the `errorparam` input argument. The output of the function handle must be a matrix of the same size as the first input argument (simulation results).

For example, suppose you have a custom error model with a standard mean-zero and unit-variance (Gaussian) normal variable e, simulation results f, and two parameters $p1$ and $p2$: $y = f + p1 + p2 * e$. You can define the corresponding function handle as follows.

```
em = @(y,p1,p2) y+p1+p2*randn(size(y));
```

where `y` is the matrix of simulation results and `p1` and `p2` are the error parameters. The output of the function handle must be the same size as `y`, which is the same as the simulation results specified in the `inputdata` input argument. The parameters `p1` and `p2` are specified in the `errorparam` argument.

There are four built-in error models. Each model defines the error using a standard mean-zero and unit-variance (Gaussian) variable e, simulation results f, and one or two parameters a and b. The models are:

- `'constant'`: $y = f + ae$
- `'proportional'`: $y = f + b|f|e$
- `'combined'`: $y = f + (a + b|f|)e$
- `'exponential'`: $y = f * \exp(ae)$

`errorparam` — Error model parameter
scalar | vector | cell array

Error model parameter(s), specified as a scalar, vector, or cell array. If `errormodel` is `'constant'`, `'proportional'`, or `'exponential'`, then `errorparam` is specified as a numeric scalar. If it is `'combined'`, then `errorparam` is specified as a row vector with two elements `[a b]`.

If `errormodel` is a cell array, then `errorparam` must be a cell array of the same length. In other words, `errorparam` must contain N elements, where N is the number of error models in `errormodel`. Each element must have the correct number of parameters for the corresponding error model.

For example, suppose you have three columns in `inputdata`, and you are applying a different error model (`constant`, `proportional`, and `exponential` error models with error parameters `0.1`, `0.2`, and `0.5`, respectively) to each column, then `errormodel` and `errorparam` must be cell arrays with three elements as follows.

```
errormodel = {'constant','proportional','exponential'};
errorparam = {0.1,0.2,0.5};
```

Output Arguments

`noisydata` — Data with added noise
vector of `SimData` objects | matrix

Data with added noise, returned as a vector of `SimData` objects or numeric matrix. If `inputdata` is a vector of `SimData` objects, `noisydata` is also a vector of `SimData` objects, and the error is added to each column in the `inputdata.Data` property. If `inputdata` is specified as a matrix, `noisydata` is a matrix, and the error is added to each column in the matrix.

Version History

Introduced in R2014a

See Also

sbiosampleparameters | createSimFunction | SimFunction object

sbiosaveproject

Save all models in root object

Syntax

```
sbiosaveproject projFilename
sbiosaveproject projFilename variableName
sbiosaveproject projFilename variableName1 variableName2 ...
```

Description

`sbiosaveproject` *`projFilename`* saves all models in the SimBiology root object to the binary SimBiology project file named *`projFilename`*`.sbproj`. The project can be loaded with `sbioloadproject`. `sbiosaveproject` returns an error if *`projFilename`*`.sbproj` is not writable.

`sbiosaveproject` creates the binary SimBiology project file named `simbiology.sbproj`. `sbiosaveproject` returns an error if this is not writable.

`sbiosaveproject` *`projFilename variableName`* saves only *`variableName`*`.` *`variableName`* can be a SimBiology model or any MATLAB variable.

`sbiosaveproject` *`projFilename variableName1 variableName2`* `...` saves the specified variables in the project.

Use the functional form of `sbiosaveproject` when the file name or variable names are stored in a character vector. For example, if the file name is stored in the variable *`fileName`* and you want to store MATLAB variables *`variableName1`* and *`variableName2`*, type `sbiosaveproject (`*`projFileName`*`, '`*`variableName1`*`', '`*`variableName2`*`')` at the command line.

Examples

1. Import an SBML file and simulate (default configset object is used).

   ```
   modelObj = sbmlimport ('oscillator.xml');
   timeseriesObj = sbiosimulate(modelObj);
   ```

2. Save the model and the simulation results to a project.

   ```
   sbiosaveproject myprojectfile modelObj timeseriesObj
   ```

Version History

Introduced in R2006a

See Also

`sbioaddtolibrary` | `sbioloadproject` | `sbioremovefromlibrary` | `sbiowhos`

Topics

sbioloadproject on page 1-130
sbiowhos on page 1-311

sbioaddtolibrary on page 1-16
sbioremovefromlibrary on page 1-222

sbioselect

Search for objects with specified constraints

Syntax

```
Out = sbioselect('PropertyName', PropertyValue)
Out = sbioselect('Where', 'PropertyName', 'Condition', PropertyValue)
Out = sbioselect(Obj, 'PropertyName', PropertyValue)
Out = sbioselect(Obj, 'Type', 'TypeValue', 'PropertyName', PropertyValue)
Out = sbioselect(Obj, 'Where', 'PropertyName', 'Condition', PropertyValue)
Out = sbioselect(Obj, 'Where', 'PropertyNameCondition',
'PropertyNamePattern', 'Condition', PropertyValue)
Out = sbioselect(Obj, 'Where', 'PropertyName1', 'Condition1', PropertyValue1,
'Where', 'PropertyName2', 'Condition2', PropertyValue2,...)
Out = sbioselect(Obj, 'Where', 'PropertyName1', 'Condition1',
PropertyValue1,Bool_Operator, 'Where', 'PropertyName2', 'Condition2',
PropertyValue2,...)
Out = sbioselect(Obj, 'Depth', DepthValue,...)
```

Arguments

Out	Object or array of objects returned by the `sbioselect` function. *Out* might contain a mixture of object types (for example, species and parameters), depending on the selection you specify. If *PropertyValue* is a cell array, then the function returns all objects with the property '*PropertyName*' that matches any element of *PropertyValue*.
Obj	SimBiology object or array of objects to search. If an object is not specified, `sbioselect` searches the root.
PropertyName	Any property of the object being searched.
PropertyValue	Specify *PropertyValue* to include in the selection criteria.
TypeValue	Type of object to include in the selection, for example, `sbiomodel`, `species`, `reaction`, or `kineticlaw`.
Condition	The search condition. See the table under “Description” on page 1-246 for a list of conditions.
PropertyNameCondition	Search condition that applies only to the name property. See the table listing “Conditions for Names” below.
PropertyNamePattern	Character vector or string used to select the property name according to the condition imposed by *PropertyNameCondition*.
DepthValue	Specify the depth number to search. Valid numbers are positive integer values and `inf`. If *DepthValue* is `inf`, `sbioselect` searches *Obj* and all of its children. If *DepthValue* is `1`, `sbioselect` only searches *Obj* and not its children. By default, *DepthValue* is `inf`.

Description

`sbioselect` searches for objects with specified constraints.

`Out` = `sbioselect('`*`PropertyName`*`', `*`PropertyValue`*`)` searches the root object (including all model objects contained by the root object) and returns the objects with the property name (*`PropertyName`*) and property value (*`PropertyValue`*) contained by the root object.

`Out` = `sbioselect('Where', '`*`PropertyName`*`', '`*`Condition`*`', `*`PropertyValue`*`)` searches the root object and finds objects that have a property name (*`PropertyName`*) and value (*`PropertyValue`*) that matches the condition (*`Condition`*).

`Out` = `sbioselect(`*`Obj`*`, '`*`PropertyName`*`', `*`PropertyValue`*`)` returns the objects with the property name (*`PropertyName`*) and property value (*`PropertyValue`*) found in any object (*`Obj`*). If the property name in a property-value pair contains either a `'?'` or `'*'`, then the name is automatically interpreted as a wildcard expression, equivalent to the where clause `('Where', 'wildcard', 'PropertyName', '==', PropertyValue)`.

`Out` = `sbioselect(`*`Obj`*`, 'Type', '`*`TypeValue`*`', '`*`PropertyName`*`', `*`PropertyValue`*`)` finds the objects of type (`TypeValue`), with the property name (*`PropertyName`*) and property value (*`PropertyValue`*) found in any object (*`Obj`*). *`TypeValue`* is the type of SimBiology object to be included in the selection, for example, `species`, `reaction`, or `kineticlaw`.

`Out` = `sbioselect(`*`Obj`*`, 'Where', '`*`PropertyName`*`', '`*`Condition`*`', `*`PropertyValue`*`)` finds objects that have a property name (*`PropertyName`*) and value (*`PropertyValue`*) that match the condition (*`Condition`*).

If you search for a character vector property value without specifying a condition, you must use the same format as `get` returns. For example, if `get` returns the `Name` as `'MyObject'`, `sbioselect` will not find an object with a `Name` property value of `'myobject'`. Therefore, for this example, you must specify:

```
modelObj = sbioselect ('Name', 'MyObject')
```

Instead, if you use a condition, you can specify:

```
modelObj = sbioselect ('Where', 'Name', '==i', 'myobject')
```

Thus, conditions let you control the specificity of your selection.

`sbioselect` searches for model objects on the root in both cases.

`Out` = `sbioselect(`*`Obj`*`, 'Where', '`*`PropertyNameCondition`*`', '`*`PropertyNamePattern`*`', '`*`Condition`*`', `*`PropertyValue`*`)` finds objects with a property name that matches the pattern in (*`PropertyNamePattern`*) with the condition (*`PropertyNameCondition`*) and matches the value (*`PropertyValue`*) with the condition (*`Condition`*). Use this syntax when you want search conditions on both property names and property values.

The conditions, with examples of property names and corresponding examples of property values that you can use, are listed in the following tables. This table shows you conditions for numeric properties.

Conditions for Numeric Properties	Example Syntax

==	Search in the model object (`modelObj`), and return parameter objects that have `Value` equal to `0.5`. `sbioselect` returns parameter objects because only parameter objects have a property called `Value`.
	
	`parameterObj = sbioselect (modelObj,...`
	`'Where', 'Value', '==', 0.5)`
	
	In the case of ==, this is equivalent to omitting the condition as shown:
	
	`parameterObj = sbioselect (modelObj,...`
	`'Value', 0.5)`
	
	Search in the model object (`modelObj`), and return parameter objects that have `ConstantValue` `false` (nonconstant parameters).
	
	`parameterObj = sbioselect (modelObj,...`
	`'Where', 'ConstantValue', '==', false)`

~=	Search in the model object (`modelObj`), and return parameter objects that do not have `Value` equal to `0.5`.
	
	`parameterObj = sbioselect (modelObj,...`
	`'Where', 'Value', '~=', 0.5)`

>,<,>=,<=	Search in the model object (`modelObj`), and return species objects that have an initial amount (`InitialAmount`) greater than `50`.
	
	`speciesObj = sbioselect (modelObj, ...`
	`'Where', 'InitialAmount', '>', 50)`
	
	Search in the model object (`modelObj`), and return species objects that have an initial amount (`InitialAmount`) less than or equal to `50`.
	
	`speciesObj = sbioselect (modelObj,...`
	`'Where', 'InitialAmount', '<=', 50)`

`between`	Search in the model object (`modelObj`), and return species objects that have an initial amount (`InitialAmount`) between `200` and `300`.
	
	`speciesObj = sbioselect (modelObj,...`
	`'Where', 'InitialAmount',...`
	`'between', [200 300])`

`~between`	Search in the model object (`modelObj`), and return species objects that have an initial amount (`InitialAmount`) that is not between `200` and `300`.
	
	`speciesObj = sbioselect (modelObj,...`
	`'Where', 'InitialAmount',...`
	`'~between', [200 300])`

Conditions for Numeric Properties	Example Syntax

`equal_and_same_type`	Similar to ==, but in addition requires the property value to be of the same type.
	
	Search in the model object (`modelObj`), and return all objects containing a property of type `double` and a value equal to `0`. (Using `'=='` would also select objects containing a property with a value of false.)
	
	`zeroObj = sbioselect(modelObj, ...`
	`'Where', '*', 'equal_and_same_type', 0);`

`unequal_and_same_type`	Similar to ~=, but in addition requires the property value to be of the same type.
	
	Select all objects containing a property of type double and value not equal to 0. (Using `'~='` would also select objects containing a property with a value of true.)
	
	`nonzeroObj = sbioselect(modelObj, ...`
	`'Where', '*', 'unequal_and_same_type', 0);`

The following table shows you conditions for the name property or for properties whose values are character vectors.

Conditions for Names	Example Syntax

`==`	Search in the model object (`modelObj`), and return species objects named `'Glucose'`.
	
	`speciesObj = sbioselect (modelObj,...`
	`'Type', 'species', 'Where',...`
	`'Name', '==', 'Glucose')`

`~=`	Search in the model object (`modelObj`), and return species objects that are not named `'Glucose'`.
	
	`speciesObj = sbioselect (modelObj,...`
	`'Type', 'species', 'Where',...`
	`'Name', '~=', 'Glucose')`

`==i`	Same as ==; in addition, this is case insensitive.

`~=i`	Search in the model object (`modelObj`), and return species objects that are not named `'Glucose'`, ignoring case.
	
	`speciesObj = sbioselect (modelObj,...`
	`'Type', 'species', 'Where',...`
	`'Name', '~=i', 'glucose')`

Conditions for Names	Example Syntax

`regexp`. Supports expressions supported by the functions `regexp` and `regexpi`.	Search in the model object (`modelObj`), and return objects that have `'ese'` or `'ase'` anywhere within the name.
	
	`Obj = sbioselect (modelObj, 'Where',...`
	` 'Name', 'regexp', '[ea]se')`
	
	Search in the root, and return objects that have `kinase` anywhere within the name.
	
	`Obj = sbioselect ('Where',...`
	` 'Name', 'regexp', 'kinase')`
	
	Note that this query could result in a mixture of object types (for example, species and parameters).

`regexpi`	Same as `regexp`; in addition, this is case insensitive.

`~regexp`	Search in the model object (`modelObj`), and return objects that do not have `kinase` anywhere within the name.
	
	`Obj = sbioselect (modelObj, 'Where',...`
	` 'Name', '~regexp', 'kinase')`

`~regexpi`	Same as `~regexp`; in addition, this is case insensitive.
`wildcard`	Supports `DOS-style` wildcards ('?' matches any single character, '*' matches any number of characters, and the pattern must match the entire character vector). See `regexptranslate` for more information.
`wildcardi`	Same as `wildcard`; in addition, this is case insensitive.

`~wildcard`	Search in the model object (`modelObj`), and return objects that have names that do not begin with `kin*`.
	
	`Obj = sbioselect (modelObj, 'Where',...`
	` 'Name', '~wildcard', 'kin*')`

`~wildcardi`	Same as `~wildcard`; in addition, this is case insensitive.

Use the condition type `function` for any property. The specified value should be a function handle that, when applied to a property value, returns a boolean indicating whether there is a match. The following table shows an example of using `function`.

Condition	Example Syntax

`'function'`	Search in the model object and return reaction objects whose `Stoichiometry` property contains the specified stoichiometry.
	
	`Out = sbioselect(modelObj, 'Where',...`
	`'Stoichiometry', 'function',...`
	` @(x)any(x>2))`
	
	Select all objects with a numeric value that is even.
	
	`iseven = @(x) isnumeric(x)...`
	` && isvector(x) && mod(x, 2) == 0;`
	`evenValuedObj = sbioselect(modelObj, ...`
	`'where', 'Value', 'function', iseven);`

The condition `'contains'` can be used only for those properties whose values are an array of SimBiology objects. The following table shows an example of using `contains`.

Condition	Example Syntax

`'contains'`	Search in the model object and return reaction objects whose `Reactant` property contains the specified species.
	
	`Out = sbioselect(modelObj, 'Where',...`
	`'Reactants', 'contains',...`
	` modelObj.Species(1))`

`Out` = sbioselect(*`Obj`*, 'Where', '*`PropertyName1`*', '*`Condition1`*', *`PropertyValue1`*, 'Where', '*`PropertyName2`*', '*`Condition2`*', *`PropertyValue2`*,...) finds objects contained by `Obj` that matches all the conditions specified.

You can combine any number of property name/property value pairs and conditions in the `sbioselect` command.

`Out` = sbioselect(*`Obj`*, 'Where', '*`PropertyName1`*', '*`Condition1`*', *`PropertyValue1`*,*`Bool_Operator`*, 'Where', '*`PropertyName2`*', '*`Condition2`*', *`PropertyValue2`*,...) finds objects contained by `Obj` that matches all the conditions specified. Supported character vectors for *`Bool_Operator`* are as follows.

- `'and'` — True if (`'Where'`, `'PropertyName1'`,`'Condition1'`,`PropertyValue1`) and (`'Where'`, `'PropertyName2'`,`'Condition2'`,`PropertyValue2`) are both true.
- `'or'` — True if either (`'Where'`, `'PropertyName1'`,`'Condition1'`,`PropertyValue1`) or (`'Where'`, `'PropertyName2'`,`'Condition2'`,`PropertyValue2`) is true.
- `'xor'` — True if exactly one of (`'Where'`, `'PropertyName1'`,`'Condition1'`,`PropertyValue1`) or (`'Where'`, `'PropertyName2'`,`'Condition2'`,`PropertyValue2`) is true.
- `'not'` — True if (`'Where'`, `'PropertyName1'`,`'Condition1'`,`PropertyValue1`) is true and (`'Where'`, `'PropertyName2'`,`'Condition2'`,`PropertyValue2`) is not true.

Compound expressions with multiple boolean operators are supported. Precedence of the operators follows the order of operations for boolean algebra `not` –> `and` –> `xor` –> `or`.

`Out` = sbioselect(*`Obj`*, 'Depth', *`DepthValue`*,...) finds objects using a model search depth of *`DepthValue`*.

Note The order of results from `sbioselect` is not guaranteed. Hence, it is not recommended to depend on the order of results.

Examples

Find Species from a SimBiology Model

Import a model.

```
modelObj = sbmlimport('oscillator');
```

Find and return an object named `pA`.

```
pA = sbioselect(modelObj, 'Name', 'pA')

pA =
   SimBiology Species Array

   Index:    Compartment:    Name:    Value:    Units:
   1         unnamed         pA       100
```

Find and return species objects whose `Name` starts with `p` and have `A` or `B` as the next letter in the name.

```
speciesObjs = sbioselect(modelObj, 'Type', 'species', 'Where',...
                         'Name', 'regexp', '^p[AB]')

speciesObjs =
   SimBiology Species Array

   Index:    Compartment:    Name:        Value:    Units:
   1         unnamed         pA           100
   2         unnamed         pB           0
   3         unnamed         pA_OpB1      0
   4         unnamed         pB_OpC1      0
   5         unnamed         pA_OpB_pA    20
   6         unnamed         pA_OpB2      0
   7         unnamed         pB_OpC2      0
   8         unnamed         pB_OpC_pB    0
```

Find a cell array. Note how cell array values must be specified inside another cell array.

```
modelObj.Species(2).UserData = {'a' 'b'};
Obj = sbioselect(modelObj, 'UserData', {{'a' 'b'}})

Obj =
   SimBiology Species Array

   Index:    Compartment:    Name:    Value:    Units:
   1         unnamed         pB       0
```

Find and return objects that do not have their units set.

```
unitlessObj = sbioselect(modelObj, 'Where', 'wildcard', '*Units', '==', '');
```

Alternatively, you can do the following.

```
unitlessObj = sbioselect(modelObj, '*Units', '');
```

Version History

Introduced before R2006a

See Also

`regexp`

sbioshowunitprefixes

Show unit prefixes in library

Syntax

```
UnitPrefixObjs = sbioshowunitprefixes
[Name, Multiplier] = sbioshowunitprefixes
[Name, Multiplier, Builtin] = sbioshowunitprefixes
[Name, Multiplier, Builtin] = sbioshowunitprefixes('Name')
```

Arguments

unitPrefixObjs	Vector of unit prefix objects from the BuiltInLibrary and UserDefinedLibrary properties of the `Root`.
Name	Name of the built-in or user-defined unit prefix. Built-in prefixes are defined based on the International System of Units (SI).
Multiplier	Shows the value of `10^Exponent` that defines the relationship of the unit prefix *Name* to the base unit. For example, the multiplier in `picomole` is `10e-12`.
Builtin	An array of logical values. If *Builtin* is true for a unit prefix, the unit prefix is built in. If *Builtin* is false for a unit prefix, the unit prefix is user-defined.

Description

`sbioshowunitprefixes` returns information about unit prefixes in the SimBiology library.

UnitPrefixObjs `= sbioshowunitprefixes` returns the unit prefixes in the library as a vector of unit prefix objects in *UnitPrefixObjs*.

[*Name, Multiplier*] `= sbioshowunitprefixes` returns the multiplier for each prefix in *Name* to *Multiplier* as a cell array of character vectors.

[*Name, Multiplier, Builtin*] `= sbioshowunitprefixes` returns whether the unit prefix is built in or user defined for each unit prefix in *Name* to *Builtin*.

[*Name, Multiplier, Builtin*] `= sbioshowunitprefixes('`*Name*`')` returns the name, multiplier, and built-in status for the unit prefix with name *Name*. *Name* can be a string vector or cell array of character vectors.

Examples

```
[name, multiplier] = sbioshowunitprefixes;
[name, multiplier] = sbioshowunitprefixes('nano');
```

Version History

Introduced in R2006a

See Also

`sbioconvertunits` | `sbioshowunits` | `sbiounitprefix`

sbioshowunits

Show units in library

Note If you specify four output arguments when calling `sbioshowunits`, the function no longer returns the offset information as the fourth output. The fourth output is now a logical vector that is true for each built-in unit.

You can no longer specify five output arguments when you call `sbioshowunits`. For details, see "Compatibility Considerations".

Syntax

```
unitObjs = sbioshowunits
[Name, Composition] = sbioshowunits
[Name, Composition, Multiplier] = sbioshowunits
[Name, Composition, Multiplier, Builtin] = sbioshowunits
[___] = sbioshowunits(UnitNames)
```

Arguments

unitObjs	Vector of unit objects from the BuiltInLibrary and UserDefinedLibrary properties of the `Root`.
UnitNames	Names of the built-in or user-defined units, specified as a character vector, string, string vector, or cell array of character vectors.
Composition	Shows the combination of base and derived units that defines the unit *Name*. For example, `molarity` is `mole/liter`.
Multiplier	The numerical value that defines the relationship between the unit *Name* and the base or derived unit as a product of the *Multiplier* and the base unit or derived unit. For example, `1 mole` is `6.0221e23*molecule`. The *Multiplier* is `6.0221e23`.
Builtin	An array of logical values. If *Builtin* is true for a unit, the unit is built in. If *Builtin* is false for a unit, the unit is user-defined.

Description

unitObjs = `sbioshowunits` returns the units in the library to *unitObjs* as a vector of unit objects.

[*Name, Composition*] = `sbioshowunits` returns the composition for each unit in *Name* to *Composition* as a cell array of character vectors.

[*Name, Composition, Multiplier*] = `sbioshowunits` returns the multiplier for the unit with name *Name* to *Multiplier*.

`[Name, Composition, Multiplier, Builtin] = sbioshowunits` returns whether the unit is built in or user defined for each unit in *`Name`* to *`Builtin`*.

`[ ___ ] = sbioshowunits(UnitNames)` returns information about the units matching any of the names specified in *`UnitNames`*.

Examples

```
[name, composition] = sbioshowunits;
[name, composition] = sbioshowunits('molecule');
```

Version History

Introduced in R2006a

R2022b: `week` has been added as a built-in unit

Behavior changed in R2022b

You can now use `week` as a built-in unit and no longer have to create your own custom week unit. However, suppose that you have added a custom week unit to the user-defined (custom) library in a previous release (R2022a or earlier), installed the new version of MATLAB (R2022b or later), and your preferences from the previous release was imported (automatically by MATLAB or manually by you). When you interact with SimBiology for the first time in your latest MATLAB, SimBiology:

1. Switches to use the built-in `week` unit.
2. Renames the custom unit to `week_N`, where *N* is a positive integer.
3. Shows a one-time warning message indicating that your custom `week` unit has been renamed.

Use `sbioremovefromlibrary` at the command line or go to **Home** > **Libraries** from the **SimBiology Model Builder** app to remove the custom unit if it is no longer needed.

Tip

- Check the model component properties, namely, `Notes`, `Tag`, and `UserData`, to see if the custom unit is being referenced by these properties before removing the unit.
- Update references to use the new name (`week_N`) if the built-in `week` unit is not sufficient for your use case.

R2021a: `sbioshowunits` no longer returns offset information

Behavior changed in R2021a

If you specify four output arguments when calling `sbioshowunits`, the function no longer returns the offset information as the fourth output. The fourth output is now *`Builtin`*, that is, a logical vector that is true for each built-in unit.

R2021a: You can no longer specify five output arguments

Errors starting in R2021a

You can no longer specify five output arguments when you call `sbioshowunits`. Specify up to four output arguments instead.

R2021a: Celsius and Fahrenheit units have been removed
Errors starting in R2021a

`Celsius`, `celsius`, and `fahrenheit` units have been removed from the built-in units library. Use `kelvin` units instead.

If you have a model containing `Celsius`, `celsius`, or `fahrenheit` units, change the units to `kelvin`.

If you have a script that sets the Units property of a parameter to `'Celsius'`, `'celsius'`, or `'fahrenheit'`, set this property to `'kelvin'` and adjust the `Value` property accordingly. Similarly, if you have compound units, make appropriate changes. For example, change `joule/Celsius` to `joule/kevin`.

See Also

`sbioconvertunits` | `sbioshowunitprefixes` | `sbiounit`

sbiosimulate

Simulate SimBiology model

Syntax

```
[time,x,names] = sbiosimulate(modelObj)
[time,x,names] = sbiosimulate(modelObj,csObj)
[time,x,names] = sbiosimulate(modelObj,dvObj)
[time,x,names] = sbiosimulate(modelObj,csObj,dvObj)
[time,x,names] = sbiosimulate(modelObj,csObj,variantObj,doseObj)

simDataObj = sbiosimulate( ___ )
```

Description

`[time,x,names] = sbiosimulate(modelObj)` returns simulation results in three outputs, `time`, vector of time samples, `x`, simulation data, and `names`, column labels of simulation data `x`. This function simulates the SimBiology model `modelObj` while using the active configuration set along with its active doses and active variants if any.

`[time,x,names] = sbiosimulate(modelObj,csObj)` returns simulation results using the specified configset object `csObj`, any active variants, and any active doses. Any other configsets are ignored. If you set `csObj` to empty `[]`, the function uses the active configset.

`[time,x,names] = sbiosimulate(modelObj,dvObj)` returns simulation results using doses or variants specified by `dvObj` and the active configset. `dvObj` can be one of the following:

- `Variant object`
- `ScheduleDose object`
- `RepeatDose object`
- Array of doses or variants

If you set `dvObj` to empty `[]`, the function uses the active configset, active variants, and active doses.

If you specify `dvObj` as variants, the function uses the specified variants and active doses. Any other variants are ignored.

If you specify `dvObj` as doses, the function uses the specified doses and active variants. Any other doses are ignored.

`[time,x,names] = sbiosimulate(modelObj,csObj,dvObj)` returns simulation results using a configset object `csObj` and dose, variant, or an array of doses or variants specified by `dvObj`.

If you set `csObj` to `[]`, then the function uses the active configset object.

If you set `dvObj` to `[]`, then the function uses no variants, but uses active doses.

If you specify `dvObj` as variants, the function uses the specified variants and active doses. Any other variants are ignored.

If you specify `dvObj` as doses, the function uses the specified doses and active variants. Any other doses are ignored.

`[time,x,names] = sbiosimulate(modelObj,csObj,variantObj,doseObj)` returns simulation results using a configset object `csObj`, variant object or variant array specified by `variantObj`, and dose object or dose array specified by `doseObj`.

If you set `csObj` to `[]`, then the function uses the active configset object.

If you set `variantObj` to `[]`, then the function uses no variants.

If you set `doseObj` to `[]`, then the function uses no doses.

`simDataObj = sbiosimulate( ___ )` returns simulation results in a `SimData object simDataObj` using any of the input arguments in the preceding syntaxes.

Examples

Simulate a SimBiology Model

Load a sample SimBiology model.

```
sbioloadproject radiodecay.sbproj
```

Change the simulation stop time to 15 seconds.

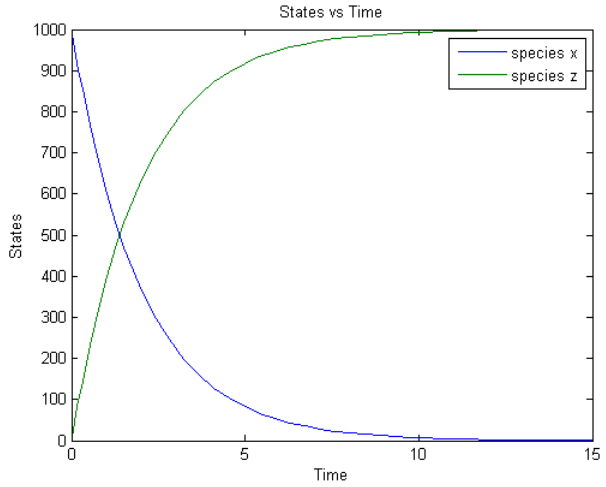
```
csObj = getconfigset(m1,'active');
set(csObj,'Stoptime',15);
```

Simulate the model and return outputs in an array.

```
[t,x,n] = sbiosimulate(m1);
```

Plot the simulated results for species `x` and `z`.

```
figure;
plot(t,x)
xlabel('Time')
ylabel('States')
title('States vs Time')
legend('species x','species z')
```

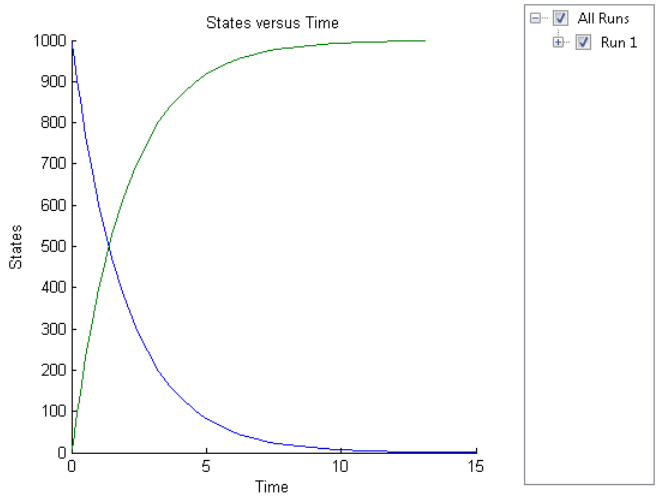


You can also return the results to a `SimData object` .

```
simData = sbiosimulate(m1);
```

Plot the simulated results.

```
sbioplot(simData);
```



Simulate a SimBiology Model Using an Array of Dose Objects

Load a sample SimBiology model.

```
sbioloadproject radiodecay.sbproj
```

Add two doses of 100 molecules each for species `x`, scheduled at 2 and 4 seconds respectively.

```
dObj1 = adddose(m1,'d1','schedule');
dObj1.Amount = 100;
dObj1.AmountUnits = 'molecule';
```

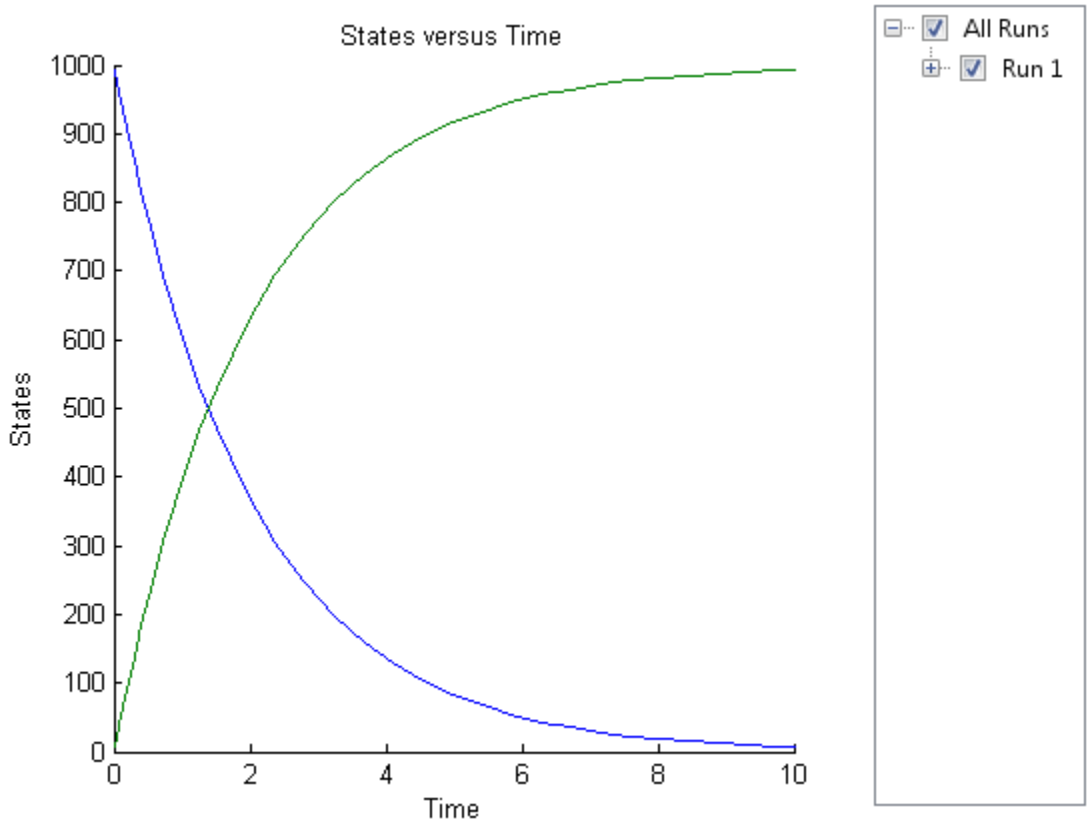
```
dObj1.TimeUnits = 'second';
dObj1.Time = 2;
dObj1.TargetName = 'unnamed.x';

dObj2 = adddose(m1,'d2','schedule');
dObj2.Amount = 100;
dObj2.AmountUnits = 'molecule';
dObj2.TimeUnits = 'second';
dObj2.Time = 4;
dObj2.TargetName = 'unnamed.x';
```

Simulate the model using no dose or any subset of the dose array.

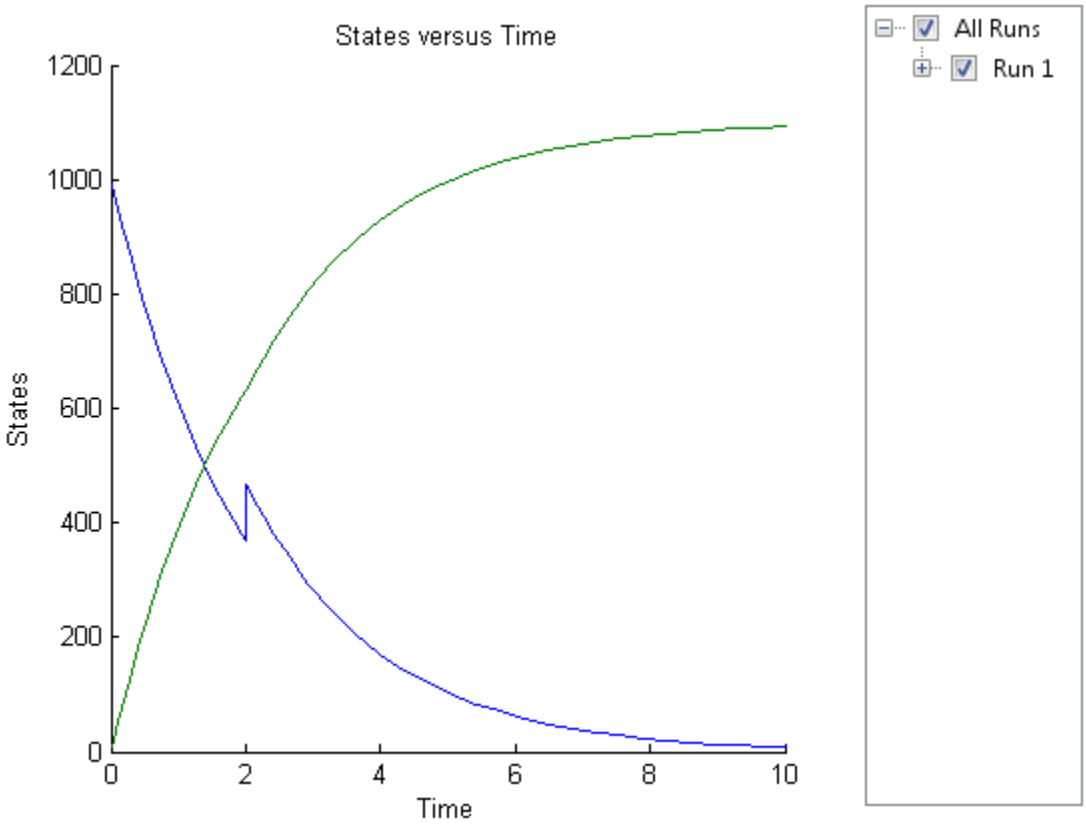
```
sim1 = sbiosimulate(m1);
sim2 = sbiosimulate(m1,dObj1);
sim3 = sbiosimulate(m1,dObj2);
sim4 = sbiosimulate(m1,[dObj1,dObj2]);
```

Plot the results.

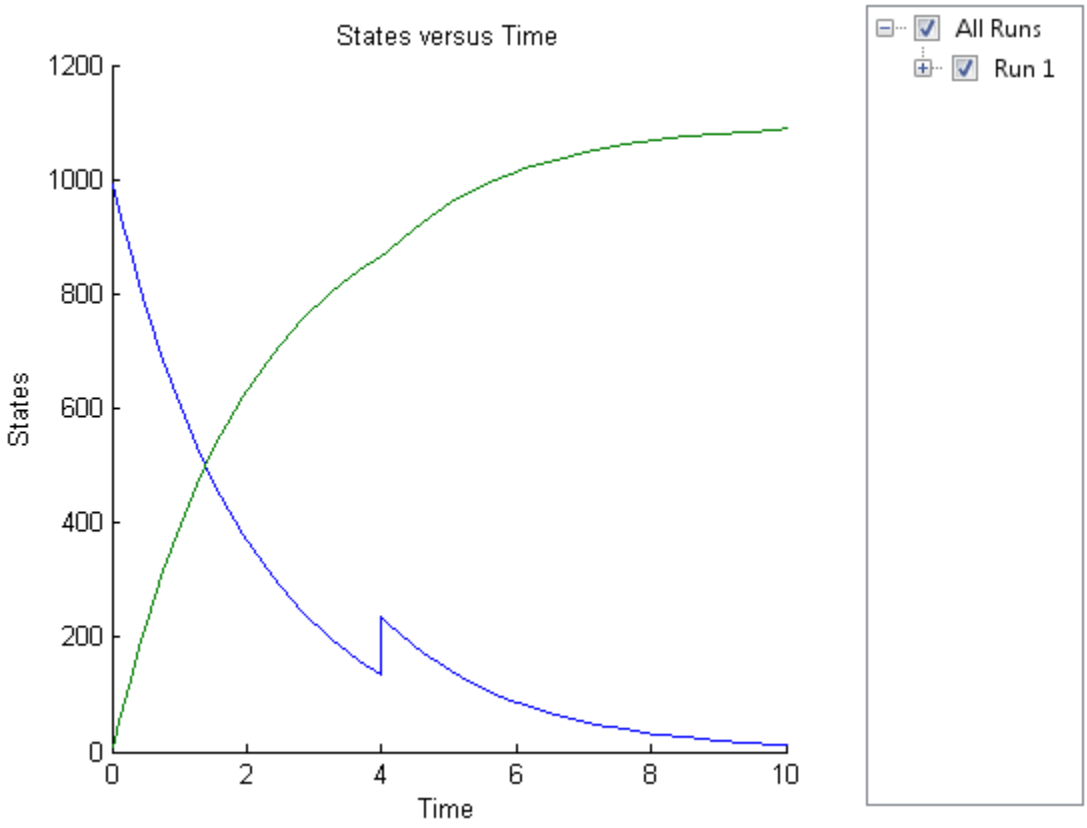
```
sbioplot(sim1)
```



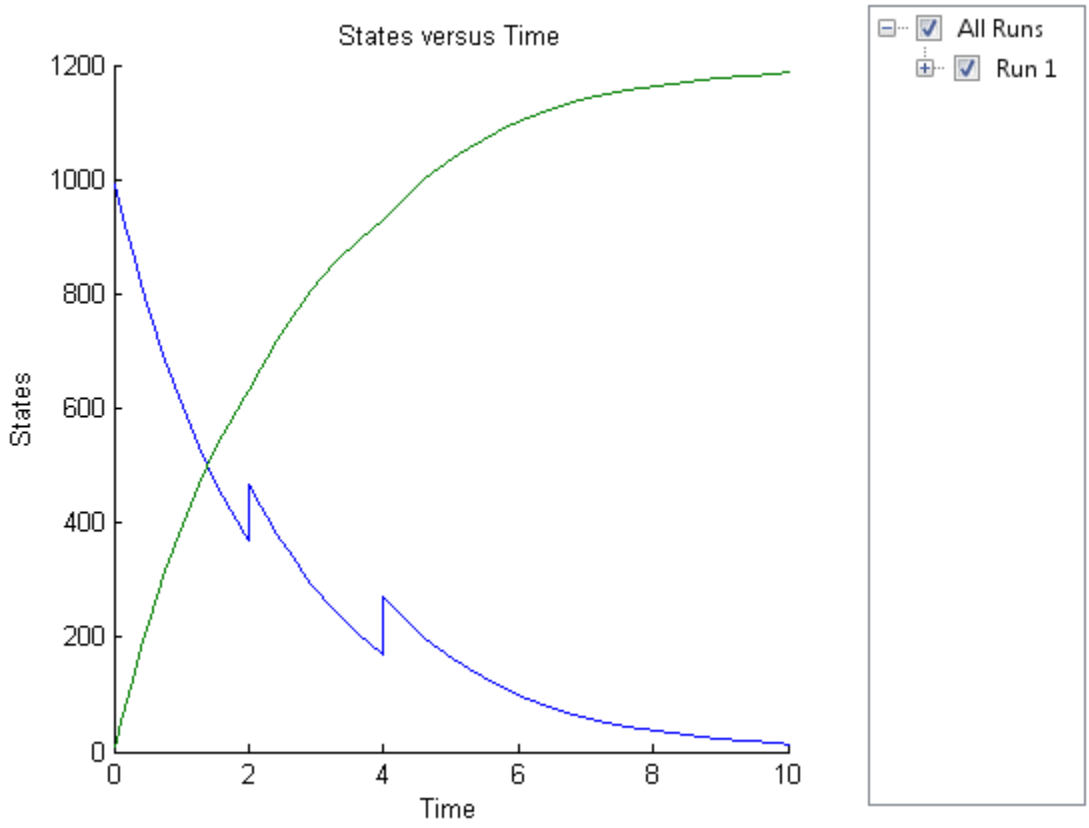

```
sbioplot(sim2)
```




```
sbioplot(sim3)
```




```
sbioplot(sim4)
```



Simulate a SimBiology Model Using Configset and Dose Objects

Load a sample SimBiology model.

```
sbioloadproject radiodecay.sbproj
```

Get the default configuration set from the model.

```
defaultConfigSet = getconfigset(m1,'default');
```

Add a scheduled dose of 100 molecules at 2 seconds for species `x`.

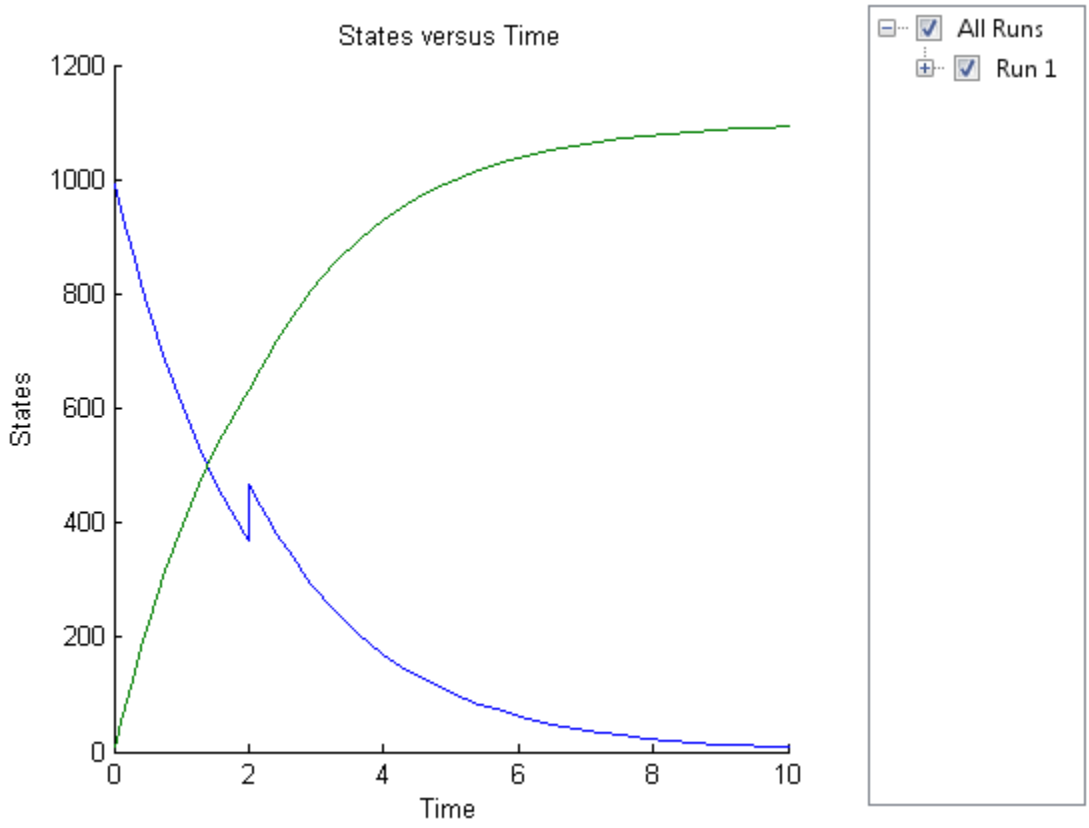
```
dObj = adddose(m1,'d1','schedule');
dObj.Amount = 100;
dObj.AmountUnits = 'molecule';
dObj.TimeUnits = 'second';
dObj.Time = 2;
dObj.TargetName = 'unnamed.x';
```

Simulate the model using configset and dose objects.

```
sim = sbiosimulate(m1,defaultConfigSet,dObj);
```

Plot the result.

```
sbioplot(sim);
```



Simulate a SimBiology Model Using Configset, Dose, and Variant Objects

Load a sample SimBiology model.

```
sbioloadproject radiodecay.sbproj
```

Add a new configuration set using a stop time of 15 seconds.

```
csObj = m1.addconfigset('newStopTimeConfigSet');
csObj.StopTime = 15;
```

Add a scheduled dose of 100 molecules at 2 seconds for species x.

```
dObj = adddose(m1,'d1','schedule');
dObj.Amount = 100;
dObj.AmountUnits = 'molecule';
dObj.TimeUnits = 'second';
dObj.Time = 2;
dObj.TargetName = 'unnamed.x';
```

Add a variant of species x using a different initial amount of 500 molecules.

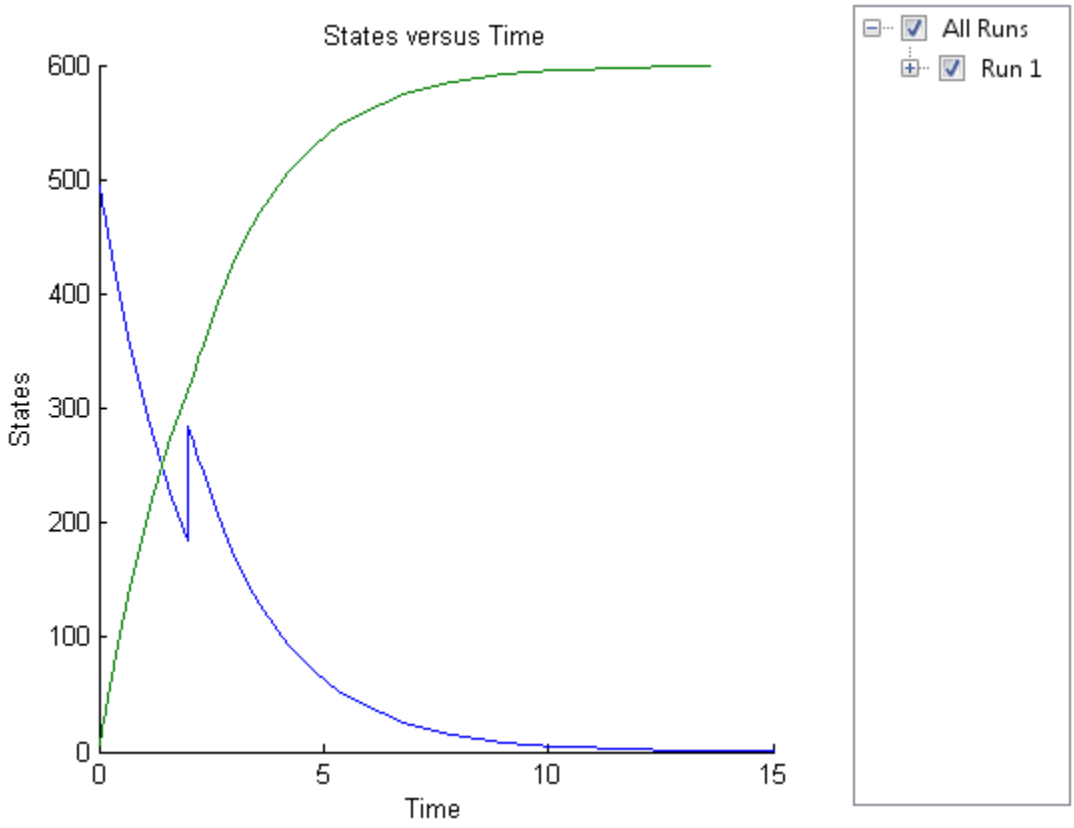
```
vObj = addvariant(m1,'v1');
addcontent(vObj,{'species','x','InitialAmount',500});
```

Simulate the model using the same configset, variant, and dose objects. Use the same order of input arguments as shown next.

```
sim = sbiosimulate(m1,csObj,vObj,dObj);
```

Plot the result.

```
sbioplot(sim);
```



Input Arguments

`modelObj` — SimBiology model

SimBiology model object

SimBiology model, specified as a SimBiology model object. The model minimally needs one reaction or rate rule for simulations.

`csObj` — Configuration set object

configset object | [ ]

Configuration set object, specified as a `configset object` that stores simulation-specific information. When you specify `csObj` as `[]`, `sbiosimulate` uses the currently active configset object.

If your model contains events, the `csObj` object cannot specify `'expltau'` or `'impltau'` for the `SolverType` property.

If your model contains doses, the `csObj` object cannot specify `'ssa'`, `'expltau'`, or `'impltau'` for the `SolverType` property.

`dvObj` — Dose or variant object
dose object or array of dose objects | variant object or array of variant objects | `[]`

Dose or variant object, specified as a `ScheduleDose object` , `RepeatDose object` , an array of dose objects, `Variant object` , or an array of variant objects.

- Use `[]` when you want to explicitly exclude any variant objects from the `sbiosimulate` function.
- When `dvObj` is a dose object, `sbiosimulate` uses the specified dose object as well as any active variant objects if available.
- When `dvObj` is a variant object, `sbiosimulate` uses the specified variant object as well as any active dose objects if available.

`variantObj` — Variant object
variant object or array of variant objects | `[]`

Variant object, specified as a `Variant object` or an array of variant objects. Use `[]` when you want to explicitly exclude any variant objects from `sbiosimulate`.

`doseObj` — Dose object
dose object or array of dose objects | `[]`

Dose object, specified as a `ScheduleDose object` , `RepeatDose object` , or an array of dose objects. A dose object defines additions that are made to species amounts or parameter values. Use `[]` when you want to explicitly exclude any dose objects from `sbiosimulate`.

Output Arguments

`time` — Vector of time samples
vector

Vector of time samples, returned as an `n-by-1` vector containing the simulation time steps. `n` is the number of time samples.

`x` — Simulation data
array

Simulation data, returned as an `n-by-m` data array, where `n` is the number of time samples and `m` is the number of states logged in the simulation. Each column of `x` describes the variation in the quantity of a species, compartment, or parameter over time.

`names` — Names of species, compartments, or parameters
cell array of character vectors

Names of species, compartments, or parameters, returned as an `m-by-1` cell array of character vectors. In other words, `names` contains the column labels of the simulation data, `x`. If the species are in multiple compartments, species names are qualified with the compartment name in the form `compartmentName.speciesName`.

`simDataObj` — Simulation data
SimData object

Simulation data, returned as a `SimData object` that holds time and state data as well as metadata, such as the types and names for the logged states or the configuration set used during simulation. You can access time, data, and names stored in a `SimData object` by using its properties.

Version History

Introduced before R2006a

See Also

`addconfigset` | `sbioaccelerate` | `sbiomodel` | `SimData object` | `Configset object` | `getconfigset` | `setactiveconfigset` | `Variant object` | `ScheduleDose object` | `RepeatDose object` | `Model object`

Topics

“Model Simulation”
“Derive ODEs from SimBiology Reactions”

sbiosobol

Perform global sensitivity analysis by computing first- and total-order Sobol indices (requires Statistics and Machine Learning Toolbox)

Syntax

```
sobolResults = sbiosobol(modelObj,params,observables)
sobolResults = sbiosobol(modelObj,scenarios,observables)
sobolResults = sbiosobol(modelObj,params,observables,Name,Value)
```

Description

`sobolResults = sbiosobol(modelObj,params,observables)` performs global sensitivity analysis [1] on a SimBiology model `modelObj` by decomposing the variances of `observables` with respect to the sensitivity inputs `params`.

`sobolResults = sbiosobol(modelObj,scenarios,observables)` uses samples from `scenarios`, a `SimBiology.Scenarios` object, to perform the analysis.

`sobolResults = sbiosobol(modelObj,params,observables,Name,Value)` uses additional options specified by one or more name-value pair arguments.

Examples

Perform Global Sensitivity Analysis by Computing First- and Total-Order Sobol Indices

Load the “Tumor Growth Model”.

```
sbioloadproject tumor_growth_vpop_sa.sbproj
```

Get a variant with the estimated parameters and the dose to apply to the model.

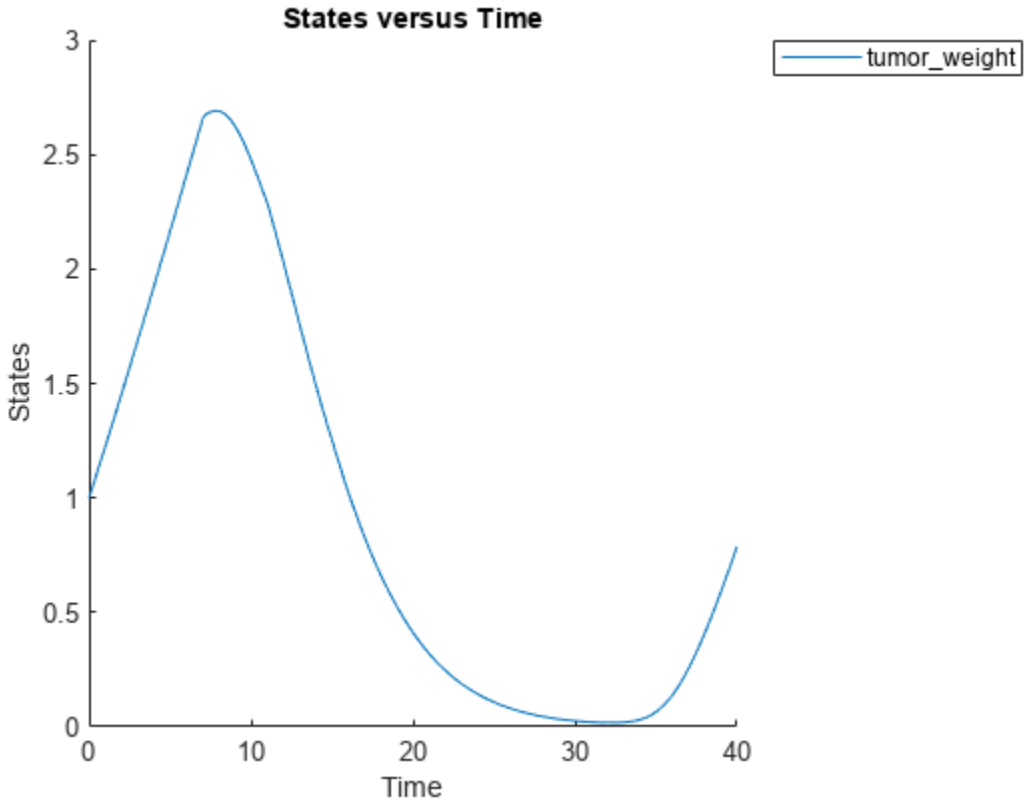
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

Get the active configset and set the tumor weight as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'tumor_weight';
```

Simulate the model and plot the tumor growth profile.

```
sbioplot(sbiosimulate(m1,cs,v,d));
```



Perform global sensitivity analysis (GSA) on the model to find the model parameters that the tumor growth is sensitive to.

First, retrieve model parameters of interest that are involved in the pharmacodynamics of the tumor growth. Define the model response as the tumor weight.

```
modelParamNames = {'L0','L1','w0','k1','k2'};
outputName = 'tumor_weight';
```

Then perform GSA by computing the first- and total-order Sobol indices using `sbiosobol`. Set `'ShowWaitBar'` to `true` to show the simulation progress. By default, the function uses 1000 parameter samples to compute the Sobol indices [1].

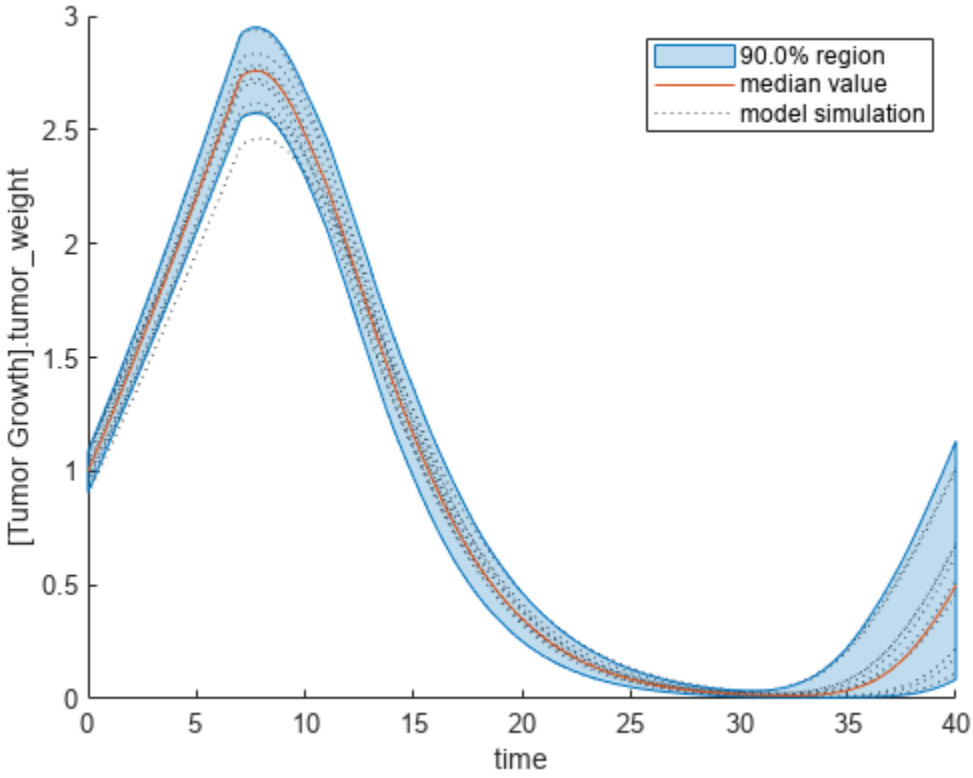
```
rng('default');
sobolResults = sbiosobol(m1,modelParamNames,outputName,Variants=v,Doses=d,ShowWaitBar=true)
```

```
sobolResults =
  Sobol with properties:

               Time: [444x1 double]
       SobolIndices: [5x1 struct]
           Variance: [444x1 table]
   ParameterSamples: [1000x5 table]
        Observables: {'[Tumor Growth].tumor_weight'}
     SimulationInfo: [1x1 struct]
```

You can change the number of samples by specifying the `'NumberSamples'` name-value pair argument. The function requires a total of `(number of input parameters + 2) * NumberSamples` model simulations.

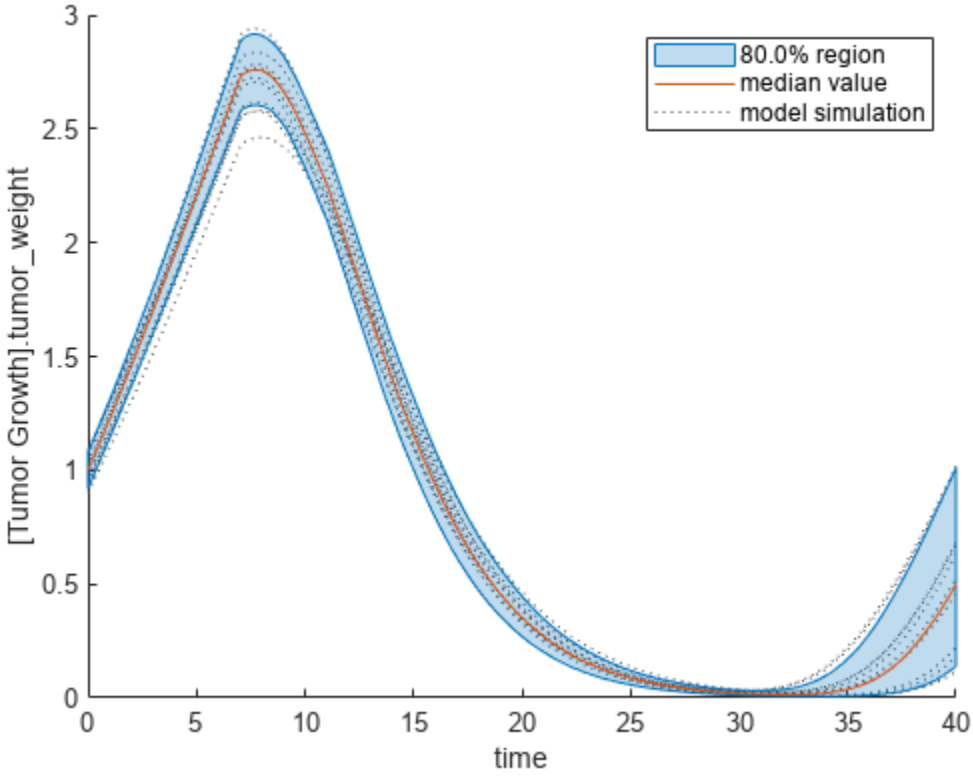
Show the mean model response, the simulation results, and a shaded region covering 90% of the simulation results.

```
plotData(sobolResults,ShowMedian=true,ShowMean=false);
```



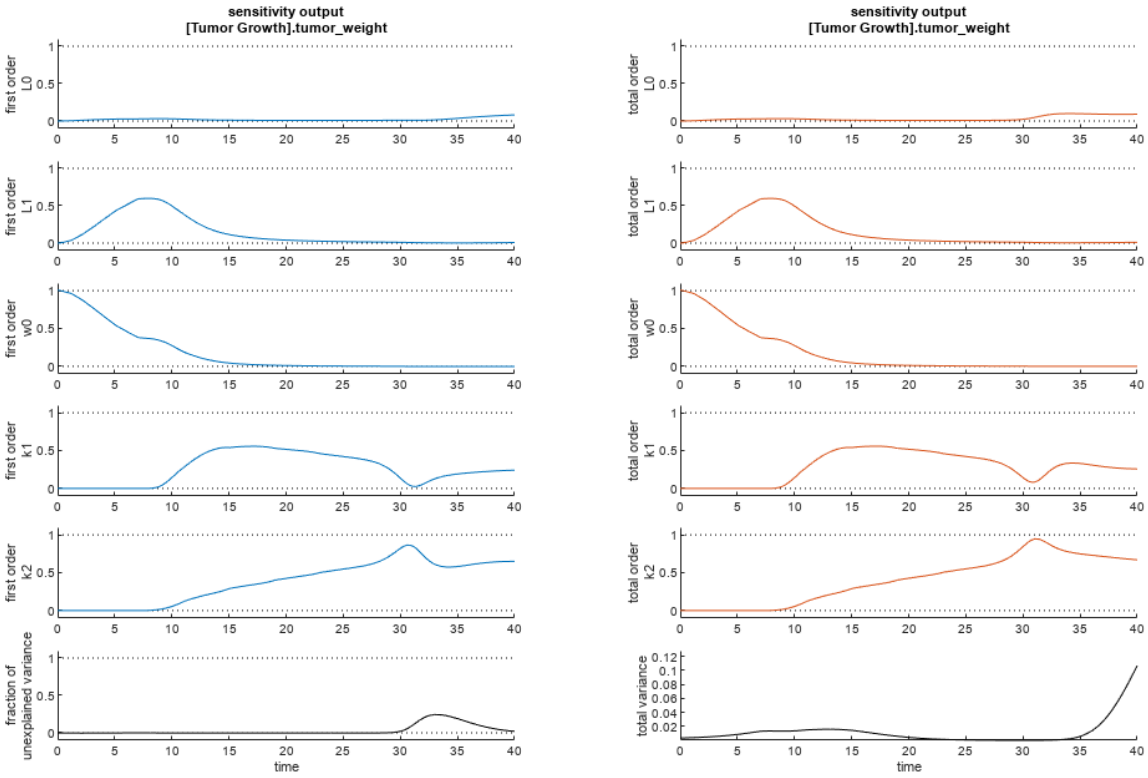
You can adjust the quantile region to a different percentage by specifying `'Alphas'` for the lower and upper quantiles of all model responses. For instance, an alpha value of 0.1 plots a shaded region between the `100 * alpha` and `100 * (1 - alpha)` quantiles of all simulated model responses.

```
plotData(sobolResults,Alphas=0.1,ShowMedian=true,ShowMean=false);
```



Plot the time course of the first- and total-order Sobol indices.

```
h = plot(sobolResults);
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```

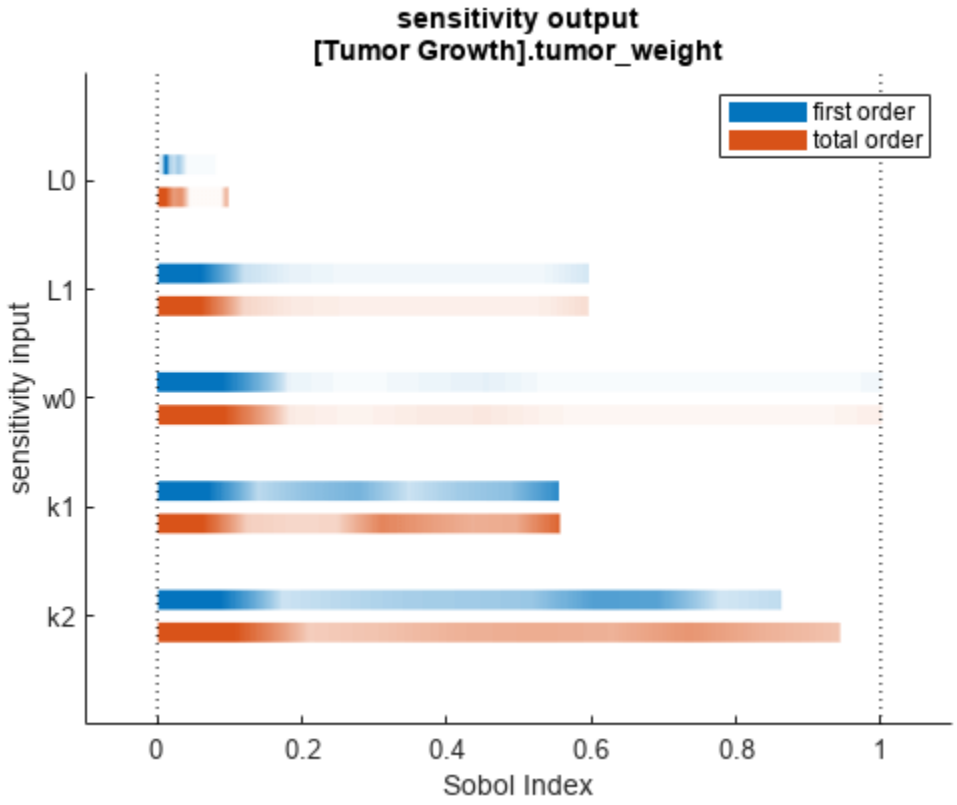


The first-order Sobol index of an input parameter gives the fraction of the overall response variance that can be attributed to variations in the input parameter alone. The total-order index gives the fraction of the overall response variance that can be attributed to any joint parameter variations that include variations of the input parameter.

From the Sobol indices plots, parameters `L1` and `w0` seem to be the most sensitive parameters to the tumor weight before the dose was applied at t = 7. But after the dose is applied, `k1` and `k2` become more sensitive parameters and contribute most to the after-dosing stage of the tumor weight. The total variance plot also shows a larger variance for the after-dose stage at t > 35 than for the before-dose stage of the tumor growth, indicating that `k1` and `k2` might be more important parameters to investigate further. The fraction of unexplained variance shows some variance at around t = 33, but the total variance plot shows little variance at t = 33, meaning the unexplained variance could be insignificant. The fraction of unexplained variance is calculated as 1 - (sum of all the first-order Sobol indices), and the total variance is calculated using `var(response)`, where `response` is the model response at every time point.

You can also display the magnitudes of the sensitivities in a bar plot. Darker colors mean that those values occur more often over the whole time course.

```
bar(sobolResults);
```



You can specify more samples to increase the accuracy of the Sobol indices, but the simulation can take longer to finish. Use `addsamples` to add more samples. For example, if you specify 1500 samples, the function performs `1500 * (2 + number of input parameters)` simulations.

```
gsaMoreSamples = addsamples(gsaResults,1500)
```

The "SimulationInfo" on page 2-0 property of the result object contains various information for computing the Sobol indices. For instance, the model simulation data (SimData) for each simulation using a set of parameter samples is stored in the `SimData` field of the property. This field is an array of `SimData` objects.

```
sobolResults.SimulationInfo.SimData
```

```
SimBiology SimData Array : 1000-by-7

Index:    Name:         ModelName:         DataCount:
1           -           Tumor Growth Model 1
2           -           Tumor Growth Model 1
3           -           Tumor Growth Model 1
...
7000        -           Tumor Growth Model 1
```

You can find out if any model simulation failed during the computation by checking the `ValidSample` field of `SimulationInfo`. In this example, the field shows no failed simulation runs.

```
all(sobolResults.SimulationInfo.ValidSample)
```

```
ans = 1x7 logical array

   1   1   1   1   1   1   1
```

`SimulationInfo.ValidSample` is a table of logical values. It has the same size as `SimulationInfo.SimData`. If `ValidSample` indicates that any simulations failed, you can get more information about those simulation runs and the samples used for those runs by extracting information from the corresponding column of `SimulationInfo.SimData`. Suppose that the fourth column contains one or more failed simulation runs. Get the simulation data and sample values used for that simulation using `getSimulationResults`.

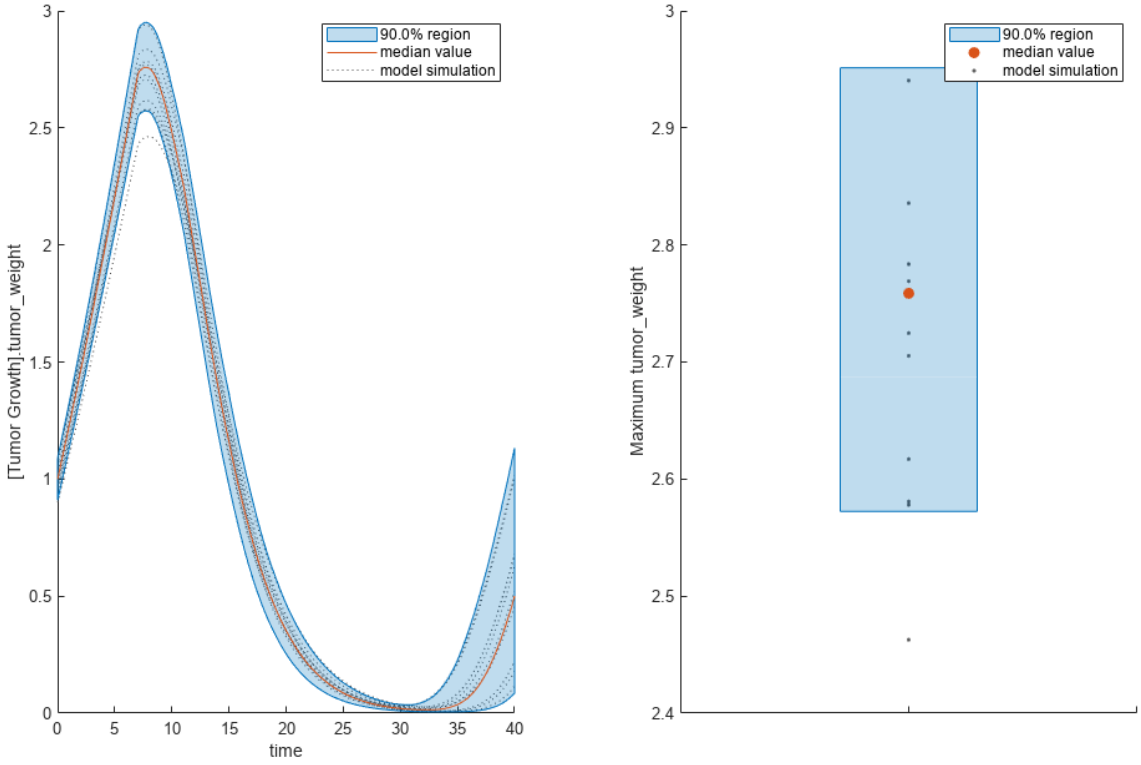
```
[samplesUsed,sd,validruns] = getSimulationResults(sobolResults,4);
```

You can add custom expressions as observables and compute Sobol indices for the added observables. For example, you can compute the Sobol indices for the maximum tumor weight by defining a custom expression as follows.

```
% Suppress an information warning that is issued during simulation.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
% Add the observable expression.
sobolObs = addobservable(sobolResults,'Maximum tumor_weight','max(tumor_weight)','Units','gram');
```

Plot the computed simulation results showing the 90% quantile region.

```
h2 = plotData(sobolObs,ShowMedian=true,ShowMean=false);
h2.Position(:) = [100 100 1280 800];
```



You can also remove the observable by specifying its name.

```
gsaNoObs = removeobservable(sobolObs,'Maximum tumor_weight');
```

Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

`modelObj` — SimBiology model

SimBiology model object

SimBiology model, specified as a SimBiology `model object`.

`params` — Names of model parameters, species, or compartments

character vector | string | string vector | cell array of character vectors

Names of model parameters, species, or compartments, specified as a character vector, string, string vector, or cell array of character vectors.

Example: `["k1","k2"]`

Data Types: `char` | `string` | `cell`

`observables` — Model responses

character vector | string | string vector | cell array of character vectors

Model responses, specified as a character vector, string, string vector, or cell array of character vectors. Specify the names of species, parameters, compartments, or `observables`.

Example: `["tumor_growth"]`

Data Types: `char` | `string` | `cell`

`scenarios` — Source for drawing samples

`SimBiology.Scenarios` object

Source for drawing samples, specified as a `SimBiology.Scenarios` object.

- You must combine entries of the object elementwise.
- Entries must be independent random variables. If there are multiple entries, they must be uncorrelated.
- `SamplingMethod` of any entry must not be `copula`.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `sobolResults = sbiosobol(modelObj,params,observables,'ShowWaitbar',true)` specifies to show a simulation progress bar.

Bounds — Parameter bounds
numeric matrix

Parameter bounds, specified as a numeric matrix with two columns. The first column contains the lower bounds and the second column contains the upper bounds. The number of rows must be equal to the number of parameters in `params`.

If a parameter has a nonzero value, the default bounds are ±10% of the value. If the parameter value is zero, the default bounds are `[0 1]`.

Example: `[0.5 5]`

Data Types: `double`

Doses — Doses to use during simulations
`ScheduleDose` object | `RepeatDose` object | vector of dose objects

Doses to use during model simulations, specified as a `ScheduleDose` or `RepeatDose` object or a vector of dose objects.

Variants — Variants to apply before simulations
variant object | vector of variant objects

Variants to apply before model simulations, specified as a variant object or vector of variant objects.

When you specify multiple variants with duplicate specifications for a property's value, the last occurrence for the property value in the array of variants is used during simulation.

NumberSamples — Number of samples to compute Sobol indices
`1000` (default) | positive integer

Number of samples to compute Sobol indices, specified as the comma-separated pair consisting of `'NumberSamples'` and a positive integer. The function requires `(number of input params + 2) * NumberSamples` model simulations to compute the first- and total-order Sobol indices.

Data Types: `double`

Distributions — Probability distributions
`prob.UniformDistribution` (default) | `prob.ProbabilityDistribution` object | vector of `prob.ProbabilityDistribution` objects

Probability distributions used to draw samples, specified as a `prob.ProbabilityDistribution` object or vector of these objects. Specify a scalar `prob.ProbabilityDistribution` or vector of length *N*, where *N* is the number of input parameters. You can create distribution objects to sample from various distributions, such as uniform, normal, or lognormal distributions, using `makedist`.

If you specify a scalar `prob.ProbabilityDistribution` object, and there are multiple input parameters, `sbiosobol` uses the same distribution object to draw samples for each parameter.

You cannot specify this argument together with “Bounds” on page 1-0 .

You cannot specify this argument when a `SimBiology.Scenarios` object is an input.

SamplingMethod — Method to generate parameter samples
`'Sobol'` (default) | character vector | string

Method to generate parameter samples, specified as a character vector or string. Valid options are:

- `'Sobol'` — Use the low-discrepancy Sobol sequence to generate samples.
- `'Halton'` — Use the low-discrepancy Halton sequence to generate samples.
- `'lhs'` — Use the low-discrepancy Latin hypercube samples.
- `'random'` — Use uniformly distributed random samples.

Data Types: `char` | `string`

`SamplingOptions` — Options for sampling method
struct

Options for the sampling method, specified as a scalar struct. The options differ depending on the sampling method: `sobol`, `halton`, or `lhs`.

For `sobol` and `halton`, specify each field name and value of the structure according to each name-value argument of the `sobolset` or `haltonset` function. SimBiology uses the default value of `1` for the `Skip` argument for both methods. For all other name-value arguments, the software uses the same default values of `sobolset` or `haltonset`. For instance, set up a structure for the `Leap` and `Skip` options with nondefault values as follows.

```
s1.Leap = 50;
s1.Skip = 0;
```

For `lhs`, there are three samplers that support different sampling options.

- If you specify a covariance matrix, SimBiology uses `lhsnorm` for sampling. `SamplingOptions` argument is not allowed.
- Otherwise, use the field name `UseLhsdesign` to select a sampler.
  - If the value is `true`, SimBiology uses `lhsdesign`. You can use the name-value arguments of `lhsdesign` to specify the field names and values.
  - If the value is `false` (default), SimBiology uses a nonconfigurable Latin hypercube sampler that is different from `lhsdesign`. This sampler does not require Statistics and Machine Learning Toolbox. `SamplingOptions` cannot contain any other options, except `UseLhsdesign`.

For instance, set up a structure to use `lhsdesign` with the `Criterion` and `Iterations` options.

```
s2.UseLhsdesign  = true;
s2.Criterion     = "correlation";
s2.Iterations    = 10;
```

You cannot specify this argument when a `SimBiology.Scenarios` object is an input.

`StopTime` — Simulation stop time
nonnegative scalar

Simulation stop time, specified as a nonnegative scalar. If you specify neither `StopTime` nor `OutputTimes`, the function uses the stop time from the active configuration set of the model. You cannot specify both `StopTime` and `OutputTimes`.

Data Types: `double`

`OutputTimes` — Simulation output times
numeric vector

Simulation output times, specified as the comma-separated pair consisting of `'OutputTimes'` and a numeric vector. The function computes the Sobol indices at these output time points. You cannot specify both `StopTime` and `OutputTimes`. By default, the function uses the output times of the first model simulation.

Example: `[0 1 2 3.5 4 5 5.5]`

Data Types: `double`

`UseParallel` — Flag to run model simulations in parallel
`false` (default) | `true`

Flag to run model simulations in parallel, specified as `true` or `false`. When the value is `true` and Parallel Computing Toolbox is available, the function runs simulations in parallel.

Data Types: `logical`

`Accelerate` — Flag to turn on model acceleration
`true` (default) | `false`

Flag to turn on model acceleration, specified as `true` or `false`.

Data Types: `logical`

`InterpolationMethod` — Method for interpolation of model simulations
`"interp1q"` (default) | character vector | string

Method for interpolation of model responses to a common set of output times, specified as a character vector or string. The valid options follow.

- `"interp1q"` — Use the `interp1q` function.
- Use the `interp1` function by specifying one of the following methods:
  - `"nearest"`
  - `"linear"`
  - `"spline"`
  - `"pchip"`
  - `"v5cubic"`
- `"zoh"` — Specify zero-order hold.

Data Types: `char` | `string`

`ShowWaitbar` — Flag to show progress of model simulations
`false` (default) | `true`

Flag to show the progress of model simulations by displaying a progress bar, specified as the comma-separated pair consisting of `'ShowWaitbar'` and `true` or `false`. By default, no wait bar is displayed.

Data Types: `logical`

Output Arguments

`sobolResults` — Results containing Sobol indices
`SimBiology.gsa.Sobol` object

Results containing the first- and total-order Sobol indices, returned as a `SimBiology.gsa.Sobol` object. The object also contains the parameter sample values and model simulation data used to compute the Sobol indices.

The results object can contain a significant amount of simulation data (SimData). The size of the object exceeds `(1 + number of observables) * number of output time points * (2 + number of parameters) * number of samples * 8` bytes. For example, if you have one observable, 500 output time points, 8 parameters, and 100,000 samples, the object size is `(1 + 1) * 500 * (2 + 8) * 100000 * 8` bytes = 8 GB. If you need to save such large objects, use this syntax:

```
save(fileName,variableName,'-v7.3');
```

For details, see MAT-file version.

More About

Saltelli Method to Compute Sobol Indices

`sbiosobol` implements the Saltelli method [1] to compute Sobol indices.

Consider a SimBiology model response Y expressed as a mathematical model $Y = f(X_1, X_2, X_3, ..., X_k)$, where X_i is a model parameter and `i = 1,…,k`.

The first-order Sobol index (S_i) gives the fraction of the overall response variance `V(Y)` that can be attributed to variations in X_i alone. S_i is defined as follows.

$$S_i = \frac{V_{X_i}\left(E_{X\sim i}(Y|X_i)\right)}{V(Y)}$$

The total-order Sobol index (S_{Ti}) gives the fraction of the overall response variance `V(Y)` that can be attributed to any joint parameter variations that include variations of X_i. S_{Ti} is defined as follows.

$$S_{Ti} = 1 - \frac{V_{X\sim i}\left(E_{X_i}(Y|X\sim i)\right)}{V(Y)} = \frac{E_{X\sim i}\left(V_{X_i}(Y|X\sim i)\right)}{V(Y)}$$

To compute individual values for Y corresponding to samples of parameters X_1, X_1, ..., X_k, consider two independent sampling matrices A and B.

$$A = \begin{pmatrix} X_{11} & X_{12} & \dots & X_{1k} \\ X_{21} & X_{22} & \dots & X_{2k} \\ \dots & \dots & \dots & \dots \\ X_{n1} & X_{n2} & \dots & X_{nk} \end{pmatrix}$$

$$B = \begin{pmatrix} X'_{11} & X'_{12} & \dots & X'_{1k} \\ X'_{21} & X'_{22} & \dots & X'_{2k} \\ \dots & \dots & \dots & \dots \\ X'_{n1} & X'_{n2} & \dots & X'_{nk} \end{pmatrix}$$

n is the sample size. Each row of the matrices A and B corresponds to one parameter sample set, which is a single realization of model parameter values.

Estimates for S_i and S_{Ti} are obtained from model simulation results using sample values from the matrices A, B, and A_B^i, which is a matrix where all columns are from A except the ith column, which is from B for `i = 1, 2, …, params`.

$$A_B^i = \begin{pmatrix} X_{11} & X_{12} & \dots & X'_{1i} & \dots & X_{1k} \\ X_{21} & X_{22} & \dots & X'_{2i} & \dots & X_{2k} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ X_{n1} & X_{n2} & \dots & X'_{ni} & \dots & X_{nk} \end{pmatrix}$$

The formulas to approximate the first- and total-order Sobol indices are as follows.

$$\widehat{S}_i = \frac{\frac{1}{n}\sum_{j=1}^{n} f(B)_j \left(f\left(A_B^i\right)_j - f(A)_j \right)}{V(Y)}$$

$$\widehat{S}_{Ti} = \frac{\frac{1}{2n}\sum_{j=1}^{n} \left(f(A)_j - f\left(A_B^i\right)_j \right)^2}{V(Y)}$$

`f(A)`, `f(B)`, and $f\left(A_B^i\right)_j$ are the model simulation results using the parameter sample values from matrices A, B, and A_B^i.

The matrix A corresponds to the `ParameterSamples` property of the Sobol results object (`resultsObj.ParameterSamples`). The matrix B corresponds to the `SupportSamples` property (`resultsObj.SimulationInfo.SupportSamples`).

The A_B^i matrices are stored in the `SimData` structure of the `SimulationInfo` on page 2-0 property (`resultsObj.SimulationInfo.SimData`). The size of `SimulationInfo.SimData` is *`NumberSamples`*`-by-`*`params`*` + 2`, where *NumberSamples* on page 1-0 is the number of samples and *param on page 1-0* is the number of input parameters. The number of columns is `2 + `*`params`* because the first column of `SimulationInfo.SimData` contains the model simulation results using the sample matrix A. The second column contains simulation results using `SupportSamples`, which is another sample matrix B. The rest of the columns contain simulation results using A_B^1, A_B^2, …, A_B^i, …, A_B^{params}. See `getSimulationResults` to retrieve the model simulation results and samples for a specified ith index (A_B^i) from the `SimulationInfo.SimData` array.

Version History

Introduced in R2020a

References

[1] Saltelli, Andrea, Paola Annoni, Ivano Azzini, Francesca Campolongo, Marco Ratto, and Stefano Tarantola. “Variance Based Sensitivity Analysis of Model Output. Design and Estimator for the

Total Sensitivity Index." *Computer Physics Communications* 181, no. 2 (February 2010): 259–70. https://doi.org/10.1016/j.cpc.2009.09.018.

See Also

`SimBiology.gsa.Sobol` | `sbiompgsa` | `sbioelementaryeffects` | `Observable`

Topics

"Sensitivity Analysis in SimBiology"

sbiosteadystate

Find steady state of SimBiology model

Syntax

```
[success, variant_out] = sbiosteadystate(model)
[success, variant_out] = sbiosteadystate(model, variant_in)
[success, variant_out] = sbiosteadystate(model, variant_in, scheduleDose)
[success, variant_out, model_out] = sbiosteadystate(model, ___ )
[success, variant_out, model_out, exitInfo] = sbiosteadystate(model, ___ )
[ ___ ] = sbiosteadystate( ___ , Name,Value)
```

Description

`[success, variant_out] = sbiosteadystate(model)` attempts to find a steady state of a SimBiology model, `model`. The function returns `success`, which is `true` if a steady state was found, and a SimBiology `Variant object`, `variant_out`, with all nonconstant species, compartments, and parameters of the model having the steady-state values. If a steady state was not found, then the `success` is `false` and `variant_out` contains the last values found by the algorithm.

`[success, variant_out] = sbiosteadystate(model, variant_in)` applies the alternate quantity values stored in a variant object or vector of objects, `variant_in`, to the model before trying to find the steady-state values.

`[success, variant_out] = sbiosteadystate(model, variant_in, scheduleDose)` also applies a `ScheduleDose` on page 2-802 object or vector of schedule doses `scheduleDose` to the corresponding model quantities before trying to find the steady state values. Only doses at time = 0 are allowed, that is, the dose time of each dose object must be 0. To specify a dose without specifying a variant, set `variant_in` to an empty array, `[]`.

`[success, variant_out, model_out] = sbiosteadystate(model, ___ )` also returns a SimBiology model, `model_out` that is a copy of the input `model` with the states set to the steady-state solution that was found. Also, `model_out` has all initial assignment rules disabled.

`[success, variant_out, model_out, exitInfo] = sbiosteadystate(model, ___ )` also returns the exit information about the steady state computation.

`[ ___ ] = sbiosteadystate( ___ , Name,Value)` uses additional options specified by one or more `Name,Value` pair arguments.

Examples

Find a Steady State of a Simple Gene Regulation Model

This example shows how to find a steady state of a simple gene regulation model, where the protein product from translation controls transcription.

Load the sample SimBiology project containing the model, m1. The model has five reactions and four species.

```
sbioloadproject('gene_reg.sbproj','m1')
```

Display the model reactions.

```
m1.Reactions
```

```
ans =
   SimBiology Reaction Array

   Index:    Reaction:
   1         DNA -> DNA + mRNA
   2         mRNA -> mRNA + protein
   3         DNA + protein <-> DNA_protein
   4         mRNA -> null
   5         protein -> null
```

A steady state calculation attempts to find the steady state values of non-constant quantities. To find out which model quantities are non-constant in this model, use `sbioselect`.

```
sbioselect(m1,'Where','Constant*','==',false)
```

```
ans =
   SimBiology Species Array

   Index:    Compartment:    Name:          Value:    Units:
   1         unnamed         DNA            50        molecule
   2         unnamed         DNA_protein    0         molecule
   3         unnamed         mRNA           0         molecule
   4         unnamed         protein        0         molecule
```

There are four species that are not constant, and the initial amounts of three of them are set to zero.

Use `sbiosteadystate` to find the steady state values for those non-constant species.

```
[success,variantOut] = sbiosteadystate(m1)
```

```
success = logical
   1


variantOut =
   SimBiology Variant - SteadyState (inactive)

   ContentIndex:     Type:        Name:             Property:          Value:
   1                 compartment  unnamed           Capacity           1.0
   2                 species      DNA               InitialAmount      8.7902390...
   3                 species      DNA_protein       InitialAmount      41.209760...
   4                 species      mRNA              InitialAmount      1.1720318...
   5                 species      protein           InitialAmount      23.440637...
   6                 parameter    Transcription.k1  Value              .2
   7                 parameter    Translation.k2    Value              20.0
   8                 parameter    [Binding/Unbin... Value              .2
   9                 parameter    [Binding/Unbin... Value              1.0
   10                parameter    [mRNA Degradat... Value              1.5
   11                parameter    [Protein Degra... Value              1.0
```

The initial amounts of all species of the model have been set to the steady-state values. `DNA` is a conserved species since the total of `DNA` and `DNA_protein` is equal to 50.

You can also use a variant to store alternate initial amounts and use them during the steady state calculation. For instance, you could set the initial amount of DNA to 100 molecules instead of 50.

```
variantIn = sbiovariant('v1');
addcontent(variantIn,{'species','DNA','InitialAmount',100});
[success2,variantOut2,m2] = sbiosteadystate(m1,variantIn)
```

```
success2 = logical
   1


variantOut2 =
   SimBiology Variant - SteadyState (inactive)

   ContentIndex:     Type:        Name:             Property:          Value:
   1                 compartment  unnamed           Capacity           1.0
   2                 species      DNA               InitialAmount      12.787619...
   3                 species      DNA_protein       InitialAmount      87.212380...
   4                 species      mRNA              InitialAmount      1.7050159...
   5                 species      protein           InitialAmount      34.100318...
   6                 parameter    Transcription.k1  Value              .2
   7                 parameter    Translation.k2    Value              20.0
   8                 parameter    [Binding/Unbin... Value              .2
   9                 parameter    [Binding/Unbin... Value              1.0
   10                parameter    [mRNA Degradat... Value              1.5
   11                parameter    [Protein Degra... Value              1.0


m2 =
   SimBiology Model - cell

   Model Components:
     Compartments:      1
     Events:            0
     Parameters:        6
     Reactions:         5
     Rules:             0
     Species:           4
     Observables:       0
```

Since the algorithm has found a steady state, the third output `m2` is the steady state model, where the values of non-constant quantities have been set to steady state values. In this example, the initial amounts of all four species have been updated to steady state values.

```
m2.Species
```

```
ans =
   SimBiology Species Array

   Index:    Compartment:    Name:          Value:     Units:
   1         unnamed         DNA            12.7876    molecule
   2         unnamed         DNA_protein    87.2124    molecule
   3         unnamed         mRNA           1.70502    molecule
   4         unnamed         protein        34.1003    molecule
```

Input Arguments

`model` — SimBiology model

SimBiology model object

SimBiology model, specified as a SimBiology `Model object`.

`variant_in` — SimBiology variant

`[]` | variant object | vector of variant objects

SimBiology variant, specified as an empty array `[]`, a `Variant object` or vector of variant objects. The alternate quantity values stored in the variants are applied to the model before finding the steady state. If there are duplicate specifications for a property value, the last occurrence for the property value in the array of variants is used.

`scheduleDose` — Dosing information

`[]` | `ScheduleDose` object | vector of `ScheduleDose` objects

Dosing information, specified as an empty array `[]`, a `ScheduleDose` on page 2-802 object or vector of `ScheduleDose` objects. The dose must be bolus, that is, there must be no time lag or administration time for the dose. In other words, its `LagParameterName` and `DurationParameterName` properties must be empty, and the dose time (the `Time` property) must be 0. For details on how to create a bolus dose, see “Creating Doses Programmatically”.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `'AbsTol',1e-6` specifies to use the absolute tolerance value of 10^{-6}.

`Method` — Method to compute steady state

`'auto'` (default) | `'simulation'` | `'algebraic'`

Method to compute the steady state of `model`, specified as the comma-separated pair consisting of `'Method'` and a character vector `'auto'`, `'simulation'`, or `'algebraic'`. The default (`'auto'`) behavior is to use the `'algebraic'` method first. If that method is unsuccessful, the function uses the `'simulation'` method.

For the simulation method, the function simulates the model and uses finite differencing to detect a steady state. For details, see “Simulation Method” on page 1-287.

For the algebraic method, the function computes a steady state by finding a root of the flux function algebraically. For nonlinear models, this method requires Optimization Toolbox. For details, see “Algebraic Method” on page 1-287.

Note The steady state returned by the algebraic method is not guaranteed to be the same as the one found by the simulation method. The algebraic method is faster since it involves no simulation, but the simulation method might be able to find a steady state when the algebraic method could not.

Example: `'Method','algebraic'`

`AbsTol` — Absolute tolerance to detect convergence
`1e-8` (default) | positive, real scalar

Absolute tolerance to detect convergence, specified as the comma-separated pair consisting of `'AbsTol'` and a positive, real scalar.

When you use the algebraic method, the absolute tolerance is used to specify optimization settings and detect convergence. For details, see “Algebraic Method” on page 1-287.

When you use the simulation method, the absolute tolerance is used to determine convergence when finding a steady state solution by forward integration as follows: $\left(\left\|\frac{d\vec{S}}{dt}\right\| < AbsTol\right) or \left(\left\|\frac{d\vec{S}}{dt}\right\| < RelTol * \left\|\vec{S}\right\|\right)$, where $\vec{S}$ is a vector of nonconstant species, parameters, and compartments.

`RelTol` — Relative tolerance to detect convergence
`1e-6` (default) | positive, real scalar

Relative tolerance to detect convergence, specified as the comma-separated pair consisting of `'RelTol'` and a positive, real scalar. This name-value pair argument is used for the `simulation` method only. The algorithm converges and reports a steady state if the algorithm finds model states by forward integration, such that $\left(\left\|\frac{d\vec{S}}{dt}\right\| < AbsTol\right) or \left(\left\|\frac{d\vec{S}}{dt}\right\| < RelTol * \left\|\vec{S}\right\|\right)$, where $\vec{S}$ is a vector of non-constant species, parameters, and compartments.

`MaxStopTime` — Maximum amount of simulation time to take before terminating without a steady state
`100000` (default) | positive integer

Maximum amount of simulation time to take before terminating without a steady state, specified as the comma-separated pair consisting of `'MaxStopTime'` and a positive integer. This name-value pair argument is used for the `simulation` method only.

`MinStopTime` — Minimum amount of simulation time to take before searching for a steady state
`1` (default) | positive integer

Minimum amount of simulation time to take before searching for a steady state, specified as the comma-separated pair consisting of `'MinStopTime'` and a positive integer. This name-value pair argument is used for the `simulation` method only.

Output Arguments

`success` — Flag to indicate if a steady state of the model is found
`true` | `false`

Flag to indicate if a steady state of the model is found, returned as `true` or `false`.

`variant_out` — SimBiology variant
variant object

SimBiology variant, returned as a variant object. The variant includes all species, parameters, and compartments of the model with the non-constant quantities having the steady-state values.

`model_out` — SimBiology model at the steady state
model object

SimBiology model at the steady state, returned as a model object. `model_out` is a copy of the input `model`, with the non-constant species, parameters, and compartments set to the steady-state values. Also, `model_out` has all initial assignment rules disabled. Simulating the model at steady state requires that initial assignment rules be inactive, since these rules can modify the values in `variant_out`.

Note

- If you decide to commit the `variant_out` to the input `model` that has initial assignment rules, then `model` is not expected to be at the steady state because the rules perturb the system when you simulate the `model`.
- `model_out` is at steady state only if simulated without any doses.

`exitInfo` — Exit information about steady state computation
character vector

Exit information about the steady state computation, returned as a character vector. The information contains different messages for corresponding exit conditions.

- `Steady state found (simulation)` – A steady state is found using the simulation method.
- `Steady state found (algebraic)` – A steady state is found using the algebraic method.
- `Steady state found (unstable)` – An unstable steady state is found using the algebraic method.
- `Steady state found (possibly underdetermined)` – A steady state that is, possibly, not asymptotically stable is found using the algebraic method.
- `No Steady state found` – No steady state is found.
- `Optimization Toolbox (TM) is missing` – The method is set to `'algebraic'` for nonlinear models and Optimization Toolbox is missing.

More About

Simulation Method

`sbiosteadystate` simulates the model until `MaxStopTime` on page 1-0 . During the simulation, the function approximates the gradient using finite differencing (forward difference) over time to detect a steady state.

Algebraic Method

`sbiosteadystate` tries to find a steady state of the model algebraically by finding a root of the flux function v. The flux function includes reaction equations, rate rules, and algebraic equations, that is, `v(X,P) = 0`, where X and P are nonconstant quantities and parameters of the model. Thereby the mass conservation imposed by the reaction equations is respected.

For nonlinear models, `sbiosteadystate` uses `fmincon` to get an initial guess for the root. The solution found by `fmincon` is then improved by `fsolve`. To detect convergence, `sbiosteadystate` uses the absolute tolerance (`'AbsTol'`). In other words, `OptimalityTolerance`, `FunctionTolerance`, and `StepTolerance` options of the corresponding optimization function are set to the `'AbsTol'` value.

For linear models, `sbiosteadystate` finds the roots of the flux function *v* by solving a linear system defined by the reaction and conservation equations. For linear models, there are no rate or algebraic equations.

Version History

Introduced in R2016a

See Also

`sbiosimulate` | `sbiovariant` | `sbiomodel` | `sbioaccelerate` | `Model object` | `ScheduleDose object` | `Variant object` | `commit`

sbiosubplot

Plot simulation results in subplots

Syntax

```
sbiosubplot(sd)
sbiosubplot(sd,fcnHandle,xArgs,yArgs)
sbiosubplot(sd,fcnHandle,xArgs,yArgs,showLegend)
sbiosubplot(sd,fcnHandle,xArgs,yArgs,showLegend,Name,Value)
```

Description

`sbiosubplot(sd)` plots each simulation run from `sd`, a `SimData` object or array of objects, into its own subplot. The subplot is a time plot of each state in `sd`.

`sbiosubplot(sd,fcnHandle,xArgs,yArgs)` plots simulation results by calling the function handle `fcnHandle` with inputs `sd`, `xArgs`, and `yArgs`. The inputs `xArgs` and `yArgs` must be cell arrays of the names of the states to plot.

`sbiosubplot(sd,fcnHandle,xArgs,yArgs,showLegend)` also specifies whether to show the legend in the plot. If `true`, the function shows `yArgs` as the legend.

`sbiosubplot(sd,fcnHandle,xArgs,yArgs,showLegend,Name,Value)` also uses additional options specified by one or more name-value pair arguments. For example, you can specify the x-label and y-label of the plot.

Examples

Plot Selected States from Simulation Data in Subplots

Plot the prey versus predator data from the stochastically simulated lotka model in separate subplots by using a custom function (`plotXY`).

Load the model. Set the solver type to SSA to perform stochastic simulations, and set the stop time to 3.

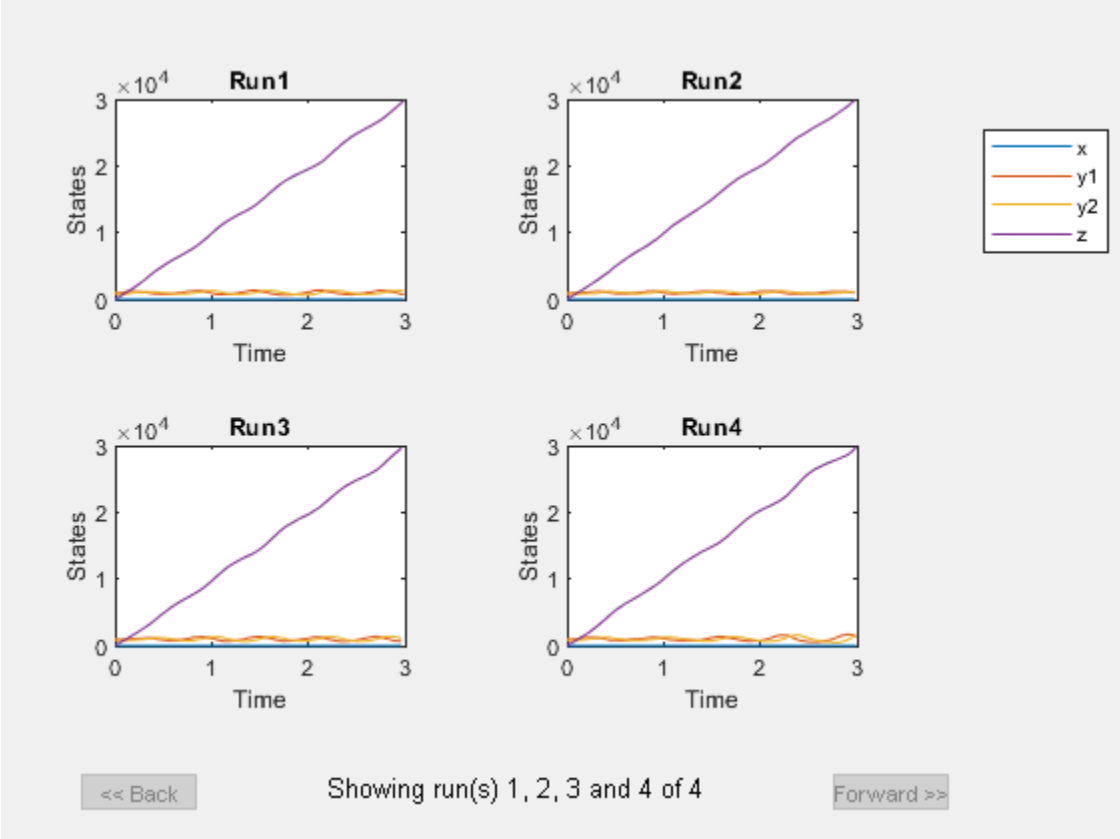
```
sbioloadproject lotka;
cs              = getconfigset(m1);
cs.SolverType   = 'SSA';
cs.StopTime     = 3;
rng('default') % For reproducibility
```

Set the number of runs and use `sbioensemblerun` for simulation.

```
numRuns = 4;
sd      = sbioensemblerun(m1,numRuns);
```

Plot each simulation run in a separate subplot. By default, `sbiosubplot` shows the time plot of each species for each run per subplot.

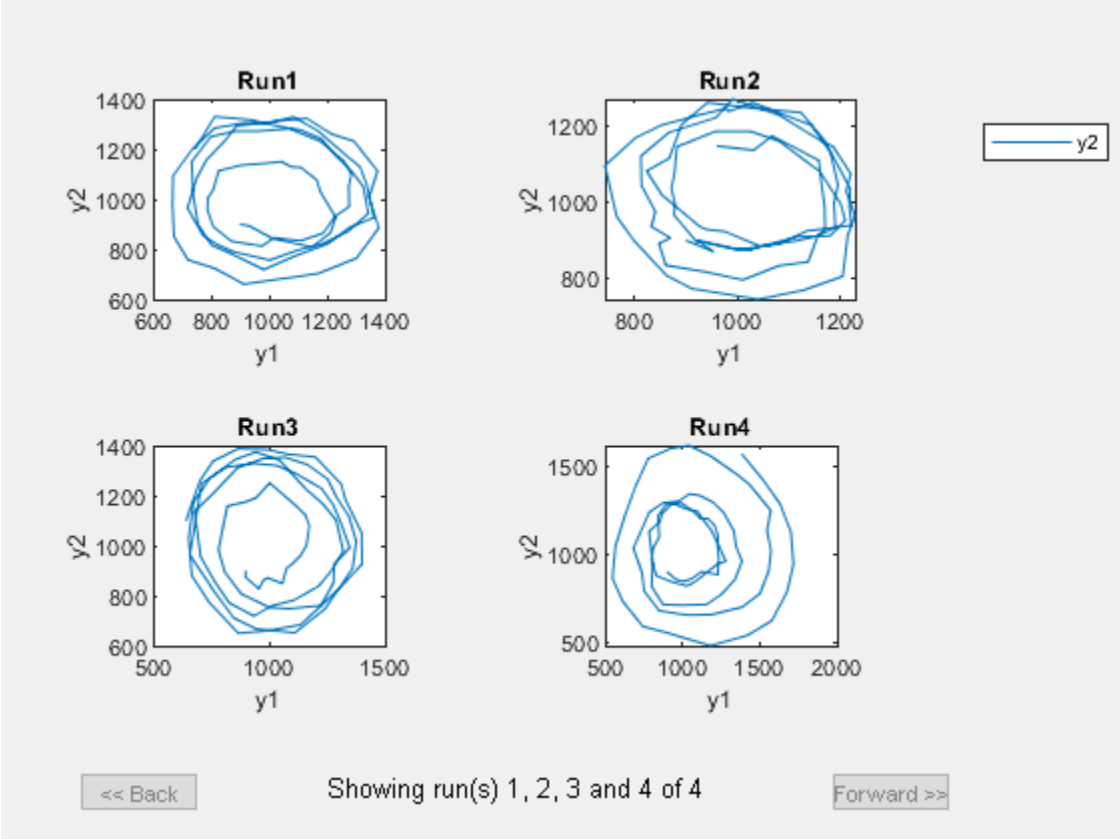
```
sbiosubplot(sd);
```



Plot selected states against each other; in this case, plot the prey population versus the predator population in separate subplots for each run. Use the function `plotXY` (shown at the end of this example) to plot the simulated y1 (prey) data versus the y2 (predator). Specify the function as a function handle in the `sbiosubplot` call to plot each run in its own subplot. In this case, the fifth input argument (`showLegend`) is set to `true`, which means the fourth input argument (`yArgs`) is shown as the legend.

If you use the live script file for this example, the `plotXY` function is already included at the end of the file. Otherwise, you must define the `plotXY` function at the end of your .m or .mlx file or add it as a file on the MATLAB path.

```
sbiosubplot(sd,@plotXY,{'y1'},{'y2'},true,'xlabel','y1','ylabel','y2')
```



Define plotXY Function

sbiosubplot accepts a function handle of a function with the signature:

`function functionName(sd,xArgs,yArgs)`.

The `plotXY` function plots two selected states against each other. The first input `sd` is the simulation data (SimBiology `SimData` object or vector of objects). In this example, `xArgs` is a cell array containing the name of the species to be plotted on the x-axis, and yArgs is a cell array containing the name of the species to be plotted on the y-axis. However, you can use the inputs xArgs and yArgs in any way in *your* custom plotting function. No output from the function is necessary.

```
function plotXY(sd,xArgs,yArgs)
% Select simulation data for each state from each run.
xData = selectbyname(sd,xArgs);
yData = selectbyname(sd,yArgs);
% Plot the species against each other.
plot(xData.Data,yData.Data);
end
```

Input Arguments

sd — Simulation results

`SimData` object

Simulation results, specified as a `SimData` object or vector of `SimData` objects.

This argument corresponds to the first input of the function referenced by `fcnHandle`.

Example: `simdata`

`fcnHandle` — Function to generate line plots
function handle

Function to generate line plots, specified as a function handle. For an example of a custom function to plot selected species from simulation data, see Plot Selected States from Simulation Data in Subplots on page 1-289.

The function must have the signature:

`function functionName(sd,xArgs,yArgs)`.

The inputs `sd`, `xArgs`, and `yArgs` are the same inputs that you pass in when you call `sbiosubplot`. No output from the function is necessary.

Example: `@plotXY`

Data Types: `function_handle`

`xArgs` — State names
string vector | cell array of character vectors

State names to plot, specified as a string vector or cell array of character vectors. For instance, you can use `xArgs` to represent the states to be plotted on the *x*-axis of your custom plot.

This argument corresponds to the second input of the function referenced by `fcnHandle`.

Example: `{'y1'}`

Data Types: `cell`

`yArgs` — State names
string vector | cell array of character vectors

State names to plot, specified as a string vector or cell array of character vectors. For instance, you can use `yArgs` to represent the states to be plotted on the *y*-axis of your custom plot.

This argument corresponds to the third input of the function referenced by `fcnHandle`.

Example: `{'y2','z'}`

Data Types: `cell`

`showLegend` — Logical flag to show plot legend
`false` (default) | `true`

Logical flag to show the plot legend, specified as `true` or `false`. If `true`, the function shows `yArgs` as the legend.

Example: `true`

Data Types: `logical`

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `'xlabel','Species A'` specifies the x-label of the plot.

`xlabel` — Label for *x*-axis
character vector | string

Label for the *x*-axis of the plot, specified as the comma-separated pair consisting of `'xlabel'` and a character vector or string.

Example: `'xlabel','y1'`

Data Types: `char` | `string`

`ylabel` — Label for *y*-axis
character vector | string

Label for the *y*-axis of the plot, specified as the comma-separated pair consisting of `'ylabel'` and a character vector or string.

Example: `'ylabel','y2'`

Data Types: `char` | `string`

Version History
Introduced in R2008a

See Also
`sbioplot` | `SimData`

sbiotrellis

Plot data or simulation results in trellis plot

Syntax

```
trellisplot = sbiotrellis(data,groupCol,xCol,yCol)
trellisplot = sbiotrellis(data,groupCol,xCol,yCol,Name,Value)
trellisplot = sbiotrellis(data,fcnHandle,groupCol,xCol,yCol)
trellisplot = sbiotrellis(simData,fcnHandle,xCol,yCol)
```

Description

`trellisplot = sbiotrellis(data,groupCol,xCol,yCol)` plots each group in `data` as defined by the group column variable `groupCol` into its own subplot. The data defined by column `xCol` is plotted against the data defined by column(s) `yCol`.

`trellisplot = sbiotrellis(data,groupCol,xCol,yCol,Name,Value)` uses additional options specified by one or more `Name,Value` pair arguments that are supported by the `plot` command.

`trellisplot = sbiotrellis(data,fcnHandle,groupCol,xCol,yCol)` plots each group in `data` as defined by the group column variable `groupCol` into its own subplot. `sbiotrellis` creates the subplot by calling the function handle, `fcnHandle`, with input arguments defined by the `data` columns `xCol` and `yCol`. The `fcnHandle` cannot be empty and must be specified.

The `fcnHandle` must have the signature `fcnHandle(x,y)`, where `x` is a numeric column vector, and `y` is a matrix with the same number of rows as `x`.

For instance, if you want to create a trellis plot with a logarithmic *y*-axis, use `@semilogy` as the function handle, where `semilogy` is the function that plots data with logarithmic scale for the *y*-axis.

`trellisplot = sbiotrellis(simData,fcnHandle,xCol,yCol)` plots each group in `simData` into its own subplot. `sbiotrellis` creates the subplot by calling the function handle, `fcnHandle` with input arguments defined by the columns `xCol` and `yCol`. The `fcnHandle` can be empty (`''` or `[]`). If empty, the default time plot is created using the handle `@plot`.

The `fcnHandle` must have the signature `fcnHandle(simDataI,xCol,yCol)`, where `simDataI` is a single `SimData` object, and `xCol` and `yCol` are the corresponding input arguments to `sbiotrellis`.

Tip Use the `plot` method of a sbiotrellis object to overlay a `SimData` object or a `dataset` on an existing `sbiotrellis` plot. For example, `plot(trellisplot,...)` adds a plot to the object `trellisplot`. The `SimData` or `dataset` that is being plotted must have the same number of elements or groups as the `trellisplot` object. The `plot` method has the same input arguments as `sbiotrellis`.

Examples

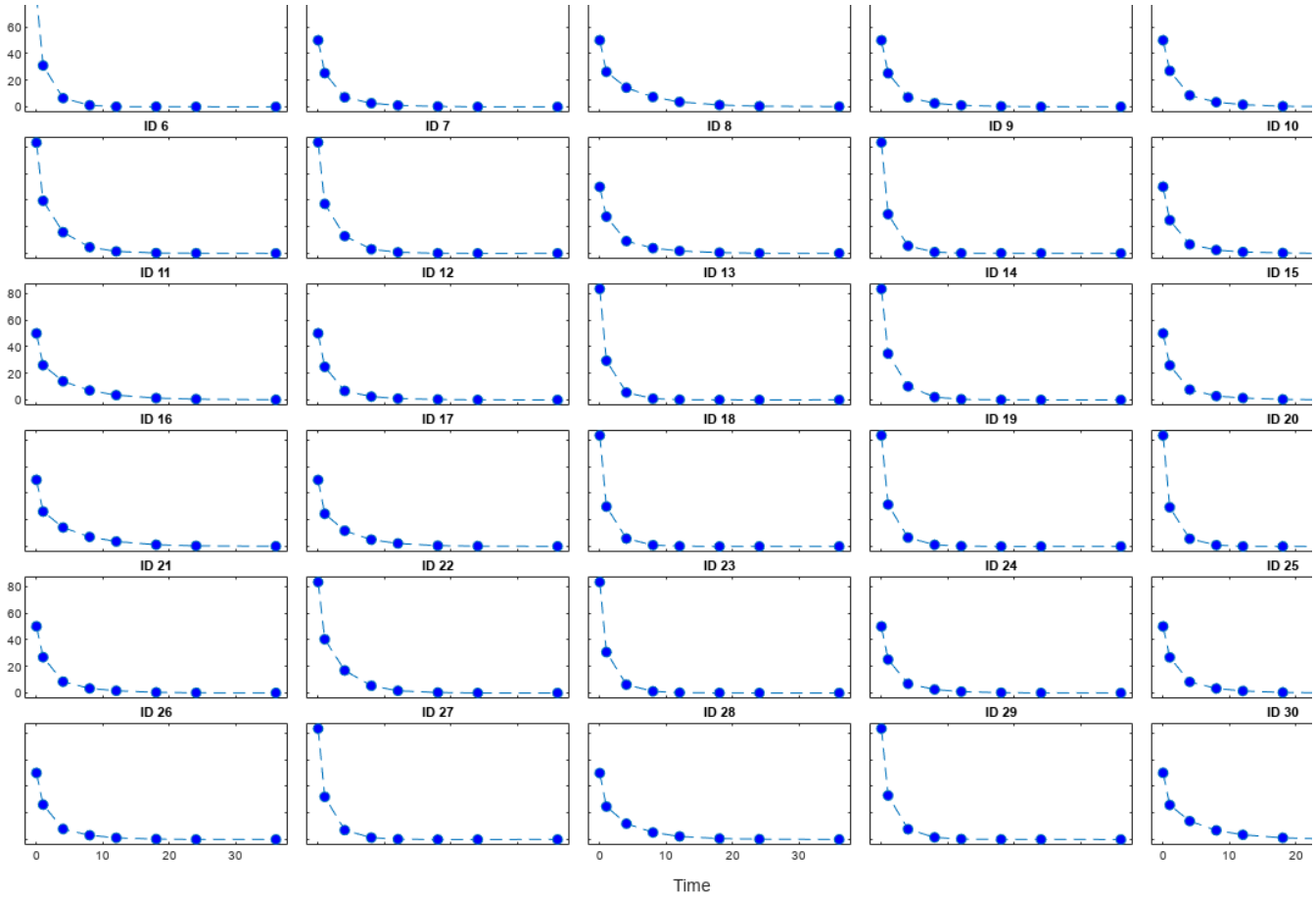
Create a Trellis Plot for Grouped Data

Load a sample dataset. The data contains measurements of drug concentration in the central and peripheral compartments for 30 subjects.

```
load('sd5_302RAgeSex.mat');
```

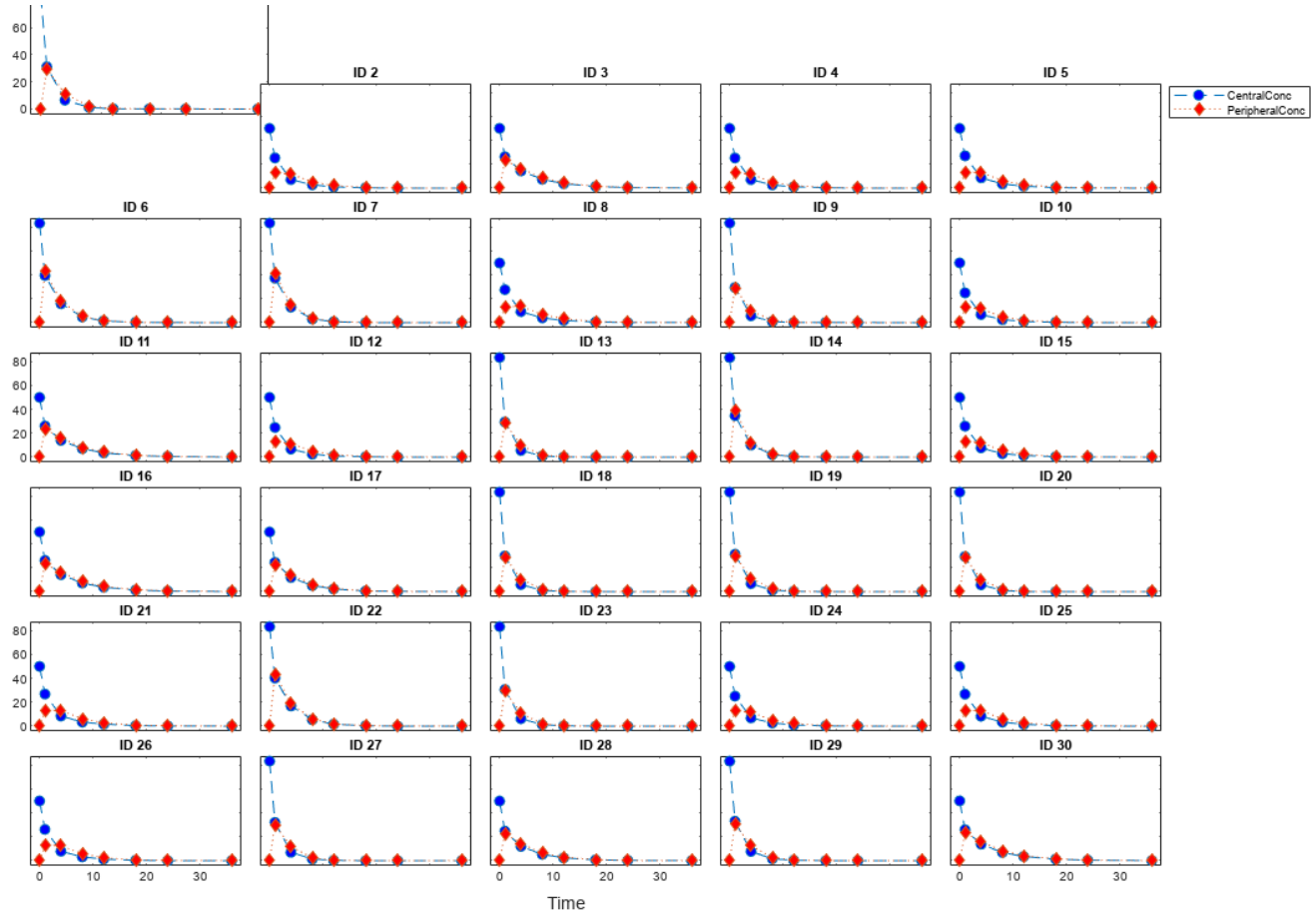
Create a trellis plot of the Central concentrations for each subject.

```
t = sbiotrellis(data, 'ID', 'Time', 'CentralConc',...
                'Marker', 'o','LineStyle','--','MarkerFaceColor','b');
% Resize the figure.
t.hFig.Position(:) = [100 100 1200 800];
```



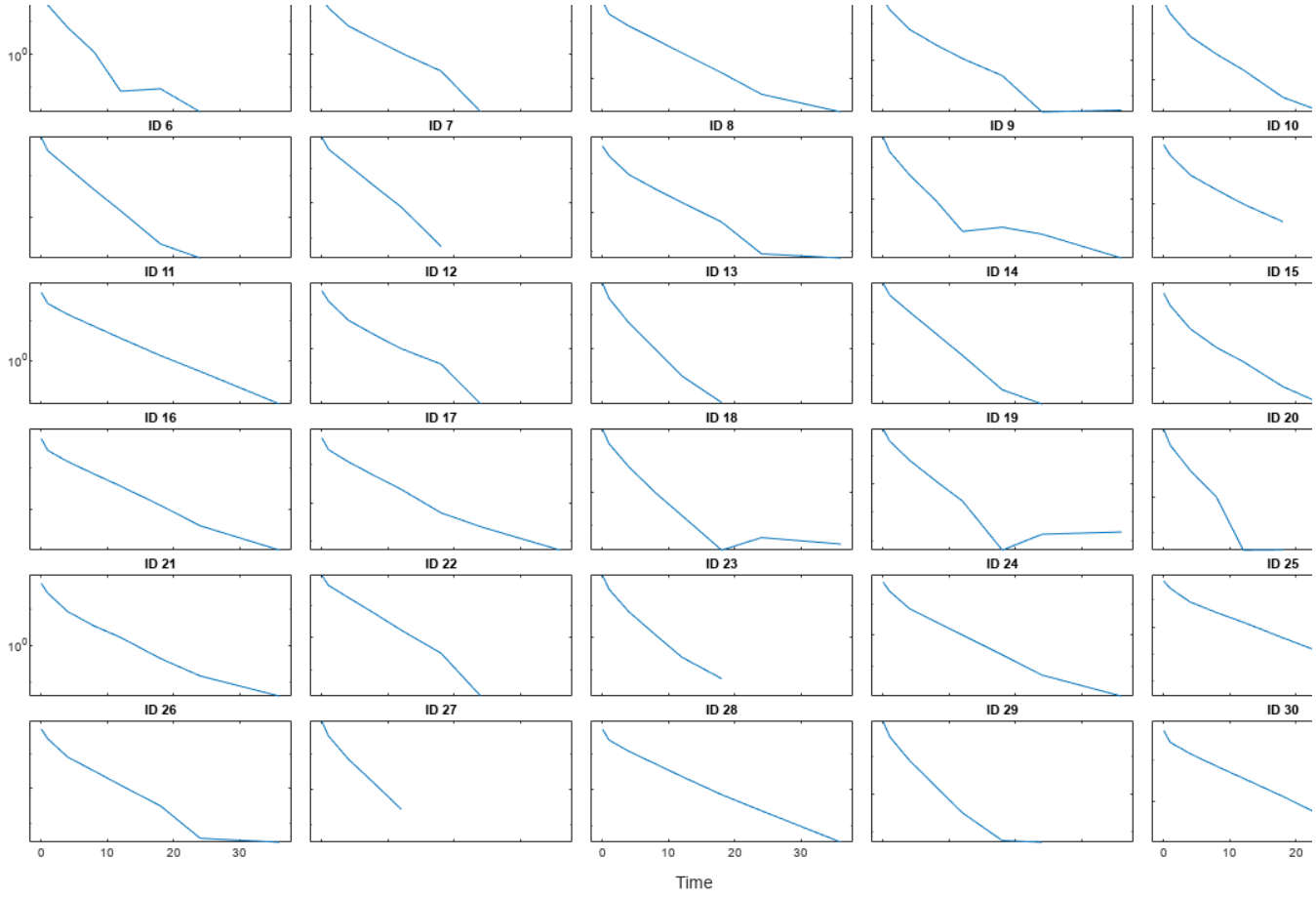
Use the `plot` method of the sbiotrellis object to overlay the peripheral concentration data on the same plot.

```
plot(t,data,'ID','Time','PeripheralConc','Marker','d',...
            'LineStyle',':','MarkerFaceColor','r');
```

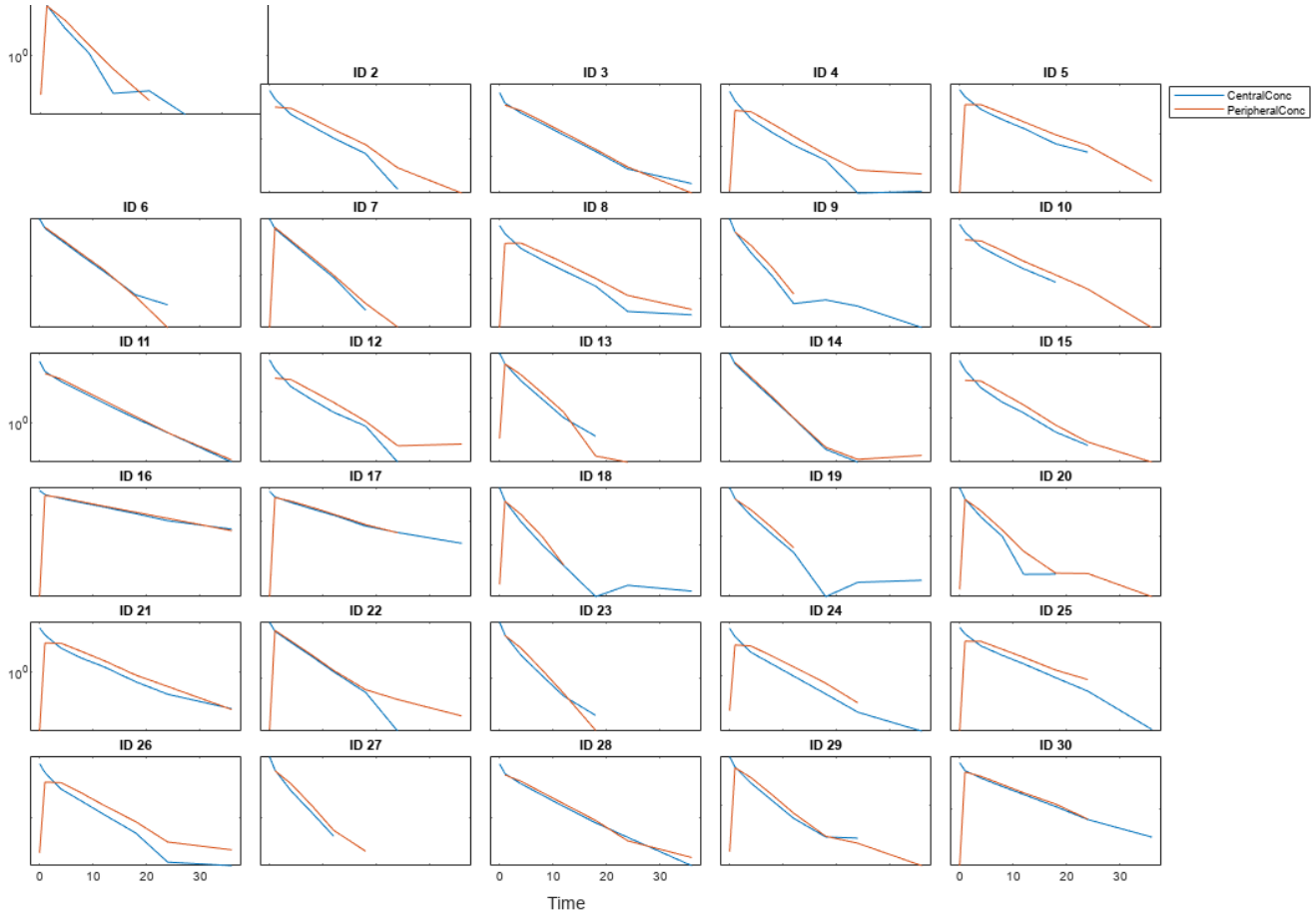


Specify the function handle `@semilogy` to change the y-axis to log scale.

```
t2 = sbiotrellis(data,@semilogy,'ID','Time','CentralConc');
%Resize the figure
t2.hFig.Position(:) = [100 100 1200 800];
```




```
plot(t2,data,@semilogy,'ID','Time','PeripheralConc');
```



Input Arguments

`data` — Data

dataset | groupedData object | table

Data, specified as a `dataset` containing grouped data, a `groupedData object`, or a `table`.

`groupCol` — Group column name

character vector | string

Group column name, specified as a character vector or string which is the name of a column in `data` that contains grouping information or an empty name `''` or `""`which implies there is only one group in `data`.

`xCol` — Name of a column to plot on the x-axis

character vector | string

Name of a column to plot on the *x*-axis, specified as a character vector or string.

If `data` is `groupedData`, then `xCol` can also be an empty name `''` or `""`, and the x-coordinates of the data are determined by the variable specified in `DATA.Properties.IndependentVariableName`.

If `data` is `dataset` or `table`, then `xCol` cannot be empty.

`yCol` — Name of a column to plot on the y-axis
character vector | string | string vector | cell array of character vectors

Name of a column to plot on the *y*-axis, specified as a character vector, string, string vector, or cell array of character vectors.

`fcnHandle` — Handle to a function
function handle

Handle to a function, specified as a function handle.

If the first argument is a `dataset` or `groupedData object`, the `fcnHandle` must have the signature `fcnHandle(x,y)`, where `x` is a numeric column vector, and `y` is a matrix with the same number of rows as `x`.

If it is a `SimData object`, the `fcnHandle` must have the signature `fcnHandle(simDataI,xCol,yCol)`, where `simDataI` is a single `SimData` object, and `xCol` and `yCol` are the corresponding input arguments to `sbiotrellis`.

`simData` — Simulation data
`SimData` object

Simulation data, specified as a `SimData object`.

Output Arguments

`trellisplot` — Plot object
sbiotrellis object

Plot object, specified as a sbiotrellis object. The object has the following properties.

- `hFig` – This is a MATLAB figure object. Use this object to control the appearance and behavior of the figure. For instance, to change the figure window background color to white, enter `trellisplot.hFig.Color = 'white'`. For the list of properties, see the Figure properties.
- `nPlots` – This property tells you the total number of plots in the figure.
- `plots` – This is a vector of axes objects with length equal to `nPlots`. Use this property to control the appearance and behavior of axes objects. For example, if you want to change the *y*-axis to a log scale, enter `set(trellisplot.plots,'YScale','log')`. For the list of properties, see the Axes properties.

Version History

Introduced in R2009a

See Also

`sbioplot` | `sbiosubplot`

sbiounit

Create user-defined unit

Note You can no longer specify an offset as an input when you call `sbiounit`. Use an absolute unit that does not require an offset. For details, see “Compatibility Considerations”.

Syntax

```
unitObject = sbiounit('NameValue')
unitObject = sbiounit('NameValue', 'CompositionValue')
unitObject = sbiounit('NameValue','CompositionValue',MultiplierValue)
unitObject = sbiounit('NameValue','CompositionValue',...'PropertyName',
PropertyValue...)
```

Arguments

NameValue	Name of the user-defined unit. *NameValue* must begin with characters and can contain characters, underscores, or numbers. *NameValue* can be any valid MATLAB variable name.
CompositionValue	Shows the combination of base and derived units that defines the unit *NameValue*. For example `molarity` is `mole/liter`. Base units are the set of units used to define all unit quantity equations. Derived units are defined using base units or mixtures of base and derived units.
MultiplierValue	Numerical value that defines the relationship between the user-defined unit *NameValue* and the base unit as a product of the *MultiplierValue* and the base unit. For example, `1 mole` is `6.0221e23*molecule`. The *MultiplierValue* is `6.0221e23`.
PropertyName	Name of the unit object property, for example, `'Notes'`.
PropertyValue	Value of the unit object property, for example, `'New unit for GPCR model'`.

Description

`unitObject = sbiounit('NameValue')` constructs a SimBiology unit object named *NameValue*. Valid names must begin with a letter, and be followed by letters, underscores, or numbers.

`unitObject = sbiounit('NameValue', 'CompositionValue')` allows you to specify the name and the composition of the unit.

`unitObject = sbiounit('NameValue','CompositionValue',MultiplierValue)` creates a unit with the name *NameValue* where the unit is defined as `MultiplierValue*CompositionValue`.

unitObject = sbiounit('*NameValue*','*CompositionValue*',...'*PropertyName*', *PropertyValue*...) defines optional properties. The name-value pairs can be in any format supported by the function `set`.

In order to use *unitObject*, you must add it to the user-defined library with the `sbioaddtolibrary` function. To get the unit object into the user-defined library, use the following command:

```
sbioaddtolibrary(unitObject);
```

You can view additional *unitObject* properties with the `get` command. You can modify additional properties with the `set` command. For more information about unit object properties and methods, see Unit object.

Use the `sbiowhos` function to list the units available in the user-defined library.

Examples

This example shows you how to create a user-defined unit, add it to the user-defined library, and query the library.

1. Create units for the rate constants of a first-order and a second-order reaction.

   ```
   unitObj1 = sbiounit('firstconstant', '1/second', 1);
   unitObj2 = sbiounit('secondconstant', '1/molarity*second', 1);
   ```

2. Add the unit to the user-defined library.

   ```
   sbioaddtolibrary(unitObj1);
   sbioaddtolibrary(unitObj2);
   ```

3. Query the user-defined library in the root object.

   ```
   rootObj = sbioroot;
   rootObj.UserDefinedLibrary.Units
   ```

   ```
   ans =

      SimBiology Unit Array

      Index:    Library:       Name:             Composition:         Multiplier:
      1         UserDefined    firstconstant     1/second             1
      2         UserDefined    secondconstant    1/molarity*second    1
   ```

   Alternatively, use the `sbiowhos` command.

   ```
   sbiowhos -userdefined -unit
   ```

   ```
      SimBiology UserDefined Units

      Index:  Name:           Composition:             Multiplier:
      1       firstconstant   1/second                 1.000000
      2       secondconstant  1/molarity*second        1.000000
   ```

Version History

Introduced in R2008a

R2022b: `week` has been added as a built-in unit

Behavior changed in R2022b

You can now use `week` as a built-in unit and no longer have to create your own custom week unit. However, suppose that you have added a custom week unit to the user-defined (custom) library in a previous release (R2022a or earlier), installed the new version of MATLAB (R2022b or later), and your preferences from the previous release was imported (automatically by MATLAB or manually by you). When you interact with SimBiology for the first time in your latest MATLAB, SimBiology:

1. Switches to use the built-in `week` unit.
2. Renames the custom unit to `week_N`, where *N* is a positive integer.
3. Shows a one-time warning message indicating that your custom `week` unit has been renamed.

Use `sbioremovefromlibrary` at the command line or go to **Home** > **Libraries** from the **SimBiology Model Builder** app to remove the custom unit if it is no longer needed.

Tip

- Check the model component properties, namely, `Notes`, `Tag`, and `UserData`, to see if the custom unit is being referenced by these properties before removing the unit.
- Update references to use the new name (`week_N`) if the built-in `week` unit is not sufficient for your use case.

R2021a: `sbiounits` no longer accepts offset as an input

Behavior changed in R2021a

You can no longer specify an offset information as an input when you call `sbiounits`. The `Offset` property of a unit object has been removed. Use an absolute unit that does not require an offset, such as kelvin instead of Celsius.

R2021a: Celsius and Fahrenheit units have been removed

Errors starting in R2021a

`Celsius`, `celsius`, and `fahrenheit` units have been removed from the built-in units library. Use `kelvin` units instead.

If you have a model containing `Celsius`, `celsius`, or `fahrenheit` units, change the units to `kelvin`.

If you have a script that sets the Units property of a parameter to `'Celsius'`, `'celsius'`, or `'fahrenheit'`, set this property to `'kelvin'` and adjust the `Value` property accordingly. Similarly, if you have compound units, make appropriate changes. For example, change `joule/Celsius` to `joule/kevin`.

See Also

`sbioaddtolibrary` | `sbioshowunits` | `sbiounitprefix` | `sbiowhos`

sbiounitcalculator

Convert value between units

Syntax

```
result = sbiounitcalculator('fromUnits', 'toUnits', Value)
```

Description

`result = sbiounitcalculator('fromUnits', 'toUnits', Value)` converts the value, `Value`, which is defined in the units, `fromUnits`, to the value, `result`, which is defined in the units, `toUnits`.

Examples

```
result = sbiounitcalculator('mile/hour','meter/second',1)
```

Version History

Introduced in R2006a

See Also

`sbioshowunits`

sbiounitprefix

Create user-defined unit prefix

Syntax

```
unitprefixObject = sbiounitprefix(prefixName)
unitprefixObject = sbiounitprefix(prefixName,exponentValue)
unitprefixObject = sbiounitprefix( ___ ,Name=Value)
```

Description

`unitprefixObject = sbiounitprefix(prefixName)` constructs a SimBiology unit prefix object with the name `prefixName`.

In order to use the unit prefix defined by `unitprefixObject` , you must add it to the user-defined library using `sbioaddtolibrary`. Use `sbioshowunitprefixes` to list the units available in the user-defined library.

`unitprefixObject = sbiounitprefix(prefixName,exponentValue)` also specifies a multiplicative factor of `10^exponentValue`.

`unitprefixObject = sbiounitprefix( ___ ,Name=Value)` also sets the `unitprefixObject` properties using one or more name-value arguments, where `Name` is the object property name and `Value` is the corresponding value. For a list of the object properties, see `UnitPrefix`.

Examples

Create a Custom Unit Prefix and Add to Library

Create a unit prefix `peta` with the exponent value of 15.

```
petaPrefix = sbiounitprefix("peta",15);
```

Add the unit prefix to the library.

```
sbioaddtolibrary(petaPrefix);
```

Check the library of unit prefixes. Note that `peta` has been added as a user-defined unit prefix.

```
sbioshowunitprefixes
```

```
ans =
   SimBiology Unit Prefix Array

   Index:    Library:       Name:    Exponent:
   1         BuiltIn        centi    -2
   2         BuiltIn        deci     -1
   3         BuiltIn        deka     1
   4         BuiltIn        femto    -15
   5         BuiltIn        giga     9
   6         BuiltIn        hecto    2
```

```
   7         BuiltIn        kilo     3
   8         BuiltIn        mega     6
   9         BuiltIn        micro    -6
   10        BuiltIn        milli    -3
   11        BuiltIn        nano     -9
   12        UserDefined    peta     15
   13        BuiltIn        pico     -12
   14        BuiltIn        tera     12
```

Alternatively, you can use `sbiowhos` or the root object.

```
sbiowhos -userdefined -unitprefix

   SimBiology UserDefined Unit Prefixes

   Index:  Name:           Multiplier:
   1       peta            1000000000000000
```

```
rootObj = sbioroot;
rootObj.UserDefinedLibrary.UnitPrefixes

ans =
   SimBiology Unit Prefix Array

   Index:    Library:       Name:    Exponent:
   1         UserDefined    peta     15
```

Input Arguments

`prefixName` — Name of unit prefix

character vector | string

Name of the unit prefix, specified as a character vector or string. Valid names must begin with a letter and be followed by letters, underscores, or numbers.

Data Types: `char` | `string`

`exponentValue` — Exponent value

integer

Exponent value, specified as an integer. It shows the value of `10^exponentValue`. For example, for the unit picomole, the `exponentValue` is -12.

Data Types: `double`

Output Arguments

`unitprefixObject` — Unit prefix

`UnitPrefix` object

Unit prefix, returned as a `UnitPrefix` object.

Version History

Introduced in R2008a

See Also

`sbioaddtolibrary` | `sbioshowunits` | `sbiounit` | `sbiowhos`

sbiovariant

Construct variant object

Syntax

```
variantObj = sbiovariant(vName)
variantObj = sbiovariant(vName,vContent)
variantObj = sbiovariant( ___ ,Name,Value)
```

Description

`variantObj = sbiovariant(vName)` creates a variant object named `vName`.

`variantObj = sbiovariant(vName,vContent)` creates a variant object and sets its `Content` property to the cell array of data, `vContent`.

`variantObj = sbiovariant( ___ ,Name,Value)` uses any of the input arguments in the previous syntaxes and additional options specified by one or more `Name,Value` pair arguments. Each name-value pair represents a property and corresponding value of a variant object. To view all the properties for a variant object, use the `get` function.

To append more data to an existing content of a variant, use `addcontent`. To replace existing data in the `Content` property, use the `set` function or dot notation.

Examples

Create Variant with Alternate Model Values

Load the G protein model.

```
sbioloadproject gprotein
```

The model already has a variant for a mutant strain.

```
getvariant(m1)
```

```
ans =
   SimBiology Variant - mutant (inactive)

   ContentIndex:     Type:        Name:            Property:          Value:
   1                 parameter    kGd              Value              .004
```

Create another variant with the `kGd` value of 0.5, and initial amount of 5000 for the `G` species.

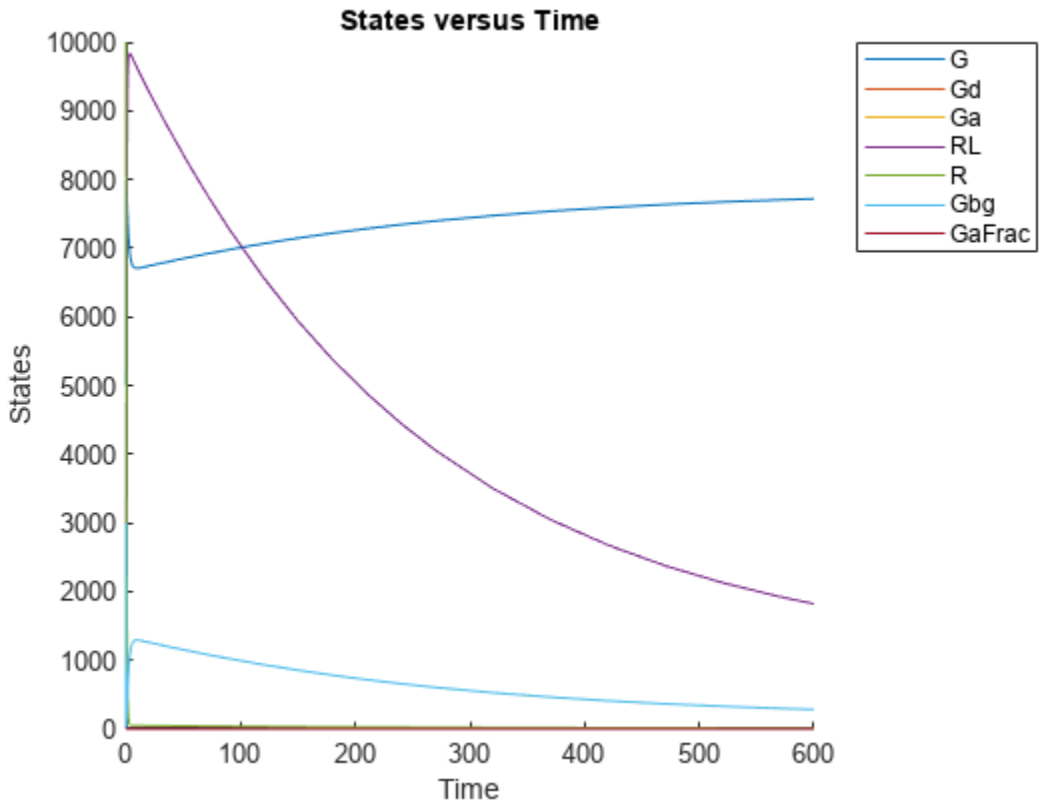
```
v2 = sbiovariant('v2');
v2.Content = {{'parameter','kGd','Value',0.5},...
              {'species','G','InitialAmount',5000}}
```

```
v2 =
   SimBiology Variant - v2 (inactive)
```

```
ContentIndex:     Type:        Name:            Property:          Value:
1                 parameter    kGd              Value              .5
2                 species      G                InitialAmount      5000.0
```

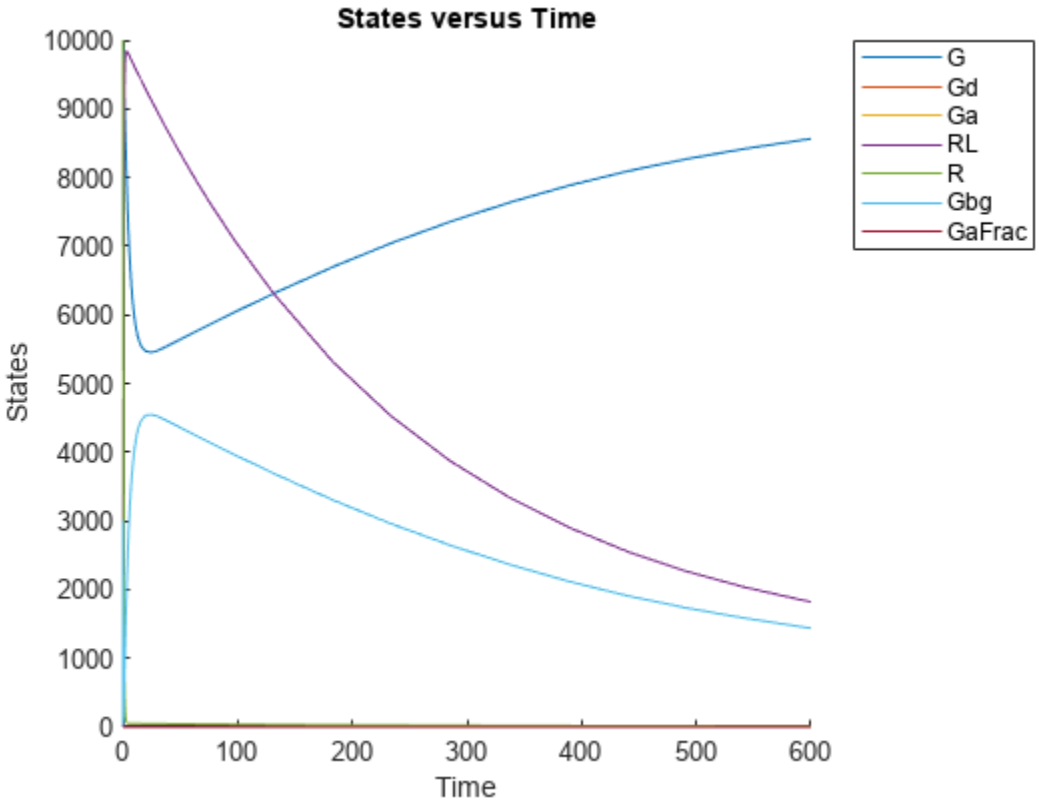
Simulate the model using the initial conditions specified in v2.

```
sbioplot(sbiosimulate(m1,v2));
```



Simulate the wild-type (original) model to compare.

```
sbioplot(sbiosimulate(m1));
```



Input Arguments

`vName` — Name of variant object

character vector

Name of a variant object, specified as a character vector.

Example: `'cancerPatient'`

`vContent` — Variant content

cell array | cell array of cell arrays

Variant content, specified as a cell array or cell array of cell arrays. Each cell array must have four values in this order: the type of model element, its name, its property name, and the alternate value of the property. For instance, `{'species','A','InitialAmount',5}` specifies to store an alternate initial amount of 5 for the species *A*.

Example: `{'parameter','ka','Value',0.3}`

Output Arguments

`variantObj` — Variant with alternate model values

variant object

Variant with alternate model values, specified as a `Variant object`.

Version History

Introduced in R2008a

See Also

`addvariant` | `getvariant` | `delete` | `get` | `set`

Topics

“Simulate Biological Variability of the Yeast G Protein Cycle Using Wild-Type and Mutant Strains”
“Simulate Model of Glucose-Insulin Response with Different Initial Conditions”
“Variants in SimBiology Models”

sbiowhos

Show contents of project file, library file, or SimBiology root object

Syntax

```
sbiowhos flag
sbiowhos ('flag')
sbiowhos flag1 flag2...
sbiowhos FileName
```

Description

`sbiowhos` shows contents of the SimBiology root object. This includes the built-in and user-defined kinetic laws, units, and unit prefixes.

`sbiowhos flag` shows specific information about the SimBiology root object as defined by `flag`. Valid flags are described in this table.

Flag	Description
`-builtin`	Built-in kinetic laws, units, and unit prefixes
`-data`	Data saved in file
`-kineticlaw`	Built-in and user-defined kinetic laws
`-unit`	Built-in and user-defined units
`-unitprefix`	Built-in and user-defined unit prefixes
`-userdefined`	User-defined kinetic laws, units, and unit prefixes

You can also specify the functional form `sbiowhos ('flag')`.

`sbiowhos flag1 flag2...` shows information about the SimBiology root object as defined by `flag1, flag2,...`.

`sbiowhos FileName` shows the contents of the SimBiology project or library defined by `Name`.

Examples

```
% Show contents of the SimBiology root object
  sbiowhos

% Show kinetic laws on the SimBiology root object
  sbiowhos -kineticlaw

% Show the builtin units of the SimBiology root object.
  sbiowhos -builtin -unit

% Show all contents of project file.
  sbiowhos myprojectfile

% Show kinetic laws from a library file.
```

```
  sbiowhos -kineticlaw mylibraryfile

% Show all contents of multiple files.
  sbiowhos myfile1 myfile2
```

Version History

Introduced in R2006a

See Also

whos

sbmlexport

Export SimBiology model to SBML file

Syntax

```
sbmlexport(modelObj)
sbmlexport(modelObj, 'FileName')
```

Arguments

modelObj	Model object. Enter a variable name for a model object.
FileName	XML file with a Systems Biology Markup Language (SBML) format. Enter either a file name or a path and file name supported by your operating system. If the file name does not have the extension `.xml`, then `.xml` is appended to end of the file name.

Description

`sbmlexport(modelObj)` exports a SimBiology model object (`modelObj`) to a file with a Systems Biology Markup Language (SBML) Level 2 Version 4 format. The default file extension is `.xml` and the file name matches the model name.

`sbmlexport(modelObj, 'FileName')` exports a SimBiology model object (`modelObj`) to an SBML file named *FileName*. The default file extension is `.xml`.

A SimBiology model can also be written to a SimBiology project with the `sbiosaveproject` function to save features not supported by SBML.

For more information about features that are supported by SimBiology but not by SBML or vice visa, see “SBML Support”.

Examples

Export a model (`modelObj`) to a file (`gene_regulation.xml`) in the current working directory.

```
sbmlexport(modelObj,'gene_regulation.xml');
```

Version History

Introduced before R2006a

References

Finney, A., Hucka, M., (2003), *Systems Biology Markup Language (SBML) Level 2: Structures and facilities for model definitions*.

See Also

`sbiomodel` | `sbiosaveproject` | `sbmlimport`

Topics

“Export a SimBiology Model to SBML Format”
“SBML Support”
sbiomodel on page 1-131
sbiosaveproject on page 1-243

sbmlimport

Import SBML-formatted file

Syntax

`modelObj = sbmlimport(File)`

Description

`modelObj = sbmlimport(File)` imports *`File`*, a Systems Biology Markup Language (SBML)-formatted file, into MATLAB and creates a model object `modelObj`.

`File` is a character vector or string specifying a file name or a path and file name supported by your operating system. *`File`* extensions are `.sbml` or `.xml`.*`File`* can also be a URL, if you have the Java® programming language.

`sbmlimport` supports SBML Level 3 Version 1 and earlier.

For functional characteristics and limitations, see “SBML Support”.

Input Arguments

`File`

Character vector or string specifying either of the following:

- File name or path and file name supported by your operating system
- URL

Examples

Import SBML model:

```
sbmlobj = sbmlimport('oscillator.xml');
```

Version History

Introduced before R2006a

R2017b: `sbmlimport` adds initial assignment rule when importing some SBML models

Behavior changed in R2017b

- `sbmlimport` adds an initial assignment rule when importing SBML models with the following conditions.
  - If an SBML model has a species *s* initialized to *X* using `initialAmount` and has the attribute setting `hasOnlySubstanceUnits = false`:
    - SimBiology sets the initial amount of *s* to *X*.

    - If the model does not already have an initial assignment or repeated assignment rule for *s*, SimBiology adds an initial assignment rule `s = X / V`, where *V* is the compartment volume (capacity). This rule ensures that the initial amount of *s* is a concentration unit.
    - If the model already has an initial assignment or repeated assignment rule for *s*, then SimBiology does not use the value *X*. Instead, SimBiology evaluates the rule and sets the appropriate initial amount.
  - If an SBML model has a species *s* initialized to *X* using `initialConcentration` and has the attribute setting `hasOnlySubstanceUnits = true`:
    - SimBiology sets the initial amount of *s* to *X*.
    - If the model does not already have an initial assignment or repeated assignment rule for *s*, SimBiology adds an initial assignment rule `s = X * V`, where *V* is the compartment volume (capacity). This rule ensures that the initial amount of *s* is an amount unit.
    - If the model already has an initial assignment or repeated assignment rule for *s*, then SimBiology does not use the value *X*. Instead, SimBiology evaluates the rule and sets the appropriate initial amount.
- If a species *s* in an SBML model has the attribute setting `hasOnlySubstanceUnits` = true without any units defined, SimBiology issues a warning and sets the species amount unit to a default unit (mole) to ensure it is interpreted as an amount, not a concentration. The imported SimBiology model has the `DimensionalAnalysis` property set to false to prevent dimensional analysis errors.

R2022a: Support for URL schemes other than HTTP and HTTPS has been removed
Errors starting in R2022a

Support for passing in a URL that is not `HTTP` and `HTTPS` has been removed in a future release. Download the file locally first and then use the file name as an input to `sbmlimport` instead.

References

Finney, A., Hucka, M., (2003). *Systems Biology Markup Language (SBML) Level 2: Structures and facilities for model definitions*.

See Also

`get` | `sbiosimulate` | `sbmlexport` | `set` | DimensionalAnalysis

Topics
“SBML Support”
“Import from SBML Files”

simbiology

Open SimBiology Model Builder

Syntax

```
simbiology
simbiology(m1)
simbiology(prjFile)
```

Description

`simbiology` opens the **SimBiology Model Builder** app.

`simbiology(m1)` opens the SimBiology model `m1` in the **SimBiology Model Builder** app.

If the **SimBiology Model Builder** or **SimBiology Model Analyzer** app is already open, you cannot load a model or project from the command line. Load the model from the app directly.

`simbiology(prjFile)` opens the project file `prjFile` in the **SimBiology Model Builder** app.

If the **SimBiology Model Builder** or **SimBiology Model Analyzer** app is already open, you cannot load a model or project from the command line. Load the model from the app directly.

Examples

Open SimBiology Model Builder

Open the PK/PD model for an antibacterial agent as described in “Perform PK/PD Modeling and Simulation to Guide Dosing Strategy for Antibiotics”.

```
simbiology('AntibacterialPKPD.sbproj');
```

Input Arguments

`m1` — SimBiology model

model object

SimBiology model, specified as a SimBiology `Model` object.

`prjFile` — SimBiology project file name

character vector | string

SimBiology project file name, specified as a character vector or string. Specify a file name or path and file name of a SimBiology project (SBPROJ) file. If you specify only a file name, the file must be on the MATLAB search path or in the current folder.

Data Types: `char` | `string`

Version History

Introduced in R2009a

R2020b: Load a project or model from the command line when the app is open
Behavior changed in R2020b

If the **SimBiology Model Builder** or **SimBiology Model Analyzer** app is open, you cannot load a project or model from the command line using `simbiology`. Load the project or model from the app directly.

See Also

SimBiology Model Builder | **SimBiology Model Analyzer** | `sbioreset` | `sbioroot` | `Model`

SimBiology.export.Dose Properties

Exported SimBiology model dose object

Description

`SimBiology.export.Dose` is the object property for modifiable export dose objects. An export dose is either of object type `SimBiology.export.RepeatDose` or `SimBiology.export.ScheduleDose`.

Export dose objects are created by the `export` function for SimBiology models. By default, all active doses are export doses, but you can specify which doses to export using the optional `editdoses` input argument to `export`. For example, see “Exported SimBiology Model Dose Objects” on page 2-283.

Properties

Export Dose

`Amount` — Amount of dose
nonnegative scalar

Amount of dose, specified as a nonnegative scalar value. This property is read-only if it is parameterized in the export model.

`AmountUnits` — Dose amount units
character vector

This property is read-only.

Dose amount units, specified as a character vector.

`DurationParameterName` — Parameter specifying length of time to administer a dose
character vector

This property is read-only.

Parameter specifying length of time to administer a dose, specified as a character vector.

`EventMode` — Determine how events that change dose parameters affect in-progress dosing
`'stop'` (default) | `'continue'`

This property is read-only.

Determine how events that change dose parameters affect in-progress dosing, specified as `'stop'` or `'continue'`.

`LagParameterName` — Parameter specifying time lag for the dose
character vector

This property is read-only.

Parameter specifying time lag for the dose, specified as a character vector.

`Name` — Name of dose object
character vector

This property is read-only.

Name of dose object, specified as a character vector.

`Notes` — Text describing dose object
character vector

This property is read-only.

Text describing dose object, specified as a character vector.

`Parent` — Name of the parent export model
SimBiology component object | empty array

This property is read-only.

Name of the parent export model, specified as a SimBiology component object or an empty array.

`Rate` — Rate of dose
nonnegative scalar

Rate of dose, specified as a nonnegative scalar value. The default value is `0` (`RepeatDose`) or `[]` (`ScheduleDose`), that is, the dose is interpreted as a bolus (instantaneous) dose. This property is read-only if it is parameterized in the export model.

`RateUnits` — Units for dose rate
character vector

This property is read-only.

Units for dose rate, specified as a character vector.

`TargetName` — Species receiving dose
character vector

This property is read-only.

Species receiving dose, specified as a character vector.

`TimeUnits` — Time units for dosing
character vector

This property is read-only.

Time units for dosing, specified as a character vector.

Version History

Introduced in R2012b

See Also

`SimBiology.export.RepeatDose` | `SimBiology.export.ScheduleDose` | `export`

Topics

“Perform PK/PD Modeling and Simulation to Guide Dosing Strategy for Antibiotics”
“Deploy a SimBiology Exported Model”

SimBiology.export.ExplicitTauSimulationOptions Properties

Settings for explicit tau-leaping solver of exported SimBiology model

Description

`SimBiology.export.ExplicitTauSimulationOptions` is the object property of simulation options associated with the explicit tau-leaping solver of an export model.

Explicit tau simulation options are created by the `export` function for SimBiology models with a stochastic `SolverType` set to `'expltau'`.

Properties

Explicit Tau Simulation Options

`ErrorTolerance` — Error tolerance
scalar value in the range (0,1)

Error tolerance, specified as a scalar value in the range (0,1).

`LogDecimation` — Frequency to log stochastic simulation output
positive integer

Frequency to log stochastic simulation output, specified as a positive integer value.

`MaximumNumberofLogs` — Maximum number of logs criterion to stop simulation
positive scalar

Maximum number of logs criterion to stop simulation, specified as a positive scalar value.

`MaximumWallClock` — Maximum elapsed wall clock time criterion to stop simulation
positive scalar

Maximum elapsed wall clock time criterion to stop simulation, specified as a positive scalar value.

`RandomState` — Random number generator
positive integer

Random number generator, specified as a positive integer value.

`SolverType` — Solver type to use for simulation
`'expltau'`

This property is read-only.

Solver type to use for simulation, specified as `'expltau'`.

`StopTime` — Simulation time criterion to stop simulation
nonnegative scalar

Simulation time criterion to stop simulation, specified as a nonnegative scalar value.

`TimeUnits` — Time units for simulation
character vector

This property is read-only.

Time units for simulation, specified as a character vector.

Version History

Introduced in R2012b

See Also

`SimBiology.export.StochasticSimulationOptions` | `SimBiology.export.ImplicitTauSimulationOptions` | `SimBiology.export.SimulationOptions` | `SimBiology.export.ODESimulationOptions` | `export`

SimBiology.export.ImplicitTauSimulationOptions Properties

Settings for implicit tau-leaping stochastic simulation of exported SimBiology model

Description

`SimBiology.export.ImplicitTauSimulationOptions` is the object property of simulation options associated with the implicit tau-leaping solver of an export model.

Implicit tau-leaping simulation options are created by the `export` function for SimBiology models with a stochastic `SolverType` set to `'impltau'`.

Properties

Implicit Tau-Leaping Simulation Options

`ErrorTolerance` — Error tolerance
scalar value in the range (0,1)

Error tolerance, specified as a scalar value in the range (0,1).

`LogDecimation` — Frequency to log stochastic simulation output
positive integer

Frequency to log stochastic simulation output, specified as a positive integer value.

`MaxIterations` — Nonlinear solver maximum number of iterations
positive integer

Nonlinear solver maximum number of iterations, specified as a positive integer value.

`MaximumNumberofLogs` — Maximum number of logs criterion to stop simulation
positive scalar

Maximum number of logs criterion to stop simulation, specified as a positive scalar value.

`MaximumWallClock` — Maximum elapsed wall clock time criterion to stop simulation
positive scalar

Maximum elapsed wall clock time criterion to stop simulation, specified as a positive scalar value.

`RandomState` — Random number generator
positive integer

Random number generator, specified as a positive integer value.

`SolverType` — Solver type to use for simulation
`'impltau'`

This property is read-only.

Solver type to use for simulation, specified as `'impltau'`.

`StopTime` — Simulation time criterion to stop simulation
nonnegative scalar

Simulation time criterion to stop simulation, specified as a nonnegative scalar value.

`TimeUnits` — Time units for simulation
character vector

This property is read-only.

Time units for simulation, specified as a character vector.

Version History

Introduced in R2012b

See Also

`SimBiology.export.StochasticSimulationOptions` | `SimBiology.export.ExplicitTauSimulationOptions` | `SimBiology.export.SimulationOptions` | `SimBiology.export.ODESimulationOptions` | `export`

SimBiology.export.Model

Exported SimBiology model object

Description

Exported SimBiology models are limited-access models that can be simulated and accelerated. You can speedup simulation of exported models using Parallel Computing Toolbox, and deploy exported models using MATLAB Compiler™.

By default, all active dose objects, species, parameters, and compartments export with a SimBiology model, and are editable in the exported model object. You can limit which doses, species, parameters, and compartments are editable using additional options during export. Reactions, rules, and events are never editable in an exported model.

Creation

Use the `export` function to export a SimBiology model.

Properties

`DependentFiles` — Function files the model depends on
cell array of character vectors

This property is read-only.

Function files the model depends on, specified as a cell array of character vectors.

`ExportNotes` — Text with additional information
character vector

This property is read-only.

Text with additional information associated with the exported model, specified as a character vector.

`ExportTime` — Creation time of the exported model
character vector

This property is read-only.

Creation time of the exported model, specified as a character vector.

`InitialValues` — Initial values for modifiable species, compartments, and parameters
vector of values

Initial values for modifiable species, compartments, and parameters, specified as a vector of values.

`Name` — Name of the exported model
character vector

This property is read-only.

Name of the exported model, specified as a character vector.

`Notes` — HTML text describing the exported model object
character vector

This property is read-only.

HTML text describing the exported model object, specified as a character vector.

`SimulationOptions` — Simulation options
`SimBiology.export.SimulationOptions` object

Simulation options, specified as a `SimBiology.export.SimulationOptions` object.

`ValueInfo` — Modifiable value components
array of `SimBiology.export.ValueInfo` objects

Modifiable value components, specified as an array of `SimBiology.export.ValueInfo` objects of modifiable species, parameters, and compartments.

Object Functions

accelerate	Prepare exported SimBiology model for acceleration
getIndex	Get indices into ValueInfo and InitialValues properties
getdose	Return exported SimBiology model dose object
isAccelerated	Determine whether an exported SimBiology model is accelerated
simulate	Simulate exported SimBiology model

Examples

Export SimBiology Model Object

Load a sample SimBiology model object, and export.

```
modelObj = sbmlimport('lotka');
em = export(modelObj)
```

```
em =
  Model with properties:

           Name: 'lotka'
     ExportTime: '03-Mar-2023 08:42:22'
    ExportNotes: ''
```

Display the editable values (compartments, species, and parameters) information.

```
em.ValueInfo
```

```
ans=8×1 object
  8x1 ValueInfo array with properties:

    Constant
```

```
    InitialValue
    Name
    Parent
    QualifiedName
    Tag
    Type
    Units
```

There are 8 editable values. Display the names of the editable values.

```
{em.ValueInfo.Name}
```

```
ans = 1x8 cell
    {'unnamed'}    {'x'}    {'y1'}    {'y2'}    {'z'}    {'c1'}    {'c2'}    {'c3'}
```

Display the exported model simulation options.

```
em.SimulationOptions
```

```
ans =
  ODESimulationOptions with properties:

            AbsoluteTolerance: 1.0000e-06
     AbsoluteToleranceScaling: 1
    AbsoluteToleranceStepSize: [0x1 double]
                      MaxStep: [0x1 double]
                  OutputTimes: [0x1 double]
            RelativeTolerance: 1.0000e-03
                   SolverType: 'ode15s'
          MaximumNumberOfLogs: Inf
             MaximumWallClock: Inf
                     StopTime: 10
                    TimeUnits: 'second'
```

Version History

Introduced in R2012b

See Also

`SimBiology.export.Dose` | `SimBiology.export.SimulationOptions` | `SimBiology.export.ValueInfo` | `export`

Topics

“Perform PK/PD Modeling and Simulation to Guide Dosing Strategy for Antibiotics”
“Deploy a SimBiology Exported Model”
Class Attributes
Property Attributes

SimBiology.export.ODESimulationOptions Properties

Settings for deterministic, ordinary differential equation simulation of exported SimBiology model

Description

`SimBiology.export.ODESimulationOptions` is the object property of simulation options associated with deterministic, ordinary differential equation (ODE) solvers.

Deterministic simulation options are created by the `export` function for SimBiology models with a deterministic `SolverType` (for example, `sundials` or `ode15s`).

Properties

Deterministic Simulation Options

`AbsoluteTolerance` — Absolute error tolerance applied to state value
positive scalar

Absolute error tolerance applied to state value during simulation, specified as a positive scalar value.

`AbsoluteToleranceScaling` — Control scaling of absolute error tolerance
logical value

Control scaling of absolute error tolerance, specified as a logical value.

`AbsoluteToleranceStepSize` — Initial guess for time step size for scaling of absolute error tolerance
empty array | scalar

Initial guess for time step size for scaling of absolute error tolerance, specified as an empty array `[]` or a scalar value.

`MaximumNumberofLogs` — Maximum number of logs criterion to stop simulation
positive scalar

Maximum number of logs criterion to stop simulation, specified as a positive scalar value.

`MaximumWallClock` — Maximum elapsed wall clock time criterion to stop simulation
positive scalar

Maximum elapsed wall clock time criterion to stop simulation, specified as a positive scalar value.

`MaxStep` — Upper bound on ODE solver step size
empty array | positive scalar

Upper bound on ODE solver step size, specified as an empty array `[]` or a positive scalar value.

`OutputTimes` — Times to log in simulation output
vector of sorted nonnegative values

Times to log in simulation output, specified as a vector of sorted nonnegative values.

`RelativeTolerance` — Allowable error tolerance relative to state
scalar value in the range (0,1)

Allowable error tolerance relative to state value during simulation, specified as a scalar value in the range (0,1).

`SolverType` — Solver type to use for simulation
`'sundials'` | `'ode15s'` | `'ode23t'` | `'ode45'`

Solver type to use for simulation, specified as a character vector. Possible deterministic solver types are:

- `'sundials'`
- `'ode15s'`
- `'ode23t'`
- `'ode45'`

`StopTime` — Simulation time criterion to stop simulation
nonnegative scalar

Simulation time criterion to stop simulation, specified as a nonnegative scalar value.

`TimeUnits` — Time units for simulation
character vector

This property is read-only.

Time units for simulation, specified as a character vector.

Version History

Introduced in R2012b

See Also

`SimBiology.export.SimulationOptions` |
`SimBiology.export.StochasticSimulationOptions` | `export`

SimBiology.export.RepeatDose Properties

Repeated doses for exported SimBiology model

Description

`SimBiology.export.RepeatDose` is the object property for export repeat doses.

Export repeat dose properties are created by the `export` function for SimBiology models. By default, all active repeat doses are export repeat doses, but you can specify which repeat doses to export using the optional `editdoses` input argument to `export`.

Properties

Export Repeat Dose

`Amount` — Amount of dose
nonnegative scalar | character vector

Amount of dose, specified as a nonnegative scalar value or the name (character vector) of a model-scoped parameter. This property is read-only if it is parameterized in the export model.

`AmountUnits` — Dose amount units
character vector

This property is read-only.

Dose amount units, specified as a character vector.

`DurationParameterName` — Parameter specifying length of time to administer a dose
character vector

This property is read-only.

Parameter specifying length of time to administer a dose, specified as a character vector.

`EventMode` — Determine how events that change dose parameters affect in-progress dosing
`'stop'` (default) | `'continue'`

This property is read-only.

Determine how events that change dose parameters affect in-progress dosing, specified as `'stop'` or `'continue'`.

`Interval` — Time between doses
nonnegative scalar | character vector

Time between doses, specified as a nonnegative scalar value or the name of a model-scoped parameter. This property is read-only if it is parameterized in the export model.

`LagParameterName` — Parameter specifying time lag for the dose
character vector

This property is read-only.

Parameter specifying time lag for the dose, specified as a character vector.

`Name` — Name of dose object
character vector

This property is read-only.

Name of dose object, specified as a character vector.

`Notes` — Text describing dose object
character vector

This property is read-only.

Text describing dose object, specified as a character vector.

`Parent` — Name of the parent export model
SimBiology component object | empty array

This property is read-only.

Name of the parent export model, specified as a SimBiology component object or an empty array.

`Rate` — Rate of dose
nonnegative scalar | string scalar | character vector

Rate of dose, specified as a nonnegative scalar value or the name (string or character vector) of a model-scoped parameter. This property is read-only if it is parameterized in the export model. The default value is `0`, that is, the dose is interpreted as a bolus (instantaneous) dose.

Note You cannot change the `Rate` property of `RepeatDose` for exported SimBiology model if *all* of the following conditions are true:

- The UnitConversion property of the model is already set to `true`.
- The `Rate` property is empty or set to zero.
- The `RateUnits` is set to empty.

To change the `Rate`, do one of the following:

- `Set` the UnitConversion property of the original model to `false`. Then `export` the model again.
- Set the `RateUnits` appropriately.

`RateUnits` — Units for dose rate
character vector

This property is read-only.

Units for dose rate, specified as a character vector.

`RepeatCount` — Dose repetitions
nonnegative integer | string scalar | character vector

Dose repetitions, specified as a nonnegative integer value or the name (string or character vector) of a model-scoped parameter. This property is read-only if it is parameterized in the export model.

`StartTime` — Start time for initial dose
nonnegative scalar | string scalar | character vector

Start time for initial dose, specified as a nonnegative scalar value or the name (string or character vector) of a model-scoped parameter. This property is read-only if it is parameterized in the export model.

`TargetName` — Species receiving dose
character vector

This property is read-only.

Species receiving dose, specified as a character vector.

`TimeUnits` — Time units for dosing
character vector

This property is read-only.

Time units for dosing, specified as a character vector.

Version History

Introduced in R2012b

See Also

`SimBiology.export.Dose` | `SimBiology.export.ScheduleDose` | `export`

SimBiology.export.ScheduleDose Properties

Schedule dose for exported SimBiology model

Description

`SimBiology.export.ScheduleDose` is the object property for export schedule doses.

Export schedule dose properties are created by the `export` function for SimBiology models. By default, all active schedule doses are export schedule doses, but you can specify which schedule doses to export using the optional `editdoses` input argument to `export`.

Properties

Export Schedule Dose

`Amount` — Amount of dose
nonnegative scalar

Amount of dose, specified as a nonnegative scalar value.

`AmountUnits` — Dose amount units
character vector

This property is read-only.

Dose amount units, specified as a character vector.

`DurationParameterName` — Parameter specifying length of time to administer a dose
character vector

This property is read-only.

Parameter specifying length of time to administer a dose, specified as a character vector.

`EventMode` — Determine how events that change dose parameters affect in-progress dosing
`'stop'` (default) | `'continue'`

This property is read-only.

Determine how events that change dose parameters affect in-progress dosing, specified as `'stop'` or `'continue'`.

`LagParameterName` — Parameter specifying time lag for the dose
character vector

This property is read-only.

Parameter specifying time lag for the dose, specified as a character vector.

`Name` — Name of dose object
character vector

This property is read-only.

Name of dose object, specified as a character vector.

`Notes` — Text describing dose object

character vector

This property is read-only.

Text describing dose object, specified as a character vector.

`Parent` — Name of the parent export model

SimBiology component object | empty array

This property is read-only.

Name of the parent export model, specified as a SimBiology component object or an empty array.

`Rate` — Rate of dose

empty array (default) | nonnegative scalar

Rate of dose, specified as a nonnegative scalar value. Default is `[]`, that is, the dose is interpreted as a bolus (instantaneous) dose. For a schedule dose, you can create a combination of bolus and infusion doses by setting the `rate` property to a vector containing zeros and non-zeros.

Note You cannot change the `Rate` property of `ScheduleDose` for exported SimBiology model if *all* of the following conditions are true:

- The UnitConversion property of the model is already set to `true`.
- The `Rate` property is empty or set to zero.
- The `RateUnits` is set to empty.

To change the `Rate`, do one of the following:

- `Set` the UnitConversion property of the original model to `false`. Then `export` the model again.
- Set the `RateUnits` appropriately.

`RateUnits` — Units for dose rate

character vector

This property is read-only.

Units for dose rate, specified as a character vector.

`TargetName` — Species receiving dose

character vector

This property is read-only.

Species receiving dose, specified as a character vector.

`Time` — Schedule dose times

vector of nonnegative values

Schedule dose times, specified as a vector of nonnegative values.

`TimeUnits` — Time units for dosing
character vector

This property is read-only.

Time units for dosing, specified as a character vector.

Version History

Introduced in R2012b

See Also

`SimBiology.export.Dose` | `SimBiology.export.RepeatDose` | `export`

SimBiology.export.SimulationOptions Properties

Simulation settings for exported SimBiology model

Description

`SimBiology.export.SimulationOptions` is the object property of simulation options for exported models. Simulation options are either of object type `SimBiology.export.ODESimulationOptions` for deterministic solvers, or `SimBiology.export.StochasticSimulationOptions` for stochastic solvers.

Simulation options are created by the `export` function for SimBiology models.

Properties

Simulation Options

`MaximumNumberofLogs` — Maximum number of logs criterion to stop simulation
positive scalar

Maximum number of logs criterion to stop simulation, specified as a positive scalar value.

`MaximumWallClock` — Maximum elapsed wall clock time criterion to stop simulation
positive scalar

Maximum elapsed wall clock time criterion to stop simulation, specified as a positive scalar value.

`StopTime` — Simulation time criterion to stop simulation
nonnegative scalar

Simulation time criterion to stop simulation, specified as a nonnegative scalar value.

`TimeUnits` — Time units for simulation
character vector

This property is read-only.

Time units for simulation, specified as a character vector.

Version History

Introduced in R2012b

See Also

`SimBiology.export.ODESimulationOptions` | `SimBiology.export.StochasticSimulationOptions` | `export`

SimBiology.export.StochasticSimulationOptions Properties

Settings for stochastic simulation of exported SimBiology model

Description

`SimBiology.export.StochasticSimulationOptions` is the object property of simulation options associated with stochastic solvers. The object types of `SimBiology.export.StochasticSimulationOptions` are `SimBiology.export.ExplicitTauSimulationOptions` and `SimBiology.export.ImplicitTauSimulationOptions`.

Stochastic simulation options are created by the `export` function for SimBiology models with a stochastic `SolverType` (`ssa`, `expltau`, or `impltau`).

Properties

Stochastic Simulation Options

`LogDecimation` — Frequency to log stochastic simulation output
positive integer

Frequency to log stochastic simulation output, specified as a positive integer value.

`MaximumNumberofLogs` — Maximum number of logs criterion to stop simulation
positive scalar

Maximum number of logs criterion to stop simulation, specified as a positive scalar value.

`MaximumWallClock` — Maximum elapsed wall clock time criterion to stop simulation
positive scalar

Maximum elapsed wall clock time criterion to stop simulation, specified as a positive scalar value.

`RandomState` — Random number generator
positive integer

Random number generator, specified as a positive integer value.

`SolverType` — Solver type to use for simulation
`'ssa'` | `'expltau'` | `'impltau'`

This property is read-only.

Solver type to use for simulation, specified as a character vector. The stochastic solver type is one of:

- `'ssa'`
- `'expltau'`

- `'impltau'`

`StopTime` — Simulation time criterion to stop simulation
nonnegative scalar

Simulation time criterion to stop simulation, specified as a nonnegative scalar value.

`TimeUnits` — Time units for simulation
character vector

This property is read-only.

Time units for simulation, specified as a character vector.

Version History

Introduced in R2012b

See Also

`SimBiology.export.SimulationOptions` | `SimBiology.export.ODESimulationOptions` | `SimBiology.export.ExplicitTauSimulationOptions` | `SimBiology.export.ImplicitTauSimulationOptions` | `export`

updateDuplicateNames

Disambiguate duplicate component names in SimBiology model

Syntax

```
updateDuplicateNames(model)
[isUpdated,changes,modelBackup] = updateDuplicateNames(model)
```

Description

`updateDuplicateNames(model)` renames components with same names in a SimBiology `model`. Use this function to disambiguate duplicate model component names in your model if any. In a future release, within a single model, model components will be required to have unique names even when they are of different types with the following two exceptions:

- Species in different compartments can have the same name.
- Parameters can have the same name if they are scoped to different parents. Specifically, you can use the same name for a model-scoped parameter and reaction-scoped parameters, where each reaction-scoped parameter belongs to a different reaction.

For details, see “Guidelines for Naming Model Components”.

`[isUpdated,changes,modelBackup] = updateDuplicateNames(model)` returns additional information about the changes made to the model, including the logical flag `isUpdated` that indicates whether any updates were made to the model, a list of `changes`, and a backup copy `modelBackup` of your model without any changes made.

Examples

Update Duplicate Component Names in SimBiology Model

Suppose that you have a species and parameter with the same name as the model.

```
model = sbiomodel('m1');
compartment = addcompartment(model,'comp');
s1 = addspecies(compartment,'x');
p1 = addparameter(model,'x');
```

```
Warning: Model 'm1' contains components with the following duplicated names: x. <a href="matlab:
```

To avoid the warning, use `updateDuplicatNames` to automatically disambiguate the duplicate names.

```
[isUpdated, changes, modelBackup] = updateDuplicateNames(model);
```

Open the Comparison Tool to see the name changes. In this example, the function updated the parameter name from *x* to *x_1*.

```
visdiff(changes);
```

In a future release, within a single model, model components will be required to have unique names even when they are of different types with the following two exceptions:

- Species in different compartments can have the same name.
- Parameters can have the same name if they are scoped to different parents. Specifically, you can use the same name for a model-scoped parameter and reaction-scoped parameters, where each reaction-scoped parameter belongs to a different reaction.

To illustrate the first exception, add another species named *x* to a different compartment.

```
compartment2 = addcompartment(model,'comp2');
s2 = addspecies(compartment2,'x');
```

Note that no warning is issued for two species (*s1* and *s2*) with the same name because they belong to different compartments.

To give an example of the second exception, add two reaction-scoped parameters with the same name *param* to two different reactions *r1* and *r2*.

```
r1 = addreaction(model,'comp.x -> comp.y');
kl1 = addkineticlaw(r1,'MassAction');
p2 = addparameter(kl1,'param');
kl1.ParameterVariableNames = 'param';

r2 = addreaction(model,'comp2.x -> comp2.y');
kl2 = addkineticlaw(r2,'MassAction');
p3 = addparameter(kl2,'param');
kl2.ParameterVariableNames = 'param';
```

Note that no warning is issued for two parameters (*p2* and *p3*) with the same name because they are scoped to different reactions.

Input Arguments

`model` — Input model

scalar SimBiology `Model` object

Input model, specified as a scalar SimBiology `Model` object.

Output Arguments

`isUpdated` — Flag indicating whether the model was updated

`true` or 1 | `false` or 0

Flag indicating whether model was updated by the function, returned as a logical 1 (true) or 0 (false).

`changes` — List of changes

`SimBiology.DiffResults`

List of changes made to the model, returned as a `SimBiology.DiffResults` object. Use the `visdiff` function to inspect the changes in the Comparison Tool.

`modelBackup` — Copy of the input model

scalar SimBiology `Model` object

Copy of the input model before changes were made to it by the function, returned as a scalar SimBiology `Model` object.

Version History

Introduced in R2022b

See Also

`Model` | `SimBiology.DiffResults`

Topics

“Guidelines for Naming Model Components”

updateInitialAssignments

Update initial assignment rules to remove order dependencies

Syntax

```
updateInitialAssignments(model)
[tfUpdated, ruleChanges, newParameters, modelBackup] =
updateInitialAssignments(model)
```

Description

`updateInitialAssignments(model)` updates the active initial assignment rules in a SimBiology `model` to recover the same simulation results at time = 0, as in R2017a or earlier when the initial assignment rules were evaluated according to the order appeared in the model. As of R2017b, the order in which the initial assignment rules appear in the model has no effect on the simulation results. For details, see “Evaluation Order of Rules”.

`[tfUpdated, ruleChanges, newParameters, modelBackup] = updateInitialAssignments(model)` returns a boolean indicating whether the model is updated, `tfUpdated`, a table of changes made to the rules, `ruleChanges`, a vector of newly added parameters, `newParameters`, and a backup copy of the original model, appending the text `" (copy)"` to the original model name.

Examples

Remove Rule Order Dependencies in SimBiology Model

Load a sample model.

```
sbioloadproject lotka
```

Show the list of species and their initial amounts.

```
m1.Species
```

```
ans =
   SimBiology Species Array

   Index:    Compartment:    Name:    Value:    Units:
   1         unnamed         x        1
   2         unnamed         y1       900
   3         unnamed         y2       900
   4         unnamed         z        0
```

Add two initial assignment rules that can result in different outcomes depending on the order of the rules that appear in the model.

```
addrule(m1,'x = z','initialAssignment');
addrule(m1,'z = 100','initialAssignment');
```

Display the rules.

```
m1.Rules
```

```
ans =
   SimBiology Rule Array

   Index:    RuleType:            Rule:
   1         initialAssignment    x = z
   2         initialAssignment    z = 100
```

Remove the rule order dependencies from the model. `tf` is a boolean indicating whether the model was updated, `ruleChanges` is a summary table of changes made to the rules, and `newParas` is a vector of newly added parameter objects. `backup` is the copy of the original (unchanged) model.

```
[tf,ruleChanges,newParas,backup] = updateInitialAssignments(m1)
```

```
tf = logical
   1


ruleChanges=1×3 table
        UpdatedRule        OldAssignment    NewAssignment
    ___________________    _____________    _____________

    1x1 SimBiology.Rule       "x = z"          "x = z0"


newParas =
   SimBiology Parameter Array

   Index:    Name:    Value:    Units:
   1         z0       0


backup =
   SimBiology Model - lotka (copy)

   Model Components:
     Compartments:      1
     Events:            0
     Parameters:        3
     Reactions:         3
     Rules:             2
     Species:           4
     Observables:       0
```

In order to remove order dependencies, SimBiology updated the initial assignment expression `x = z` to `x = z0`, where `z0` is a newly added parameter.

Input Arguments

`model` — SimBiology model

model object (default)

SimBiology model, specified as a Model on page 2-439 object.

Example: `m1`

Output Arguments

`tfUpdated` — Whether model is updated
`true` | `false`

Whether the model is updated, returned as `true` or `false`.

`ruleChanges` — Table of changes made to rules
table

Table of changes made to initial assignment rules, returned as a table with one row per rule. The table contains the following columns.

Column	Description
`UpdatedRule`	Vector of the updated rule objects in the model.
`OldAssignment`	String vector of the original Rule property values in the model.
`NewAssignment`	String vector of the new Rule property values in the model.

`newParameters` — Newly added parameters
vector

Newly added parameters, returned as a vector of Parameter on page 2-488 objects that are referenced in the updated rules.

`modelBackup` — Backup copy of original model
model object

Backup copy of the original model, returned as a model object.

Version History

Introduced in R2017b

See Also

Model on page 2-439 | Parameter on page 2-488

Topics
“Evaluation Order of Rules”

SimBiology.export.ValueInfo Properties

Modifiable species, compartments, or parameters in exported SimBiology model

Description

`SimBiology.export.ValueInfo` is the object property that describes the modifiable value components in a `SimBiology.export.Model`, including species, parameters, and compartments.

`ValueInfo` properties are created by the `export` function for SimBiology models. By default, all model species, parameters, and compartments are `ValueInfo` properties, but you can specify which value components to export using the optional `editvals` input argument to `export`.

Properties

Object Properties

`Constant` — Display whether value is constant or time-varying
logical value

This property is read-only.

Display whether value is constant or time-varying, specified as a logical value.

`InitialValue` — Initial value for the component
scalar

Initial value for the component, specified as a scalar value.

`Name` — Name of species, compartment, or parameter
character vector

This property is read-only.

Name of a species, compartment, or parameter, specified as a character vector.

`Parent` — Name of parent model, compartment, or reaction
character vector

This property is read-only.

Name of parent model, compartment, or reaction, specified as a character vector.

`QualifiedName` — Qualified name of species, compartment, or parameter
character vector

This property is read-only.

Qualified name of species, compartment, or parameter, specified as a character vector.

- For compartments and model-scoped parameters, the qualified name is the same as the name.

- For species, the qualified name is `CompartmentName.SpeciesName`.
- For reaction-scoped parameters, the qualified name is `ReactionName.ParameterName`.

Tag — Label for species, compartment, or parameter
character vector

This property is read-only.

Label for species, compartment, or parameter, specified as a character vector.

Type — Type of value
`'species'` | `'parameter'` | `'compartment'`

This property is read-only.

Type of value, specified as `'species'`, `'parameter'`, or `'compartment'`.

`Units` — Value units
character vector

This property is read-only.

Value units, specified as a character vector.

Version History

Introduced in R2012b

See Also

`SimBiology.export.Model` | `export`

simbio.complexstep.abs

`abs` function for SimBiology local sensitivity analysis

Syntax

```
M = simbio.complexstep.abs(X)
```

Description

`M = simbio.complexstep.abs(X)` returns `M`, where `M = abs(real(X)) + 1i*imag(X)`. `simbio.complexstep.abs` is equivalent to `abs` when the input is real.

- When you have a SimBiology model with a custom function that calls `abs` and you are performing local sensitivity analysis on the model, replace `abs` with `simbio.complexstep.abs` in your custom function.
- You do not need to update SimBiology expressions (such as reaction rates or rules) that directly call `abs`. SimBiology automatically replaces `abs` with `simbio.complexstep.abs` whenever:
  - You calculate local sensitivities using `sbiosimulate`, a `SimFunctionSensitivity on page 2-220` object, or the **Calculate Sensitivities** program.
  - `sbiofit` or `fitproblem` uses local sensitivity analysis to determine the gradients of the objective function during parameter estimation.
- `simbio.complexstep.abs` is not differentiable when the real part of the input is 0 [1]. For more information, see “Local Sensitivity Analysis (LSA)”.

Examples

Use Replacements for abs, min, and max in Custom Functions for SimBiology Local Sensitivity Analysis

This example shows how to use replacements for `abs`, `min`, and `max` in some custom functions so that the model becomes compatible with local sensitivity analysis (LSA). The replacement functions are `simbio.complexstep.abs`, `simbio.complexstep.min`, and `simbio.complexstep.max`. Specifically, one of the custom functions used by this example computes the net amount of a drug species moved between two compartments. The other custom function sets the thresholds for the forward and reverse reaction fluxes.

Create a model.

```
model       = sbiomodel("model");
c1          = addcompartment(model,"c1");
c2          = addcompartment(model,"c2");
s1          = addspecies(c1,"Drug",2);
s2          = addspecies(c2,"Drug");
netFlux     = addspecies(c1,"netFlux");
reaction    = addreaction(model,"c1.Drug <-> c2.Drug");
kf          = addparameter(model,"kf",1.0);
kr          = addparameter(model,"kr",1.5);
```

```
fluxMin     = addparameter(model,"fluxMin",0.1);
fluxMax     = addparameter(model,"fluxMax",10);
```

Define the net amount of drug species moved between two compartments using a custom function `calculateNetFlux` based on the constrained forward and reverse reaction fluxes, which are defined later.

```
rule = addrule(model,"netFlux = calculateNetFlux(boundedForwardFlux,boundedReverseFlux)","rate");
```

calculateNetFlux uses `simbio.complexstep.abs`, and the function is already saved in the provided file named calculateNetFlux`.m`.

```
type calculateNetFlux.m
```

```
function netFlux = calculateNetAmount(forwardFlux,reverseFlux)
    netFlux   = simbio.complexstep.abs(forwardFlux-reverseFlux);
end
```

Define the forward and reverse fluxes of the reaction. Set the thresholds on the fluxes using the `imposeBounds` custom function.

```
boundedForwardFlux = addparameter(model,"boundedForwardFlux","Constant",false);
boundedReverseFlux = addparameter(model,"boundedReverseFlux","Constant",false);
forwardFlux        = addparameter(model,"forwardFlux","Constant",false);
reverseFlux        = addparameter(model,"reverseFlux","Constant",false);

forwardFlux        = addrule(model,"forwardFlux = kf*c1.Drug","repeatedAssignment");
reverseFlux        = addrule(model,"reverseFlux = kr*c2.Drug","repeatedAssignment");
boundedForwardFlux = addrule(model,"boundedForwardFlux = imposeBounds(forwardFlux,fluxMin,fluxMax
boundedReverseFlux = addrule(model,"boundedReverseFlux = imposeBounds(reverseFlux,fluxMin,fluxMax
reaction.ReactionRate = "boundedForwardFlux - boundedReverseFlux";
```

`imposeBounds` uses `simbio.complexstep.min` and `simbio.complexstep.max` to set the lower and upper limits for the reaction flux.

```
type imposeBounds.m
```

```
function boundedFlux = imposeBounds(fluxInput,fluxMin,fluxMax)
    fm             = simbio.complexstep.max(fluxMin,fluxInput);
    boundedFlux    = simbio.complexstep.min(fluxMax,fm);
end
```

Enable local sensitivity analysis.

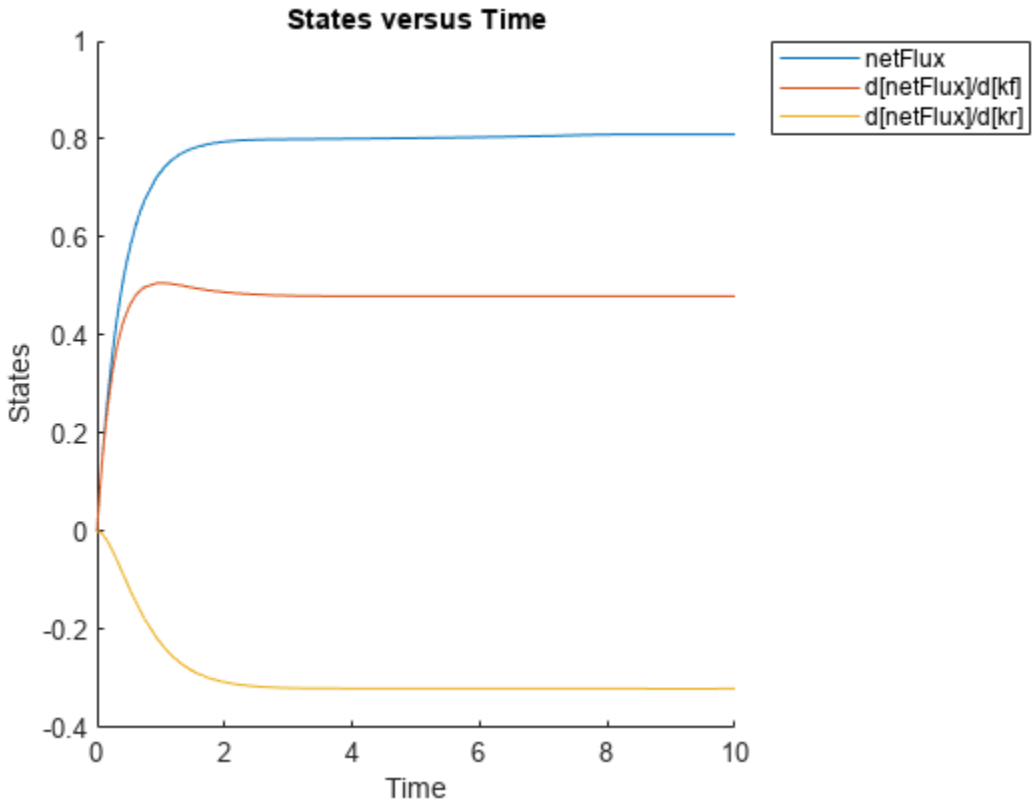
```
configset = getconfigset(model);
configset.RuntimeOptions.StatesToLog        = "netFlux";
configset.SolverOptions.SensitivityAnalysis = true;
sensitivityOptions          = configset.SensitivityAnalysisOptions;
sensitivityOptions.Inputs   = [kf,kr];
sensitivityOptions.Outputs  = netFlux;
```

Temporarily disable the warning about unsupported functions. The warning is safe to ignore.

```
warnState  = warning("off","SimBiology:senscsverify:UnsupportedFunction");
cleanupobj = onCleanup(@()warning(warnState));
```

Simulate the model and perform sensitivity analysis.

```
simdata = sbiosimulate(model);
sbioplot(simdata);
```




```
delete(cleanupobj);
```

Input Arguments

X — Input array

scalar | vector | matrix | multidimensional array

Input array, specified as a numeric scalar, vector, matrix, or multidimensional array.

Data Types: `double`
Complex Number Support: Yes

Output Arguments

M — Output array

scalar | vector | matrix | multidimensional array

Output array, returned as a numeric scalar, vector, matrix, or multidimensional array. The size of the output array is the same as the input array.

- For a complex number `x` with a nonnegative real part, `simbio.complexstep.abs(x) = x`.

- For a complex number `x` with a negative real part, `simbio.complexstep.abs(x) = -real(x) + 1i*imag(X)`.

Version History

Introduced in R2022b

References

[1] Martins, Joaquim, Ilan Kroo, and Juan Alonso. "An Automated Method for Sensitivity Analysis Using Complex Variables." In *38th Aerospace Sciences Meeting and Exhibit*. Reno, NV, U.S.A.: American Institute of Aeronautics and Astronautics, 2000. https://doi.org/10.2514/6.2000-689.

See Also

`simbio.complexstep.max` | `simbio.complexstep.min` | `abs`

Topics

"Local Sensitivity Analysis (LSA)"

simbio.complexstep.max

max function for SimBiology local sensitivity analysis

Syntax

```
M = simbio.complexstep.max(X,Y)
```

Description

`M = simbio.complexstep.max(X,Y)` returns `X` if `real(X)` is greater than `real(Y)`. Otherwise, the function returns `Y`. `simbio.complexstep.max` is equivalent to `max` when both inputs are real.

- When you have a SimBiology model with a custom function that calls `max` and you are performing local sensitivity analysis on the model, replace `max` with `simbio.complexstep.max` in your custom function.
- You do not need to update SimBiology expressions (such as reaction rates or rules) that directly call `max`. SimBiology automatically replaces `max` with `simbio.complexstep.max` whenever:
  - You calculate local sensitivities using `sbiosimulate`, a `SimFunctionSensitivity on page 2-220` object, or the **Calculate Sensitivities** program.
  - `sbiofit` or `fitproblem` uses local sensitivity analysis to determine the gradients of the objective function during parameter estimation.
- `simbio.complexstep.max` is not differentiable when the real parts of `X` and `Y` are equal [1]. For more information, see “Local Sensitivity Analysis (LSA)”.

Examples

Use Replacements for abs, min, and max in Custom Functions for SimBiology Local Sensitivity Analysis

This example shows how to use replacements for `abs`, `min`, and `max` in some custom functions so that the model becomes compatible with local sensitivity analysis (LSA). The replacement functions are `simbio.complexstep.abs`, `simbio.complexstep.min`, and `simbio.complexstep.max`. Specifically, one of the custom functions used by this example computes the net amount of a drug species moved between two compartments. The other custom function sets the thresholds for the forward and reverse reaction fluxes.

Create a model.

```
model       = sbiomodel("model");
c1          = addcompartment(model,"c1");
c2          = addcompartment(model,"c2");
s1          = addspecies(c1,"Drug",2);
s2          = addspecies(c2,"Drug");
netFlux     = addspecies(c1,"netFlux");
reaction    = addreaction(model,"c1.Drug <-> c2.Drug");
kf          = addparameter(model,"kf",1.0);
kr          = addparameter(model,"kr",1.5);
```

```
fluxMin     = addparameter(model,"fluxMin",0.1);
fluxMax     = addparameter(model,"fluxMax",10);
```

Define the net amount of drug species moved between two compartments using a custom function `calculateNetFlux` based on the constrained forward and reverse reaction fluxes, which are defined later.

```
rule = addrule(model,"netFlux = calculateNetFlux(boundedForwardFlux,boundedReverseFlux)","rate");
```

calculateNetFlux uses `simbio.complexstep.abs`, and the function is already saved in the provided file named calculateNetFlux.m.

```
type calculateNetFlux.m
```

```
function netFlux = calculateNetAmount(forwardFlux,reverseFlux)
    netFlux   = simbio.complexstep.abs(forwardFlux-reverseFlux);
end
```

Define the forward and reverse fluxes of the reaction. Set the thresholds on the fluxes using the `imposeBounds` custom function.

```
boundedForwardFlux = addparameter(model,"boundedForwardFlux","Constant",false);
boundedReverseFlux = addparameter(model,"boundedReverseFlux","Constant",false);
forwardFlux        = addparameter(model,"forwardFlux","Constant",false);
reverseFlux        = addparameter(model,"reverseFlux","Constant",false);

forwardFlux        = addrule(model,"forwardFlux = kf*c1.Drug","repeatedAssignment");
reverseFlux        = addrule(model,"reverseFlux = kr*c2.Drug","repeatedAssignment");
boundedForwardFlux = addrule(model,"boundedForwardFlux = imposeBounds(forwardFlux,fluxMin,fluxMax
boundedReverseFlux = addrule(model,"boundedReverseFlux = imposeBounds(reverseFlux,fluxMin,fluxMax
reaction.ReactionRate = "boundedForwardFlux - boundedReverseFlux";
```

`imposeBounds` uses `simbio.complexstep.min` and `simbio.complexstep.max` to set the lower and upper limits for the reaction flux.

```
type imposeBounds.m
```

```
function boundedFlux = imposeBounds(fluxInput,fluxMin,fluxMax)
    fm             = simbio.complexstep.max(fluxMin,fluxInput);
    boundedFlux    = simbio.complexstep.min(fluxMax,fm);
end
```

Enable local sensitivity analysis.

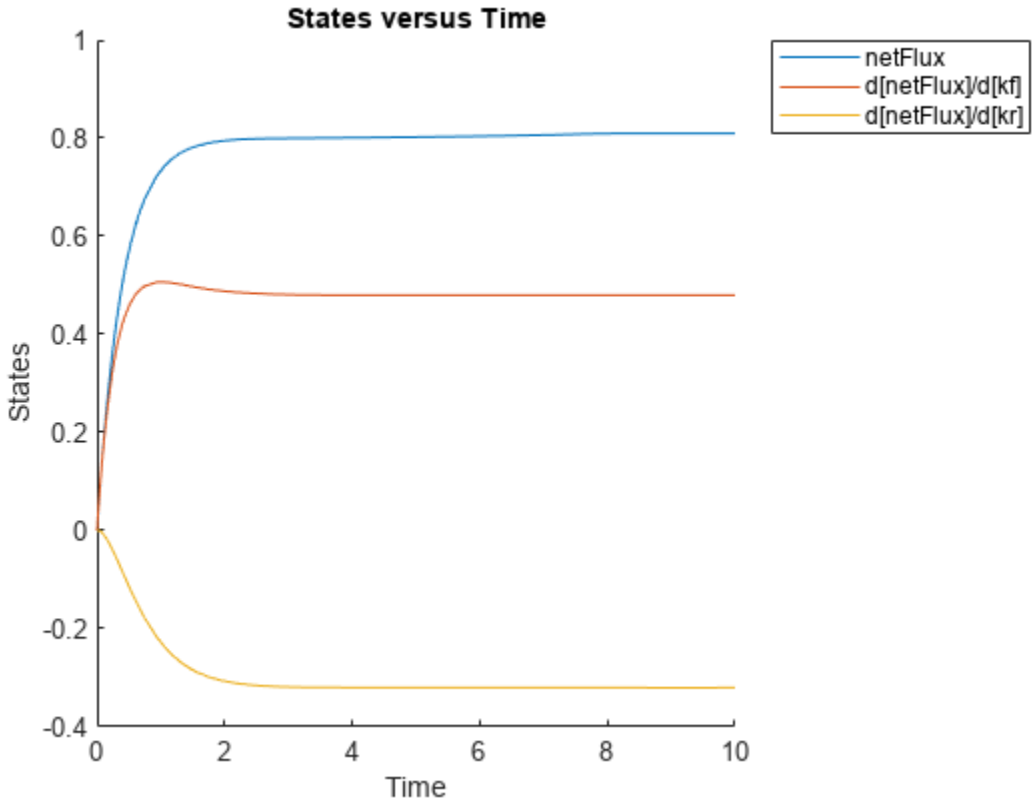
```
configset = getconfigset(model);
configset.RuntimeOptions.StatesToLog        = "netFlux";
configset.SolverOptions.SensitivityAnalysis = true;
sensitivityOptions          = configset.SensitivityAnalysisOptions;
sensitivityOptions.Inputs   = [kf,kr];
sensitivityOptions.Outputs  = netFlux;
```

Temporarily disable the warning about unsupported functions. The warning is safe to ignore.

```
warnState  = warning("off","SimBiology:senscsverify:UnsupportedFunction");
cleanupobj = onCleanup(@()warning(warnState));
```

Simulate the model and perform sensitivity analysis.

```
simdata = sbiosimulate(model);
sbioplot(simdata);
```




```
delete(cleanupobj);
```

Input Arguments

X — First input

scalar

First input, specified as a numeric scalar.

Data Types: `double`
Complex Number Support: Yes

Y — Second input

scalar

Second input, specified as a numeric scalar.

Data Types: `double`
Complex Number Support: Yes

Version History

Introduced in R2022b

References

[1] Martins, Joaquim, Ilan Kroo, and Juan Alonso. “An Automated Method for Sensitivity Analysis Using Complex Variables.” In *38th Aerospace Sciences Meeting and Exhibit*. Reno, NV, U.S.A.: American Institute of Aeronautics and Astronautics, 2000. https://doi.org/10.2514/6.2000-689.

See Also

`simbio.complexstep.abs` | `simbio.complexstep.min` | `max`

Topics

“Local Sensitivity Analysis (LSA)”

simbio.complexstep.min

`min` function for SimBiology local sensitivity analysis

Syntax

```
M = simbio.complexstep.min(X,Y)
```

Description

`M = simbio.complexstep.min(X,Y)` returns `X` if `real(X)` is less than `real(Y)`. Otherwise, the function returns `Y`. `simbio.complexstep.min` is equivalent to `min` when both inputs are real.

- When you have a SimBiology model with a custom function that calls `min` and you are performing local sensitivity analysis on the model, replace `min` with `simbio.complexstep.min` in your custom function.
- You do not need to update SimBiology expressions (such as reaction rates or rules) that directly call `min`. SimBiology automatically replaces `min` with `simbio.complexstep.min` whenever:
  - You calculate local sensitivities using `sbiosimulate`, a `SimFunctionSensitivity on page 2-220` object, or the **Calculate Sensitivities** program.
  - `sbiofit` or `fitproblem` uses local sensitivity analysis to determine the gradients of the objective function during parameter estimation.
- `simbio.complexstep.min` is not differentiable when the real parts of `X` and `Y` are equal [1]. For more information, see “Local Sensitivity Analysis (LSA)”.

Examples

Use Replacements for abs, min, and max in Custom Functions for SimBiology Local Sensitivity Analysis

This example shows how to use replacements for `abs`, `min`, and `max` in some custom functions so that the model becomes compatible with local sensitivity analysis (LSA). The replacement functions are `simbio.complexstep.abs`, `simbio.complexstep.min`, and `simbio.complexstep.max`. Specifically, one of the custom functions used by this example computes the net amount of a drug species moved between two compartments. The other custom function sets the thresholds for the forward and reverse reaction fluxes.

Create a model.

```
model       = sbiomodel("model");
c1          = addcompartment(model,"c1");
c2          = addcompartment(model,"c2");
s1          = addspecies(c1,"Drug",2);
s2          = addspecies(c2,"Drug");
netFlux     = addspecies(c1,"netFlux");
reaction    = addreaction(model,"c1.Drug <-> c2.Drug");
kf          = addparameter(model,"kf",1.0);
kr          = addparameter(model,"kr",1.5);
```

```
fluxMin     = addparameter(model,"fluxMin",0.1);
fluxMax     = addparameter(model,"fluxMax",10);
```

Define the net amount of drug species moved between two compartments using a custom function `calculateNetFlux` based on the constrained forward and reverse reaction fluxes, which are defined later.

```
rule = addrule(model,"netFlux = calculateNetFlux(boundedForwardFlux,boundedReverseFlux)","rate");
```

calculateNetFlux uses `simbio.complexstep.abs`, and the function is already saved in the provided file named calculateNetFlux.m.

```
type calculateNetFlux.m
```

```
function netFlux = calculateNetAmount(forwardFlux,reverseFlux)
    netFlux   = simbio.complexstep.abs(forwardFlux-reverseFlux);
end
```

Define the forward and reverse fluxes of the reaction. Set the thresholds on the fluxes using the `imposeBounds` custom function.

```
boundedForwardFlux = addparameter(model,"boundedForwardFlux","Constant",false);
boundedReverseFlux = addparameter(model,"boundedReverseFlux","Constant",false);
forwardFlux        = addparameter(model,"forwardFlux","Constant",false);
reverseFlux        = addparameter(model,"reverseFlux","Constant",false);

forwardFlux        = addrule(model,"forwardFlux = kf*c1.Drug","repeatedAssignment");
reverseFlux        = addrule(model,"reverseFlux = kr*c2.Drug","repeatedAssignment");
boundedForwardFlux = addrule(model,"boundedForwardFlux = imposeBounds(forwardFlux,fluxMin,fluxMax
boundedReverseFlux = addrule(model,"boundedReverseFlux = imposeBounds(reverseFlux,fluxMin,fluxMax
reaction.ReactionRate = "boundedForwardFlux - boundedReverseFlux";
```

`imposeBounds` uses `simbio.complexstep.min` and `simbio.complexstep.max` to set the lower and upper limits for the reaction flux.

```
type imposeBounds.m
```

```
function boundedFlux = imposeBounds(fluxInput,fluxMin,fluxMax)
    fm             = simbio.complexstep.max(fluxMin,fluxInput);
    boundedFlux    = simbio.complexstep.min(fluxMax,fm);
end
```

Enable local sensitivity analysis.

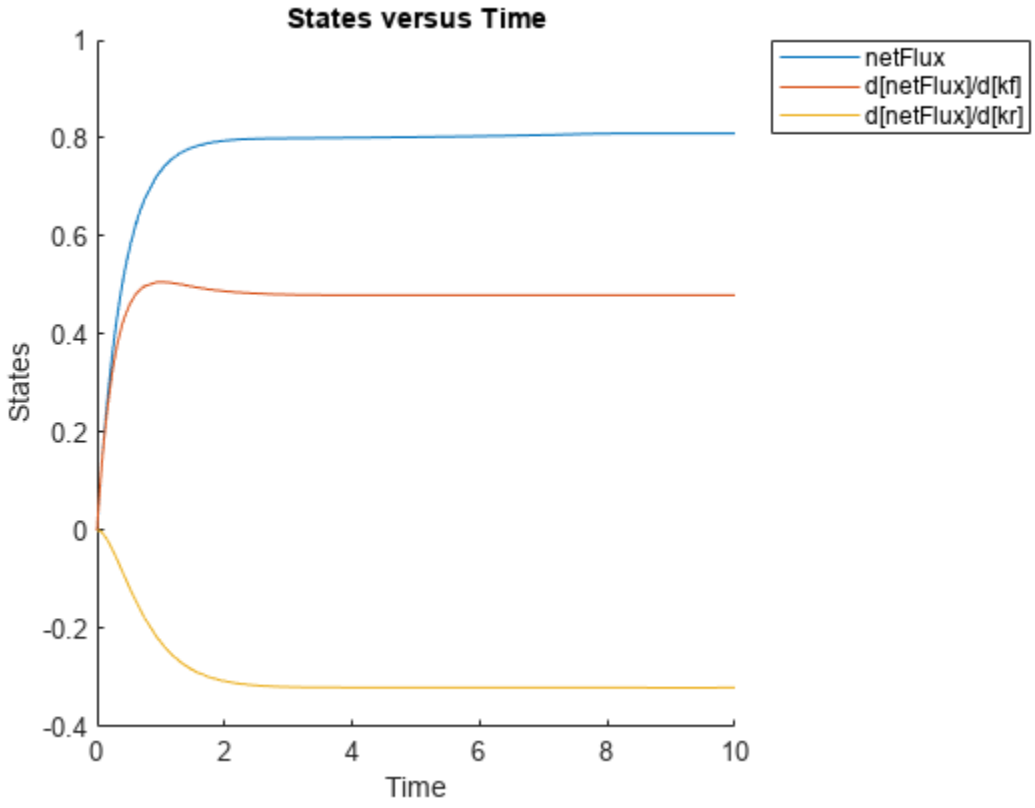
```
configset = getconfigset(model);
configset.RuntimeOptions.StatesToLog        = "netFlux";
configset.SolverOptions.SensitivityAnalysis = true;
sensitivityOptions          = configset.SensitivityAnalysisOptions;
sensitivityOptions.Inputs   = [kf,kr];
sensitivityOptions.Outputs  = netFlux;
```

Temporarily disable the warning about unsupported functions. The warning is safe to ignore.

```
warnState  = warning("off","SimBiology:senscsverify:UnsupportedFunction");
cleanupobj = onCleanup(@()warning(warnState));
```

Simulate the model and perform sensitivity analysis.

```
simdata = sbiosimulate(model);
sbioplot(simdata);
```




```
delete(cleanupobj);
```

Input Arguments

X — First input

scalar

First input, specified as a numeric scalar.

Data Types: `double`
Complex Number Support: Yes

Y — Second input

scalar

Second input, specified as a numeric scalar.

Data Types: `double`
Complex Number Support: Yes

Version History

Introduced in R2022b

References

[1] Martins, Joaquim, Ilan Kroo, and Juan Alonso. “An Automated Method for Sensitivity Analysis Using Complex Variables.” In *38th Aerospace Sciences Meeting and Exhibit*. Reno, NV, U.S.A.: American Institute of Aeronautics and Astronautics, 2000. https://doi.org/10.2514/6.2000-689.

See Also

`simbio.complexstep.abs` | `simbio.complexstep.max` | `min`

Topics

“Local Sensitivity Analysis (LSA)”

simbio.diagram.getBlock

Package: `simbio.diagram`

Get SimBiology diagram block properties

Syntax

```
SV = simbio.diagram.getBlock(sObj)
SV = simbio.diagram.getBlock(speciesObj,exprObj)
QV = simbio.diagram.getBlock(sObj,propertyNames)
QV = simbio.diagram.getBlock(speciesObj,exprObj,propertyNames)
simbio.diagram.getBlock( ___ )
```

Description

`simbio.diagram.getBlock` returns properties of diagram blocks shown in **SimBiology Model Builder**.

Before you run the function at the command line:

1. Open the corresponding SimBiology model in the **SimBiology Model Builder** app.
2. Export the model from the app to MATLAB workspace by selecting **Export > Export Model to MATLAB Workspace** on the **Home** tab of the app.

You can query and configure only the properties of the objects shown in the **Diagram** tab of the app. The objects shown in the diagram are compartments, species, reactions, rate rules, repeated assignment rules, and parameters that are on the left-hand side of a rate rule, a repeated assignment rule, or an event function.

`SV = simbio.diagram.getBlock(sObj)` returns the names and current values of the block properties of a SimBiology object `sObj` as a structure `SV`.

`SV = simbio.diagram.getBlock(speciesObj,exprObj)` returns the names and current values of the block properties of the species object `speciesObj` that is connected to an expression (reaction, rate rule, or repeated assignment rule) object `exprObj`. You can use this syntax to configure the `Position`, `Pin`, and `Visible` properties of a specific cloned block when you have multiple clones of the same species. Clones have the same values for all the other properties.

`QV = simbio.diagram.getBlock(sObj,propertyNames)` returns the values of the specified block properties `propertyNames` of a SimBiology object `sObj`.

`QV = simbio.diagram.getBlock(speciesObj,exprObj,propertyNames)` returns the names and current values of the specified block properties `propertyNames` of the species object `speciesObj` that is connected to an expression object `exprObj`.

`simbio.diagram.getBlock( ___ )` displays the names and values of block properties. Use this syntax with any of the input arguments in the previous syntaxes.

Examples

Configure SimBiology Diagram Block Properties

You can programmatically adjust the appearances and locations of diagram blocks of a SimBiology model.

Open the `lotka` model in the **SimBiology Model Builder** app.

```
simBiologyModelBuilder('lotka')
```

The app opens and shows the model in the **Diagram** tab.

On the **Home** tab of the app, select **Export > Export Model to MATLAB Workspace**.

In the **SimBiology Model Export** dialog, click **OK** to export the model with the variable name *m1*.

Go to the MATLAB command line and confirm that the model *m1* is in the workspace. Get a list of species of the model.

```
m1.Species
```

```
ans =

   SimBiology Species Array

   Index:    Compartment:    Name:    Value:    Units:
   1         unnamed         x        1
   2         unnamed         y1       900
   3         unnamed         y2       900
   4         unnamed         z        0
```

Get the current block shape of species *x*.

```
x = m1.Species(1);
v = simbio.diagram.getBlock(x,'Shape')
```

```
v =

    'rounded rectangle'
```

Get a list of all possible shapes for the species block.

```
simbio.diagram.setBlock(x,'Shape')
```

```
ans =

  8×1 cell array

    {'rounded rectangle'}
    {'rectangle'        }
    {'oval'             }
    {'triangle'         }
    {'hexagon'          }
    {'chevron'          }
    {'parallelogram'    }
    {'diamond'          }
```

Set the shape of the species block to an oval.

```
simbio.diagram.setBlock(x,'Shape','oval')
```

Get the current position of the block. The first two numbers represent the x and y coordinates with respect to the top left corner ($x = 0$, $y = 0$) of the diagram. The last two numbers represent the width and height of the block.

```
simbio.diagram.getBlock(x,'Position')
```

```
ans =

   223   137    30    15
```

Set the position to a new location.

```
simbio.diagram.setBlock(x,'Position',[260 130 30 15])
```

You can also configure multiple properties.

```
simbio.diagram.setBlock(x,'FaceColor','yellow','FontSize',20,'TextLocation','center')
```

Configure Cloned Species Block Properties

When you have multiple cloned blocks for the same species in a SimBiology diagram, you can programmatically adjust the position and visibility of a specific clone by specifying the expression block that the cloned species is connected to. In other words, you can change the `Position`, `Pin`, and `Visible` properties specific to an individual clone. All the other properties have the same values across all clones of the same species.

Open the `gprotein` model in the **SimBiology Model Builder** app.

```
simBiologyModelBuilder('gprotein');
```

The app opens and shows the model in the **Diagram** tab.

On the **Home** tab of the app, select **Export > Export Model to MATLAB Workspace**.

In the **SimBiology Model Export** dialog, click **OK** to export the model with the variable name *m1*.

Go to the MATLAB command line and confirm that the model *m1* is in the workspace. Get a list of species of the model.

```
m1.Species
```

```
ans =

   SimBiology Species Array

   Index:    Compartment:    Name:    Value:       Units:
   1         unnamed         G        7000
   2         unnamed         Gd       3000
   3         unnamed         Ga       0
   4         unnamed         RL       0
   5         unnamed         L        6.022e+17
   6         unnamed         R        10000
   7         unnamed         Gbg      3000
```

The species block *Gbg* is cloned and connected to two reactions: `G protein activation` and `G protein complex formation`. Get the current position of the cloned block connected to the second reaction.

```
Gbg = m1.Species(7);
r2 = m1.Reaction(2);
simbio.diagram.getBlock(Gbg,r2,'Position')
```

```
ans =

   393   307    30    15
```

Unpin the cloned block and move it to another position.

```
simbio.diagram.setBlock(Gbg,r2,'Pin',false,'Position',[391 340 30 15])
```

Input Arguments

`sObj` — SimBiology object

`Compartment` object | `Species` object | `Reaction` object | `Rule` object | `Parameter` object | array of objects

SimBiology object, specified as a `Compartment`, `Species`, `Reaction`, `Rule`, or `Parameter` object, or as an array of objects.

`propertyNames` — Names of block properties

character vector | string | string vector | cell array of character vectors

Names of block properties, specified as a character vector, string, string vector, or cell array of character vectors. You can specify multiple property names as an 1-by-*N* or *N*-by-1 cell array of names.

Available block properties follow.

Property Name	Description
`Connections`	Read-only property that lists the objects connected to the input block
`Cloned`	Read-only flag indicating if more than one block exists for the input object. You can clone only species blocks.
`EdgeColor`	Block edge color, specified as one of these values: • RGB triplet, such as `[1 1 0]` • Character vector or string representing the color name, such as `'y'` or `'yellow'`
`ExpressionLines`	Flag to show lines from the expression block to other model components referenced by the expression, specified as `'show'` or `'hide'`. You can set this property for reactions or rules.
`FaceColor`	Block face color, specified as one of these values: • RGB triplet, such as `[1 1 0]` • Character vector or string representing the color name, such as `'y'` or `'yellow'`

Property Name	Description
`FontName`	Block text font, specified as a character vector or string. Valid options are: • `'Arial'` • `'Arial Black'` • `'Arial Narrow'` • `'Comic Sans MS'` • `'Courier'` • `'Courier New'` • `'Georgia'` • `'Helvetica'` • `'Impact'` • `'Times New Roman'` • `'Trebuchet MS'` • `'Verdana'`
`FontSize`	Block text font size, specified as a positive scalar
`FontWeight`	Block text font thickness, specified as `'plain'`, `'bold'`, `'italic'`, or `'bold italic'`
`Object`	Read-only property that lists the corresponding SimBiology object of the block
`Pin`	Flag to indicate if a block can be moved or not. Set the property to `false` to allow moving the block in the diagram.
`Position`	Position and size of the block, specified as a four-element vector `[x,y,width,height]`. The position of the upper-left corner of the diagram is equal to x = 0 and y = 0. SimBiology configures all block positions relative to that corner. You can configure block positions to negative positions.
`Rotate`	Block rotation, specified as a scalar between 0 and 360. You cannot rotate compartment blocks.
`Shape`	Block shape, specified as a character vector or string. Valid options are: • `'rounded rectangle'` • `'rectangle'` • `'oval'` • `'triangle'` • `'hexagon'` • `'chevron'` • `'parallelogram'` • `'diamond'` Compartment blocks must be `'rounded rectangle'` or `'rectangle'`.

Property Name	Description
`TextColor`	Block text color, specified as one of these values: • RGB triplet, such as `[1 1 0]` • Character vector or string representing the color name, such as `'y'` or `'yellow'`
`TextLocation`	Block text location relative to the block, specified as one of the following: `'top'`, `'left'`, `'bottom'`, `'right'`, `'center'`, or `'none'`
`Visible`	Flag to indicate if the block is visible in the diagram. Set the property to false to hide the block. **Warning** Starting in R2022a, this property for all compartment blocks is always set to 1 and you can no longer hide compartments.

Example: `'Position'`

Data Types: `double` | `char` | `string` | `cell`

`speciesObj` — Species object
`Species` object

Species object, specified as a SimBiology `Species` object. `speciesObj` must be scalar.

`exprObj` — Expression object
`Reaction` object | `Rule` object

Expression object, specified as a `Reaction` or `Rule` object. The rule object can be a rate rule or repeated assignment rule. `exprObj` must be a scalar.

Output Arguments

`QV` — Values of queried properties
numeric vector | character vector | logical scalar | object | cell array

Values of queried properties, returned as a numeric vector, character vector, logical scalar, SimBiology object, or cell array.

If `sObj` is an array of objects, `QV` is an *M*-by-`1` cell array of values where *M* equals to the length of `sObj`.

If you also specify an *N*-by-`1` or `1`-by-*N* cell array for `propertyNames`, `QV` is an *M*-by-*N* cell array of values, where *N* is the number of properties.

`SV` — Structure of property names and values
structure | structure array

Structure of property names and values, returned as a structure or structure array. The field names are the object property names and values are the current values of the corresponding properties.

If `sObj` is an array of objects, `SV` is an array of structures. The function returns one structure per block. If `sObj` has multiple cloned blocks, `SV` contains a structure for each cloned block.

Version History

Introduced in R2021a

See Also

SimBiology Model Builder | `simbio.diagram.setBlock` | `simbio.diagram.getLine` | `simbio.diagram.setLine` | `simbio.diagram.splitBlock` | `simbio.diagram.joinBlock`

Topics

“Create Model of Receptor-Ligand Kinetics”
“Incorporate SGLT2 Inhibition into Physiologically Based Glucose-Insulin Model Using SimBiology Model Builder”

simbio.diagram.getLine

Package: `simbio.diagram`

Get SimBiology diagram line properties

Syntax

```
SV = simbio.diagram.getLine(sObj)
SV = simbio.diagram.getLine(obj1,obj2)
QV = simbio.diagram.getLine(sObj,propertyNames)
QV = simbio.diagram.getLine(obj1,obj2,propertyNames)
simbio.diagram.getLine( ___ )
```

Description

`simbio.diagram.getLine` returns properties of diagram lines shown in **SimBiology Model Builder**.

Before you run the function at the command line:

1. Open the corresponding SimBiology model in the **SimBiology Model Builder** app.
2. Export the model from the app to MATLAB workspace by selecting **Export > Export Model to MATLAB Workspace** on the **Home** tab of the app.

You can query and configure only the properties of the objects shown in the **Diagram** tab of the app. The objects shown in the diagram are compartments, species, reactions, rate rules, repeated assignment rules, and parameters that are on the left-hand side of a rate rule, a repeated assignment rule, or an event function.

`SV = simbio.diagram.getLine(sObj)` returns the names and current values of all properties of all lines connected to a SimBiology object `sObj` as a structure `SV`.

`SV = simbio.diagram.getLine(obj1,obj2)` returns all the properties of a line that connects two SimBiology objects `obj1` and `obj2` as a structure `SV`. `obj1` and `obj2` must be scalar.

`QV = simbio.diagram.getLine(sObj,propertyNames)` returns the values of the specified properties `propertyNames` of the lines connected to a SimBiology object `sObj`.

`QV = simbio.diagram.getLine(obj1,obj2,propertyNames)` returns the values of the specified properties of a line that connects two SimBiology objects `obj1` and `obj2`. `obj1` and `obj2` must be scalar.

`simbio.diagram.getLine( ___ )` displays the names and values of all line properties. Use this syntax with any of the input arguments in the previous syntaxes.

Examples

Configure SimBiology Diagram Line Properties

You can programmatically adjust the appearance of lines connected to blocks in a diagram.

Open the `lotka` model in the **SimBiology Model Builder** app.

```
simBiologyModelBuilder('lotka');
```

The app opens and shows the model in the **Diagram** tab.

On the **Home** tab of the app, select **Export > Export Model to MATLAB Workspace**.

In the **SimBiology Model Export** dialog, click **OK** to export the model with the variable name *m1*.

Go to the MATLAB command line and confirm that the model *m1* is in the workspace. Get a list of species of the model.

```
m1.Species
```

```
ans =

   SimBiology Species Array

   Index:    Compartment:    Name:    Value:    Units:
   1         unnamed         x        1
   2         unnamed         y1       900
   3         unnamed         y2       900
   4         unnamed         z        0
```

Get the current property values of the line connected to species *x*. If multiple lines are connected to the species, the function returns an array of structures containing one structure per line.

```
x = m1.Species(1);
sv = simbio.diagram.getLine(x)
```

```
sv =

  struct with fields:

          Color: [66 66 66]
    Connections: [1×2 SimBiology.ModelComponent]
          Width: 1
```

Change the line color to red and increase the line width.

```
simbio.diagram.setLine(x,'Color','red','Width',2)
```

You can also query properties of a line that connects two objects. For example, get the property values of the line that connects species `y1` and `Reaction1`.

```
y1 = m1.Species(2);
r1 = m1.Reactions(1);
simbio.diagram.getLine(y1,r1)
```

```
ans =

  struct with fields:

          Color: [66 66 66]
```

```
    Connections: [1×2 SimBiology.ModelComponent]
          Width: 1
```

Change the line color to a new RGB value and increase the line width.

```
simbio.diagram.setLine(y1,r1,'Color',[0.6 0.2 0.6],'Width',3)
```

Input Arguments

`sObj` — SimBiology object

`Compartment` object | `Species` object | `Reaction` object | `Rule` object | `Parameter` object | array of objects

SimBiology object, specified as a `Compartment`, `Species`, `Reaction`, `Rule`, or `Parameter` object, or as an array of objects.

`propertyNames` — Names of line properties

character vector | string | string vector | cell array of character vectors

Names of line properties, specified as a character vector, string, string vector, or cell array of character vectors. You can specify multiple property names as a 1-by-*N* or *N*-by-1 cell array of names.

Available line properties follow.

Property Name	Description
`Color`	Line color, specified as one of these values: • RGB triplet, such as `[1 1 0]` • Character vector or string representing the color name, such as `'y'` or `'yellow'`
`Connections`	Read-only property that lists the objects connected by the line
`Width`	Line width, specified as a positive scalar

Example: `'Width'`

Data Types: `char` | `string` | `cell`

`obj1` — SimBiology object

`Compartment` object | `Species` object | `Reaction` object | `Rule` object | `Parameter` object

SimBiology object, specified as a `Compartment`, `Species`, `Reaction`, `Rule`, or `Parameter` object.

`obj2` — SimBiology object

`Compartment` object | `Species` object | `Reaction` object | `Rule` object | `Parameter` object

SimBiology object, specified as a `Compartment`, `Species`, `Reaction`, `Rule`, or `Parameter` object.

Output Arguments

`QV` — Values of queried properties

numeric vector | character vector | object | cell array

Values of queried properties, returned as a numeric vector, character vector, SimBiology object, or cell array.

If multiple lines are connected to the SimBiology object `sObj` or if `sObj` is an array of objects, `QV` is an *M*-by-`1` cell array of values where *M* equals the total number of lines connected to each object in `sObj`.

If you also specify an *N*-by-`1` or `1`-by-*N* cell array for `propertyNames`, `QV` is an *M*-by-*N* cell array of values, where *N* is the number of properties.

`SV` — Structure of property names and values
structure | structure array

Structure of property names and values, returned as a structure or structure array. The field names are the object property names and the values are the current values of the corresponding properties.

If multiple lines are connected to the SimBiology object `sObj` or if `sObj` is an array of objects, `SV` is an array of structures. The function returns one structure per line.

Version History

Introduced in R2021a

See Also

SimBiology Model Builder | `simbio.diagram.getBlock` | `simbio.diagram.setBlock` | `simbio.diagram.setLine` | `simbio.diagram.splitBlock` | `simbio.diagram.joinBlock`

Topics

“Create Model of Receptor-Ligand Kinetics”
“Incorporate SGLT2 Inhibition into Physiologically Based Glucose-Insulin Model Using SimBiology Model Builder”

simbio.diagram.joinBlock

Package: `simbio.diagram`

Combine copies of SimBiology species block in diagram

Syntax

```
simbio.diagram.joinBlock(speciesObj)
simbio.diagram.joinBlock(speciesObj,exprObj)
simbio.diagram.joinBlock(speciesObj,exprObj1,exprObj2)
```

Description

`simbio.diagram.joinBlock` combines cloned blocks of a species block into one block in **SimBiology Model Builder**.

Before you run the function at the command line:

1. Open the corresponding SimBiology model in the **SimBiology Model Builder** app.
2. Export the model from the app to MATLAB workspace by selecting **Export > Export Model to MATLAB Workspace** on the **Home** tab of the app.

You can query and configure only the properties of the objects shown in the **Diagram** tab of the app. The objects shown in the diagram are compartments, species, reactions, rate rules, repeated assignment rules, and parameters that are on the left-hand side of a rate rule, a repeated assignment rule, or an event function.

`simbio.diagram.joinBlock(speciesObj)` combines all copies of the SimBiology species `speciesObj` block into one block in the model diagram. `speciesObj` must be scalar.

`simbio.diagram.joinBlock(speciesObj,exprObj)` combines all copies of the species `speciesObj` block into one block and keeps the block that is connected to the expression object `exprObj` in the diagram. Both `speciesObj` and `exprObj` must be scalar.

`simbio.diagram.joinBlock(speciesObj,exprObj1,exprObj2)` combines cloned species blocks connected to the expression objects `exprObj1` and `exprObj2` into one block. `speciesObj`, `exprObj1`, and `exprObj2` must be scalar.

Examples

Join and Split Species Blocks

Open the `gprotein` model in the **SimBiology Model Builder** app.

```
simBiologyModelBuilder('gprotein');
```

The app opens and shows the model in the **Diagram** tab.

On the **Home** tab of the app, select **Export > Export Model to MATLAB Workspace**.

In the **SimBiology Model Export** dialog, click **OK** to export the model with the variable name *m1*.

Go to the MATLAB command line and confirm that the model *m1* is in the workspace. Get a list of species of the model.

```
m1.Species
```

```
ans =

   SimBiology Species Array

   Index:    Compartment:    Name:    Value:       Units:
   1         unnamed         G        7000
   2         unnamed         Gd       3000
   3         unnamed         Ga       0
   4         unnamed         RL       0
   5         unnamed         L        6.022e+17
   6         unnamed         R        10000
   7         unnamed         Gbg      3000
```

The model diagram already has a copy for each expression that references the species `Gbg`. In this case, calling `simbio.diagram.splitBlock` does not split the block again, but returns the list of expressions that the species is connected to. In this case, `Gbg` is used in two reactions.

```
Gbg = m1.Species(7);
expr = simbio.diagram.splitBlock(Gbg)
```

```
expr =

   SimBiology Reaction Array

   Index:    Reaction:
   1         Gd + Gbg -> G
   2         G + RL -> Ga + Gbg + RL
```

Join all the cloned blocks so that there is only one block for `Gbg`. In this case, keep the copy of the block that is connected to the G protein activation reaction (`G + RL -> Ga + Gbg + RL`). Note that the order of reactions returned in `expr` can change.

```
simbio.diagram.joinBlock(Gbg,expr(2));
```

Input Arguments

`speciesObj` — Species object

`Species` object

Species object, specified as a SimBiology `Species` object. `speciesObj` must be scalar.

`exprObj` — Expression object

`Reaction` object | `Rule` object

Expression object, specified as a `Reaction` or `Rule` object. The rule object can be a rate rule or repeated assignment rule. `exprObj` must be a scalar.

`exprObj1` — Expression object

`Reaction` object | `Rule` object

Expression object, specified as a `Reaction` or `Rule` object. The rule object can be a rate rule or repeated assignment rule. `exprObj1` must be a scalar.

`exprObj2` — Expression object
`Reaction` object | `Rule` object

Expression object, specified as a `Reaction` or `Rule` object. The rule object can be a rate rule or repeated assignment rule. `exprObj2` must be a scalar.

Version History

Introduced in R2021a

See Also

SimBiology Model Builder | `simbio.diagram.getBlock` | `simbio.diagram.setBlock` | `simbio.diagram.getLine` | `simbio.diagram.setLine` | `simbio.diagram.splitBlock`

Topics

“Create Model of Receptor-Ligand Kinetics”
“Incorporate SGLT2 Inhibition into Physiologically Based Glucose-Insulin Model Using SimBiology Model Builder”

simbio.diagram.setBlock

Package: `simbio.diagram`

Set SimBiology diagram block properties

Syntax

```
simbio.diagram.setBlock(sObj,propertyNames,propertyValues)
simbio.diagram.setBlock(sObj,S)
simbio.diagram.setBlock(sObj,Name,Value)
simbio.diagram.setBlock(sObj)
outStruct = simbio.diagram.setBlock(sObj)
CV = simbio.diagram.setBlock(sObj,propertyName)
simbio.diagram.setBlock(speciesObj,exprObj, ___ )
simbio.diagram.setBlock(speciesObj,exprObj)
```

Description

`simbio.diagram.setBlock` sets properties of diagram blocks shown in **SimBiology Model Builder**. The changes are instantly reflected in the app.

Before you run the function at the command line:

1. Open the corresponding SimBiology model in the **SimBiology Model Builder** app.
2. Export the model from the app to MATLAB workspace by selecting **Export > Export Model to MATLAB Workspace** on the **Home** tab of the app.

You can query and configure only the properties of the objects shown in the **Diagram** tab of the app. The objects shown in the diagram are compartments, species, reactions, rate rules, repeated assignment rules, and parameters that are on the left-hand side of a rate rule, a repeated assignment rule, or an event function.

`simbio.diagram.setBlock(sObj,propertyNames,propertyValues)` sets the values of specified block properties of a SimBiology object or array of objects `sObj`.

`simbio.diagram.setBlock(sObj,S)` sets the property values of `sObj` using a structure `S`. The field names of `S` are the property names and the field values are the property values.

`simbio.diagram.setBlock(sObj,Name,Value)` sets the property values specified by one or more name-value arguments.

`Name` is the property name and `Value` is the corresponding value. `Name` must appear inside quotes. You can specify several name and value pair arguments in any order as `Name1,Value1,...,NameN,ValueN`.

You can specify a mixture of name-value arguments, structures, and cell array pairs of property names and values in the same function call.

`simbio.diagram.setBlock(sObj)` displays the names and possible values of configurable block properties of a SimBiology object `sObj`. `sObj` must be scalar.

`outStruct = simbio.diagram.setBlock(sObj)` returns a structure `outStruct` containing the names and possible values of configurable block properties of a SimBiology object `sObj`. `sObj` must be scalar.

`CV = simbio.diagram.setBlock(sObj,propertyName)` returns a cell array of possible values `CV` for the block property `propertyName`. `sObj` must be scalar.

`simbio.diagram.setBlock(speciesObj,exprObj, ___ )` sets the values of the specified block properties of a species object `speciesObj` that is connected to an expression object `exprObj`. You can specify any combination of `Name,Value` pairs, structures, and cell array pairs of property names and values as shown in previous syntaxes.

Use this syntax to configure the `Position`, `Pin`, and `Visible` properties of a specific cloned block when you have multiple clones of the same species. Clones have the same values for all the other properties.

`simbio.diagram.setBlock(speciesObj,exprObj)` displays the names of configurable block properties of a species object `speciesObj` that is connected to an expression (reaction, rate rule, or repeated assignment rule) object `exprObj`.

Use this syntax to check the properties of a specific cloned block when you have multiple clones of the same species.

Examples

Configure SimBiology Diagram Block Properties

You can programmatically adjust the appearance and locations of diagram blocks of a SimBiology model.

Open the `lotka` model in the **SimBiology Model Builder** app.

```
simBiologyModelBuilder('lotka')
```

The app opens and shows the model in the **Diagram** tab.

On the **Home** tab of the app, select **Export > Export Model to MATLAB Workspace**.

In the **SimBiology Model Export** dialog, click **OK** to export the model with the variable name *m1*.

Go to the MATLAB command line and confirm that the model *m1* is in the workspace. Get a list of species of the model.

```
m1.Species
```

```
ans =

   SimBiology Species Array

   Index:    Compartment:    Name:    Value:    Units:
   1         unnamed         x        1
   2         unnamed         y1       900
   3         unnamed         y2       900
   4         unnamed         z        0
```

Get the current block shape of species *x*.

```
x = m1.Species(1);
v = simbio.diagram.getBlock(x,'Shape')
```

```
v =

    'rounded rectangle'
```

Get a list of all possible shapes for the species block.

```
simbio.diagram.setBlock(x,'Shape')
```

```
ans =

  8×1 cell array

    {'rounded rectangle'}
    {'rectangle'        }
    {'oval'             }
    {'triangle'         }
    {'hexagon'          }
    {'chevron'          }
    {'parallelogram'    }
    {'diamond'          }
```

Set the shape of the species block to an oval.

```
simbio.diagram.setBlock(x,'Shape','oval')
```

Get the current position of the block. The first two numbers represent the x and y coordinates with respect to the top left corner ($x = 0$, $y = 0$) of the diagram. The last two numbers represent the width and height of the block.

```
simbio.diagram.getBlock(x,'Position')
```

```
ans =

   223   137    30    15
```

Set the position to a new location.

```
simbio.diagram.setBlock(x,'Position',[260 130 30 15])
```

You can also configure multiple properties.

```
simbio.diagram.setBlock(x,'FaceColor','yellow','FontSize',20,'TextLocation','center')
```

Configure Cloned Species Block Properties

When you have multiple cloned blocks for the same species in a SimBiology diagram, you can programmatically adjust the position and visibility of a specific clone by specifying the expression block that the cloned species is connected to. In other words, you can change the `Position`, `Pin`, and `Visible` properties specific to an individual clone. All the other properties have the same values across all clones of the same species.

Open the `gprotein` model in the **SimBiology Model Builder** app.

```
simBiologyModelBuilder('gprotein');
```

The app opens and shows the model in the **Diagram** tab.

On the **Home** tab of the app, select **Export > Export Model to MATLAB Workspace**.

In the **SimBiology Model Export** dialog, click **OK** to export the model with the variable name *m1*.

Go to the MATLAB command line and confirm that the model *m1* is in the workspace. Get a list of species of the model.

```
m1.Species
```

```
ans =

   SimBiology Species Array

   Index:    Compartment:    Name:    Value:       Units:
   1         unnamed         G        7000
   2         unnamed         Gd       3000
   3         unnamed         Ga       0
   4         unnamed         RL       0
   5         unnamed         L        6.022e+17
   6         unnamed         R        10000
   7         unnamed         Gbg      3000
```

The species block *Gbg* is cloned and connected to two reactions: `G protein activation` and `G protein complex formation`. Get the current position of the cloned block connected to the second reaction.

```
Gbg = m1.Species(7);
r2 = m1.Reaction(2);
simbio.diagram.getBlock(Gbg,r2,'Position')
```

```
ans =

   393   307    30    15
```

Unpin the cloned block and move it to another position.

```
simbio.diagram.setBlock(Gbg,r2,'Pin',false,'Position',[391 340 30 15])
```

Input Arguments

`sObj` — SimBiology object

`Compartment` object | `Species` object | `Reaction` object | `Rule` object | `Parameter` object | array of objects

SimBiology object, specified as a `Compartment`, `Species`, `Reaction`, `Rule`, or `Parameter` object, or as an array of objects.

`propertyName` — Property name

character vector | string

Property name of the block, specified as a character vector or string. You can specify only one property name.

Example: `'FontName'`

Data Types: `char` | `string`

`propertyNames` — Names of block properties
character vector | string | string vector | cell array of character vectors

Names of block properties, specified as a character vector, string, string vector, or cell array of character vectors. You can specify multiple property names as an 1-by-*N* or *N*-by-1 cell array of names.

Available block properties follow.

Property Name	Description
`Connections`	Read-only property that lists the objects connected to the input block
`Cloned`	Read-only flag indicating if more than one block exists for the input object. You can clone only species blocks.
`EdgeColor`	Block edge color, specified as one of these values: • RGB triplet, such as `[1 1 0]` • Character vector or string representing the color name, such as `'y'` or `'yellow'`
`ExpressionLines`	Flag to show lines from the expression block to other model components referenced by the expression, specified as `'show'` or `'hide'`. You can set this property for reactions or rules.
`FaceColor`	Block face color, specified as one of these values: • RGB triplet, such as `[1 1 0]` • Character vector or string representing the color name, such as `'y'` or `'yellow'`
`FontName`	Block text font, specified as a character vector or string. Valid options are: • `'Arial'` • `'Arial Black'` • `'Arial Narrow'` • `'Comic Sans MS'` • `'Courier'` • `'Courier New'` • `'Georgia'` • `'Helvetica'` • `'Impact'` • `'Times New Roman'` • `'Trebuchet MS'` • `'Verdana'`
`FontSize`	Block text font size, specified as a positive scalar

Property Name	Description
`FontWeight`	Block text font thickness, specified as `'plain'`, `'bold'`, `'italic'`, or `'bold italic'`
`Object`	Read-only property that lists the corresponding SimBiology object of the block
`Pin`	Flag to indicate if a block can be moved or not. Set the property to `false` to allow moving the block in the diagram.
`Position`	Position and size of the block, specified as a four-element vector `[x,y,width,height]`. The position of the upper-left corner of the diagram is equal to x = 0 and y = 0. SimBiology configures all block positions relative to that corner. You can configure block positions to negative positions.
`Rotate`	Block rotation, specified as a scalar between 0 and 360. You cannot rotate compartment blocks.
`Shape`	Block shape, specified as a character vector or string. Valid options are: • `'rounded rectangle'` • `'rectangle'` • `'oval'` • `'triangle'` • `'hexagon'` • `'chevron'` • `'parallelogram'` • `'diamond'` Compartment blocks must be `'rounded rectangle'` or `'rectangle'`.
`TextColor`	Block text color, specified as one of these values: • RGB triplet, such as `[1 1 0]` • Character vector or string representing the color name, such as `'y'` or `'yellow'`
`TextLocation`	Block text location relative to the block, specified as one of the following: `'top'`, `'left'`, `'bottom'`, `'right'`, `'center'`, or `'none'`
`Visible`	Flag to indicate if the block is visible in the diagram. Set the property to false to hide the block. **Warning** Starting in R2022a, this property for all compartment blocks is always set to 1 and you can no longer hide compartments.

Example: `'Position'`

Data Types: `double` | `char` | `string` | `cell`

`propertyValues` — Property values

character vector | string | string vector | numeric vector | logical scalar | cell array

Property values to set, specified as a character vector, string, string vector, numeric vector, logical scalar, or cell array.

If `propertyNames` is a cell array of 1-by-*N* or *N*-by-1, `propertyValues` can be a cell array of the same length containing the corresponding values for each property in `propertyNames`.

If `sObj` is a vector and `propertyNames` contains a single property name and `propertyValues` contains a single value, the function updates the specified property of all objects to the specified value.

If `sObj` is a vector containing *M* objects, and `propertyNames` is a cell array of 1-by-*N* or *N*-by-1, `propertyValues` can be a cell array of *M*-by-*N* such that each object is updated with a different set of values for the list of properties in `propertyNames`.

Example: `[140 210 30 15]`

Data Types: `double` | `logical` | `char` | `string` | `cell`

`S` — Property names and corresponding values
structure | structure array

Property names and corresponding values to set, specified as a structure or structure array. Each field name corresponds to a property name, and the field value is the property value.

If `sObj` is a vector and `S` is a scalar structure, the function configures all objects to have the same property values.

You can specify a different set of property values for each object. To do so, specify `S` as an array of the same length as `sObj`.

Data Types: `structure`

`speciesObj` — Species object
`Species` object

Species object, specified as a SimBiology `Species` object. `speciesObj` must be scalar.

`exprObj` — Expression object
`Reaction` object | `Rule` object

Expression object, specified as a `Reaction` or `Rule` object. The rule object can be a rate rule or repeated assignment rule. `exprObj` must be a scalar.

Output Arguments

`CV` — Possible property values
cell array

Possible property values, returned as a cell array of values. `CV` is an empty cell array if the property does not have a finite set of possible values.

`outStruct` — Configurable property names and their possible values
structure

Configurable property names and their possible values, returned as a structure. Each field name is a property name and the value is a cell array of possible values or an empty cell array if the property does not have a finite set of possible values.

Version History

Introduced in R2021a

See Also

SimBiology Model Builder | `simbio.diagram.getBlock` | `simbio.diagram.getLine` | `simbio.diagram.setLine` | `simbio.diagram.splitBlock` | `simbio.diagram.joinBlock`

Topics

“Create Model of Receptor-Ligand Kinetics”
“Incorporate SGLT2 Inhibition into Physiologically Based Glucose-Insulin Model Using SimBiology Model Builder”

simbio.diagram.setLine

Package: `simbio.diagram`

Set SimBiology diagram line properties

Syntax

```
simbio.diagram.setLine(sObj,propertyNames,propertyValues)
simbio.diagram.setLine(sObj,S)
simbio.diagram.setLine(sObj,Name,Value)
simbio.diagram.setLine(sObj)
outStruct = simbio.diagram.setLine(sObj)
CV = simbio.diagram.setLine(sObj,propertyName)
simbio.diagram.setLine(obj1,obj2,___)
simbio.diagram.setLine(obj1,obj2)
```

Description

`simbio.diagram.setLine` sets properties of diagram lines shown in **SimBiology Model Builder**. The changes are instantly reflected in the app.

Before you run the function at the command line:

1. Open the corresponding SimBiology model in the **SimBiology Model Builder** app.
2. Export the model from the app to MATLAB workspace by selecting **Export > Export Model to MATLAB Workspace** on the **Home** tab of the app.

You can query and configure only the properties of the objects shown in the **Diagram** tab of the app. The objects shown in the diagram are compartments, species, reactions, rate rules, repeated assignment rules, and parameters that are on the left-hand side of a rate rule, a repeated assignment rule, or an event function.

`simbio.diagram.setLine(sObj,propertyNames,propertyValues)` sets the values of specified properties for the lines connected to a SimBiology object or array of objects `sObj`.

`simbio.diagram.setLine(sObj,S)` sets the property values of `sObj` using a structure `S`. The field names of `S` are the property names and the field values are the property values.

`simbio.diagram.setLine(sObj,Name,Value)` sets the property values specified by one or more name-value arguments.

`Name` is the property name and `Value` is the corresponding value. `Name` must appear inside quotes. You can specify several name and value pair arguments in any order as `Name1,Value1,...,NameN,ValueN`.

You can specify a mixture of name-value arguments, structures, and cell array pairs of property names and values in the same function call.

`simbio.diagram.setLine(sObj)` displays the names and possible values of configurable properties of a line connected to a SimBiology object `sObj`. This syntax requires that only one line is

connected to `sObj`. If there are multiple lines connected to `sObj`, specify the line by providing two objects as inputs that are connected by the line. The functions returns an empty cell array when the property does not have a finite set of possible values. `sObj` must be scalar.

`outStruct = simbio.diagram.setLine(sObj)` returns a structure `outStruct` containing the names and possible values of configurable properties of a line connected to a SimBiology object `sObj`. `sObj` must be scalar.

`CV = simbio.diagram.setLine(sObj,propertyName)` returns a cell array of possible values `CV` for the line property `propertyName`. `sObj` must be scalar.

`simbio.diagram.setLine(obj1,obj2, ___ )` sets the properties of the line that connects the SimBiology objects `obj1` and `obj2` using any of the previous input arguments. `obj1` and `obj2` must be scalar.

`simbio.diagram.setLine(obj1,obj2)` displays the configurable properties of the line that connects the SimBiology objects `obj1` and `obj2`. `obj1` and `obj2` must be scalar.

Examples

Configure SimBiology Diagram Line Properties

You can programmatically adjust the appearance of lines connected to blocks in a diagram.

Open the `lotka` model in the **SimBiology Model Builder** app.

```
simBiologyModelBuilder('lotka');
```

The app opens and shows the model in the **Diagram** tab.

On the **Home** tab of the app, select **Export > Export Model to MATLAB Workspace**.

In the **SimBiology Model Export** dialog, click **OK** to export the model with the variable name *m1*.

Go to the MATLAB command line and confirm that the model *m1* is in the workspace. Get a list of species of the model.

```
m1.Species
```

```
ans =

   SimBiology Species Array

   Index:    Compartment:    Name:    Value:    Units:
   1         unnamed         x        1
   2         unnamed         y1       900
   3         unnamed         y2       900
   4         unnamed         z        0
```

Get the current property values of the line connected to species *x*. If multiple lines are connected to the species, the function returns an array of structures containing one structure per line.

```
x = m1.Species(1);
sv = simbio.diagram.getLine(x)
```

```
sv =

  struct with fields:

          Color: [66 66 66]
    Connections: [1×2 SimBiology.ModelComponent]
          Width: 1
```

Change the line color to red and increase the line width.

```
simbio.diagram.setLine(x,'Color','red','Width',2)
```

You can also query properties of a line that connects two objects. For example, get the property values of the line that connects species `y1` and `Reaction1`.

```
y1 = m1.Species(2);
r1 = m1.Reactions(1);
simbio.diagram.getLine(y1,r1)
```

```
ans =

  struct with fields:

          Color: [66 66 66]
    Connections: [1×2 SimBiology.ModelComponent]
          Width: 1
```

Change the line color to a new RGB value and increase the line width.

```
simbio.diagram.setLine(y1,r1,'Color',[0.6 0.2 0.6],'Width',3)
```

Input Arguments

`sObj` — SimBiology object

`Compartment` object | `Species` object | `Reaction` object | `Rule` object | `Parameter` object | array of objects

SimBiology object, specified as a `Compartment`, `Species`, `Reaction`, `Rule`, or `Parameter` object, or as an array of objects.

`propertyName` — Property name

character vector | string

Property name of the line, specified as a character vector or string. You can specify only one property name.

Example: `'Color'`

Data Types: `char` | `string`

`propertyNames` — Names of line properties

character vector | string | string vector | cell array of character vectors

Names of line properties, specified as a character vector, string, string vector, or cell array of character vectors. You can specify multiple property names as a 1-by-*N* or *N*-by-1 cell array of names.

Available line properties follow.

Property Name	Description
`Color`	Line color, specified as one of these values: • RGB triplet, such as `[1 1 0]` • Character vector or string representing the color name, such as `'y'` or `'yellow'`
`Connections`	Read-only property that lists the objects connected by the line
`Width`	Line width, specified as a positive scalar

Example: `'Width'`

Data Types: `char` | `string` | `cell`

`propertyValues` — Property values
character vector | string | string vector | numeric vector | cell array

Property values to set, specified as a character vector, string, string vector, numeric vector, or cell array.

If `propertyNames` is a cell array of 1-by-*N* or *N*-by-1, `propertyValues` can be a cell array of the same length containing the corresponding values for each property in `propertyNames`.

If `sObj` is a vector and `propertyNames` contains a single property name and `propertyValues` contains a single value, the function updates the property of all lines connected to `sObj` to the specified value.

If `sObj` is a vector containing *M* objects, and `propertyNames` is a cell array of 1-by-*N* or *N*-by-1, `propertyValues` can be a cell array of *M*-by-*N* so that each object is updated with a different set of values for the list of properties in `propertyNames`.

Example: `'green'`

Data Types: `double` | `char` | `string` | `cell`

`S` — Property names and corresponding values
structure | structure array

Property names and corresponding values to set, specified as a structure or structure array. Each field name corresponds to a property name, and the field value is the property value.

If `sObj` is a vector and `S` is a scalar structure, the function configures all objects to have the same property values.

You can specify a different set of property values for each object. To do so, specify `S` as an array of the same length as `sObj`.

Data Types: `structure`

`obj1` — SimBiology object
`Compartment` object | `Species` object | `Reaction` object | `Rule` object | `Parameter` object

SimBiology object, specified as a `Compartment`, `Species`, `Reaction`, `Rule`, or `Parameter` object.

obj2 — SimBiology object
`Compartment` object | `Species` object | `Reaction` object | `Rule` object | `Parameter` object

SimBiology object, specified as a `Compartment`, `Species`, `Reaction`, `Rule`, or `Parameter` object.

Output Arguments

CV — Possible property values
cell array

Possible property values, returned as a cell array of values. `CV` is an empty cell array if the property does not have a finite set of possible values.

outStruct — Configurable property names and their possible values
structure

Configurable property names and their possible values, returned as a structure. Each field name is a property name and the value is a cell array of possible values or an empty cell array if the property does not have a finite set of possible values.

Version History

Introduced in R2021a

See Also

SimBiology Model Builder | `simbio.diagram.getBlock` | `simbio.diagram.setBlock` | `simbio.diagram.getLine` | `simbio.diagram.splitBlock` | `simbio.diagram.joinBlock`

Topics
“Create Model of Receptor-Ligand Kinetics”
“Incorporate SGLT2 Inhibition into Physiologically Based Glucose-Insulin Model Using SimBiology Model Builder”

simbio.diagram.splitBlock

Package: `simbio.diagram`

Split SimBiology species block in diagram

Syntax

```
expr = simbio.diagram.splitBlock(speciesObj)
```

Description

`simbio.diagram.splitBlock` splits a species block so that each expression that references the species is connected to a different copy of the species block in **SimBiology Model Builder**. The changes are instantly reflected in the app.

Before you run the function at the command line:

1. Open the corresponding SimBiology model in the **SimBiology Model Builder** app.
2. Export the model from the app to MATLAB workspace by selecting **Export > Export Model to MATLAB Workspace** on the **Home** tab of the app.

You can query and configure only the properties of the objects shown in the **Diagram** tab of the app. The objects shown in the diagram are compartments, species, reactions, rate rules, repeated assignment rules, and parameters that are on the left-hand side of a rate rule, a repeated assignment rule, or an event function.

`expr = simbio.diagram.splitBlock(speciesObj)` makes copies of a SimBiology species `speciesObj` block so that each expression that references `speciesObj` is connected to a different copy of the species block and returns a list of expression objects `expr` that are connected to `speciesObj`. Use this function to make the diagram look less cluttered and clearer.

Examples

Create Copies of Species Block

Open the `gprotein` model in the **SimBiology Model Builder** app.

```
simBiologyModelBuilder('gprotein');
```

The app opens and shows the model in the **Diagram** tab.

On the **Home** tab of the app, select **Export > Export Model to MATLAB Workspace**.

In the **SimBiology Model Export** dialog, click **OK** to export the model with the variable name *m1*.

Go to the MATLAB command line and confirm that the model *m1* is in the workspace. Get a list of species of the model.

```
m1.Species
```

```
ans =

   SimBiology Species Array

   Index:    Compartment:    Name:    Value:       Units:
   1         unnamed         G        7000
   2         unnamed         Gd       3000
   3         unnamed         Ga       0
   4         unnamed         RL       0
   5         unnamed         L        6.022e+17
   6         unnamed         R        10000
   7         unnamed         Gbg      3000
```

The model diagram already has a copy for each expression that the species Gbg is being referenced. In this case, calling `simbio.diagram.splitBlock` does not split the block again, but returns the list of expressions that the species is connected to. In this case, `Gbg` is used in two reactions.

```
Gbg = m1.Species(7);
expr = simbio.diagram.splitBlock(Gbg)
```

```
expr =

   SimBiology Reaction Array

   Index:    Reaction:
   1         Gd + Gbg -> G
   2         G + RL -> Ga + Gbg + RL
```

Join all the cloned blocks so that there is only one block for `Gbg`. In this case, keep the copy of the block that is connected to the G Protein activation reaction (`G + RL -> Ga + Gbg + RL`). Note that the order of reactions returned in `expr` can change.

```
simbio.diagram.joinBlock(Gbg,expr(2))
```

Input Arguments

`speciesObj` — Species object

`Species` object

Species object, specified as a SimBiology `Species` object. `speciesObj` must be scalar.

Output Arguments

`expr` — List of expressions

`Reaction` object | `Rule` object | array of objects

List of expressions that species is connected to, returned as a `Reaction`, `Rule` object or array of objects. The rule object can be a rate rule or repeated assignment rule.

Version History

Introduced in R2021a

See Also

SimBiology Model Builder | `simbio.diagram.getBlock` | `simbio.diagram.setBlock` | `simbio.diagram.getLine` | `simbio.diagram.setLine` | `simbio.diagram.joinBlock`

Topics

“Create Model of Receptor-Ligand Kinetics”
“Incorporate SGLT2 Inhibition into Physiologically Based Glucose-Insulin Model Using SimBiology Model Builder”

SimBiology Model Analyzer

Analyze QSP, PK/PD, and mechanistic systems biology models

Description

The **SimBiology Model Analyzer** app lets you analyze models of dynamic systems such as metabolic networks, signaling pathways, quantitative systems pharmacology (QSP) models, and pharmacokinetic/pharmacodynamic (PK/PD) models of drugs. It provides several methods to analyze models and various plots to visualize the results.

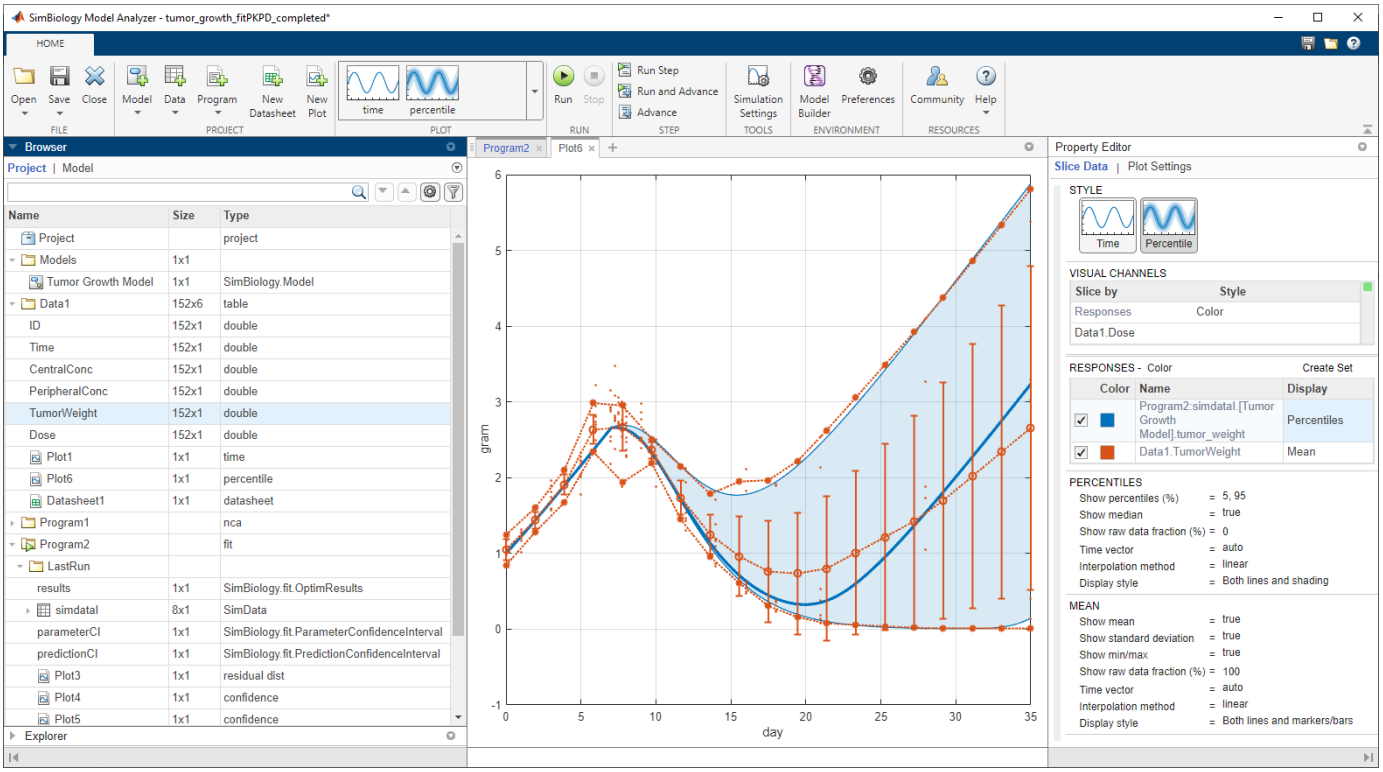
Using the app, you can:

- Simulate a model to see its dynamic behavior over time.
- Explore biological variability by simulating alternate scenarios such as virtual patients.
- Estimate model parameters using nonlinear regression and nonlinear mixed-effects methods.
- Perform parameter scans and sensitivity analysis to investigate the influence of model parameters and initial conditions on model behavior.
- Specify units and let the app automatically convert the matching physical quantities to one consistent unit system.
- Explore various dosing regimens.
- Perform noncompartmental analysis (NCA) to compute PK parameters of a drug from its PK data.
- View analysis results in various plots.

Available Plots

The app lets you visualize the analysis results using various plots, including:

- Time course of model quantities
- Sensitivity matrix
- Overlay of estimated results on experimental data
- Plots to measure fit quality, such as confidence interval plots, residuals plots, residual distribution plots, actual-versus-predicted plots, and box plots
- Scatter plot matrix
- Percentile plot



Open the SimBiology Model Analyzer App

- MATLAB toolstrip: On the **Apps** tab, under **Computational Biology**, click the app icon.
- MATLAB command prompt: Enter `simBiologyModelAnalyzer`.

Examples

- “Calculate NCA Parameters and Fit Model to PK/PD Data Using SimBiology Model Analyzer”
- “Find Important Tumor Growth Parameters with Local Sensitivity Analysis Using SimBiology Model Analyzer”
- “Explore Biological Variability with Virtual Patients Using SimBiology Model Analyzer”
- “Scan Dosing Regimens Using SimBiology Model Analyzer App”
- “Generate Report for SimBiology Program Results”
- “View and Run Program Code Generated by SimBiology Model Analyzer”
- “Simulate Groups Using Doses and Variants from Data Set”
- “Percentile Plot”
- “Keyboard Shortcuts for SimBiology Model Analyzer”

Programmatic Use

`simBiologyModelAnalyzer` opens the **SimBiology Model Analyzer** app.

`simBiologyModelAnalyzer(m1)` opens the SimBiology model `m1` in the **SimBiology Model Analyzer** app. If you also have the **SimBiology Model Builder** app open at the same time, both apps share the same model.

If the **SimBiology Model Builder** or **SimBiology Model Analyzer** app is already open, you cannot load a model or project from the command line. Load the model from the app directly.

`simBiologyModelAnalyzer(sbprojFile)` opens the SimBiology project file `sbprojFile` in the **SimBiology Model Analyzer** app. `sbprojFile` is a string or character vector specifying a file name or path and file name of a SimBiology project SBPROJ file. If you specify only a file name, the file must be on the MATLAB search path or in the current folder. If you also have the **SimBiology Model Builder** app open at the same time, both apps share the same project.

If the **SimBiology Model Builder** or **SimBiology Model Analyzer** app is already open, you cannot load a model or project from the command line. Load the model from the app directly.

Version History

Introduced in R2019b

R2020b: Load a project or model from the command line when the app is open
Behavior changed in R2020b

If the **SimBiology Model Builder** or **SimBiology Model Analyzer** app is open, you cannot load a project or model from the command line using the `simBiologyModelBuilder` or `simBiologyModelAnalyzer` functions. Load the project or model from the app directly.

See Also

Apps
SimBiology Model Builder

Functions
`sbiosimulate` | `sbionca` | `sbiosteadystate` | `sbiofit` | `sbioparameterci` | `sbiopredictionci`

Topics
“Calculate NCA Parameters and Fit Model to PK/PD Data Using SimBiology Model Analyzer”
“Find Important Tumor Growth Parameters with Local Sensitivity Analysis Using SimBiology Model Analyzer”
“Explore Biological Variability with Virtual Patients Using SimBiology Model Analyzer”
“Scan Dosing Regimens Using SimBiology Model Analyzer App”
“Generate Report for SimBiology Program Results”
“View and Run Program Code Generated by SimBiology Model Analyzer”
“Simulate Groups Using Doses and Variants from Data Set”
“Percentile Plot”
“Keyboard Shortcuts for SimBiology Model Analyzer”
“Model Simulation”
“Noncompartmental Analysis”
“Sensitivity Analysis in SimBiology”
“Nonlinear Regression”
“Nonlinear Mixed-Effects Modeling”

SimBiology Model Builder

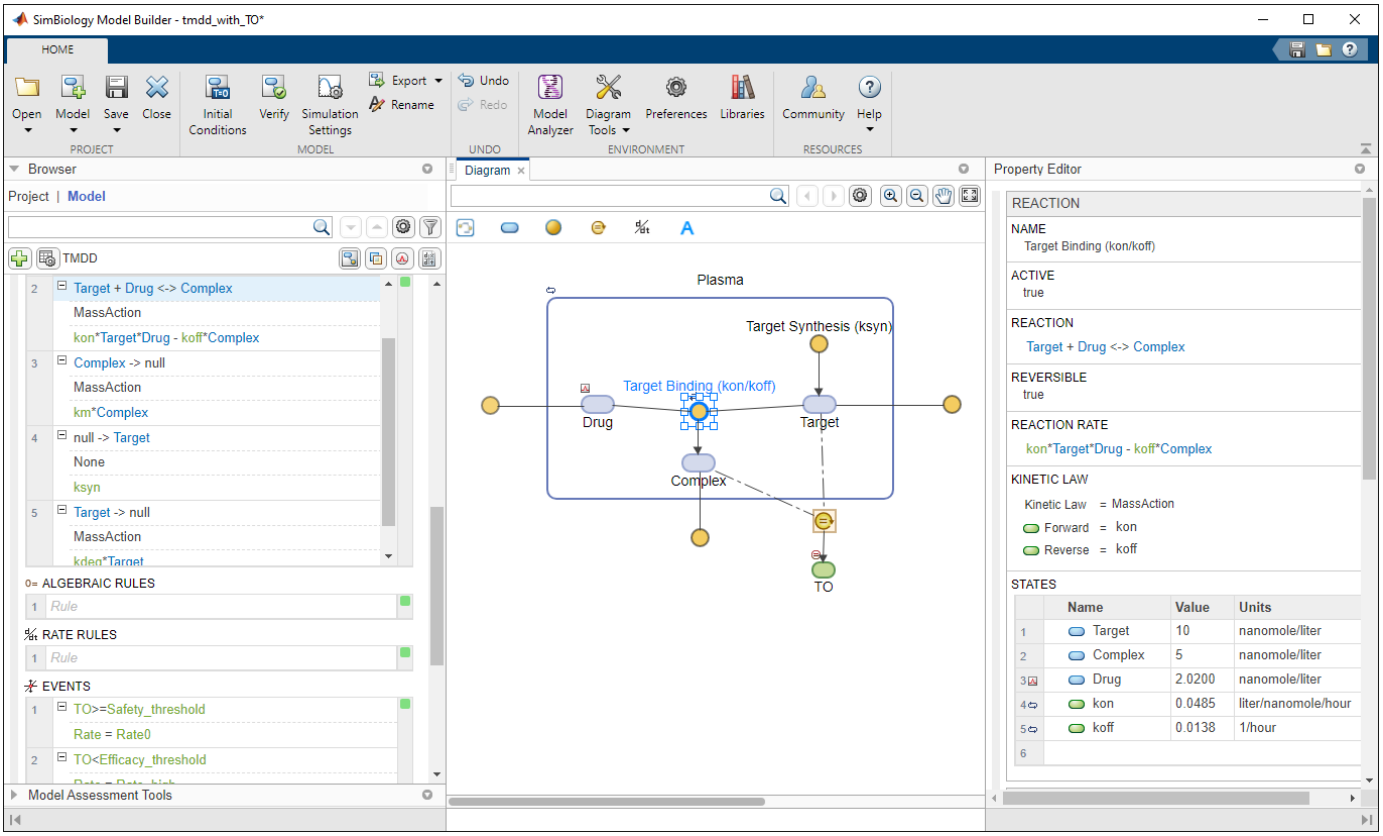
Build QSP, PK/PD, and mechanistic systems biology models interactively

Description

The **SimBiology Model Builder** app lets you build models of dynamic systems such as quantitative systems pharmacology (QSP) models, pharmacokinetic/pharmacodynamic (PK/PD) models, and systems biology models interactively. It provides a block diagram editor to build the model reaction schematic by using built-in blocks.

Using the app, you can:

- Build a variety of dynamic systems such as metabolic networks, signaling pathways, QSP models, PBPK models, and PK/PD models.
- Create standard compartmental PK models from the built-in library.
- View your model as a graphical representation or as mathematical equations.
- Use variants to store a set of parameter values or initial conditions that are different from the base model configuration.
- Create an array of doses to explore different dosing regimens.
- Import or export SimBiology models to and from the MATLAB workspace or from a Systems Biology Markup Language (SBML) file.



Open the SimBiology Model Builder App

- MATLAB toolstrip: On the **Apps** tab, under **Computational Biology**, click the app icon.
- MATLAB command prompt: Enter `simBiologyModelBuilder`.

Examples

- "Create Model of Receptor-Ligand Kinetics"
- "Incorporate SGLT2 Inhibition into Physiologically Based Glucose-Insulin Model Using SimBiology Model Builder"
- "Generate SimBiology Model Report"

Programmatic Use

`simBiologyModelBuilder` opens the app.

`simBiologyModelBuilder(m1)` opens the SimBiology model `m1` in the **SimBiology Model Builder** app. If you also have the **SimBiology Model Analyzer** app open at the same time, both apps share the same model.

If the **SimBiology Model Builder** or **SimBiology Model Analyzer** app is already open, you cannot load a model or project from the command line. Load the model from the app directly.

`simBiologyModelBuilder(sbprojFile)` opens the SimBiology project file `sbprojFile` in the **SimBiology Model Builder** app. `sbprojFile` is a string or character vector specifying a file name or path and file name of a SimBiology project SBPROJ file. If you specify only a file name, the file must be on the MATLAB search path or in the current folder. If you also have the **SimBiology Model Analyzer** app open at the same time, both apps share the same project.

If the **SimBiology Model Builder** or **SimBiology Model Analyzer** app is already open, you cannot load a model or project from the command line. Load the model from the app directly.

Version History

Introduced in R2020b

R2020b: Load a project or model from the command line when the app is open
Behavior changed in R2020b

If the **SimBiology Model Builder** or **SimBiology Model Analyzer** app is open, you cannot load a project or model from the command line using the `simBiologyModelBuilder` or `simBiologyModelAnalyzer` functions. Load the project or model from the app directly.

See Also

Apps
SimBiology Model Analyzer

Functions
`sbioloadproject` | `sbmlimport` | `sbiomodel` | `sbiodose` | `sbiovariant` | `sbioreset`

Topics
“Create Model of Receptor-Ligand Kinetics”
“Incorporate SGLT2 Inhibition into Physiologically Based Glucose-Insulin Model Using SimBiology Model Builder”
“Generate SimBiology Model Report”
“Copy SimBiology Blocks”
“Keyboard Shortcuts for SimBiology Model Builder”
“Message Indicator Icons in SimBiology Model Builder”
“What is a SimBiology Model?”
“Doses in SimBiology Models”
“Variants in SimBiology Models”

Methods

The object that the methods apply to are listed in parenthesis after the method name.

accelerate(SimFunction)

Prepare SimFunction object for accelerated simulations

Syntax

```
accelerate(F)
```

Input Arguments

F	`SimFunction object` created by the `createSimFunction` method of a SimBiology model.

Description

`accelerate(F)` prepares `SimFunction object` `F` for accelerated simulations.

Note `F` is automatically accelerated at the first function execution. However, manually accelerate the object if you want it accelerated in your deployment applications.

Examples

Simulate SimFunction Object

This example uses the Lotka-Volterra (predator-prey) model described by Gillespie [1].

Load the sample project containing the lotka model.

```
sbioloadproject lotka;
```

Create a SimFunction object `f` with `c1` and `c2` as input parameters to be scanned, and `y1` and `y2` as the output of the function with no dose.

```
f = createSimFunction(m1,{'Reaction1.c1', 'Reaction2.c2'},{'y1', 'y2'}, [])
```

```
f =

SimFunction

Parameters:

         Name          Value       Type
    _______________    _____    ___________

    'Reaction1.c1'       10     'parameter'
    'Reaction2.c2'     0.01     'parameter'

Observables:
```

```
    Name       Type
    ____    _________

    'y1'    'species'
    'y2'    'species'

Dosed: None
```

The `SimFunction` object `f` is not set for acceleration at the time of creation. But it will be automatically accelerated when executed.

```
f.isAccelerated
```

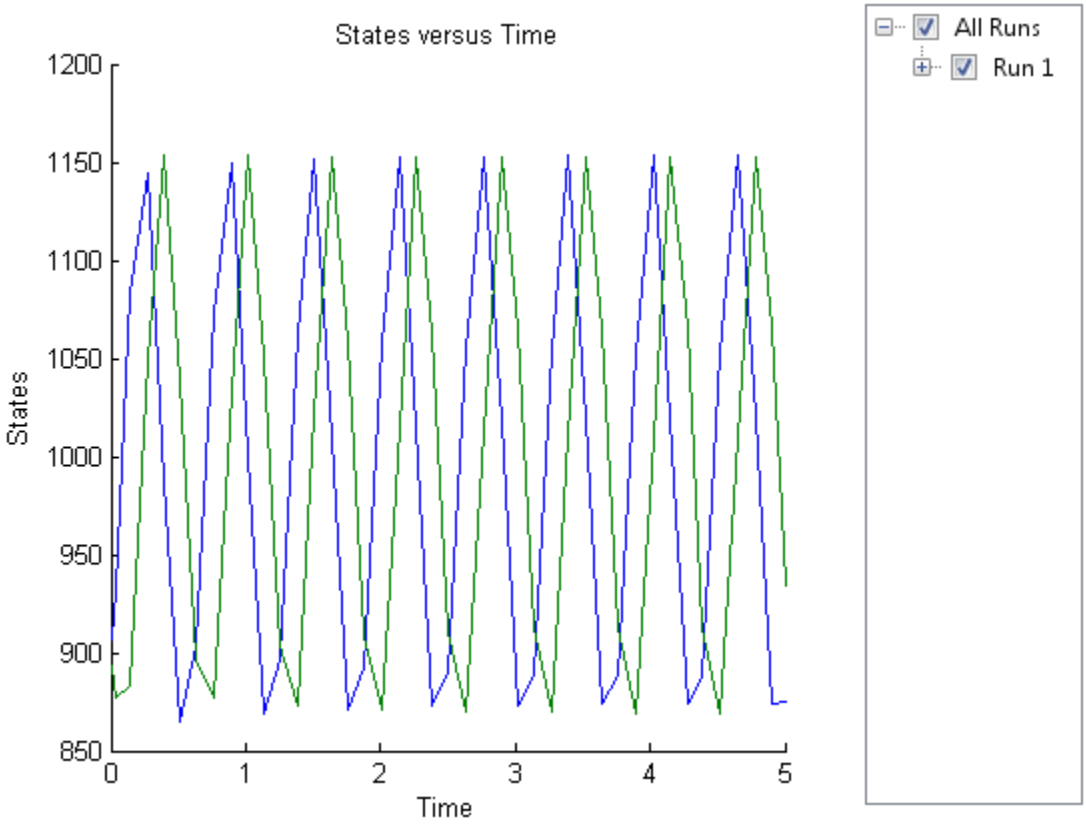
```
ans =

     0
```

Define an input matrix that contains parameter values for `c1` and `c2`.

```
phi = [10 0.01];
```

Run simulations until the stop time is 5 and plot the simulation results.

```
sbioplot(f(phi,5))
```



Confirm the `SimFunction` object `f` was accelerated during execution.

```
f.isAccelerated
```

```
ans =

     1
```

See Also

`createSimFunction`, `SimFunction object`

Version History

Introduced in R2014a

References

[1] Gillespie D.T. "Exact Stochatic Simulation of Coupled Chemical Reactions," (1977) The Journal of Physical Chemistry, 81(25), 2340-2361.

accelerate

Prepare exported SimBiology model for acceleration

Syntax

```
accelerate(model)
```

Description

`accelerate(model)` prepares the exported model for acceleration on the current type of computer.

Note Microsoft® Visual Studio® 2010 run-time libraries must be available on any computer running accelerated models generated using Microsoft Windows® SDK. If you plan to redistribute your accelerated models to other MATLAB users, be sure they have the run-time libraries.

Examples

Accelerate Exported SimBiology Model

Load a sample SimBiology model object, and export.

```
modelObj = sbmlimport('lotka');
em = export(modelObj)
```

```
em =
  Model with properties:

           Name: 'lotka'
     ExportTime: '03-Mar-2023 08:33:02'
    ExportNotes: ''
```

Accelerate the exported model.

```
accelerate(em);
em.isAccelerated
```

```
ans = logical
   1
```

The logical value 1 indicates that the exported model is accelerated.

Input Arguments

`model` — Input model

`SimBiology.export.Model` object

Input model, specified as a `SimBiology.export.Model` object.

Version History

Introduced in R2012b

See Also

`SimBiology.export.Model` | `isAccelerated` | `export`

Topics

“Perform PK/PD Modeling and Simulation to Guide Dosing Strategy for Antibiotics”
“Deploy a SimBiology Exported Model”

AbstractKineticLaw object

Kinetic law information in library

Description

The abstract kinetic law object represents a *kinetic law definition*, which provides a mechanism for applying a rate law to multiple reactions. The information in this object acts as a mapping template for the reaction rate. The kinetic law definition specifies a mathematical relationship that defines the rate at which reactant species are produced and product species are consumed in the reaction. The expression is shown in the `Expression` property. The species variables are defined in the `SpeciesVariables` property, and the parameter variables are defined in the `ParameterVariables` property of the abstract kinetic law object. For an explanation of how the kinetic law definition relates to the kinetic law object, see `KineticLaw object`.

Create your own kinetic law definition and add it to the kinetic law library with the `sbioaddtolibrary` function. You can then use the kinetic law to define a reaction rate. To retrieve a kinetic law definition from the user-defined library, first create a root object using `sbioroot`, then use the command `get(rootObj.UserDefinedLibrary, 'KineticLaws')`.

See “Property Summary” on page 2-8 for links to abstract kinetic law object property reference pages.

Properties define the characteristics of an object. For example, an abstract kinetic law object includes properties for the expression, the name of the law, parameter variables, and species variables. Use the `get` and `set` commands to list object properties and change their values at the command line. You can graphically change object properties in the **SimBiology Model Builder** app.

Constructor Summary

sbioabstractkineticlaw	Create kinetic law definition

Method Summary

delete	Delete SimBiology object
display	Display summary of SimBiology object
findUsages	Find out how an `AbstractKineticLaw` object is used
get	Get SimBiology object properties
rename	Rename object and update expressions
set	Set SimBiology object properties

Property Summary

Expression	Expression to determine reaction rate equation or expression of observable object
Name	Specify name of object
Notes	HTML text describing SimBiology object
ParameterVariables	Parameters in kinetic law definition
Parent	Indicate parent object
SpeciesVariables	Species in abstract kinetic law
Tag	Specify label for SimBiology object
Type	Display SimBiology object type
UserData	Specify data to associate with object

See Also

`Configset object`, `KineticLaw object`, `Model object`, `Parameter object`, `Reaction object`, `Root object`, `Rule object`, `Species object`

Version History

Introduced in R2006b

add

Add quantity values, doses, or variants to `SimBiology.Scenarios` object

Syntax

```
sObj = add(sObj,combination,name,content)
sObj = add(sObj,combination,quantityNames,probDist,Name,Value)
sObj = add(sObj,combination,sObj2)
```

Description

`sObj = add(sObj,combination,name,content)` adds an entry on page 2-799 to the `SimBiology.Scenarios` object `sObj`. The input argument `name` is the entry name and `content` is the entry content. `combination` specifies how to combine the new entry with the existing entries of `sObj`.

`sObj = add(sObj,combination,quantityNames,probDist,Name,Value)` specifies to generate the sample values for one or more model quantities `quantityNames` from the joint probability distribution `probDist`. Specify additional options for the probability distributions and sampling method using one or more name-value pair arguments. To use probability distributions, you must have Statistics and Machine Learning Toolbox.

`sObj = add(sObj,combination,sObj2)` adds entries from the `SimBiology.Scenarios` object `sObj2` to `sObj`. The function combines the entries from `sObj2` with the existing entries from `sObj` using the specified `combination` method.

Examples

Generate Different Simulation Scenarios for Glucose-Insulin Response

Load the model of glucose-insulin response. For details about the model, see the **Background** section in “Simulate the Glucose-Insulin Response”.

```
sbioloadproject('insulindemo','m1');
```

The model contains different parameter values and initial conditions that represents different insulin impairments (such as Type 2 diabetes, low insulin sensitivity, and so on) stored in five variants.

```
variants = getvariant(m1)
```

```
variants =
   SimBiology Variant Array

   Index:  Name:             Active:
   1       Type 2 diabetic   false
   2       Low insulin se... false
   3       High beta cell... false
   4       Low beta cell ... false
   5       High insulin s... false
```

Suppress an informational warning that is issued during simulations.

```
warnSettings = warning('off','SimBiology:DimAnalysisNotDone_MatlabFcn_Dimensionless');
```

Select a dose that represents a single meal of 78 grams of glucose.

```
singleMeal = sbioselect(m1,'Name','Single Meal');
```

Create a `Scenarios` object to represent different initial conditions combined with the dose. That is, create a `scenario` object where each variant is paired (or combined) with the dose, for a total of five simulation scenarios.

```
sObj = SimBiology.Scenarios;
add(sObj,'cartesian','variants',variants);
add(sObj,'cartesian','dose',singleMeal)
```

```
ans =
  Scenarios (5 scenarios)

                  Name            Content          Number
                ________    ____________________    ______

    Entry 1     variants    SimBiology variants      5
    x Entry 2   dose        SimBiology dose          1

  See also Expression property.
```

`sObj` contains two entries. Use the `generate` function to combine the entries and generate five scenarios. The function returns a scenarios table, where each row represents a scenario and each column represents an entry of the `Scenarios` object.

```
scenariosTbl = generate(sObj)
```

```
scenariosTbl=5×2 table
           variants                    dose
    ________________________    ____________________________

    1x1 SimBiology.Variant      1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant      1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant      1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant      1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant      1x1 SimBiology.RepeatDose
```

Change the entry name of the first entry.

```
rename(sObj,1,'Insulin Impairements')
```

```
ans =
  Scenarios (5 scenarios)

                       Name                 Content          Number
                ____________________    ____________________    ______

    Entry 1     Insulin Impairements    SimBiology variants      5
    x Entry 2   dose                    SimBiology dose          1
```

```
  See also Expression property.
```

Create a `SimFunction` object to simulate the generated scenarios. Use the `Scenarios` object as the input and specify the plasma glucose and insulin concentrations as reponses (outputs of the function to be plotted). Specify `[]` for the dose input argument since the `Scenarios` object already has the dosing information.

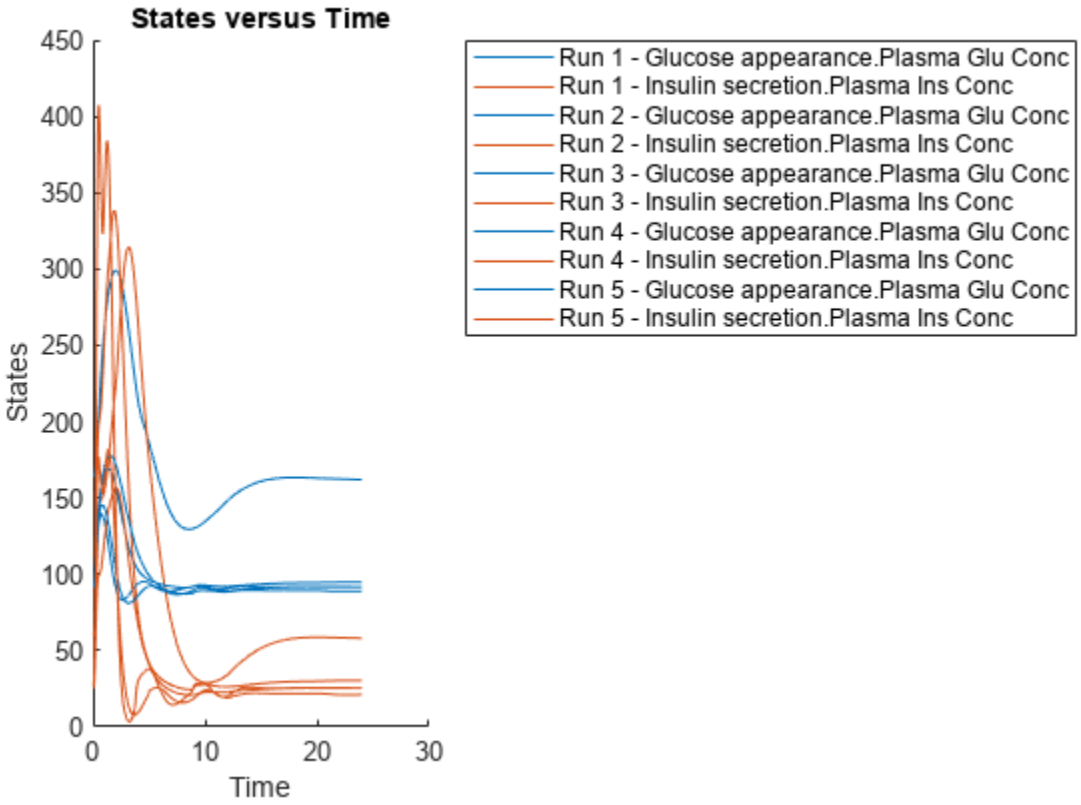
```
f = createSimFunction(m1,sObj,{'[Plasma Glu Conc]','[Plasma Ins Conc]'},[])
```

```
f = 
SimFunction

Parameters:

              Name                  Value        Type                       Units                
    _________________________    ______    _____________    _____________________________________

    {'Plasma Volume (Glu)'  }      1.88    {'parameter'}    {'deciliter'                          
    {'k1'                   }     0.065    {'parameter'}    {'1/minute'                           
    {'k2'                   }     0.079    {'parameter'}    {'1/minute'                           
    {'Plasma Volume (Ins)'  }      0.05    {'parameter'}    {'liter'                              
    {'m1'                   }      0.19    {'parameter'}    {'1/minute'                           
    {'m2'                   }     0.484    {'parameter'}    {'1/minute'                           
    {'m4'                   }    0.1936    {'parameter'}    {'1/minute'                           
    {'m5'                   }    0.0304    {'parameter'}    {'minute/picomole'                    
    {'m6'                   }    0.6469    {'parameter'}    {'dimensionless'                      
    {'Hepatic Extraction'   }       0.6    {'parameter'}    {'dimensionless'                      
    {'kmax'                 }    0.0558    {'parameter'}    {'1/minute'                           
    {'kmin'                 }     0.008    {'parameter'}    {'1/minute'                           
    {'kabs'                 }    0.0568    {'parameter'}    {'1/minute'                           
    {'kgri'                 }         0    {'parameter'}    {'1/minute'                           
    {'f'                    }       0.9    {'parameter'}    {'dimensionless'                      
    {'a'                    }         0    {'parameter'}    {'1/milligram'                        
    {'b'                    }      0.82    {'parameter'}    {'dimensionless'                      
    {'c'                    }         0    {'parameter'}    {'1/milligram'                        
    {'d'                    }      0.01    {'parameter'}    {'dimensionless'                      
    {'kp1'                  }       2.7    {'parameter'}    {'milligram/minute'                   
    {'kp2'                  }    0.0021    {'parameter'}    {'1/minute'                           
    {'kp3'                  }     0.009    {'parameter'}    {'(milligram/minute)/(picomole/liter
    {'kp4'                  }    0.0618    {'parameter'}    {'(milligram/minute)/picomole'        
    {'ki'                   }    0.0079    {'parameter'}    {'1/minute'                           
    {'[Ins Ind Glu Util]'   }         1    {'parameter'}    {'milligram/minute'                   
    {'Vm0'                  }    2.5129    {'parameter'}    {'milligram/minute'                   
    {'Vmx'                  }     0.047    {'parameter'}    {'(milligram/minute)/(picomole/liter
    {'Km'                   }    225.59    {'parameter'}    {'milligram'                          
    {'p2U'                  }    0.0331    {'parameter'}    {'1/minute'                           
    {'K'                    }      2.28    {'parameter'}    {'picomole/(milligram/deciliter)'     
    {'alpha'                }      0.05    {'parameter'}    {'1/minute'                           
    {'beta'                 }      0.11    {'parameter'}    {'(picomole/minute)/(milligram/decil
    {'gamma'                }       0.5    {'parameter'}    {'1/minute'                           
    {'ke1'                  }    0.0005    {'parameter'}    {'1/minute'                           
    {'ke2'                  }       339    {'parameter'}    {'milligram'                          
    {'Basal Plasma Glu Conc'}     91.76    {'parameter'}    {'milligram/deciliter'                
    {'Basal Plasma Ins Conc'}     25.49    {'parameter'}    {'picomole/liter'                     

Observables:
```

```
          Name                Type                Units
    ______________________    ________    ____________________________

    {'[Plasma Glu Conc]'}    {'species'}    {'milligram/deciliter'}
    {'[Plasma Ins Conc]'}    {'species'}    {'picomole/liter'     }

Dosed:

    TargetName       TargetDimension
    __________    ____________________

     {'Dose'}     {'Mass (e.g., gram)'}


TimeUnits: hour
```

Simulate the model for 24 hours and plot the simulation data. The data contains five runs, where each run represents a scenario in the Scenarios object.

```
sd = f(sObj,24);
sbioplot(sd)
```




```
ans =
  Axes (SbioPlot) with properties:

            XLim: [0 30]
            YLim: [0 450]
          XScale: 'linear'
```

```
          YScale: 'linear'
    GridLineStyle: '-'
         Position: [0.0920 0.1100 0.2956 0.8150]
            Units: 'normalized'

  Show all properties
```

If you have Statistics and Machine Learning Toolbox™, you can also draw sample values for model quantities from various probability distributions. For instance, suppose that the parameters `Vmx` and `kp3`, which are known for the low and high insulin sensitivity, follow the lognormal distribution. You can generate sample values for these parameters from such a distribution, and perform a scan to explore model behavior.

Define the lognormal probability distribution object for `Vmx`.

```
pd_Vmx = makedist('lognormal')
```

```
pd_Vmx =
  LognormalDistribution

  Lognormal distribution
       mu = 0
    sigma = 1
```

By definition, the parameter `mu` is the mean of logarithmic values. To vary the parameter value around the base (model) value of the parameter, set `mu` to `log(`*`model_value`*`)`. Set the standard deviation (*sigma*) to 0.2. For a small *sigma* value, the mean of a lognormal distribtion is approximately equal to `log(`*`model_value`*`)`. For details, see “Lognormal Distribution” (Statistics and Machine Learning Toolbox).

```
Vmx = sbioselect(m1,'Name','Vmx');
pd_Vmx.mu = log(Vmx.Value);
pd_Vmx.sigma = 0.2
```

```
pd_Vmx =
  LognormalDistribution

  Lognormal distribution
       mu = -3.05761
    sigma =      0.2
```

Similarly define the probability distribution for kp3.

```
pd_kp3 = makedist('lognormal');
kp3 = sbioselect(m1,'Name','kp3');
pd_kp3.mu = log(kp3.Value);
pd_kp3.sigma = 0.2
```

```
pd_kp3 =
  LognormalDistribution

  Lognormal distribution
       mu = -4.71053
    sigma =      0.2
```

Now define a joint probability distribution to draw sample values for Vmx and kp3, with a rank correlation to specify some correlation between these two parameters. Note that this correlation assumption is for the illustration purposes of this example only and may not be biologically relevant.

First remove the variants entry (entry 1) from `sObj`.

```
remove(sObj,1)
```

```
ans =
  Scenarios (1 scenarios)

               Name        Content        Number
               ____    _______________    ______

    Entry 1    dose    SimBiology dose      1

  See also Expression property.
```

Add an entry that defines the joint probability distribution with a rank correlation matrix.

```
add(sObj,'cartesian',["Vmx","kp3"],[pd_Vmx, pd_kp3],'RankCorrelation',[1,0.5;0.5,1])
```

```
ans =
  Scenarios (2 scenarios)

                    Name           Content              Number
                    ____    ____________________    ___________

    Entry 1         dose    SimBiology dose           1
    x (Entry 2.1    Vmx     Lognormal distribution    2 (default)
    + Entry 2.2)    kp3     Lognormal distribution    2 (default)

  See also Expression property.
```

By default, the number of samples to draw from the joint distribution is set to 2. Increase the number of samples.

```
updateEntry(sObj,2,'Number',50)
```

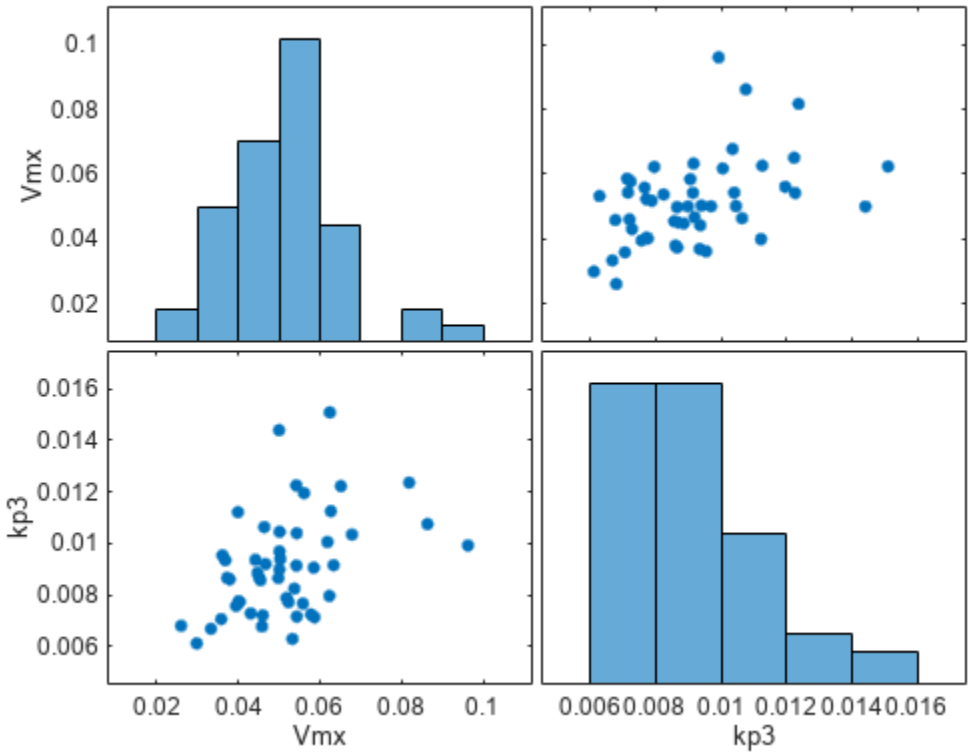
```
ans =
  Scenarios (50 scenarios)

                    Name           Content            Number
                    ____    ____________________    ______

    Entry 1         dose    SimBiology dose           1
    x (Entry 2.1    Vmx     Lognormal distribution    50
    + Entry 2.2)    kp3     Lognormal distribution    50

  See also Expression property.
```

Verify that the `Scenarios` object can be simulated with the model. The `verify` function throws an error if any entry does not resolve uniquely to an object in the model or the entry contents have inconsistent lengths (sample sizes). The function throws a warning if multiple entries resolve to the same object in the model.

```
verify(sObj,m1)
```

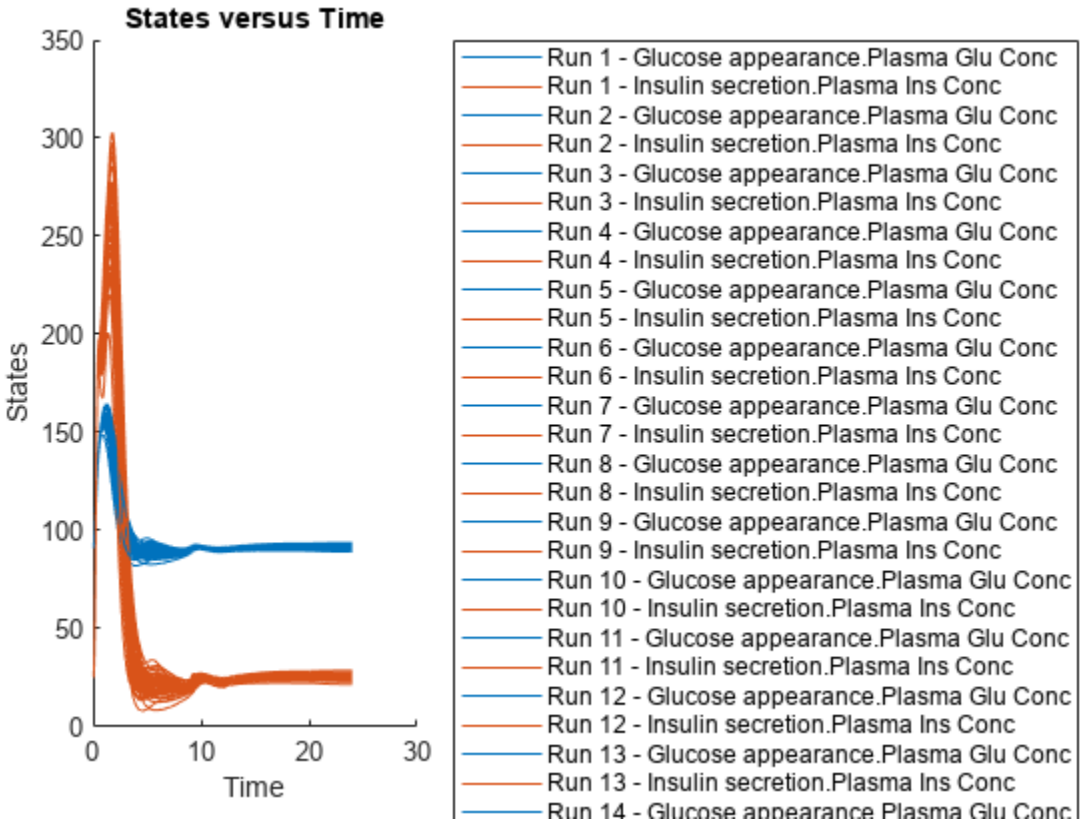
Generate the simulation scenarios. Plot the sample values using `plotmatrix`. You can see the value of `Vmx` is varied around its model value 0.047 and that of `kp3` around 0.009.

```
sTbl = generate(sObj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl.Vmx,sTbl.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
ax(2,1).XLabel.String = "Vmx";
ax(2,2).XLabel.String = "kp3";
```



Simulate the scenarios using the same SimFunction you created previously. You do not need to create a new SimFunction object even though the Scenarios object has been updated.

```
sd2 = f(sObj,24);
sbioplot(sd2);
```



By default, SimBiology uses the random sampling method. You can change it to the Latin hypercube sampling (or sobol or halton) for a more systematic space-filling approach.

```
entry2struct = getEntry(sObj,2)
```

```
entry2struct = struct with fields:
               Name: {'Vmx'  'kp3'}
            Content: [2x1 prob.LognormalDistribution]
             Number: 50
    RankCorrelation: [2x2 double]
         Covariance: []
     SamplingMethod: 'random'
    SamplingOptions: [0x0 struct]
```

```
entry2struct.SamplingMethod = 'lhs'
```

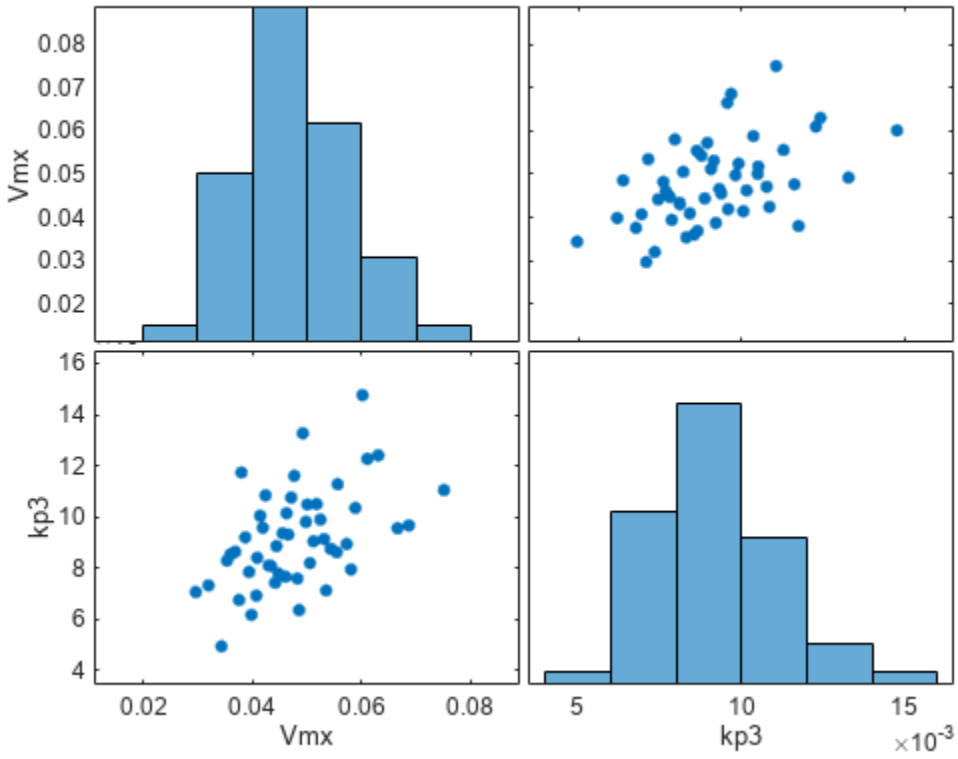
```
entry2struct = struct with fields:
               Name: {'Vmx'  'kp3'}
            Content: [2x1 prob.LognormalDistribution]
             Number: 50
    RankCorrelation: [2x2 double]
         Covariance: []
     SamplingMethod: 'lhs'
    SamplingOptions: [0x0 struct]
```

You can now use the updated structure to modify entry 2.

```
updateEntry(sObj,2,entry2struct)

ans =
  Scenarios (50 scenarios)

                    Name           Content             Number
                    ____    ____________________      ______

    Entry 1         dose    SimBiology dose             1
    x (Entry 2.1    Vmx     Lognormal distribution      50
    + Entry 2.2)    kp3     Lognormal distribution      50

  See also Expression property.
```

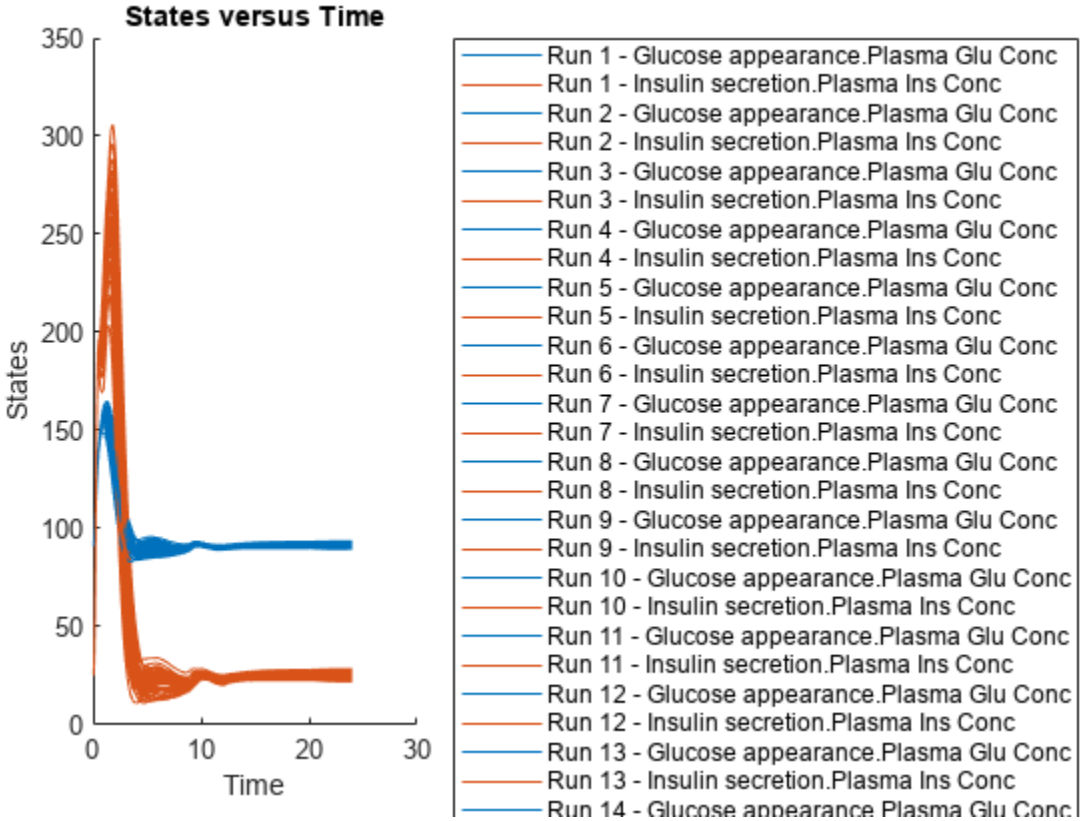
Visualize the sample values.

```
sTbl2 = generate(sObj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl2.Vmx,sTbl2.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
ax(2,1).XLabel.String = "Vmx";
ax(2,2).XLabel.String = "kp3";
```



Simulate the scenarios.

```
sd3 = f(sObj,24);
sbioplot(sd3);
```



Restore warning settings.

```
warning(warnSettings);
```

Input Arguments

`sObj` — Simulation scenarios

`SimBiology.Scenarios` object

Simulation scenarios, specified as a `SimBiology.Scenarios` object.

`sObj2` — Simulation scenarios

`SimBiology.Scenarios` object

Simulation scenarios, specified as a `SimBiology.Scenarios` object.

`name` — Entry name

character vector | string

Entry name, specified as a character vector or string.

You can set the entry name to the name of a model quantity (species, parameter, or compartment). Alternatively, you can define a name for a group of doses or variants to be included in the sample (scenarios) generation.

Example: `"k1"`

Data Types: `char` | `string`

`content` — Model quantity values or vector of doses or variants
numeric vector | vector of `RepeatDose` or `ScheduleDose` objects | vector of variant objects

Model quantity values, or a vector of doses or variants, specified as a numeric vector, vector of `RepeatDose` or `ScheduleDose` objects, or vector of `variant` objects.

If you specify a quantity name for the `name` input argument, set `content` to a numeric vector.

If you specify a name for a group of doses or variants, set `content` to a vector of dose objects or vector of variant objects.

Example: `[0.5,1,1.5]`

`combination` — Method to combine entries
`'cartesian'` | `'elementwise'`

Method to combine entries, specified as one of the following:

- `'cartesian'` – Combine entries by taking the Cartesian product of the corresponding sample values. This is denoted by the cross symbol `x`.
- `'elementwise'` – Combine entries one to one (elementwise), that is, the first element from the first entry is paired with the first element from the second entry and so on. This is denoted by the plus symbol `+`. The entries must have the same number of sample values (elements) for this method.

For details, see “Combine Simulation Scenarios in SimBiology”.

`quantityNames` — Names of model quantities
character vector | string | string vector | cell array of character vectors

Names of model quantities for the sample (scenario) generation, specified as a character vector, string, string vector, or cell array of character vectors.

Example: `["k12","k21"]`

Data Types: `char` | `string` | `cell`

`probDist` — Probability distributions
vector of probability distribution objects | character vector | string | string vector | cell array of character vectors

Probability distributions to generate sample values for model quantities, specified as a vector of probability distribution objects, character vector, string, string vector, or cell array of character vectors containing the names of supported probability distributions. To specify the probability distributions, you must have Statistics and Machine Learning Toolbox.

Use the `makedist` function to create distribution objects. For a list of supported distributions, see “distname” (Statistics and Machine Learning Toolbox).

Example: `[pd1,pd2]`

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `'Number',10` specifies to generate 10 samples.

`Number` — Number of samples

`[]` (default) | positive scalar

Number of samples to draw from probability distributions, specified as the comma-separated pair consisting of `'Number'` and a positive scalar. The default value `[]` means that the function infers the number of samples from other entries. If the number cannot be inferred, the number is set to `2`.

Example: `'Number',5`

`RankCorrelation` — Rank correlation matrix

`[]` (default) | numeric matrix

Rank correlation matrix for the joint probability distribution, specified as the comma-separated pair consisting of `'RankCorrelation'` and a numeric matrix. The default behavior is that when both `'RankCorrelation'` and `'Covariance'` are set to `[]`, `SimBiology.Scenarios` draws uncorrelated samples from the joint probability distribution.

You cannot specify `'RankCorrelation'` if `'Covariance'` is set. The number of columns in the matrix must match the number of specified distributions. The matrix must be symmetric with diagonal values of 1. All of its eigenvalues must also be positive.

Example: `'RankCorrelation',[1 0.3;0.3 1]`

`Mean` — Mean values

numeric vector

Mean values of quantities, specified as the comma-separated pair consisting of `'Mean'` and a numeric vector.

You can specify mean values for normal distributions only. The number of mean values must equal the number of specified probability distributions.

Example: `'Mean',[0.5,1.5]`

`Covariance` — Covariance matrix

`[]` (default) | numeric matrix

Covariance matrix for the joint probability distribution, specified as the comma-separated pair consisting of `'Covariance'` and a numeric matrix. The default behavior is that if both `'RankCorrelation'` and `'Covariance'` are set to `[]`, `SimBiology.Scenarios` draws uncorrelated samples from the joint probability distribution. You cannot specify `'Covariance'` if you specify `'RankCorrelation'`.

You can specify the covariance matrix for normal distributions only. The number of columns in the matrix must match the number of specified distributions. All of its eigenvalues must also be nonnegative.

Example: `'Covariance',[0.25 0.15;0.15 0.25]`

`SamplingMethod` — Sampling method
`'random'` (default) | `'lhs'` | `'copula'` | `'sobol'` | `'halton'`

Sampling method, specified as the comma-separated pair consisting of `'SamplingMethod'` and a character vector or string. Depending on whether probability distributions with `'RankCorrelation'` or normal distributions with `'Covariance'` are specified, the sampling techniques differ.

If an entry contains a (joint) normal distribution with `Covariance` specified, the sampling methods are:

- `'random'` – Draw random samples from the specified normal distribution using `mvnrnd`.
- `'lhs'` – Draw Latin hypercube samples from the specified normal distributions using `lhsnorm`. For details, see “Generating Quasi-Random Numbers” (Statistics and Machine Learning Toolbox).

If an entry contains a (joint) distribution with no `Covariance` specified, the sampling methods are:

- `'random'` – Draw random samples from the specified probability distributions using `random`.
- `'lhs'` – Draw Latin hypercube samples from the specified probability distributions using an algorithm similar to `lhsdesign`. This approach is a more systematic space-filling approach than random sampling. For details, see “Generating Quasi-Random Numbers” (Statistics and Machine Learning Toolbox).
- `'copula'` – Draw random samples using a copula (Statistics and Machine Learning Toolbox). Use this option to impose correlations between samples using copulas.
- `'sobol'` – Use the sobol sequence (`sobolset`) which is transformed using the inverse cumulative distribution function (`icdf`) of the specified probability distributions. Use this method for highly systematic space-filling. For details, see “Generating Quasi-Random Numbers” (Statistics and Machine Learning Toolbox).
- `'halton'` – Use the halton sequence (`haltonset`) which is transformed using the inverse cumulative distribution function (`icdf`) of the specified probability distributions. For details, see “Generating Quasi-Random Numbers” (Statistics and Machine Learning Toolbox).

If no `Covariance` is specified, `SimBiology.Scenarios` essentially performs two steps. The first step is to generate samples using one of the above sampling methods. For `lhs`, `sobol`, and `halton` methods, the generated uniform samples are transformed to samples from the specified distribution using the inverse cumulative distribution function `icdf`. Then, as the second step, the samples are correlated using the Iman-Conover algorithm if `RankCorrelation` is specified. For `random`, the samples are drawn directly from the specified distributions and the samples are then correlated using the Iman-Conover algorithm.

Example: `'SamplingMethod','lhs'`

`SamplingOptions` — Options for sampling method
struct

Options for the sampling method, specified as a scalar struct. The options differ depending on the sampling method: `sobol`, `halton`, or `lhs`.

For `sobol` and `halton`, specify each field name and value of the structure according to each name-value argument of the `sobolset` or `haltonset` function. SimBiology uses the default value of `1` for the `Skip` argument for both methods. For all other name-value arguments, the software uses the

same default values of `sobolset` or `haltonset`. For instance, set up a structure for the `Leap` and `Skip` options with nondefault values as follows.

```
s1.Leap = 50;
s1.Skip = 0;
```

For `lhs`, there are three samplers that support different sampling options.

- If you specify a covariance matrix, SimBiology uses `lhsnorm` for sampling. `SamplingOptions` argument is not allowed.
- Otherwise, use the field name `UseLhsdesign` to select a sampler.
  - If the value is `true`, SimBiology uses `lhsdesign`. You can use the name-value arguments of `lhsdesign` to specify the field names and values.
  - If the value is `false` (default), SimBiology uses a nonconfigurable Latin hypercube sampler that is different from `lhsdesign`. This sampler does not require Statistics and Machine Learning Toolbox. `SamplingOptions` cannot contain any other options, except `UseLhsdesign`.

For instance, set up a structure to use `lhsdesign` with the `Criterion` and `Iterations` options.

```
s2.UseLhsdesign  = true;
s2.Criterion     = "correlation";
s2.Iterations    = 10;
```

Example: `'SamplingOptions',struct("Skip",5)`

Data Types: `struct`

Output Arguments

`sObj` — Simulation scenarios

`Scenarios` object

Simulation scenarios, returned as a `Scenarios` object.

Version History

Introduced in R2019b

See Also

`SimBiology.Scenarios` | `SimFunction object` | `createSimFunction (model)`

Topics

“SimBiology.Scenarios Terminology” on page 2-799
“Combine Simulation Scenarios in SimBiology”

addcompartment (model, compartment)

Create compartment object

Syntax

```
compartmentObj = addcompartment(modelObj, 'NameValue')
compartmentObj = addcompartment(owningCompObj, 'NameValue')
compartmentObj = addcompartment(modelObj, 'NameValue', CapacityValue)

compartmentObj = addcompartment(...'PropertyName', PropertyValue...)
```

Arguments

modelObj	`Model object`
owningCompObj	Compartment object that contains the newly created compartment object.
NameValue	Name for a compartment object. Enter a character vector unique to the model object. For information on naming compartments, see Name.
CapacityValue	Capacity value for the compartment object. Enter `double`. Positive real number, default = `1`.
PropertyName	Enter the name of a valid property. Valid property names are listed in “Property Summary” on page 2-24.
PropertyValue	Enter the value for the property specified in *PropertyName*. Valid property values are listed on each property reference page.

Description

compartmentObj = addcompartment(*modelObj*, '*NameValue*') creates a compartment object and returns the compartment object (*compartmentObj*). In the compartment object, this method assigns a value (*NameValue*) to the property `Name`, and assigns the `model object` (*modelObj*) to the property `Parent`. In the model object, this method assigns the compartment object to the property `Compartments`.

compartmentObj = addcompartment(*owningCompObj*, '*NameValue*') in addition to the above, adds the newly created compartment within a compartment object (*owningCompObj*), and assigns this compartment object (*owningCompObj*) to the `Owner` property of the newly created compartment object (*compartmentObj*). The parent model is the model that contains the owning compartment (*owningCompObj*).

compartmentObj = addcompartment(*modelObj*, '*NameValue*', *CapacityValue*), in addition to the above, this method assigns capacity *(CapacityValue)* for the compartment.

If you define a reaction within a model object (`modelObj`) that does not contain any compartments, the process of adding a reaction generates a default compartment object and assigns the reaction

species to the compartment. If there is more than one compartment, you must specify which compartment the species should be assigned to using the format *`CompartmentName`*.*`SpeciesName`*.

`compartmentObj` `= addcompartment(...'`*`PropertyName`*`', `*`PropertyValue`*`...)` defines optional properties. “Property Summary” on page 2-24 lists the properties. The `Owner` property is one exception; you cannot set the `Owner` property in the `addcompartment` syntax because, `addcompartment` requires the owning model or compartment to be specified as the first argument and uses this information to set the `Owner` property.

Method Summary

Methods for compartment objects

addcompartment (model, compartment)	Create compartment object
addspecies (model, compartment)	Create species object and add to compartment object within model object
copyobj	Copy SimBiology object and its children
delete	Delete SimBiology object
display	Display summary of SimBiology object
findUsages	Find out how a species, parameter, or compartment is used in a model
get	Get SimBiology object properties
move	Move SimBiology compartment object to new owner
rename	Rename object and update expressions
reorder (model, compartment, kinetic law)	Reorder component lists
set	Set SimBiology object properties

Property Summary

Properties for compartment objects

Capacity	Compartment capacity
CapacityUnits	Compartment capacity units
Compartments	Array of compartments in model or compartment
Constant	Specify variable or constant species amount, parameter value, or compartment capacity
ConstantCapacity	Specify variable or constant compartment capacity
Name	Specify name of object
Notes	HTML text describing SimBiology object
Owner	Owning compartment
Parent	Indicate parent object
Species	Array of species in compartment object
Tag	Specify label for SimBiology object
Type	Display SimBiology object type
Units	Units for species amount, parameter value, compartment capacity, observable expression
UserData	Specify data to associate with object
Value	Value of species, compartment, or parameter object

Examples

Add Compartments

This example shows how to add compartments to a SimBiology model.

Create a SimBiology model which is named `m1`.

```
model = sbiomodel('m1');
```

Add two compartments to the model, which are named as `Central` and `Peripheral` respectively.

```
comp1 = addcompartment(model,'Central');
comp2 = addcompartment(model,'Peripheral');
```

Change the compartment capacities and units.

```
comp1.Capacity = 2;
comp1.CapacityUnits = 'liter';
comp2.Capacity = 1;
comp2.CapacityUnits = 'liter';
```

Display all the compartments of the model.

```
model.Compartments
```

```
ans =
   SimBiology Compartment Array

   Index:    Name:         Value:    Units:
   1         Central       2         liter
```

```
2         Peripheral    1         liter
```

Version History

Introduced in R2007b

R2022b: Having duplicate model component names issues a warning

Warns starting in R2022b

- SimBiology issues a warning if multiple model components (model, compartment, species, parameter, reaction, rule, event, observable, dose, and variant) have the same name. In a future release, within a single model, these components will be required to have unique names even when they are of different types with the following two exceptions:
  - Species in different compartments can have the same name.
  - Parameters can have the same name if they are scoped to different parents. Specifically, you can use the same name for a model-scoped parameter and reaction-scoped parameters, where each reaction-scoped parameter belongs to a different reaction.

  The purpose of this naming restriction is to ensure that every model component can be unambiguously referenced by its unique name within a model. For details on how to reference model component names in expressions, see “Guidelines for Referencing Names in Expressions”.
- To disambiguate duplicate names from your model, use the `updateDuplicateNames` function at the command line. The function takes in a SimBiology model as an input and updates the component names as necessary. You can also specify optional outputs, such as a logical flag to check whether any update occurred, a list of model changes, and a copy of the original model before any updates were made.
- The `updateDuplicateNames` function disambiguates the duplicate names by adding a suffix `"_N"`, where *N* is the first positive integer that results in a unique name. If there is an existing suffix, *N* will be incremented from that suffix. For example, if there are two model components named *x_3*, the function updates one of the names to *x_4*. If the existing suffix has leading zeros, the function omits the zeros in the new name. For instance, if *x_003* is a duplicate name, it gets renamed to *x_4*. However, the function assumes that names with leading zeros and without leading zeros are different. For instance, *x_005* and *x_5* are considered to be different names.

R2022a: Having duplicate model component names will not be allowed in a future release

Behavior change in future release

SimBiology will not allow you to have duplicate names for model components within a model.

See Also

`model object` | `addproduct` | `addreactant` | `addreaction` | `addspecies`

addCompartment (PKModelDesign)

Add compartment to `PKModelDesign` object

Syntax

```
PKCompartmentObj = addCompartment(PKModelDesignObj, CompObjName)
PKCompartmentObj = addCompartment(PKModelDesignObj, CompObjName, Name, Value)
```

Description

`PKCompartmentObj = addCompartment(PKModelDesignObj, CompObjName)` constructs a PK compartment with the specified name and adds it to *`PKModelDesignObj`*, a `PKModelDesign` object.

`PKCompartmentObj = addCompartment(PKModelDesignObj, CompObjName, Name, Value)` constructs a PK compartment with the specified name, and with additional options specified by one or more `Name,Value` pair arguments.

Input Arguments

`PKModelDesignObj`	`PKModelDesign object` to which you want to add a compartment
`CompObjName`	Name of the `PKCompartment` object that is constructed, specified as a character vector or string.

Name-Value Pair Arguments

Optional comma-separated pairs of *`Name, Value`* arguments, where *`Name`* is the argument name and *`Value`* is the corresponding value. *`Name`* must appear inside single quotes (`''`). You can specify several name-value pair arguments in any order as `Name1,Value1,…,NameN,ValueN`.

`DosingType`	Character vector (or string) specifying the mechanism for drug absorption. Choices are: • `'Bolus'` • `'Infusion'` • `'ZeroOrder'` • `'FirstOrder'` • `''` (default) For more information, see “Dosing Types”.

`EliminationType`	Character vector (or string) specifying the mechanism for drug elimination. Choices are: • `'Linear'` • `'Linear-Clearance'` • `'Enzymatic'` • `''` (default) For more information, see “Elimination Types”.
`HasResponseVariable`	Logical indicating if the drug concentration in this compartment is reported. Multiple compartments in a model can have this property set to `true`. Default is `false`. **Note** If you perform a parameter fit on a model, at least one compartment in the model must have a `HasResponseVariable` property set to `true`.
`HasLag`	Logical indicating if any dose targeting this compartment have a lag associated with them. Default is `false`.

These optional name-value pair arguments set the corresponding property of the `PKCompartment` object. You can also set these properties after creating the `PKCompartment` object by using the following syntax:

```
PKCompartmentObj.PropertyName = Value
```

For example:

```
PKCompartmentObj.DosingType = 'Bolus'
```

Output Arguments

`PKCompartmentObj`	`PKCompartment object`

Method Summary

delete	Delete SimBiology object
display	Display summary of SimBiology object
get	Get SimBiology object properties
set	Set SimBiology object properties

Property Summary

DosingType	Drug dosing type in compartment
EliminationType	Drug elimination type from compartment
HasLag	Lag associated with dose targeting compartment
HasResponseVariable	Compartment drug concentration reported
Name	Specify name of object

See Also

“Create a Pharmacokinetic Model Using the Command Line”, `HasLag`, `HasResponseVariable`, `PKCompartment object`, `PKModelDesign object`

Version History

Introduced in R2009a

addconfigset (model)

Create configuration set object and add to model object

Syntax

```
configsetObj = addconfigset(modelObj, 'NameValue')

configsetObj = addconfigset(..., 'PropertyName', PropertyValue, ...)
```

Arguments

modelObj	`Model object`. Enter a variable name.
NameValue	Descriptive name for a configuration set object. Reserved words `'active'` and `'default'` are not allowed.
configsetObj	`Configset object`.

Description

`configsetObj = addconfigset(modelObj, 'NameValue')` creates a configuration set object and returns to *configsetObj*.

In the configuration set object, this method assigns a value (*NameValue*) to the property `Name`.

`configsetObj = addconfigset(..., 'PropertyName', PropertyValue, ...)` constructs a configuration set object, *configsetObj*, and configures *configsetObj* with property value pairs. The *configsetObj* properties are listed in “Property Summary” on page 2-31.

A configuration set stores simulation specific information. A model object can contain multiple configuration sets, with one being active at any given time. The active configuration set contains the settings that are used during a simulation. *configsetObj* is not automatically set to active. Use the function `setactiveconfigset` to define the active `configset` for `modelObj`.

Use the method `copyobj` to copy a `configset` object and add it to the `modelObj`.

Method Summary

Methods for configuration set objects

copyobj	Copy SimBiology object and its children
delete	Delete SimBiology object
display	Display summary of SimBiology object
get	Get SimBiology object properties
set	Set SimBiology object properties

Property Summary

Properties for configuration set objects

Active	Indicate object in use during simulation
AmountUnits	Amount unit used internally during simulation when UnitConversion is on
CompileOptions	Dimensional analysis and unit conversion options
MassUnits	Mass unit used internally during simulation when UnitConversion is on
MaximumNumberOfLogs	Maximum number of logs criteria to stop simulation
MaximumWallClock	Maximum elapsed wall clock time to stop simulation
Name	Specify name of object
Notes	HTML text describing SimBiology object
RuntimeOptions	Options for logged species
SensitivityAnalysisOptions	Specify sensitivity analysis options
SolverType	Select solver type for simulation
StopTime	Simulation time criteria to stop simulation
TimeUnits	Show time units for dosing and simulation
Type	Display SimBiology object type

Examples

Add a Configuration Set Object

This example shows how to add a configset object to a SimBiology model and set it up for simulation.

Load the sample radiodecay model `m1`, and add a `Configset` object to the model.

```
sbioloadproject radiodecay;
configsetObj = addconfigset(m1, 'myset');
```

Configure the simulation stop criteria by setting the `StopTime` property.

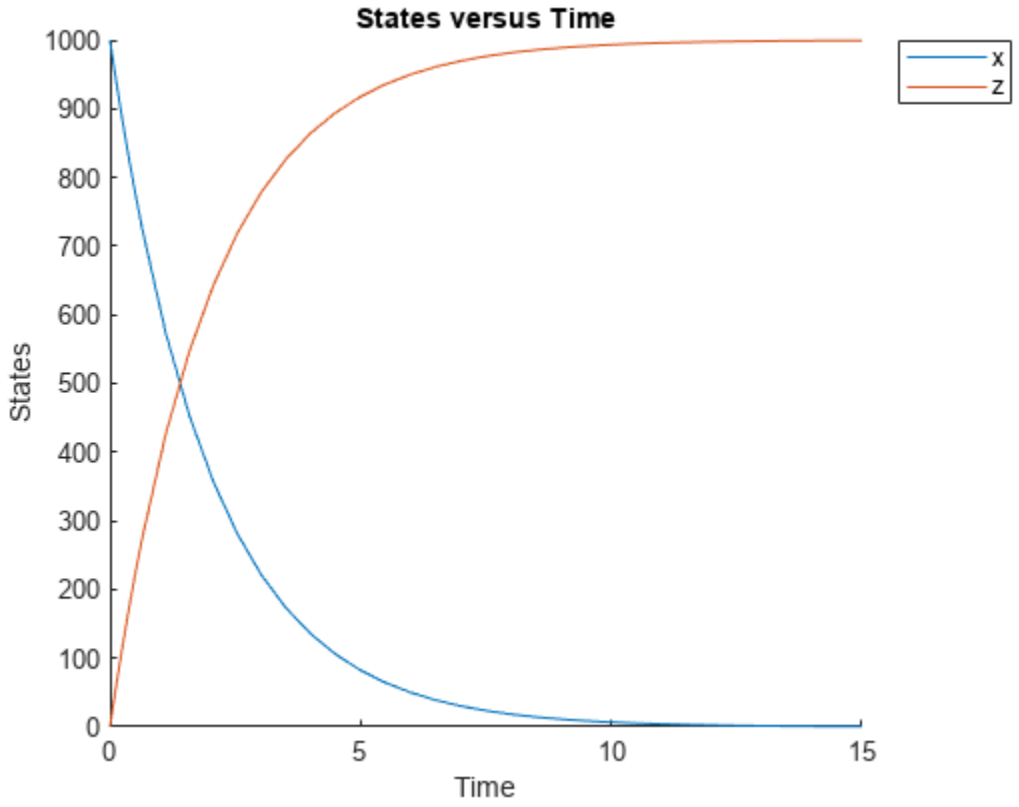
```
configsetObj.StopTime = 15;
```

Set the configset object to be active so that its settings are used during simulation.

```
setactiveconfigset(m1,configsetObj);
```

Simulate the model and plot results.

```
simdata = sbiosimulate(m1);
sbioplot(simdata);
```



See Also

`model object`, `configset object`, `getconfigset`, `removeconfigset`, `setactiveconfigset`

Version History

Introduced in R2006a

addcontent (variant)

Append content to variant object

Syntax

`addcontent(variantObj, contents)`

`addcontent(variantObj1, variantObj2)`

Arguments

variantObj	Specify the variant object to which you want to append data. The `Content` property is modified to add the new data.
contents	Specify the data you want to add to a variant object. Contents can either be a cell array or an array of cell arrays. A valid cell array should have the form `{'Type', 'Name', 'PropertyName', PropertyValue}`, where *PropertyValue* is the new value to be applied for the *PropertyName*. Valid *Type*, *Name*, and *PropertyName* values are as follows.

'*Type*'	'*Name*'	'*PropertyName*'
`'species'`	Name of the species. If there are multiple species in the model with the same name, specify the species as [`compartmentName.speciesName`], where `compartmentName` is the name of the compartment containing the species.	`'InitialAmount'`
`'parameter'`	If the parameter scope is a model, specify the parameter name. If the parameter scope is a kinetic law, specify [`reactionName.parameterName`].	`'Value'`
`'compartment'`	Name of the compartment.	`'Capacity'`

Description

`addcontent(variantObj, contents)` adds the data stored in the variable *contents* to the variant object (*variantObj*).

`addcontent(variantObj1, variantObj2)` appends the data in the `Content` property of the variant object *variantObj2* to the `Content` property of variant object *variantObj1*.

Note Remember to use the `addcontent` method instead of using the `set` method on the `Content` property because the `set` method replaces the data in the `Content` property, whereas `addcontent` appends the data.

Examples

1 Create a model containing one species.

```
modelObj = sbiomodel('mymodel');
compObj = addcompartment(modelObj, 'comp1');
speciesObj = addspecies(compObj, 'A');
```

2 Add a variant object that varies the `InitialAmount` property of a species named A.

```
variantObj = addvariant(modelObj, 'v1');
addcontent(variantObj, {'species', 'A', 'InitialAmount', 5});
```

See Also

`addvariant`, `rmcontent`, `sbiovariant`

Version History

Introduced in R2007b

adddose (model)

Add dose object to model

Syntax

```
doseObj2 = adddose(modelObj, 'DoseName')
doseObj2 = adddose(modelObj, 'DoseName', 'DoseType')
doseObj2 = adddose(modelObj, doseObj)
```

Arguments

modelObj	`Model object` to which you add a dose object.
DoseName	Name of a dose object to construct and add to a model object. *DoseName* is the value of the dose object property `Name`.
DoseType	Type of dose object to construct and add to a model object. Enter either `'schedule'` or `'repeat'`.
doseObj	Dose object to add to a model object. Created with the constructor `sbiodose`.

Outputs

doseObj2	`ScheduleDose object` or `RepeatDose object`. A `RepeatDose` or `ScheduleDose` object defines an increase (dose) to a species amount during a simulation.

Description

Before using a dose object in a simulation, use the `adddose` method to add the dose object to a SimBiology `model object`. Then, set the `Active` dose object property to `true`.

doseObj2 = `adddose(`*modelObj*`, '`*DoseName*`')` constructs a SimBiology RepeatDose object (*doseObj2*), assigns *DoseName* to the property `Name`, adds the dose object to a SimBiology model object (*modelObj*), and assigns *modelObj* to the property `Parent`.

doseObj2 = `adddose(`*modelObj*`, '`*DoseName*`', '`*DoseType*`')` constructs either a SimBiology `ScheduleDose` object or `RepeatDose` object (*doseObj*).

doseObj2 = `adddose(`*modelObj*`, `*doseObj*`)` adds a SimBiology dose object (*doseObj*) to a SimBiology model object (*modelObj*), copies the dose object to a second dose object (*doseObj2*), and assigns *modelObj* to the property `Parent`. The `Active` property of *doseObj2* is set to `false` by default.

Note Alternatively, you can create a dose object using `sbiodose` as a standalone dose object, which you can apply to different models. For details, see “Creating Doses Programmatically”.

Examples

Add an Infusion Dose

This example shows how to add a constant-rate infusion dose to a one-compartment model.

Background

Suppose you have a one-compartment model with a species named `drug` that represents the total amount of drug in the body. The drug is removed from the body via the first-order elimination represented by the reaction `drug -> null`, with the elimination rate constant `ke`. In other words, the drug concentration versus the time profile follows the monoexponential decline $C_t = C_0 e^{-k_e t}$, where C_t is the drug concentration at time t, C_0 is the initial concentration, and `ke` is the elimination rate constant. This example shows how to set up such a one-compartment model and add an infusion dose at a constant rate of 10 mg/hour for the total dose amount of 250 mg.

Create a One-Compartment Model

Create a SimBiology model named `onecomp`.

```
m1 = sbiomodel('onecomp');
```

Define the elimination of the drug from the system by adding a reaction `drug -> null` to the model.

```
r1 = addreaction(m1,'drug -> null');
```

The species `drug` is automatically created and added to the compartment. The `null` species is a reserved species that acts as a sink in this reaction.

Add a mass action kinetic law to the reaction. This kinetic law defines the drug elimination to follow the first-order kinetics.

```
k1 = addkineticlaw(r1,'MassAction');
```

Define the elimination rate parameter `ke` and add it to the kinetic law.

```
p1 = addparameter(k1,'ke','Value',1.0,'ValueUnits','1/hour');
```

Specify the rate parameter `ke` as the forward rate parameter of the reaction by setting the `ParameterVariableNames` property of kinetic law object `k1`. This allows SimBiology to determine the reaction rate for `drug -> null` reaction.

```
k1.ParameterVariableNames = 'ke';
```

Set Up an Infusion Dose

Add a dose object to the model using the `adddose` method. Specify the amount of the dose (`Amount`), the dose target (`TargetName`), and the infusion rate (`Rate`). You also need to set the `Active` property of the dose object to `true` so that the dose is applied to the model during simulation.

```
d1 = adddose(m1,'InfusionDose');
d1.Amount = 250;
d1.TargetName = 'drug';
d1.Rate = 10;
d1.RateUnits = 'milligram/hour';
d1.Active = true;
```

Simulate the Model

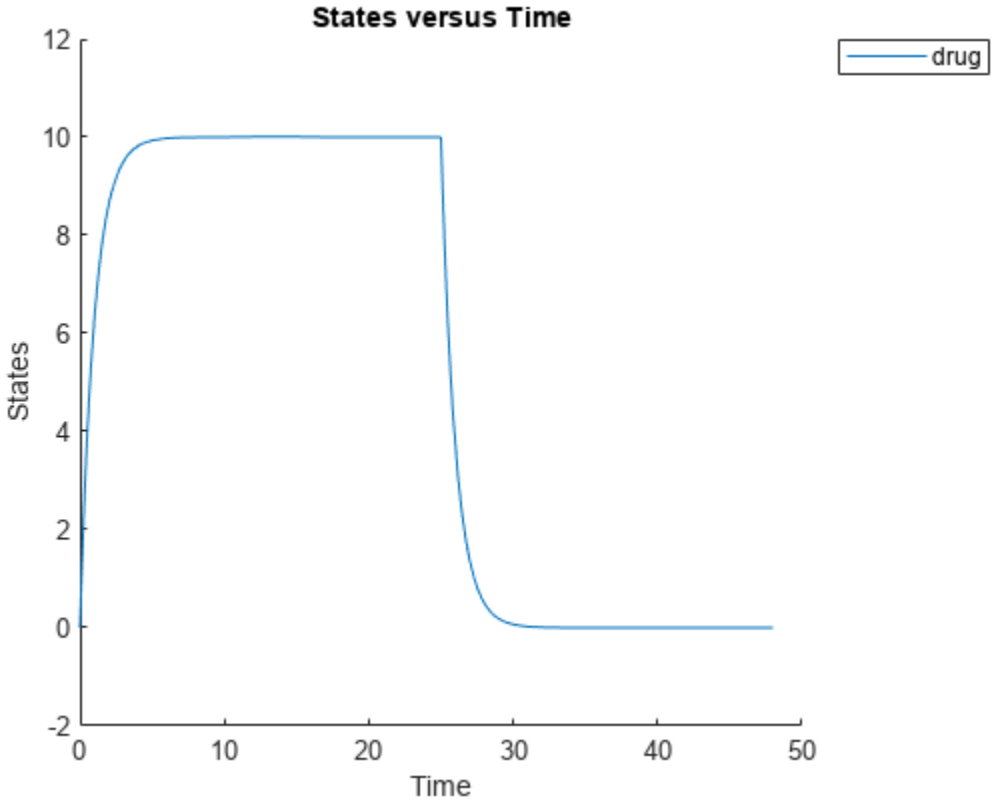
Change the simulation stop time to 48 hours to see the complete time course.

```
cs = getconfigset(m1);
cs.StopTime = 48;
cs.TimeUnits = 'hour';
sd = sbiosimulate(m1);
```

Plot Results

Plot the concentration versus the time profile of the drug in the system.

```
sbioplot(sd);
```



Version History

Introduced in R2010a

R2022b: Having duplicate model component names issues a warning

Warns starting in R2022b

- SimBiology issues a warning if multiple model components (model, compartment, species, parameter, reaction, rule, event, observable, dose, and variant) have the same name. In a future release, within a single model, these components will be required to have unique names even when they are of different types with the following two exceptions:

  - Species in different compartments can have the same name.
  - Parameters can have the same name if they are scoped to different parents. Specifically, you can use the same name for a model-scoped parameter and reaction-scoped parameters, where each reaction-scoped parameter belongs to a different reaction.

  The purpose of this naming restriction is to ensure that every model component can be unambiguously referenced by its unique name within a model. For details on how to reference model component names in expressions, see “Guidelines for Referencing Names in Expressions”.
- To disambiguate duplicate names from your model, use the `updateDuplicateNames` function at the command line. The function takes in a SimBiology model as an input and updates the component names as necessary. You can also specify optional outputs, such as a logical flag to check whether any update occurred, a list of model changes, and a copy of the original model before any updates were made.
- The `updateDuplicateNames` function disambiguates the duplicate names by adding a suffix `"_N"`, where *N* is the first positive integer that results in a unique name. If there is an existing suffix, *N* will be incremented from that suffix. For example, if there are two model components named *x_3*, the function updates one of the names to *x_4*. If the existing suffix has leading zeros, the function omits the zeros in the new name. For instance, if *x_003* is a duplicate name, it gets renamed to *x_4*. However, the function assumes that names with leading zeros and without leading zeros are different. For instance, *x_005* and *x_5* are considered to be different names.

R2022a: Having duplicate model component names will not be allowed in a future release
Behavior change in future release

SimBiology will not allow you to have duplicate names for model components within a model.

See Also

`model object` | `getdose` | `removedose` | `sbiodose` | `RepeatDose object` | `ScheduleDose object`

Topics
“Doses in SimBiology Models”

addevent (model)

Add event object to model object

Syntax

```
eventObj = addevent(modelObj, 'TriggerValue', 'EventFcnsValue')

eventObj = addevent(...'PropertyName', PropertyValue...)
```

Arguments

modelObj	`Model object`.
TriggerValue	Required property to specify a trigger condition. Must be a MATLAB expression that evaluates to a logical value. Use the keyword `'time'` to specify that an event occurs at a specific time during the simulation. For more information, see `Trigger`.
EventFcnsValue	Character vector or a cell array of character vectors, each of which specifies an assignment of the form `'objectname = expression'`, where *objectname* is the name of a valid object. Defines what occurs when the event is triggered. For more information, see `EventFcns`.
PropertyName	Property name for an event object from “Property Summary” on page 2-40.
PropertyValue	Property value. For more information on property values, see the property reference for each property listed in “Property Summary” on page 2-40.

Description

`eventObj = addevent(modelObj, 'TriggerValue', 'EventFcnsValue')` creates an `Event object` (*eventObj*) and adds the event to the model (*modelObj*). In the event object, this method assigns a value (*TriggerValue*) to the property `TriggerCondition`, assigns a value (*EventFcnsValue*) to the property `EventFcns`, and assigns the `model object` (*modelObj*) to the property `Parent`. In the model object, this method appends the event object to the property `Events`.

When the trigger expression in the property `Trigger` changes from false to true, the assignments in `EventFcns` are executed during simulation.

For details on how events are handled during a simulation, see “Events in SimBiology Models”.

`eventObj = addevent(...'PropertyName', PropertyValue...)` defines optional properties. The property name and property value pairs can be any format supported by the function `set`.

Property Summary

Active	Indicate object in use during simulation
EventFcns	Event expression
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Tag	Specify label for SimBiology object
Trigger	Event trigger
Type	Display SimBiology object type
UserData	Specify data to associate with object

Examples

Add an Event

This example shows how to add an event to a SimBiology model.

Create a simple model with a mass action reaction `A -> B`, where A and B are species. Also add the reaction rate parameter, p1, with the parameter value of 0.5.

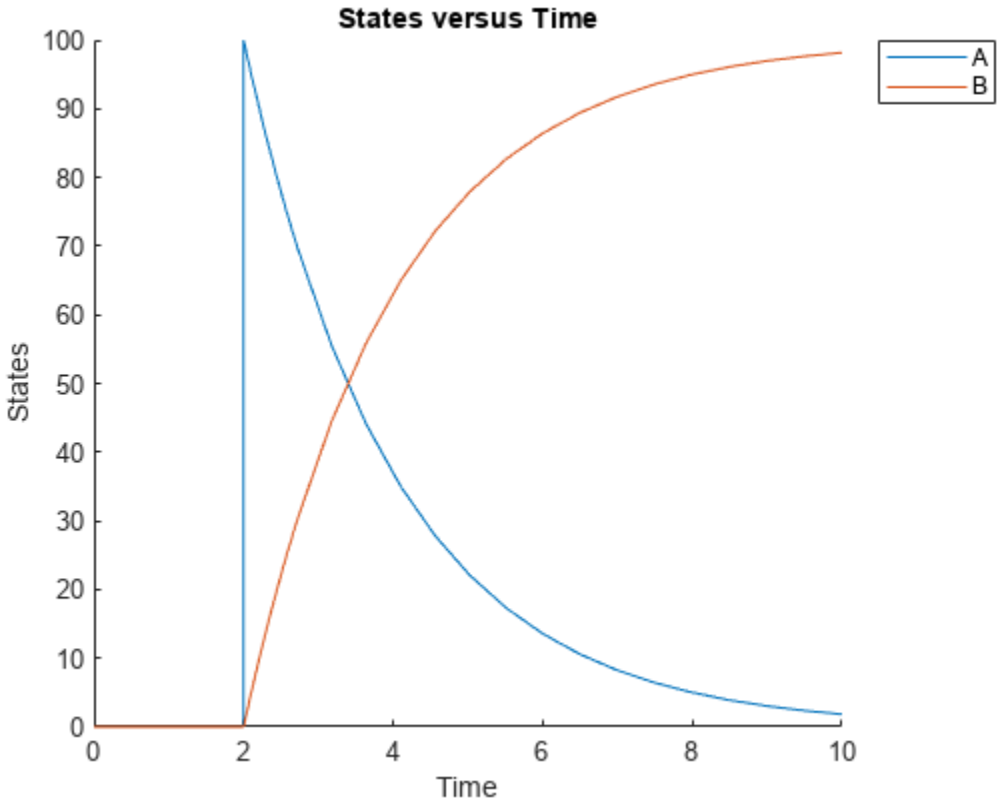
```
model       = sbiomodel('example');
r1          = addreaction(model,'A -> B');
kl          = addkineticlaw(r1,'MassAction');
p1          = addparameter(model,'p1',0.5);
kl.ParameterVariableNames = 'p1';
```

Increase the amount of species A to 100 at time = 2. You can do this by adding an event object to the model. You must specify the event trigger (`time >= 2`), and also the event function, which defines what happens when the event is triggered. In this example, the event function is `A = 100`.

```
e1 = addevent(model,'time>=2','A = 100');
```

Simulate the model, and plot the result.

```
sd = sbiosimulate(model);
sbioplot(sd);
```



Version History

Introduced in R2007b

R2022b: Having duplicate model component names issues a warning

Warns starting in R2022b

- SimBiology issues a warning if multiple model components (model, compartment, species, parameter, reaction, rule, event, observable, dose, and variant) have the same name. In a future release, within a single model, these components will be required to have unique names even when they are of different types with the following two exceptions:

  - Species in different compartments can have the same name.
  - Parameters can have the same name if they are scoped to different parents. Specifically, you can use the same name for a model-scoped parameter and reaction-scoped parameters, where each reaction-scoped parameter belongs to a different reaction.

  The purpose of this naming restriction is to ensure that every model component can be unambiguously referenced by its unique name within a model. For details on how to reference model component names in expressions, see “Guidelines for Referencing Names in Expressions”.
- To disambiguate duplicate names from your model, use the `updateDuplicateNames` function at the command line. The function takes in a SimBiology model as an input and updates the component names as necessary. You can also specify optional outputs, such as a logical flag to

check whether any update occurred, a list of model changes, and a copy of the original model before any updates were made.

- The `updateDuplicateNames` function disambiguates the duplicate names by adding a suffix `"_N"`, where *N* is the first positive integer that results in a unique name. If there is an existing suffix, *N* will be incremented from that suffix. For example, if there are two model components named *x_3*, the function updates one of the names to *x_4*. If the existing suffix has leading zeros, the function omits the zeros in the new name. For instance, if *x_003* is a duplicate name, it gets renamed to *x_4*. However, the function assumes that names with leading zeros and without leading zeros are different. For instance, *x_005* and *x_5* are considered to be different names.

R2022a: Having duplicate model component names will not be allowed in a future release
Behavior change in future release

SimBiology will not allow you to have duplicate names for model components within a model.

See Also

Topics
“Deterministic Simulation of a Model Containing a Discontinuity”
“Events in SimBiology Models”

addkineticlaw (reaction)

Create kinetic law object and add to reaction object

Syntax

```
kineticlawObj = addkineticlaw(reactionObj, 'KineticLawNameValue')

kineticlawObj= addkineticlaw(..., 'PropertyName', PropertyValue, ...)
```

Arguments

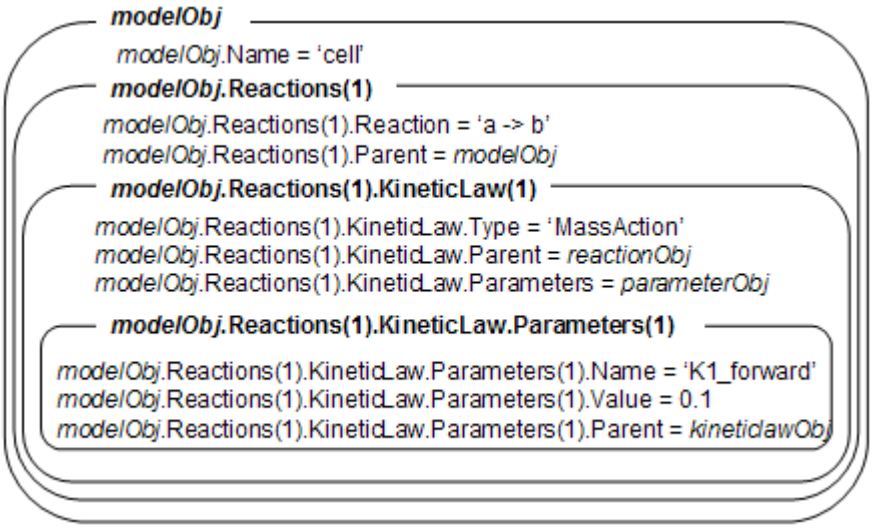
reactionObj	Reaction object. Enter a variable name for a reaction object.
KineticLawNameValue	Property to select the type of kinetic law object to create. For built-in kinetic law, valid values are: `'Unknown'`, `'MassAction'`, `'Henri-Michaelis-Menten'`, `'Henri-Michaelis-Menten-Reversible'`, `'Hill-Kinetics'`, `'Iso-Uni-Uni'`, `'Ordered-Bi-Bi'`, `'Ping-Pong-Bi-Bi'`, `'Competitive-Inhibition'`, `'NonCompetitive-Inhibition'`, and `'UnCompetitive-Inhibition'`. Find valid *KineticLawNameValue* by using `sbioroot` to create a SimBiology root object, then query the object with the commands `rootObj.BuiltinLibrary.KineticLaws` and `rootObj.UserDefinedLibrary.KineticLaws`. `sbiowhos -kineticlaw` lists kinetic laws in the SimBiology root, which includes kinetic laws from both the `BuiltInLibrary` and the `UserDefinedLibrary`.

Description

kineticlawObj = addkineticlaw(*reactionObj*, '*KineticLawNameValue*') creates and adds a `KineticLaw object` to the *reactionObj*.

In the kinetic law object, this method assigns a name (*KineticLawNameValue*) to the property `KineticLawName` and assigns the reaction object to the property `Parent`. In the reaction object, this method assigns the kinetic law object to the property `KineticLaw`.

```
modelObj = sbiomodel('cell');
reactionObj = addreaction(modelObj, 'a -> b');
kineticlawObj = addkineticlaw(reactionObj, 'MassAction');
parameterObj = addparameter(kineticlawObj, 'K1_forward', 0.1);
set(kineticlawObj, ParameterVariableName, 'K1_forward');
```



`KineticLawNameValue` is any valid kinetic law definition. See “Kinetic Law Definition” on page 3-58 for a definition of kinetic laws and more information about how they are used to get the reaction rate expression.

`kineticlawObj``= addkineticlaw(..., '`*`PropertyName`*`', `*`PropertyValue`*`, ...)` constructs a kinetic law object, *`kineticlawObj`*, and configures *`kineticlawObj`* with property value pairs. The property name/property value pairs can be in any format supported by the function `set`. The `kineticlawObj` properties are listed in “Property Summary” on page 2-44.

Note To define a Hill kinetic rate equation with a non-integer exponent that is compatible with DimensionalAnalysis, see “Define a Custom Hill Kinetic Law that Works with Dimensional Analysis” on page 3-117.

Property Summary

Properties for kinetic law objects

Expression	Expression to determine reaction rate equation or expression of observable object
KineticLawName	Name of kinetic law applied to reaction
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parameters	Array of parameter objects
ParameterVariableNames	Cell array of reaction rate parameters
ParameterVariables	Parameters in kinetic law definition
Parent	Indicate parent object
SpeciesVariableNames	Cell array of species in reaction rate equation
SpeciesVariables	Species in abstract kinetic law
Tag	Specify label for SimBiology object
Type	Display SimBiology object type
UserData	Specify data to associate with object

Examples

Convert Substrate into Product Using Henri-Michaelis-Menten Kinetics

This example shows how to simulate the conversion of a substrate into a product using the Henri-Michaelis-Menten enzyme kinetics.

Create a model named `mymodel`.

```
model = sbiomodel('mymodel');
```

Add a reaction that represents the conversion of a substrate to a product.

```
reaction = addreaction(model,'Substrate -> Product');
```

Add the built-in Henri-Michaelis-Menten kinetic law to the reaction.

```
kineticLaw = addkineticlaw(reaction,'Henri-Michaelis-Menten');
kineticLaw.Expression
```

```
ans =
'Vm*S/(Km + S)'
```

The kinetic law has two parameters and a species that you need to define. View these parameters.

```
kineticLaw.ParameterVariables
```

```
ans = 2x1 cell
    {'Vm'}
    {'Km'}
```

```
kineticLaw.SpeciesVariables
```

```
ans = 1x1 cell array
    {'S'}
```

To define the parameters, create two parameter objects and set parameter values.

```
Vm_param = addparameter(kineticLaw,'Vm_param','Value',6.0);
Km_param = addparameter(kineticLaw,'Km_param','Value',1.25);
```

Map the parameters accordingly by setting the `ParameterVariableNames` property. This associates the parameters in the expression with the two parameters you just created using a one-to-one mapping in the order given.

```
kineticLaw.ParameterVariableNames = {'Vm_param','Km_param'};
```

Also associate the `Substrate` species with the species `S` in the expression.

```
kineticLaw.SpeciesVariableNames = {'Substrate'};
```

Verify the mapping by looking at the reaction rate and checking the parameters and species are correctly substituted according to the expression.

```
reaction.ReactionRate
```

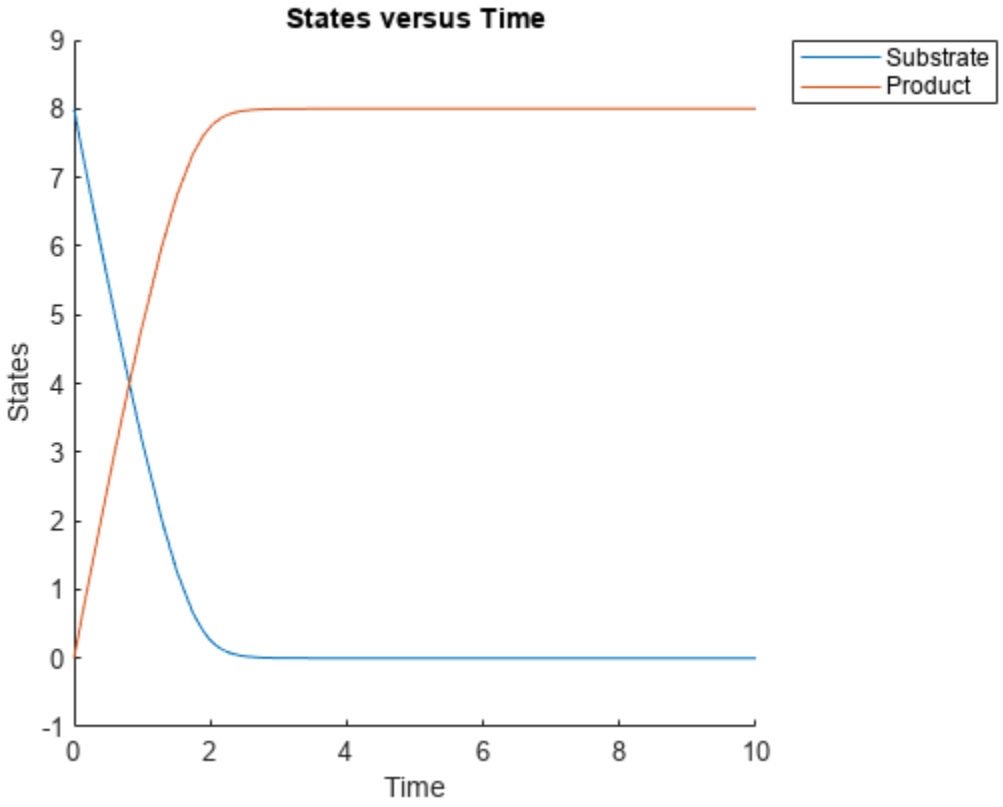
```
ans =
'Vm_param*Substrate/(Km_param+Substrate)'
```

Enter the initial amount of the substrate species for simulation.

```
model.Species(1).InitialAmount  = 8;
```

Simulate the model and plot results.

```
simdata  = sbiosimulate(model);
sbioplot(simdata);
```



See Also

`addreaction`, `setparameter`

Version History

Introduced in R2006a

addobservable

Add observable object to SimBiology model

Syntax

```
obsObj = addobservable(modelObj,obsName,obsExpression)
obsObj = addobservable(modelObj,obsName,obsExpression,Name,Value)
```

Description

`obsObj = addobservable(modelObj,obsName,obsExpression)` adds an `observable` object to a SimBiology model `modelObj`. The inputs `obsName` and `obsExpression` are the observable object name and its expression, respectively.

`obsObj = addobservable(modelObj,obsName,obsExpression,Name,Value)` sets the property values of `obsObj` using one or more name-value pair arguments. `Name` is the property name and `Value` is the corresponding value `Name` must appear inside quotes. You can specify several name and value pair arguments in any order as `Name1,Value1,...,NameN,ValueN`. For a list of properties, see observable object properties on page 2-471.

Examples

Calculate Statistics After Model Simulation Using Observables

Load the "Target-Mediated Drug Disposition (TMDD) Model".

```
sbioloadproject tmdd_with_TO.sbproj
```

Set the target occupancy (`TO`) as a response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'TO';
```

Get the dosing information.

```
d = getdose(m1,'Daily Dose');
```

Scan over different dose amounts using a `SimBiology.Scenarios` object. To do so, first parameterize the `Amount` property of the dose. Then vary the corresponding parameter value using the `Scenarios` object.

```
amountParam = addparameter(m1,'AmountParam','Units',d.AmountUnits);
d.Amount = 'AmountParam';
d.Active = 1;
doseSamples = SimBiology.Scenarios('AmountParam',linspace(0,300,31));
```

Create a `SimFunction` to simulate the model. Set `TO` as the simulation output.

```
% Suppress informational warnings that are issued during simulation.
warning('off','SimBiology:SimFunction:DOSES_NOT_EMPTY');
f = createSimFunction(m1,doseSamples,'TO',d)
```

```
f =
SimFunction

Parameters:

        Name          Value        Type           Units
    ______________    _____    _____________    ___________

    {'AmountParam'}      1      {'parameter'}    {'nanomole'}

Observables:

     Name         Type              Units
    ______    _____________    _________________

    {'T0'}    {'parameter'}    {'dimensionless'}

Dosed:

      TargetName                TargetDimension                    Amount          AmountValue    A
    ______________    ____________________________________    ______________    ___________    _

    {'Plasma.Drug'}    {'Amount (e.g., mole or molecule)'}    {'AmountParam'}         1         

TimeUnits: day
```

```
warning('on','SimBiology:SimFunction:DOSES_NOT_EMPTY');
```

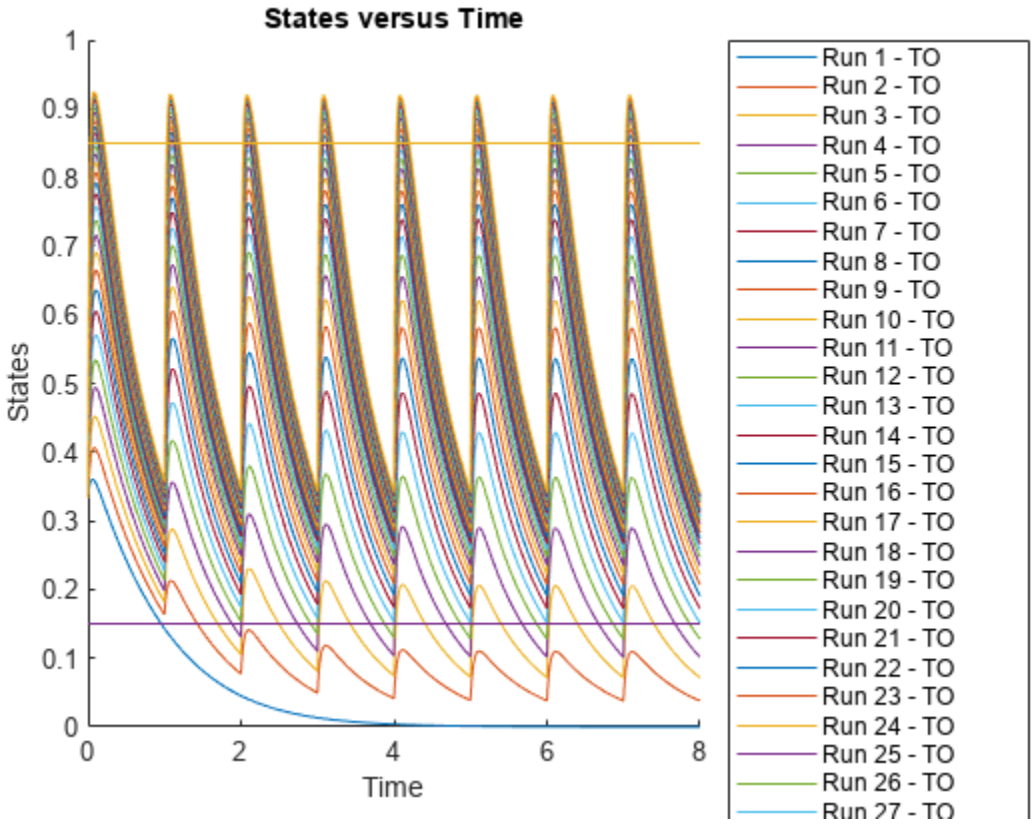
Simulate the model using the dose amounts generated by the `Scenarios` object. In this case, the object generates 31 different doses; hence the model is simulated 31 times and generates a `SimData` array.

```
doseTable = getTable(d);
sd = f(doseSamples,cs.StopTime,doseTable)
```

```
   SimBiology Simulation Data Array: 31-by-1

   ModelName:        TMDD
   Logged Data:
     Species:        0
     Compartment:    0
     Parameter:      1
     Sensitivity:    0
     Observable:     0
```

Plot the simulation results. Also add two reference lines that represent the safety and efficacy thresholds for `T0`. In this example, suppose that any `T0` value above 0.85 is unsafe, and any `T0` value below 0.15 has no efficacy.

```
h = sbioplot(sd);
time = sd(1).Time;
h.NextPlot = 'add';
safetyThreshold = plot(h,[min(time), max(time)],[0.85, 0.85],'DisplayName','Safety Threshold');
efficacyThreshold = plot(h,[min(time), max(time)],[0.15, 0.15],'DisplayName','Efficacy Threshold
```



Postprocess the simulation results. Find out which dose amounts are effective, corresponding to the `TO` responses within the safety and efficacy thresholds. To do so, add an observable expression to the simulation data.

```
% Suppress informational warnings that are issued during simulation.
warning('off','SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
newSD = addobservable(sd,'stat1','max(TO) < 0.85 & min(TO) > 0.15','Units','dimensionless')
```

```
SimBiology Simulation Data Array: 31-by-1

ModelName:        TMDD
Logged Data:
  Species:        0
  Compartment:    0
  Parameter:      1
  Sensitivity:    0
  Observable:     1
```

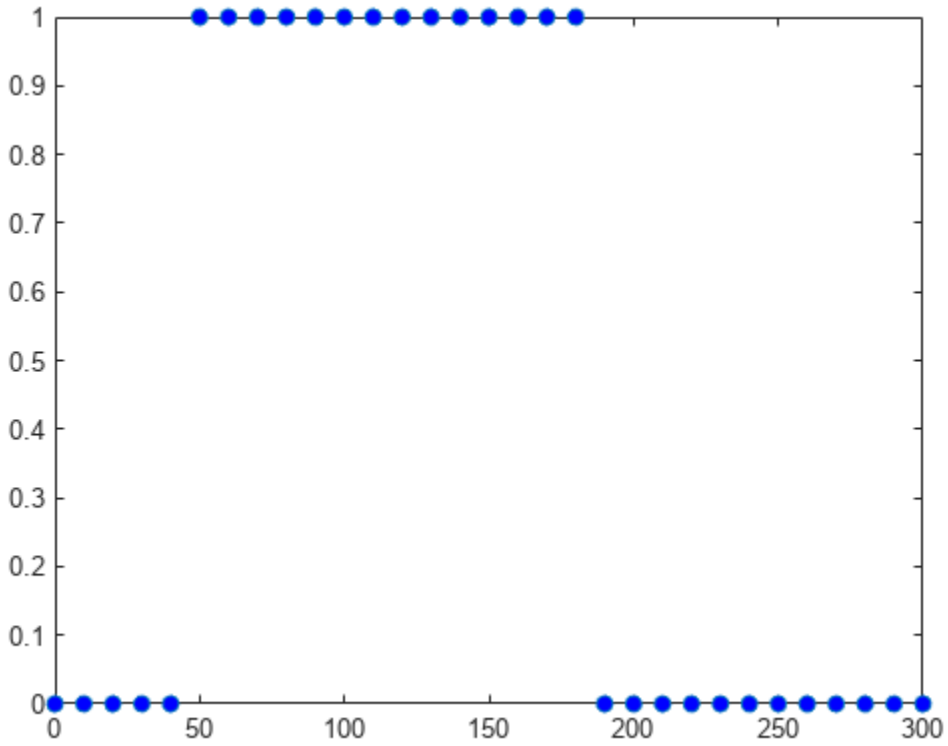
The addobservable function evaluates the new observable expression for each `SimData` in `sd` and returns the evaluated results as a new `SimData` array, `newSD`, which now has the added observable (`stat1`).

SimBiology stores the observable results in two different properties of a `SimData` object. If the results are scalar-valued, they are stored in `SimData.ScalarObservables`. Otherwise, they are

stored in `SimData.VectorObservables`. In this example, the `stat1` observable expression is scalar-valued.

Extract the scalar observable values and plot them against the dose amounts.

```
scalarObs = vertcat(newSD.ScalarObservables);
doseAmounts = generate(doseSamples);
figure
plot(doseAmounts.AmountParam,scalarObs.stat1,'o','MarkerFaceColor','b')
```



The plot shows that dose amounts ranging from 50 to 180 nanomoles provide `T0` responses that lie within the target efficacy and safety thresholds.

You can update the observable expression with different threshold amounts. The function recalculates the expression and returns the results in a new `SimData` object array.

```
newSD2 = updateobservable(newSD,'stat1','max(T0) < 0.75 & min(T0) > 0.30');
```

Rename the observable expression. The function renames the observable, updates any expressions that reference the renamed observable (if applicable), and returns the results in a new `SimData` object array.

```
newSD3 = renameobservable(newSD2,'stat1','EffectiveDose');
```

Restore the warning settings.

```
warning('on','SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
```

Input Arguments

`modelObj` — SimBiology model
SimBiology model object

SimBiology model, specified as a SimBiology `model object`.

`obsName` — Name of observable object
character vector | string

Name of the observable object, specified as a character vector or string.

The name

- Cannot contain the characters `[ ]`, `->`, or `<->`.
- Cannot be empty, the word *time*, the word *null*, or all whitespace.
- Must be unique in a model, meaning no observable object can have the same name as another observable, species, compartment, parameter, reaction, variant, or dose in the model.

For details, see “Guidelines for Naming Model Components”.

Example: `'AUC_obs'`

Data Types: `char` | `string`

`obsExpression` — Expression of observable object
character vector | string

Expression of the observable object, specified as a character vector or string.

Example: `'trapz(time,drug)'`

Data Types: `char` | `string`

Output Arguments

`obsObj` — Observable object
`Observable` object

Observable object, returned as an `observable` object.

Version History

Introduced in R2020a

R2022b: Having duplicate model component names issues a warning
Warns starting in R2022b

- SimBiology issues a warning if multiple model components (model, compartment, species, parameter, reaction, rule, event, observable, dose, and variant) have the same name. In a future release, within a single model, these components will be required to have unique names even when they are of different types with the following two exceptions:
  - Species in different compartments can have the same name.

- Parameters can have the same name if they are scoped to different parents. Specifically, you can use the same name for a model-scoped parameter and reaction-scoped parameters, where each reaction-scoped parameter belongs to a different reaction.

The purpose of this naming restriction is to ensure that every model component can be unambiguously referenced by its unique name within a model. For details on how to reference model component names in expressions, see “Guidelines for Referencing Names in Expressions”.

- To disambiguate duplicate names from your model, use the `updateDuplicateNames` function at the command line. The function takes in a SimBiology model as an input and updates the component names as necessary. You can also specify optional outputs, such as a logical flag to check whether any update occurred, a list of model changes, and a copy of the original model before any updates were made.
- The `updateDuplicateNames` function disambiguates the duplicate names by adding a suffix "*_N*", where *N* is the first positive integer that results in a unique name. If there is an existing suffix, *N* will be incremented from that suffix. For example, if there are two model components named *x_3*, the function updates one of the names to *x_4*. If the existing suffix has leading zeros, the function omits the zeros in the new name. For instance, if *x_003* is a duplicate name, it gets renamed to *x_4*. However, the function assumes that names with leading zeros and without leading zeros are different. For instance, *x_005* and *x_5* are considered to be different names.

R2022a: Having duplicate model component names will not be allowed in a future release
Behavior change in future release

SimBiology will not allow you to have duplicate names for model components within a model.

See Also

`Observable` | `addobservable(SimData)` | `updateobservable(SimData)` | `renameobservable(SimData)`

addobservable

Add observable expressions to SimData

Syntax

```
sdout = addobservable(sdin,obsNames,obsExpressions)
sdout = addobservable(sdin,obsNames,obsExpressions,'Units',units)
```

Description

`sdout = addobservable(sdin,obsNames,obsExpressions)` returns a new `SimData` object (or array of objects) `sdout` after adding the specified observables to the input `SimData` `sdin`. The inputs `obsNames` and `obsExpressions` are the observable names and their corresponding expressions. The number of expressions must match the number of observable names.

`sdout = addobservable(sdin,obsNames,obsExpressions,'Units',units)` specifies `units` for the observable expressions. The number of units must match the number of observable names.

Examples

Calculate Statistics After Model Simulation Using Observables

Load the "Target-Mediated Drug Disposition (TMDD) Model".

```
sbioloadproject tmdd_with_TO.sbproj
```

Set the target occupancy (`TO`) as a response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'TO';
```

Get the dosing information.

```
d = getdose(m1,'Daily Dose');
```

Scan over different dose amounts using a `SimBiology.Scenarios` object. To do so, first parameterize the `Amount` property of the dose. Then vary the corresponding parameter value using the `Scenarios` object.

```
amountParam = addparameter(m1,'AmountParam','Units',d.AmountUnits);
d.Amount = 'AmountParam';
d.Active = 1;
doseSamples = SimBiology.Scenarios('AmountParam',linspace(0,300,31));
```

Create a `SimFunction` to simulate the model. Set `TO` as the simulation output.

```
% Suppress informational warnings that are issued during simulation.
warning('off','SimBiology:SimFunction:DOSES_NOT_EMPTY');
f = createSimFunction(m1,doseSamples,'TO',d)
```

```
f =
SimFunction
```

```
Parameters:

        Name          Value        Type           Units
    ______________    _____    _____________    ___________

    {'AmountParam'}      1      {'parameter'}    {'nanomole'}

Observables:

     Name         Type              Units
    ______    _____________    _________________

    {'T0'}    {'parameter'}    {'dimensionless'}

Dosed:

      TargetName                TargetDimension                    Amount          AmountValue    A
    ______________    ____________________________________    _______________    ___________    -

    {'Plasma.Drug'}    {'Amount (e.g., mole or molecule)'}    {'AmountParam'}         1         -

TimeUnits: day
```

```
warning('on','SimBiology:SimFunction:DOSES_NOT_EMPTY');
```

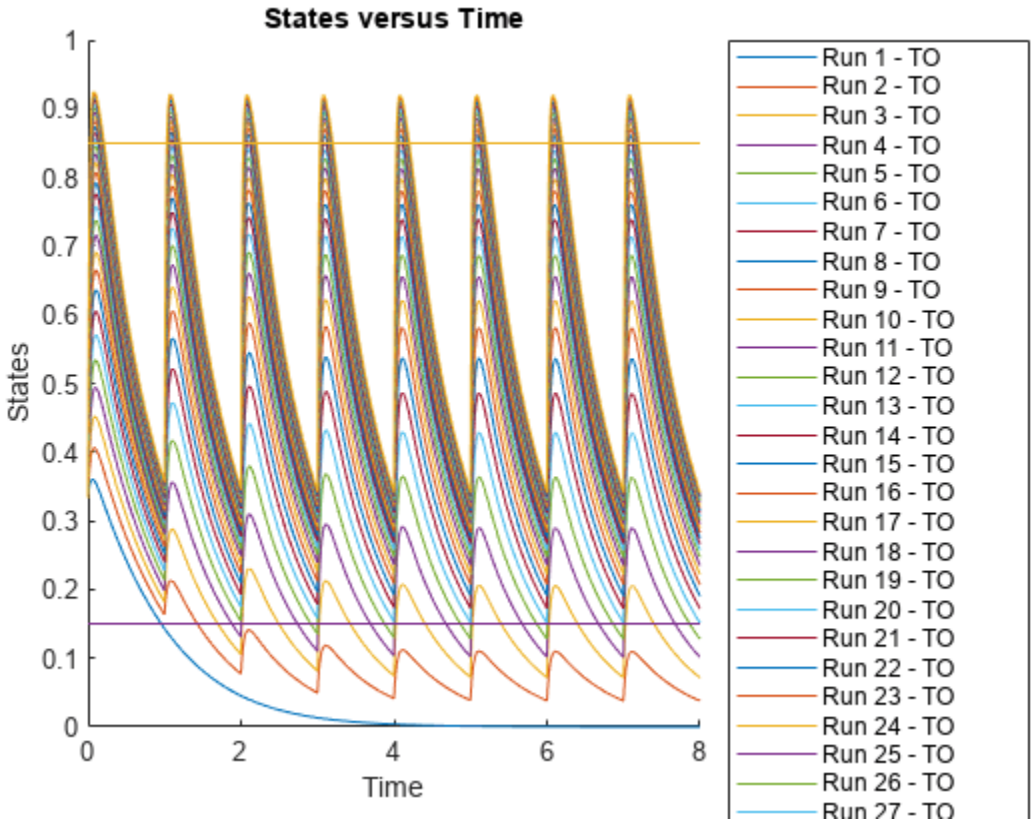
Simulate the model using the dose amounts generated by the `Scenarios` object. In this case, the object generates 31 different doses; hence the model is simulated 31 times and generates a `SimData` array.

```
doseTable = getTable(d);
sd = f(doseSamples,cs.StopTime,doseTable)
```

```
   SimBiology Simulation Data Array: 31-by-1

   ModelName:        TMDD
   Logged Data:
     Species:        0
     Compartment:    0
     Parameter:      1
     Sensitivity:    0
     Observable:     0
```

Plot the simulation results. Also add two reference lines that represent the safety and efficacy thresholds for `T0`. In this example, suppose that any `T0` value above 0.85 is unsafe, and any `T0` value below 0.15 has no efficacy.

```
h = sbioplot(sd);
time = sd(1).Time;
h.NextPlot = 'add';
safetyThreshold = plot(h,[min(time), max(time)],[0.85, 0.85],'DisplayName','Safety Threshold');
efficacyThreshold = plot(h,[min(time), max(time)],[0.15, 0.15],'DisplayName','Efficacy Threshold
```



Postprocess the simulation results. Find out which dose amounts are effective, corresponding to the `TO` responses within the safety and efficacy thresholds. To do so, add an observable expression to the simulation data.

```
% Suppress informational warnings that are issued during simulation.
warning('off','SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
newSD = addobservable(sd,'stat1','max(TO) < 0.85 & min(TO) > 0.15','Units','dimensionless')
```

```
SimBiology Simulation Data Array: 31-by-1

ModelName:        TMDD
Logged Data:
  Species:        0
  Compartment:    0
  Parameter:      1
  Sensitivity:    0
  Observable:     1
```

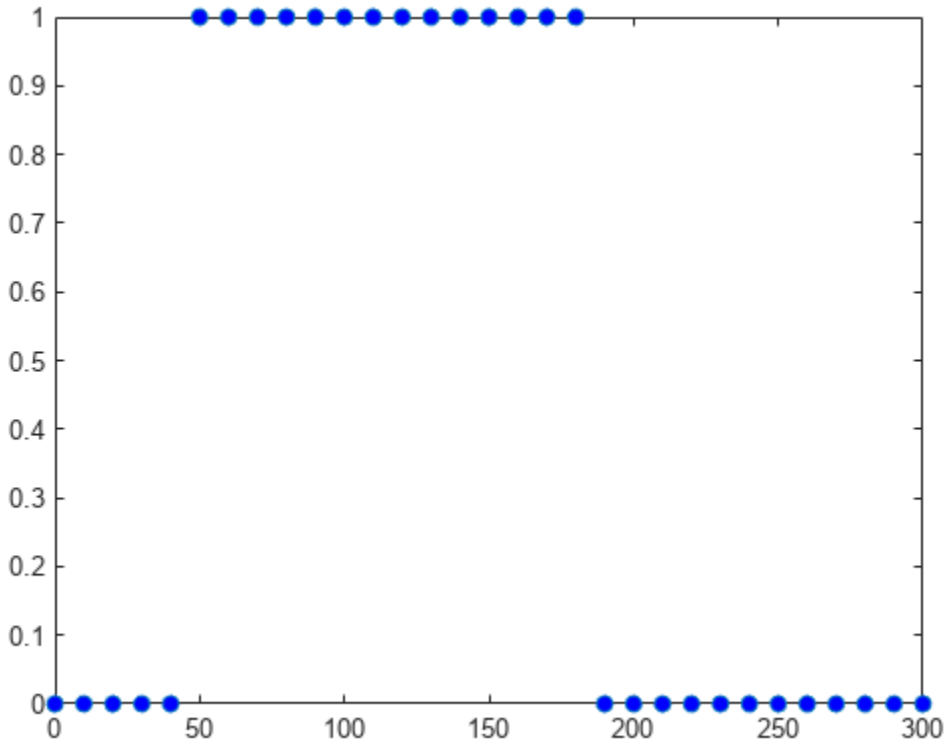
The addobservable function evaluates the new observable expression for each `SimData` in `sd` and returns the evaluated results as a new `SimData` array, `newSD`, which now has the added observable (`stat1`).

SimBiology stores the observable results in two different properties of a `SimData` object. If the results are scalar-valued, they are stored in `SimData.ScalarObservables`. Otherwise, they are

stored in `SimData.VectorObservables`. In this example, the `stat1` observable expression is scalar-valued.

Extract the scalar observable values and plot them against the dose amounts.

```
scalarObs = vertcat(newSD.ScalarObservables);
doseAmounts = generate(doseSamples);
figure
plot(doseAmounts.AmountParam,scalarObs.stat1,'o','MarkerFaceColor','b')
```



The plot shows that dose amounts ranging from 50 to 180 nanomoles provide `T0` responses that lie within the target efficacy and safety thresholds.

You can update the observable expression with different threshold amounts. The function recalculates the expression and returns the results in a new `SimData` object array.

```
newSD2 = updateobservable(newSD,'stat1','max(T0) < 0.75 & min(T0) > 0.30');
```

Rename the observable expression. The function renames the observable, updates any expressions that reference the renamed observable (if applicable), and returns the results in a new `SimData` object array.

```
newSD3 = renameobservable(newSD2,'stat1','EffectiveDose');
```

Restore the warning settings.

```
warning('on','SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
```

Input Arguments

`sdin` — Input simulation data

`SimData` object | array of `SimData` objects

Input simulation data, specified as a `SimData` object or array of objects.

`obsNames` — Names of observable expressions

character vector | string | string vector | cell array of character vectors

Names of the observable expressions, specified as a character vector, string, string vector, or cell array of character vectors.

Each name must be unique in the `SimData` object, meaning it cannot match the name of any other observable, species, compartment, parameter, or reaction referenced in the `SimData` object.

Example: `{'max_drug','mean_drug'}`

Data Types: `char` | `string` | `cell`

`obsExpressions` — Observable expressions

character vector | string | string vector | cell array of character vectors

Observable expressions, specified as a character vector, string, string vector, or cell array of character vectors. The number of expressions must match the number of observable names.

Example: `{'max(drug)','mean(drug)'}`

Data Types: `char` | `string` | `cell`

`units` — Units for observable expressions

character vector | string | string vector | cell array of character vectors

Units for the observable expressions, specified as a character vector, string, string vector, or cell array of character vectors. The number of units must match the number of observable names.

Example: `{'nanomole/liter','nanomole/liter'}`

Data Types: `char` | `string` | `cell`

Output Arguments

`sdout` — Simulation data with observable results

`SimData` object | array of `SimData` objects

Simulation data with observable results, returned as a `SimData` object or array of objects.

Version History

Introduced in R2020a

See Also

`SimData` | `updateobservable` | `renameobservable`

addobservable

Compute Sobol indices or elementary effects for new observable expression

Syntax

```
results = addobservable(gsaObj,obsNames,obsExpressions)
results = addobservable(gsaObj,obsNames,obsExpressions,'Units',units)
```

Description

`results = addobservable(gsaObj,obsNames,obsExpressions)` computes Sobol indices or elementary effects for the new observables specified by `obsNames` with the corresponding expressions `obsExpressions`.

`results = addobservable(gsaObj,obsNames,obsExpressions,'Units',units)` specifies units for the new observable expressions. The function performs unit conversion for the observable expressions only if you set `UnitConversion` to `true`.

Examples

Perform Global Sensitivity Analysis by Computing First- and Total-Order Sobol Indices

Load the “Tumor Growth Model”.

```
sbioloadproject tumor_growth_vpop_sa.sbproj
```

Get a variant with the estimated parameters and the dose to apply to the model.

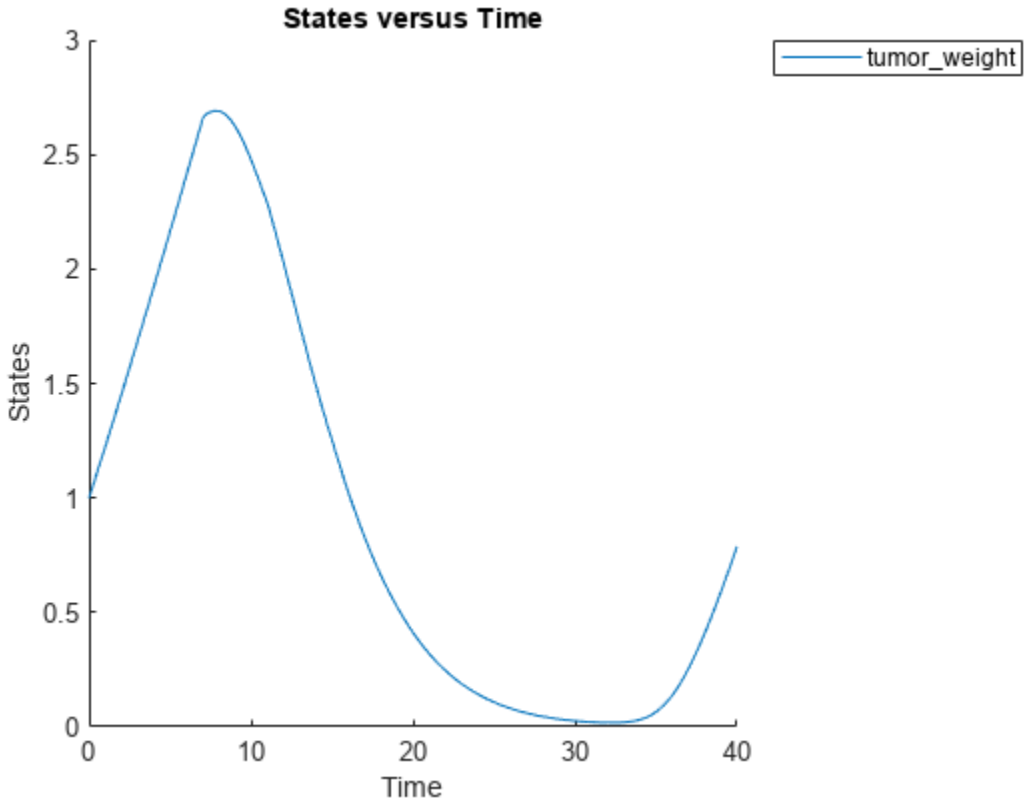
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

Get the active configset and set the tumor weight as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'tumor_weight';
```

Simulate the model and plot the tumor growth profile.

```
sbioplot(sbiosimulate(m1,cs,v,d));
```



Perform global sensitivity analysis (GSA) on the model to find the model parameters that the tumor growth is sensitive to.

First, retrieve model parameters of interest that are involved in the pharmacodynamics of the tumor growth. Define the model response as the tumor weight.

```
modelParamNames = {'L0','L1','w0','k1','k2'};
outputName = 'tumor_weight';
```

Then perform GSA by computing the first- and total-order Sobol indices using `sbiosobol`. Set `'ShowWaitBar'` to `true` to show the simulation progress. By default, the function uses 1000 parameter samples to compute the Sobol indices [1].

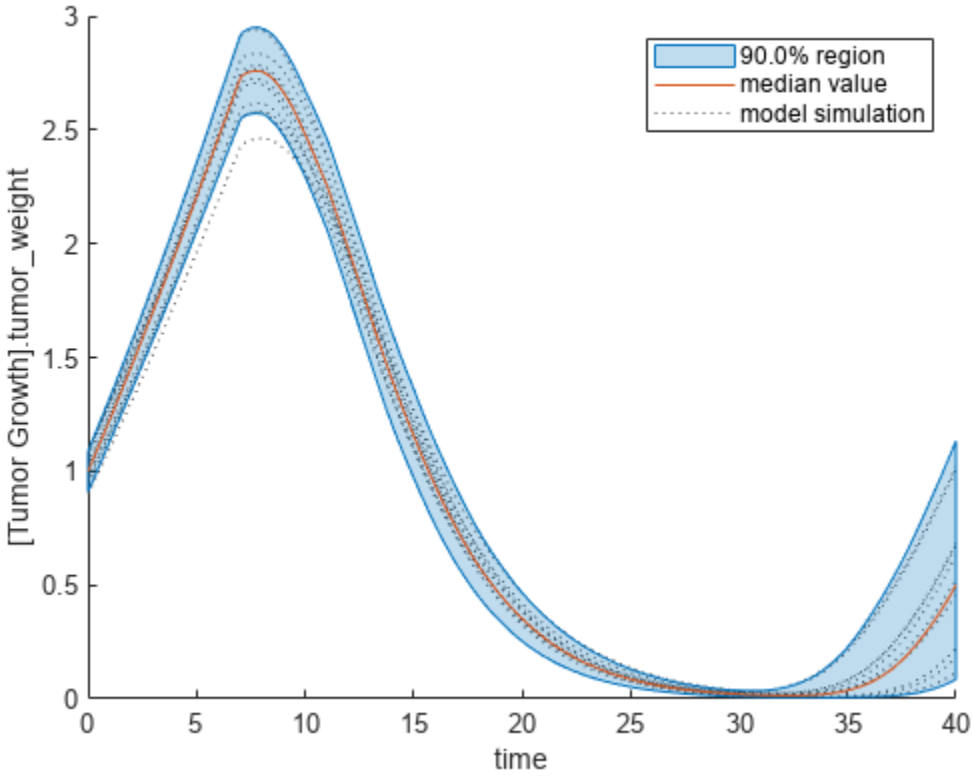
```
rng('default');
sobolResults = sbiosobol(m1,modelParamNames,outputName,Variants=v,Doses=d,ShowWaitBar=true)
```

```
sobolResults =
  Sobol with properties:

                Time: [444x1 double]
        SobolIndices: [5x1 struct]
            Variance: [444x1 table]
    ParameterSamples: [1000x5 table]
         Observables: {'[Tumor Growth].tumor_weight'}
      SimulationInfo: [1x1 struct]
```

You can change the number of samples by specifying the `'NumberSamples'` name-value pair argument. The function requires a total of `(number of input parameters + 2) * NumberSamples` model simulations.

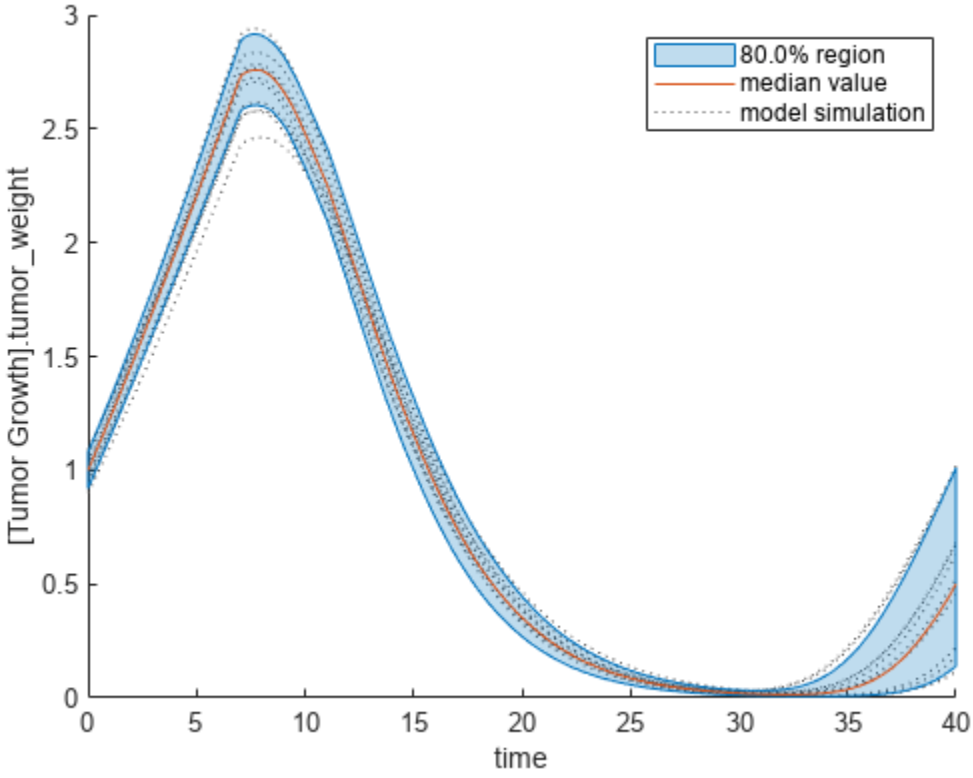
Show the mean model response, the simulation results, and a shaded region covering 90% of the simulation results.

```
plotData(sobolResults,ShowMedian=true,ShowMean=false);
```



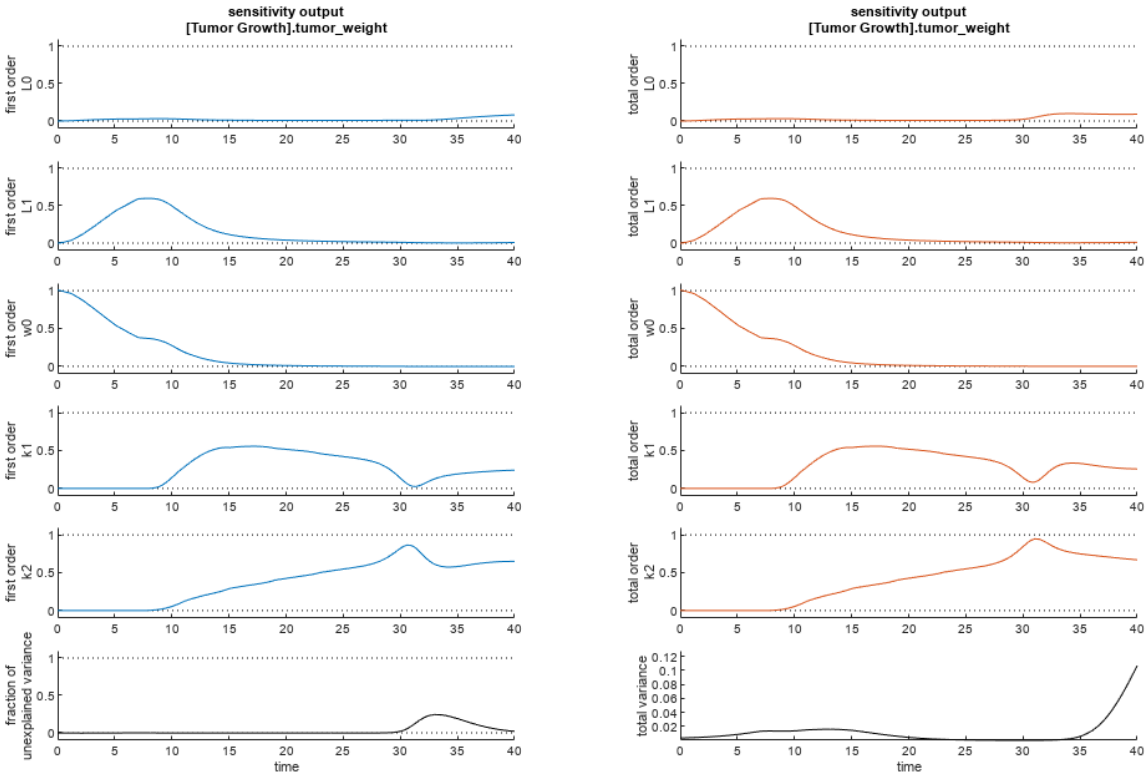
You can adjust the quantile region to a different percentage by specifying `'Alphas'` for the lower and upper quantiles of all model responses. For instance, an alpha value of 0.1 plots a shaded region between the `100 * alpha` and `100 * (1 - alpha)` quantiles of all simulated model responses.

```
plotData(sobolResults,Alphas=0.1,ShowMedian=true,ShowMean=false);
```



Plot the time course of the first- and total-order Sobol indices.

```
h = plot(sobolResults);
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```

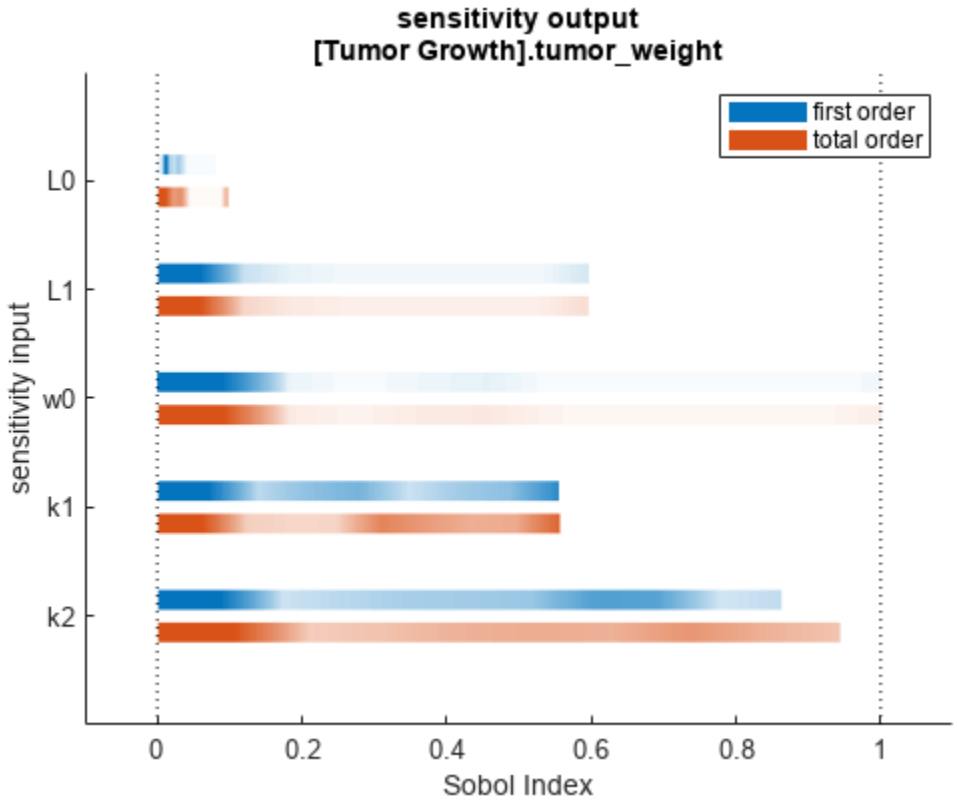


The first-order Sobol index of an input parameter gives the fraction of the overall response variance that can be attributed to variations in the input parameter alone. The total-order index gives the fraction of the overall response variance that can be attributed to any joint parameter variations that include variations of the input parameter.

From the Sobol indices plots, parameters `L1` and `w0` seem to be the most sensitive parameters to the tumor weight before the dose was applied at t = 7. But after the dose is applied, `k1` and `k2` become more sensitive parameters and contribute most to the after-dosing stage of the tumor weight. The total variance plot also shows a larger variance for the after-dose stage at t > 35 than for the before-dose stage of the tumor growth, indicating that `k1` and `k2` might be more important parameters to investigate further. The fraction of unexplained variance shows some variance at around t = 33, but the total variance plot shows little variance at t = 33, meaning the unexplained variance could be insignificant. The fraction of unexplained variance is calculated as 1 - (sum of all the first-order Sobol indices), and the total variance is calculated using `var(response)`, where `response` is the model response at every time point.

You can also display the magnitudes of the sensitivities in a bar plot. Darker colors mean that those values occur more often over the whole time course.

```
bar(sobolResults);
```



You can specify more samples to increase the accuracy of the Sobol indices, but the simulation can take longer to finish. Use `addsamples` to add more samples. For example, if you specify 1500 samples, the function performs `1500 * (2 + number of input parameters)` simulations.

```
gsaMoreSamples = addsamples(gsaResults,1500)
```

The “SimulationInfo” on page 2-0 property of the result object contains various information for computing the Sobol indices. For instance, the model simulation data (SimData) for each simulation using a set of parameter samples is stored in the `SimData` field of the property. This field is an array of `SimData` objects.

```
sobolResults.SimulationInfo.SimData
```

```
SimBiology SimData Array : 1000-by-7

Index:    Name:         ModelName:         DataCount:
1           -           Tumor Growth Model 1
2           -           Tumor Growth Model 1
3           -           Tumor Growth Model 1
...
7000        -           Tumor Growth Model 1
```

You can find out if any model simulation failed during the computation by checking the `ValidSample` field of `SimulationInfo`. In this example, the field shows no failed simulation runs.

```
all(sobolResults.SimulationInfo.ValidSample)
```

```
ans = 1x7 logical array

   1   1   1   1   1   1   1
```

`SimulationInfo.ValidSample` is a table of logical values. It has the same size as `SimulationInfo.SimData`. If `ValidSample` indicates that any simulations failed, you can get more information about those simulation runs and the samples used for those runs by extracting information from the corresponding column of `SimulationInfo.SimData`. Suppose that the fourth column contains one or more failed simulation runs. Get the simulation data and sample values used for that simulation using `getSimulationResults`.

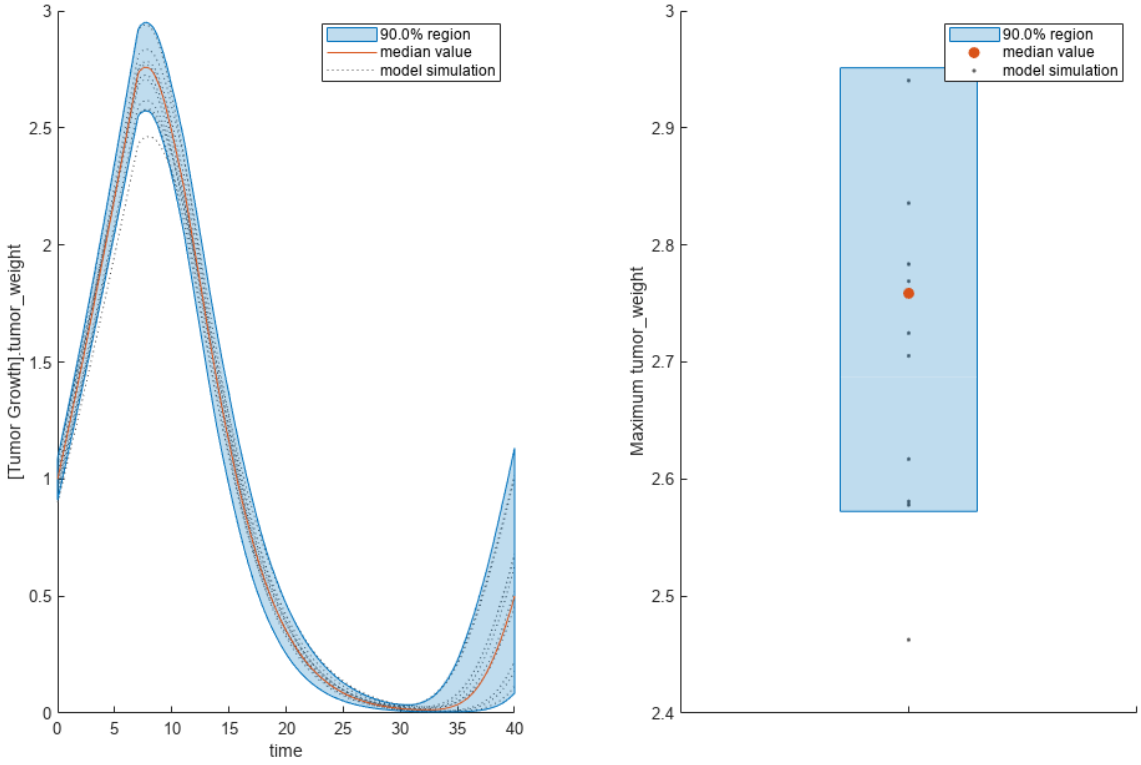
```
[samplesUsed,sd,validruns] = getSimulationResults(sobolResults,4);
```

You can add custom expressions as observables and compute Sobol indices for the added observables. For example, you can compute the Sobol indices for the maximum tumor weight by defining a custom expression as follows.

```
% Suppress an information warning that is issued during simulation.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
% Add the observable expression.
sobolObs = addobservable(sobolResults,'Maximum tumor_weight','max(tumor_weight)','Units','gram');
```

Plot the computed simulation results showing the 90% quantile region.

```
h2 = plotData(sobolObs,ShowMedian=true,ShowMean=false);
h2.Position(:) = [100 100 1280 800];
```



You can also remove the observable by specifying its name.

```
gsaNoObs = removeobservable(sobolObs,'Maximum tumor_weight');
```

Restore the warning settings.

```
warning(warnSettings);
```

Perform GSA by Computing Elementary Effects

Load the “Tumor Growth Model”.

```
sbioloadproject tumor_growth_vpop_sa.sbproj
```

Get a variant with estimated parameters and the dose to apply to the model.

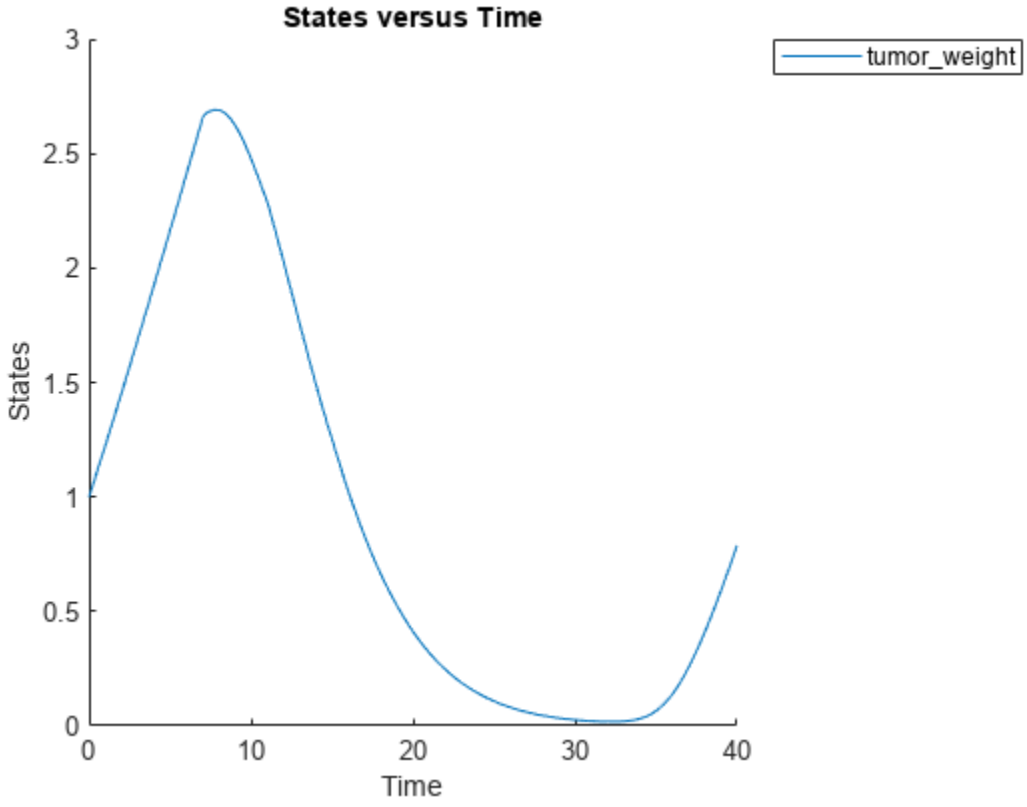
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

Get the active configset and set the tumor weight as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'tumor_weight';
```

Simulate the model and plot the tumor growth profile.

```
sbioplot(sbiosimulate(m1,cs,v,d));
```



Perform global sensitivity analysis (GSA) on the model to find the model parameters that the tumor growth is sensitive to.

First, define model parameters of interest, which are involved in the pharmacodynamics of the tumor growth. Define the model response as the tumor weight.

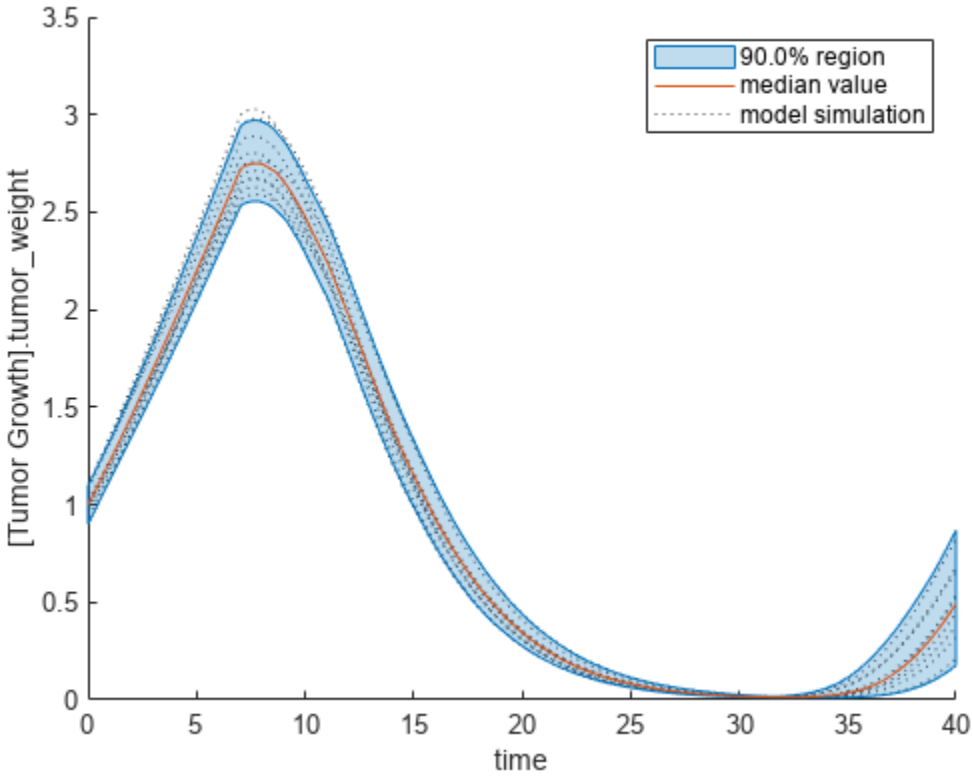
```
modelParamNames = {'L0','L1','w0','k1'};
outputName = 'tumor_weight';
```

Then perform GSA by computing the elementary effects using `sbioelementaryeffects`. Use `100` as the number of samples and set `ShowWaitBar` to `true` to show the simulation progress.

```
rng('default');
eeResults = sbioelementaryeffects(m1,modelParamNames,outputName,Variants=v,Doses=d,NumberSamples=
```

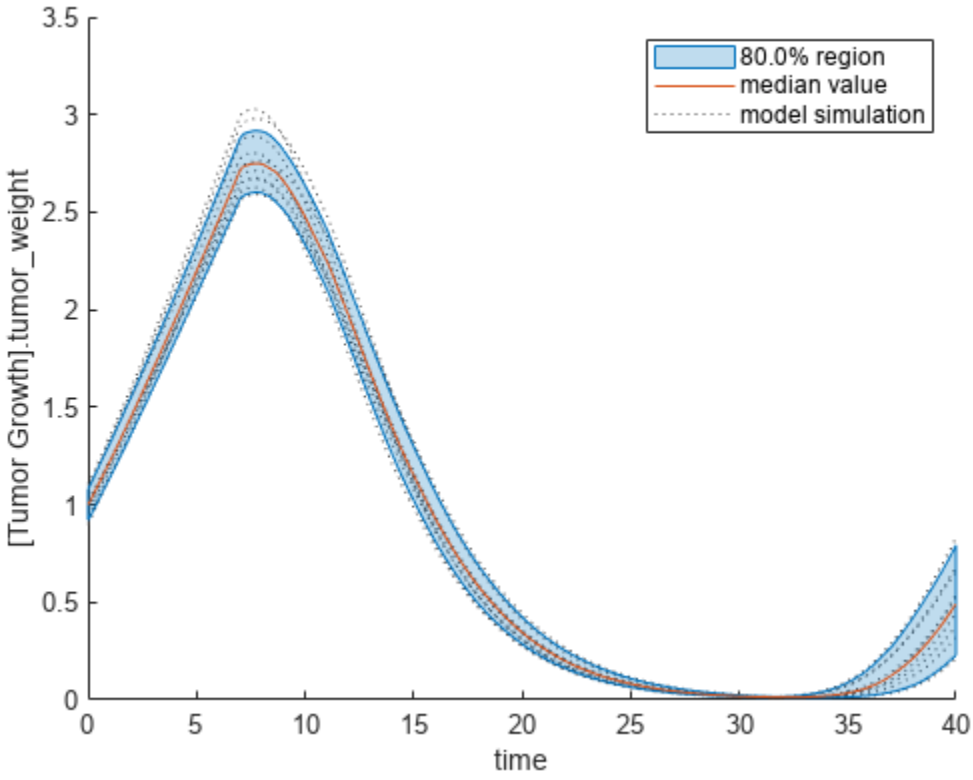
Show the median model response, the simulation results, and a shaded region covering 90% of the simulation results.

```
plotData(eeResults,ShowMedian=true,ShowMean=false);
```



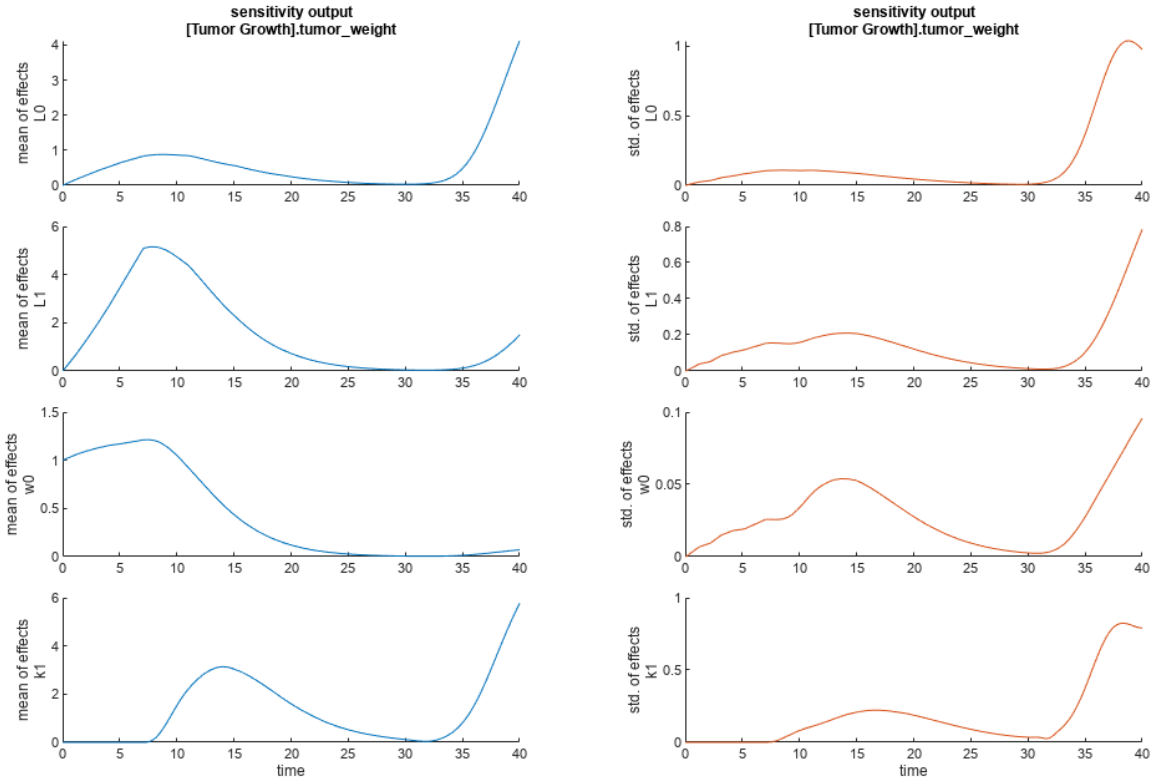
You can adjust the quantile region to a different percentage by specifying `Alphas` for the lower and upper quantiles of all model responses. For instance, an `alpha` value of 0.1 plots a shaded region between the `100*alpha` and `100*(1-alpha)` quantiles of all simulated model responses.

```
plotData(eeResults,Alphas=0.1,ShowMedian=true,ShowMean=false);
```



Plot the time course of the means and standard deviations of the elementary effects.

```
h = plot(eeResults);
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```

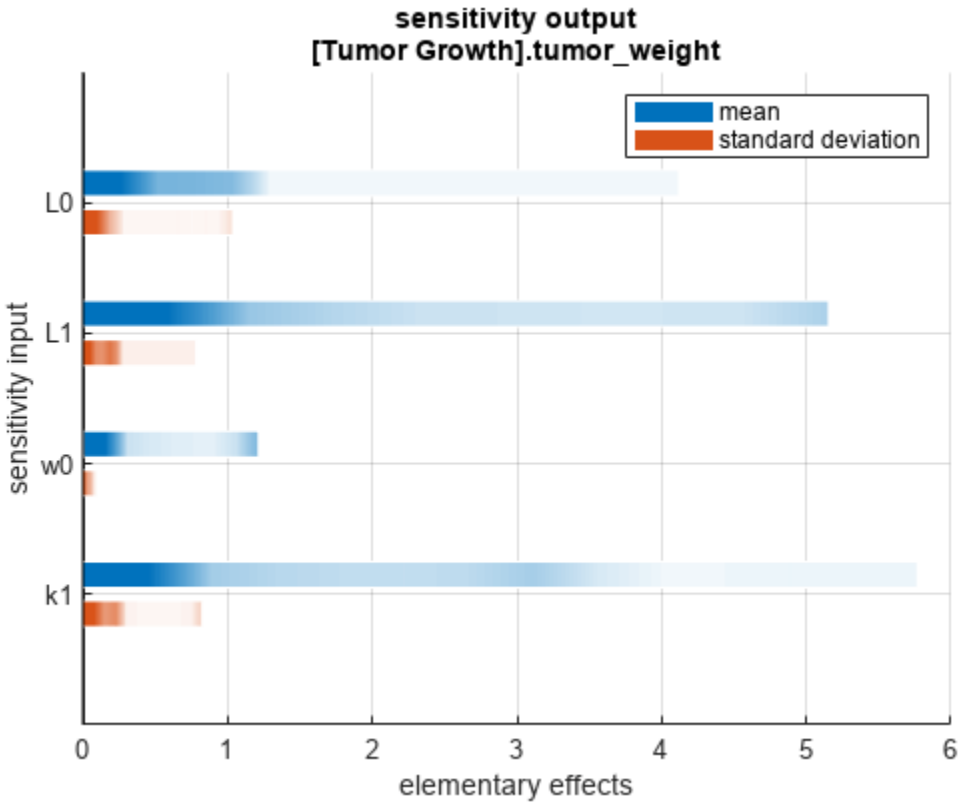


The mean of effects explains whether variations in input parameter values have any effect on the tumor weight response. The standard deviation of effects explains whether the sensitivity change is dependent on the location in the parameter domain.

From the mean of effects plots, parameters `L1` and `w0` seem to be the most sensitive parameters to the tumor weight before the dose is applied at t = 7. But, after the dose is applied, `k1` and `L0` become more sensitive parameters and contribute most to the after-dosing stage of the tumor weight. The plots of standard deviation of effects show more deviations for the larger parameter values in the later stage (t > 35) than for the before-dose stage of the tumor growth.

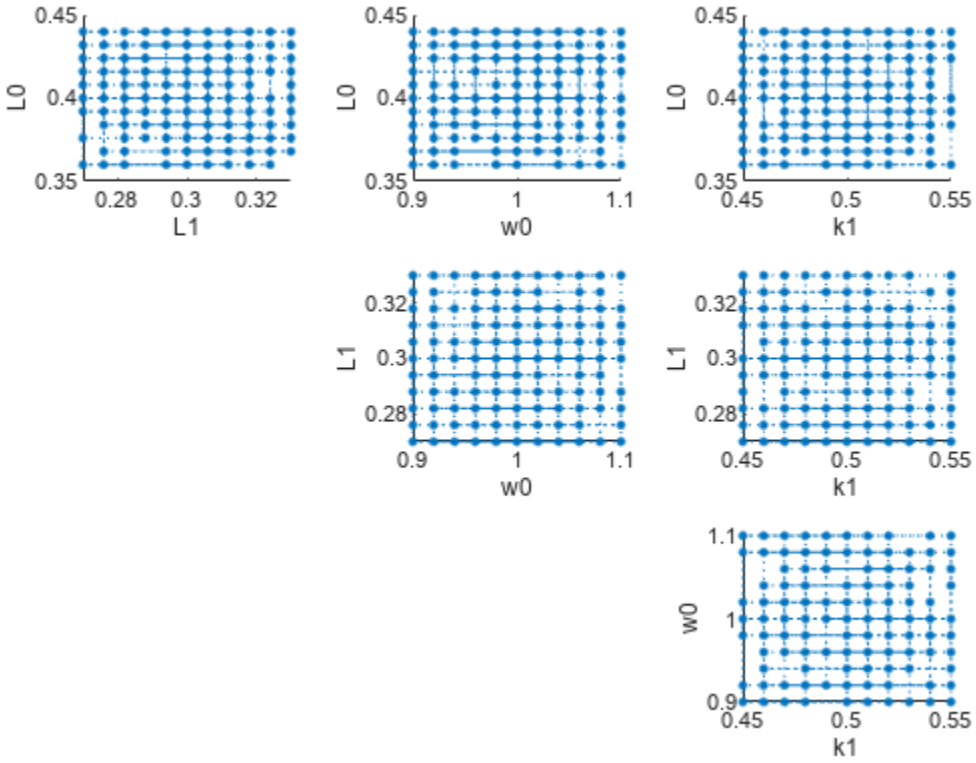
You can also display the magnitudes of the sensitivities in a bar plot. Each color shading represents a histogram representing values at different times. Darker colors mean that those values occur more often over the whole time course.

```
bar(eeResults);
```



You can also plot the parameter grids and samples used to compute the elementary effects.

```
plotGrid(eeResults)
```



You can specify more samples to increase the accuracy of the elementary effects, but the simulation can take longer to finish. Use `addsamples` to add more samples.

```
eeResults2 = addsamples(eeResults,200);
```

The `SimulationInfo` property of the result object contains various information for computing the elementary effects. For instance, the model simulation data (SimData) for each simulation using a set of parameter samples is stored in the `SimData` field of the property. This field is an array of `SimData` objects.

```
eeResults2.SimulationInfo.SimData
```

```
SimBiology SimData Array : 1500-by-1

Index:    Name:         ModelName:         DataCount:
1           -           Tumor Growth Model 1
2           -           Tumor Growth Model 1
3           -           Tumor Growth Model 1
...
1500        -           Tumor Growth Model 1
```

You can find out if any model simulation failed during the computation by checking the `ValidSample` field of `SimulationInfo`. In this example, the field shows no failed simulation runs.

```
all(eeResults2.SimulationInfo.ValidSample)
```

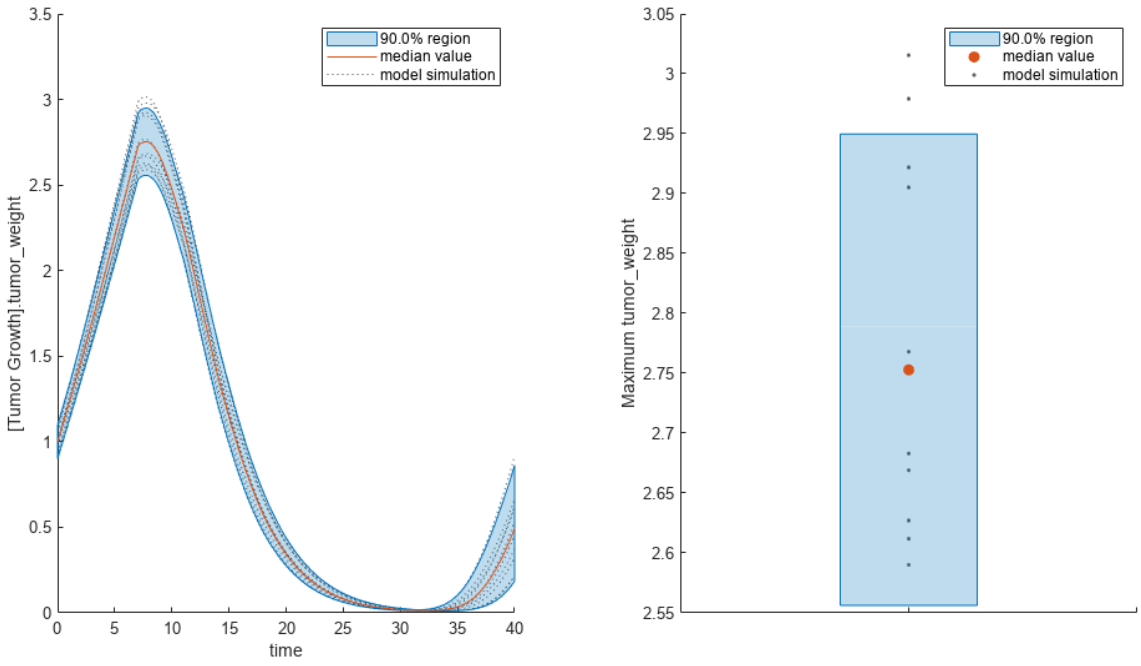
```
ans = logical
   1
```

You can add custom expressions as observables and compute the elementary effects of the added observables. For example, you can compute the effects for the maximum tumor weight by defining a custom expression as follows.

```
% Suppress an information warning that is issued.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
% Add the observable expression.
eeObs = addobservable(eeResults2,'Maximum tumor_weight','max(tumor_weight)','Units','gram');
```

Plot the computed simulation results showing the 90% quantile region.

```
h2 = plotData(eeObs,ShowMedian=true,ShowMean=false);
h2.Position(:) = [100 100 1500 800];
```



You can also remove the observable by specifying its name.

```
eeNoObs = removeobservable(eeObs,'Maximum tumor_weight');
```

Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

gsaObj — Results from global sensitivity analysis

`SimBiology.gsa.Sobol` object | `SimBiology.gsa.ElementaryEffects` object

Results from global sensitivity analysis, specified as a `SimBiology.gsa.Sobol` or `SimBiology.gsa.ElementaryEffects` object.

`obsNames` — Names of observable expressions
character vector | string | string vector | cell array of character vector

Names of observable expressions, specified as a character vector, string, string vector, or cell array of character vectors.

Data Types: `char` | `string` | `cell`

`obsExpressions` — Observable expressions
character vector | string | string vector | cell array of character vector

Observable expressions, specified as a character vector, string, string vector, or cell array of character vectors.

Data Types: `char` | `string` | `cell`

`units` — Observable units
character vector | string | string vector | cell array of character vector

Observable units, specified as a character vector, string, string vector, or cell array of character vectors.

Data Types: `char` | `string` | `cell`

Output Arguments

`results` — Computed Sobol indices or elementary effects for observables
`SimBiology.gsa.Sobol` | `SimBiology.gsa.ElementaryEffects`

Computed Sobol indices or elementary effects for added observables, returned as a `SimBiology.gsa.Sobol` or `SimBiology.gsa.ElementaryEffects` object.

Version History

Introduced in R2020a

References

[1] Saltelli, Andrea, Paola Annoni, Ivano Azzini, Francesca Campolongo, Marco Ratto, and Stefano Tarantola. “Variance Based Sensitivity Analysis of Model Output. Design and Estimator for the Total Sensitivity Index.” *Computer Physics Communications* 181, no. 2 (February 2010): 259–70. https://doi.org/10.1016/j.cpc.2009.09.018.

[2] Morris, Max D. “Factorial Sampling Plans for Preliminary Computational Experiments.” *Technometrics* 33, no. 2 (May 1991): 161–74.

[3] Sohier, Henri, Jean-Loup Farges, and Helene Piet-Lahanier. “Improvement of the Representativity of the Morris Method for Air-Launch-to-Orbit Separation.” *IFAC Proceedings Volumes* 47, no. 3 (2014): 7954–59.

See Also

`SimBiology.gsa.Sobol` | `SimBiology.gsa.ElementaryEffects` | `sbiosobol` | `sbioelementaryeffects`

Topics

“Sensitivity Analysis in SimBiology”

addparameter (model, kineticlaw)

Create parameter object and add to model or kinetic law object

Syntax

```
parameterObj = addparameter(Obj, 'NameValue')
parameterObj = addparameter(Obj, 'NameValue', ValueValue)

parameterObj = addparameter(...'PropertyName', PropertyValue...)
```

Arguments

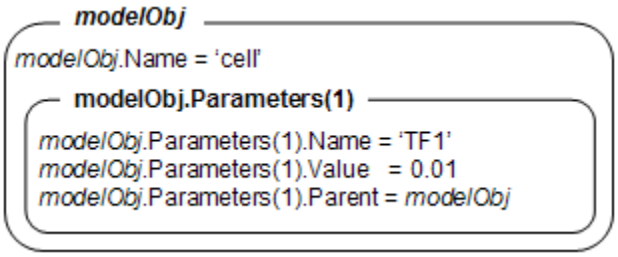
Obj	`Model object` or `kineticlaw object`. Enter a variable name for the object.
NameValue	Property for a parameter object. Enter a unique character vector. Since objects can use this property to reference a parameter, a parameter object must have a unique name at the level it is created. For example, a kinetic law object cannot contain two parameter objects named `kappa`. However, the model object that contains the kinetic law object can contain a parameter object named `kappa` along with the kinetic law object. For information on naming parameters, see Name.
ValueValue	Property for a parameter object. Enter a number.

Description

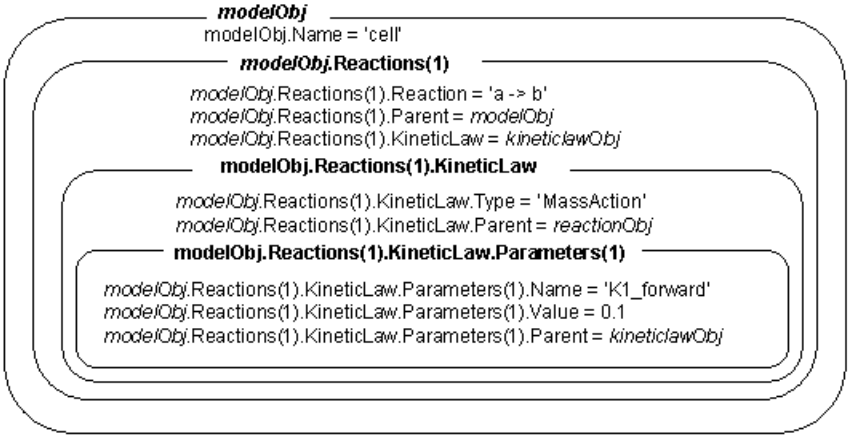
`parameterObj = addparameter(Obj, 'NameValue')` creates a parameter object and returns the object (*parameterObj*). In the parameter object, this method assigns a value (*NameValue*) to the property `Name`, assigns a value `1` to the property `Value`, and assigns the model or kinetic law object to the property `Parent`. In the model or kinetic law object, (*Obj*), this method assigns the parameter object to the property `Parameters`.

A parameter object defines an assignment that a model or a kinetic law can use. The scope of the parameter is defined by the parameter parent. If a parameter is defined with a kinetic law object, then only the kinetic law object and objects within the kinetic law object can use the parameter. If a parameter object is defined with a model object as its parent, then all objects within the model (including all rules, events and kinetic laws) can use the parameter.

```
modelObj = sbiomodel('cell')
parameterObj = addparameter(modelObj, 'TF1', 0.01)
```




```
modelObj = sbiomodel('cell')
reactionObj = addreaction(modelObj, 'a -> b')
kineticlawObj = addkineticlaw (reactionObj, 'MassAction')
parameterObj = addparameter(kineticlawObj, 'K1_forward', 0.1)
```



`parameterObj = addparameter(Obj, '`*`NameValue`*`', `*`ValueValue`*`)` creates a parameter object, assigns a value (*`NameValue`*) to the property `Name`, assigns the value (*`ValueValue`*) to the property `Value`, and assigns the `model object` or the `kineticlaw object` to the property `Parent`. In the model or kinetic law object (`Obj`), this method assigns the parameter object to the property `Parameters`, and returns the parameter object to a variable (`parameterObj`).

`parameterObj = addparameter(...'`*`PropertyName`*`', `*`PropertyValue`*`...)` defines optional property values. The name-value pairs can be in any format supported by the function `set`.

Scope of a parameter — A parameter can be *scoped* to either a model or a kinetic law.

- When a kinetic law searches for a parameter in its expression, it first looks in the parameter list of the kinetic law. If the parameter isn't found there, it moves to the model that the kinetic law object is in and looks in the model parameter list. If the parameter isn't found there, it moves to the model parent.
- When a rule searches for a parameter in its expression, it looks in the parameter list for the model. If the parameter isn't found there, it moves to the model parent. A rule cannot use a parameter that is scoped to a kinetic law. So for a parameter to be used in both a reaction rate equation and a rule, the parameter should be *scoped* to a model.

Additional parameter object properties can be viewed with the `get` command. Additional parameter object properties can be modified with the `set` command. The parameters of `Obj` can be viewed with `get(`*`Obj`*`, 'Parameters')`.

A SimBiology parameter object can be copied to a SimBiology model or kinetic law object with `copyobj`. A SimBiology parameter object can be removed from a SimBiology model or kinetic law object with `delete`.

Method Summary

Methods for parameter objects

copyobj	Copy SimBiology object and its children
delete	Delete SimBiology object
display	Display summary of SimBiology object
findUsages	Find out how a species, parameter, or compartment is used in a model
get	Get SimBiology object properties
move	Move SimBiology species or parameter object to new parent
rename	Rename object and update expressions
set	Set SimBiology object properties

Property Summary

Properties for parameter objects

Constant	Specify variable or constant species amount, parameter value, or compartment capacity
ConstantValue	Specify variable or constant parameter value
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Tag	Specify label for SimBiology object
Type	Display SimBiology object type
Units	Units for species amount, parameter value, compartment capacity, observable expression
UserData	Specify data to associate with object
Value	Value of species, compartment, or parameter object
ValueUnits	Parameter value units

Example

1. Create a model object, and then add a reaction object.

```
modelObj = sbiomodel ('my_model');
reactionObj = addreaction (modelObj, 'a + b -> c + d');
```

2. Define a kinetic law for the reaction object.

```
kineticlawObj = addkineticlaw(reactionObj, 'MassAction');
```

3. Add a parameter and assign it to the kinetic law object (`kineticlawObj`); add another parameter and assign to the model object (`modelObj`).

```
% Add parameter to kinetic law object
parameterObj1 = addparameter (kineticlawObj, 'K1');

get (kineticlawObj, 'Parameters')
```

MATLAB returns:

```
SimBiology Parameter Array

Index:    Name:    Value:    ValueUnits:
 1         K1       1
```

```
% Add parameter with value 0.9 to model object
parameterObj1 = addparameter (modelObj, 'K2', 0.9);

get (modelObj, 'Parameters')
```

MATLAB returns:

```
SimBiology Parameter Array

 Index:    Name:    Value:    ValueUnits:
   1         K2       1
```

Version History

Introduced in R2006a

R2022b: Having duplicate model component names issues a warning

Warns starting in R2022b

- SimBiology issues a warning if multiple model components (model, compartment, species, parameter, reaction, rule, event, observable, dose, and variant) have the same name. In a future release, within a single model, these components will be required to have unique names even when they are of different types with the following two exceptions:
  - Species in different compartments can have the same name.
  - Parameters can have the same name if they are scoped to different parents. Specifically, you can use the same name for a model-scoped parameter and reaction-scoped parameters, where each reaction-scoped parameter belongs to a different reaction.

  The purpose of this naming restriction is to ensure that every model component can be unambiguously referenced by its unique name within a model. For details on how to reference model component names in expressions, see “Guidelines for Referencing Names in Expressions”.
- To disambiguate duplicate names from your model, use the `updateDuplicateNames` function at the command line. The function takes in a SimBiology model as an input and updates the component names as necessary. You can also specify optional outputs, such as a logical flag to check whether any update occurred, a list of model changes, and a copy of the original model before any updates were made.
- The `updateDuplicateNames` function disambiguates the duplicate names by adding a suffix "*_N*", where *N* is the first positive integer that results in a unique name. If there is an existing suffix, *N* will be incremented from that suffix. For example, if there are two model components named *x_3*, the function updates one of the names to *x_4*. If the existing suffix has leading zeros, the function omits the zeros in the new name. For instance, if *x_003* is a duplicate name, it gets

renamed to *x_4*. However, the function assumes that names with leading zeros and without leading zeros are different. For instance, *x_005* and *x_5* are considered to be different names.

R2022a: Having duplicate model component names will not be allowed in a future release
Behavior change in future release

SimBiology will not allow you to have duplicate names for model components within a model.

See Also

`model object` | `kineticlaw object` | `addreaction`

addproduct (reaction)

Add product species object to reaction object

Syntax

```
speciesObj = addproduct(reactionObj, 'NameValue')
speciesObj = addproduct(reactionObj, speciesObj)
speciesObj = addproduct(reactionObj, 'NameValue', Stoichcoefficient)
speciesObj = addproduct(reactionObj, speciesObj, Stoichcoefficient)
```

Arguments

reactionObj	Reaction object. Enter a name for the reaction object.
NameValue	Names of species objects. Enter a character vector or cell array of character vectors. A species object can be referenced by other objects using its name. You can use the function `sbioselect` on page 1-245 to find an object with a name specified by `NameValue`.
speciesObj	Species object or vector of species objects.
Stoichcoeffieient	Stoichiometric coefficients for products. Enter a positive scalar or vector of positive doubles. If vector, it must have the same number of elements as the number of species specified by *NameValue* or *speciesObj*.

Description

speciesObj = addproduct(*reactionObj*, '*NameValue*') creates a species object (if it does not exist already in the model) and returns the species object (*speciesObj*). In the species object, this method assigns the value (*NameValue*) to the property `Name`. In the reaction object, this method assigns the species object to the property `Products`, modifies the reaction equation in the property `Reaction` to include the new species, and adds the stoichiometric coefficient `1` to the property `Stoichiometry`.

When you define a reaction with a new species:

- If no compartment objects exist in the model, the method creates a compartment object (called '*unnamed*') in the model and adds the newly created species to that compartment.
- If only one compartment object (`compObj`) exists in the model, the method creates a species object in that compartment.
- If there is more than one compartment object (`compObj`) in the model, you must qualify the species name with the compartment name.

  For example, `cell.glucose` denotes that you want to put the species named `glucose` into a compartment named `cell`. Additionally, if the compartment named `cell` does not exist, the process of adding the reaction creates the compartment and names it `cell`.

Create and add a species object to a compartment object with the method `addspecies` on page 2-108.

`speciesObj` `= addproduct(`*`reactionObj`*`, `*`speciesObj`*`)`, in the species object (*`speciesObj`*), assigns the parent object of the *`reactionObj`* to the species property `Parent`. In the reaction object (`reactionObj`), it assigns the species object to the property `Products`, modifies the reaction equation in the property `Reaction` to include the new species, and adds the stoichiometric coefficient `1` to the property `Stoichiometry`.

`speciesObj` `= addproduct(`*`reactionObj`*`, '`*`NameValue`*`', `*`Stoichcoefficient`*`)`, in addition to the description above, adds the stoichiometric coefficient (`Stoichcoefficient`) to the property `Stoichiometry`. If `NameValue` is a cell array of species names, then `Stoichcoefficient` must be a vector of doubles with the same length as `NameValue`.

`speciesObj` `= addproduct(`*`reactionObj`*`, `*`speciesObj`*`, `*`Stoichcoefficient`*`)`, in addition to the description above, adds the stoichiometric coefficient (`Stoichcoefficient`) to the property `Stoichiometry`.

Species names are referenced by reaction objects, kinetic law objects, and model objects. If you change the `Name` of a species the reaction also uses the new name. You must however configure all other applicable elements such as rules that use the species, and the kinetic law object.

Examples

1. Create a model object, and then add a reaction object.

```
modelObj = sbiomodel('my_model');
reactionObj = addreaction(modelObj, 'A + C -> U');
```

2. Modify the reaction of the `reactionObj` from `A + C -> U` to `A + C -> U + 2 H`.

```
speciesObj = addproduct(reactionObj, 'H', 2);
```

See Also

`addspecies`

Version History

Introduced in R2006a

addreactant (reaction)

Add species object as reactant to reaction object

Syntax

```
speciesObj = addreactant(reactionObj, 'NameValue')
speciesObj = addreactant(reactionObj, speciesObj)
speciesObj = addreactant(reactionObj, speciesObj, StoichCoefficient)
speciesObj = addreactant(reactionObj, 'NameValue', StoichCoefficient)
```

Arguments

reactionObj	Reaction object.
NameValue	Names of species objects. Enter a character vector or cell array of character vectors. A species object can be referenced by other objects using its name. You can use the function `sbioselect` on page 1-245 to find an object with a name specified by `NameValue`.
speciesObj	Species object or vector of species objects.
StoichCoefficient	Stoichiometric coefficients for reactants. Enter a positive scalar or vector of positive doubles. If vector, it must have the same number of elements as the number of species specified by *NameValue* or *speciesObj*.

Description

speciesObj = addreactant(*reactionObj*, '*NameValue*') creates a species object (if it does not exist already in the model) and returns the species object (*speciesObj*). In the species object, this method assigns the value (*NameValue*) to the property `Name`. In the reaction object, this method assigns the species object to the property `Reactants`, modifies the reaction equation in the property `Reaction` to include the new species, and adds the stoichiometric coefficient `-1` to the property `Stoichiometry`.

When you define a reaction with a new species:

- If no compartment objects exist in the model, the method creates a compartment object (called '*unnamed*') in the model and adds the newly created species to that compartment.
- If only one compartment object (`compObj`) exists in the model, the method creates a species object in that compartment.
- If there is more than one compartment object (`compObj`) in the model, you must qualify the species name with the compartment name.

  For example, `cell.glucose` denotes that you want to put the species named `glucose` into a compartment named `cell`. Additionally, if the compartment named `cell` does not exist, the process of adding the reaction creates the compartment and names it `cell`.

Create and add a species object to a compartment object with the method `addspecies` on page 2-108.

`speciesObj` `= addreactant(`*`reactionObj`*`, `*`speciesObj`*`)`, in the species object (*`speciesObj`*), assigns the parent object of the *`reactionObj`* to the species property `Parent`. In the reaction object (`reactionObj`), it assigns the species object to the property `Reactants`, modifies the reaction equation in the property `Reaction` to include the new species, and adds the stoichiometric coefficient `1` to the property `Stoichiometry`.

`speciesObj` `= addreactant(`*`reactionObj`*`, `*`speciesObj`*`, `*`StoichCoefficient`*`)`, in the species object (`speciesObj`), assigns the parent object to the `speciesObj` property `Parent`. In the reaction object (`reactionObj`), it assigns the species object to the property `Reactants`, modifies the reaction equation in the property `Reaction` to include the new species, and adds the stoichiometric coefficient `-1` to the property `Stoichiometry`. If `speciesObj` is a cell array of species objects, then *`StoichCoefficient`* must be a vector of doubles with the same length as `speciesObj`.

`speciesObj` `= addreactant(`*`reactionObj`*`, '`*`NameValue`*`', `*`StoichCoefficient`*`)`, in addition to the description above, adds the stoichiometric coefficient (*`StoichCoefficient`*) to the property `Stoichiometry`. If *`NameValue`* is a cell array of species names, then *`StoichCoefficient`* must be a vector of doubles with the same length as *`NameValue`*.

Species names are referenced by reaction objects, kinetic law objects, and model objects. If you change the `Name` of a species the reaction also uses the new name. You must, however, configure all other applicable elements such as rules that use the species, and the kinetic law object.

See “Specifying Species Names in SimBiology” for more information on species names.

Example

1. Create a model object, and then add a reaction object.

```
modelObj = sbiomodel('my_model');
reactionObj = addreaction(modelObj, 'A -> U');
```

2. Modify the `reaction` of `the reactionObj` from `A -> U` to be `A + 3 C -> U`.

```
speciesObj = addreactant(reactionObj, 'C', 3);
```

See Also

`addspecies`

Version History

Introduced in R2006a

addreaction (model)

Create reaction object and add to model object

Syntax

```
reactionObj = addreaction(modelObj,'ReactionValue')
reactionObj = addreaction(modelObj, 'ReactantsValue', 'ProductsValue')
reactionObj = addreaction(modelObj, 'ReactantsValue', RStoichCoefficients,
'ProductsValue', PStoichCoefficients)

reactionObj = addreaction(...'PropertyName', PropertyValue...)
```

Arguments

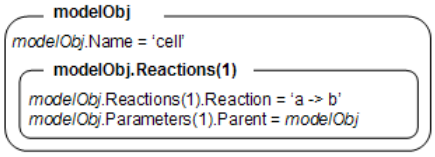
modelObj	SimBiology `model object`.
ReactionValue	Specify the reaction equation. Enter a character vector. A hyphen preceded by a space and followed by a right angle bracket (`->`) indicates reactants going forward to products. A hyphen with left and right angle brackets (`<->`) indicates a reversible reaction. Coefficients before reactant or product names must be followed by a space. Examples are `'A -> B'`, `'A + B -> C'`, `'2 A + B -> 2 C'`, and `'A <-> B'`. Enter reactions with spaces between the species. If there are multiple compartments, or to specify the compartment name, use *compartmentName.speciesName* to qualify the species name. Examples are `'cytoplasm.A -> cytoplasm.B'`, `'cytoplasm.A -> nucleus.A'`, and `'cytoplasm.A + cytoplasm.B -> nucleus.AB'`.
ReactantsValue	Character vector defining the species name, a cell array of character vectors, a species object, or an array of species objects. If using names, qualify with compartment names if there are multiple compartments.
ProductsValue	Character vector defining the species name, a cell array of character vectors, a species object, or an array of species objects. If using names, qualify with compartment names if there are multiple compartments.
RStoichCoefficients	Stoichiometric coefficients for reactants, length of array equal to length of *ReactantsValue*.
PStoichCoefficients	Stoichiometric coefficients for products, length of array equal to length of *ProductsValue*.

Note If you qualify any species name with a compartment name, then you must qualify every species with the corresponding compartment name.

Description

reactionObj = addreaction(*modelObj*,'*ReactionValue*') creates a reaction object, assigns a value (*ReactionValue*) to the property Reaction, assigns reactant species object(s) to the property Reactants, assigns the product species object(s) to the property Products, and assigns the model object to the property Parent. In the Model object (modelObj), this method assigns the reaction object to the property Reactions, and returns the reaction object (reactionObj).

```
reactionObj = addreaction(modelObj, 'a -> b')
```



When you define a reaction with a new species:

- If no compartment objects exist in the model, the method creates a compartment object (called '*unnamed*') in the model and adds the newly created species to that compartment.
- If only one compartment object (compObj) exists in the model, the method creates a species object in that compartment.
- If there is more than one compartment object (compObj) in the model, you must qualify the species name with the compartment name.

  For example, cell.glucose denotes that you want to put the species named glucose into a compartment named cell. Additionally, if the compartment named cell does not exist, the process of adding the reaction creates the compartment and names it cell.

You can manually add a species to a compartment object with the method addspecies.

You can add species to a reaction object using the methods addreactant or addproduct. You can remove species from a reaction object with the methods rmreactant or rmproduct. The property Reaction is modified by adding or removing species from the reaction equation.

You can copy a SimBiology reaction object to a model object with the function copyobj. You can remove the SimBiology reaction object from a SimBiology model object with the function delete.

You can view additional reaction object properties with the get command. For example, the reaction equation of reactionObj can be viewed with the command get(*reactionObj*, 'Reaction'). You can modify additional reaction object properties with the command set.

reactionObj = addreaction(*modelObj*, '*ReactantsValue*', '*ProductsValue*') creates a reaction object, assigns a value to the property Reaction using the reactant (*ReactantsValue*) and product (*ProductsValue*) names, assigns the species objects to the properties Reactants and Products, and assigns the model object to the property Parent. In the model object (modelObj), this method assigns the reaction object to the property Reactions, and returns the reaction object (reactionObj). The stoichiometric values are assumed to be 1.

`reactionObj = addreaction(modelObj, 'ReactantsValue', RStoichCoefficients, 'ProductsValue', PStoichCoefficients)` adds stoichiometric coefficients (*`RStoichCoefficients`*) for reactant species, and stoichiometric coefficients (`PStoichCoefficients`) for product species to the property `Stoichiometry` on page 3-143. The length of `Reactants` and `RCoefficients` must be equal, and the length of `Products` and `PCoefficients` must be equal.

`reactionObj` `= addreaction(...'PropertyName', PropertyValue...)` defines optional properties. The property name/property value pairs can be in any format supported by the function `set`.

Note If you use the `addreaction` method to create a reaction rate expression that is not continuous and differentiable, see “Using Events to Address Discontinuities in Rule and Reaction Rate Expressions” before simulating your model.

Method Summary

Methods for reaction objects

addkineticlaw (reaction)	Create kinetic law object and add to reaction object
addproduct (reaction)	Add product species object to reaction object
addreactant (reaction)	Add species object as reactant to reaction object
copyobj	Copy SimBiology object and its children
delete	Delete SimBiology object
display	Display summary of SimBiology object
get	Get SimBiology object properties
rename	Rename object and update expressions
rmproduct (reaction)	Remove species object from reaction object products
rmreactant (reaction)	Remove species object from reaction object reactants
set	Set SimBiology object properties

Property Summary

Properties for reaction objects

Active	Indicate object in use during simulation
KineticLaw	Show kinetic law used for `ReactionRate`
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Products	Array of reaction products
Reactants	Array of reaction reactants
Reaction	Reaction object reaction
ReactionRate	Reaction rate equation in reaction object
Reversible	Specify whether reaction is reversible or irreversible
Stoichiometry	Species coefficients in reaction
Tag	Specify label for SimBiology object
Type	Display SimBiology object type
UserData	Specify data to associate with object

Examples

Create a model, add a reaction object, and assign the expression for the reaction rate equation.

1. Create a model object, and then add a reaction object.

```
modelObj = sbiomodel('my_model');
reactionObj = addreaction(modelObj, 'a -> c + d');
```

2. Create a kinetic law object for the reaction object, of the type `'Henri-Michaelis-Menten'`.

```
kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
```

`reactionObj` `KineticLaw` property is configured to `kineticlawObj`.

3. The `'Henri-Michaelis-Menten'` kinetic law has two parameter variables (`Vm` and `Km`) and one species variable (`S`) that should to be set. To set these variables, first create the parameter variables as parameter objects (`parameterObj1, parameterObj2`) with names `Vm_d`, and `Km_d`, and assign the objects `Parent` property value to the `kineticlawObj`.

```
parameterObj1 = addparameter(kineticlawObj, 'Vm_d');
parameterObj2 = addparameter(kineticlawObj, 'Km_d');
```

4. Set the variable names for the kinetic law object.

```
set(kineticlawObj,'ParameterVariableNames', {'Vm_d' 'Km_d'});
set(kineticlawObj,'SpeciesVariableNames', {'a'});
```

5. Verify that the reaction rate is expressed correctly in the reaction object `ReactionRate` property.

```
get (reactionObj, 'ReactionRate')
```

MATLAB returns:

```
ans =

Vm_d*a/(Km_d+a)
```

Version History

Introduced in R2006a

R2022b: Having duplicate model component names issues a warning
Warns starting in R2022b

- SimBiology issues a warning if multiple model components (model, compartment, species, parameter, reaction, rule, event, observable, dose, and variant) have the same name. In a future release, within a single model, these components will be required to have unique names even when they are of different types with the following two exceptions:
  - Species in different compartments can have the same name.
  - Parameters can have the same name if they are scoped to different parents. Specifically, you can use the same name for a model-scoped parameter and reaction-scoped parameters, where each reaction-scoped parameter belongs to a different reaction.

  The purpose of this naming restriction is to ensure that every model component can be unambiguously referenced by its unique name within a model. For details on how to reference model component names in expressions, see “Guidelines for Referencing Names in Expressions”.
- To disambiguate duplicate names from your model, use the `updateDuplicateNames` function at the command line. The function takes in a SimBiology model as an input and updates the component names as necessary. You can also specify optional outputs, such as a logical flag to check whether any update occurred, a list of model changes, and a copy of the original model before any updates were made.
- The `updateDuplicateNames` function disambiguates the duplicate names by adding a suffix `"_N"`, where *N* is the first positive integer that results in a unique name. If there is an existing suffix, *N* will be incremented from that suffix. For example, if there are two model components named *x_3*, the function updates one of the names to *x_4*. If the existing suffix has leading zeros, the function omits the zeros in the new name. For instance, if *x_003* is a duplicate name, it gets renamed to *x_4*. However, the function assumes that names with leading zeros and without leading zeros are different. For instance, *x_005* and *x_5* are considered to be different names.

R2022a: Having duplicate model component names will not be allowed in a future release
Behavior change in future release

SimBiology will not allow you to have duplicate names for model components within a model.

See Also

`model object` | `addkineticlaw` | `addproduct` | `addreactant` | `rmproduct` | `rmreactant`

addrule (model)

Create rule object and add to model object

Syntax

```
ruleObj = addrule(modelObj, Rule)
ruleObj = addrule(modelObj, Rule, RuleType)

ruleObj = addrule(..., 'PropertyName', PropertyValue,...)
```

Arguments

modelObj	`Model object` to which to add the rule.
Rule	Character vector specifying the rule. For example, enter the algebraic rule `'Va*Ea + Vi*Ei - K2'`.
RuleType	Character vector specifying the type of rule. Choices are: • `'algebraic'` • `'initialAssignment'` • `'repeatedAssignment'` • `'rate'` For more information, see RuleType

Description

A rule is a mathematical expression that changes the amount of a species or the value of a parameter. It also defines how species and parameters interact with one another.

`ruleObj = addrule(modelObj, Rule)` constructs and returns *ruleObj*, a rule object. In *ruleObj*, the rule object, this method assigns the *modelObj* input argument to the `Parent` property, assigns the *Rule* input argument to the `Rule` property, and assigns `'initialAssignment'` or `'algebraic'` to the `RuleType` property. (This method assigns `'initialAssignment'` for all assignment rules and `'algebraic'` for all other rules.) In *modelObj*, the `model object`, this method assigns *ruleObj*, the rule object, to the `Rules` property.

`ruleObj = addrule(modelObj, Rule, RuleType)` in addition to the assignments above, assigns the *RuleType* input argument to the `RuleType` property. For more information on the types of rules, see RuleType.

`ruleObj = addrule(..., 'PropertyName', PropertyValue,...)` defines optional properties. The property name/property value pairs can be in any format supported by the function `set`.

View additional rule properties with the function `get`, and modify rule properties with the function `set`. Copy a rule object to a model with the function `copyobj on page 2-185`, or delete a rule object from a model with the function `delete on page 2-239`.

Note If you use the `addrule` method to create an algebraic rule, rate rule, or repeated assignment rule, and the rule expression is not continuous and differentiable, see “Using Events to Address Discontinuities in Rule and Reaction Rate Expressions” before simulating your model.

Method Summary

Methods for rule objects

copyobj	Copy SimBiology object and its children
delete	Delete SimBiology object
display	Display summary of SimBiology object
get	Get SimBiology object properties
rename	Rename object and update expressions
set	Set SimBiology object properties

Property Summary

Properties for rule objects

Active	Indicate object in use during simulation
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Rule	Specify species and parameter interactions
RuleType	Specify type of rule for rule object
Tag	Specify label for SimBiology object
Type	Display SimBiology object type
UserData	Specify data to associate with object

Examples

Add a rule with the default `RuleType`.

1 Create a model object, and then add a rule object.

```
modelObj = sbiomodel('cell');
ruleObj = addrule(modelObj, '0.1*B-A')
```

2 Get a list of properties for a rule object.

```
get(modelObj.Rules(1)) or get(ruleObj)
```

MATLAB displays a list of rule properties.

```
    Active: 1
    Annotation: ''
          Name: ''
```

```
          Notes: ''
         Parent: [1x1 SimBiology.Model]
           Rule: '0.1*B-A'
       RuleType: 'algebraic'
            Tag: ''
           Type: 'rule'
       UserData: []
```

Add a rule with the `RuleType` property set to `rate`.

1. Create model object, and then add a reaction object.

   ```
   modelObj = sbiomodel ('my_model');
   reactionObj = addreaction (modelObj, 'a -> b');
   ```

2. Add a rule which defines that the quantity of a species `c`. In the rule expression, `k` is the rate constant for `a -> b`.

   ```
   ruleObj = addrule(modelObj, 'c = k*(a+b)')
   ```

3. Change the `RuleType` from default (`'algebraic'`) to `'rate'`, and verify using the `get` command.

   ```
   set(ruleObj, 'RuleType', 'rate');
   get(ruleObj)
   ```

   MATLAB returns all the properties for the rule object.

   ```
       Active: 1
   Annotation: ''
         Name: ''
        Notes: ''
       Parent: [1x1 SimBiology.Model]
         Rule: 'c = k*(a+b)'
     RuleType: 'rate'
          Tag: ''
         Type: 'rule'
     UserData: []
   ```

Version History

Introduced in R2006a

R2022b: Having duplicate model component names issues a warning

Warns starting in R2022b

- SimBiology issues a warning if multiple model components (model, compartment, species, parameter, reaction, rule, event, observable, dose, and variant) have the same name. In a future release, within a single model, these components will be required to have unique names even when they are of different types with the following two exceptions:

  - Species in different compartments can have the same name.
  - Parameters can have the same name if they are scoped to different parents. Specifically, you can use the same name for a model-scoped parameter and reaction-scoped parameters, where each reaction-scoped parameter belongs to a different reaction.

The purpose of this naming restriction is to ensure that every model component can be unambiguously referenced by its unique name within a model. For details on how to reference model component names in expressions, see “Guidelines for Referencing Names in Expressions”.

- To disambiguate duplicate names from your model, use the `updateDuplicateNames` function at the command line. The function takes in a SimBiology model as an input and updates the component names as necessary. You can also specify optional outputs, such as a logical flag to check whether any update occurred, a list of model changes, and a copy of the original model before any updates were made.
- The `updateDuplicateNames` function disambiguates the duplicate names by adding a suffix `"_N"`, where *N* is the first positive integer that results in a unique name. If there is an existing suffix, *N* will be incremented from that suffix. For example, if there are two model components named *x_3*, the function updates one of the names to *x_4*. If the existing suffix has leading zeros, the function omits the zeros in the new name. For instance, if *x_003* is a duplicate name, it gets renamed to *x_4*. However, the function assumes that names with leading zeros and without leading zeros are different. For instance, *x_005* and *x_5* are considered to be different names.

R2022a: Having duplicate model component names will not be allowed in a future release
Behavior change in future release

SimBiology will not allow you to have duplicate names for model components within a model.

See Also

`model object` | `copyobj` | `delete` | `sbiomodel`

addsamples

Add additional samples to increase accuracy of Sobol indices or elementary effects analysis

Syntax

```
results = addsamples(gsaObj,numSamples)
results = addobservable(gsaObj,numSamples,'ShowWaitbar',tf)
```

Description

`results = addsamples(gsaObj,numSamples)` adds the specified number of new samples to increase the accuracy of the variance decomposition (Sobol indices) or the accuracy of elementary effects analysis. For the Sobol indices, the function simulates the model `numSamples * (2 + number of parameters)` times. For details, see “Saltelli Method to Compute Sobol Indices” on page 2-876. For the elementary effects analysis, the function simulates the model `numSamples * (1 + number of parameters)` times. For details, see “Elementary Effects for Global Sensitivity Analysis” on page 1-51.

`results = addobservable(gsaObj,numSamples,'ShowWaitbar',tf)` specifies whether to show the simulation progress in a graphic.

Examples

Perform Global Sensitivity Analysis by Computing First- and Total-Order Sobol Indices

Load the “Tumor Growth Model”.

```
sbioloadproject tumor_growth_vpop_sa.sbproj
```

Get a variant with the estimated parameters and the dose to apply to the model.

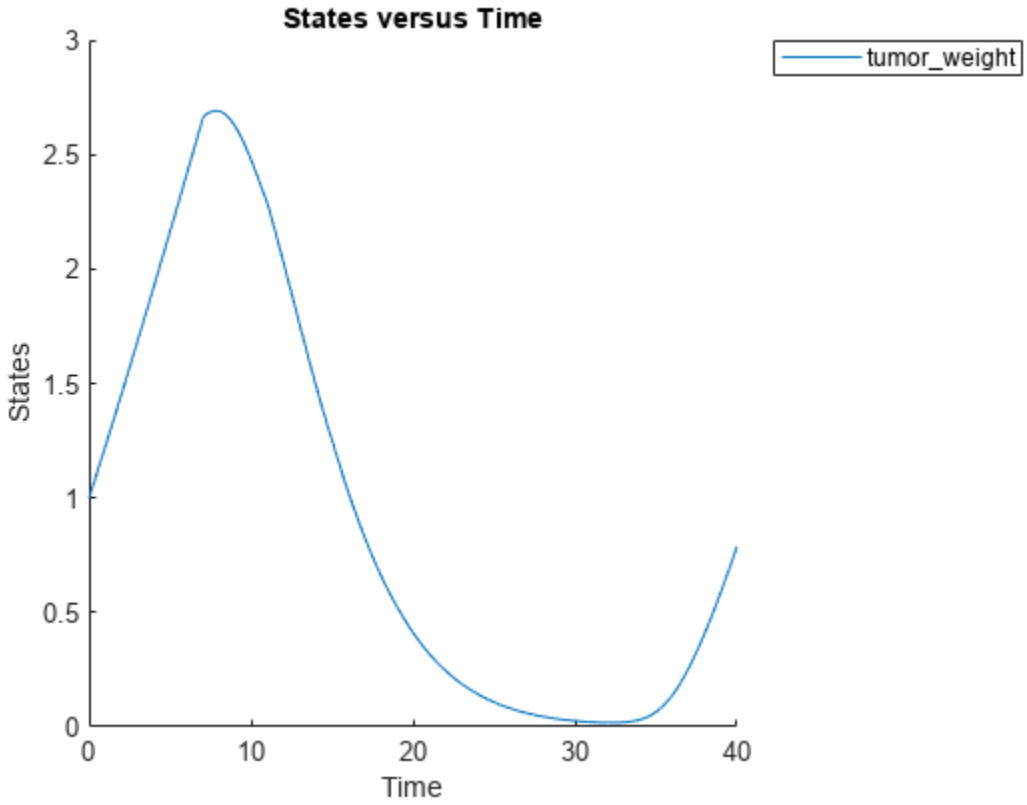
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

Get the active configset and set the tumor weight as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'tumor_weight';
```

Simulate the model and plot the tumor growth profile.

```
sbioplot(sbiosimulate(m1,cs,v,d));
```



Perform global sensitivity analysis (GSA) on the model to find the model parameters that the tumor growth is sensitive to.

First, retrieve model parameters of interest that are involved in the pharmacodynamics of the tumor growth. Define the model response as the tumor weight.

```
modelParamNames = {'L0','L1','w0','k1','k2'};
outputName = 'tumor_weight';
```

Then perform GSA by computing the first- and total-order Sobol indices using `sbiosobol`. Set `'ShowWaitBar'` to `true` to show the simulation progress. By default, the function uses 1000 parameter samples to compute the Sobol indices [1].

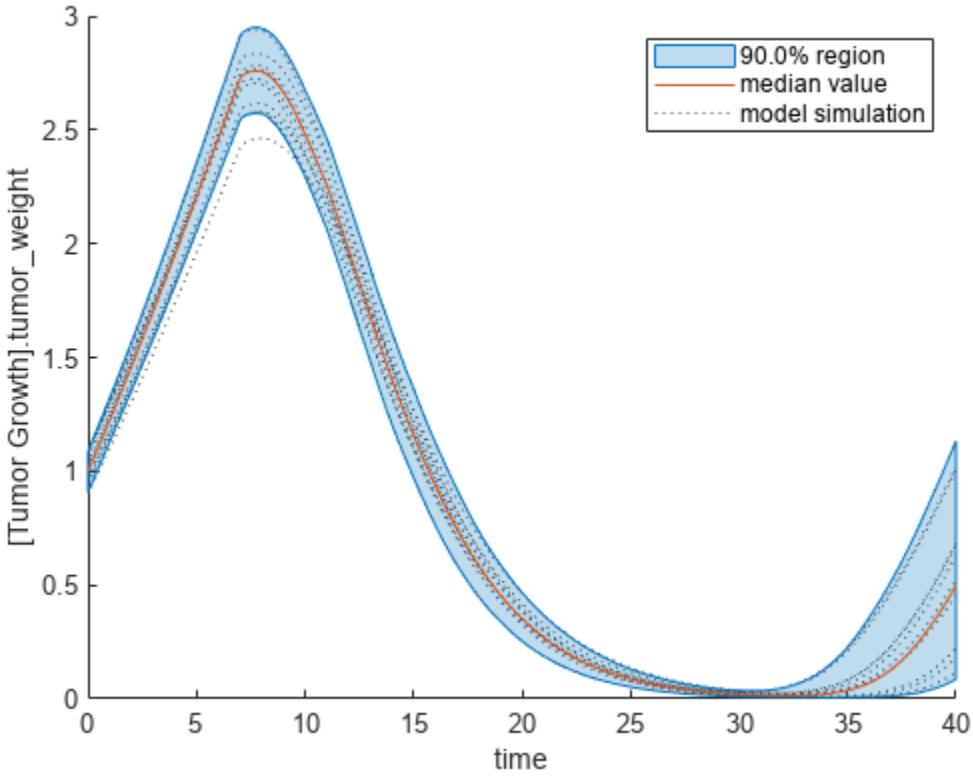
```
rng('default');
sobolResults = sbiosobol(m1,modelParamNames,outputName,Variants=v,Doses=d,ShowWaitBar=true)
```

```
sobolResults =
  Sobol with properties:

                Time: [444x1 double]
        SobolIndices: [5x1 struct]
            Variance: [444x1 table]
    ParameterSamples: [1000x5 table]
         Observables: {'[Tumor Growth].tumor_weight'}
      SimulationInfo: [1x1 struct]
```

You can change the number of samples by specifying the `'NumberSamples'` name-value pair argument. The function requires a total of `(number of input parameters + 2) * NumberSamples` model simulations.

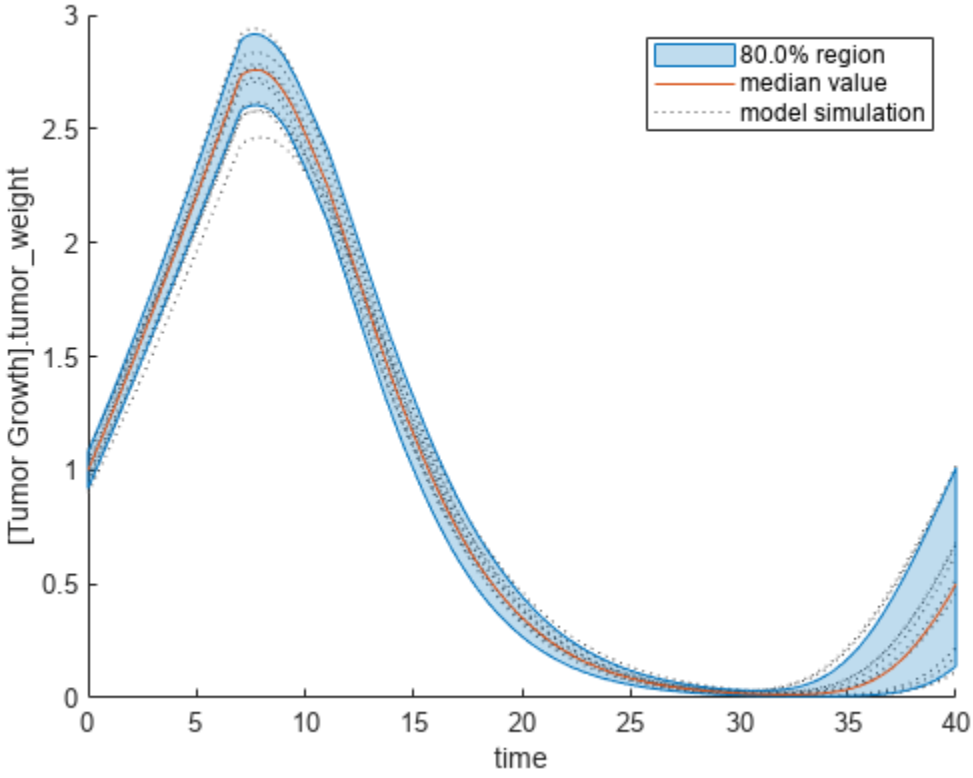
Show the mean model response, the simulation results, and a shaded region covering 90% of the simulation results.

```
plotData(sobolResults,ShowMedian=true,ShowMean=false);
```



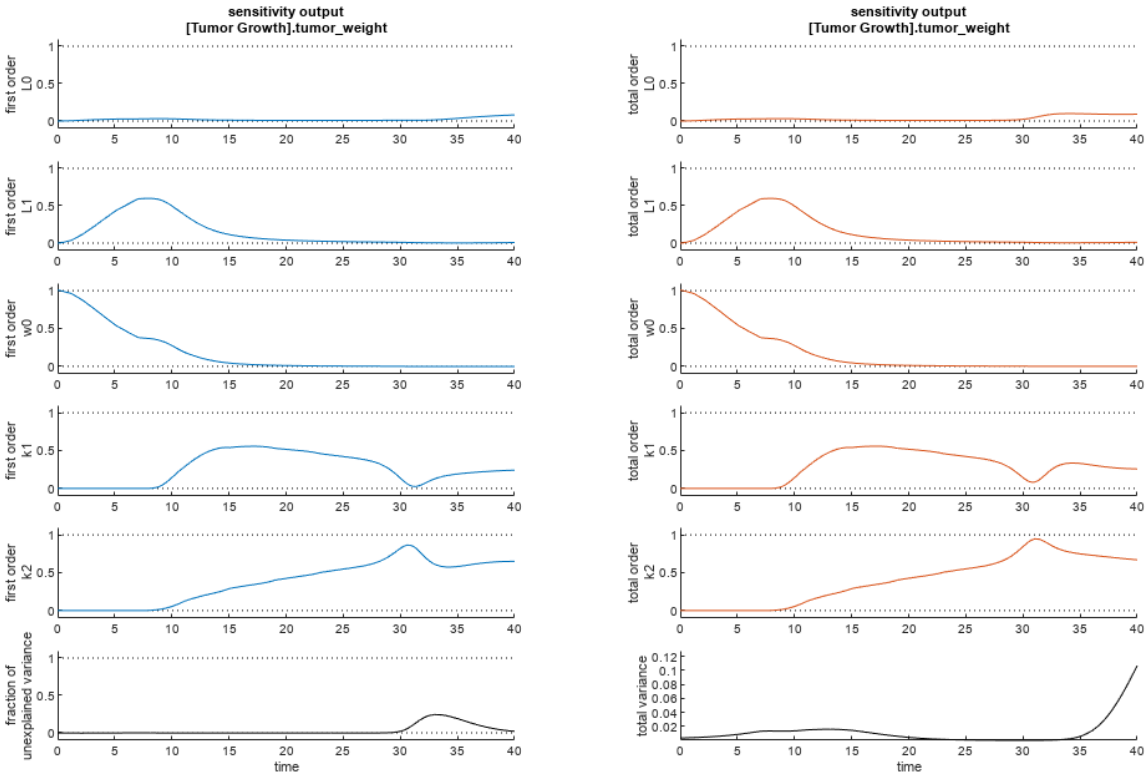
You can adjust the quantile region to a different percentage by specifying `'Alphas'` for the lower and upper quantiles of all model responses. For instance, an alpha value of 0.1 plots a shaded region between the `100 * alpha` and `100 * (1 - alpha)` quantiles of all simulated model responses.

```
plotData(sobolResults,Alphas=0.1,ShowMedian=true,ShowMean=false);
```



Plot the time course of the first- and total-order Sobol indices.

```
h = plot(sobolResults);
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```

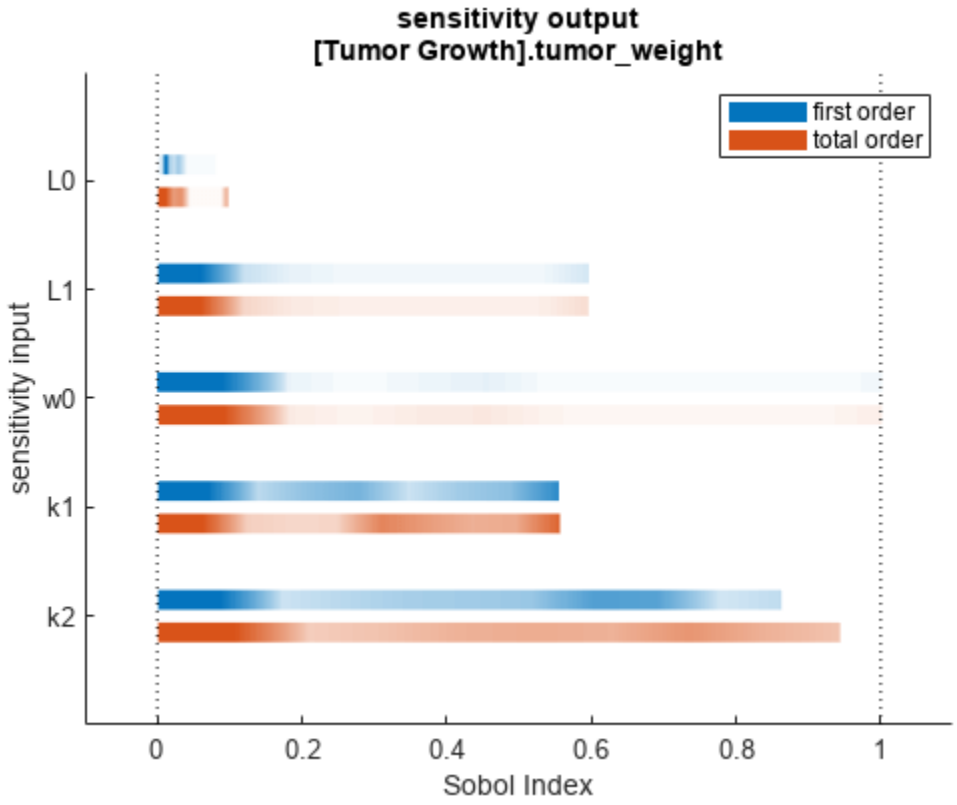


The first-order Sobol index of an input parameter gives the fraction of the overall response variance that can be attributed to variations in the input parameter alone. The total-order index gives the fraction of the overall response variance that can be attributed to any joint parameter variations that include variations of the input parameter.

From the Sobol indices plots, parameters `L1` and `w0` seem to be the most sensitive parameters to the tumor weight before the dose was applied at t = 7. But after the dose is applied, `k1` and `k2` become more sensitive parameters and contribute most to the after-dosing stage of the tumor weight. The total variance plot also shows a larger variance for the after-dose stage at t > 35 than for the before-dose stage of the tumor growth, indicating that `k1` and `k2` might be more important parameters to investigate further. The fraction of unexplained variance shows some variance at around t = 33, but the total variance plot shows little variance at t = 33, meaning the unexplained variance could be insignificant. The fraction of unexplained variance is calculated as 1 - (sum of all the first-order Sobol indices), and the total variance is calculated using `var(response)`, where `response` is the model response at every time point.

You can also display the magnitudes of the sensitivities in a bar plot. Darker colors mean that those values occur more often over the whole time course.

```
bar(sobolResults);
```



You can specify more samples to increase the accuracy of the Sobol indices, but the simulation can take longer to finish. Use `addsamples` to add more samples. For example, if you specify 1500 samples, the function performs `1500 * (2 + number of input parameters)` simulations.

```
gsaMoreSamples = addsamples(gsaResults,1500)
```

The “SimulationInfo” on page 2-0 property of the result object contains various information for computing the Sobol indices. For instance, the model simulation data (SimData) for each simulation using a set of parameter samples is stored in the `SimData` field of the property. This field is an array of `SimData` objects.

```
sobolResults.SimulationInfo.SimData
```

```
SimBiology SimData Array : 1000-by-7

Index:    Name:         ModelName:         DataCount:
1           -           Tumor Growth Model 1
2           -           Tumor Growth Model 1
3           -           Tumor Growth Model 1
...
7000        -           Tumor Growth Model 1
```

You can find out if any model simulation failed during the computation by checking the `ValidSample` field of `SimulationInfo`. In this example, the field shows no failed simulation runs.

```
all(sobolResults.SimulationInfo.ValidSample)
```

```
ans = 1x7 logical array

   1   1   1   1   1   1   1
```

`SimulationInfo.ValidSample` is a table of logical values. It has the same size as `SimulationInfo.SimData`. If `ValidSample` indicates that any simulations failed, you can get more information about those simulation runs and the samples used for those runs by extracting information from the corresponding column of `SimulationInfo.SimData`. Suppose that the fourth column contains one or more failed simulation runs. Get the simulation data and sample values used for that simulation using `getSimulationResults`.

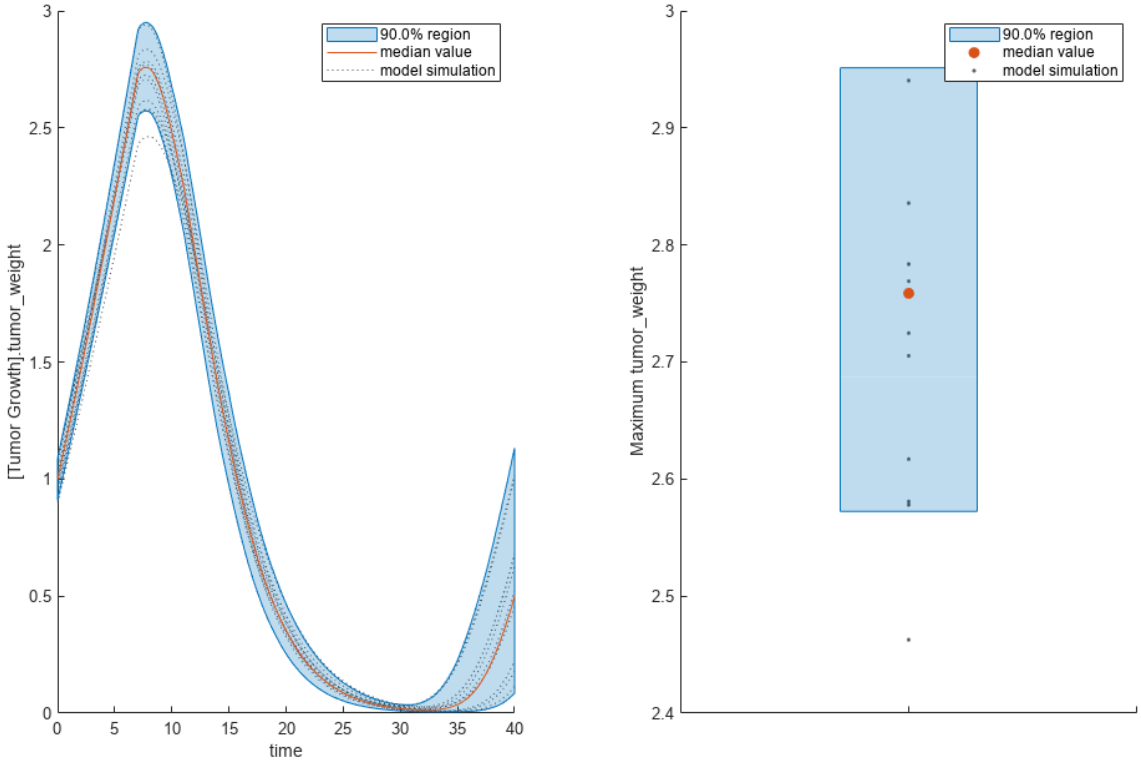
```
[samplesUsed,sd,validruns] = getSimulationResults(sobolResults,4);
```

You can add custom expressions as observables and compute Sobol indices for the added observables. For example, you can compute the Sobol indices for the maximum tumor weight by defining a custom expression as follows.

```
% Suppress an information warning that is issued during simulation.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
% Add the observable expression.
sobolObs = addobservable(sobolResults,'Maximum tumor_weight','max(tumor_weight)','Units','gram');
```

Plot the computed simulation results showing the 90% quantile region.

```
h2 = plotData(sobolObs,ShowMedian=true,ShowMean=false);
h2.Position(:) = [100 100 1280 800];
```



You can also remove the observable by specifying its name.

```
gsaNoObs = removeobservable(sobolObs,'Maximum tumor_weight');
```

Restore the warning settings.

```
warning(warnSettings);
```

Perform GSA by Computing Elementary Effects

Load the “Tumor Growth Model”.

```
sbioloadproject tumor_growth_vpop_sa.sbproj
```

Get a variant with estimated parameters and the dose to apply to the model.

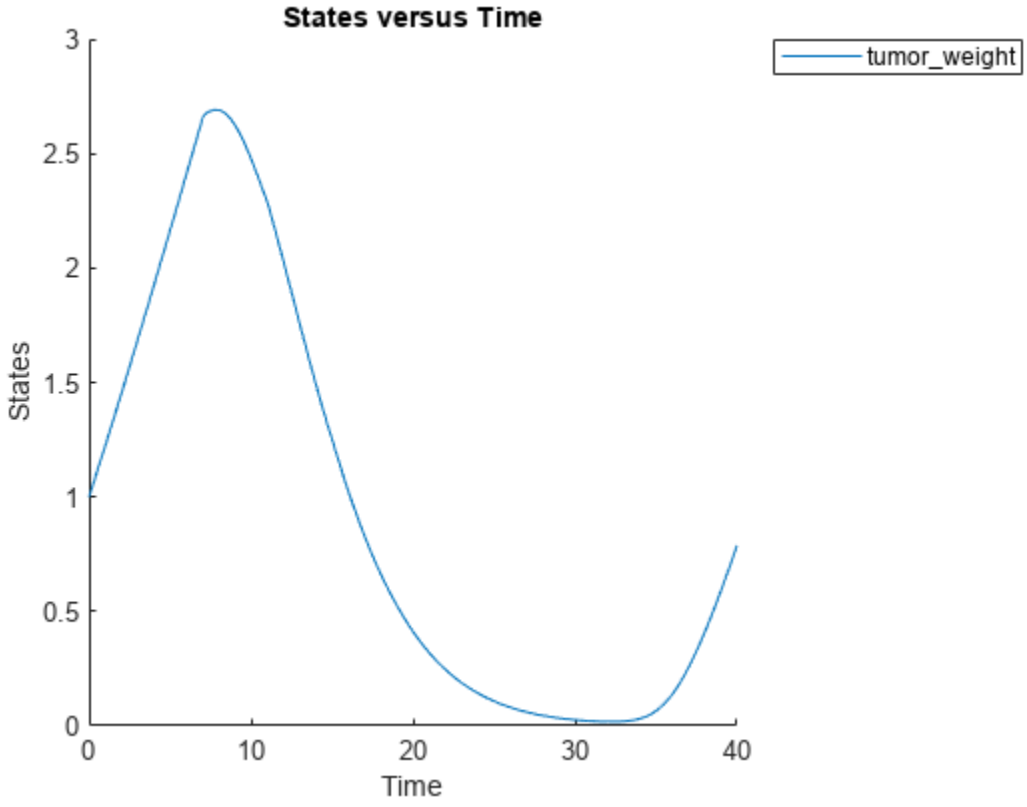
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

Get the active configset and set the tumor weight as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'tumor_weight';
```

Simulate the model and plot the tumor growth profile.

```
sbioplot(sbiosimulate(m1,cs,v,d));
```



Perform global sensitivity analysis (GSA) on the model to find the model parameters that the tumor growth is sensitive to.

First, define model parameters of interest, which are involved in the pharmacodynamics of the tumor growth. Define the model response as the tumor weight.

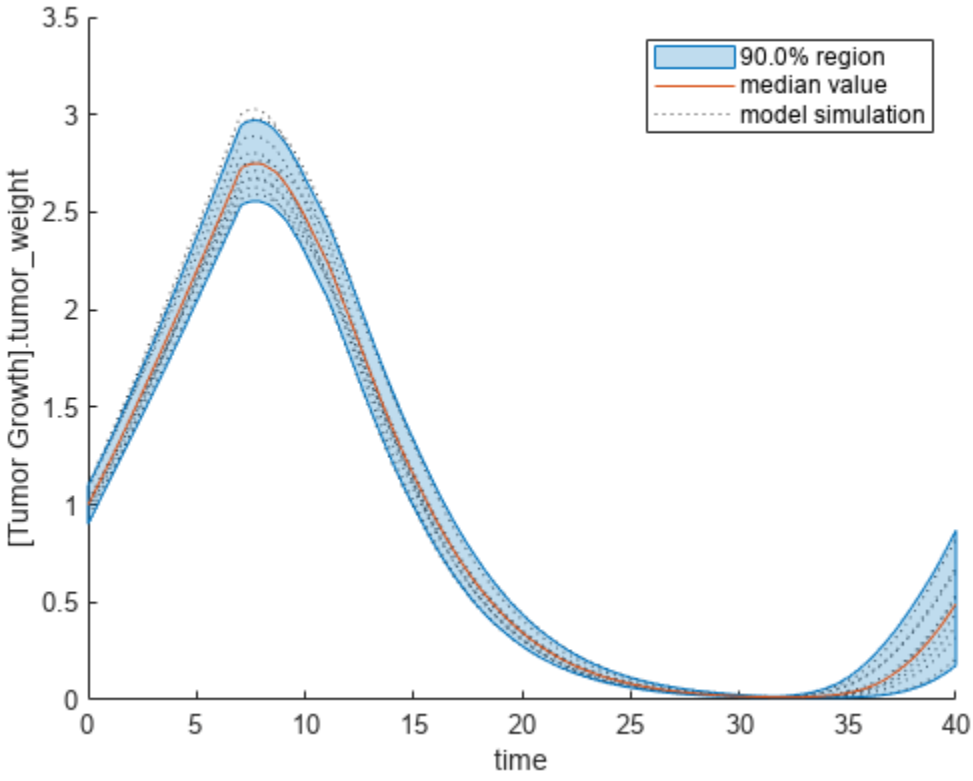
```
modelParamNames = {'L0','L1','w0','k1'};
outputName = 'tumor_weight';
```

Then perform GSA by computing the elementary effects using `sbioelementaryeffects`. Use `100` as the number of samples and set `ShowWaitBar` to `true` to show the simulation progress.

```
rng('default');
eeResults = sbioelementaryeffects(m1,modelParamNames,outputName,Variants=v,Doses=d,NumberSamples=
```

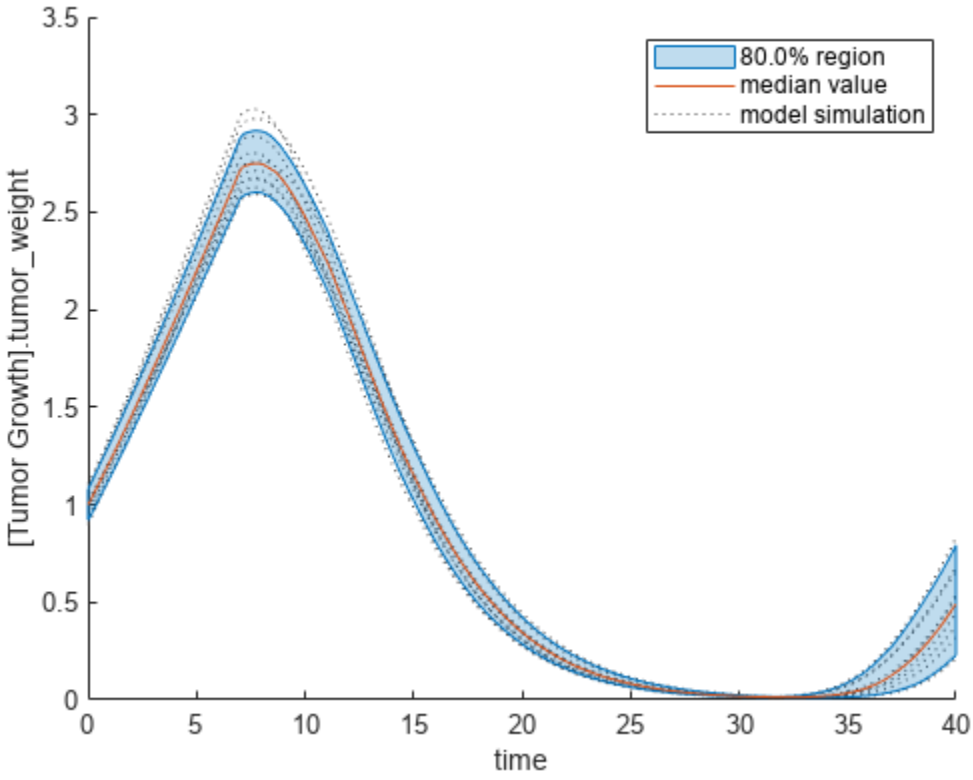
Show the median model response, the simulation results, and a shaded region covering 90% of the simulation results.

```
plotData(eeResults,ShowMedian=true,ShowMean=false);
```



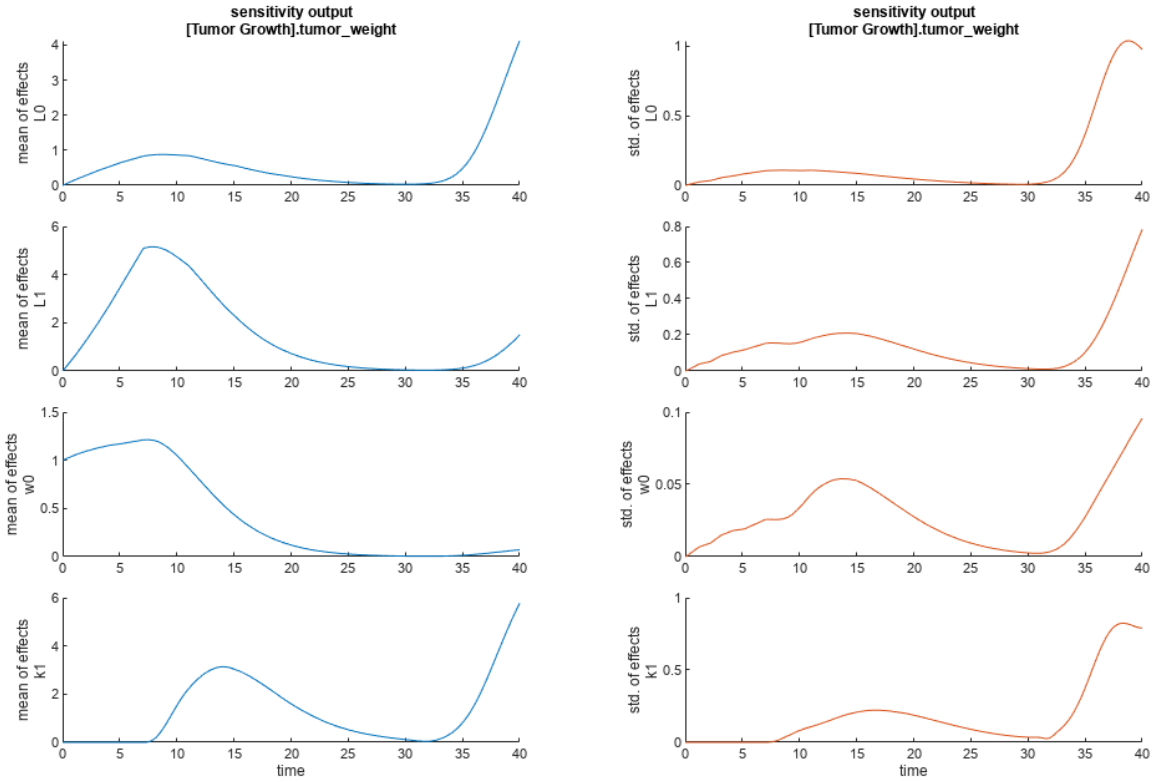
You can adjust the quantile region to a different percentage by specifying `Alphas` for the lower and upper quantiles of all model responses. For instance, an `alpha` value of 0.1 plots a shaded region between the `100*alpha` and `100*(1-alpha)` quantiles of all simulated model responses.

```
plotData(eeResults,Alphas=0.1,ShowMedian=true,ShowMean=false);
```



Plot the time course of the means and standard deviations of the elementary effects.

```
h = plot(eeResults);
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```

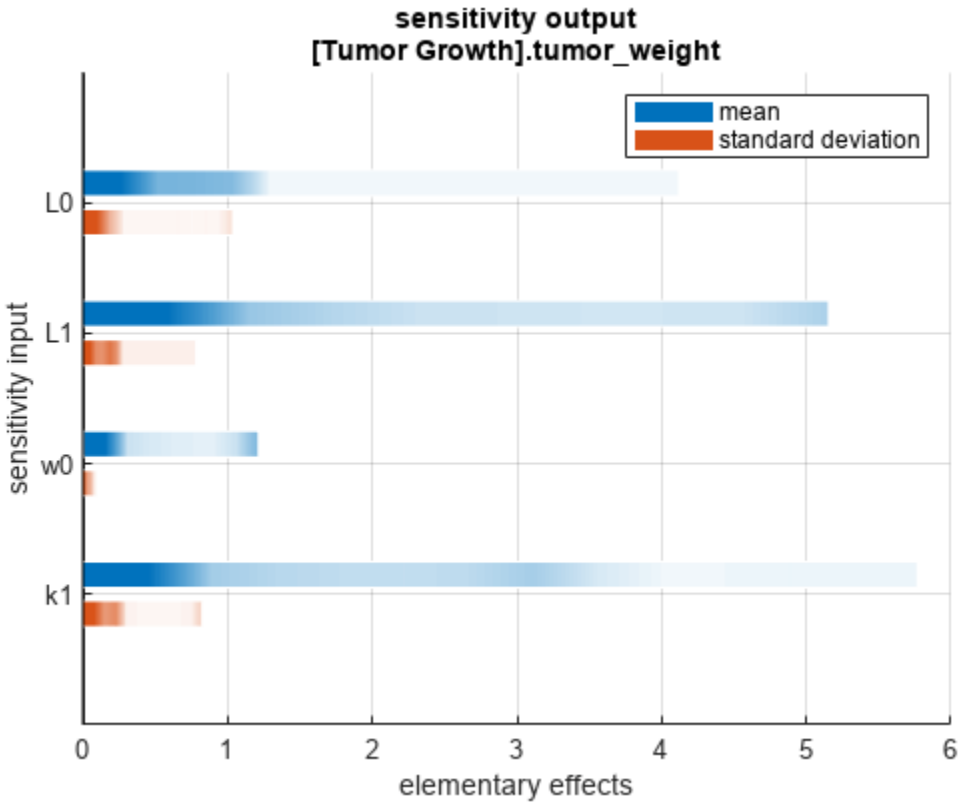


The mean of effects explains whether variations in input parameter values have any effect on the tumor weight response. The standard deviation of effects explains whether the sensitivity change is dependent on the location in the parameter domain.

From the mean of effects plots, parameters `L1` and `w0` seem to be the most sensitive parameters to the tumor weight before the dose is applied at t = 7. But, after the dose is applied, `k1` and `L0` become more sensitive parameters and contribute most to the after-dosing stage of the tumor weight. The plots of standard deviation of effects show more deviations for the larger parameter values in the later stage (t > 35) than for the before-dose stage of the tumor growth.

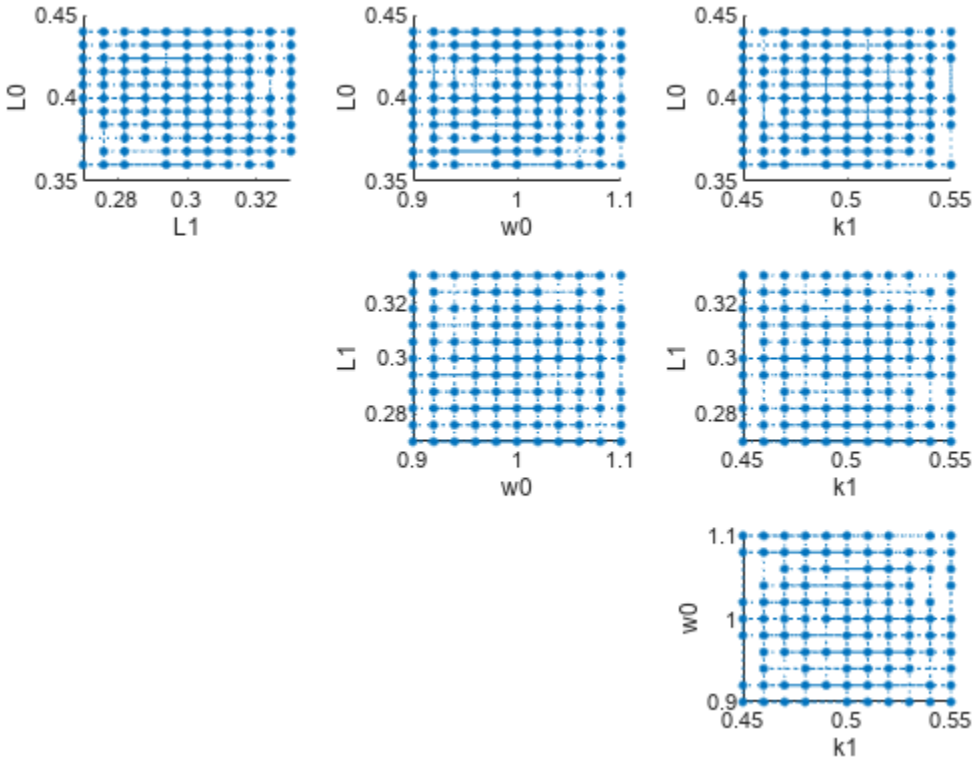
You can also display the magnitudes of the sensitivities in a bar plot. Each color shading represents a histogram representing values at different times. Darker colors mean that those values occur more often over the whole time course.

```
bar(eeResults);
```



You can also plot the parameter grids and samples used to compute the elementary effects.

```
plotGrid(eeResults)
```



You can specify more samples to increase the accuracy of the elementary effects, but the simulation can take longer to finish. Use `addsamples` to add more samples.

```
eeResults2 = addsamples(eeResults,200);
```

The `SimulationInfo` property of the result object contains various information for computing the elementary effects. For instance, the model simulation data (SimData) for each simulation using a set of parameter samples is stored in the `SimData` field of the property. This field is an array of `SimData` objects.

```
eeResults2.SimulationInfo.SimData
```

```
SimBiology SimData Array : 1500-by-1

Index:    Name:         ModelName:         DataCount:
1           -           Tumor Growth Model 1
2           -           Tumor Growth Model 1
3           -           Tumor Growth Model 1
...
1500        -           Tumor Growth Model 1
```

You can find out if any model simulation failed during the computation by checking the `ValidSample` field of `SimulationInfo`. In this example, the field shows no failed simulation runs.

```
all(eeResults2.SimulationInfo.ValidSample)
```

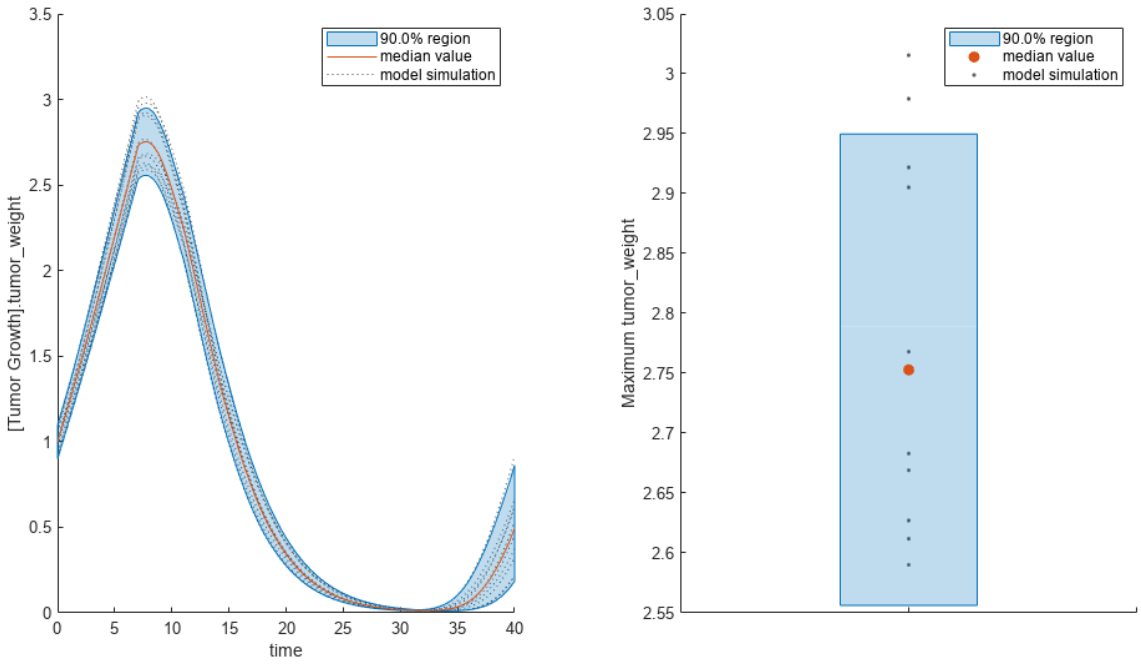
```
ans = logical
   1
```

You can add custom expressions as observables and compute the elementary effects of the added observables. For example, you can compute the effects for the maximum tumor weight by defining a custom expression as follows.

```
% Suppress an information warning that is issued.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
% Add the observable expression.
eeObs = addobservable(eeResults2,'Maximum tumor_weight','max(tumor_weight)','Units','gram');
```

Plot the computed simulation results showing the 90% quantile region.

```
h2 = plotData(eeObs,ShowMedian=true,ShowMean=false);
h2.Position(:) = [100 100 1500 800];
```



You can also remove the observable by specifying its name.

```
eeNoObs = removeobservable(eeObs,'Maximum tumor_weight');
```

Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

gsaObj — Results from global sensitivity analysis

`SimBiology.gsa.Sobol` object | `SimBiology.gsa.ElementaryEffects` object

Results from global sensitivity analysis, specified as a `SimBiology.gsa.Sobol` or `SimBiology.gsa.ElementaryEffects` object.

`numSamples` — Number of new samples
positive integer

Number of new samples to add, specified a positive integer.

Data Types: `double`

`tf` — Flag to show simulation progress
false (default) | true

Flag to show the simulation progress graphically, specified as `true` or `false`.

Data Types: `logical`

Output Arguments

`results` — Computed Sobol indices or elementary effects
`SimBiology.gsa.Sobol` | `SimBiology.gsa.ElementaryEffects`

Computed Sobol indices or elementary effects after adding more samples, returned as a `SimBiology.gsa.Sobol` or `SimBiology.gsa.ElementaryEffects` object.

Version History

Introduced in R2020a

References

[1] Saltelli, Andrea, Paola Annoni, Ivano Azzini, Francesca Campolongo, Marco Ratto, and Stefano Tarantola. “Variance Based Sensitivity Analysis of Model Output. Design and Estimator for the Total Sensitivity Index.” *Computer Physics Communications* 181, no. 2 (February 2010): 259–70. https://doi.org/10.1016/j.cpc.2009.09.018.

[2] Morris, Max D. “Factorial Sampling Plans for Preliminary Computational Experiments.” *Technometrics* 33, no. 2 (May 1991): 161–74.

[3] Sohier, Henri, Jean-Loup Farges, and Helene Piet-Lahanier. “Improvement of the Representativity of the Morris Method for Air-Launch-to-Orbit Separation.” *IFAC Proceedings Volumes* 47, no. 3 (2014): 7954–59.

See Also

`SimBiology.gsa.Sobol` | `SimBiology.gsa.ElementaryEffects` | `sbioelementaryeffects`

Topics
“Sensitivity Analysis in SimBiology”

addspecies (model, compartment)

Create species object and add to compartment object within model object

Syntax

```
speciesObj = addspecies(compObj, 'NameValue')
speciesObj = addspecies(compObj, 'NameValue', InitialAmountValue)
speciesObj = addspecies(modelObj, 'NameValue')
speciesObj = addspecies(modelObj, 'NameValue', InitialAmountValue)

speciesObj = addspecies(...'PropertyName', PropertyValue...)
```

Arguments

compObj	`Compartment object`.
modelObj	`Model object` containing zero or one compartment.
NameValue	Name for a species object. Enter a character vector unique among species within *modelObj* or *compObj*. Species objects are identified by name within the `Event`, `ReactionRate`, and `Rule` properties. For information on naming species, see Name. You can use the function `sbioselect on page 1-245` to find an object with a specific `Name` property value.
InitialAmountValue	Initial amount value for the species object. Enter `double`. Positive real number, default is `0`.
PropertyName	Enter the name of a valid property. Valid property names are listed in “Property Summary” on page 2-110.
PropertyValue	Enter the value for the property specified in *PropertyName*. Valid property values are listed on each property reference page.

Description

speciesObj = addspecies(*compObj*, '*NameValue*') creates `speciesObj`, a species object, and adds it to *compObj*, a compartment object. In the species object, this method assigns *NameValue* to the `Name` property, assigns *compObj* to the `Parent` property, and assigns `0` to the `InitialAmount` property. In the compartment object, this method adds the species object to the `Species` property.

speciesObj = addspecies(*compObj*, '*NameValue*', *InitialAmountValue*), in addition to the above, assigns *InitialAmountValue* to the `InitialAmount` property for the species object.

speciesObj = addspecies(*modelObj*, '*NameValue*') creates `speciesObj`, a species object, and adds it to *compObj*, the compartment object in *modelObj*, a `Model object`. If *modelObj* does not contain any compartments, it creates *compObj* with a `Name` property of `'unnamed'`. In the species object, this method assigns *NameValue* to the `Name` property, assigns *compObj* to the

`Parent` property, and assigns `0` to the `InitialAmount` property. In the compartment object, this method adds the species object to the `Species` property.

`speciesObj` `= addspecies(`*`modelObj`*`, '`*`NameValue`*`', `*`InitialAmountValue`*`)`, in addition to the above, assigns *`InitialAmountValue`* to the `InitialAmount` property for the species object.

You can also add a species to a reaction using the methods `addreactant on page 2-82` and `addproduct on page 2-80`.

A species object must have a unique name at the level at which it is created. For example, a compartment object cannot contain two species objects named `H2O`. However, another compartment can have a species named `H2O`.

View properties for a species object with the `get` command, and modify properties for a species object with the `set` command. You can view a summary table of species objects in a compartment (`compObj`) with `get(compObj, 'Species')` or the properties of the first species with `get(compObj.Species(1))`.

`speciesObj` `= addspecies(...'`*`PropertyName`*`', `*`PropertyValue`*`...)` defines optional properties. The property name/property value pairs can be in any format supported by the function `set` (for example, name-value pairs, structures, and name-value cell array pairs). The property summary on this page shows the list of properties.

If there is more than one compartment object (`compObj`) in the model, you must qualify the species name with the compartment name. For example, `cell.glucose` denotes that you want to put the species named `glucose` into a compartment named `cell`. Additionally, if the compartment named `cell` does not exist, the process of adding the reaction creates the compartment and names it `cell`.

If you change the name of a species you must configure all applicable elements, such as events and rules that use the species, any user-specified ReactionRate, or the kinetic law object property SpeciesVariableNames. Use the method `setspecies` to configure `SpeciesVariableNames`.

To update species names in the SimBiology graphical user interface, access each appropriate pane through the **Project Explorer**. You can also use the **Find** feature to locate the names that you want to update. The **Output** pane opens with the results of **Find**. Double-click a result row to go to the location of the model component.

Species names are automatically updated for reactions that use `MassAction` kinetic law.

Method Summary

Methods for species objects

copyobj	Copy SimBiology object and its children
delete	Delete SimBiology object
display	Display summary of SimBiology object
findUsages	Find out how a species, parameter, or compartment is used in a model
get	Get SimBiology object properties
move	Move SimBiology species or parameter object to new parent
rename	Rename object and update expressions
set	Set SimBiology object properties

Property Summary

Properties for species objects

BoundaryCondition	Indicate species boundary condition
Constant	Specify variable or constant species amount, parameter value, or compartment capacity
ConstantAmount	Specify variable or constant species amount
InitialAmount	Species initial amount
InitialAmountUnits	Species initial amount units
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Tag	Specify label for SimBiology object
Type	Display SimBiology object type
Units	Units for species amount, parameter value, compartment capacity, observable expression
UserData	Specify data to associate with object
Value	Value of species, compartment, or parameter object

Examples

Add two species to a model, where one is a reactant and the other is the enzyme catalyzing the reaction.

1 Create a model object named `my_model` and add a compartment object.

```
modelObj = sbiomodel ('my_model');
compObj = addcompartment(modelObj, 'comp1');
```

2 Add two species objects named `glucose_6_phosphate` and `glucose_6_phosphate_dehydrogenase`.

```
speciesObj1 = addspecies (compObj, 'glucose_6_phosphate');
speciesObj2 = addspecies (compObj, ...
                          'glucose_6_phosphate_dehydrogenase');
```

3 Set the initial amount of `glucose_6_phosphate` to `100` and verify.

```
set (speciesObj1, 'InitialAmount',100);
get (speciesObj1, 'InitialAmount')
```

MATLAB returns:

```
ans =

   100
```

4 Use `get` to note that `modelObj` contains the species object array.

```
get(compObj, 'Species')
```

MATLAB returns:

```
SimBiology Species Array

Index: Name:                           InitialAmount: InitialAmountUnits:
 1     glucose_6_phosphate              100
 2     glucose_6_phosphate_dehydrogenase  0
```

5 Retrieve information about the first species in the array.

```
get(compObj.Species(1))
            Annotation: ''
     BoundaryCondition: 0
        ConstantAmount: 0
         InitialAmount: 100
    InitialAmountUnits: ''
                  Name: 'glucose_6_phosphate'
                 Notes: ''
                Parent: [1x1 SimBiology.Compartment]
                   Tag: ''
                  Type: 'species'
              UserData: []
```

Version History

Introduced in R2006a

R2022b: Having duplicate model component names issues a warning

Warns starting in R2022b

- SimBiology issues a warning if multiple model components (model, compartment, species, parameter, reaction, rule, event, observable, dose, and variant) have the same name. In a future release, within a single model, these components will be required to have unique names even when they are of different types with the following two exceptions:

  - Species in different compartments can have the same name.
  - Parameters can have the same name if they are scoped to different parents. Specifically, you can use the same name for a model-scoped parameter and reaction-scoped parameters, where each reaction-scoped parameter belongs to a different reaction.

  The purpose of this naming restriction is to ensure that every model component can be unambiguously referenced by its unique name within a model. For details on how to reference model component names in expressions, see “Guidelines for Referencing Names in Expressions”.

- To disambiguate duplicate names from your model, use the `updateDuplicateNames` function at the command line. The function takes in a SimBiology model as an input and updates the

component names as necessary. You can also specify optional outputs, such as a logical flag to check whether any update occurred, a list of model changes, and a copy of the original model before any updates were made.

- The `updateDuplicateNames` function disambiguates the duplicate names by adding a suffix `"_N"`, where *N* is the first positive integer that results in a unique name. If there is an existing suffix, *N* will be incremented from that suffix. For example, if there are two model components named *x_3*, the function updates one of the names to *x_4*. If the existing suffix has leading zeros, the function omits the zeros in the new name. For instance, if *x_003* is a duplicate name, it gets renamed to *x_4*. However, the function assumes that names with leading zeros and without leading zeros are different. For instance, *x_005* and *x_5* are considered to be different names.

R2022a: Having duplicate model component names will not be allowed in a future release
Behavior change in future release

SimBiology will not allow you to have duplicate names for model components within a model.

See Also

`Model object` | `Compartment object` | `addcompartment` | `addproduct` | `addreactant` | `addreaction`

addvariant (model)

Add variant to model

Syntax

```
variantObj = addvariant(modelObj, 'NameValue')
variantObj2 = addvariant(modelObj, variantObj)
```

Arguments

modelObj	Specify the `Model object` to which you want add a variant.
variantObj	`Variant object` to create and add to the model object.
NameValue	Name of the variant object. *NameValue* is assigned to the `Name` property of the variant object.

Description

variantObj = `addvariant(`*modelObj*`, '`*NameValue*`')` creates a SimBiology variant object (*variantObj*) with the name *NameValue* and adds the variant object to the SimBiology `Model object` *modelObj*. The variant object `Parent` property is assigned the value of *modelObj*.

A SimBiology variant object stores alternate values for properties on a SimBiology model. For more information on variants, see `Variant object`.

variantObj2 = `addvariant(`*modelObj*`, `*variantObj*`)` adds a SimBiology variant object (*variantObj*) to the SimBiology model object and returns another variant object *variantObj2*. The variant object *variantObj2* `Parent` property is assigned the value of *modelObj*. The `Active` property of *variantObj2* is set to `false` by default.

View properties for a variant object with the `get` command, and modify properties for a variant object with the `set` command.

Note

- Remember to use the `addcontent` method instead of using the `set` method on the `Content` property, because the `set` method replaces the data in the `Content` property, whereas `addcontent` appends the data.
- When there are multiple active variant objects on a model, if there are duplicate specifications for a property's value, the last occurrence for the property value in the array of variants, is used during simulation.

To view the variants stored on a model object, use the `getvariant` method. To copy a variant object to another model, use `copyobj`. To remove a variant object from a SimBiology model, use the `delete` method.

Examples

1. Create a model containing one species.

```
modelObj = sbiomodel('mymodel');
compObj = addcompartment(modelObj, 'comp1');
speciesObj = addspecies(compObj, 'A');
```

2. Add a variant object that varies the `InitialAmount` property of a species named A.

```
variantObj = addvariant(modelObj, 'v1');
addcontent(variantObj, {'species', 'A', 'InitialAmount', 5});
```

Version History

Introduced in R2007b

R2022b: Having duplicate model component names issues a warning

Warns starting in R2022b

- SimBiology issues a warning if multiple model components (model, compartment, species, parameter, reaction, rule, event, observable, dose, and variant) have the same name. In a future release, within a single model, these components will be required to have unique names even when they are of different types with the following two exceptions:
  - Species in different compartments can have the same name.
  - Parameters can have the same name if they are scoped to different parents. Specifically, you can use the same name for a model-scoped parameter and reaction-scoped parameters, where each reaction-scoped parameter belongs to a different reaction.

  The purpose of this naming restriction is to ensure that every model component can be unambiguously referenced by its unique name within a model. For details on how to reference model component names in expressions, see “Guidelines for Referencing Names in Expressions”.
- To disambiguate duplicate names from your model, use the `updateDuplicateNames` function at the command line. The function takes in a SimBiology model as an input and updates the component names as necessary. You can also specify optional outputs, such as a logical flag to check whether any update occurred, a list of model changes, and a copy of the original model before any updates were made.
- The `updateDuplicateNames` function disambiguates the duplicate names by adding a suffix `"_N"`, where *N* is the first positive integer that results in a unique name. If there is an existing suffix, *N* will be incremented from that suffix. For example, if there are two model components named *x_3*, the function updates one of the names to *x_4*. If the existing suffix has leading zeros, the function omits the zeros in the new name. For instance, if *x_003* is a duplicate name, it gets renamed to *x_4*. However, the function assumes that names with leading zeros and without leading zeros are different. For instance, *x_005* and *x_5* are considered to be different names.

R2022a: Having duplicate model component names will not be allowed in a future release

Behavior change in future release

SimBiology will not allow you to have duplicate names for model components within a model.

See Also

`Model object` | `Variant object` | `addcontent` | `commit` | `copyobj` | `delete` | `getvariant`

bar

Create bar plot of multiparametric global sensitivity analysis statistics

Syntax

```
h = bar(mpgsaObj)
h = bar(mpgsaObj,Name,Value)
```

Description

`h = bar(mpgsaObj)` creates a bar plot of the Kolmogorov-Smirnov statistic (Statistics and Machine Learning Toolbox) (K-S statistic) from multiparametric global sensitivity analysis (MPGSA) and returns the figure handle `h`.

- The function plots `o` for each input parameter if all of its parameter samples are classified in one category (accepted or rejected).
- The function plots `x` for negligible p-values smaller than 0.001.
- The function plots two solid vertical lines at x = 0 and x = 1 as limiting reference lines because K-S statistic values are always between 0 and 1.

`h = bar(mpgsaObj,Name,Value)` uses additional options specified by one or more name-value pair arguments.

Examples

Perform Multiparametric Global Sensitivity Analysis (MPGSA)

Load the “Target-Mediated Drug Disposition (TMDD) Model”.

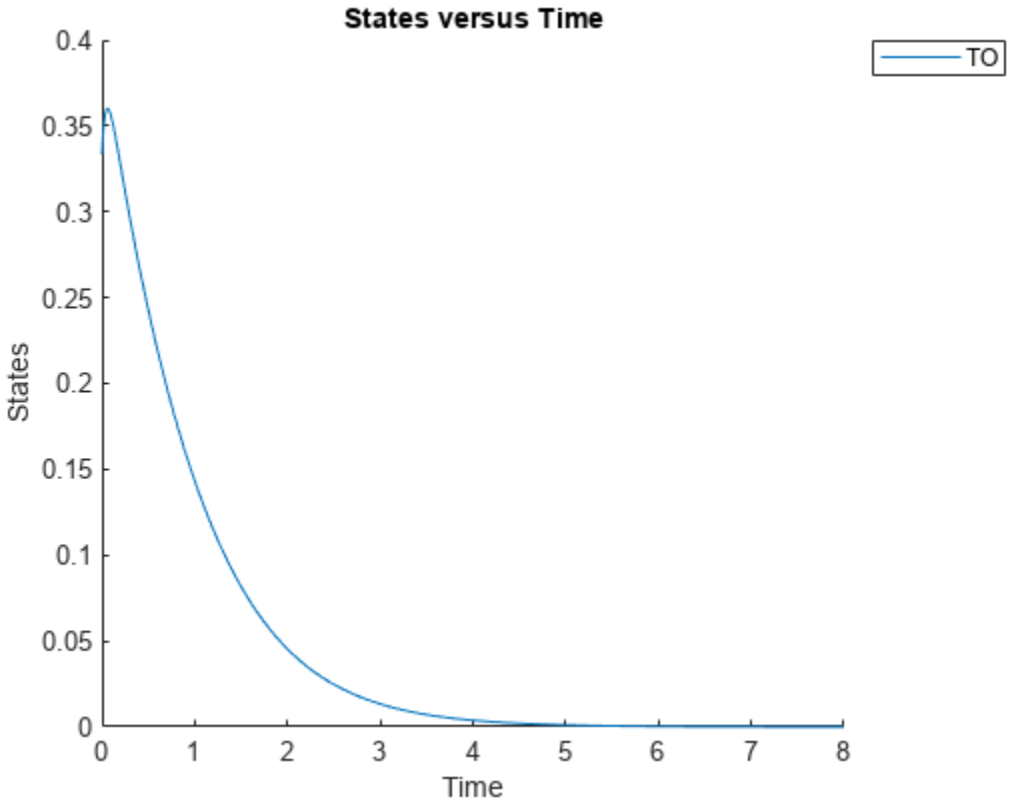
```
sbioloadproject tmdd_with_T0.sbproj
```

Get the active configset and set the target occupancy (`T0`) as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'T0';
```

Simulate the model and plot the `T0` profile.

```
sbioplot(sbiosimulate(m1,cs));
```



Define an exposure (area under the curve of the TO profile) threshold for the target occupancy.

```
classifier = 'trapz(time,TO) <= 0.1';
```

Perform MPGSA to find sensitive parameters with respect to the TO. Vary the parameter values between predefined bounds to generate 10,000 parameter samples.

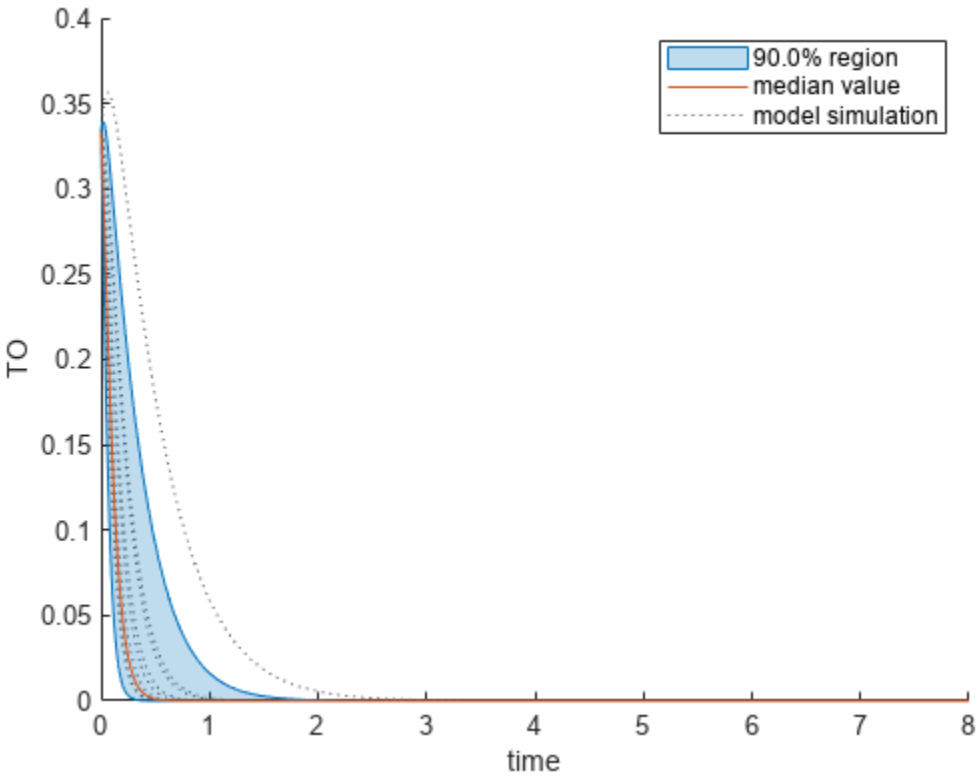
```
% Suppress an information warning that is issued during simulation.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
rng(0,'twister'); % For reproducibility
params = {'kel','ksyn','kdeg','km'};
bounds = [0.1, 1;
          0.1, 1;
          0.1, 1;
          0.1, 1];
mpgsaResults = sbiompgsa(m1,params,classifier,Bounds=bounds,NumberSamples=10000)
```

```
mpgsaResults =
  MPGSA with properties:

                  Classifiers: {'trapz(time,TO) <= 0.1'}
    KolmogorovSmirnovStatistics: [4x1 table]
                    ECDFData: {4x4 cell}
             SignificanceLevel: 0.0500
                      PValues: [4x1 table]
             SupportHypothesis: [10000x1 table]
              ParameterSamples: [10000x4 table]
                   Observables: {'TO'}
```

```
    SimulationInfo: [1x1 struct]
```

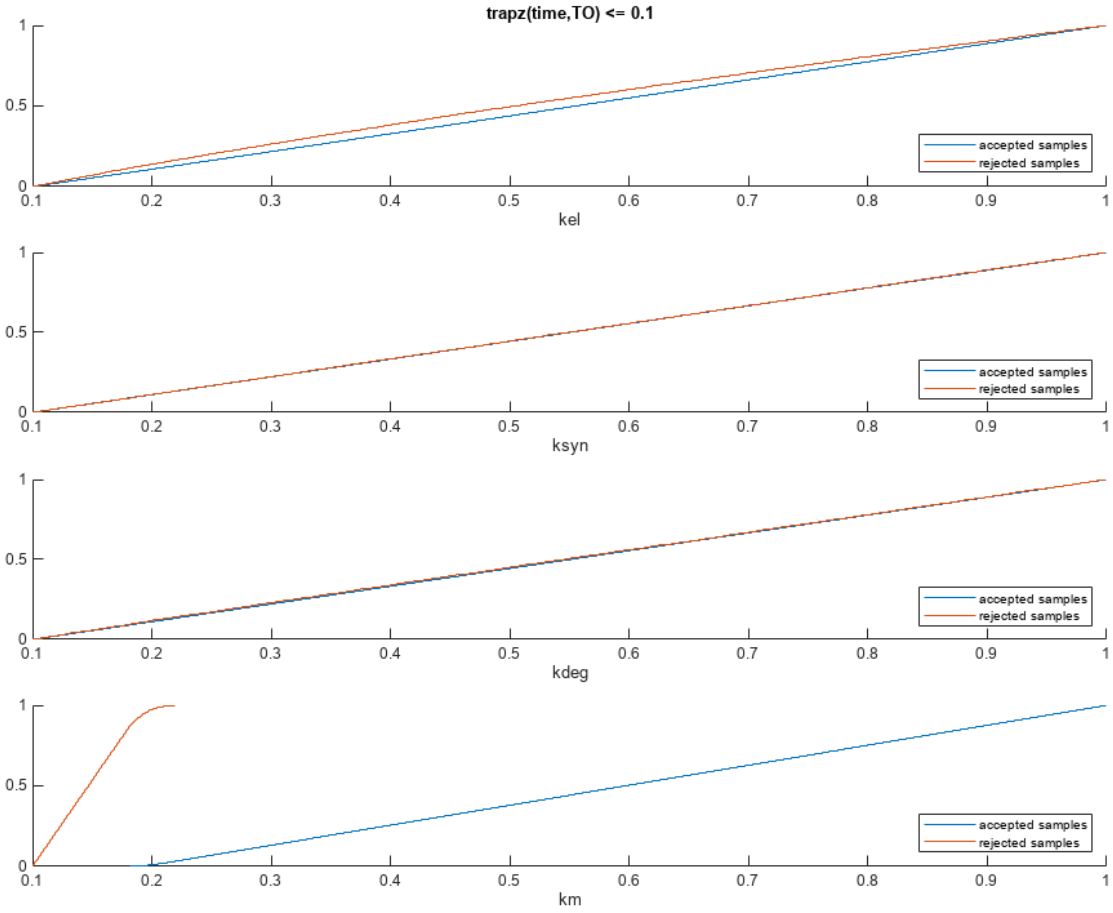
Plot the quantiles of the simulated model response.

```
plotData(mpgsaResults,ShowMedian=true,ShowMean=false);
```



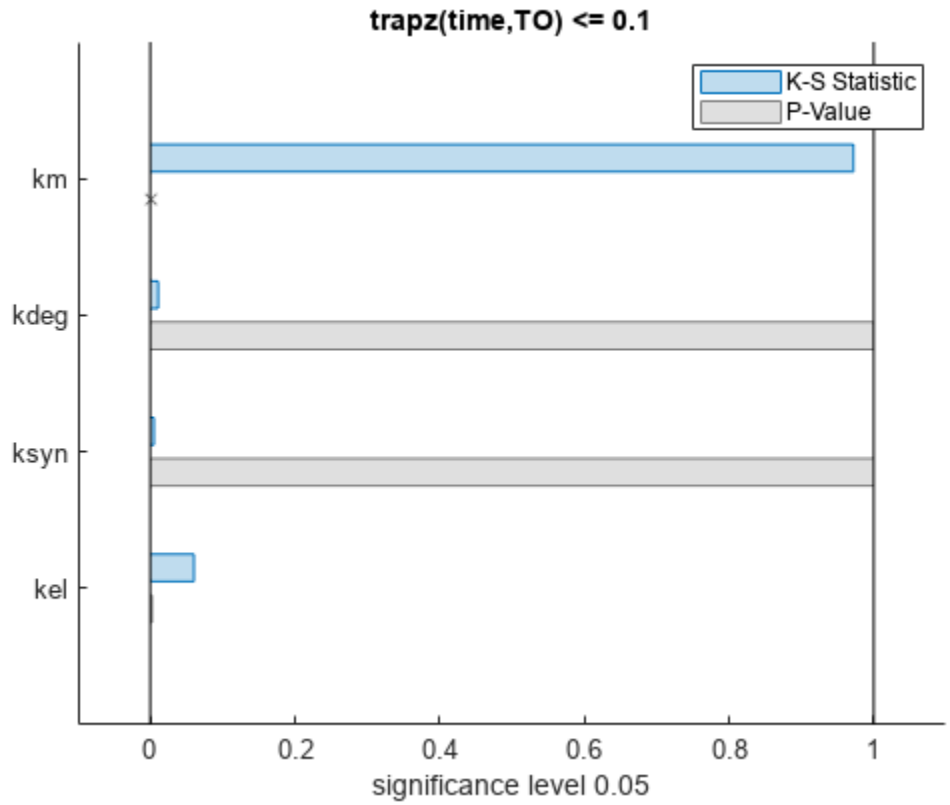
Plot the empirical cumulative distribution functions (eCDFs) of the accepted and rejected samples. Except for `km`, none of the parameters shows a significant difference in the eCDFs for the accepted and rejected samples. The `km` plot shows a large Kolmogorov-Smirnov (K-S) distance between the eCDFs of the accepted and rejected samples. The K-S distance is the maximum absolute distance between two eCDFs curves.

```
h = plot(mpgsaResults);
% Resize the figure.
pos = h.Position(:);
h.Position(:) = [pos(1) pos(2) pos(3)*2 pos(4)*2];
```



To compute the K-S distance between the two eCDFs, SimBiology uses a two-sided test based on the null hypothesis that the two distributions of accepted and rejected samples are equal. See `kstest2` (Statistics and Machine Learning Toolbox) for details. If the K-S distance is large, then the two distributions are different, meaning that the classification of the samples is sensitive to variations in the input parameter. On the other hand, if the K-S distance is small, then variations in the input parameter do not affect the classification of samples. The results suggest that the classification is insensitive to the input parameter. To assess the significance of the K-S statistic rejecting the null-hypothesis, you can examine the p-values.

```
bar(mpgsaResults)
```



The bar plot shows two bars for each parameter: one for the K-S distance (K-S statistic) and another for the corresponding p-value. You reject the null hypothesis if the p-value is less than the significance level. A cross (`x`) is shown for any p-value that is almost 0. You can see the exact p-value corresponding to each parameter.

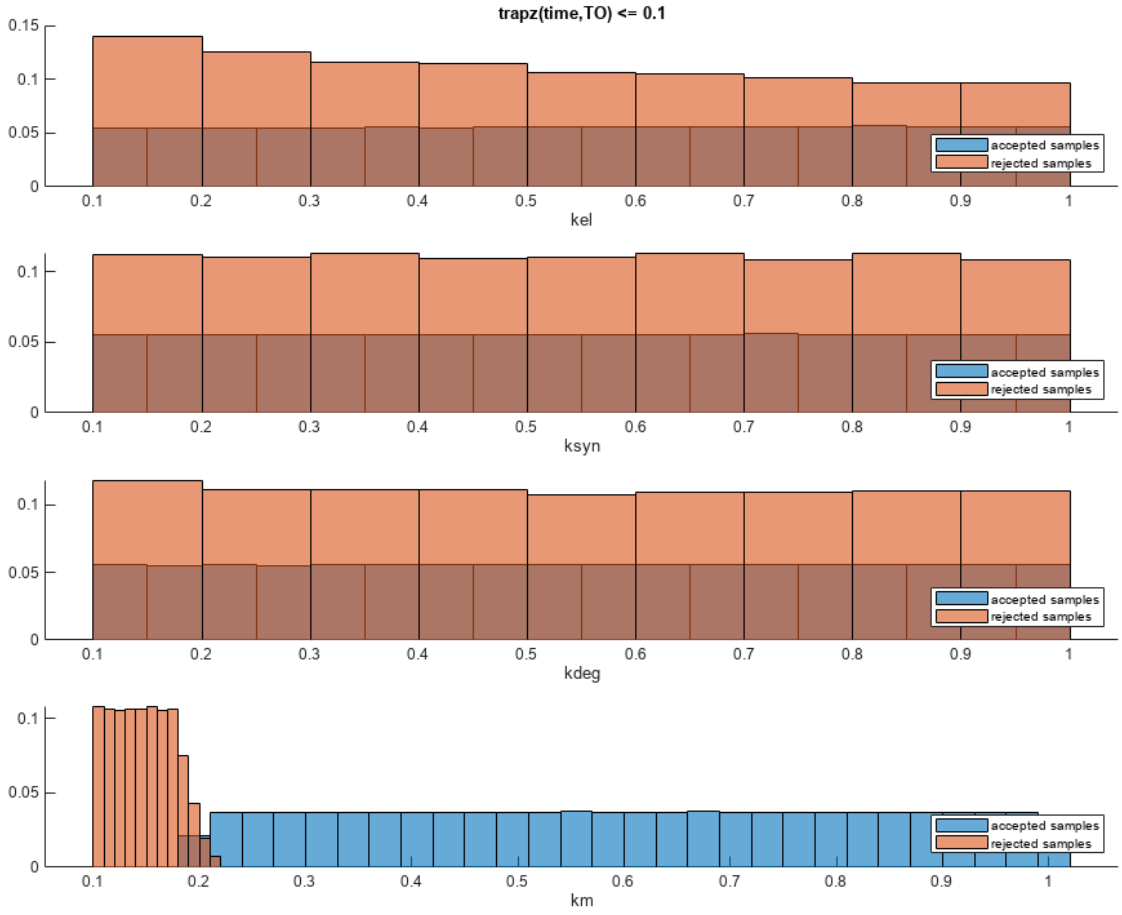
```
[mpgsaResults.ParameterSamples.Properties.VariableNames',mpgsaResults.PValues]
```

```
ans=4×2 table
      Var1      trapz(time,TO) <= 0.1
    ________    _____________________

    {'kel' }          0.0021877
    {'ksyn'}                  1
    {'kdeg'}            0.99983
    {'km'  }                  0
```

The p-values of `km` and `kel` are less than the significance level (0.05), supporting the alternative hypothesis that the accepted and rejected samples come from different distributions. In other words, the classification of the samples is sensitive to `km` and `kel` but not to other parameters (`kdeg` and `ksyn`).

You can also plot the histograms of accepted and rejected samples. The historgrams let you see trends in the accepted and rejected samples. In this example, the histogram of `km` shows that there are more accepted samples for larger `km` values, while the `kel` histogram shows that there are fewer rejected samples as `kel` increases.

```
h2 = histogram(mpgsaResults);
% Resize the figure.
pos = h2.Position(:);
h2.Position(:) = [pos(1) pos(2) pos(3)*2 pos(4)*2];
```



Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

`mpgsaObj` — Multiparametric global sensitivity analysis results

`SimBiology.gsa.MPGSA` object

Multiparametric global sensitivity analysis results, specified as a `SimBiology.gsa.MPGSA` object.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `h = bar(results,'Classifier',1)` specifies to create a bar plot of the MPGSA results of the first classifier.

`Parameters` — Input model quantities to plot

character vector | string | string vector | cell array of character vectors | vector of positive integers

Input model quantities, namely parameters, species, or compartments, to plot, specified as a character vector, string, string vector, cell array of character vectors, or a vector of positive integers indexing into the columns of the `mpgsaObj.ParameterSamples` table.

Example: `'Parameters','k1'`

Data Types: `double` | `char` | `string` | `cell`

`Classifiers` — Classifiers to plot

character vector | string | string vector | cell array of character vectors | vector of positive integers

Classifiers to plot, specified as a character vector, string, string vector, cell array of character vectors, or a vector of positive integers.

Specify the expressions of classifiers to plot as a character vector, string, string vector, cell array of character vectors. Alternatively, you can specify a vector of positive integers indexing into `mpgsaObj.Classifiers`.

Example: `'Classifiers',[1 3]`

Data Types: `double` | `char` | `string` | `cell`

`Color` — Color of Kolmogorov-Smirnov statistic

three-element row vector | hexadecimal color code | color name

Color of Kolmogorov-Smirnov statistic (K-S Statistic), specified as a three-element row vector, hexadecimal color code, color name, or a short name. By default, the function uses the first MATLAB default color. To view the default color order, enter `get(groot,'defaultAxesColorOrder')` or see the “ColorOrder” property.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see “Specify Plot Colors”.

Example: `'Color',[0.4,0.3,0.2]`

Data Types: `double`

`PValueColor` — Color of p-values

`[0.5,0.5,0.5]` (default) | three-element row vector | hexadecimal color code | color name

Color of *p*-values, specified as a three-element row vector, hexadecimal color code, color name, or a short name. The default color is gray `[0.5,0.5,0.5]`.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see “Specify Plot Colors”.

Example: `'PValueColor',[0.4,0.3,0.2]`

Data Types: `double`

Output Arguments

h — Handle

figure handle

Handle to the figure, specified as a figure handle.

Version History

Introduced in R2020a

References

[1] Tiemann, Christian A., Joep Vanlier, Maaike H. Oosterveer, Albert K. Groen, Peter A. J. Hilbers, and Natal A. W. van Riel. “Parameter Trajectory Analysis to Identify Treatment Effects of Pharmacological Interventions.” Edited by Scott Markel. *PLoS Computational Biology* 9, no. 8 (August 1, 2013): e1003166. https://doi.org/10.1371/journal.pcbi.1003166.

See Also

`SimBiology.gsa.MPGSA` | `sbiompgsa` | `plotData` | `histogram` | `kstest2` | `ecdf`

bar

Plot magnitudes of means and standard deviations of elementary effects

Syntax

```
h = bar(eeObj)
h = bar(eeObj,Name=Value)
```

Description

`h = bar(eeObj)` plots the means and standard deviations of elementary effects as a bar graph and returns the figure handle `h`. The color shading of each bar represents a histogram representing values at different times. Darker colors mean that those values occur more often over the whole time course. The plot shows a single dot for scalar or constant model responses instead of a bar.

`h = bar(eeObj,Name=Value)` uses additional options specified by one or more name-value arguments.

Examples

Perform GSA by Computing Elementary Effects

Load the “Tumor Growth Model”.

```
sbioloadproject tumor_growth_vpop_sa.sbproj
```

Get a variant with estimated parameters and the dose to apply to the model.

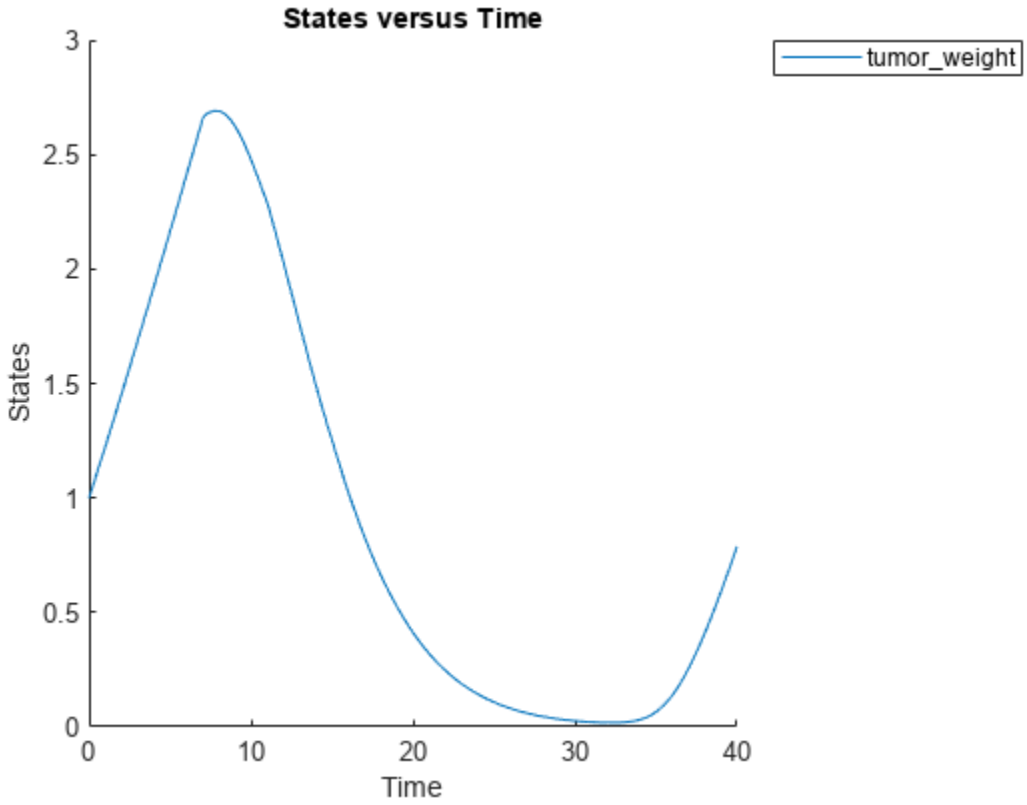
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

Get the active configset and set the tumor weight as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'tumor_weight';
```

Simulate the model and plot the tumor growth profile.

```
sbioplot(sbiosimulate(m1,cs,v,d));
```



Perform global sensitivity analysis (GSA) on the model to find the model parameters that the tumor growth is sensitive to.

First, define model parameters of interest, which are involved in the pharmacodynamics of the tumor growth. Define the model response as the tumor weight.

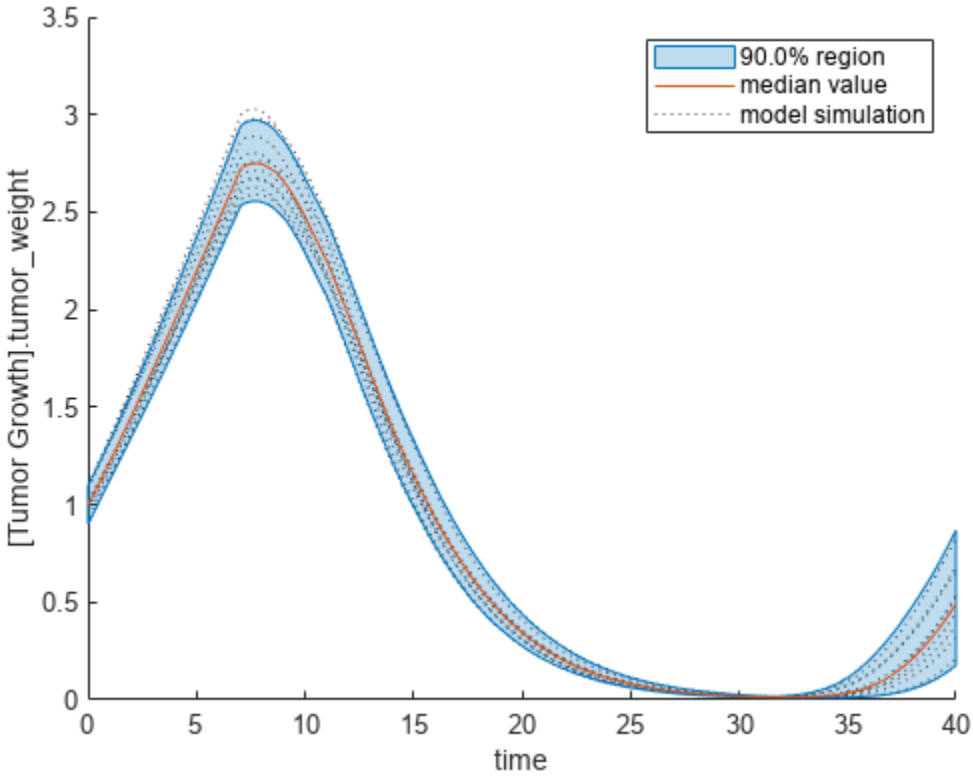
```
modelParamNames = {'L0','L1','w0','k1'};
outputName = 'tumor_weight';
```

Then perform GSA by computing the elementary effects using `sbioelementaryeffects`. Use `100` as the number of samples and set `ShowWaitBar` to `true` to show the simulation progress.

```
rng('default');
eeResults = sbioelementaryeffects(m1,modelParamNames,outputName,Variants=v,Doses=d,NumberSamples=
```

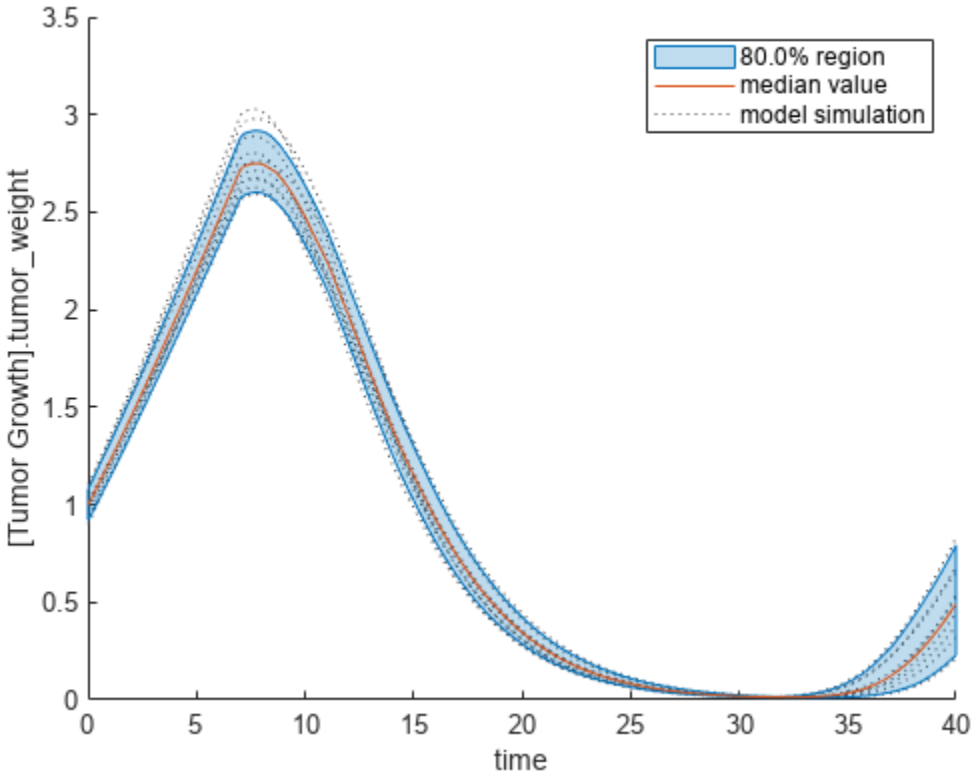
Show the median model response, the simulation results, and a shaded region covering 90% of the simulation results.

```
plotData(eeResults,ShowMedian=true,ShowMean=false);
```



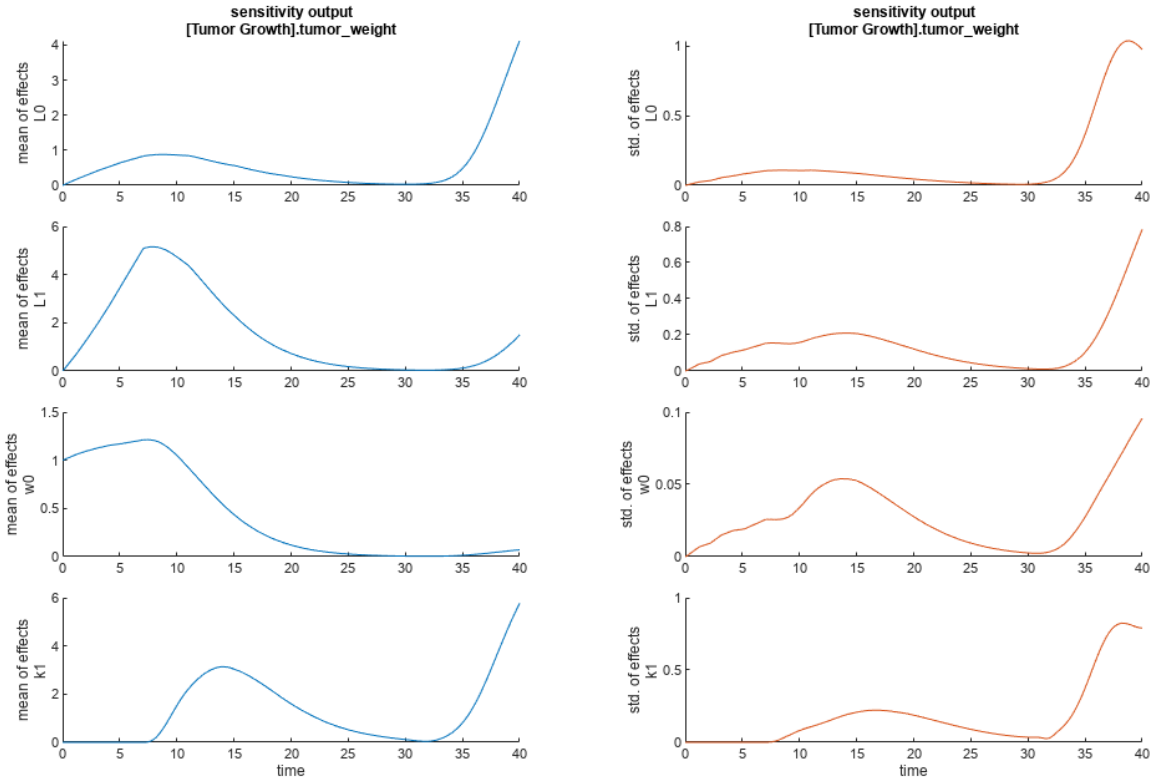
You can adjust the quantile region to a different percentage by specifying `Alphas` for the lower and upper quantiles of all model responses. For instance, an `alpha` value of 0.1 plots a shaded region between the `100*alpha` and `100*(1-alpha)` quantiles of all simulated model responses.

```
plotData(eeResults,Alphas=0.1,ShowMedian=true,ShowMean=false);
```



Plot the time course of the means and standard deviations of the elementary effects.

```
h = plot(eeResults);
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```

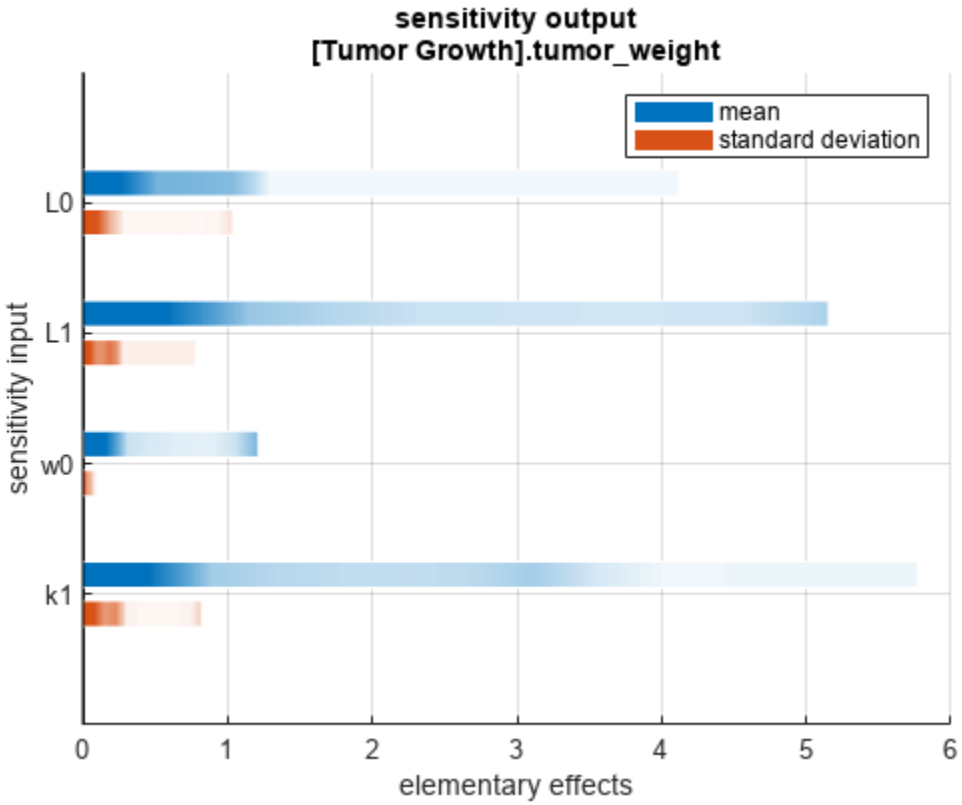


The mean of effects explains whether variations in input parameter values have any effect on the tumor weight response. The standard deviation of effects explains whether the sensitivity change is dependent on the location in the parameter domain.

From the mean of effects plots, parameters `L1` and `w0` seem to be the most sensitive parameters to the tumor weight before the dose is applied at t = 7. But, after the dose is applied, `k1` and `L0` become more sensitive parameters and contribute most to the after-dosing stage of the tumor weight. The plots of standard deviation of effects show more deviations for the larger parameter values in the later stage (t > 35) than for the before-dose stage of the tumor growth.

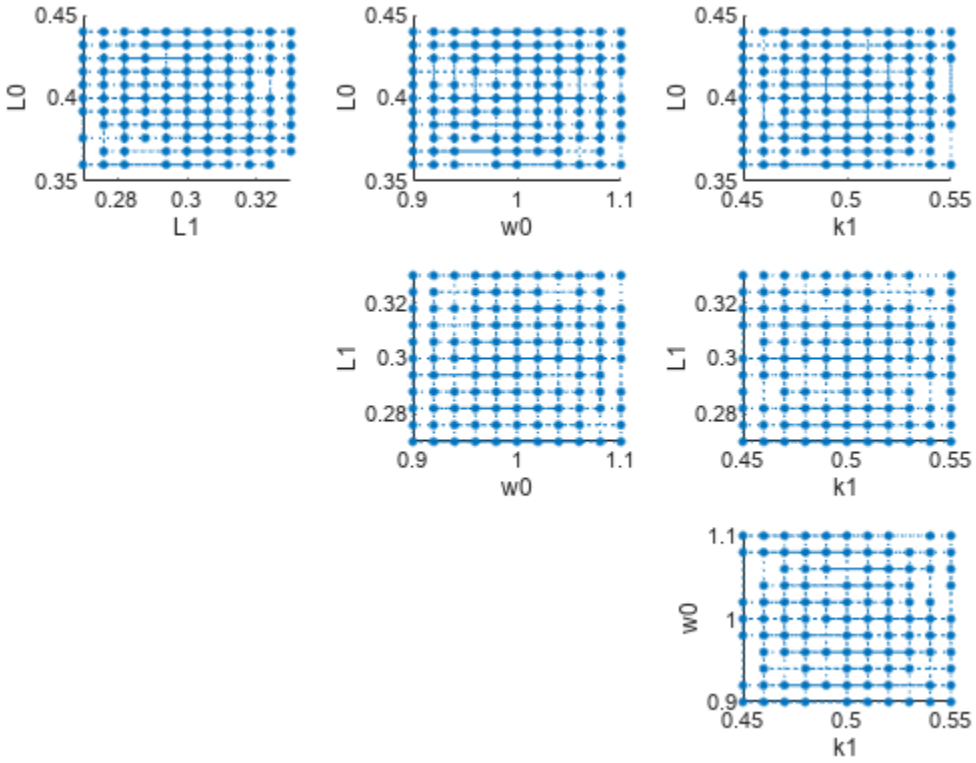
You can also display the magnitudes of the sensitivities in a bar plot. Each color shading represents a histogram representing values at different times. Darker colors mean that those values occur more often over the whole time course.

```
bar(eeResults);
```



You can also plot the parameter grids and samples used to compute the elementary effects.

```
plotGrid(eeResults)
```



You can specify more samples to increase the accuracy of the elementary effects, but the simulation can take longer to finish. Use `addsamples` to add more samples.

```
eeResults2 = addsamples(eeResults,200);
```

The `SimulationInfo` property of the result object contains various information for computing the elementary effects. For instance, the model simulation data (SimData) for each simulation using a set of parameter samples is stored in the `SimData` field of the property. This field is an array of `SimData` objects.

```
eeResults2.SimulationInfo.SimData
```

```
SimBiology SimData Array : 1500-by-1

Index:    Name:         ModelName:         DataCount:
1           -           Tumor Growth Model 1
2           -           Tumor Growth Model 1
3           -           Tumor Growth Model 1
...
1500        -           Tumor Growth Model 1
```

You can find out if any model simulation failed during the computation by checking the `ValidSample` field of `SimulationInfo`. In this example, the field shows no failed simulation runs.

```
all(eeResults2.SimulationInfo.ValidSample)
```

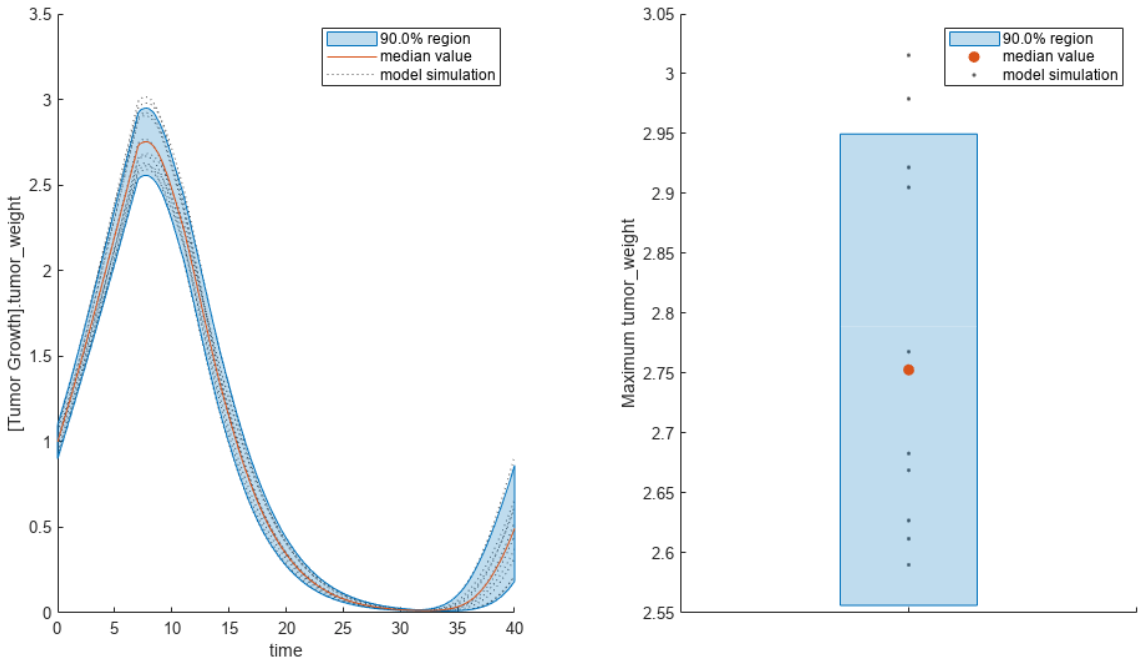
```
ans = logical
   1
```

You can add custom expressions as observables and compute the elementary effects of the added observables. For example, you can compute the effects for the maximum tumor weight by defining a custom expression as follows.

```
% Suppress an information warning that is issued.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
% Add the observable expression.
eeObs = addobservable(eeResults2,'Maximum tumor_weight','max(tumor_weight)','Units','gram');
```

Plot the computed simulation results showing the 90% quantile region.

```
h2 = plotData(eeObs,ShowMedian=true,ShowMean=false);
h2.Position(:) = [100 100 1500 800];
```



You can also remove the observable by specifying its name.

```
eeNoObs = removeobservable(eeObs,'Maximum tumor_weight');
```

Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

eeObj — Results containing means and standard deviations of elementary effects

`SimBiology.gsa.ElementaryEffects` object

Results containing the means and standard deviations of elementary effects, specified as a `SimBiology.gsa.ElementaryEffects` object.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Example: `h = bar(results,Observables='tumor_weight')` specifies to plot the bar graph of the mean and standard deviation of elementary effects corresponding to the tumor weight response.

`Parameters` — Input parameters to plot

character vector | string | string vector | cell array of character vectors | vector of positive integers

Input parameters to plot, specified as a character vector, string, string vector, cell array of character vectors, or vector of positive integers indexing into the columns of the `resultsObject.ParameterSamples` table. Use this name-value argument to select parameters and plot their corresponding GSA results. By default, all input parameters are included in the plot.

Data Types: `double` | `char` | `string` | `cell`

`Observables` — Model responses or observables to plot

character vector | string | string vector | cell array of character vectors | vector of positive integers

Model responses or observables to plot, specified as a character vector, string, string vector, cell array of character vectors, or vector of positive integers indexing into `resultsObject.Observables`. By default, the function plots GSA results for all model responses or observables.

Data Types: `double` | `char` | `string` | `cell`

`ShowMean` — Flag to plot means of elementary effects

`true` (default) | `false`

Flag to plot the means of elementary effects, specified as `true` or `false`.

Data Types: `logical`

`ShowStandardDeviation` — Flag to plot standard deviations of elementary effects

`true` (default) | `false`

Flag to plot the standard deviations of elementary effects, specified as `true` or `false`.

Data Types: `logical`

`MeanColor` — Color of means of elementary effects

three-element row vector | hexadecimal color code | color name

Color of the means of elementary effects, specified as a three-element row vector, hexadecimal color code, color name, or a short name. By default, the function uses the first MATLAB default color. To view the default color order, enter `get(groot,'defaultAxesColorOrder')` or see the "ColorOrder" property.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see "Specify Plot Colors".

Data Types: `double`

`StandardDeviationColor` — Color of standard deviations of elementary effects
three-element row vector | hexadecimal color code | color name

Color of the standard deviations of elementary effects, specified as a three-element row vector, hexadecimal color code, color name, or a short name. By default, the function uses the second MATLAB default color. To view the default color order, enter `get(groot,'defaultAxesColorOrder')` or see the “ColorOrder” property.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see “Specify Plot Colors”.

Data Types: `double`

Output Arguments

h — Handle
figure handle

Handle to the figure, specified as a figure handle.

Version History

Introduced in R2021b

See Also

`SimBiology.gsa.Sobol` | `SimBiology.gsa.ElementaryEffects` | `sbioelementaryeffects`

Topics
“Sensitivity Analysis in SimBiology”

bar

Create bar plot of first- and total-order Sobol indices

Syntax

```
h = bar(sobolObj)
h = bar(sobolObj,Name,Value)
```

Description

`h = bar(sobolObj)` plots the first- and total-order Sobol indices as a bar plot and returns the figure handle `h`. The color shading of each bar represents a histogram representing values at different times. Darker colors mean that those values occur more often over the whole time course. The plot shows a single dot for scalar or constant model responses instead of a bar.

`h = bar(sobolObj,Name,Value)` uses additional options specified by one or more name-value pair arguments.

Examples

Perform Global Sensitivity Analysis by Computing First- and Total-Order Sobol Indices

Load the “Tumor Growth Model”.

```
sbioloadproject tumor_growth_vpop_sa.sbproj
```

Get a variant with the estimated parameters and the dose to apply to the model.

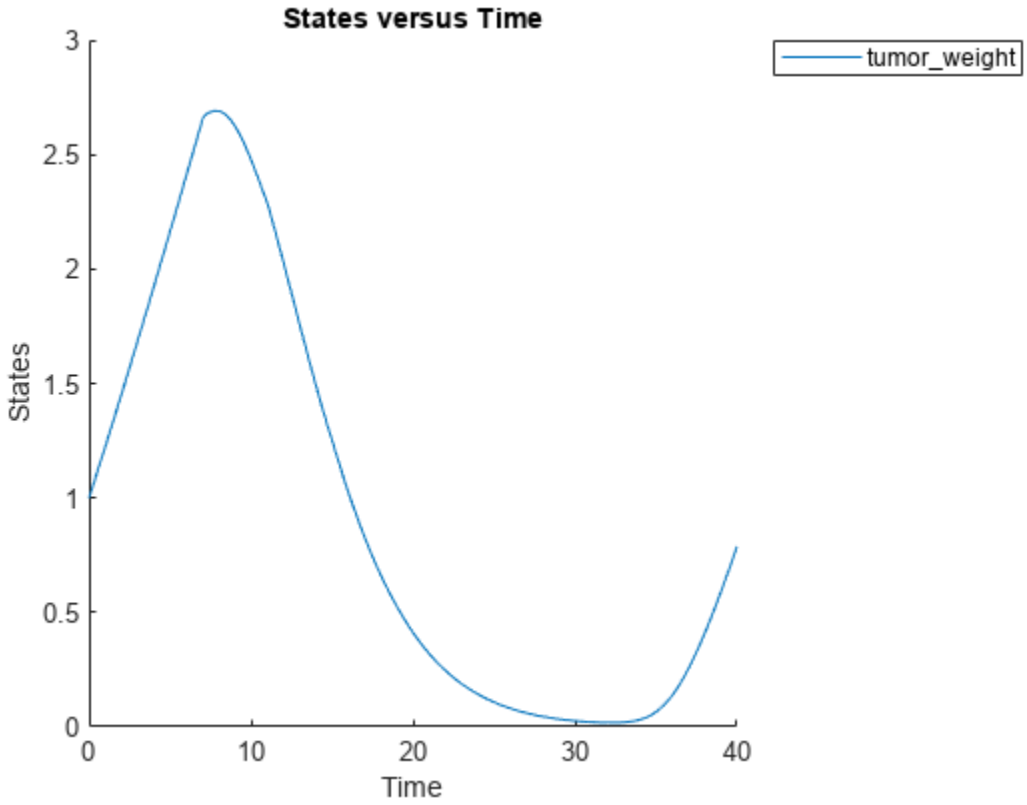
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

Get the active configset and set the tumor weight as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'tumor_weight';
```

Simulate the model and plot the tumor growth profile.

```
sbioplot(sbiosimulate(m1,cs,v,d));
```



Perform global sensitivity analysis (GSA) on the model to find the model parameters that the tumor growth is sensitive to.

First, retrieve model parameters of interest that are involved in the pharmacodynamics of the tumor growth. Define the model response as the tumor weight.

```
modelParamNames = {'L0','L1','w0','k1','k2'};
outputName = 'tumor_weight';
```

Then perform GSA by computing the first- and total-order Sobol indices using `sbiosobol`. Set `'ShowWaitBar'` to `true` to show the simulation progress. By default, the function uses 1000 parameter samples to compute the Sobol indices [1].

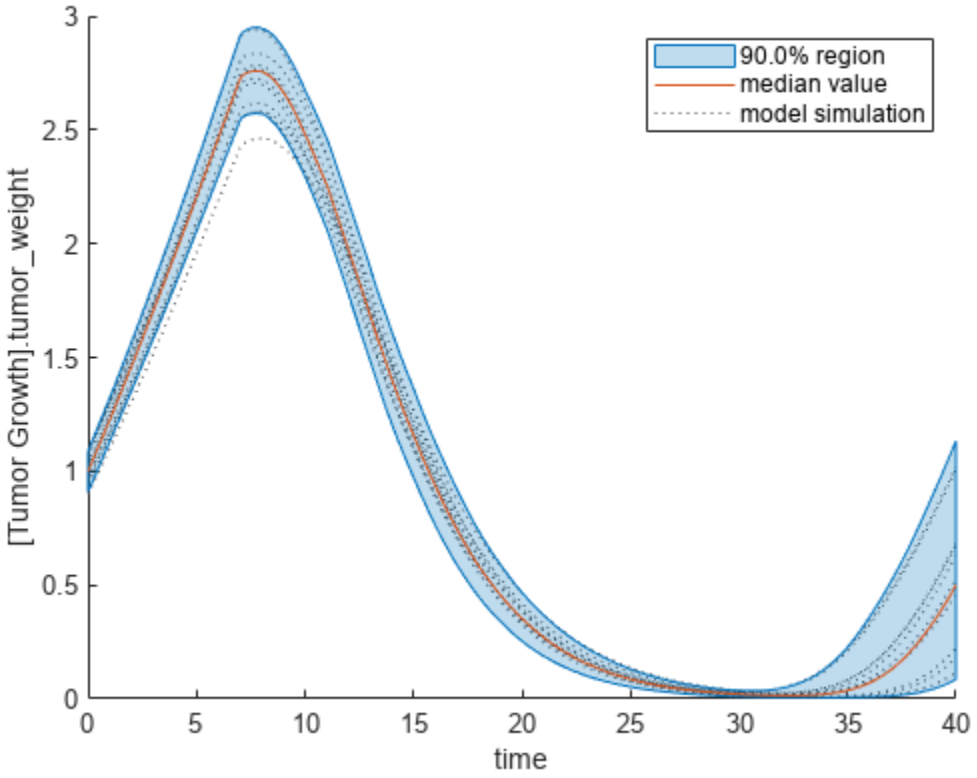
```
rng('default');
sobolResults = sbiosobol(m1,modelParamNames,outputName,Variants=v,Doses=d,ShowWaitBar=true)
```

```
sobolResults =
  Sobol with properties:

                Time: [444x1 double]
        SobolIndices: [5x1 struct]
            Variance: [444x1 table]
    ParameterSamples: [1000x5 table]
         Observables: {'[Tumor Growth].tumor_weight'}
      SimulationInfo: [1x1 struct]
```

You can change the number of samples by specifying the `'NumberSamples'` name-value pair argument. The function requires a total of `(number of input parameters + 2) * NumberSamples` model simulations.

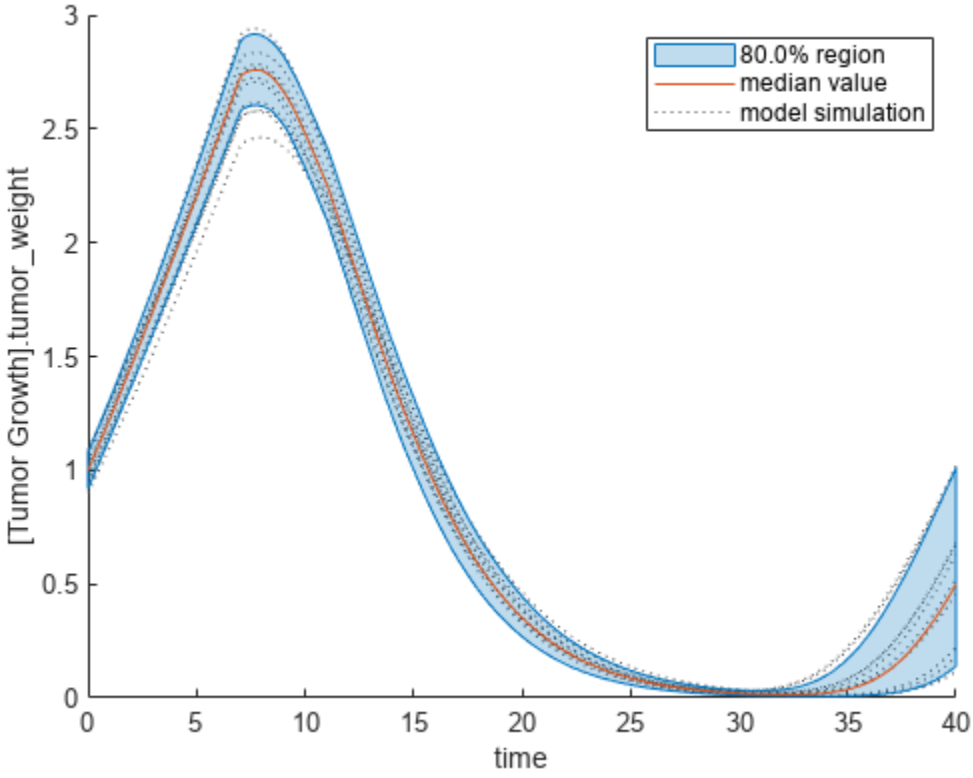
Show the mean model response, the simulation results, and a shaded region covering 90% of the simulation results.

```
plotData(sobolResults,ShowMedian=true,ShowMean=false);
```



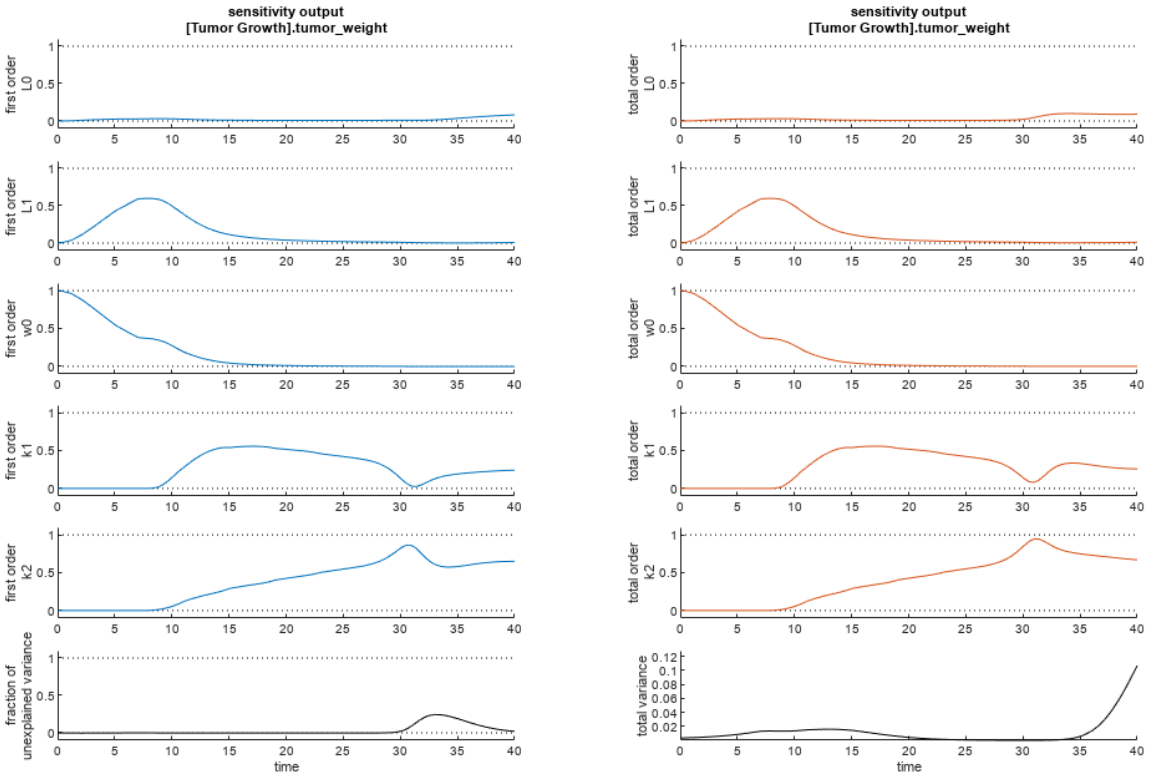
You can adjust the quantile region to a different percentage by specifying `'Alphas'` for the lower and upper quantiles of all model responses. For instance, an alpha value of 0.1 plots a shaded region between the `100 * alpha` and `100 * (1 - alpha)` quantiles of all simulated model responses.

```
plotData(sobolResults,Alphas=0.1,ShowMedian=true,ShowMean=false);
```



Plot the time course of the first- and total-order Sobol indices.

```
h = plot(sobolResults);
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```

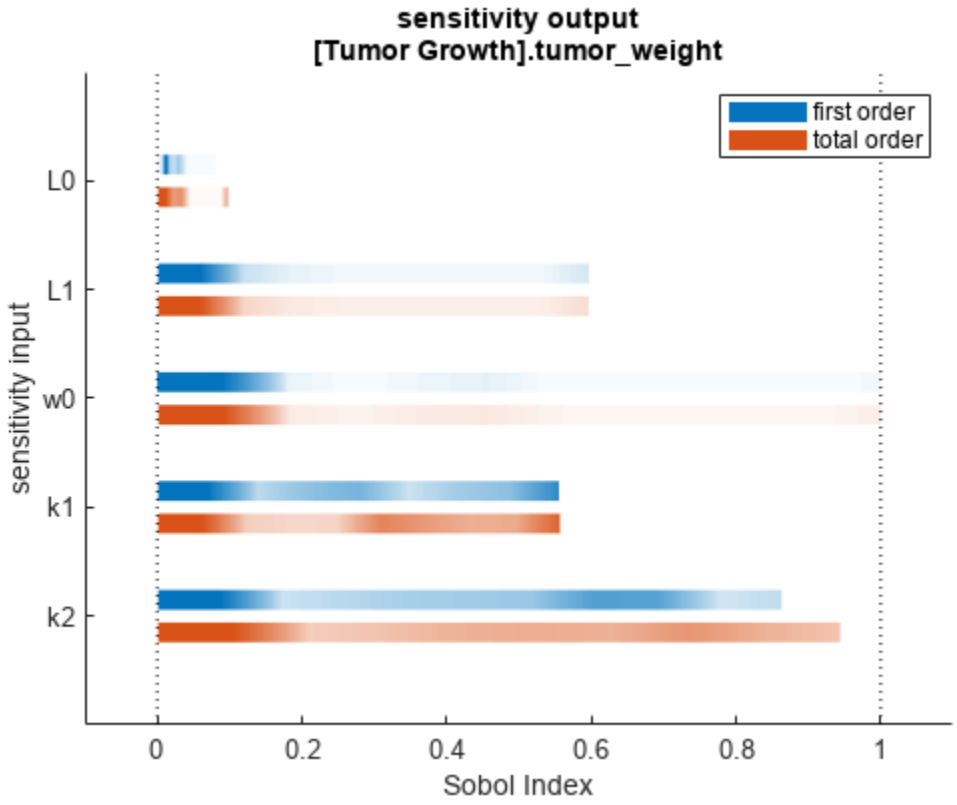


The first-order Sobol index of an input parameter gives the fraction of the overall response variance that can be attributed to variations in the input parameter alone. The total-order index gives the fraction of the overall response variance that can be attributed to any joint parameter variations that include variations of the input parameter.

From the Sobol indices plots, parameters `L1` and `w0` seem to be the most sensitive parameters to the tumor weight before the dose was applied at t = 7. But after the dose is applied, `k1` and `k2` become more sensitive parameters and contribute most to the after-dosing stage of the tumor weight. The total variance plot also shows a larger variance for the after-dose stage at t > 35 than for the before-dose stage of the tumor growth, indicating that `k1` and `k2` might be more important parameters to investigate further. The fraction of unexplained variance shows some variance at around t = 33, but the total variance plot shows little variance at t = 33, meaning the unexplained variance could be insignificant. The fraction of unexplained variance is calculated as 1 - (sum of all the first-order Sobol indices), and the total variance is calculated using `var(response)`, where `response` is the model response at every time point.

You can also display the magnitudes of the sensitivities in a bar plot. Darker colors mean that those values occur more often over the whole time course.

```
bar(sobolResults);
```



You can specify more samples to increase the accuracy of the Sobol indices, but the simulation can take longer to finish. Use `addsamples` to add more samples. For example, if you specify 1500 samples, the function performs `1500 * (2 + number of input parameters)` simulations.

```
gsaMoreSamples = addsamples(gsaResults,1500)
```

The “SimulationInfo” on page 2-0 property of the result object contains various information for computing the Sobol indices. For instance, the model simulation data (SimData) for each simulation using a set of parameter samples is stored in the `SimData` field of the property. This field is an array of `SimData` objects.

```
sobolResults.SimulationInfo.SimData
```

```
SimBiology SimData Array : 1000-by-7

Index:    Name:         ModelName:         DataCount:
1           -           Tumor Growth Model 1
2           -           Tumor Growth Model 1
3           -           Tumor Growth Model 1
...
7000        -           Tumor Growth Model 1
```

You can find out if any model simulation failed during the computation by checking the `ValidSample` field of `SimulationInfo`. In this example, the field shows no failed simulation runs.

```
all(sobolResults.SimulationInfo.ValidSample)
```

```
ans = 1x7 logical array

   1   1   1   1   1   1   1
```

`SimulationInfo.ValidSample` is a table of logical values. It has the same size as `SimulationInfo.SimData`. If `ValidSample` indicates that any simulations failed, you can get more information about those simulation runs and the samples used for those runs by extracting information from the corresponding column of `SimulationInfo.SimData`. Suppose that the fourth column contains one or more failed simulation runs. Get the simulation data and sample values used for that simulation using `getSimulationResults`.

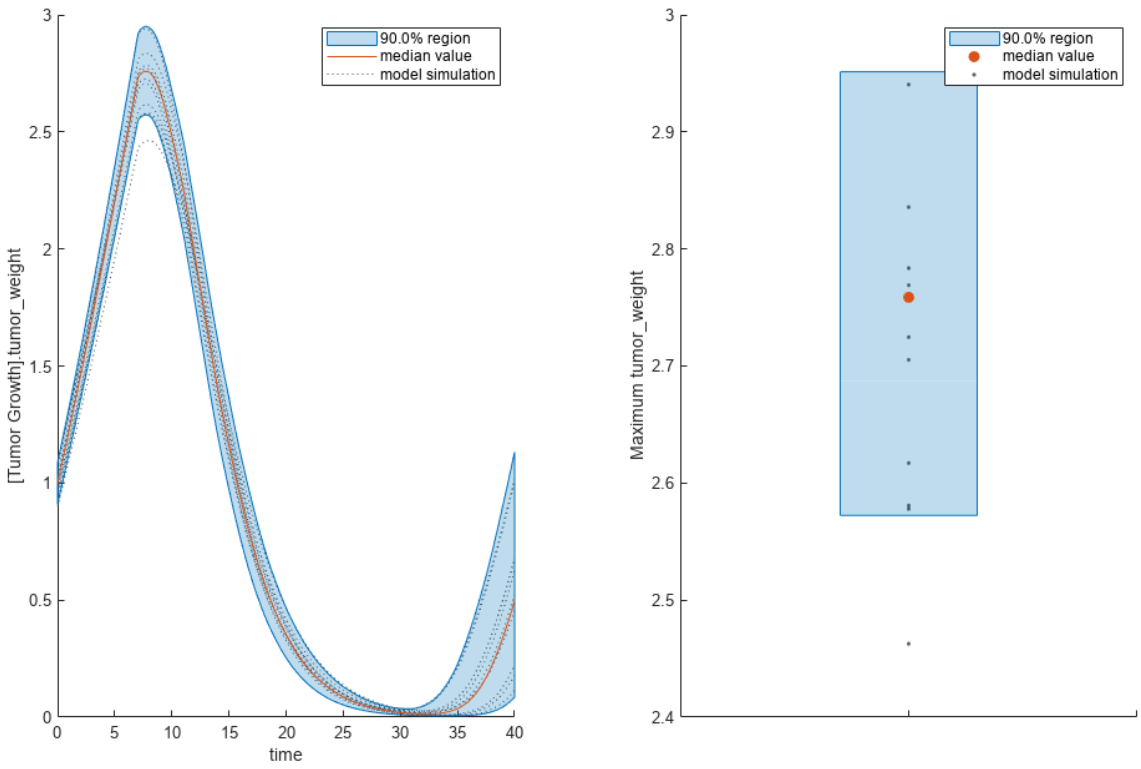
```
[samplesUsed,sd,validruns] = getSimulationResults(sobolResults,4);
```

You can add custom expressions as observables and compute Sobol indices for the added observables. For example, you can compute the Sobol indices for the maximum tumor weight by defining a custom expression as follows.

```
% Suppress an information warning that is issued during simulation.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
% Add the observable expression.
sobolObs = addobservable(sobolResults,'Maximum tumor_weight','max(tumor_weight)','Units','gram');
```

Plot the computed simulation results showing the 90% quantile region.

```
h2 = plotData(sobolObs,ShowMedian=true,ShowMean=false);
h2.Position(:) = [100 100 1280 800];
```



You can also remove the observable by specifying its name.

```
gsaNoObs = removeobservable(sobolObs,'Maximum tumor_weight');
```

Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

`sobolObj` — Results containing Sobol indices

`SimBiology.gsa.Sobol` object

Results containing the first- and total-order Sobol indices, specified as a `SimBiology.gsa.Sobol` object.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `h = bar(results,'Observables','tumor_weight')` creates a bar plot of the Sobol indices corresponding to the tumor weight response.

`Parameters` — Input parameters to plot

character vector | string | string vector | cell array of character vectors | vector of positive integers

Input parameters to plot, specified as a character vector, string, string vector, cell array of character vectors, or vector of positive integers indexing into the columns of the `resultsObject.ParameterSamples` table. Use this name-value argument to select parameters and plot their corresponding GSA results. By default, all input parameters are included in the plot.

Data Types: `double` | `char` | `string` | `cell`

`Observables` — Model responses or observables to plot

character vector | string | string vector | cell array of character vectors | vector of positive integers

Model responses or observables to plot, specified as a character vector, string, string vector, cell array of character vectors, or vector of positive integers indexing into `resultsObject.Observables`. By default, the function plots GSA results for all model responses or observables.

Data Types: `double` | `char` | `string` | `cell`

`FirstOrderColor` — Color first-order Sobol indices

three-element row vector | hexadecimal color code | color name

Color of the first-order Sobol indices, specified as a three-element row vector, hexadecimal color code, color name, or a short name. By default, the function uses the first MATLAB default color. To view the default color order, enter `get(groot,'defaultAxesColorOrder')` or see the “ColorOrder” property.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see “Specify Plot Colors”.

Example: `'FirstOrderColor',[0.4,0.3,0.2]`

Data Types: `double`

`TotalOrderColor` — Color of total-order Sobol indices
three-element row vector | hexadecimal color code | color name

Color of the total-order Sobol indices, specified as a three-element row vector, hexadecimal color code, color name, or a short name. By default, the function uses the second MATLAB default color. To view the default color order, enter `get(groot,'defaultAxesColorOrder')` or see the “ColorOrder” property.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see “Specify Plot Colors”.

Example: `'TotalOrderColor',[0.2,0.5,0.8]`

Data Types: `double`

Output Arguments

h — Handle
figure handle

Handle to the figure, specified as a figure handle.

Version History

Introduced in R2020a

References

[1] Saltelli, Andrea, Paola Annoni, Ivano Azzini, Francesca Campolongo, Marco Ratto, and Stefano Tarantola. “Variance Based Sensitivity Analysis of Model Output. Design and Estimator for the Total Sensitivity Index.” *Computer Physics Communications* 181, no. 2 (February 2010): 259–70. https://doi.org/10.1016/j.cpc.2009.09.018.

See Also

`SimBiology.gsa.Sobol` | `sbiosobol` | `plot` | `plotData`

boxplot

Create box plot showing the variation of estimated SimBiology model parameters

Syntax

```
boxplot(resultsObj)
```

Description

`boxplot(resultsObj)` creates a box plot showing the variation of the estimated SimBiology model parameters.

Examples

Estimate Two-Compartment PK Parameters

Load the sample data set.

```
load data10_32R.mat
gData = groupedData(data);
gData.Properties.VariableUnits = ["","hour","milligram/liter","milligram/liter"];
```

Create a two-compartment PK model.

```
pkmd                 = PKModelDesign;
pkc1                 = addCompartment(pkmd,"Central");
pkc1.DosingType      = "Infusion";
pkc1.EliminationType = "linear-clearance";
pkc1.HasResponseVariable = true;
pkc2                 = addCompartment(pkmd,"Peripheral");
model                = construct(pkmd);
configset            = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
responseMap = ["Drug_Central = CentralConc","Drug_Peripheral = PeripheralConc"];
```

Provide model parameters to estimate.

```
paramsToEstimate   = ["log(Central)","log(Peripheral)","Q12","Cl_Central"];
estimatedParam     = estimatedInfo(paramsToEstimate,'InitialValue',[1 1 1 1]);
```

Assume every individual receives an infusion dose at time = 0, with a total infusion amount of 100 mg at a rate of 50 mg/hour.

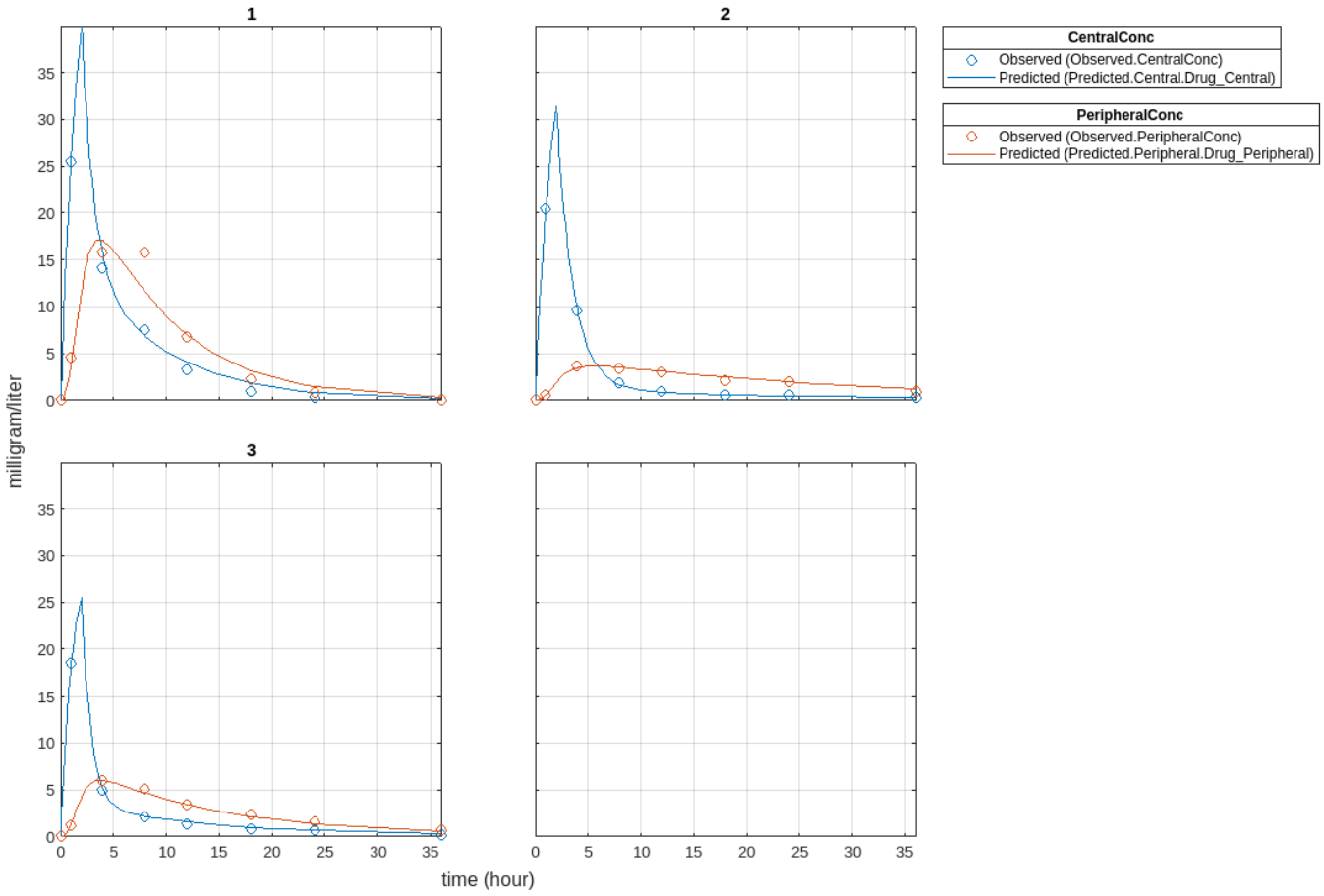
```
dose             = sbiodose("dose","TargetName","Drug_Central");
dose.StartTime   = 0;
dose.Amount      = 100;
dose.Rate        = 50;
dose.AmountUnits = "milligram";
dose.TimeUnits   = "hour";
dose.RateUnits   = "milligram/hour";
```

Estimate model parameters. By default, the function estimates a set of parameter for each individual (unpooled fit).

```
fitResults =  sbiofit(model,gData,responseMap,estimatedParam,dose);
```

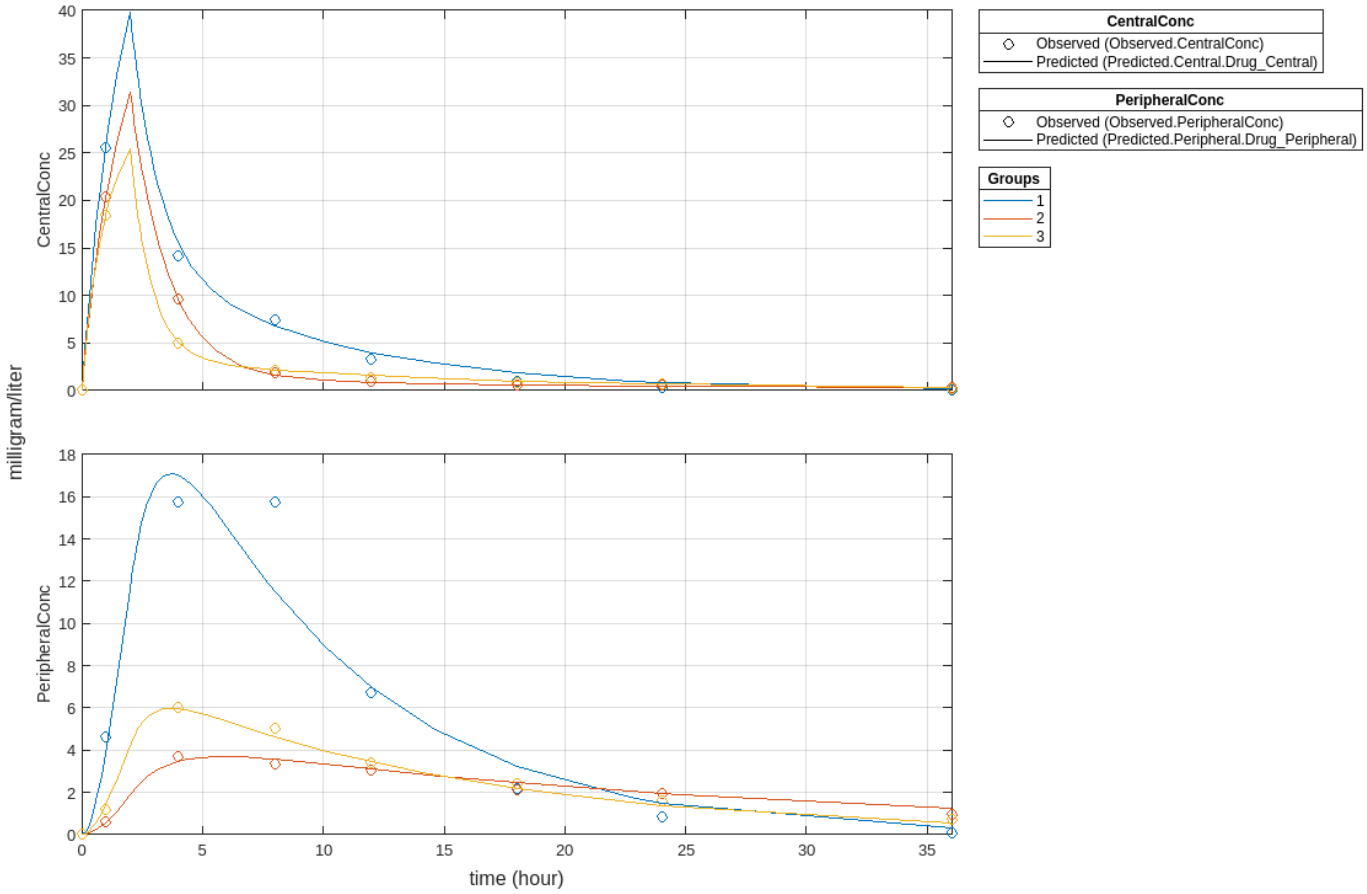
Plot the results.

```
plot(fitResults);
```



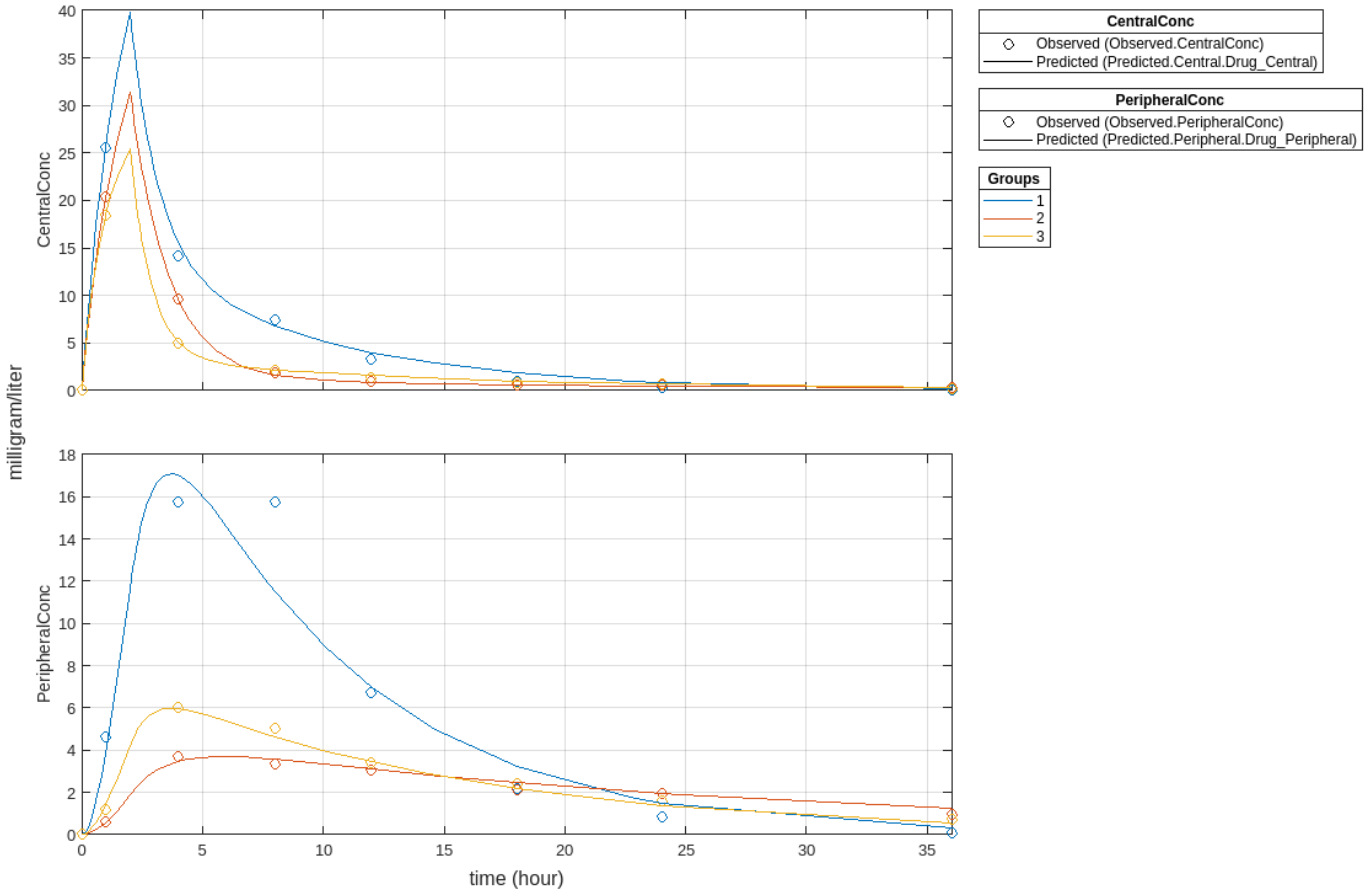
Plot all groups in one plot.

```
plot(fitResults,"PlotStyle","one axes");
```



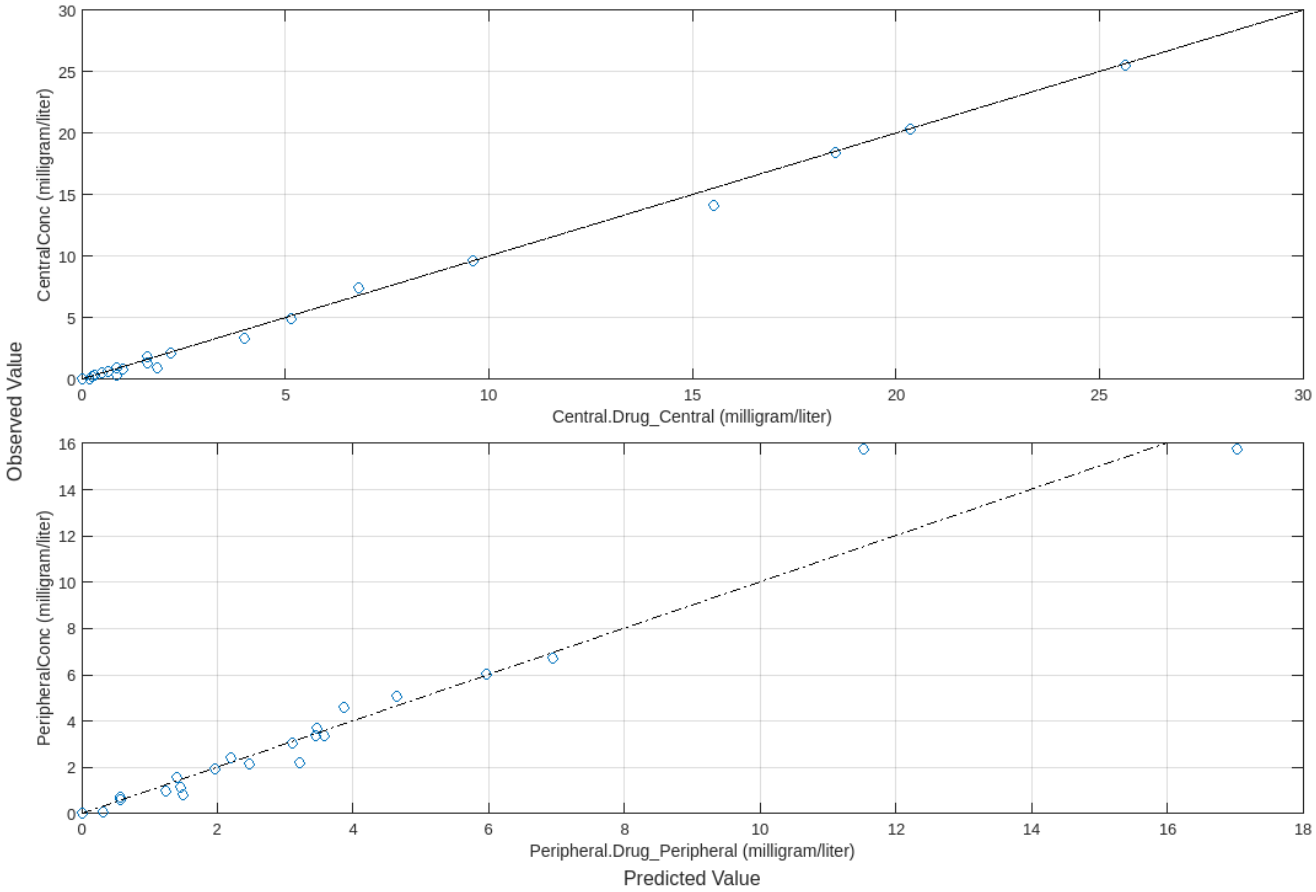
Change some axes properties.

```
s = struct;
s.Properties.XGrid = "on";
s.Properties.YGrid = "on";
plot(fitResults,"PlotStyle","one axes","AxesStyle",s);
```



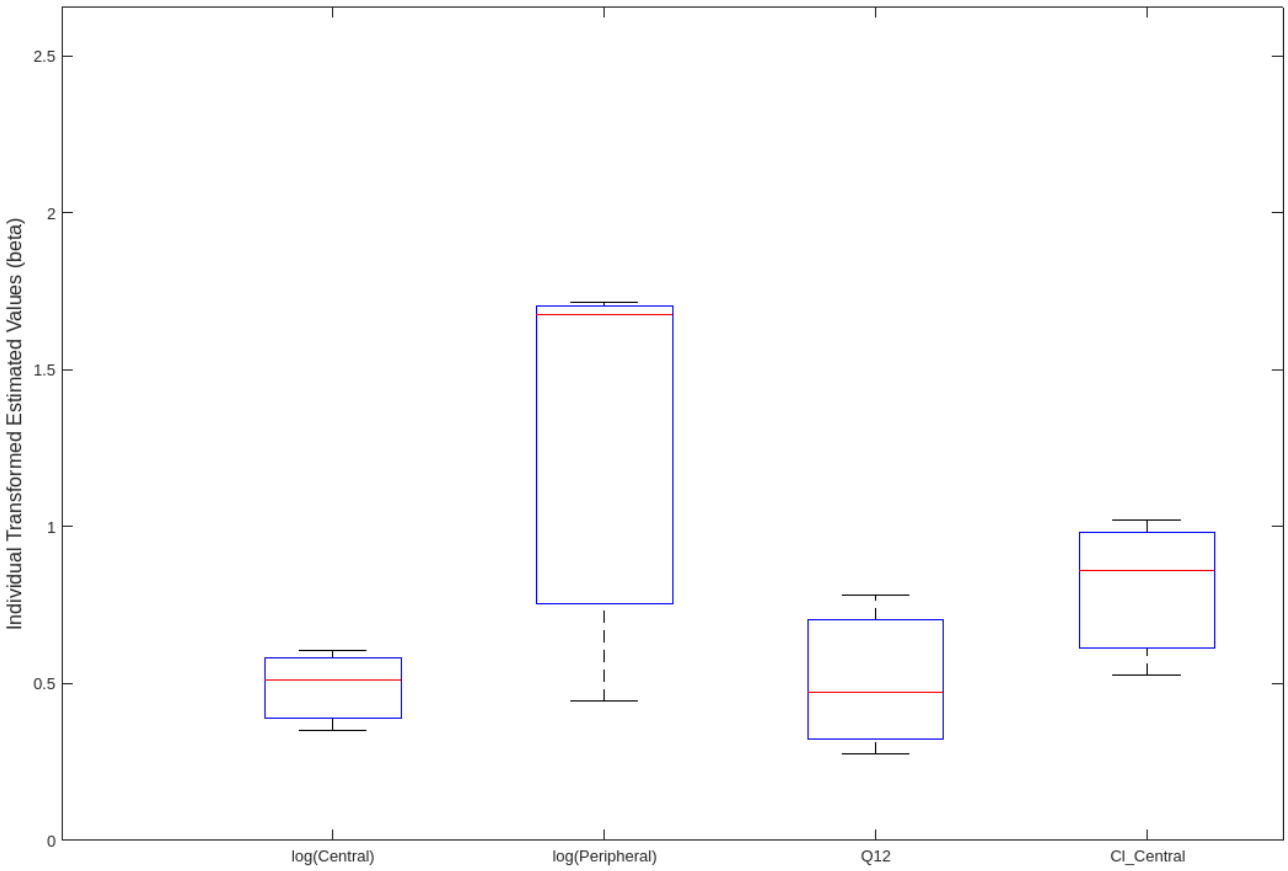
Compare the model predictions to the actual data.

```
plotActualVersusPredicted(fitResults)
```



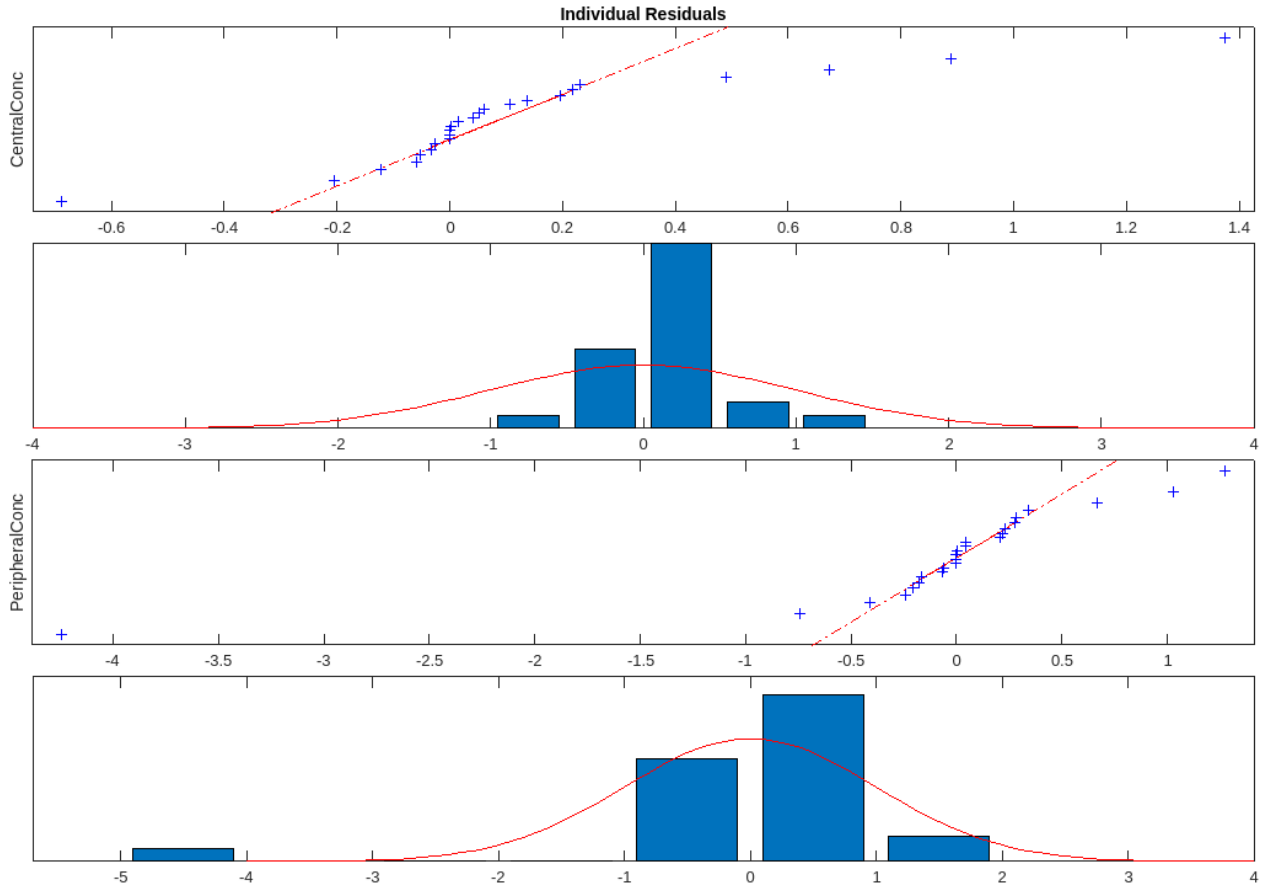
Use `boxplot` to show the variation of estimated model parameters.

```
boxplot(fitResults)
```



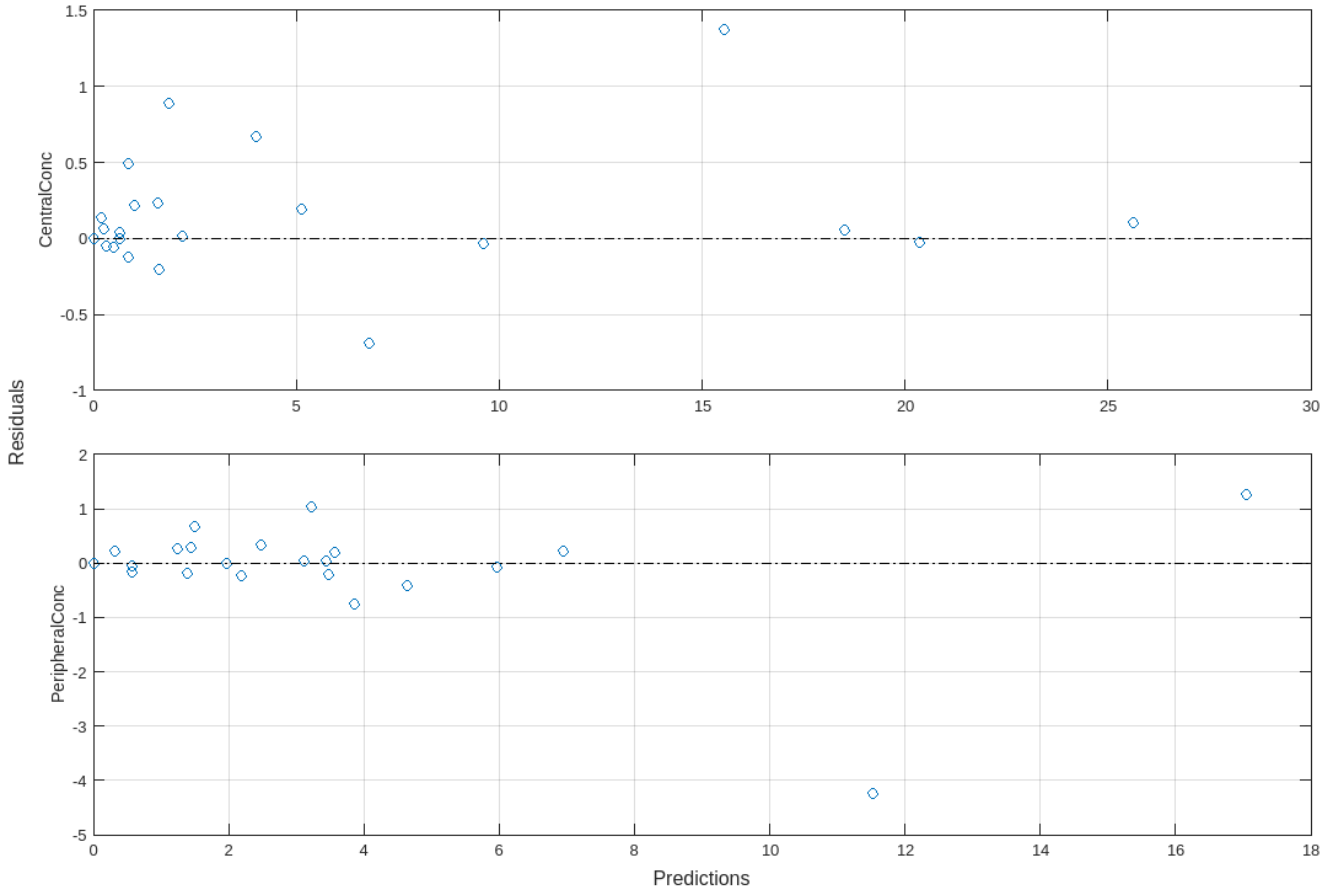
Plot the distribution of residuals. This normal probability plot shows the deviation from normality and the skewness on the right tail of the distribution of residuals. The default (constant) error model might not be the correct assumption for the data being fitted.

```
plotResidualDistribution(fitResults)
```



Plot residuals for each response using the model predictions on *x*-axis.

```
plotResiduals(fitResults,"Predictions")
```



Get the summary of the fit results. `stats.Name` contains the name for each table from `stats.Table`, which contains a list of tables with estimated parameter values and fit quality statistics.

```
stats = summary(fitResults);
stats.Name
```

```
ans =
'Unpooled Parameter Estimates'

ans =
'Statistics'

ans =
'Unpooled Beta'

ans =
'Residuals'

ans =
'Covariance Matrix'

ans =
'Error Model'
```

```
stats.Table
```

```
ans=3×9 table
    Group    Central Estimate    Central StandardError    Peripheral Estimate    Peripheral Stand
    _____    ________________    _____________________    ___________________    ________________

    {'1'}          1.422               0.12334                1.5619                0.36355
    {'2'}         1.8322              0.019672                5.3364                0.65327
    {'3'}         1.6657              0.038529                5.5632                0.37063


ans=3×7 table
    Group      AIC        BIC      LogLikelihood    DFE      MSE         SSE
    _____    _______    _______    _____________    ___    ________    _______

    {'1'}     60.961     64.051       -26.48        12        2.138     25.656
    {'2'}    -7.8379    -4.7475       7.9189        12     0.029012    0.34814
    {'3'}    -1.4336     1.6567       4.7168        12     0.043292     0.5195


ans=3×9 table
    Group    Central Estimate    Central StandardError    Peripheral Estimate    Peripheral Stand
    _____    ________________    _____________________    ___________________    ________________

    {'1'}        0.35208              0.086736               0.44589                0.23277
    {'2'}        0.60551              0.010737                1.6746                0.12242
    {'3'}        0.51027               0.02313                1.7162                0.06662


ans=24×4 table
    ID    Time    CentralConc    PeripheralConc
    __    ____    ___________    ______________

    1       0              0              0
    1       1        0.10646        -0.74394
    1       4         1.3745          1.2726
    1       8       -0.68825         -4.2435
    1      12        0.67383         0.21806
    1      18        0.88823          1.0269
    1      24        0.48941         0.66755
    1      36        0.13632         0.22948
    2       0              0              0
    2       1      -0.026731      -0.058311
    2       4      -0.033299       -0.20544
    2       8       -0.20466        0.20696
    2      12       -0.12223       0.045409
    2      18       0.041224        0.33883
    2      24      -0.059498      0.0036257
    2      36      -0.051645        0.27616
      ⋮


ans=12×6 table
    Group        Parameters          log(Central)    log(Peripheral)        Q12        Cl_Central
    _____    __________________    _____________    _______________    ___________    __________

    {'1'}    {'log(Central)'   }       0.015213        -0.022539       -0.0086672       0.00115
    {'1'}    {'log(Peripheral)'}      -0.022539          0.13217         0.045746     -0.007313
    {'1'}    {'Q12'            }     -0.0086672         0.045746         0.023092     -0.002148
    {'1'}    {'Cl_Central'     }       0.001159       -0.0073135       -0.0021484      0.001367
    {'2'}    {'log(Central)'   }     0.00038701        -0.002161      -0.00010177     9.7448e-05
```

```
    {'2'}    {'log(Peripheral)'}      -0.002161          0.42676          0.019101      -0.01575
    {'2'}    {'Q12'            }    -0.00010177         0.019101         0.00094857    -0.0007332
    {'2'}    {'Cl_Central'     }     9.7448e-05         -0.015755        -0.00073328     0.0006894
    {'3'}    {'log(Central)'   }      0.0014845        -0.0054648         -0.0013216     0.0001663
    {'3'}    {'log(Peripheral)'}     -0.0054648          0.13737           0.016903     -0.007272
    {'3'}    {'Q12'            }     -0.0013216         0.016903          0.0034406    -0.0008253
    {'3'}    {'Cl_Central'     }      0.00016639       -0.0072722        -0.00082538     0.0007458
```

```
ans=3×5 table
    Group     Response      ErrorModel        a        b
    _____    __________    ____________    _______    ___

    {'1'}    {0×0 char}    {'constant'}     1.2663    NaN
    {'2'}    {0×0 char}    {'constant'}    0.14751    NaN
    {'3'}    {0×0 char}    {'constant'}    0.18019    NaN
```

Input Arguments

`resultsObj` — Estimation results

`OptimResults` object | `NLINResults` object | vector of results objects

Estimation results, specified as an `OptimResults object` or `NLINResults object`, or vector of results objects which contains estimation results from running `sbiofit`.

Version History

Introduced in R2014a

See Also

`NLINResults object` | `OptimResults object` | `sbiofit`

boxplot

Create box plot showing the variation of estimated SimBiology model parameters

Syntax

```
boxplot(resultsObj)
```

Description

`boxplot(resultsObj)` creates a box plot showing the variation of the estimated SimBiology model parameters.

Input Arguments

`resultsObj` — Estimation results
`NLMEResults` object

Estimation results, specified as an `NLMEResults object`, which contains estimation results from running `sbiofitmixed`.

Version History

Introduced in R2014a

See Also

`NLMEResults object` | `sbiofitmixed`

ci2table

Package: `SimBiology.fit`

Return summary table of confidence interval results

Syntax

```
tbl = ci2table(paraCI)
```

Description

`tbl = ci2table(paraCI)` returns a summary table of confidence interval results from `paraCI`, a `ParameterConfidenceInterval` object or vector of objects.

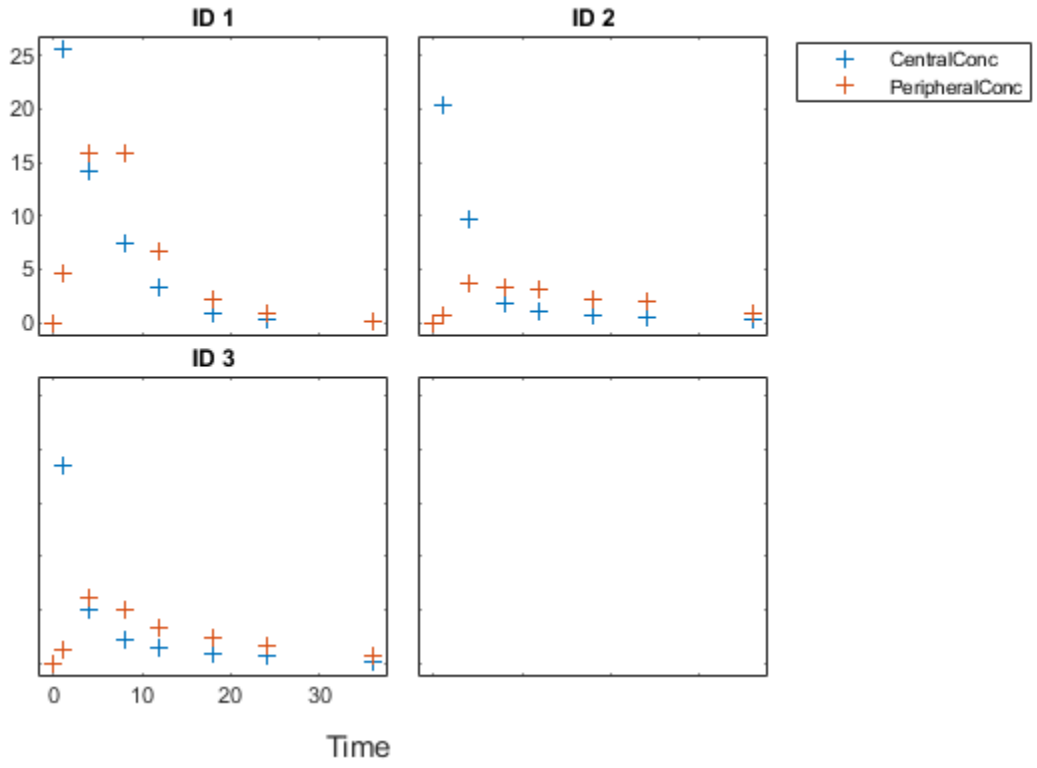
Examples

Compute Confidence Intervals for Estimated PK Parameters and Model Predictions

Load Data

Load the sample data to fit. The data is stored as a table with variables *ID* , *Time* , *CentralConc* , and *PeripheralConc*. This synthetic data represents the time course of plasma concentrations measured at eight different time points for both central and peripheral compartments after an infusion dose for three individuals.

```
load data10_32R.mat
gData = groupedData(data);
gData.Properties.VariableUnits = {'','hour','milligram/liter','milligram/liter'};
sbiotrellis(gData,'ID','Time',{'CentralConc','PeripheralConc'},'Marker','+',...
            'LineStyle','none');
```



Create Model

Create a two-compartment model.

```
pkmd                 = PKModelDesign;
pkc1                 = addCompartment(pkmd,'Central');
pkc1.DosingType      = 'Infusion';
pkc1.EliminationType = 'linear-clearance';
pkc1.HasResponseVariable = true;
pkc2                 = addCompartment(pkmd,'Peripheral');
model                = construct(pkmd);
configset            = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
```

Define Dosing

Define the infusion dose.

```
dose             = sbiodose('dose','TargetName','Drug_Central');
dose.StartTime   = 0;
dose.Amount      = 100;
dose.Rate        = 50;
dose.AmountUnits = 'milligram';
dose.TimeUnits   = 'hour';
dose.RateUnits   = 'milligram/hour';
```

Define Parameters

Define the parameters to estimate. Set the parameter bounds for each parameter. In addition to these explicit bounds, the parameter transformations (such as log, logit, or probit) impose implicit bounds.

```
responseMap = {'Drug_Central = CentralConc','Drug_Peripheral = PeripheralConc'};
paramsToEstimate   = {'log(Central)','log(Peripheral)','Q12','Cl_Central'};
estimatedParam     = estimatedInfo(paramsToEstimate,...
                                   'InitialValue',[1 1 1 1],...
                                   'Bounds',[0.1 3;0.1 10;0 10;0.1 2]);
```

Fit Model

Perform an unpooled fit, that is, one set of estimated parameters for each patient.

```
unpooledFit = sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',false);
```

Perform a pooled fit, that is, one set of estimated parameters for all patients.

```
pooledFit = sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',true);
```

Compute Confidence Intervals for Estimated Parameters

Compute 95% confidence intervals for each estimated parameter in the unpooled fit.

```
ciParamUnpooled = sbioparameterci(unpooledFit);
```

Display Results

Display the confidence intervals in a table format. For details about the meaning of each estimation status, see “Parameter Confidence Interval Estimation Status” on page 2-666.

```
ci2table(ciParamUnpooled)
```

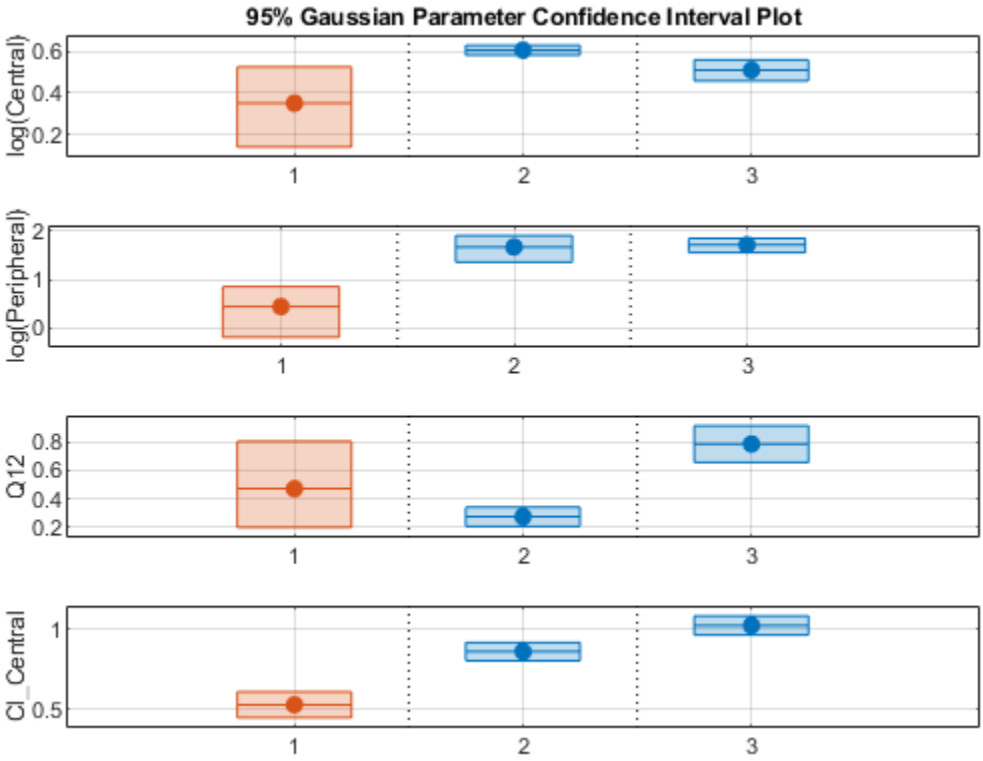
```
ans =

  12x7 table

    Group         Name         Estimate    ConfidenceInterval      Type      Alpha      Status
    _____    _____________    ________    __________________    ________    _____    __________

      1      {'Central'   }      1.422      1.1533     1.6906    Gaussian    0.05     estimable
      1      {'Peripheral'}     1.5629     0.83143     2.3551    Gaussian    0.05     constrained
      1      {'Q12'       }    0.47159     0.20093    0.80247    Gaussian    0.05     constrained
      1      {'Cl_Central'}    0.52898     0.44842    0.60955    Gaussian    0.05     estimable
      2      {'Central'   }     1.8322      1.7893     1.8751    Gaussian    0.05     success
      2      {'Peripheral'}     5.3368      3.9133     6.7602    Gaussian    0.05     success
      2      {'Q12'       }    0.27641      0.2093    0.34351    Gaussian    0.05     success
      2      {'Cl_Central'}    0.86034     0.80313    0.91755    Gaussian    0.05     success
      3      {'Central'   }     1.6657      1.5818     1.7497    Gaussian    0.05     success
      3      {'Peripheral'}     5.5632      4.7557     6.3708    Gaussian    0.05     success
      3      {'Q12'       }    0.78361     0.65581    0.91142    Gaussian    0.05     success
      3      {'Cl_Central'}     1.0233     0.96375     1.0828    Gaussian    0.05     success
```

Plot the confidence intervals. If the estimation status of a confidence interval is `success`, it is plotted in blue (the first default color). Otherwise, it is plotted in red (the second default color), which

indicates that further investigation into the fitted parameters may be required. If the confidence interval is `not estimable`, then the function plots a red line with a centered cross. If there are any transformed parameters with estimated values 0 (for the log transform) and 1 or 0 (for the probit or logit transform), then no confidence intervals are plotted for those parameter estimates. To see the color order, type `get(groot,'defaultAxesColorOrder')`.

Groups are displayed from left to right in the same order that they appear in the `GroupNames` property of the object, which is used to label the x-axis. The y-labels are the transformed parameter names.

```
plot(ciParamUnpooled)
```



Compute the confidence intervals for the pooled fit.

```
ciParamPooled = sbioparameterci(pooledFit);
```

Display the confidence intervals.

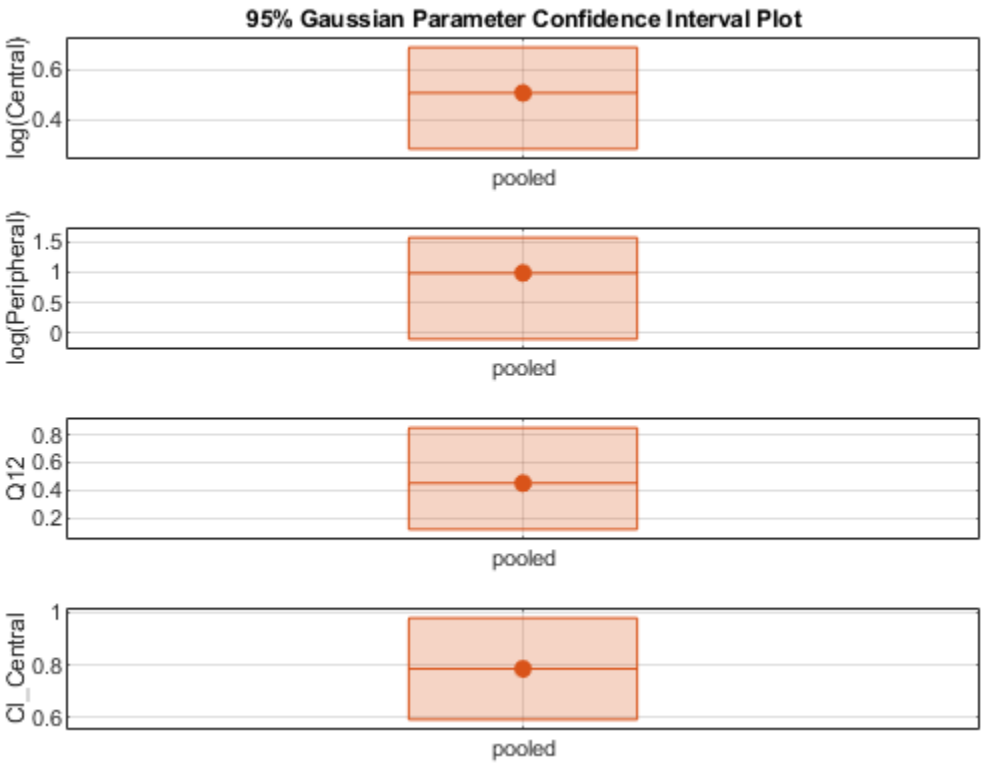
```
ci2table(ciParamPooled)
```

```
ans =

  4x7 table

    Group          Name          Estimate    ConfidenceInterval      Type       Alpha      Status
    ______    _______________    ________    __________________    ________    _____    __________
```

```
pooled    {'Central'   }     1.6626      1.3287      1.9965    Gaussian    0.05     estimable
pooled    {'Peripheral'}      2.687     0.89848      4.8323    Gaussian    0.05     constraine
pooled    {'Q12'       }    0.44956     0.11445     0.85152    Gaussian    0.05     constraine
pooled    {'Cl_Central'}    0.78493     0.59222     0.97764    Gaussian    0.05     estimable
```

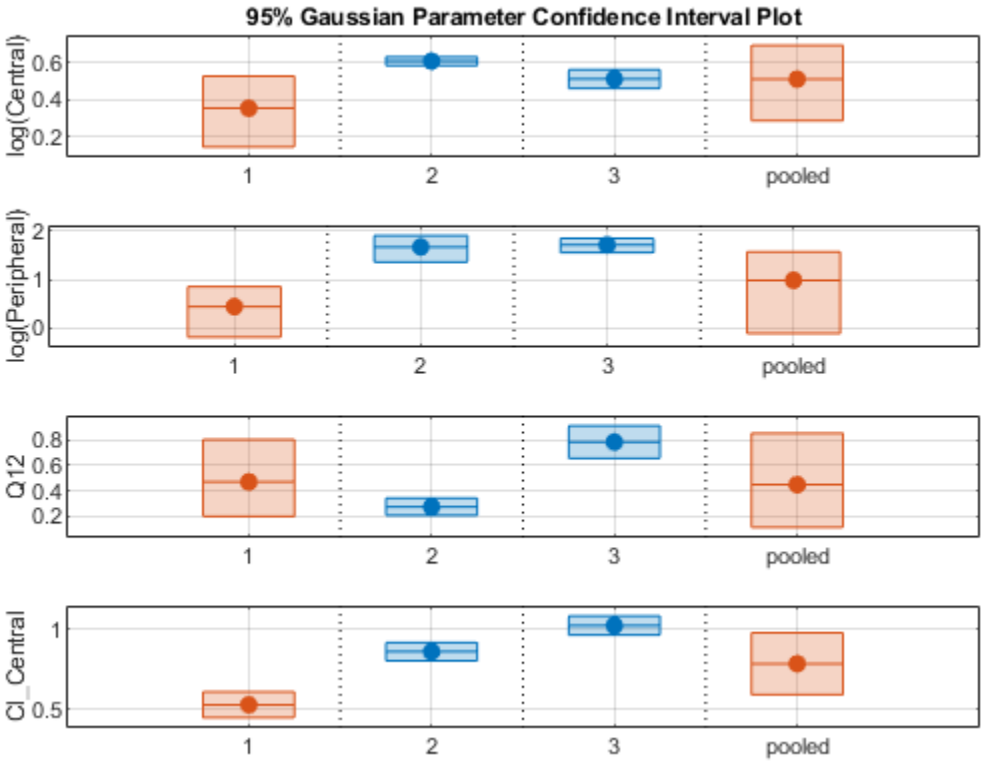
Plot the confidence intervals. The group name is labeled as "pooled" to indicate such fit.

```
plot(ciParamPooled)
```



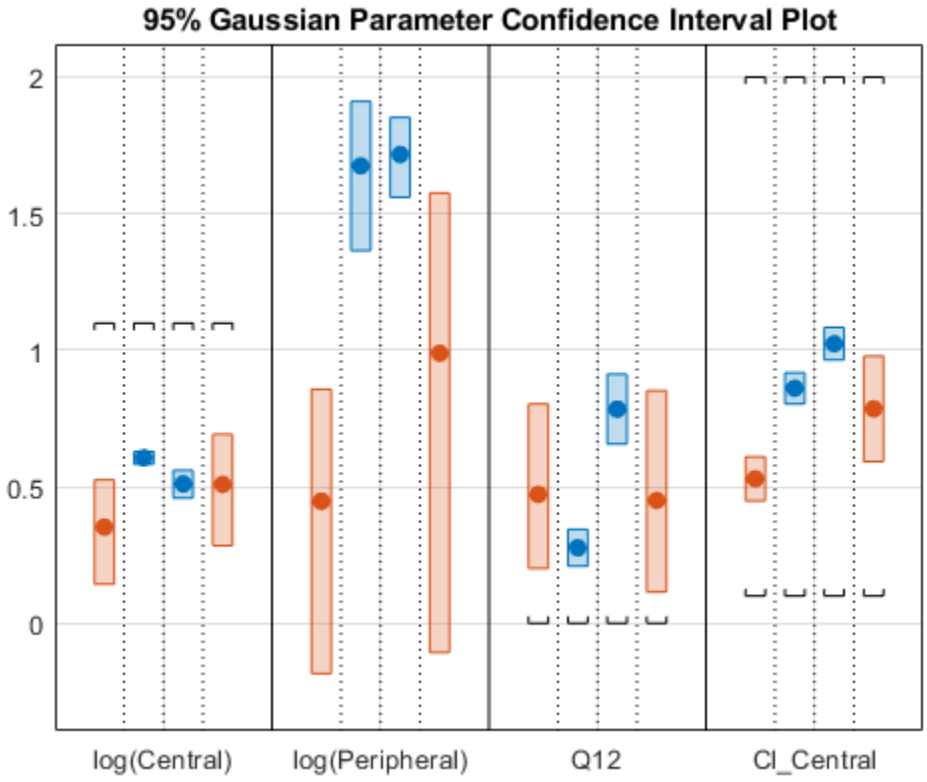
Plot all the confidence interval results together. By default, the confidence interval for each parameter estimate is plotted on a separate axes. Vertical lines group confidence intervals of parameter estimates that were computed in a common fit.

```
ciAll = [ciParamUnpooled;ciParamPooled];
plot(ciAll)
```



You can also plot all confidence intervals in one axes grouped by parameter estimates using the 'Grouped' layout.

```
plot(ciAll,'Layout','Grouped')
```



In this layout, you can point to the center marker of each confidence interval to see the group name. Each estimated parameter is separated by a vertical black line. Vertical dotted lines group confidence intervals of parameter estimates that were computed in a common fit. Parameter bounds defined in the original fit are marked by square brackets. Note the different scales on the y-axis due to parameter transformations. For instance, the y-axis of `Q12` is in the linear scale, but that of `Central` is in the log scale due to its log transform.

Compute Confidence Intervals for Model Predictions

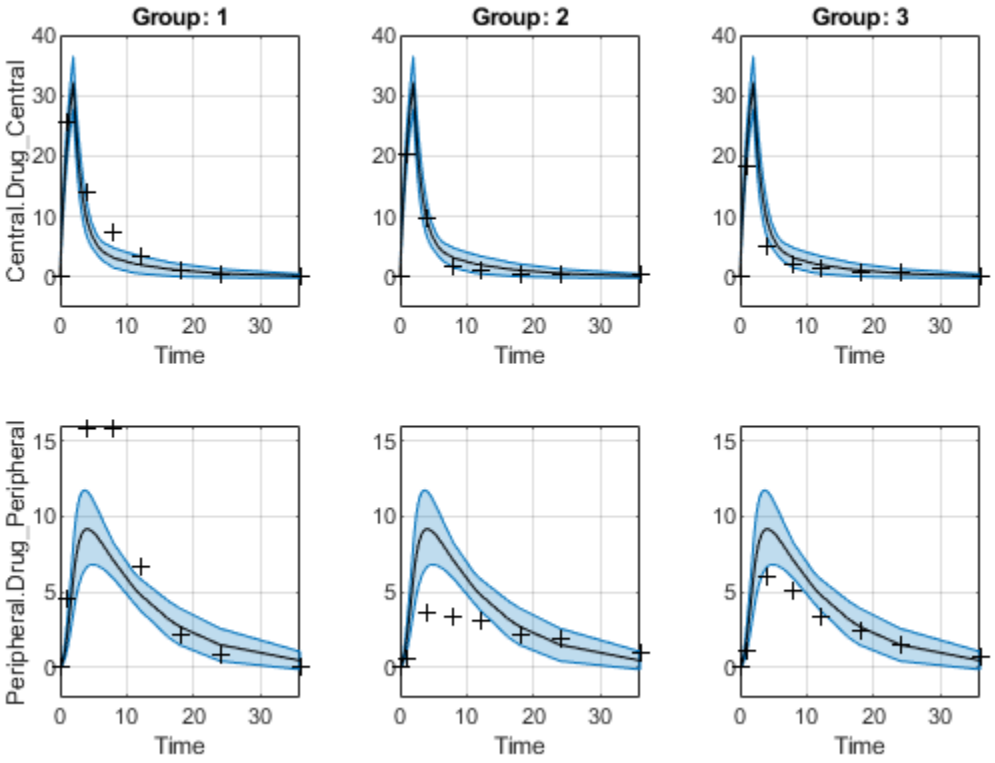
Calculate 95% confidence intervals for the model predictions, that is, simulation results using the estimated parameters.

```
% For the pooled fit
ciPredPooled = sbiopredictionci(pooledFit);
% For the unpooled fit
ciPredUnpooled = sbiopredictionci(unpooledFit);
```

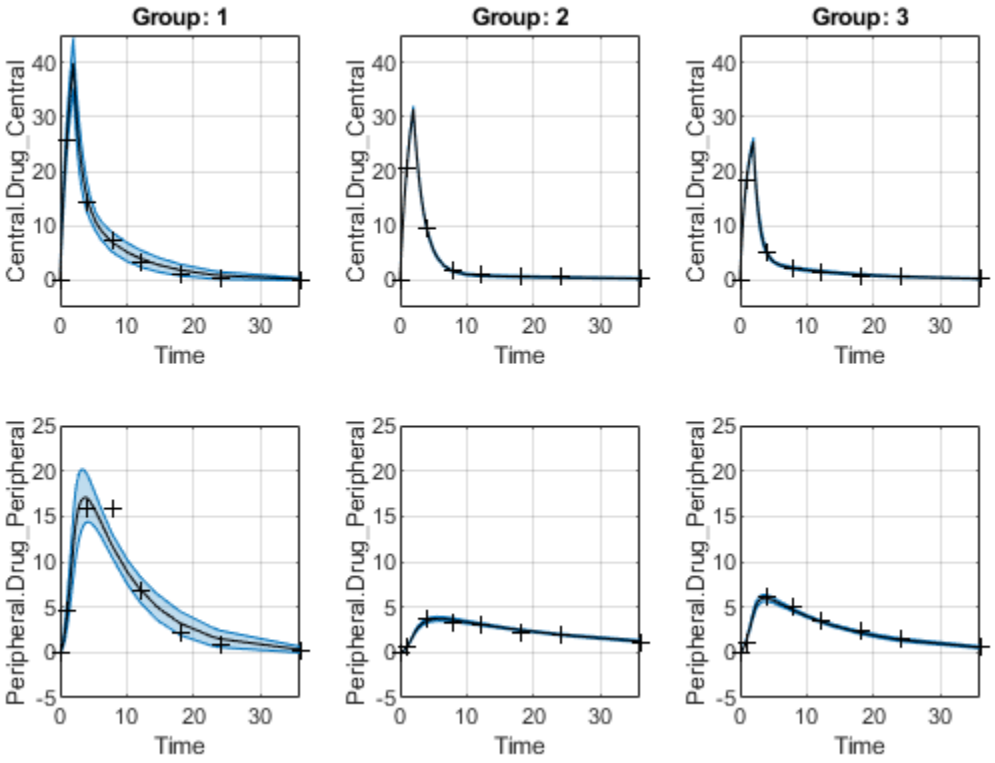
Plot Confidence Intervals for Model Predictions

The confidence interval for each group is plotted in a separate column, and each response is plotted in a separate row. Confidence intervals limited by the bounds are plotted in red. Confidence intervals not limited by the bounds are plotted in blue.

```
plot(ciPredPooled)
```




```
plot(ciPredUnpooled)
```



Input Arguments

`paraCI` — Parameter confidence interval results

`ParameterConfidenceInterval` object | vector

Parameter confidence interval results, specified as a `ParameterConfidenceInterval` object or a vector of objects.

Output Arguments

`tbl` — Summary table for confidence interval results

Summary table for confidence interval results, returned as a `table`. The table contains the following columns.

Column Name	Description
Group	Group name
Name	Estimated parameter name
Estimate	Estimated parameter value
ConfidenceInterval	Confidence interval values
Type	Confidence interval type

Column Name	Description
Alpha	Confidence level
Status	Confidence interval estimation status (for details, see “Parameter Confidence Interval Estimation Status” on page 2-666)

Version History

Introduced in R2017b

See Also

`ParameterConfidenceInterval` | `sbioparameterci`

commit (variant)

Commit variant contents to model

Syntax

`commit(`*`variantObj`*`, `*`modelObj`*`)`

Arguments

`modelObj`	Specify the model object to which you want to commit a variant.
`variantObj`	Variant object to commit to the model object.

Description

`commit(`*`variantObj`*`, `*`modelObj`*`)` commits the `Contents` property of a SimBiology variant object (*`variantObj`*) to the model object *`modelObj`*. The property values stored in the variant object replace the values stored in the model.

A SimBiology variant object stores alternate values for properties on a SimBiology model. For more information on variants, see `Variant object`.

The `Contents` are set on the model object in order of occurrence, with duplicate entries overwriting. If the `commit` method finds an incorrectly specified entry, an error occurs and the remaining properties defined in the `Contents` property are not set.

Examples

1. Create a model containing one species.

```
modelObj = sbiomodel('mymodel');
compObj = addcompartment(modelObj, 'comp1');
speciesObj = addspecies(compObj, 'A', 10);
```

2. Add a variant object that varies the `InitialAmount` property of a species named A.

```
variantObj = addvariant(modelObj, 'v1');
addcontent(variantObj, {'species', 'A', 'InitialAmount', 5});
```

3. Commit the contents of the variant (*`variantObj`*).

```
commit (variantObj, modelObj);
```

See Also

`addvariant`, `Variant object`

Version History

Introduced in R2007b

Compartment object

Object containing compartment information

Description

The SimBiology compartment object represents a container for species in a model. Compartment size can vary or remain constant during a simulation. All models must have at least one compartment and all species in a model must be assigned to a compartment. Compartment names must be unique within a model.

Compartments allow you to define the size (`Capacity`) of physically isolated regions that may affect simulation, and associate pools of species within those regions. You can specify or change `Capacity` using rules, events, and variants, similar to species amounts or parameter values.

The model object stores compartments as a flat list. Each compartment stores information on its own organization; in other words a compartment has information on which compartment it lives within (`Owner`) and who it contains (`Compartments`).

The flat list of compartments in the model object lets you vary the way compartments are organized in your model without invalidating any expressions.

To add species that participate in reactions, add the reaction to the model using the `addreaction` method. When you define a reaction with a new species:

- If no compartment objects exist in the model, the `addreaction` method creates a compartment object (called `'unnamed'`) in the model and adds the newly created species to that compartment.
- If only one compartment object exists in the model, the method creates a species object in that compartment.
- If there is more than one compartment object in the model, you must qualify the species name with the compartment name.

  For example, `cell.glucose` denotes that you want to put the species named `glucose` into a compartment named `cell`. Additionally, if the compartment named `cell` does not exist, the process of adding the reaction creates the compartment and names it `cell`.

Alternatively, create and add a species object to a compartment object, using the `addspecies` method at the command line.

When you use the SimBiology desktop to create a new model, it adds an empty compartment (*unnamed*), to which you can add species.

You can specify reactions that cross compartments using the syntax *compartment1Name*`.`*species1Name* `->` *compartment2Name*`.`*species2Name*. If you add a reaction that contains species from different compartments, and the reaction rate dimensions are concentration/time, all reactants should be from the same compartment.

In addition, if the reaction is reversible then there are two cases:

- If the kinetic law is `MassAction`, and the reaction rate reaction rate dimensions are concentration/time, then the products must be from the same compartment.

- If the kinetic law is not `MassAction`, then both reactants and products must be in the same compartment.

See “Property Summary” on page 2-166 for links to compartment property reference pages.
Properties define the characteristics of an object. Use the `get` and `set` commands to list object properties and change their values at the command line. You can graphically change object properties in the graphical user interface.

Constructor Summary

addcompartment (model, compartment)	Create compartment object

Method Summary

Methods for compartment objects

addcompartment (model, compartment)	Create compartment object
addspecies (model, compartment)	Create species object and add to compartment object within model object
copyobj	Copy SimBiology object and its children
delete	Delete SimBiology object
display	Display summary of SimBiology object
findUsages	Find out how a species, parameter, or compartment is used in a model
get	Get SimBiology object properties
move	Move SimBiology compartment object to new owner
rename	Rename object and update expressions
reorder (model, compartment, kinetic law)	Reorder component lists
set	Set SimBiology object properties

Property Summary

Properties for compartment objects

Capacity	Compartment capacity
CapacityUnits	Compartment capacity units
Compartments	Array of compartments in model or compartment
Constant	Specify variable or constant species amount, parameter value, or compartment capacity
ConstantCapacity	Specify variable or constant compartment capacity
Name	Specify name of object
Notes	HTML text describing SimBiology object
Owner	Owning compartment
Parent	Indicate parent object
Species	Array of species in compartment object
Tag	Specify label for SimBiology object
Type	Display SimBiology object type
Units	Units for species amount, parameter value, compartment capacity, observable expression
UserData	Specify data to associate with object
Value	Value of species, compartment, or parameter object

See Also

`AbstractKineticLaw object`, `Configset object`, `KineticLaw object`, `Model object`, `Parameter object`, `Reaction object`, `Root object`, `Rule object`

Version History

Introduced in R2008a

ConfidenceInterval

Object containing confidence interval results

Description

The `ConfidenceInterval` object is a superclass of two confidence interval objects: `PredictionConfidenceInterval` and `ParameterConfidenceInterval`. These objects contain confidence interval results computed with `sbiopredictionci` and `sbioparameterci`, respectively.

Properties

Type — Confidence interval type

`'gaussian'` | `'profilelikelihood'` | `'bootstrap'`

This property is read-only.

Confidence interval type, specified as `'gaussian'`, `'profileLikelihood'` (for `ParameterConfidenceInterval` only), or `'bootstrap'`

Example: `'bootstrap'`

GroupNames — Original group names from data used for fitting

cell array of character vectors

This property is read-only.

Original group names from the data used for fitting the model, specified as a cell array of character vectors. Each cell contains the name of a group.

Example: `{'1'}{'2'}{'3'}`

Alpha — Confidence level

positive scalar

This property is read-only.

Confidence level, `(1-`*`Alpha`*`) * 100%`, specified as a positive scalar between 0 and 1.

Example: `0.01`

Results — Confidence interval data

table

This property is read-only.

Confidence interval data, specified as a table.

ExitFlags — Exit flags returned during calculation of bootstrap confidence intervals

vector

This property is read-only.

Exit flags returned during the calculation of `bootstrap` confidence intervals only, specified as a vector of integers. Each integer is an exit flag returned by the estimation function (except `nlinfit`) used to fit parameters during bootstrapping. The same estimation function used in the original fit is used for bootstrapping.

Each flag indicates the success or failure status of the fitting performed to create a bootstrap sample. Refer to the reference page of the corresponding estimation function for the meaning of the exit flag.

If the estimation function does not return an exit flag, `ExitFlags` is set to `[]`. For the `gaussian` and `profileLikelihood` confidence intervals, `ExitFlags` is not supported and is always set to `[]`.

Version History

Introduced in R2017b

See Also

`sbioparameterci` | `sbiopredictionci` | `ParameterConfidenceInterval` | `PredictionConfidenceInterval`

Configset object

Solver settings information for model simulation

Description

The SimBiology configset object, also known as the configuration set object, contains the options that the solver uses during simulation of the model object. The configuration set object contains the following options for you to choose:

- Type of solver
- Stop time for the simulation
- Solver error tolerances, and for ode solvers — the maximum time step the solver should take
- Whether to perform sensitivity analysis during simulation
- Whether to perform dimensional analysis and unit conversion during simulation
- Species and parameter input factors for sensitivity analysis

A SimBiology model can contain multiple configsets with one being active at any given time. The active configset contains the settings that are used during the simulation. Use the method `setactiveconfigset` to define the active configset. Use the method `getconfigset` to return a list of configsets contained by a model. Use the method `addconfigset` to add a new configset to a model.

Warning The `Active` property of the `configset object` will be removed in a future release. Explicitly specify a `configset object` as an input argument when you simulate a model using `sbiosimulate`.

See “Property Summary” on page 2-171 for links to configset object property reference pages.

Properties define the characteristics of an object. Use the `get` and `set` commands to list object properties and change their values at the command line. You can graphically change object properties in the SimBiology desktop.

Constructor Summary

addconfigset (model)	Create configuration set object and add to model object

Method Summary

copyobj	Copy SimBiology object and its children
delete	Delete SimBiology object
display	Display summary of SimBiology object
get	Get SimBiology object properties
set	Set SimBiology object properties

Property Summary

Active	Indicate object in use during simulation
AmountUnits	Amount unit used internally during simulation when UnitConversion is on
CompileOptions	Dimensional analysis and unit conversion options
MassUnits	Mass unit used internally during simulation when UnitConversion is on
MaximumNumberOfLogs	Maximum number of logs criteria to stop simulation
MaximumWallClock	Maximum elapsed wall clock time to stop simulation
Name	Specify name of object
Notes	HTML text describing SimBiology object
RuntimeOptions	Options for logged species
SensitivityAnalysisOptions	Specify sensitivity analysis options
SolverType	Select solver type for simulation
StopTime	Simulation time criteria to stop simulation
TimeUnits	Show time units for dosing and simulation
Type	Display SimBiology object type

See Also

`AbstractKineticLaw object`, `KineticLaw object`, `Model object`, `Parameter object`, `Reaction object`, `Root object`, `Rule object`, `Species object`

Version History

Introduced in R2006b

construct (PKModelDesign)

Construct SimBiology model from `PKModelDesign` object

Syntax

```
[modelObj, pkModelMapObject] = construct(pkModelDesignObject)
[modelObj, pkModelMapObject, CovModelObj] = construct(pkModelDesignObject)
```

Arguments

modelObj	SimBiology model object specifying a pharmacokinetic model.
pkModelMapObject	Defines the roles of the components in *modelObj*. For details, see `PKModelMap object`.
CovModelObj	Defines the relationship between parameters and covariates. For details, see `CovariateModel`.

Description

`[modelObj, pkModelMapObject] = construct(pkModelDesignObject)` constructs a SimBiology model object, *modelObj*, containing the model components (such as compartments, species, reactions, and rules) required to represent the pharmacokinetic model specified in *pkModelDesignObject*. It also constructs *pkModelMapObject*, a `PKModelMap` object, which defines the roles of the model components.

The newly constructed model object, *modelObj*, is named `'Generated Model'` (which you can change). It contains one compartment for each compartment specified in the `PKCompartment` property of *pkModelDesignObject*. Each compartment contains a species that represents a drug concentration. The compartments are connected with reversible reactions that models flux between compartments.

`[modelObj, pkModelMapObject, CovModelObj] = construct(pkModelDesignObject)` constructs *CovModelObj*, a `CovariateModel` object, which defines the relationship between parameters and covariates. Within the `Expression` property of *CovModelObj*, each parameter being estimated has an expression of the form `parameterName = exp(theta1 + eta1)` (without covariate dependencies), where `theta1` is a fixed effect, and `eta1` is a random effect. You can modify the expressions to add covariate dependencies. For details, see `CovariateModel`.

Version History

Introduced in R2009a

See Also

`PKModelDesign object` | `PKModelMap object` | `CovariateModel`

Topics

“Create a Pharmacokinetic Model Using the Command Line”
“Model the Population Pharmacokinetics of Phenobarbital in Neonates”

“Specify a Covariate Model”

constructDefaultFixedEffectValues

Create structure containing initial estimates fixed effects needed for fit

Syntax

```
FEInitEstimates = constructDefaultFixedEffectValues(CovModel)
```

Description

`FEInitEstimates = constructDefaultFixedEffectValues(CovModel)` returns `FEInitEstimates`, a structure containing the initial estimates for the fixed effects in `CovModel`, a `CovariateModel` object. By default, the values of initial estimates are set to zero.

Examples

Specify a Covariate Model

Create an empty `CovariateModel` object.

```
covModel = CovariateModel;
```

Set its Expression property to define the relationships between parameters (*Cl*, *V*, and *k*) and covariate (*w*). You must use `theta` as a prefix for all fixed effects and `eta` for random effects.

```
covModel.Expression = ["Cl = theta1 + theta2*w + eta1","V = theta3 + eta2","k = theta4 + eta3"];
```

Display the names of fixed effects.

```
covModel.FixedEffectNames
```

```
ans = 4x1 cell
    {'theta1'}
    {'theta3'}
    {'theta4'}
    {'theta2'}
```

The `FixedEffectDescription` property displays which fixed effects correspond to which parameter. For instance, *theta1* is the fixed effect for the *Cl* parameter, and *theta2* is the fixed effect for the weight covariate that has a correlation with *Cl* parameter, denoted as *Cl/w*.

```
covModel.FixedEffectDescription
```

```
ans = 4x1 cell
    {'Cl'  }
    {'V'   }
    {'k'   }
    {'Cl/w'}
```

Specify initial estimates for the fixed effects. Create a default structure containing initial estimates using the `constructDefaultFixedEffectValues` function.

```
initialEstimates = constructDefaultFixedEffectValues(covModel)
```

```
initialEstimates = struct with fields:
    theta1: 0
    theta3: 0
    theta4: 0
    theta2: 0
```

Update the initial estimate value of each fixed effects.

```
initialEstimates.theta1 = 1.20;
initialEstimates.theta2 = 0.30;
initialEstimates.theta3 = 0.90;
initialEstimates.theta4 = 0.10;
```

Update the `FixedEffectValues` property to use the updated initial estimates.

```
covModel.FixedEffectValues = initialEstimates;
```

Check the covariate model for errors.

```
verify(covModel)
```

Perform Nonlinear Mixed-Effects Estimation

Estimate nonlinear mixed-effects parameters using clinical pharmacokinetic data collected from 59 infants. Evaluate the fitted model given new data or dosing information.

Load Data

This example uses data collected on 59 preterm infants given phenobarbital during the first 16 days after birth [1]. `ds` is a table containing the concentration-time profile data and covariate information for each infant (or group).

```
load pheno.mat ds
```

Convert to groupedData

Convert the data to the groupedData format for parameter estimation.

```
data = groupedData(ds);
```

Display the first few rows of `data`.

```
data(1:5,:)
```

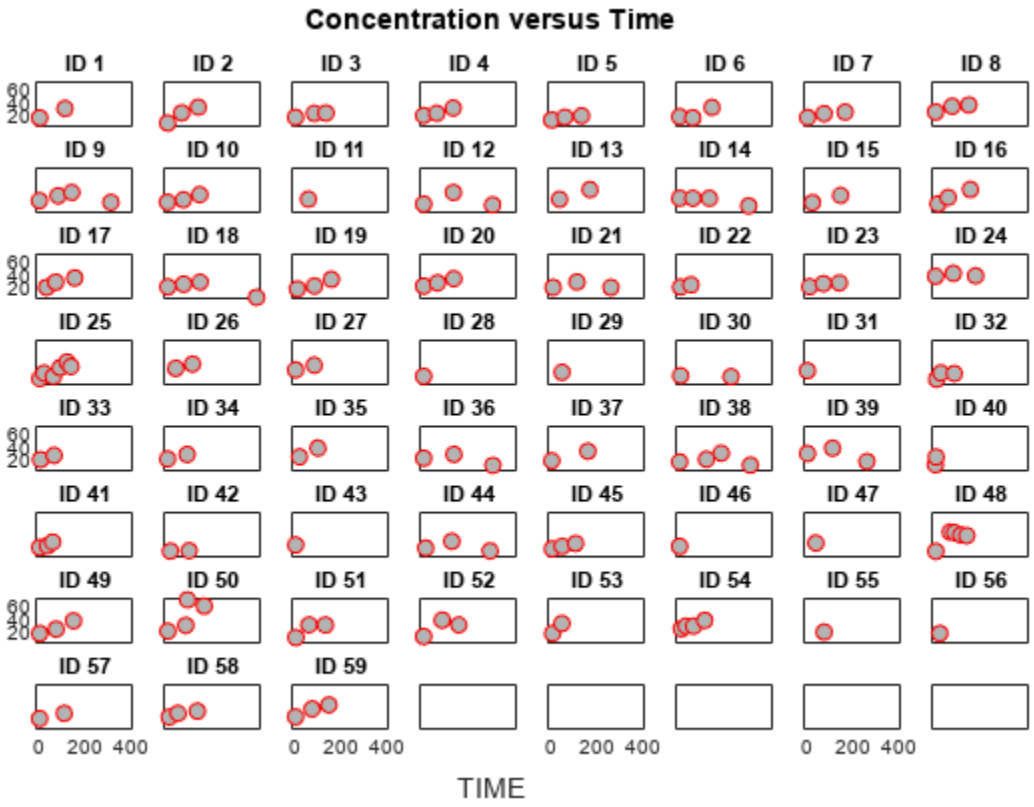
```
ans =

  5x6 groupedData

    ID    TIME    DOSE    WEIGHT    APGAR    CONC
    __    ____    ____    ______    _____    ____

    1        0     25       1.4        7       NaN
    1        2    NaN       1.4        7      17.3
```

```
    1     12.5    3.5     1.4       7       NaN
    1     24.5    3.5     1.4       7       NaN
    1       37    3.5     1.4       7       NaN
```

Visualize Data

Display the data in a trellis plot.

```
t = sbiotrellis(data, 'ID', 'TIME', 'CONC', 'marker', 'o',...
       'markerfacecolor', [.7 .7 .7], 'markeredgecolor', 'r', ...
       'linestyle', 'none');
t.plottitle = 'Concentration versus Time';
```



Create a One-Compartment PK Model

Create a simple one-compartment PK model, with bolus dose administration and linear clearance elimination, to fit the data.

```
pkmd = PKModelDesign;
addCompartment(pkmd,'Central','DosingType','Bolus',...
                    'EliminationType','linear-clearance',...
                    'HasResponseVariable',true,'HasLag',false);
onecomp = pkmd.construct;
```

Map model species to response data.

```
responseMap = 'Drug_Central = CONC';
```

Define Estimated Parameters

The parameters to estimate in this model are the volume of the central compartment (`Central`) and the clearance rate (`Cl_Central`). `sbiofitmixed` calculates fixed and random effects for each parameter. The underlying algorithm computes normally distributed random effects, which might violate constraints for biological parameters that are always positive, such as volume and clearance. Therefore, specify a transform for the estimated parameters so that the transformed parameters follow a normal distribution. The resulting model is

$$log(V_i) = log(\phi_{V,i}) = \theta_V + \eta_{V,i}$$

and

$$log(Cl_i) = log(\phi_{Cl,i}) = \theta_{Cl} + \eta_{Cl,i},$$

where θ, *eta*, and ϕ are the fixed effects, random effects, and estimated parameter values respectively, calculated for each infant (group) i. Some arbitrary initial estimates for V (volume of central compartment) and Cl (clearance rate) are used here in the absence of better empirical data.

```
estimatedParams = estimatedInfo({'log(Central)','log(Cl_Central)'},'InitialValue',[1 1]);
```

Define Dosing

All infants were given the drug, represented by the `Drug_Central` species, where the dosing schedule varies among infants. The amount of drug is listed in the data variable DOSE. You can automatically generate dose objects from the data and use them during fitting. In this example, `Drug_Central` is the target species that receives the dose.

```
sampleDose = sbiodose('sample','TargetName','Drug_Central');
doses = createDoses(data,'DOSE','',sampleDose);
```

Fit the Model

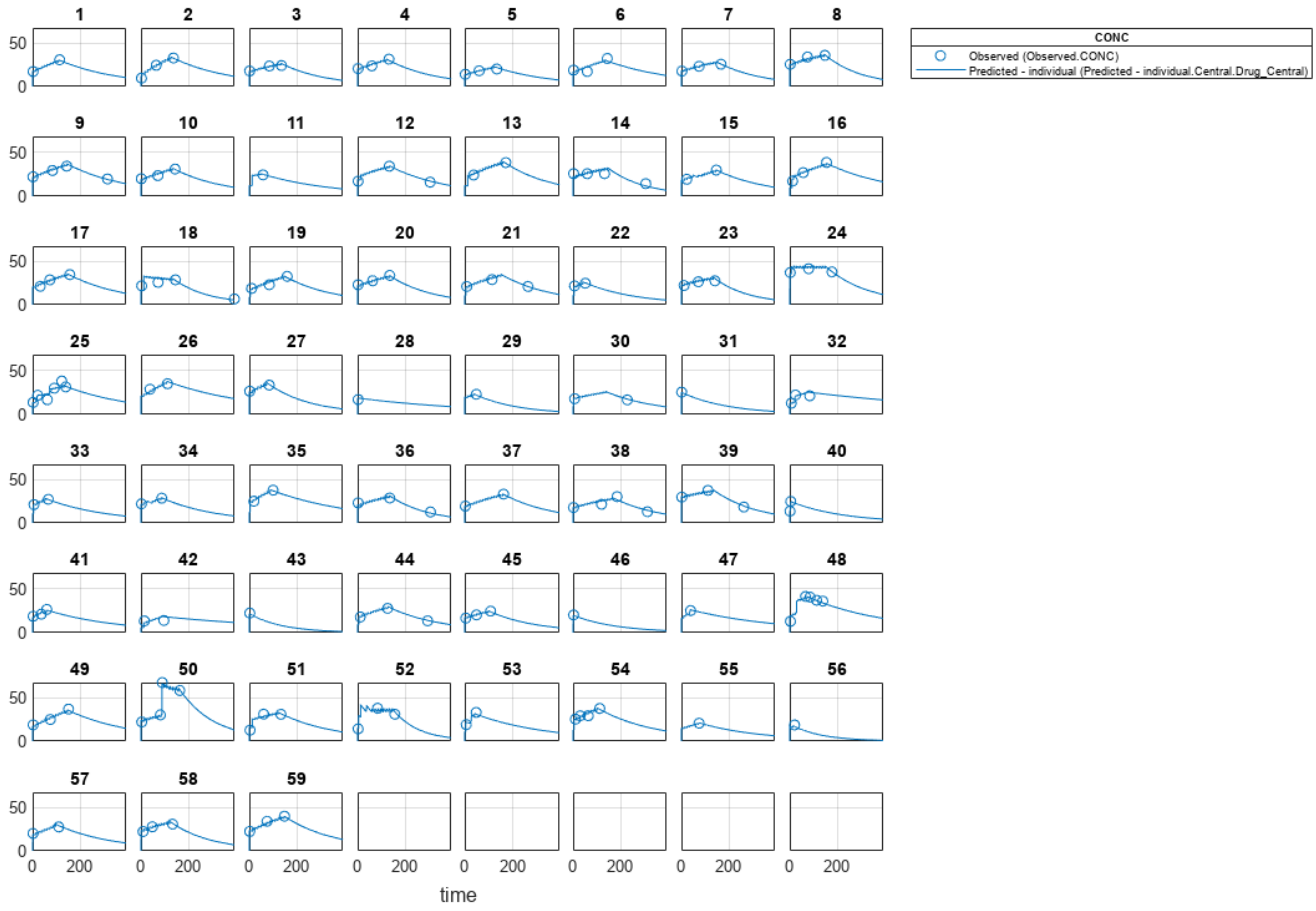
Use `sbiofitmixed` to fit the one-compartment model to the data.

```
nlmeResults = sbiofitmixed(onecomp,data,responseMap,estimatedParams,doses,'nlmefit');
```

Visualize Results

Visualize the fitted results using individual-specific parameter estimates.

```
plot(nlmeResults,'ParameterType','individual');
```



Use New Dosing Data to Simulate the Fitted Model

Suppose you want to predict how infants 1 and 2 would have responded under different dosing amounts. You can predict their responses as follows.

Create new dose objects with new dose amounts.

```
dose1 = doses(1);
dose1.Amount = dose1.Amount*2;
dose2 = doses(2);
dose2.Amount = dose2.Amount*1.5;
```

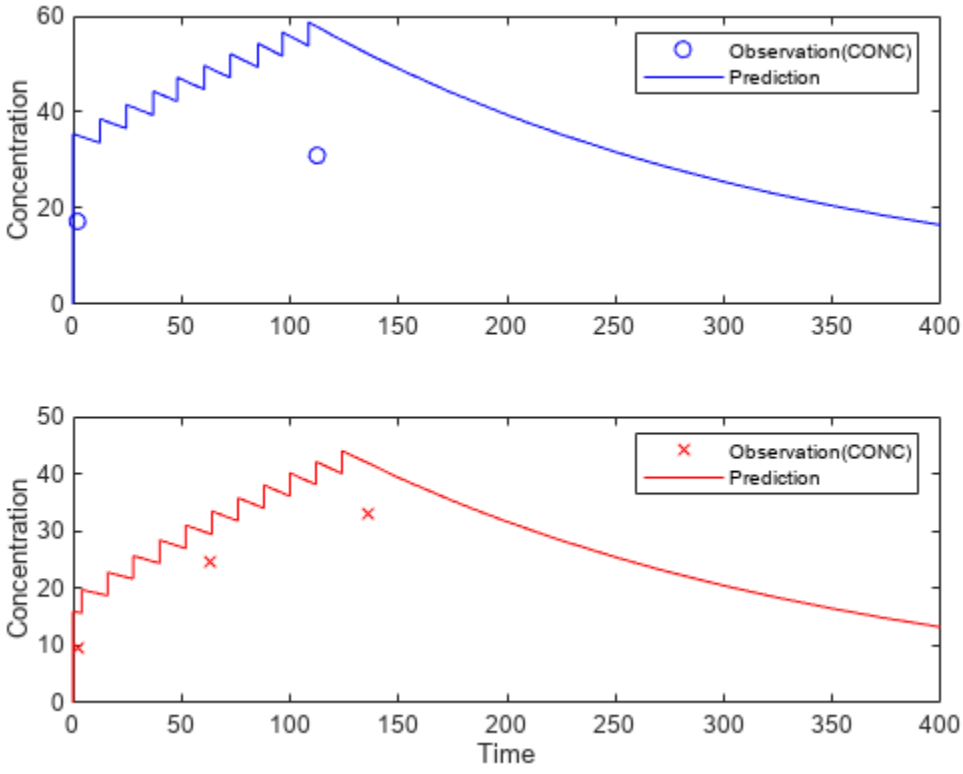
Use the `predict` function to evaluate the fitted model using the new dosing data. If you want response predictions at particular times, provide the new output time vector. Use the 'ParameterType' option to specify individual or population parameters to use. By default, `predict` uses the population parameters when you specify output times.

```
timeVec = [0:25:400];
newResults = predict(nlmeResults,timeVec,[dose1;dose2],'ParameterType','population');
```

Visualize the predicted responses while overlapping the experimental data for infants 1 and 2.

```
figure;
subplot(2,1,1)
plot(data.TIME(data.ID == 1),data.CONC(data.ID == 1),'bo')
```

```
hold on
plot(newResults(1).Time,newResults(1).Data,'b')
hold off
ylabel('Concentration')
legend('Observation(CONC)','Prediction')
subplot(2,1,2)
plot(data.TIME(data.ID == 2),data.CONC(data.ID == 2),'rx')
hold on
plot(newResults(2).Time,newResults(2).Data,'r')
hold off
legend('Observation(CONC)','Prediction')
ylabel('Concentration')
xlabel('Time')
```



Create a Covariate Model for the Covariate Dependencies

Suppose there is a correlation between volume and weight, and possibly volume and APGAR score. Consider the effect of weight by modeling two of these covariate dependencies: the volume of central (`Central`) and the clearance rate (`Cl_Central`) vary with weight. The model becomes

$$log(V_i) = log(\phi_{V,i}) = \theta_V + \theta_{V/weight} * weight_i + \eta_{V,i}$$

and

$$log(Cl_i) = log(\phi_{Cl,i}) = \theta_{Cl} + \theta_{Cl/weight} * weight_i + \eta_{Cl,i}$$

Use the `CovariateModel` object to define the covariate dependencies. For details, see “Specify a Covariate Model”.

```
covModel = CovariateModel;
covModel.Expression = ({'Central = exp(theta1 + theta2*WEIGHT + eta1)',...
                        'Cl_Central = exp(theta3 + theta4*WEIGHT + eta2)'});
```

Use `constructDefaultInitialEstimate` to create an `initialEstimates` struct.

```
initialEstimates = covModel.constructDefaultFixedEffectValues;
```

Use the `FixedEffectNames` property to display the thetas (fixed effects) defined in the model.

```
covModel.FixedEffectNames
```

```
ans = 4x1 cell
    {'theta1'}
    {'theta3'}
    {'theta2'}
    {'theta4'}
```

Use the `FixedEffectDescription` property to show the descriptions of corresponding fixed effects (thetas) used in the covariate expression. For example, `theta2` is the fixed effect for the weight covariate that correlates with the volume (`Central`), denoted as 'Central/WEIGHT'.

```
disp('Fixed Effects Description:');
```

```
Fixed Effects Description:
```

```
disp(covModel.FixedEffectDescription);
```

```
    {'Central'          }
    {'Cl_Central'       }
    {'Central/WEIGHT'   }
    {'Cl_Central/WEIGHT'}
```

Set the initial guesses for the fixed-effect parameter values for `Central` and `Cl_Central` using the values estimated from fitting the base model.

```
initialEstimates.theta1 = nlmeResults.FixedEffects.Estimate(1);
initialEstimates.theta3 = nlmeResults.FixedEffects.Estimate(2);
covModel.FixedEffectValues = initialEstimates;
```

Fit the Model

```
nlmeResults_cov = sbiofitmixed(onecomp,data,responseMap,covModel,doses,'nlmefit');
```

Display Fitted Parameters and Covariances

```
disp('Estimated Fixed Effects:');
```

```
Estimated Fixed Effects:
```

```
disp(nlmeResults_cov.FixedEffects);
```

```
       Name            Description          Estimate    StandardError
    ___________    ____________________    ________    _____________

    {'theta1'}    {'Central'          }    -0.45664      0.078933
```

```
    {'theta3'}    {'Cl_Central'       }     -5.9519        0.1177
    {'theta2'}    {'Central/WEIGHT'   }     0.52948      0.047342
    {'theta4'}    {'Cl_Central/WEIGHT'}     0.61954      0.071386
```

```
disp('Estimated Covariance Matrix:');
```

```
Estimated Covariance Matrix:
```

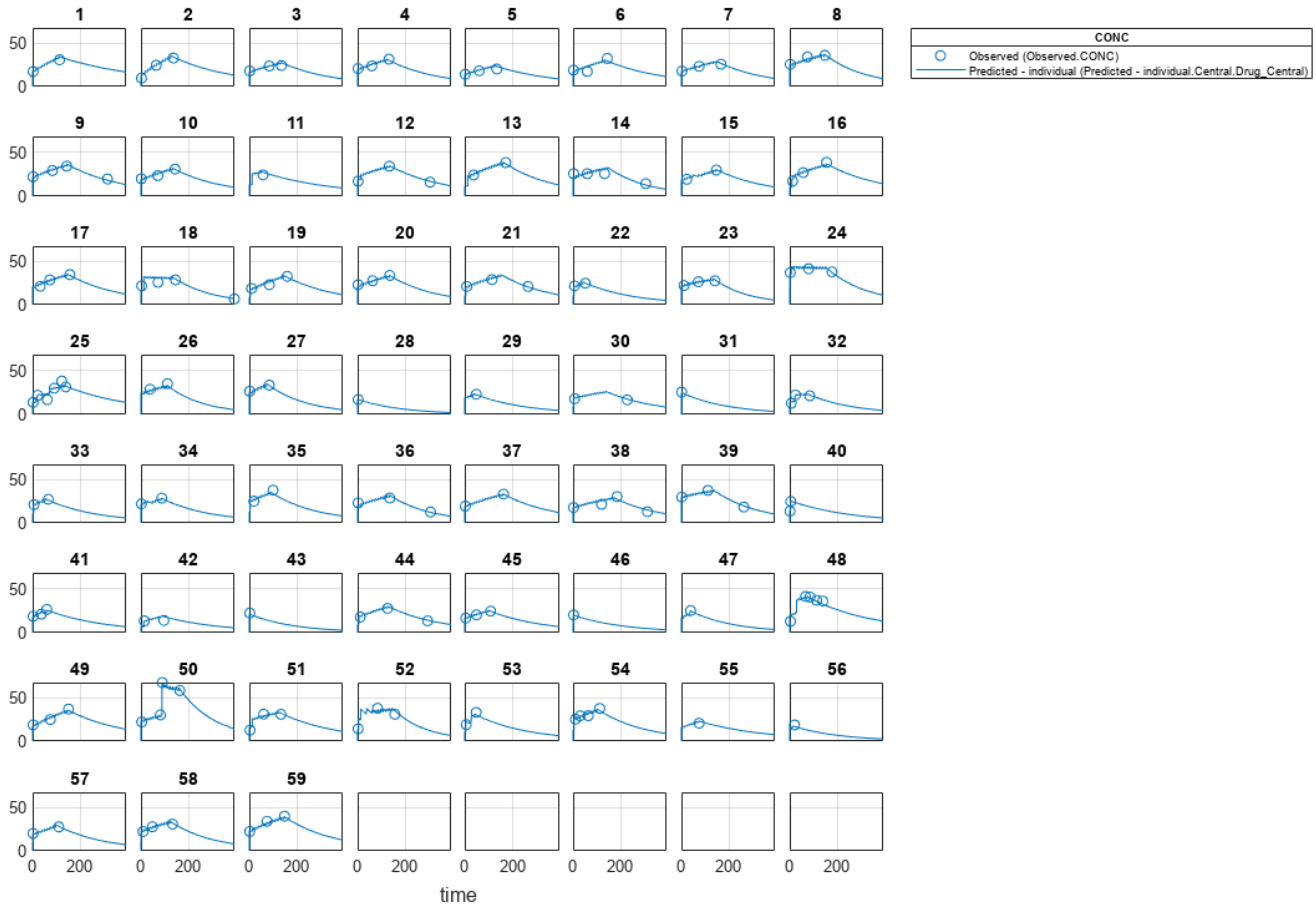
```
disp(nlmeResults_cov.RandomEffectCovarianceMatrix);
```

```
              eta1         eta2
            ________    ________

    eta1    0.046503           0
    eta2           0    0.041609
```

Visualize Results

Visualize the fitted results using individual-specific parameter estimates.

```
plot(nlmeResults_cov,'ParameterType','individual');
```



Use New Covariate Data to Evaluate the Fitted Model

Suppose you want to explore the responses of infants 1 and 2 using different covariate data, namely `WEIGHT`. You can do this by specifying the new `WEIGHT` data. The `ID` variable of the data corresponds to individual infants.

```
newData = data(data.ID == 1 | data.ID == 2,:);
newData.WEIGHT(newData.ID == 1) = 1.3;
newData.WEIGHT(newData.ID == 2) = 1.4;
```

Simulate the responses of infants 1 and 2 using the new covariate data.

```
[newResults_cov, newEstimates] = predict(nlmeResults_cov,newData,[dose1;dose2]);
```

`newEstimates` contains the updated parameter estimates for each individual (infants 1 and 2) after the model is reevaluated using the new covariate data.

```
newEstimates
```

```
newEstimates=4×3 table
    Group          Name          Estimate
    _____    _______________    _________

      1      {'Central'   }       2.5596
      1      {'Cl_Central'}    0.0065965
      2      {'Central'   }       1.7123
      2      {'Cl_Central'}    0.0064806
```

Compare to the estimated values from the original fit using the old covariate data.

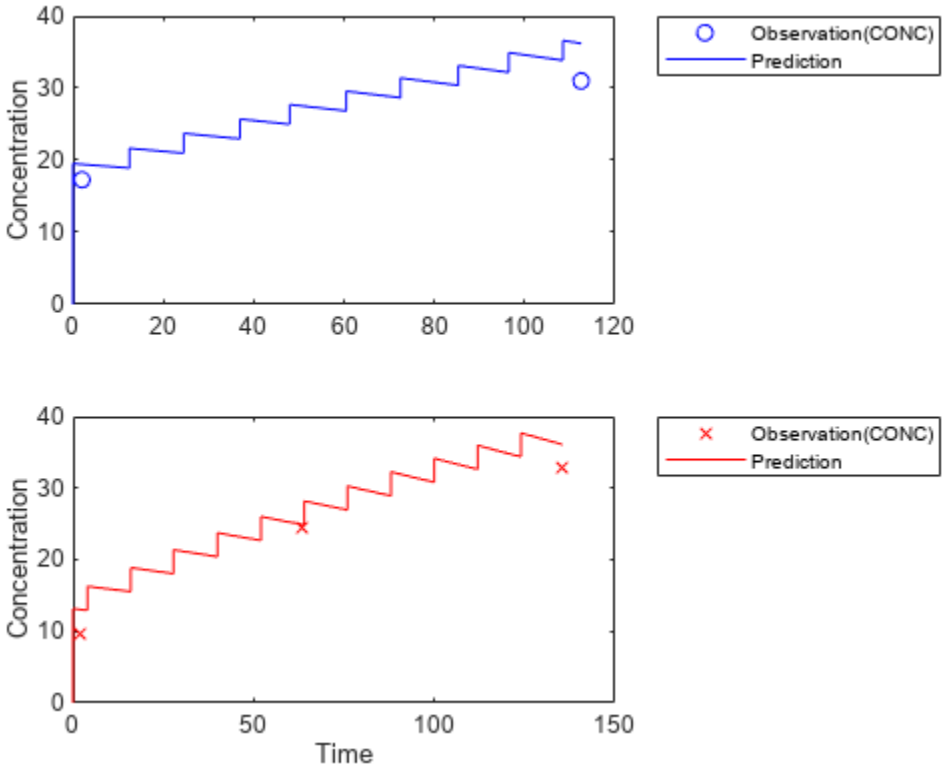
```
nlmeResults_cov.IndividualParameterEstimates( ...
            nlmeResults_cov.IndividualParameterEstimates.Group == '1' | ...
            nlmeResults_cov.IndividualParameterEstimates.Group == '2',:)
```

```
ans=4×3 table
    Group          Name          Estimate
    _____    _______________    _________

      1      {'Central'   }       2.6988
      1      {'Cl_Central'}    0.0070181
      2      {'Central'   }       1.8054
      2      {'Cl_Central'}    0.0068948
```

Visualize the new simulation results together with the experimental data for infant 1 and 2.

```
figure;
subplot(2,1,1);
plot(data.TIME(data.ID == 1),data.CONC(data.ID == 1),'bo')
hold on
plot(newResults_cov(1).Time,newResults_cov(1).Data,'b')
hold off
ylabel('Concentration')
legend('Observation(CONC)','Prediction','Location','NorthEastOutside')
subplot(2,1,2)
plot(data.TIME(data.ID == 2),data.CONC(data.ID == 2),'rx')
hold on
plot(newResults_cov(2).Time,newResults_cov(2).Data,'r')
```

```
hold off
legend('Observation(CONC)','Prediction','Location','NorthEastOutside')
ylabel('Concentration')
xlabel('Time')
```



References

[1] Grasela, T. H. Jr., and S. M. Donn. "Neonatal population pharmacokinetics of phenobarbital derived from routine clinical data." *Dev Pharmacol Ther* 1985:8(6). 374-83.

Input Arguments

`CovModel` — Covariate model

`CovariateModel` object

Covariate model, specified as a `CovariateModel` object.

Output Arguments

`FEInitEstimates` — Initial estimates for fixed effects

structure

Initial estimates for fixed effects, returned as a structure. Each field of the structure represents a fixed effect and its value. By default, the values of initial estimates are set to zero, but you can edit these estimates as needed. If you do, make sure that the number and names of the fields in the

`FEInitEstimates` structure matches the number and names of fixed effects (`theta` values) in the "Expression" on page 2-0 property of `CovModel`.

Version History

Introduced in R2011b

See Also

`CovariateModel`

Topics

"Specify a Covariate Model"
"Model the Population Pharmacokinetics of Phenobarbital in Neonates"

copyobj

Copy SimBiology object and its children

Syntax

```
copiedObj = copyobj(Obj, parentObj)
copiedObj = copyobj(modelObj)
```

Arguments

Obj	Compartment, configuration set, event, kinetic law, model, parameter, reaction, rule, species, RepeatDose, ScheduleDose, variant, or observable object. **Note** Abstract kinetic law objects cannot be copied using `copyobj`.
parentObj	**If *copiedObj* is...** / ***parentObj* must be...** configuration set, event, reaction, rule, RepeatDose, ScheduleDose, variant, or observable object — model object compartment object — compartment or model object species object — compartment object parameter object — model or kinetic law object kinetic law object — reaction object model object — `sbioroot`
modelObj	Model object to be copied.
copiedObj	Output returned by the `copyobj` method with the parent set as specified in input argument (*parentObj*).

Description

copiedObj = `copyobj(`*Obj, parentObj*`)` makes a copy of a SimBiology object (*Obj*) and returns a pointer to the copy (*copiedObj*). In the copied object (*copiedObj*), this method assigns a value (*parentObj*) to the property `Parent`.

copiedObj = `copyobj(`*modelObj*`)` makes a copy of a model object (*modelObj*) and returns the copy (*copiedObj*). In the copied model object (*copiedObj*), this method assigns the root object to the property `Parent`.

Note When the `copyobj` method copies a model, it resets the StatesToLog property to the default value. Similarly, the Inputs and Outputs properties are not copied but rather left empty. Thus, when you simulate a copied model you see results for the default states, unless you manually update these properties.

Examples

Create a reaction object separate from a model object, and then add it to a model.

1. Create a model object and add a reaction object.

```
modelObj1 = sbiomodel('cell');
reactionObj = addreaction(modelObj1, 'a -> b');
```

2. Create a copy of the `reaction object` and assign it to another `model object`.

```
modelObj2 = sbiomodel('cell2');
reactionObjCopy = copyobj(reactionObj, modelObj2);
modelObj2.Reactions

SimBiology Reaction Array

Index:    Reaction:
 1         a -> b
```

See Also

`sbiomodel`, `sbioroot`

Version History

Introduced in R2006a

CovariateModel

Define relationship between parameters and covariates

Description

A `CovariateModel` object defines the relationship between estimated parameters and covariates.

Use a `CovariateModel` object as an input argument to `sbiofitmixed` to fit a model with covariate dependencies. Before using the `CovariateModel` object, set the `FixedEffectValues` property to specify the initial estimates for the fixed effects.

Creation

Syntax

```
CovModelObj= CovariateModel
CovModelObj= CovariateModel(E)
```

Description

`CovModelObj= CovariateModel` creates an empty `CovariateModel` object.

`CovModelObj= CovariateModel(E)` creates a `CovariateModel` object with its `Expression` property set to `E`, which defines the relationships between estimated parameters and one or more covariates.

Input Arguments

E — Expression to define parameter-covariate relationships

character vector | string | string vector | cell array of character vectors

Expression to define the parameter-covariate relationships, specified as a character vector, string, string vector, or cell array of character vectors.

Denote fixed effects with the prefix `theta`, and random effects with the prefix `eta`. The expression must be in the form: `parameterName = relationship`. Here is an example, `"volume = theta1 + theta2*weight"`. For details on additional requirements, see the “Expression” on page 2-0 property.

If a model component name or covariate name is not a valid MATLAB variable name, surround it by square brackets when referring to it in the expression. For example, if the name of a species is *DNA polymerase+*, write `[DNA polymerase+]`. If a covariate name itself contains square brackets, you cannot use it in the expression.

This table illustrates expression formats for some common parameter-covariate relationships.

Parameter-Covariate Relationship	Expression Format
Linear with random effect	`Cl = theta1 + theta2*WEIGHT + eta1`
Exponential without random effect	`Cl = exp(theta_Cl + theta_Cl_WT*WEIGHT)`
Exponential, WEIGHT centered by mean, has random effect	`Cl = exp(theta1 + theta2*(WEIGHT - mean(WEIGHT)) + eta1)`
Exponential, log(WEIGHT), which is equivalent to power model	`Cl = exp(theta1 + theta2*log(WEIGHT) + eta1)`
Exponential, dependent on WEIGHT and AGE, has random effect	`Cl = exp(theta1 + theta2*WEIGHT + theta3*AGE + eta1)`
Inverse of probit, dependent on WEIGHT and AGE, has random effect	`Cl = probitinv(theta1 + theta2*WEIGHT + theta3*AGE + eta1)`
Inverse of logit, dependent on WEIGHT and AGE, has random effect	`Cl = logitinv(theta1 + theta2*WEIGHT + theta3*AGE + eta1)`

Tip To simultaneously fit data from multiple dose levels, use a `CovariateModel` object as an input argument to `sbiofitmixed`, and omit the random effect (`eta`) from the `Expression` property in the `CovariateModel` object.

Properties

`CovariateLabels` — Labels for covariates

cell array of character vectors

This property is read-only.

Labels for covariates in the `Expression` property of the object, returned as a cell array of character vectors.

Data Types: `cell`

`Expression` — Relationships between parameters being estimated and covariates

cell array of character vectors

Relationships between parameters being estimated and covariates, returned as a cell array of character vectors.

The `Expression` property must meet the following requirements:

- The expressions are valid MATLAB code.
- Each expression is linear with a transformation.
- There is exactly one expression for each parameter.
- In each expression, a covariate is used in at most one term.

- In each expression, there is at most one random effect (`eta`)
- Fixed effect (`theta`) and random effect (`eta`) names are unique within and across expressions. That is, each covariate has its own fixed effect.

For examples of some common parameter-covariate relationships, see “E” on page 2-0 .

Tip

- To simultaneously fit data from multiple dose levels, use a `CovariateModel` object as an input argument to `sbiofitmixed`, and omit the random effect (`eta`) from the `Expression` property in the `CovariateModel` object.
- Use the `getCovariateData` on page 2-355 method to view the covariate data when writing equations for the `Expression` property of a `CovariateModel` object.
- Use the `verify` on page 2-933 method to check that the `Expression` property of a `CovariateModel` object meets the conditions described previously.

Data Types: `cell`

`FixedEffectDescription` — Descriptions of fixed effects

cell array of character vectors

This property is read-only.

Descriptions of fixed effects in the `Expression` property of the object, returned as a cell array of character vectors.

Each character vector describes the role of a fixed effect in the expression equation. For example, consider the following expression: $Cl = e^{\theta_1 + \theta_2 \times WEIGHT + \theta_3 \times AGE + \eta_1}$

At the command line, you can create a `CovariateModel` object using that expression.

```
cm = CovariateModel("Cl = exp(theta1 + theta2*WEIGHT + theta3*AGE + eta1)");
cm.FixedEffectDescription
```

```
ans =

  3×1 cell array

    {'Cl'       }
    {'Cl/WEIGHT'}
    {'Cl/AGE'   }
```

In this example, the description for the fixed effect `theta1` is `'Cl'`, which indicates it is the intercept for the parameter `Cl`. Also, the description for the fixed effect `theta2` is `'Cl/WEIGHT'`, which indicates it is the slope of the line that defines the relationship between the parameter `Cl` and the covariate `WEIGHT`. The description of `theta3` is `'Cl/AGE'`.

Data Types: `cell`

`FixedEffectNames` — Names of fixed effects

cell array of character vectors

This property is read-only.

Names of fixed effects in the `Expression` property of the object, returned as a cell array of character vectors. The names are denoted with the prefix `theta`.

Data Types: `cell`

`FixedEffectValues` — Values for initial estimates of fixed effects
structure

Values for initial estimates of fixed effects in the `Expression` property of the object, returned as a structure. Each field contains the value of the initial estimate for each fixed effect (`theta`).

Tip You must set this property before using the `CovariateModel` object as input to `sbionlmefit` or `sbionlmefitsa`. Use the `constructDefaultFixedEffectValues` on page 2-174 method to create a structure of fixed-effect (`theta`) initial estimate values, which are set to a default of zero. Then edit the structure to change the initial estimate values. Then set the structure as the value of this property. For an example, see “Specify a Covariate Model”.

Data Types: `struct`

`ParameterNames` — Names of parameters
cell array of character vectors

This property is read-only.

Names of parameters in the `Expression` property of the object, returned as a cell array of character vectors.

Data Types: `cell`

`RandomEffectNames` — Names of random effects
cell array of character vectors

This property is read-only.

Names of random effects in the `Expression` property of the object, returned as a cell array of character vectors. Each name is denoted with the prefix `eta`.

Data Types: `cell`

Object Functions

constructDefaultFixedEffectValues	Create structure containing initial estimates fixed effects needed for fit
verify	Check covariate model for errors

Examples

Specify a Covariate Model

Create an empty `CovariateModel` object.

```
covModel = CovariateModel;
```

Set its Expression property to define the relationships between parameters (*Cl*, *V*, and *k*) and covariate (*w*). You must use `theta` as a prefix for all fixed effects and `eta` for random effects.

```
covModel.Expression = ["Cl = theta1 + theta2*w + eta1","V = theta3 + eta2","k = theta4 + eta3"];
```

Display the names of fixed effects.

```
covModel.FixedEffectNames
```

```
ans = 4x1 cell
    {'theta1'}
    {'theta3'}
    {'theta4'}
    {'theta2'}
```

The `FixedEffectDescription` property displays which fixed effects correspond to which parameter. For instance, *theta1* is the fixed effect for the *Cl* parameter, and *theta2* is the fixed effect for the weight covariate that has a correlation with *Cl* parameter, denoted as *Cl/w*.

```
covModel.FixedEffectDescription
```

```
ans = 4x1 cell
    {'Cl'  }
    {'V'   }
    {'k'   }
    {'Cl/w'}
```

Specify initial estimates for the fixed effects. Create a default structure containing initial estimates using the `constructDefaultFixedEffectValues` function.

```
initialEstimates = constructDefaultFixedEffectValues(covModel)
```

```
initialEstimates = struct with fields:
    theta1: 0
    theta3: 0
    theta4: 0
    theta2: 0
```

Update the initial estimate value of each fixed effects.

```
initialEstimates.theta1 = 1.20;
initialEstimates.theta2 = 0.30;
initialEstimates.theta3 = 0.90;
initialEstimates.theta4 = 0.10;
```

Update the `FixedEffectValues` property to use the updated initial estimates.

```
covModel.FixedEffectValues = initialEstimates;
```

Check the covariate model for errors.

```
verify(covModel)
```

Perform Nonlinear Mixed-Effects Estimation

Estimate nonlinear mixed-effects parameters using clinical pharmacokinetic data collected from 59 infants. Evaluate the fitted model given new data or dosing information.

Load Data

This example uses data collected on 59 preterm infants given phenobarbital during the first 16 days after birth [1]. `ds` is a table containing the concentration-time profile data and covariate information for each infant (or group).

```
load pheno.mat ds
```

Convert to groupedData

Convert the data to the groupedData format for parameter estimation.

```
data = groupedData(ds);
```

Display the first few rows of `data`.

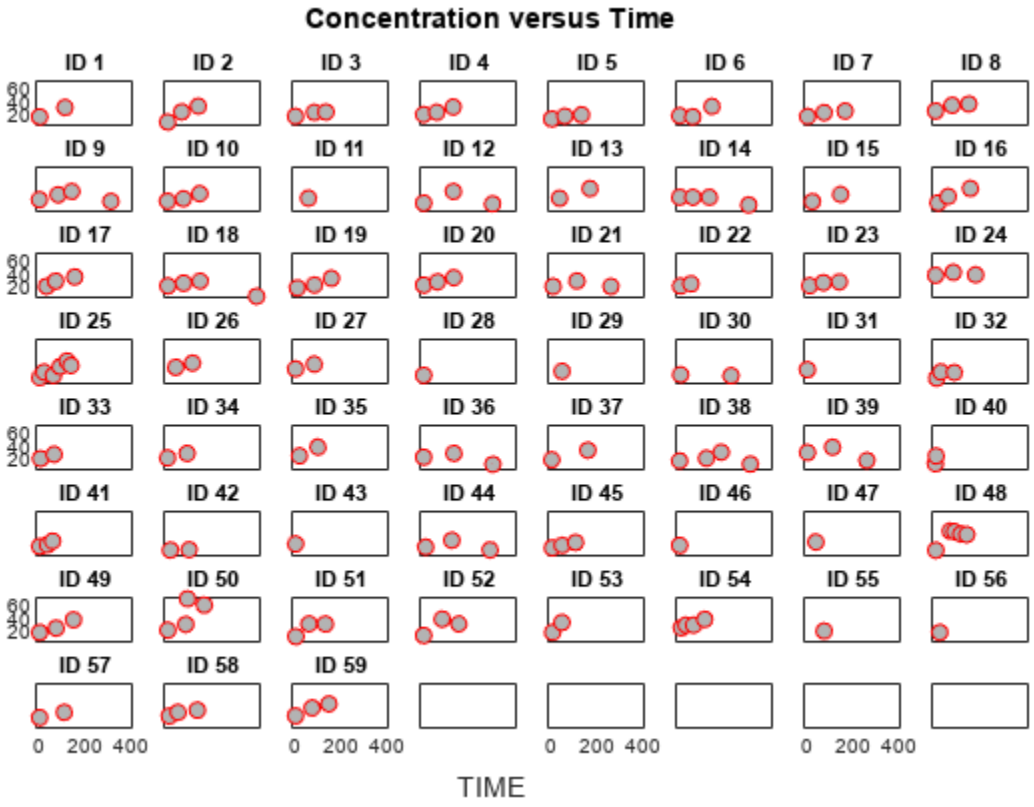
```
data(1:5,:)
```

```
ans =

  5x6 groupedData

    ID    TIME    DOSE    WEIGHT    APGAR    CONC
    __    ____    ____    ______    _____    ____

    1        0     25       1.4        7       NaN
    1        2    NaN       1.4        7      17.3
    1     12.5    3.5       1.4        7       NaN
    1     24.5    3.5       1.4        7       NaN
    1       37    3.5       1.4        7       NaN
```

Visualize Data

Display the data in a trellis plot.

```
t = sbiotrellis(data, 'ID', 'TIME', 'CONC', 'marker', 'o',...
       'markerfacecolor', [.7 .7 .7], 'markeredgecolor', 'r', ...
       'linestyle', 'none');
t.plottitle = 'Concentration versus Time';
```



Create a One-Compartment PK Model

Create a simple one-compartment PK model, with bolus dose administration and linear clearance elimination, to fit the data.

```
pkmd = PKModelDesign;
addCompartment(pkmd,'Central','DosingType','Bolus',...
                    'EliminationType','linear-clearance',...
                    'HasResponseVariable',true,'HasLag',false);
onecomp = pkmd.construct;
```

Map model species to response data.

```
responseMap = 'Drug_Central = CONC';
```

Define Estimated Parameters

The parameters to estimate in this model are the volume of the central compartment (`Central`) and the clearance rate (`Cl_Central`). `sbiofitmixed` calculates fixed and random effects for each parameter. The underlying algorithm computes normally distributed random effects, which might violate constraints for biological parameters that are always positive, such as volume and clearance. Therefore, specify a transform for the estimated parameters so that the transformed parameters follow a normal distribution. The resulting model is

$$log(V_i) = log(\phi_{V,i}) = \theta_V + \eta_{V,i}$$

and

$$log(Cl_i) = log(\phi_{Cl,i}) = \theta_{Cl} + \eta_{Cl,i},$$

where θ, *eta*, and ϕ are the fixed effects, random effects, and estimated parameter values respectively, calculated for each infant (group) i. Some arbitrary initial estimates for V (volume of central compartment) and Cl (clearance rate) are used here in the absence of better empirical data.

```
estimatedParams = estimatedInfo({'log(Central)','log(Cl_Central)'},'InitialValue',[1 1]);
```

Define Dosing

All infants were given the drug, represented by the `Drug_Central` species, where the dosing schedule varies among infants. The amount of drug is listed in the data variable DOSE. You can automatically generate dose objects from the data and use them during fitting. In this example, `Drug_Central` is the target species that receives the dose.

```
sampleDose = sbiodose('sample','TargetName','Drug_Central');
doses = createDoses(data,'DOSE','',sampleDose);
```

Fit the Model

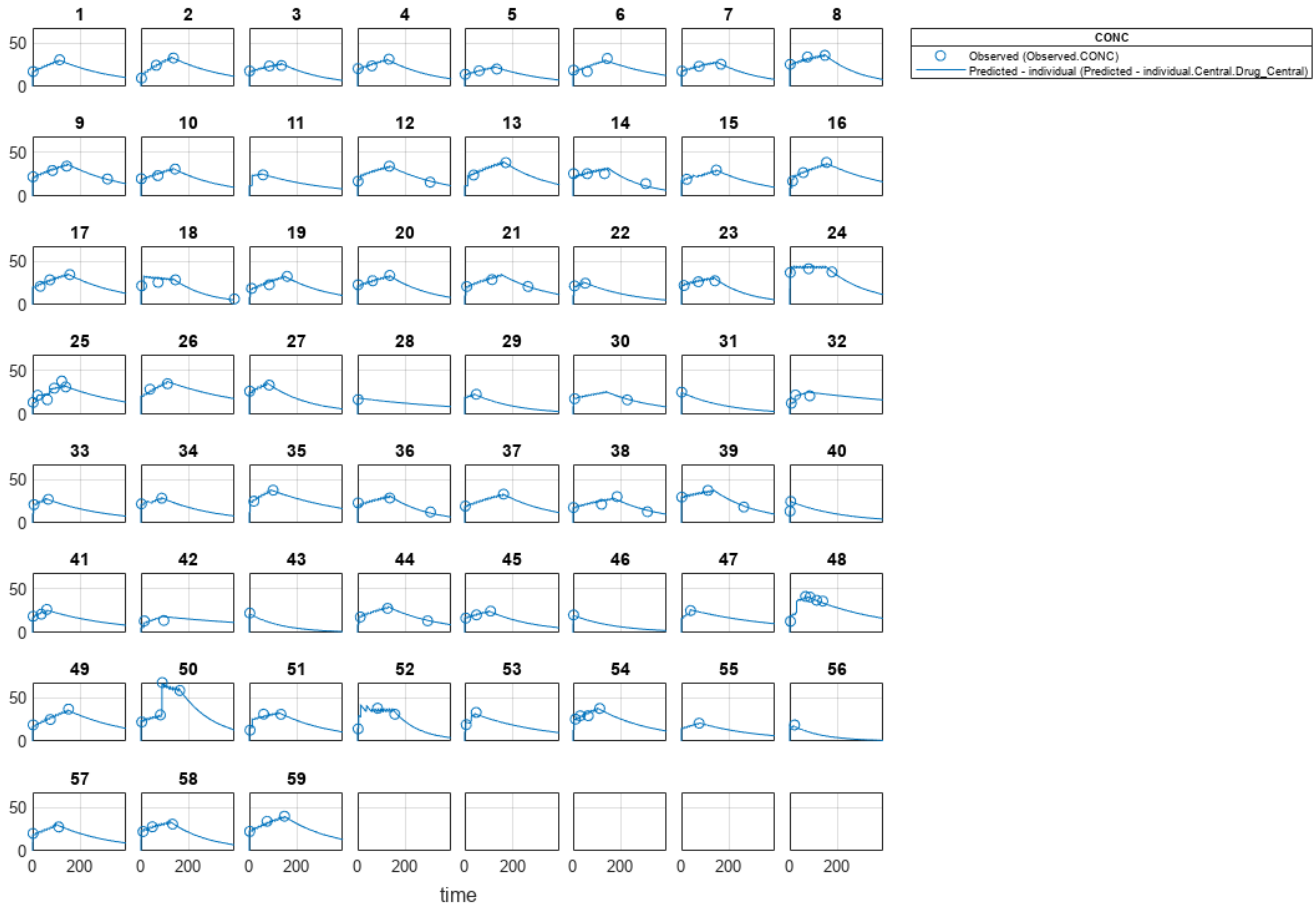
Use `sbiofitmixed` to fit the one-compartment model to the data.

```
nlmeResults = sbiofitmixed(onecomp,data,responseMap,estimatedParams,doses,'nlmefit');
```

Visualize Results

Visualize the fitted results using individual-specific parameter estimates.

```
plot(nlmeResults,'ParameterType','individual');
```



Use New Dosing Data to Simulate the Fitted Model

Suppose you want to predict how infants 1 and 2 would have responded under different dosing amounts. You can predict their responses as follows.

Create new dose objects with new dose amounts.

```
dose1 = doses(1);
dose1.Amount = dose1.Amount*2;
dose2 = doses(2);
dose2.Amount = dose2.Amount*1.5;
```

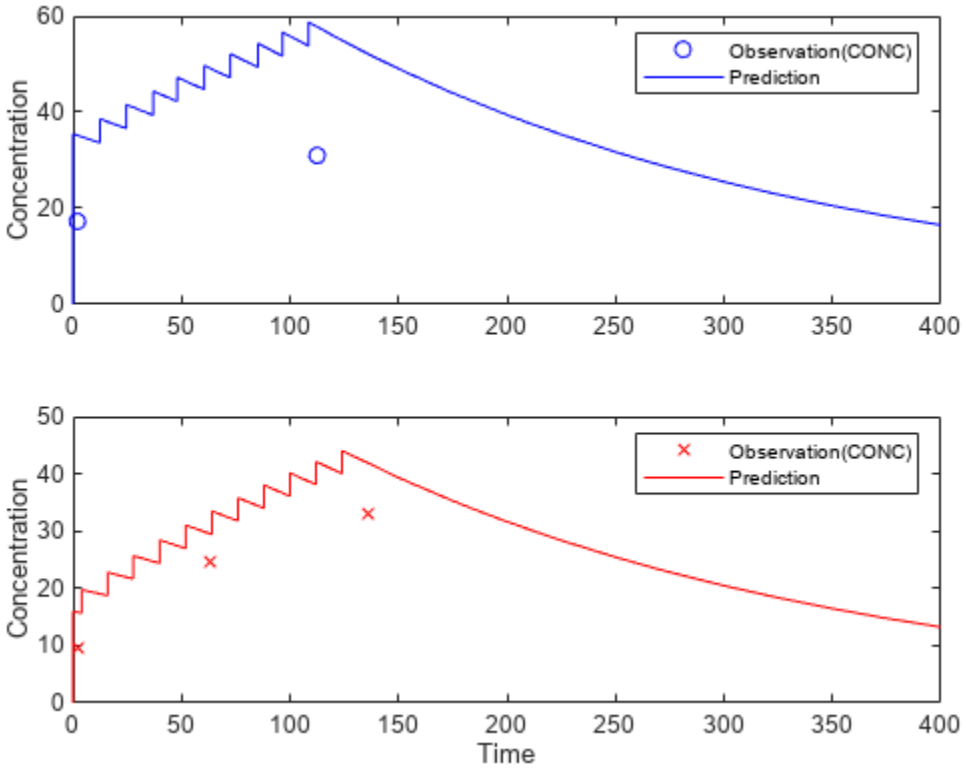
Use the `predict` function to evaluate the fitted model using the new dosing data. If you want response predictions at particular times, provide the new output time vector. Use the 'ParameterType' option to specify individual or population parameters to use. By default, `predict` uses the population parameters when you specify output times.

```
timeVec = [0:25:400];
newResults = predict(nlmeResults,timeVec,[dose1;dose2],'ParameterType','population');
```

Visualize the predicted responses while overlapping the experimental data for infants 1 and 2.

```
figure;
subplot(2,1,1)
plot(data.TIME(data.ID == 1),data.CONC(data.ID == 1),'bo')
```

```
hold on
plot(newResults(1).Time,newResults(1).Data,'b')
hold off
ylabel('Concentration')
legend('Observation(CONC)','Prediction')
subplot(2,1,2)
plot(data.TIME(data.ID == 2),data.CONC(data.ID == 2),'rx')
hold on
plot(newResults(2).Time,newResults(2).Data,'r')
hold off
legend('Observation(CONC)','Prediction')
ylabel('Concentration')
xlabel('Time')
```



Create a Covariate Model for the Covariate Dependencies

Suppose there is a correlation between volume and weight, and possibly volume and APGAR score. Consider the effect of weight by modeling two of these covariate dependencies: the volume of central (`Central`) and the clearance rate (`Cl_Central`) vary with weight. The model becomes

$$log(V_i) = log(\phi_{V,i}) = \theta_V + \theta_{V/weight} * weight_i + \eta_{V,i}$$

and

$$log(Cl_i) = log(\phi_{Cl,i}) = \theta_{Cl} + \theta_{Cl/weight} * weight_i + \eta_{Cl,i}$$

Use the `CovariateModel` object to define the covariate dependencies. For details, see “Specify a Covariate Model”.

```
covModel = CovariateModel;
covModel.Expression = ({'Central = exp(theta1 + theta2*WEIGHT + eta1)',...
                        'Cl_Central = exp(theta3 + theta4*WEIGHT + eta2)'});
```

Use `constructDefaultInitialEstimate` to create an `initialEstimates` struct.

```
initialEstimates = covModel.constructDefaultFixedEffectValues;
```

Use the `FixedEffectNames` property to display the thetas (fixed effects) defined in the model.

```
covModel.FixedEffectNames
```

```
ans = 4x1 cell
    {'theta1'}
    {'theta3'}
    {'theta2'}
    {'theta4'}
```

Use the `FixedEffectDescription` property to show the descriptions of corresponding fixed effects (thetas) used in the covariate expression. For example, `theta2` is the fixed effect for the weight covariate that correlates with the volume (`Central`), denoted as 'Central/WEIGHT'.

```
disp('Fixed Effects Description:');
```

```
Fixed Effects Description:
```

```
disp(covModel.FixedEffectDescription);
```

```
    {'Central'          }
    {'Cl_Central'       }
    {'Central/WEIGHT'   }
    {'Cl_Central/WEIGHT'}
```

Set the initial guesses for the fixed-effect parameter values for `Central` and `Cl_Central` using the values estimated from fitting the base model.

```
initialEstimates.theta1 = nlmeResults.FixedEffects.Estimate(1);
initialEstimates.theta3 = nlmeResults.FixedEffects.Estimate(2);
covModel.FixedEffectValues = initialEstimates;
```

Fit the Model

```
nlmeResults_cov = sbiofitmixed(onecomp,data,responseMap,covModel,doses,'nlmefit');
```

Display Fitted Parameters and Covariances

```
disp('Estimated Fixed Effects:');
```

```
Estimated Fixed Effects:
```

```
disp(nlmeResults_cov.FixedEffects);
```

```
       Name            Description          Estimate    StandardError
    ___________    ____________________    ________    _____________

    {'theta1'}    {'Central'          }    -0.45664      0.078933
```

```
    {'theta3'}    {'Cl_Central'       }     -5.9519        0.1177
    {'theta2'}    {'Central/WEIGHT'   }     0.52948      0.047342
    {'theta4'}    {'Cl_Central/WEIGHT'}     0.61954      0.071386
```

```
disp('Estimated Covariance Matrix:');
```

```
Estimated Covariance Matrix:
```

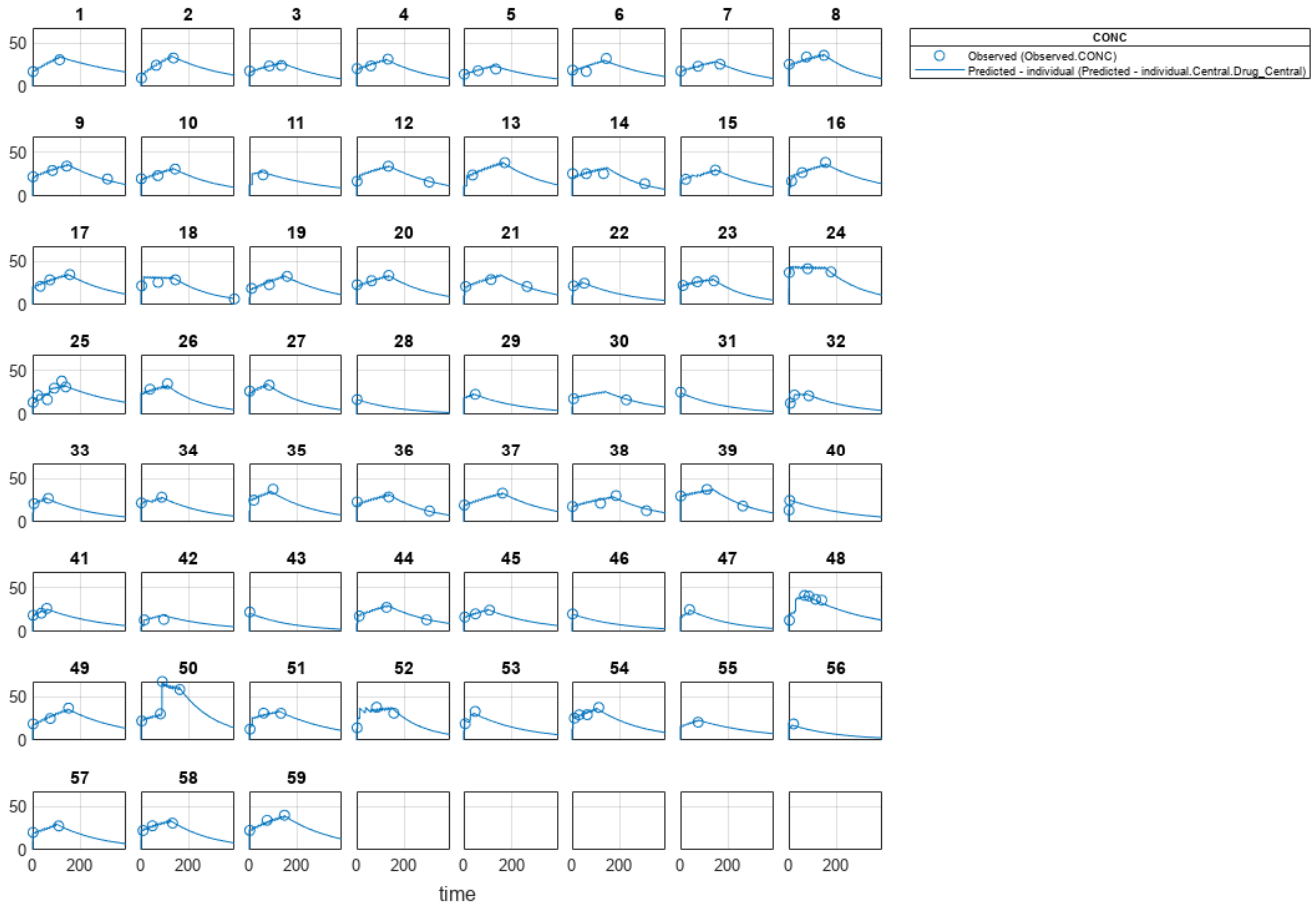
```
disp(nlmeResults_cov.RandomEffectCovarianceMatrix);
```

```
              eta1         eta2
            ________    ________

    eta1    0.046503           0
    eta2           0    0.041609
```

Visualize Results

Visualize the fitted results using individual-specific parameter estimates.

```
plot(nlmeResults_cov,'ParameterType','individual');
```



Use New Covariate Data to Evaluate the Fitted Model

Suppose you want to explore the responses of infants 1 and 2 using different covariate data, namely `WEIGHT`. You can do this by specifying the new `WEIGHT` data. The `ID` variable of the data corresponds to individual infants.

```
newData = data(data.ID == 1 | data.ID == 2,:);
newData.WEIGHT(newData.ID == 1) = 1.3;
newData.WEIGHT(newData.ID == 2) = 1.4;
```

Simulate the responses of infants 1 and 2 using the new covariate data.

```
[newResults_cov, newEstimates] = predict(nlmeResults_cov,newData,[dose1;dose2]);
```

`newEstimates` contains the updated parameter estimates for each individual (infants 1 and 2) after the model is reevaluated using the new covariate data.

```
newEstimates
```

```
newEstimates=4×3 table
    Group          Name          Estimate
    _____    _______________    _________

      1      {'Central'   }       2.5596
      1      {'Cl_Central'}    0.0065965
      2      {'Central'   }       1.7123
      2      {'Cl_Central'}    0.0064806
```

Compare to the estimated values from the original fit using the old covariate data.

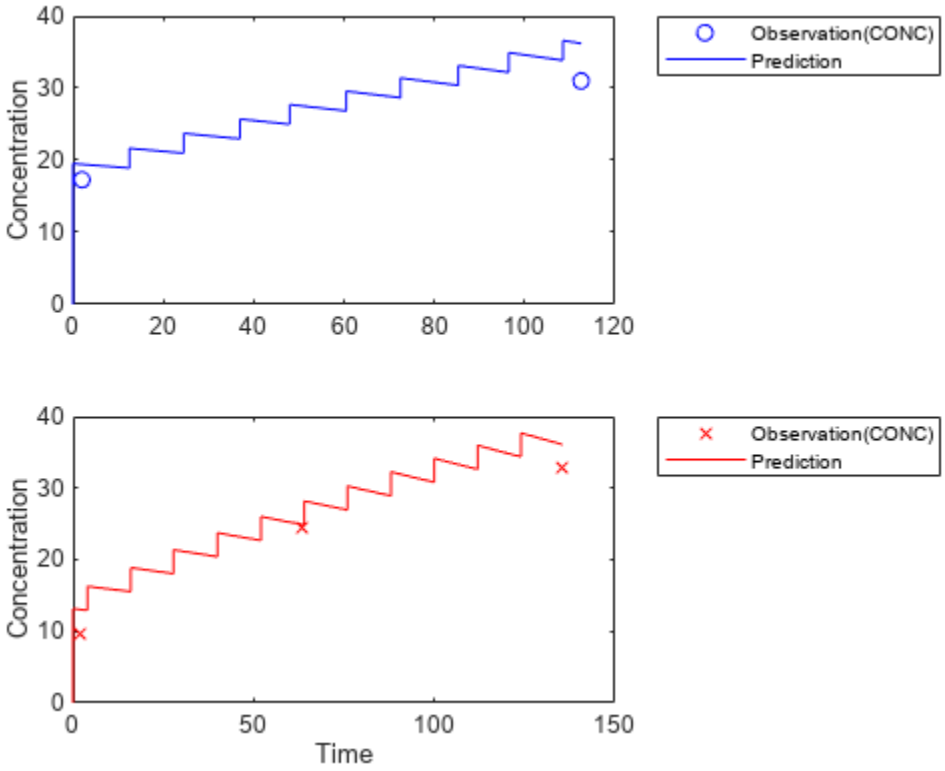
```
nlmeResults_cov.IndividualParameterEstimates( ...
            nlmeResults_cov.IndividualParameterEstimates.Group == '1' | ...
            nlmeResults_cov.IndividualParameterEstimates.Group == '2',:)
```

```
ans=4×3 table
    Group          Name          Estimate
    _____    _______________    _________

      1      {'Central'   }       2.6988
      1      {'Cl_Central'}    0.0070181
      2      {'Central'   }       1.8054
      2      {'Cl_Central'}    0.0068948
```

Visualize the new simulation results together with the experimental data for infant 1 and 2.

```
figure;
subplot(2,1,1);
plot(data.TIME(data.ID == 1),data.CONC(data.ID == 1),'bo')
hold on
plot(newResults_cov(1).Time,newResults_cov(1).Data,'b')
hold off
ylabel('Concentration')
legend('Observation(CONC)','Prediction','Location','NorthEastOutside')
subplot(2,1,2)
plot(data.TIME(data.ID == 2),data.CONC(data.ID == 2),'rx')
hold on
plot(newResults_cov(2).Time,newResults_cov(2).Data,'r')
```

```
hold off
legend('Observation(CONC)','Prediction','Location','NorthEastOutside')
ylabel('Concentration')
xlabel('Time')
```



References

[1] Grasela, T. H. Jr., and S. M. Donn. "Neonatal population pharmacokinetics of phenobarbital derived from routine clinical data." *Dev Pharmacol Ther* 1985:8(6). 374-83.

Sample Parameter Values from a Covariate Model

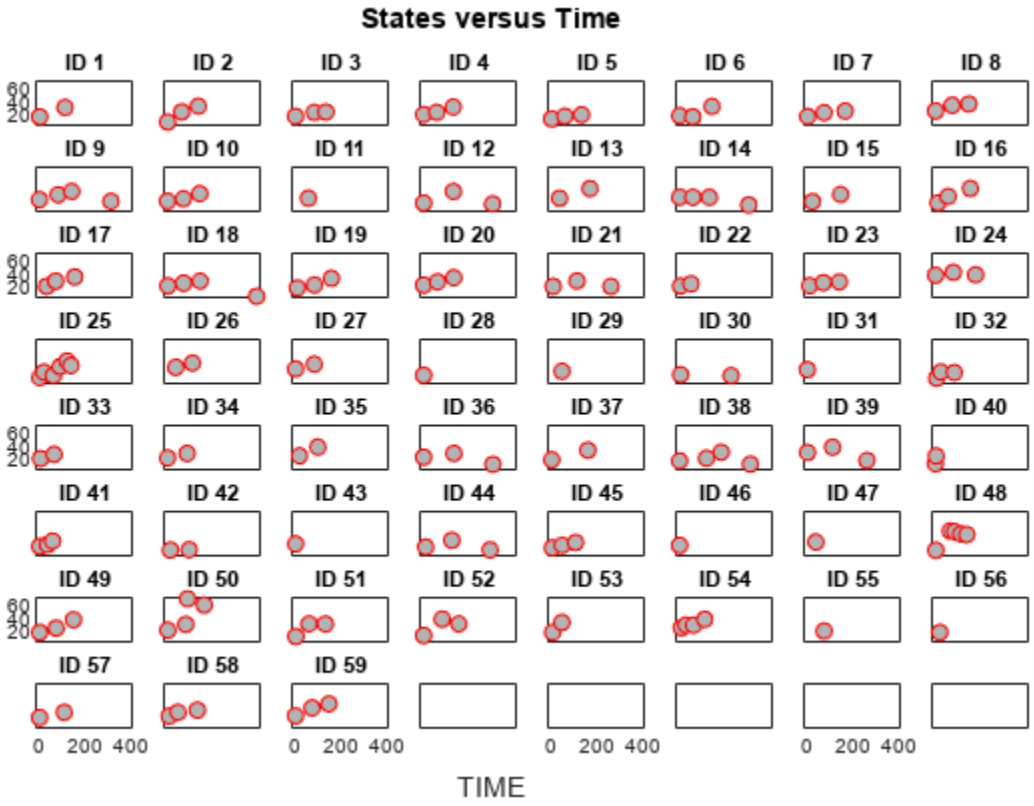
This example uses data collected on 59 preterm infants given phenobarbital during the first 16 days after birth. Each infant received an initial dose followed by one or more sustaining doses by intravenous bolus administration. A total of between 1 and 6 concentration measurements were obtained from each infant at times other than dose times, for a total of 155 measurements. Infant weights and APGAR scores (a measure of newborn health) were also recorded. Data was described in [1], a study funded by the NIH/NIBIB grant P41-EB01975.

Load the data.

```
load pheno.mat ds
```

Visualize the data.

```
t = sbiotrellis(ds,'ID','TIME','CONC','marker','o','markerfacecolor',[.7 .7 .7],'markeredgecolor
t.plottitle = 'States versus Time';
```



Create a one-compartment PK model with bolus dosing and linear clearance to model such data.

```
pkmd = PKModelDesign;
pkmd.addCompartment('Central','DosingType','Bolus','EliminationType','linear-clearance',...
                    'HasResponseVariable',true,'HasLag',false);
onecomp = pkmd.construct;
```

Suppose there is a correlation between the volume of the central compartment (`Central`) and the weight of infants. You can define this parameter-covariate relationship using a covariate model that can be described as

$$\log(V_i) = \theta_V + \theta_{V/WEIGHT} * WEIGHT_i + \eta_{V,i},$$

where, for each ith infant, `V` is the volume, θs (thetas) are fixed effects, η (eta) represents random effects, and `WEIGHT` is the covariate.

```
covM = CovariateModel;
covM.Expression = {'Central = exp(theta1+theta2*WEIGHT+eta1)'};
```

Define the fixed and random effects. The column names of each table must have the names of fixed effects and random effects, respectively.

```
thetas = table(1.4,0.05,'VariableNames',{'theta1','theta2'});
eta1 = table(0.2,'VariableNames',{'eta1'});
```

Change the group label ID to GROUP as required by the `sbiosampleparameters` function.

```
ds.Properties.VariableNames{'ID'} = 'GROUP';
```

Generate parameter values for the volumes of central compartments Central based on the covariate model for all infants in the data set.

```
phi = sbiosampleparameters(covM.Expression,thetas,eta1,ds);
```

You can then simulate the model using the sampled parameter values. For convenience, use the function-like interface provided by a SimFunction object.

First, construct a SimFunction object using the createSimFunction method, specifying the volume (Central) as the parameter, and the drug concentration in the compartment (Drug_Central) as the output of the SimFunction object, and the dosed species.

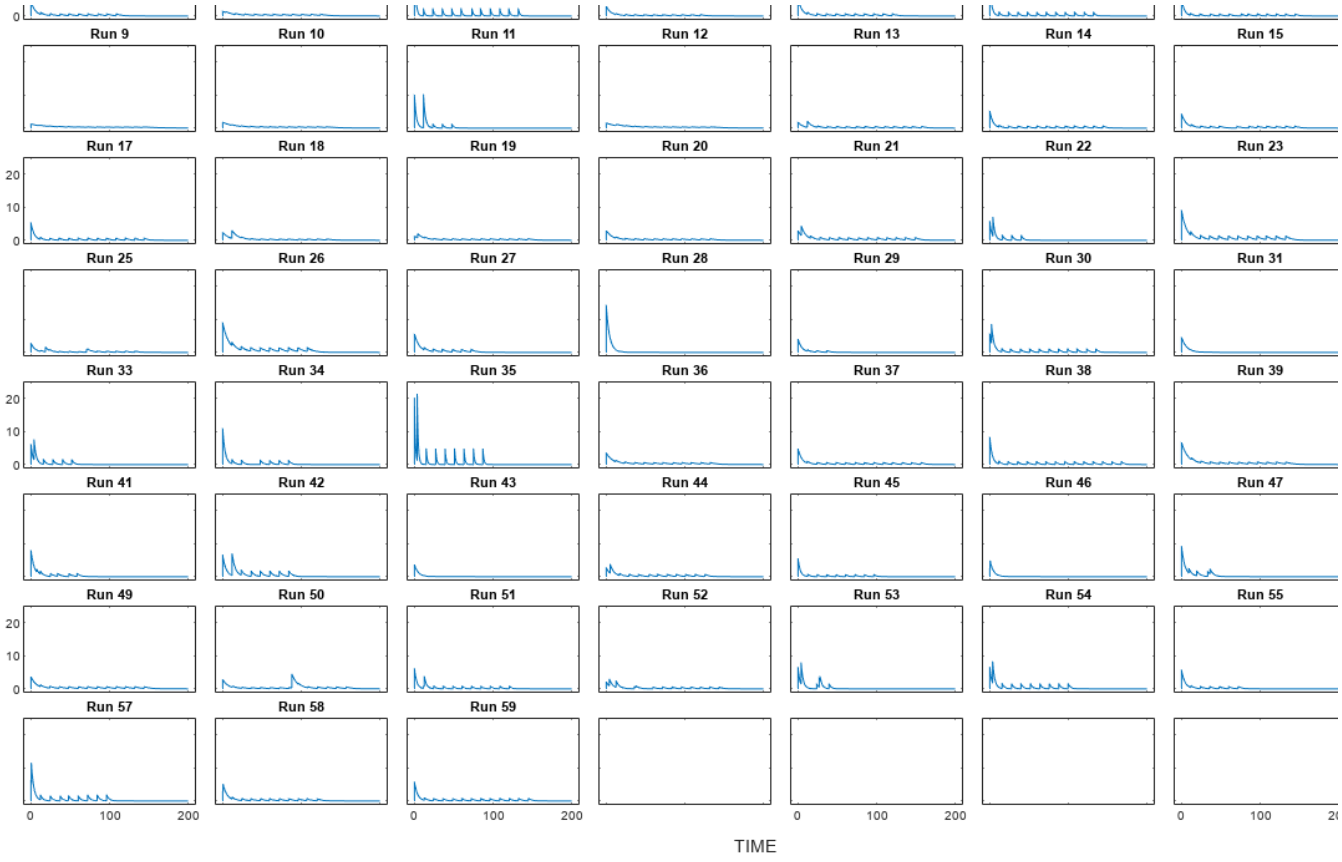
```
f = createSimFunction(onecomp,covM.ParameterNames,'Drug_Central','Drug_Central');
```

The data set ds contains dosing information for each infant, and the groupedData object provides a convenient way to extract such dosing information. Convert ds to a groupedData object and extract dosing information.

```
grpData = groupedData(ds);
doses = createDoses(grpData,'DOSE');
```

Simulate the model using the sampled parameter values from phi and the extracted dosing information of each infant, and plot the results. The ith run uses the ith parameter value in phi and dosing information of the ith infant.

```
t = sbiotrellis(f(phi,200,doses.getTable),[],'TIME','Drug_Central');
% Resize the figure.
t.hFig.Position(:) = [100 100 1280 800];
```



Version History

Introduced in R2011b

See Also

Topics

“Model the Population Pharmacokinetics of Phenobarbital in Neonates”
“Specify a Covariate Model”

covariateModel

Return a copy of the covariate model that was used for the nonlinear mixed-effects estimation using `sbiofitmixed`

Syntax

```
covmodel = covariateModel(resultsObj)
```

Description

`covmodel = covariateModel(resultsObj)` returns a copy of the covariate model that was used for the nonlinear mixed-effects estimation using `sbiofitmixed`.

Input Arguments

`resultsObj` — Estimation results
`NLMEResults` object

Estimation results, specified as an `NLMEResults object`, which contains estimation results from running `sbiofitmixed`.

Output Arguments

`covmodel` — Covariate model
`CovariateModel` object

Covariate model, returned as a `CovariateModel` object, that was used for the nonlinear mixed-effects estimation using `sbiofitmixed`. The model describes the relationship between SimBiology model parameters, fixed effects, random effects, and covariates.

Version History

Introduced in R2014a

See Also

`NLMEResults object` | `sbiofitmixed` | `CovariateModel`

createDoses

Create dose objects from groupedData object

Syntax

```
doseArray = createDoses(grpData,amountVarNames)
doseArray = createDoses(grpData,amountVarNames,rateVarNames)
doseArray = createDoses(grpData,amountVarNames,rateVarNames,tempDoses)
doseArray = createDoses(grpData,amountVarNames,rateVarNames,tempDoses,groups)
```

Description

`doseArray = createDoses(grpData,amountVarNames)` creates an array of SimBiology dose objects using dose times and amount data specified in `grpData`, with one row per group and one column per dose amount variable.

`grpData.Properties.IndependentVariable` specifies which variable contains dose times, and `amountVarNames` specifies which variables contain valid dose amounts.

`doseArray = createDoses(grpData,amountVarNames,rateVarNames)` uses dose rate variables specified by `rateVarNames`.

`doseArray = createDoses(grpData,amountVarNames,rateVarNames,tempDoses)` uses template doses specified by `tempDoses` as templates for dose objects in `doseArray`. In other words, this argument lets you copy some of the template dose properties, such as `TargetName`, `DurationParameterName`, and `LagParameterName`, to dose objects in `doseArray`.

`doseArray = createDoses(grpData,amountVarNames,rateVarNames,tempDoses,groups)` specifies which groups in `grpData` to create doses for.

Examples

Create Array of Doses from groupedData

Load the sample data set.

```
load pheno.mat ds
```

Create a `groupedData` object from the data set `ds`.

```
grpData = groupedData(ds);
```

Display the object properties.

```
grpData.Properties
```

```
ans = struct with fields:
                Description: ''
                   UserData: []
             DimensionNames: {'Observations'  'Variables'}
```

```
             VariableNames: {'ID'  'TIME'  'DOSE'  'WEIGHT'  'APGAR'  'CONC'}
       VariableDescriptions: {}
              VariableUnits: {}
        VariableContinuity: []
                   RowNames: {}
          CustomProperties: [1x1 matlab.tabular.CustomProperties]
         GroupVariableName: 'ID'
    IndependentVariableName: 'TIME'
```

`GroupVariableName` and `IndpendentVariableName` have been automatically assigned to 'ID' and 'Time', respectively.

Create an array of dose objects using the dosing information from the groupedData specified by the `DOSE` variable. Each row (dose object) represents a dosing schedule for each individual (group).

```
doseArray = createDoses(grpData,'DOSE');
```

Input Arguments

`grpData` — Grouped data

`groupedData` object

Grouped data, specified as a `groupedData` object.

Set `grpData.Properties.IndependentVariable` to a valid variable in `grpData` that specifies the dose times. `grpData.Properties.GroupVariableName` optionally identifies a grouping variable. `grpData.Properties.VariableUnits` optionally specifies units for the corresponding variables. If the specified units are invalid, a warning is issued, and the units of corresponding doses in `doseArray` are set to empty character vectors (`''`).

`amountVarNames` — Amount variable names

character vector | string | cell array of character vectors | string vector

Amount variable names, specified as a character vector, string, string vector, or cell array of character vectors that specifies variables in `grpData` that define dose amounts. Each character vector or string must specify a valid amount variable.

An amount variable is valid if it is a real, nonnegative column vector containing no infinite values.

`rateVarNames` — Rate variable names

character vector | string | cell array of character vectors | string vector

Rate variable names, specified as a character vector, string, string vector, or cell array of character vectors that specify variables in `grpData` that define dose rates. If it is empty `[]` or `{}`, it indicates that there are no dose rates. If it is not empty, it must be a character vector, string, cell array of character vectors or string vector of names of the same length as `amountVarNames`. Individual names can be empty (`''` or `""`) to indicate no dose rates for the corresponding doses or can be valid variable names in `grpData` specifying dose rates.

A rate variable is valid if it is a real, nonnegative column vector containing no infinite values. `NaN` rate values are allowed, but they are treated the same as the rate values of 0, that is, the doses are treated as bolus (instantaneous) doses.

`tempDoses` — Template doses
dose object | vector of dose object | `[]`

Template doses, specified as a dose object (`ScheduleDose object` or `RepeatDose object`), vector of dose objects, or empty array `[]`.

Use this argument to copy the following template dose properties to each dose in `doseArray`: `TargetName`, `DurationParameterName`, `LagParameterName`, `Notes`, `Tag`, and `UserData`.

If `tempDoses` is a single dose object, these properties from the object are copied to all doses in `doseArray`. If it is a vector, it must have the same length as `amountVarNames`, and these properties from each element (dose) are copied to the corresponding column of doses in `doseArray`.

The `Name` property of each dose in `doseArray` consists of the `Name` of the template dose followed by the group name in parentheses, such as `'DailyDose (Patient1)'`.

If you do not specify units in `grpData.Properties.VariableUnits`, the following template dose units properties are copied to doses in `doseArray`: `AmountUnits`, `RateUnits`, and `TimeUnits`.

`groups` — Group names
`[]` (default) | character vector | string vector | vector

Group names, specified as a character vector, string vector, an empty array `[]`, or a vector of data types that can be converted to a categorical vector. For a list of supported data types, see `categorical`.

By default, `groups` is set to `[]`, meaning the function creates doses for each group in `grpData`, with `doseArray` containing one row per group in `grpData`, in the order of the first occurrence of each group in `grpData`.

If you specify any group, the function converts those groups and the grouping variable in `grpData` to categorical vectors and compares them. The ith row of `doseArray` corresponds to the ith group specified in `groups`.

Output Arguments

`doseArray` — SimBiology dose objects
2-D matrix of dose objects

SimBiology dose objects, returned as a 2-D matrix of dose objects containing dose time and amount data from `grpData`. If dose times for a particular dose in `grpData` are regularly spaced, then the corresponding dose object in `doseArray` is a `RepeatDose object`. Otherwise, the corresponding dose object is a `ScheduleDose object`.

Note If there is a single dose time, then the dose object is represented as a `ScheduleDose object`.

Version History

Introduced in R2014a

See Also

`table` | `groupedData` | `ScheduleDose object` | `RepeatDose object`

createSimFunction (model)

Create SimFunction object

Syntax

```
F = createSimFunction(model,params,observables,dosed)
F = createSimFunction(model,params,observables,dosed, variants)
F = createSimFunction( ___ ,Name,Value)
```

Description

`F = createSimFunction(model,params,observables,dosed)` creates a `SimFunction object` `F` that you can execute like a function handle. The `params` and `observables` arguments define the inputs and outputs of the function `F` when it is executed, and `dosed` defines the dosing information of species. See `SimFunction object` for details on how to execute `F`.

`F = createSimFunction(model,params,observables,dosed, variants)` creates a `SimFunction object`, applying the values stored in `variants`, a vector of variant objects, as the model baseline values.

`F = createSimFunction( ___ ,Name,Value)` uses additional options specified by one or more `Name,Value` pair arguments.

Note

- Active doses and variants of the model are ignored when `F` is executed.
- `F` is immutable after it is created.
- `F` is automatically accelerated at the first function execution unless you set "AutoAccelerate" on page 2-0 to `false`. Manually accelerate the object if you want it accelerated in your deployment applications.

Input Arguments

`model` — SimBiology model

SimBiology model object

SimBiology model, specified as a SimBiology `model object`.

The function uses the same `configset` settings by making a copy of the `Configset` object of the `model` object. However, the function ignores the following `configset` settings: StatesToLog, OutputTimes, StopTime, and SensitivityAnalysisOptions because these settings are provided by other inputs to the function.

`params` — Inputs of SimFunction `F`

character vector | cell array of character vectors | `{}` | `SimBiology.Scenarios` object

Inputs of SimFunction `F`, specified as a character vector, cell array of character vectors, empty cell array `{}`, or `SimBiology.Scenarios` object. The character vectors represent the names of model

quantities (species, compartments, or parameters) that define the inputs of F. Use an empty cell array {} or empty Scenarios object SimBiology.Scenarios.empty() to create a SimFunction object that has no parameters.

To unambiguously name a model quantity, use the qualified name, which includes the name of the compartment. To name a reaction-scoped parameter, use the reaction name to qualify the parameter. If the name is not a valid MATLAB variable name, surround it by square brackets such as [reaction 1].[parameter 1].

observables — Outputs of SimFunction F
character vector | cell array of character vectors

Outputs of SimFunction F, specified as a character vector or cell array of character vectors. The character vectors represent the names of model quantities (species, compartments, or parameters) or observable objects that define the outputs of F.

dosed — Dosed species or dose objects
character vector | cell array of character vectors | vector of dose objects | []

Dosed species or dose objects, specified as a character vector, cell array of character vectors, vector of dose objects, or empty array [].

If it is [], no species are dosed during simulation unless you specify a Scenarios object that has doses defined in its entries.

If it is a cell array of character vectors, it must be 1-by-*N* array, where *N* is the number of dosed species names. You can use duplicate species names if you plan to use multiple doses on page 2-0 for the same species when you run the SimFunction F. Using only dosed species names contains no information on the dose properties. If you have a dose object that contains parameterized properties such as Amount, use the dose object as input instead of just species names to transfer such parameter information to the created SimFunction F.

If it is a vector of dose objects, it must be 1-by-*N* vector, where *N* is the number of dose objects. If dose objects have properties with nondefault numeric values, these values are ignored and a warning is issued. Only TargetName, DurationParameterName, LagParameterName, and parameterized properties are used to create the SimFunction object F, that is, to define the Dosed property of F. For details on how the Dosed property table is populated, see “Property Summary” on page 2-844.

The dosing information that you specify during the creation of the SimFunction object must be consistent with the dosing information you specify during the execution of the object. In other words, the number of elements in the Dosed property of SimFunction F must equal to the combined number of doses in the input Scenarios object in phi on page 2-0 and doses in the input argument u on page 2-0 when you execute the object.

variants — Alternate model values
variant object | vector of variant objects

Alternate model values, specified as a variant or vector of variant objects. These values are applied as the model baseline values when the SimFunction object is created. If there are multiple variants referring to the same model element, the last occurrence is used.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `'UseParallel',true` specifies to execute the SimFunction `F` in parallel.

`UseParallel` — Flag to execute SimFunction `F` in parallel

`false` (default) | `true`

Flag to execute SimFunction `F` in parallel, specified as the comma-separated pair consisting of `'UseParallel'` and `true` or `false`. If `true` and Parallel Computing Toolbox is available, the SimFunction `F` is executed in parallel.

Example: `'UseParallel',true`

`AutoAccelerate` — Flag to accelerate model on first evaluation of `SimFunction`

`true` (default) | `false`

Flag to accelerate the model on the first evaluation of the `SimFunction` object, specified as the comma-separated pair consisting of `'AutoAccelerate'` and `true` or `false`.

Set the value to `false` if you have a model that is fast to simulate because the acceleration of the model could take longer than the actual simulation of the model.

Example: `'AutoAccelerate',false`

`SensitivityOutputs` — Sensitivity output factors

`{}` (default) | cell array of character vectors | `'all'`

Sensitivity output factors, specified as the comma-separated pair consisting of `'SensitivityOutputs'` and a cell array of character vectors. The character vectors are the names of model quantities (species and parameters) for which you want to compute the sensitivities. The default is `{}` meaning there is no output factors. Output factors are the numerators of time-dependent derivatives explained in “Sensitivity Analysis in SimBiology”.

Use the keyword `'all'` or `"all"` to specify all model quantities as sensitivity outputs. However, `{'all'}` means a model quantity named `all` in the model. `["all","x"]` sets the sensitivity input factors or output factors to the species named `all` and `x`.

You must specify both `'SensitivityOutputs'` and `'SensitivityInputs'` name-value pair arguments for sensitivity calculations.

Example: `'SensitivityOutputs','all'`

`SensitivityInputs` — Sensitivity input factors

`{}` (default) | cell array of character vectors | `'all'`

Sensitivity input factors, specified as the comma-separated pair consisting of `'SensitivityInputs'` and a cell array of character vectors. The character vectors are the names of model quantities (species, compartments, and parameters) with respect to which you want to compute the sensitivities. The default is `{}` meaning no input factors. Input factors are the denominators of time-dependent derivatives explained in “Sensitivity Analysis in SimBiology”.

Use the keyword `'all'` or `"all"` to specify all model quantities as sensitivity outputs. However, `{'all'}` means a model quantity named `all` in the model. `["all","x"]` sets the sensitivity inputs or outputs to the species named `all` and `x`.

You must specify both `'SensitivityOutputs'` and `'SensitivityInputs'` name-value pair arguments for sensitivity calculations.

Example: `'SensitivityInputs',{'Reaction1.c1','Reaction1.c2'}`

`SensitivityNormalization` — Normalization for calculated sensitivities
`'None'` (default) | `'Half'` | `'Full'`

Normalization for calculated sensitivities, specified as the comma-separated pair consisting of `'SensitivityNormalization'` and `'None'`, `'Half'`, or `'Full'`.

- `'None'` — No normalization (default)
- `'Half'` — Normalization relative to the numerator only
- `'Full'` — Full dedimensionalization

For details, see `Normalization`.

Example: `'SensitivityNormalization','Full'`

Output Arguments

`F` — SimFunction
`SimFunction` object | `SimFunctionSensitivity` object

SimFunction, returned as a `SimFunction object` or `SimFunctionSensitivity object`. You can execute `F` like a function handle.

`F` is a `SimFunctionSensitivity object` if you specify non-empty `'SensitivityOutputs'` and `'SensitivityInputs'` name-value pair arguments.

Examples

Create a SimFunction Object

This example uses a radioactive decay model with the first-order reaction $\frac{dz}{dt} = c \cdot x$, where `x` and `z` are species and `c` is the forward rate constant.

Load the sample project containing the radioactive decay model `m1`.

```
sbioloadproject radiodecay;
```

Create a `SimFunction object`, specifying the parameter `Reaction1.c` to be scanned, and species `x` as the output of the function with no dosed species.

```
f = createSimFunction(m1, 'Reaction1.c','x', [])
```

```
f =
SimFunction
```

```
Parameters:

         Name           Value        Type            Units
    ________________    _____    _____________    ____________

    {'Reaction1.c'}      0.5     {'parameter'}    {'1/second'}

Observables:

    Name        Type           Units
    _____    ___________    ___________

    {'x'}    {'species'}    {'molecule'}

Dosed: None

TimeUnits: second
```

If the `UnitConversion` option was set to `false` when the `SimFunction` object `f` was created, the table does not display the units of the model quantities.

To illustrate this, first set the `UnitConversion` option to `false`.

```
cs = getconfigset(m1);
cs.CompileOptions.UnitConversion = false;
```

Create the `SimFunction` object as before and note that the variable named `Units` disappears.

```
f = createSimFunction(m1, {'Reaction1.c'},{'x'}, [])
```

```
f =
SimFunction

Parameters:

         Name           Value        Type
    ________________    _____    _____________

    {'Reaction1.c'}      0.5     {'parameter'}

Observables:

    Name        Type
    _____    ___________

    {'x'}    {'species'}

Dosed: None
```

If any of the species in the model is being dosed, specify the names of dosed species as the last argument. For example, if the species `x` is being dosed, specify it as the last argument.

```
f = createSimFunction(m1, {'Reaction1.c'},{'x'}, 'x')
```

```
f =
SimFunction

Parameters:
```

```
        Name          Value        Type
    ________________    _____    _____________

    {'Reaction1.c'}     0.5     {'parameter'}

Observables:

    Name        Type
    _____    ___________

    {'x'}    {'species'}

Dosed:

    TargetName
    __________

      {'x'}
```

Once the `SimFunction` object is created, you can execute it like a function handle and perform parameter scans (in parallel if Parallel Computing Toolbox™ is available), Monte Carlo simulations, and scans with multiple or vectorized doses. See `SimFunction object` for more examples.

Create a SimFunction Object with Dosing Information

This example creates a `SimFunction` object with dosing information using a `RepeatDose` or `ScheduleDose` object or a vector of these objects. However, if any dose object contains data such as `StartTime`, `Amount`, and `Rate`, such data are ignored, and a warning is issued. Only data, if available, used are `TargetName`, `LagParameterName`, and `DurationParameterName` of the dose object.

Load the sample project containing the radioactive decay model `m1`.

```
sbioloadproject radiodecay;
```

Create a `RepeatDose object` and specify its properties.

```
rdose = sbiodose('rd');
rdose.TargetName = 'x';
rdose.StartTime = 5;
rdose.TimeUnits = 'second';
rdose.Amount = 300;
rdose.AmountUnits = 'molecule';
rdose.Rate = 1;
rdose.RateUnits = 'molecule/second';
rdose.Interval = 100;
rdose.RepeatCount = 2;
```

Add a lag parameter and duration parameter to the model.

```
lagPara = addparameter(m1,'lp');
lagPara.Value = 1;
lagPara.ValueUnits = 'second';
```

```
duraPara = addparameter(m1,'dp');
duraPara.Value = 1;
duraPara.ValueUnits = 'second';
```

Set these parameters to the dose object.

```
rdose.LagParameterName = 'lp';
rdose.DurationParameterName = 'dp';
```

Create a `SimFunction` object `f` using the `RepeatDose` object `rdose` that you just created.

```
f = createSimFunction(m1,{'Reaction1.c'},{'x','z'},rdose)
```

```
Warning: Some Dose objects in DOSED had data. This data
will be ignored.
> In SimFunction>SimFunction.SimFunction at 847
  In SimFunction>SimFunction.createSimFunction at 374

f =

SimFunction

Parameters:

        Name          Value       Type          Units
    ______________    _____    ___________    __________

    'Reaction1.c'     0.5      'parameter'    '1/second'

Observables:

    Name      Type          Units
    ____    _________    __________

    'x'     'species'    'molecule'
    'z'     'species'    'molecule'

Dosed:

    TargetName            TargetDimension
    __________    ___________________________________

    'x'           'Amount(e.g. mole or molecule)'

    DurationParameterName    DurationParameterValue
    _____________________    ______________________

    'dp'                     1

    DurationParameterUnits    LagParameterName
    ______________________    ________________

    'second'                  'lp'

    LagParameterValue    LagParameterUnits
```

```
    ________________    ________________

    1                   'second'
```

A warning message appears because the `rdose` object contains data (`StartTime`, `Amount`, `Rate`) that are ignored by the `createSimFunction` method.

Scan Parameters of the Lotka-Volterra Model

This example shows how to execute different signatures of the `SimFunction object` to simulate and scan parameters of the Lotka-Volterra (predator-prey) model described by Gillespie [1].

Load the sample project containing the model `m1`.

```
sbioloadproject lotka;
```

Create a SimFunction object `f` with `c1` and `c2` as input parameters to be scanned, and `y1` and `y2` as the output of the function with no dosed species.

```
f = createSimFunction(m1,{'Reaction1.c1', 'Reaction2.c2'},{'y1', 'y2'}, [])
```

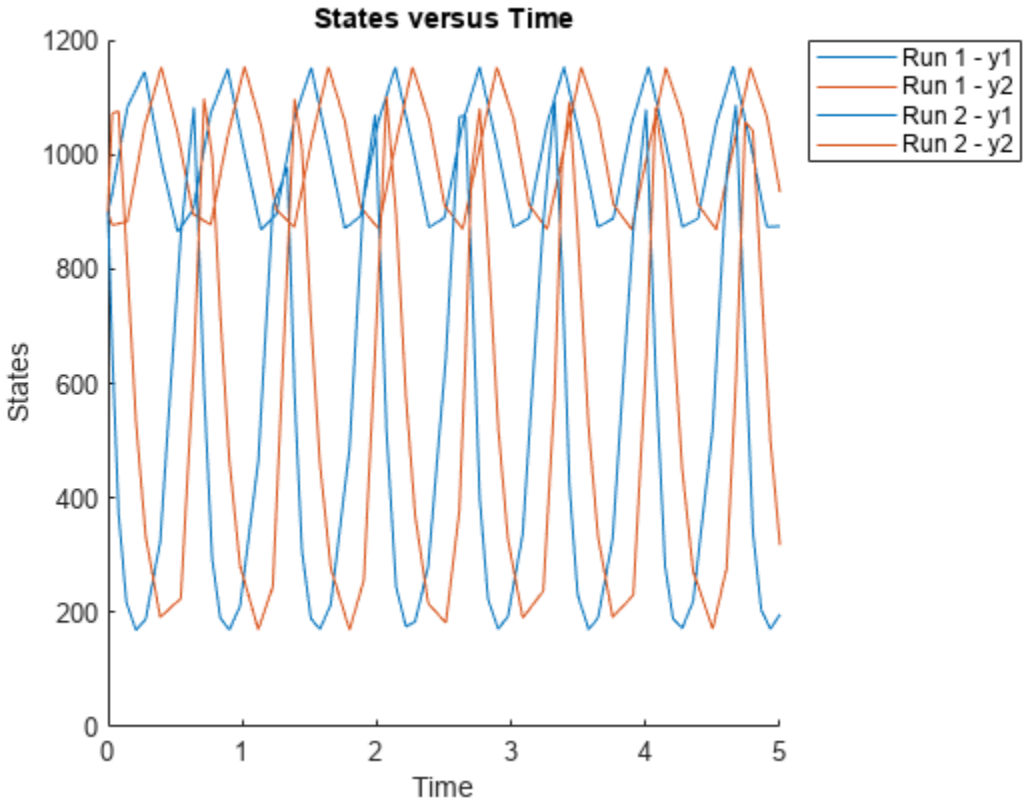
```
f =
SimFunction

Parameters:

          Name          Value        Type
    ________________    _____    _____________

    {'Reaction1.c1'}      10     {'parameter'}
    {'Reaction2.c2'}    0.01     {'parameter'}

Observables:

     Name        Type
    ______    ___________

    {'y1'}    {'species'}
    {'y2'}    {'species'}

Dosed: None
```

Define an input matrix that contains values for each parameter (`c1` and `c2`) for each simulation. The number of rows indicates the total number of simulations, and each simulation uses the parameter values specified in each row.

```
phi = [10 0.01; 10 0.02];
```

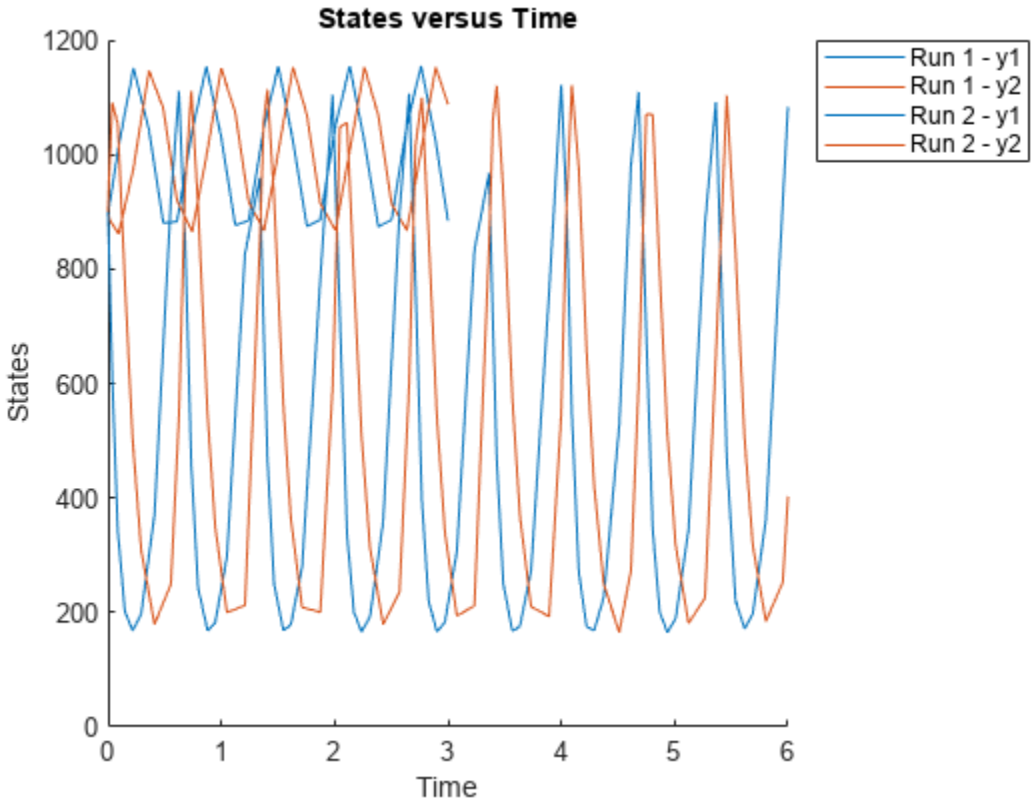
Run simulations until the stop time is 5 and plot the simulation results.

```
sbioplot(f(phi, 5));
```



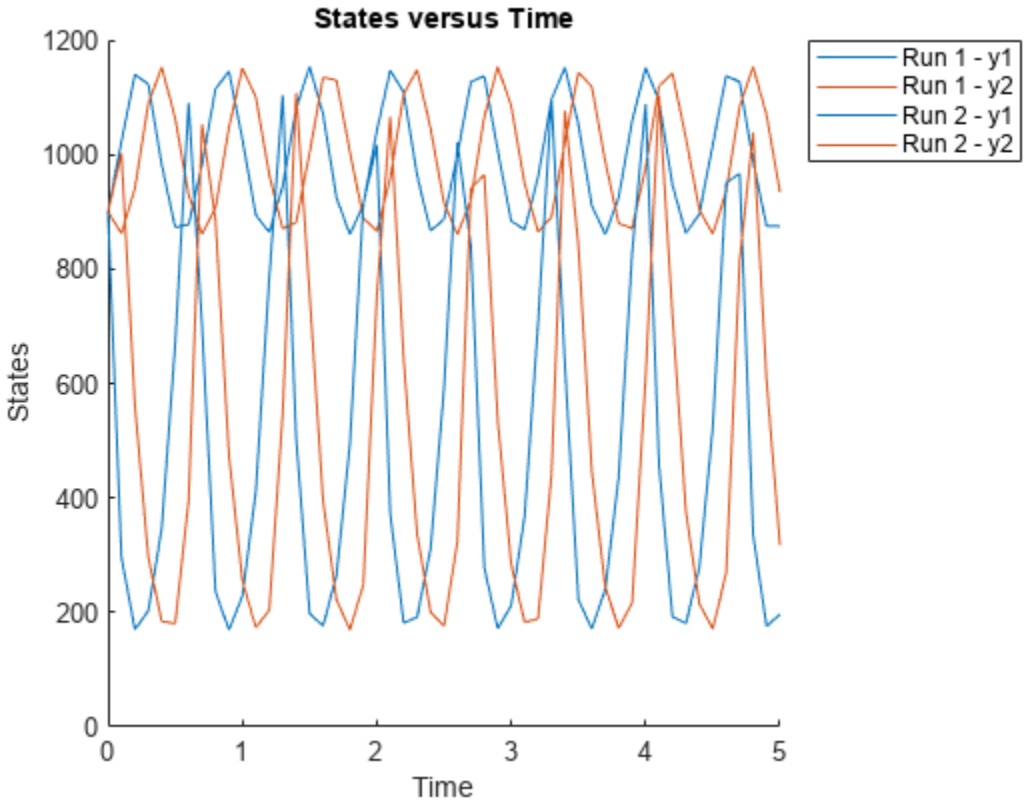
You can also specify a vector of different stop times for each simulation.

```
t_stop = [3;6];
sbioplot(f(phi, t_stop));
```



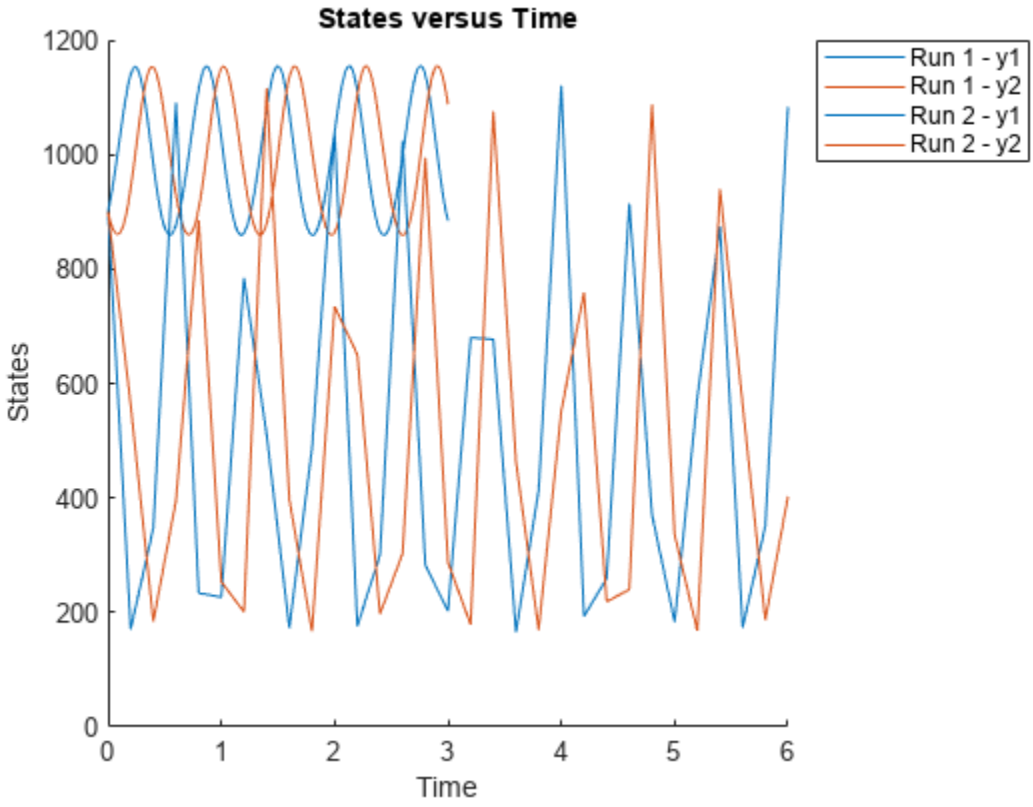
Next, specify the output times as a vector.

```
t_output = 0:0.1:5;
sbioplot(f(phi,[],[],t_output));
```



Specify output times as a cell array of vectors.

```
t_output = {0:0.01:3, 0:0.2:6};
sbioplot(f(phi, [], [], t_output));
```



Calculate Local Sensitivities Using `SimFunctionSensitivity` Object

This example shows how to calculate the local sensitivities of some species in the Lotka-Volterra model using the `SimFunctionSensitivity` object.

Load the sample project.

```
sbioloadproject lotka;
```

Define the input parameters.

```
params = {'Reaction1.c1', 'Reaction2.c2'};
```

Define the observed species, which are the outputs of simulation.

```
observables  = {'y1', 'y2'};
```

Create a `SimFunctionSensitivity` object. Set the sensitivity output factors to all species (`y1` and `y2`) specified in the `observables` argument and input factors to those in the `params` argument (`c1` and `c2`) by setting the name-value pair argument to `'all'`.

```
f = createSimFunction(m1,params,observables,[],'SensitivityOutputs','all','SensitivityInputs','a
```

```
f =
SimFunction
```

```
Parameters:

          Name          Value        Type
    ________________    _____    _____________

    {'Reaction1.c1'}      10     {'parameter'}
    {'Reaction2.c2'}    0.01     {'parameter'}

Observables:

     Name        Type
    ______    ___________

    {'y1'}    {'species'}
    {'y2'}    {'species'}

Dosed: None

Sensitivity Input Factors:

          Name              Type
    ________________    _____________

    {'Reaction1.c1'}    {'parameter'}
    {'Reaction2.c2'}    {'parameter'}

Sensitivity Output Factors:

     Name        Type
    ______    ___________

    {'y1'}    {'species'}
    {'y2'}    {'species'}

Sensitivity Normalization:

Full
```

Calculate sensitivities by executing the object with `c1` and `c2` set to 10 and 0.1, respectively. Set the output times from 1 to 10. `t` contains time points, `y` contains simulation data, and `sensMatrix` is the sensitivity matrix containing sensitivities of `y1` and `y2` with respect to `c1` and `c2`.

```
[t,y,sensMatrix] = f([10,0.1],[],[],1:10);
```

Retrieve the sensitivity information at time point 5.

```
temp = sensMatrix{:};
sensMatrix2 = temp(t{:}==5,:,:);
sensMatrix2 = squeeze(sensMatrix2)
```

```
sensMatrix2 = 2×2

   37.6987   -6.8447
  -40.2791    5.8225
```

The rows of `sensMatrix2` represent the output factors (`y1` and `y2`). The columns represent the input factors (`c1` and `c2`).

$$sensMatrix2 = \begin{bmatrix} \frac{\partial y1}{\partial c1} & \frac{\partial y1}{\partial c2} \\ \frac{\partial y2}{\partial c1} & \frac{\partial y2}{\partial c2} \end{bmatrix}$$

Set the stop time to 15, without specifying the output times. In this case, the output times are the solver time points by default.

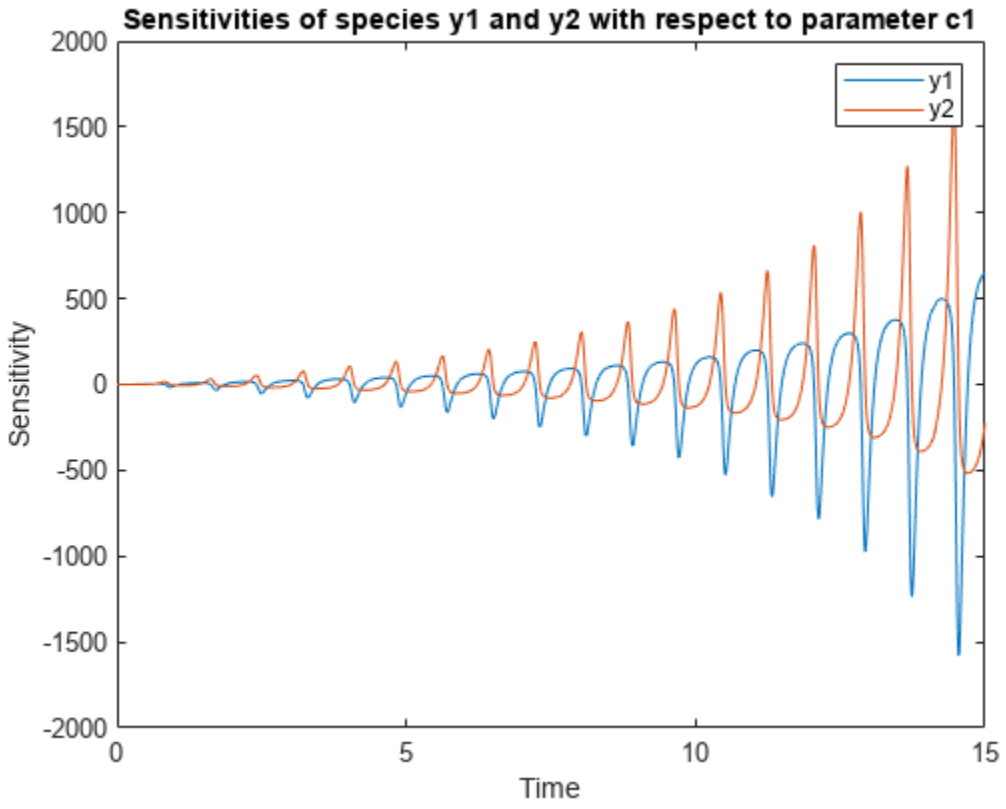
```
sd = f([10,0.1],15);
```

Retrieve the calculated sensitivities from the `SimData` object `sd`.

```
[t,y,outputs,inputs] = getsensmatrix(sd);
```

Plot the sensitivities of species `y1` and `y2` with respect to `c1`.

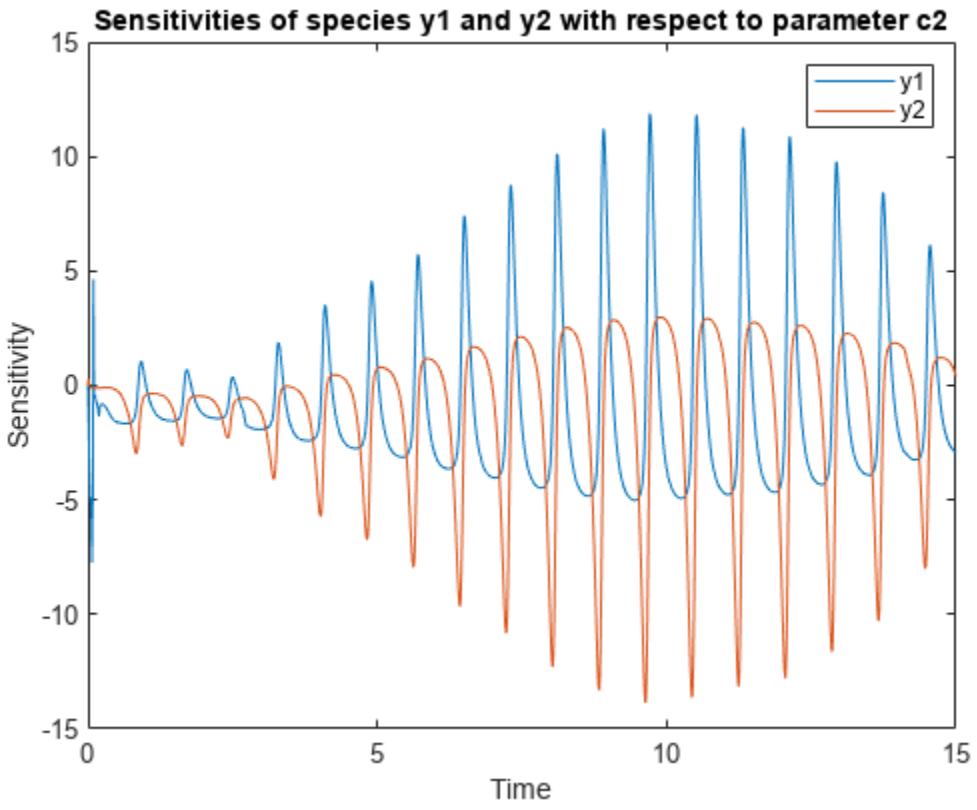
```
figure;
plot(t,y(:,:,1));
legend(outputs);
title('Sensitivities of species y1 and y2 with respect to parameter c1');
xlabel('Time');
ylabel('Sensitivity');
```



Plot the sensitivities of species `y1` and `y2` with respect to `c2`.

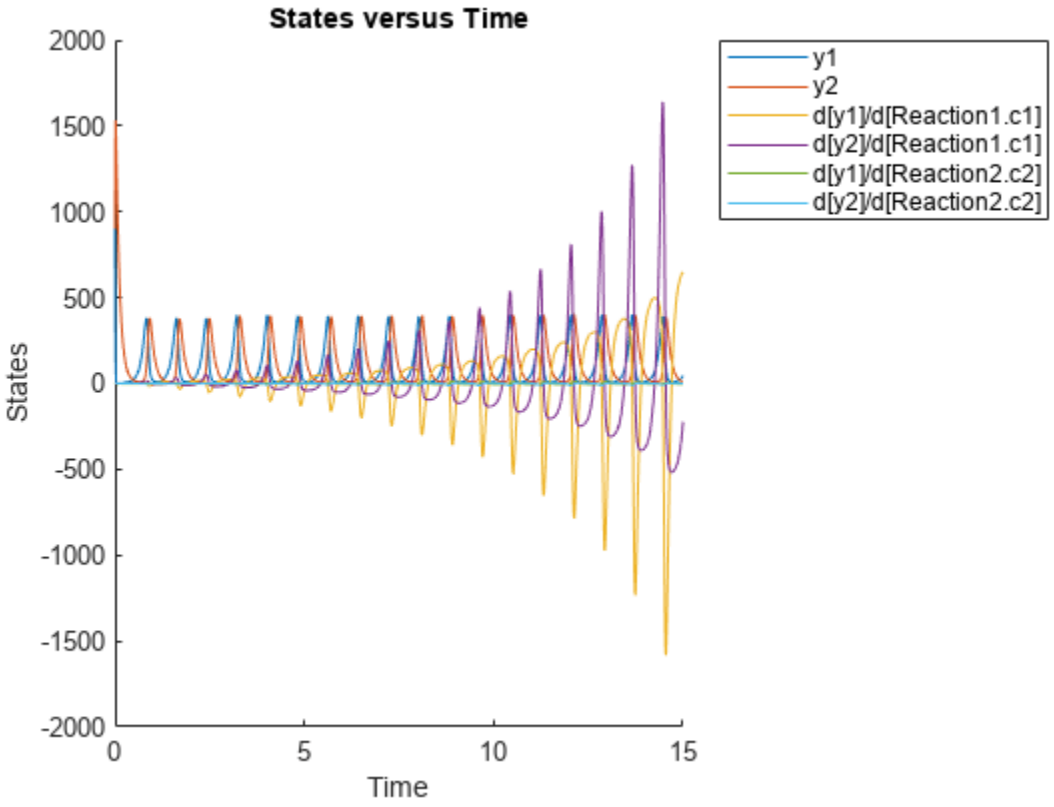
```
figure;
plot(t,y(:,:,2));
```

```
legend(outputs);
title('Sensitivities of species y1 and y2 with respect to parameter c2');
xlabel('Time');
ylabel('Sensitivity');
```



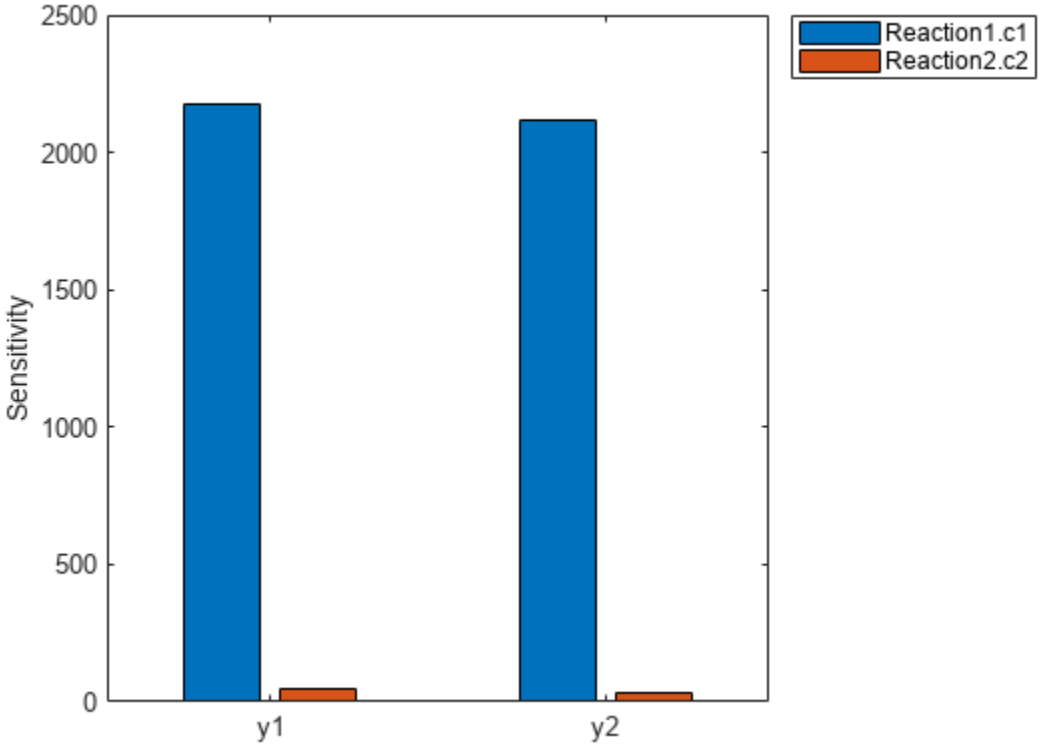
Alternatively, you can use `sbioplot`.

```
sbioplot(sd);
```



You can also plot the sensitivity matrix using the time integral for the calculated sensitivities of `y1` and `y2`. The plot indicates `y1` and `y2` are more sensitive to `c1` than `c2`.

```
[~, in, out] = size(y);
result = zeros(in, out);
for i = 1:in
    for j = 1:out
        result(i,j) = trapz(t(:),abs(y(:,i,j)));
    end
end
figure;
hbar = bar(result);
haxes = hbar(1).Parent;
haxes.XTick = 1:length(outputs);
haxes.XTickLabel = outputs;
legend(inputs,'Location','NorthEastOutside');
ylabel('Sensitivity');
```



Simulate Model of Glucose-Insulin Response with Different Initial Conditions

This example shows how to simulate the glucose-insulin responses for the normal and diabetic subjects.

Load the model of glucose-insulin response. For details about the model, see the **Background** section in “Simulate the Glucose-Insulin Response”.

```
sbioloadproject('insulindemo', 'm1')
```

The model contains different initial conditions stored in various variants.

```
variants = getvariant(m1);
```

Get the initial conditions for the type 2 diabetic patient.

```
type2 = variants(1)
```

```
type2 =
   SimBiology Variant - Type 2 diabetic (inactive)

   ContentIndex:     Type:        Name:             Property:          Value:
   1                 parameter    Plasma Volume ... Value              1.49
   2                 parameter    k1                Value              .042
   3                 parameter    k2                Value              .071
```

```
   4                parameter    Plasma Volume ... Value               .04
   5                parameter    m1                Value               .379
   6                parameter    m2                Value               .673
   7                parameter    m4                Value               .269
   8                parameter    m5                Value               .0526
   9                parameter    m6                Value               .8118
   10               parameter    Hepatic Extrac... Value               .6
   11               parameter    kmax              Value               .0465
   12               parameter    kmin              Value               .0076
   13               parameter    kabs              Value               .023
   14               parameter    kgri              Value               .0465
   15               parameter    f                 Value               .9
   16               parameter    a                 Value               6e-05
   17               parameter    b                 Value               .68
   18               parameter    c                 Value               .00023
   19               parameter    d                 Value               .09
   20               parameter    kp1               Value               3.09
   21               parameter    kp2               Value               .0007
   22               parameter    kp3               Value               .005
   23               parameter    kp4               Value               .0786
   24               parameter    ki                Value               .0066
   25               parameter    [Ins Ind Glu U... Value               1.0
   26               parameter    Vm0               Value               4.65
   27               parameter    Vmx               Value               .034
   28               parameter    Km                Value               466.21
   29               parameter    p2U               Value               .084
   30               parameter    K                 Value               .99
   31               parameter    alpha             Value               .013
   32               parameter    beta              Value               .05
   33               parameter    gamma             Value               .5
   34               parameter    ke1               Value               .0007
   35               parameter    ke2               Value               269.0
   36               parameter    Basal Plasma G... Value               164.18
   37               parameter    Basal Plasma I... Value               54.81
```

Suppress an informational warning that is issued during simulations.

```
warnSettings = warning('off','SimBiology:DimAnalysisNotDone_MatlabFcn_Dimensionless');
```

Create SimFunction objects to simulate the glucose-insulin response for the normal and diabetic subjects.

- Specify an empty array `{}` for the second input argument to denote that the model will be simulated using the base parameter values (that is, no parameter scanning will be performed).
- Specify the plasma glucose and insulin concentrations as responses (outputs of the function to be plotted).
- Specify the species `Dose` as the dosed species. This species represents the initial concentration of glucose at the start of the simulation.

```
normSim = createSimFunction(m1,{},...
            {'[Plasma Glu Conc]','[Plasma Ins Conc]'},'Dose')
```

```
normSim =
SimFunction

Parameters:
```

```
Observables:

           Name                Type                Units
    ________________________    ___________    ________________________

    {'[Plasma Glu Conc]'}    {'species'}    {'milligram/deciliter'}
    {'[Plasma Ins Conc]'}    {'species'}    {'picomole/liter'     }

Dosed:

    TargetName       TargetDimension
    __________    ____________________

     {'Dose'}     {'Mass (e.g., gram)'}


TimeUnits: hour
```

For the diabetic patient, specify the initial conditions using the variant `type2`.

```
diabSim = createSimFunction(m1,{},...
             {'[Plasma Glu Conc]','[Plasma Ins Conc]'},'Dose',type2)
```

```
diabSim =
SimFunction

Parameters:

Observables:

           Name                Type                Units
    ________________________    ___________    ________________________

    {'[Plasma Glu Conc]'}    {'species'}    {'milligram/deciliter'}
    {'[Plasma Ins Conc]'}    {'species'}    {'picomole/liter'     }

Dosed:

    TargetName       TargetDimension
    __________    ____________________

     {'Dose'}     {'Mass (e.g., gram)'}


TimeUnits: hour
```

Select a dose that represents a single meal of 78 grams of glucose at the start of the simulation.

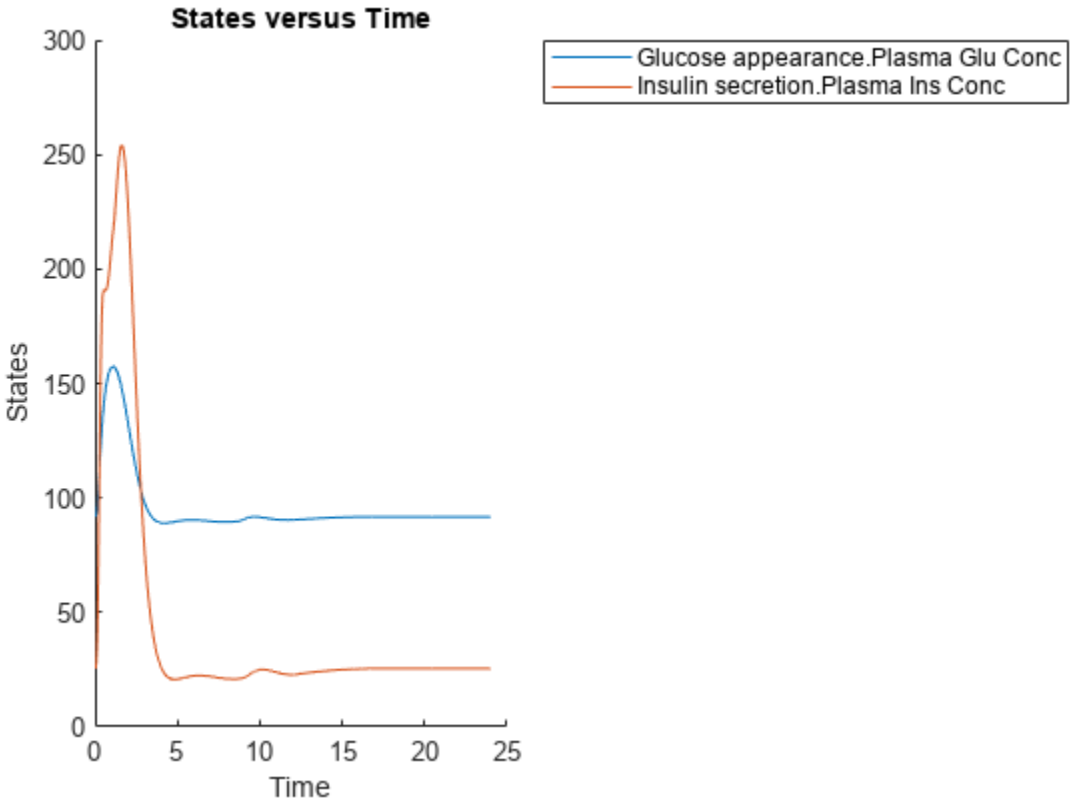
```
singleMeal = sbioselect(m1,'Name','Single Meal');
```

Convert the dosing information to the table format.

```
mealTable  = getTable(singleMeal);
```

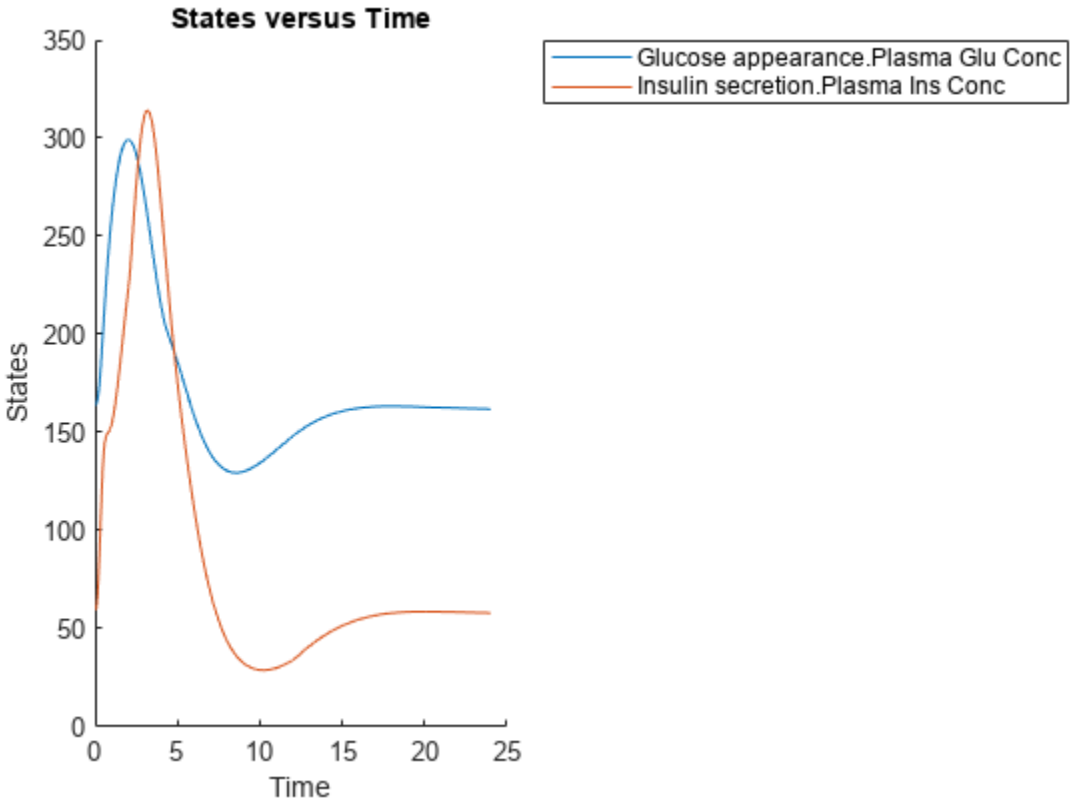
Simulate the glucose-insulin response for a normal subject for 24 hours.

```
sbioplot(normSim([],24,mealTable));
```



Simulate the glucose-insulin response for a diabetic subject for 24 hours.

```
sbioplot(diabSim([],24,mealTable));
```



Perform a Scan Using Variants

Suppose you want to perform a parameter scan using an array of variants that contain different initial conditions for different insulin impairments. For example, the model `m1` has variants that correspond to the low insulin sensitivity and high insulin sensitivity. You can simulate the model for both conditions via a single call to the SimFunction object.

Select the variants to scan.

```
varToScan = sbioselect(m1,'Name',...
                   {'Low insulin sensitivity','High insulin sensitivity'});
```

Check which model parameters are being stored in each variant.

```
varToScan(1)
```

```
ans =
   SimBiology Variant - Low insulin sensitivity (inactive)

   ContentIndex:     Type:        Name:            Property:          Value:
   1                 parameter    Vmx              Value              .0235
   2                 parameter    kp3              Value              .0045


varToScan(2)

ans =
   SimBiology Variant - High insulin sensitivity (inactive)
```

```
ContentIndex:     Type:        Name:            Property:          Value:
1                 parameter    Vmx              Value              .094
2                 parameter    kp3              Value              .018
```

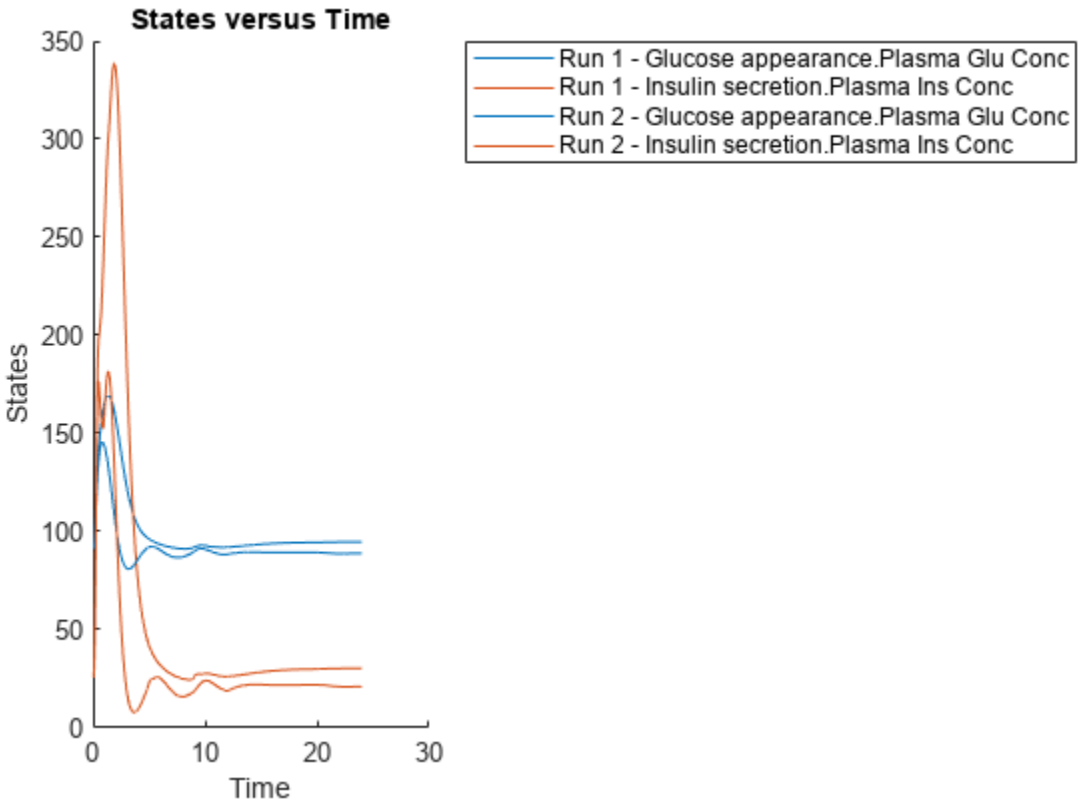
Both variants store alternate values for `Vmx` and `kp3` parameters. You need to specify them as input parameters when you create a SimFunction object.

Create a SimFunction object to scan the variants.

```
variantScan = createSimFunction(m1,{'Vmx','kp3'},...
          {'[Plasma Glu Conc]','[Plasma Ins Conc]'},'Dose');
```

Simulate the model and plot the results. `Run 1` include simulation results for the low insulin sensitivity and `Run 2` for the high insulin sensitivity.

```
sbioplot(variantScan(varToScan,24,mealTable));
```



Low insulin sensitivity lead to increased and prolonged plasma glucose concentration.

Restore warning settings.

```
warning(warnSettings);
```

Version History

Introduced in R2014a

References

[1] Gillespie, D.T. (1977). Exact Stochastic Simulation of Coupled Chemical Reactions. The Journal of Physical Chemistry. 81(25), 2340–2361.

Extended Capabilities

Automatic Parallel Support

Accelerate code by automatically running computation in parallel using Parallel Computing Toolbox™.

To run in parallel, set `'UseParallel'` to `true`.

For more information, see the `'UseParallel'` name-value pair argument.

See Also

`SimBiology.Scenarios` | `model object` | `SimFunction object` | `SimFunctionSensitivity object` | `sbiosampleerror` | `sbiosampleparameters`

Topics

“Model Simulation”

createVariants

Create variant objects from groupedData object

Syntax

```
variants = createVariants(grpData,variableNames)
variants = createVariants(grpData,variableNames,groups)
variants = createVariants( ___ ,Name=Value)
```

Description

`variants = createVariants(grpData,variableNames)` creates a column vector of variant objects for each group in `grpData` using data variables `variableNames`.

`variants = createVariants(grpData,variableNames,groups)` creates a vector of variant objects for the specified `groups`.

`variants = createVariants( ___ ,Name=Value)` uses additional options specified by one or more name-value arguments.

Examples

Create Variants from Grouped Data

Import sample data. The data contain three groups (individuals) with some time course measurement data. The `Cl_Central` and `Central` columns represent group-specific variant values.

```
tbl = readtable('sample_data_variants_simbiology.xlsx')
```

```
tbl=16×6 table
    Group    Time    CentralConc    Dose1    Cl_Central    Central
    _____    ____    ___________    _____    __________    _______

      1        0        83.378       100        0.65        0.96
      1        0            85       NaN         NaN         NaN
      1        1        31.019       NaN         NaN         NaN
      1        4        6.4875       NaN         NaN         NaN
      1        8        1.1631       NaN         NaN         NaN
      1       36             0       NaN         NaN         NaN
      2        0        49.992       100        0.55        0.67
      2        1        25.276       NaN        0.55        0.67
      2        4        7.1079       NaN        0.55        0.67
      2        8        2.7109       NaN        0.55        0.67
      2       36             0       NaN        0.55        0.67
      3        0           NaN       100        0.78         NaN
      3        1        26.269       NaN         NaN         NaN
      3        4        14.365       NaN         NaN         NaN
      3        8        7.3422       NaN         NaN         NaN
      3       36       0.18685       NaN         NaN         NaN
```

Convert to a `groupedData` object.

```
gdata = groupedData(tbl);
```

By default, the function uses the "Group" column as the group variable.

```
gdata.Properties.GroupVariableName
```

```
ans =
'Group'
```

Create a variant for each group for using the `Cl_Central` and `Central` variables from the data.

```
variants = createVariants(gdata,["Cl_Central","Central"])
```

```
variants =
   SimBiology Variant Array

   Index:  Name:             Active:
   1       1                 false
   2       2                 false
   3       3                 false
```

```
variants(1)
```

```
ans =
   SimBiology Variant - 1 (inactive)

   ContentIndex:     Type:        Name:             Property:           Value:
   1                 parameter    Cl_Central        Value               .65
   2                 parameter    Central           Value               .96
```

```
variants(2)
```

```
ans =
   SimBiology Variant - 2 (inactive)

   ContentIndex:     Type:        Name:             Property:           Value:
   1                 parameter    Cl_Central        Value               .55
   2                 parameter    Central           Value               .67
```

```
variants(3)
```

```
ans =
   SimBiology Variant - 3 (inactive)

   ContentIndex:     Type:        Name:             Property:           Value:
   1                 parameter    Cl_Central        Value               .78
```

Note that individual 3 has a variant value for `Cl_Central` but not `Central`. Hence the function created only one variant content, for `Cl_Central`.

You can also specify which group to create variants for. For example, create variants for individuals 1 and 2 only.

```
variants = createVariants(gdata,["Cl_Central","Central"],["1","2"])
```

```
variants =
   SimBiology Variant Array

   Index:  Name:             Active:
   1       1                 false
   2       2                 false


variants(1)

ans =
   SimBiology Variant - 1 (inactive)

   ContentIndex:     Type:        Name:             Property:           Value:
   1                 parameter    Cl_Central        Value               .65
   2                 parameter    Central           Value               .96


variants(2)

ans =
   SimBiology Variant - 2 (inactive)

   ContentIndex:     Type:        Name:             Property:           Value:
   1                 parameter    Cl_Central        Value               .55
   2                 parameter    Central           Value               .67
```

By default, the function assigns the type as parameter for each variable. You can specify which type (species, parameter, or compartment) by using the `Types` name-value argument. Specify `Cl_Central` as a parameter and `Central` as a compartment.

```
variants = createVariants(gdata,["Cl_Central","Central"],Types=["parameter","compartment"]);
variants(1)

ans =
   SimBiology Variant - 1 (inactive)

   ContentIndex:     Type:        Name:             Property:           Value:
   1                 parameter    Cl_Central        Value               .65
   2                 compartment  Central           Value               .96


variants(2)

ans =
   SimBiology Variant - 2 (inactive)

   ContentIndex:     Type:        Name:             Property:           Value:
   1                 parameter    Cl_Central        Value               .55
   2                 compartment  Central           Value               .67


variants(3)

ans =
   SimBiology Variant - 3 (inactive)

   ContentIndex:     Type:        Name:             Property:           Value:
```

```
   1                parameter    Cl_Central        Value               .78
```

If you know the name of model component that maps to each variable, you can use the component name to define the Name of each variant content. For example, map the data variables to the model components named "Clearance" and "Central".

```
variants = createVariants(gdata,["Cl_Central","Central"],Types=["parameter","compartment"],Names=
variants(1)

ans =
   SimBiology Variant - 1 (inactive)

   ContentIndex:     Type:        Name:             Property:           Value:
   1                 parameter    Clearance         Value               .65
   2                 compartment  Central           Value               .96


variants(2)

ans =
   SimBiology Variant - 2 (inactive)

   ContentIndex:     Type:        Name:             Property:           Value:
   1                 parameter    Clearance         Value               .55
   2                 compartment  Central           Value               .67


variants(3)

ans =
   SimBiology Variant - 3 (inactive)

   ContentIndex:     Type:        Name:             Property:           Value:
   1                 parameter    Clearance         Value               .78
```

If your data variables have the same names as the corresponding model components, you can use the model as the source and the function automatically does the mapping.

```
% Create a two-compartment model.
pkmd                                  = PKModelDesign;
pkc1                                  = addCompartment(pkmd,'Central');
pkc1.DosingType                       = 'Bolus';
pkc1.EliminationType                  = 'linear-clearance';
pkc1.HasResponseVariable              = true;
pkc2                                  = addCompartment(pkmd,'Peripheral');
model                                 = construct(pkmd);
variants = createVariants(gdata,["Cl_Central","Central"],Model=model);
variants(1)

ans =
   SimBiology Variant - 1 (inactive)

   ContentIndex:     Type:        Name:             Property:           Value:
   1                 parameter    Cl_Central        Value               .65
   2                 compartment  Central           Value               .96
```

Alternatively, if you have the corresponding model component objects, you can use them as well to map to the data variables.

```
% Extract the parameter and compartment object.
clearance = sbioselect(model,Name="Cl_Central");
centralVol = sbioselect(model,Name="Central");
% Map the data variables to these objects.
variants = createVariants(gdata,["Cl_Central","Central"],Components=[clearance,centralVol])
```

```
variants =
   SimBiology Variant Array

   Index:  Name:             Active:
   1       1                 false
   2       2                 false
   3       3                 false
```

```
variants(1)
```

```
ans =
   SimBiology Variant - 1 (inactive)

   ContentIndex:     Type:        Name:             Property:           Value:
   1                 parameter    Cl_Central        Value               .65
   2                 compartment  Central           Value               .96
```

Input Arguments

`grpData` — Grouped data

`groupedData` object

Grouped data, specified as a `groupedData` object.

`grpData.Properties.GroupVariableName` optionally identifies a grouping variable.

`variableNames` — Names of data variables

character vector | string | string vector | cell array of character vectors

Names of data variables used to generate variants, specified as a character vector, string, string vector, or cell array of character vectors.

Each variable in `variableNames` must be a numeric column vector without `Inf` values.

For each variable, the non-NaN values within a group can be repeated but they must be identical. You can use `NaN` to indicate no value for a particular row. If all values of a variable within a group are `NaN`, that variable is not included in the group variant.

`groups` — Group names

`[]` | character vector | string scalar | string vector | cell array of character vectors | vector

Group names, specified as an empty vector `[]`, character vector, string scalar, string vector, cell array of character vectors, or a vector of data types that can be converted to a categorical vector. For a list of supported data types, see `categorical`.

Use `[]` to indicate the default behavior of including variants for each group.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Example: `Types="compartment",Names="Central"` specifies the model component type as compartment and its name as `Central`.

`Types` — Model component types

`"parameter"` (default) | `"species"` | `"compartment"` | string vector | cell array of character vectors

Model component types used in the variants, specified as `"parameter"`, `"species"`, `"compartment"`, string vector, or cell array of character vectors, where each element must be one of these strings or character vectors.

If you specify only one component type, the function applies it to all variant content. If you specify more than one type, the number of types must match the number of names in `variableNames`.

You cannot specify this argument together with `'Components'` or `'Model'`.

Data Types: `char` | `string` | `cell`

`Names` — Model component names

names from `variableNames` input argument (default) | character vector | string scalar | string vector | cell array of character vectors

Model component names used in the variants, specified as a character vector, string scalar, string vector, or cell array of character vectors. If you do not specify this argument or `'Components'`, by default, the function uses the names from the `variableName` input argument as the component names.

You cannot specify this argument together with `'Components'`.

Data Types: `char` | `string` | `cell`

`Components` — Model components

vector of parameter, species, or compartment objects

Model components used in the variants, specified as a vector of parameter, species, or compartment objects. The number of components must match the number of names in `variableNames`. The types and names used in the variant contents on page 3-29 are the types and qualified names of the specified components.

You cannot specify this argument together with `'Types'`,`'Names'`, or `'Model'`.

`Model` — SimBiology model

model object

SimBiology model used to identify the model components in the variants, specified as a model object.

When you have a name that matches different quantities, the software uses the following precedence rule to decide: species > compartment > parameter. For details, see “Precedence Rules for Evaluating Quantity Names”.

You cannot specify this argument together with `'Types'` or `'Components'`.

`UnitConversion` — Flag to covert units
`"auto"` (default) | `true` | `false`

Flag to convert units of the data variable to the units specified for each model component, specified as `"auto"`, `true`, or `false`. The variable units are defined in `grpData.Properties.VariableUnits`.

When the value is `"auto"`, the function converts units for any pair of variable and component that both specify nonempty units, which are consistent with each other. Otherwise, the values in the data variables are used without unit conversion.

When the value is `true`, the function converts all values in the data variables to the units of each component. You can set the value to `true` only if you have specified the model components using either the `Model` or `Components` name-value argument.

When the value is `false`, the function uses the values in the data variables without unit conversion.

Output Arguments

`variants` — SimBiology variant objects
column vector of variant objects

SimBiology variant objects, returned as a column vector of variant objects, with one variant for each group in `grpData`. If you do not specify the `groups` input, the order of returned variants follows the order of groups in the input data. If you specify `groups`, the order of variants follows the order of specified groups.

Version History

Introduced in R2021b

See Also

`Variant object` | `table` | `groupedData` | `ScheduleDose object` | `RepeatDose object`

Topics
“Variants in SimBiology Models”

delete

Delete SimBiology object

Syntax

```
delete(sobj)
```

Description

`delete(sobj)` deletes the SimBiology object `sobj` and removes it from its parent on page 3-106 object.

Note You can also use `sbioreset` to delete all model objects from the SimBiology root object, which contains a list of model objects, available units, unit prefixes, and kinetic laws.

Examples

Delete SimBiology Objects

Load the G-protein model.

```
sbioloadproject('gprotein.sbproj');
```

Get the model-scoped parameters.

```
params = m1.Parameters
```

```
params =
   SimBiology Parameter Array

   Index:    Name:     Value:      Units:
   1         kRLm      0.01
   2         kRL       3.32e-18
   3         kRdo      0.0004
   4         kRs       4
   5         kRD1      0.004
   6         kG1       1
   7         kGa       1e-05
   8         kGd       0.11
   9         GaFrac    1
```

Delete the parameters.

```
delete(params)
```

```
m1.Parameters
```

```
ans =
  0x1 Parameter array with properties:
```

```
ValueUnits
ConstantValue
Constant
Value
Units
BoundaryCondition
Name
Parent
Notes
Tag
Type
UserData
```

Input Arguments

`sobj` — Object

SimBiology object | array of SimBiology objects

Object, specified as a SimBiology object or array of SimBiology objects.

- If `sobj` is a model object, the model is deleted from the root object. `delete` removes all references to the model at the command line and in the **SimBiology** and **SimBiology Model Analyzer** apps.
- If `sobj` is a species object used by a reaction object, the function issues a warning, and the species object is not deleted. You need to delete the reaction or remove the species from the reaction before you can delete the species object.
- If `sobj` is a parameter object used by a kinetic law object, there is no warning when the object is deleted. However, when you try to simulate your model, a error occurs because the parameter cannot be found.

- If `sobj` is a reaction object, the function deletes the object, but the species objects that were being used by the reaction object are not deleted.
- If `sobj` is an abstract kinetic law object and there is a kinetic law object referencing it, the function returns an error.
- If `sobj` is a configuration set object, and it is the active configuration set object, the function, after deleting the object, makes the default configuration set object active. Note that you cannot delete the default configuration set.
- You cannot delete the SimBiology `root` object or a `SimData` object.

Version History

Introduced in R2006a

See Also

`set`

SimBiology.DiffResults

Results of comparison between two SimBiology models and diagrams

Description

`SimBiology.DiffResults` contains the results from comparing two SimBiology models and diagram information.

Creation

Use `sbiodiff` to compare the models and the function returns `SimBiology.DiffResults` as an output.

Properties

`Comparisons` — Results of comparison between two SimBiology models and their diagrams
table

Results of comparison between two SimBiology models and their diagrams, specified as a table.

The table has the following columns:

- *Class* — Model component type specified as a string. Note that for a variant, the table shows `"Variant (`*X*`)"`, where *X* is the string `"species"`, `"compartment"`, or `"parameter"` depending on the type of the component referenced in the corresponding row of the variant content. For details on how SimBiology matches variants, see “Doses and Variants”.
- *Source* — Source component name.
  - For a species, parameter, or compartment, the column shows a qualified name (such as `cell.Ligand`).
  - For a kinetic law, it shows `"Kinetic Law (`*Y*`)"`, where *Y* is the parent reaction name.
  - For a rule, it shows the rule name. If the name is empty, it shows the value of the Rule property instead.
  - For an event, it shows the event name. If the name is empty, it shows the value of the Trigger property instead.
  - For a reaction, observable, dose, or variant, it shows the value of the Name property.
- *Target* — Target component name (see the *Source* column for details)
- *Property* — Name of the component property for which the value is shown in the *SourceValue* and *TargetValue* column.
- *SourceValue* — Value of the corresponding property of the source component
- *TargetValue* — Value of the corresponding property of the target component

The *Property*, *SourceValue*, and *TargetValue* show `<missing>` as the value for any deleted or inserted model component.

Tip The *Class*, *Source*, *Target*, and *Property* columns contain strings. You can use these columns to select specific changes by using string comparisons. For instance, to get all modifications to the value of any parameter from the table, use:

```
diffResults = sbiodiff(m1,m2);
diffTbl = diffResults.Comparisons;
param_subset = diffTbl(diffTbl.Class == "Parameter" & diffTbl.Property == "Value",:);
```

To find <missing> values, use `ismissing`.

Data Types: `table`

`Source` — Source model information

struct

Source model information, specified as a structure. The structure contains the following fields.

- `Project` — Name of the SBPROJ file that contains the source model. If you specify the corresponding model as a SimBiology model object, this field value is `""`.
- `ModelName` — SimBiology model name
- `Model` — SimBiology model object
- `LastModified` — Last modified date of the SBPROJ file. If you specify the corresponding model as a SimBiology model object, this field value is `""`.

Data Types: `struct`

`Target` — Target model information

struct

Target model information, specified as a structure. The structure contains the following fields.

- `Project` — Name of the SBPROJ file that contains the target model. If you specify the corresponding model as a SimBiology model object, this field value is `""`.
- `ModelName` — SimBiology model name
- `Model` — SimBiology model object
- `LastModified` — Last modified date of the SBPROJ file. If you specify the corresponding model as a SimBiology model object, this field value is `""`.

Data Types: `struct`

Object Functions

getComponents	Get model components associated with SimBiology model comparison results
visdiff	Visualize SimBiology model comparison results

Examples

Compare SimBiology Models

Load a source model.

```
model1      = sbmlimport("lotka");
y1          = sbioselect(model1, "Type", "species", "Name", "y1");
y1.Value    = 880;
```

Load a target model to compare against the source model.

```
model2      = sbmlimport("lotka");
y1          = sbioselect(model2, "Type", "species", "Name", "y1");
y1.Value    = 920;
```

Compare the models using `sbiodiff` and display the comparison table.

```
diffResults = sbiodiff(model1,model2);
diffTable   = diffResults.Comparisons
```

```
diffTable=1×6 table
           Class       Source    Target    Property    SourceValue    TargetValue
          _________    ______    ______    ________    ___________    ___________

    1     "Species"     "y1"      "y1"     "Value"       {[880]}        {[920]}
```

You can also view the comparison results graphically in the Comparison tool.

```
visdiff(diffResults);
```

Get a table of model components associated with the changes reported in the comparison table.

```
tbl = getComponents(diffResults)
```

```
tbl=1×2 table
                    Source                                Target
          ____________________________    ____________________________

    1     {1x1 SimBiology.Species}        {1x1 SimBiology.Species}
```

Version History

Introduced in R2022a

See Also

`Model` | `sbioloadproject` | **SimBiology Model Builder** | `sbiodiff` | `visdiff`

Topics

“Compare SimBiology Models”
“SimBiology Model Matching Policy”
“What is a SimBiology Model?”

display

Display summary of SimBiology object

Syntax

```
display(sobj)
```

Description

`display(sobj)` displays the summary information of the SimBiology object `sobj`.

Examples

Display Summary Information of SimBiology Model

Load the G-protein model.

```
sbioloadproject('gprotein.sbproj')
```

Display the summary information of the model.

```
display(m1)
```

```
m1 =
   SimBiology Model - Heterotrimeric G Protein wt

   Model Components:
     Compartments:      1
     Events:            0
     Parameters:        9
     Reactions:         6
     Rules:             1
     Species:           7
     Observables:       0
```

Input Arguments

`sobj` — Object

SimBiology object | array of SimBiology objects

Object, specified as a SimBiology object or array of SimBiology objects.

Version History

Introduced in R2006a

See Also

`set` | `SimData`

SimBiology.gsa.ElementaryEffects

Object containing results from calculation of elementary effects for global sensitivity analysis (GSA)

Description

The `SimBiology.gsa.ElementaryEffects` object contains GSA results returned by `sbioelementaryeffects`. The object contains the computed elementary effects with respect to parameter inputs.

Creation

Create a `SimBiology.gsa.ElementaryEffects` object using `sbioelementaryeffects`.

Properties

`AbsoluteEffects` — Flag to use absolute values of elementary effects
`true` (default) | `false`

Flag to use the absolute values of elementary effects, specified as `true` or `false`. By default, the function uses the absolute values of elementary effects. Using nonabsolute values can average out when calculating the mean. For details, see “Elementary Effects for Global Sensitivity Analysis” on page 1-51.

Data Types: `logical`

`Time` — Time points
column numeric vector

This property is read-only.

Time points at which elementary effects are computed, specified as a column numeric vector. The property is `[]` if all observables are scalars.

Data Types: `double`

`Results` — GSA results with elementary effects
structure array

This property is read-only.

GSA results with elementary effects, specified as a structure array. The size of the array is *params*-by-*observables*, where *params* is the number of input parameters (sensitivity inputs) and *observables* is the number of observables (sensitivity outputs).

Each structure contains the following fields.

- `Parameter` — Name of an input parameter, specified as a character vector
- `Observable` — Name of an observable, specified as a character vector

- `Mean` — Mean of absolute values of elementary effects, specified as a scalar or numeric vector
- `StandardDeviation` — Standard deviation of absolute elementary effects, specified as a scalar or numeric vector

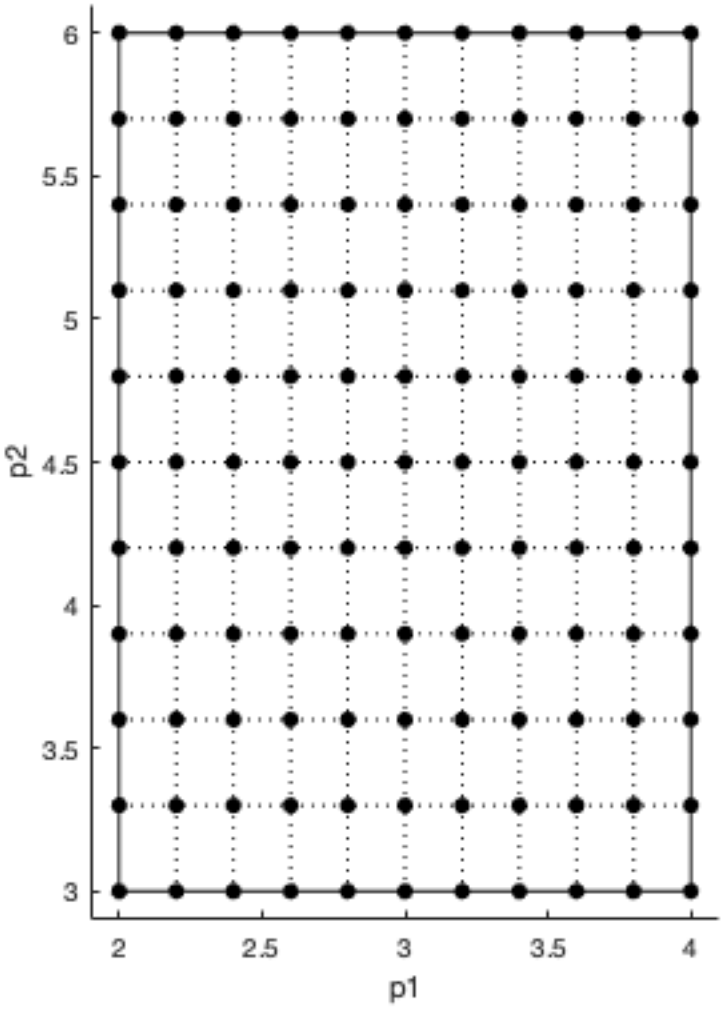
If all observables are scalar, then the `Mean` and `StandardDeviation` fields are specified as scalars. If any observables are vectors, `Mean` and `StandardDeviation` are numeric vectors of length `Time`. If some observables are scalars and some are vectors, scalar observables are scalar-expanded, where each time point has the same value.

Data Types: `struct`

`GridLevel` — Discretization level of parameter domain
`10` (default) | positive even integer

This property is read-only.

Discretization level of the parameter domain, specified as a positive even integer. This parameter defines a grid of equidistant points in the parameter domain, where each dimension is discretized using `Gridlevel+1` points. The following figure shows an example of a grid for parameters *p1* and *p2* within given parameter bounds.



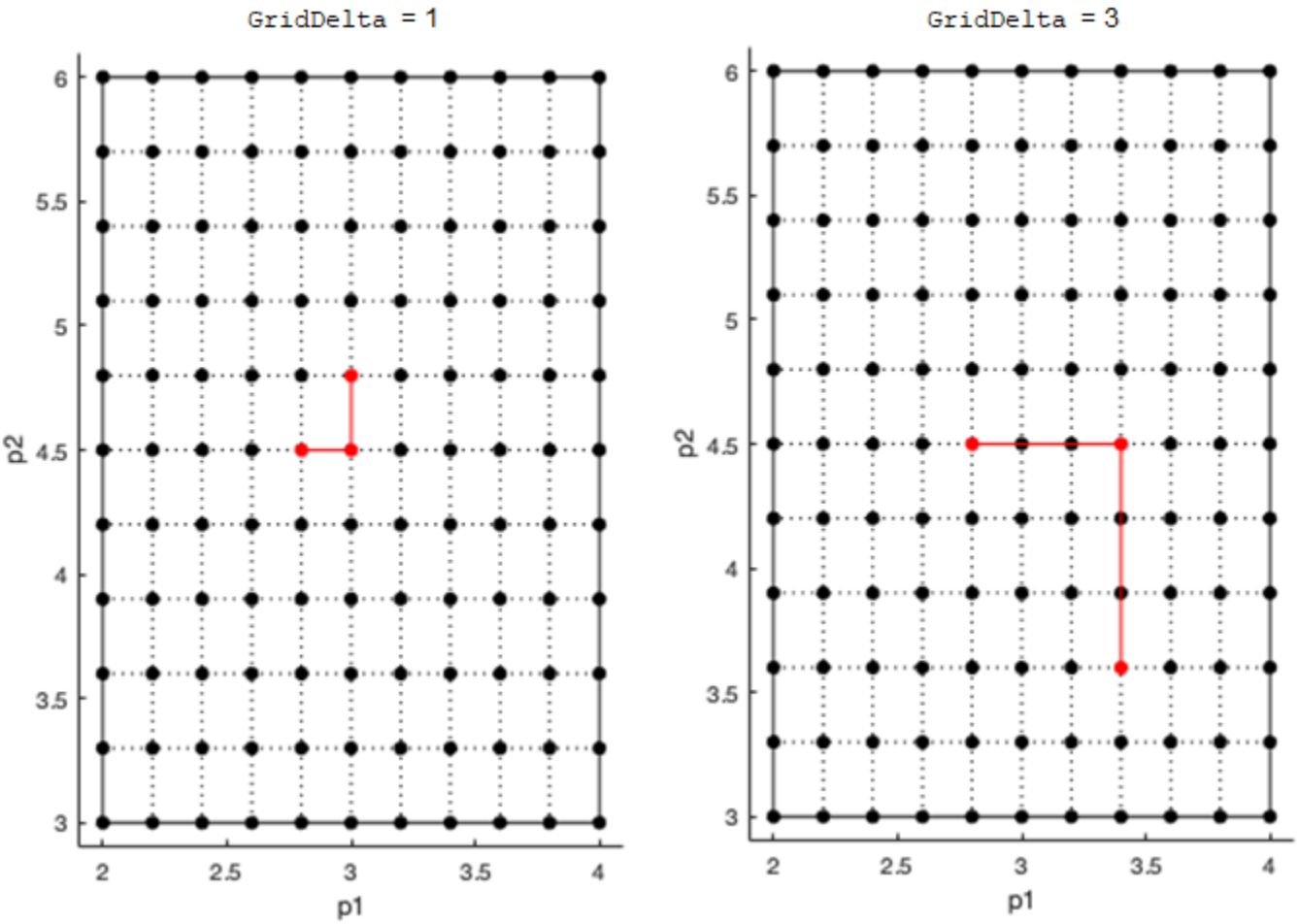
For details, see “Elementary Effects for Global Sensitivity Analysis” on page 1-51.

Data Types: `double`

`GridDelta` — Step size for computing elementary effects
`GridLevel/2` (default) | positive integer between 1 and `GridLevel`

This property is read-only.

Step size for computing elementary effects, specified as a positive integer between 1 and `GridLevel`. The step size is measured in terms of grid points between neighboring points. The following figure shows examples of different grid delta values.



For details, see “Elementary Effects for Global Sensitivity Analysis” on page 1-51.

Data Types: `double`

`PointSelection` — Method to select sample points to compute elementary effects
`"chain"` (default) | `"radial"`

This property is read-only.

Method to select sample points to compute elementary effects, specified as `"chain"` or `"radial"`. The `"chain"` point selection uses the Morris method [1]. The `"radial"` point selection uses the Sohier method [2]. For details, see “Elementary Effects for Global Sensitivity Analysis” on page 1-51.

Data Types: `double`

`ParameterSamples` — Sampled parameter values
table

This property is read-only.

Sampled parameter values, specified as a table. The table contains `(1+numel(“params” on page 1-0 ))*“NumberSamples” on page 1-0` rows and `numel(“params” on page 1-0 )` columns.

`sbioelementaryeffects` uses blocks of $k+1$ rows, where k is the number of input “params” on page 1-0 , to compute an elementary effect for each input parameter. The total number of these blocks is equal to the total number of samples. You can get the block indices by running `kron((1:NumberSamples)',ones(numel(params)+1,1))`. For details, see “Elementary Effects for Global Sensitivity Analysis” on page 1-51.

Data Types: `table`

`Observables` — Names of model responses or observables
cell array of character vectors

This property is read-only.

Names of model responses or observables, specified as a cell array of character vectors.

Data Types: `char`

`SimulationInfo` — Simulation information used for computing elementary effects
structure

This property is read-only.

Simulation information, such as simulation data and parameter samples, used for computing elementary effects, specified as a structure. The structure contains the following fields.

- `SimFunction` — `SimFunction` object used for simulating model responses or observables.
- `SimData` — `SimData` array of size `[`*`NumberSamples`*`,1]`, where *“NumberSamples” on page 1-0* is the number of samples. The array contains simulation results from `ParameterSamples`.
- `OutputTimes` — Numeric column vector containing the common time vector of all `SimData` objects.
- `Bounds` — Numeric matrix of size `[`*`params`*`,2]`. *params* is the number of input parameters. The first column contains the lower bounds and the second column contains the upper bounds for sensitivity inputs.
- `DoseTables` — Cell array of dose tables used for the `SimFunction` evaluation. `DoseTables` is the output of `getTable(doseInput)`, where *doseInput* is the value specified for the `'Doses'` name-value pair argument in the call to `sbiosobol`, `sbiompgsa`, or `sbioelementaryeffects`. If no doses are applied, this field is set to `[]`.

- `ValidSample` — Logical vector of size `[NumberSamples,1]` indicating whether a simulation for a particular sample failed. Resampling of the simulation data (`SimData`) can result in `NaN` values if the data is extrapolated. Such `SimData` are indicated as invalid.
- `InterpolationMethod` — Name of the interpolation method for `SimData`.
- `SamplingMethod` — Name of the sampling method used to draw `ParameterSamples`.
- `RandomState` — Structure containing the state of `rng` before drawing `ParameterSamples`.

Data Types: `struct`

Object Functions

resample	Resample Sobol indices or elementary effects to new time vector
addobservable	Compute Sobol indices or elementary effects for new observable expression
removeobservable	Remove Sobol indices or elementary effects of observables
addsamples	Add additional samples to increase accuracy of Sobol indices or elementary effects analysis
plotData	Plot quantile summary of model simulations from global sensitivity analysis (requires Statistics and Machine Learning Toolbox)
plot	Plot means and standard deviations of elementary effects
bar	Plot magnitudes of means and standard deviations of elementary effects
plotGrid	Plot parameter grid and points used to compute elementary effects

Examples

Perform GSA by Computing Elementary Effects

Load the “Tumor Growth Model”.

```
sbioloadproject tumor_growth_vpop_sa.sbproj
```

Get a variant with estimated parameters and the dose to apply to the model.

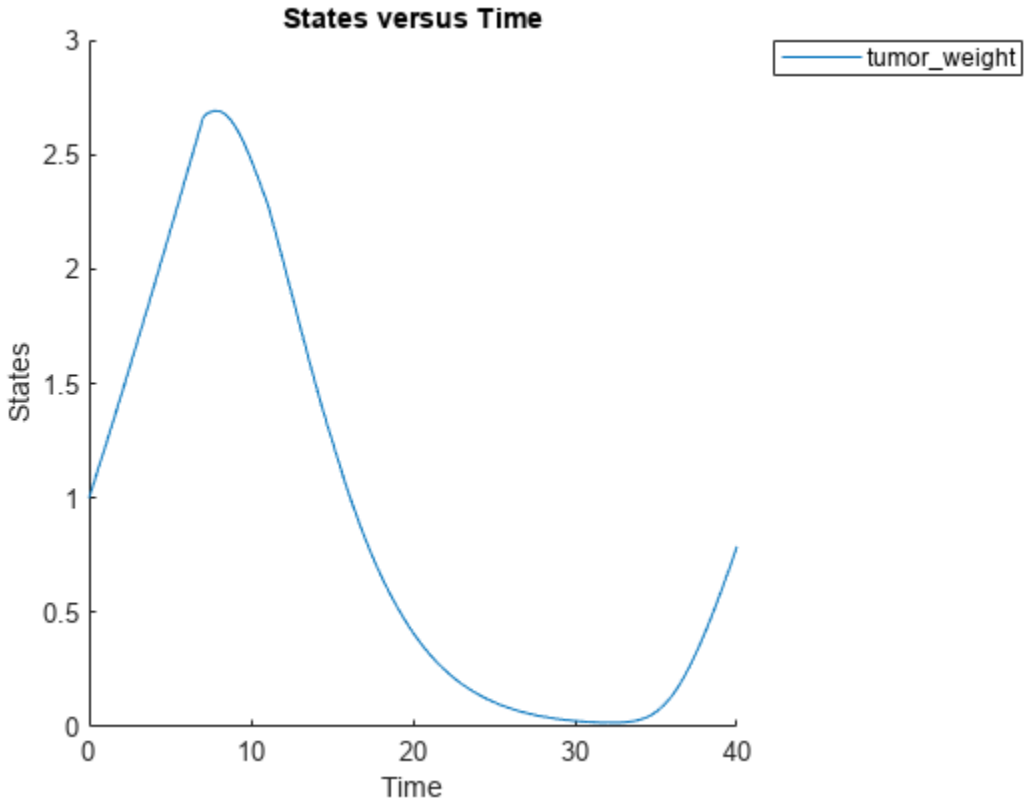
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

Get the active configset and set the tumor weight as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'tumor_weight';
```

Simulate the model and plot the tumor growth profile.

```
sbioplot(sbiosimulate(m1,cs,v,d));
```



Perform global sensitivity analysis (GSA) on the model to find the model parameters that the tumor growth is sensitive to.

First, define model parameters of interest, which are involved in the pharmacodynamics of the tumor growth. Define the model response as the tumor weight.

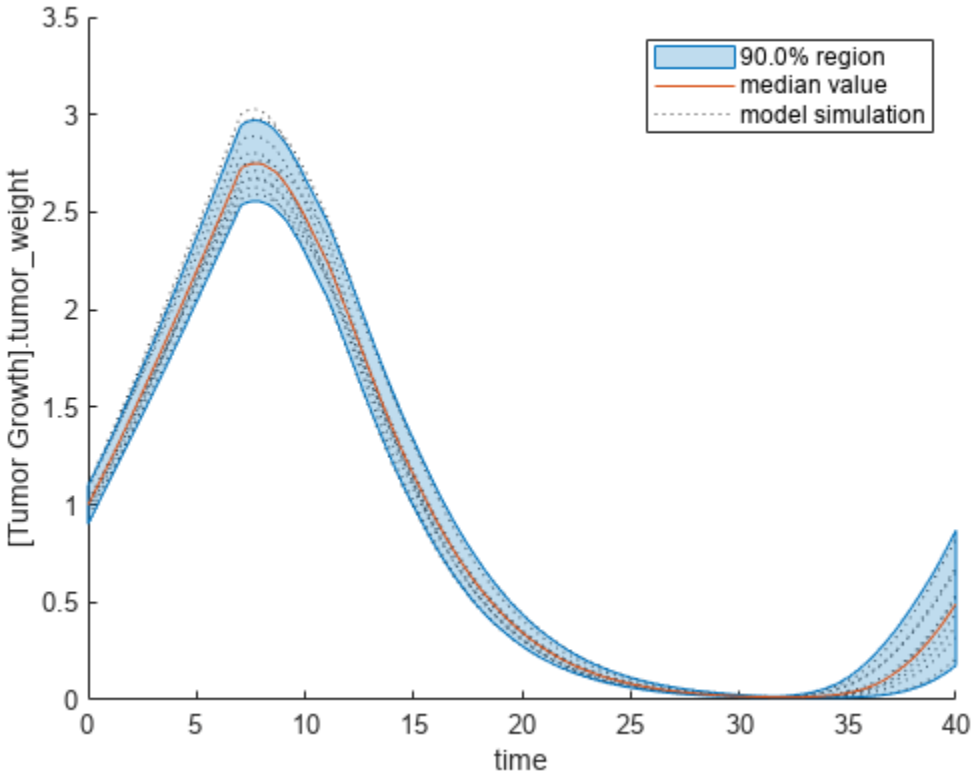
```
modelParamNames = {'L0','L1','w0','k1'};
outputName = 'tumor_weight';
```

Then perform GSA by computing the elementary effects using `sbioelementaryeffects`. Use `100` as the number of samples and set `ShowWaitBar` to `true` to show the simulation progress.

```
rng('default');
eeResults = sbioelementaryeffects(m1,modelParamNames,outputName,Variants=v,Doses=d,NumberSamples=
```

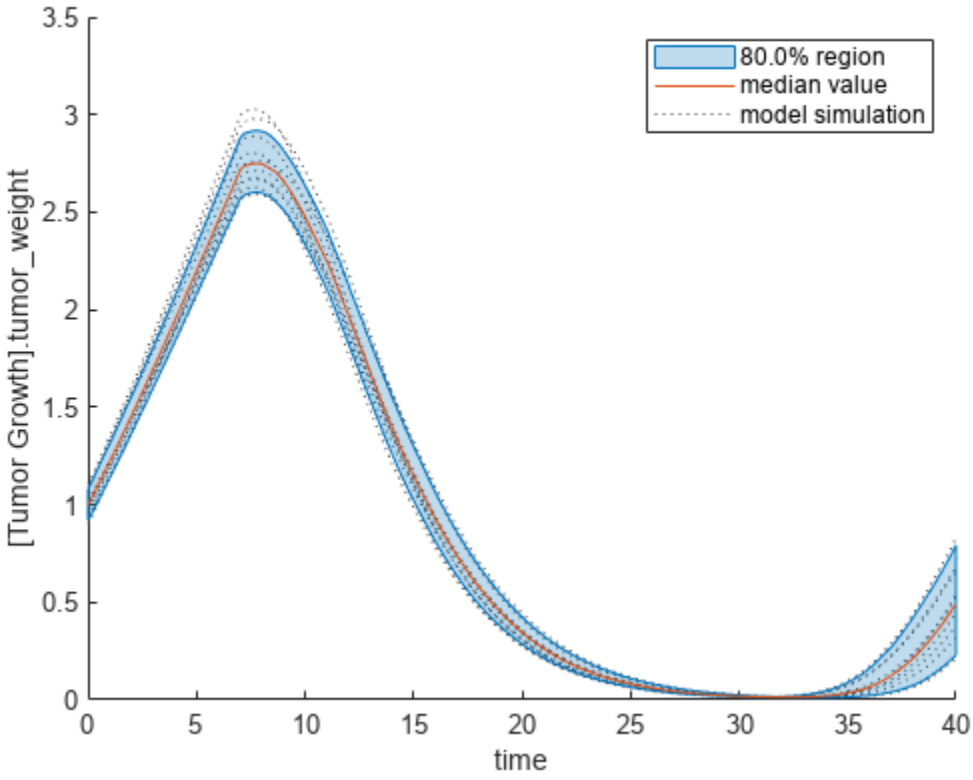
Show the median model response, the simulation results, and a shaded region covering 90% of the simulation results.

```
plotData(eeResults,ShowMedian=true,ShowMean=false);
```



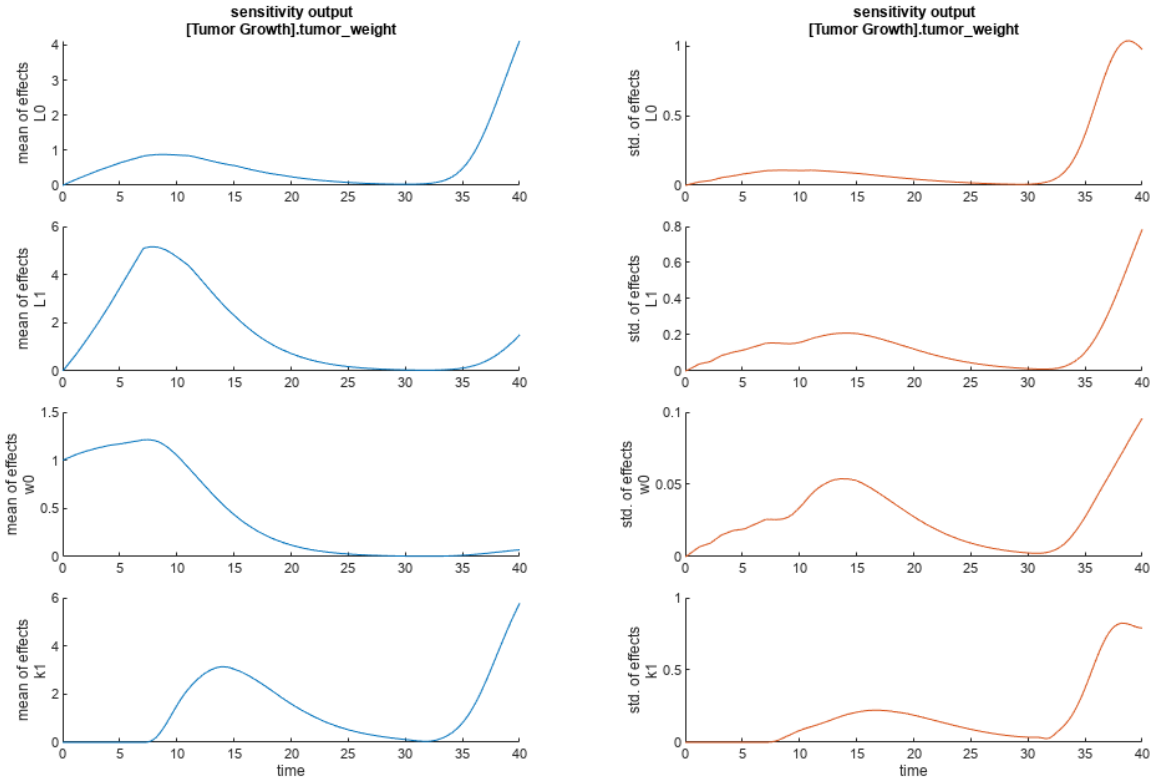
You can adjust the quantile region to a different percentage by specifying `Alphas` for the lower and upper quantiles of all model responses. For instance, an `alpha` value of 0.1 plots a shaded region between the `100*alpha` and `100*(1-alpha)` quantiles of all simulated model responses.

```
plotData(eeResults,Alphas=0.1,ShowMedian=true,ShowMean=false);
```



Plot the time course of the means and standard deviations of the elementary effects.

```
h = plot(eeResults);
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```

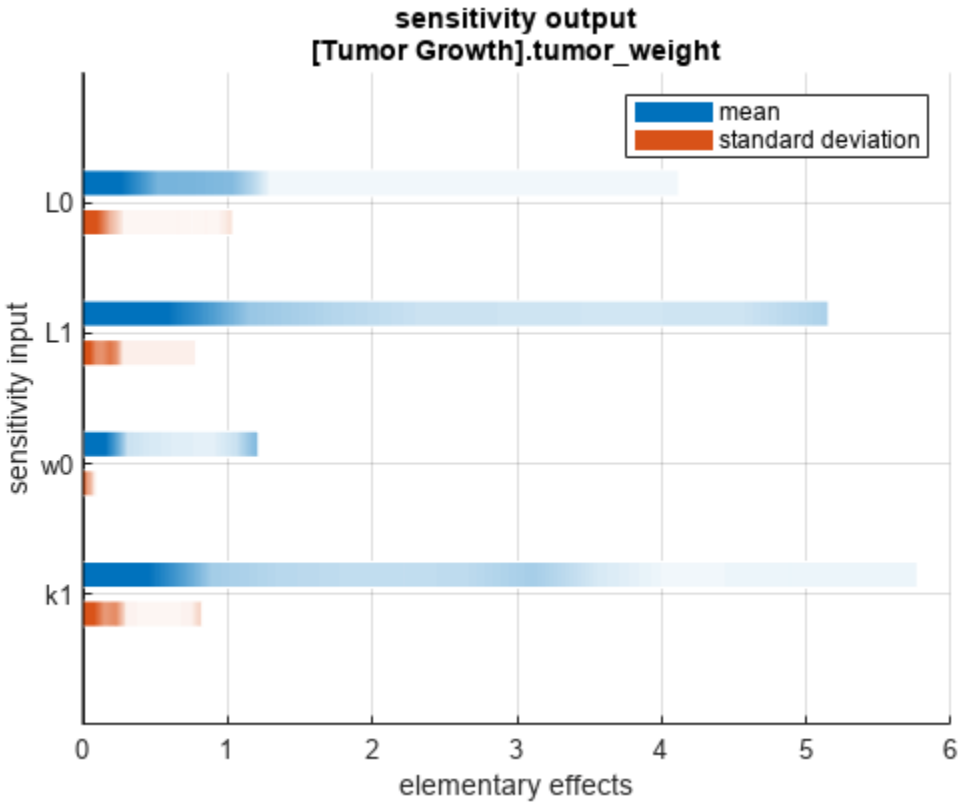


The mean of effects explains whether variations in input parameter values have any effect on the tumor weight response. The standard deviation of effects explains whether the sensitivity change is dependent on the location in the parameter domain.

From the mean of effects plots, parameters `L1` and `w0` seem to be the most sensitive parameters to the tumor weight before the dose is applied at t = 7. But, after the dose is applied, `k1` and `L0` become more sensitive parameters and contribute most to the after-dosing stage of the tumor weight. The plots of standard deviation of effects show more deviations for the larger parameter values in the later stage (t > 35) than for the before-dose stage of the tumor growth.

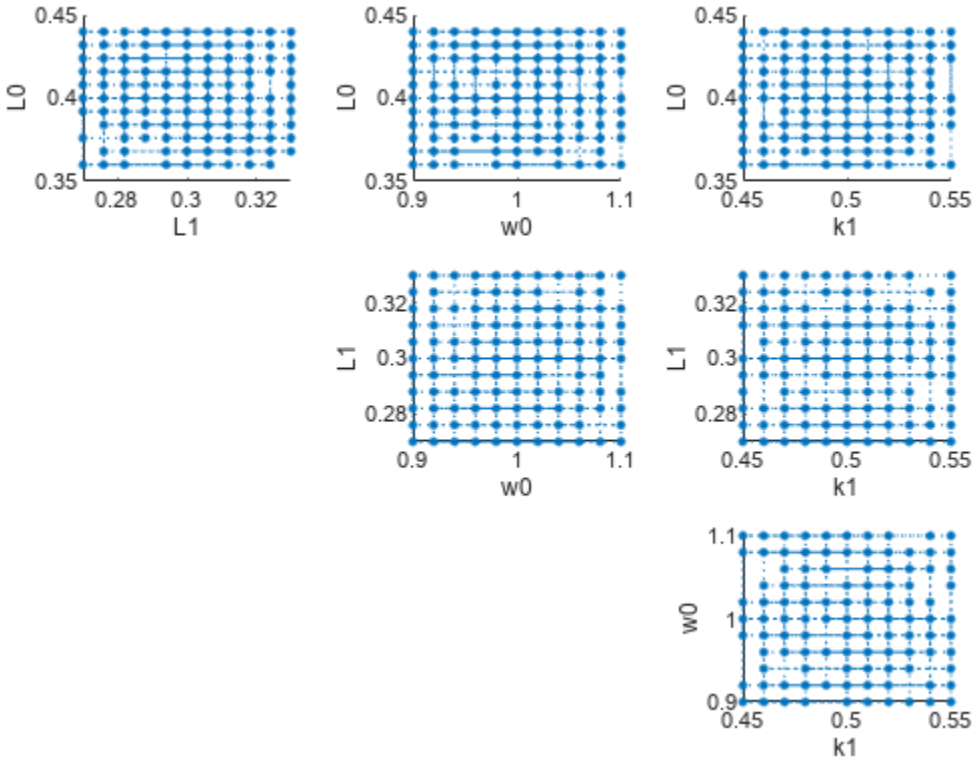
You can also display the magnitudes of the sensitivities in a bar plot. Each color shading represents a histogram representing values at different times. Darker colors mean that those values occur more often over the whole time course.

```
bar(eeResults);
```



You can also plot the parameter grids and samples used to compute the elementary effects.

```
plotGrid(eeResults)
```



You can specify more samples to increase the accuracy of the elementary effects, but the simulation can take longer to finish. Use `addsamples` to add more samples.

```
eeResults2 = addsamples(eeResults,200);
```

The `SimulationInfo` property of the result object contains various information for computing the elementary effects. For instance, the model simulation data (SimData) for each simulation using a set of parameter samples is stored in the `SimData` field of the property. This field is an array of `SimData` objects.

```
eeResults2.SimulationInfo.SimData
```

```
SimBiology SimData Array : 1500-by-1

Index:    Name:         ModelName:         DataCount:
1           -           Tumor Growth Model 1
2           -           Tumor Growth Model 1
3           -           Tumor Growth Model 1
...
1500        -           Tumor Growth Model 1
```

You can find out if any model simulation failed during the computation by checking the `ValidSample` field of `SimulationInfo`. In this example, the field shows no failed simulation runs.

```
all(eeResults2.SimulationInfo.ValidSample)
```

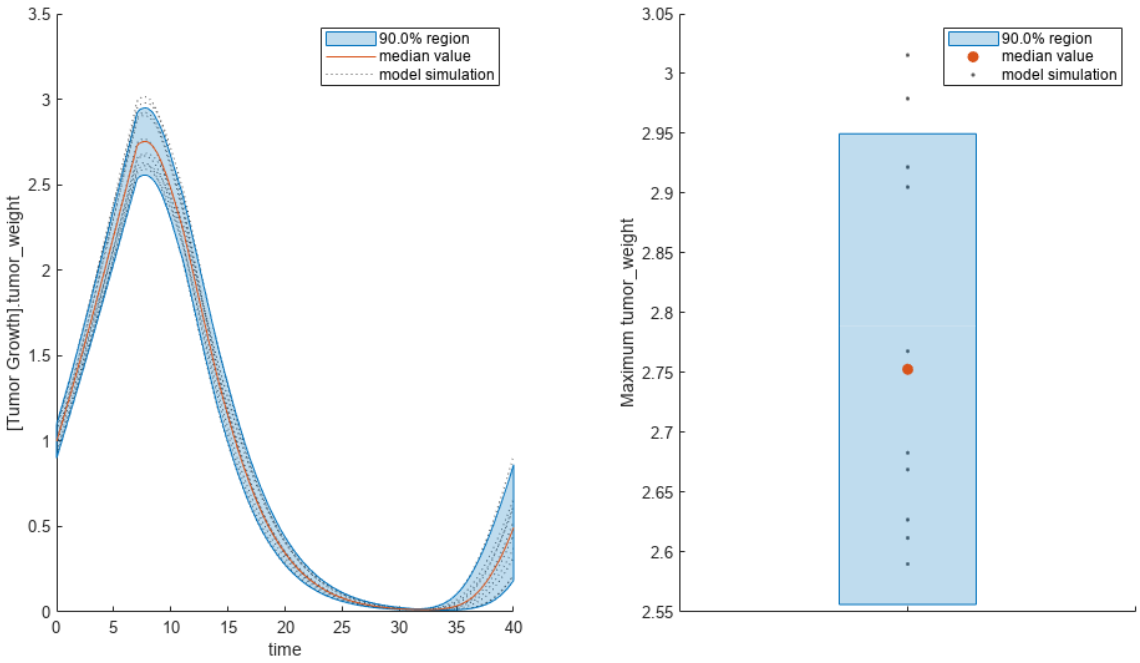
```
ans = logical
   1
```

You can add custom expressions as observables and compute the elementary effects of the added observables. For example, you can compute the effects for the maximum tumor weight by defining a custom expression as follows.

```
% Suppress an information warning that is issued.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
% Add the observable expression.
eeObs = addobservable(eeResults2,'Maximum tumor_weight','max(tumor_weight)','Units','gram');
```

Plot the computed simulation results showing the 90% quantile region.

```
h2 = plotData(eeObs,ShowMedian=true,ShowMean=false);
h2.Position(:) = [100 100 1500 800];
```



You can also remove the observable by specifying its name.

```
eeNoObs = removeobservable(eeObs,'Maximum tumor_weight');
```

Restore the warning settings.

```
warning(warnSettings);
```

Version History

Introduced in R2021b

References

[1] Morris, Max D. “Factorial Sampling Plans for Preliminary Computational Experiments.” *Technometrics* 33, no. 2 (May 1991): 161–74.

[2] Sohier, Henri, Jean-Loup Farges, and Helene Piet-Lahanier. “Improvement of the Representativity of the Morris Method for Air-Launch-to-Orbit Separation.” *IFAC Proceedings Volumes* 47, no. 3 (2014): 7954–59.

See Also

“Elementary Effects for Global Sensitivity Analysis” on page 1-51

estimatedInfo

Object containing information about estimated model quantities

Description

The `estimatedInfo` object contains information about estimated model quantities (species, parameters, or compartments). Use this object to specify which quantities in a SimBiology model are estimated, what parameter transforms are used, and optionally, the initial estimates for these quantities when using `sbiofit` or `sbiofitmixed`.

Creation

Syntax

```
estimInfo = estimatedInfo
estimInfoArray = estimatedInfo(transformedNames)
estimInfoArray = estimatedInfo( ___ ,Name,Value)
```

Description

`estimInfo = estimatedInfo` creates an empty `estimatedInfo` object.

`estimInfoArray = estimatedInfo(transformedNames)` creates a vector of `estimatedInfo` objects for quantities specified in `transformedNames`. The initial values for these quantities are obtained from the SimBiology model when you run `sbiofit` or `sbiofitmixed`.

`estimInfoArray = estimatedInfo( ___ ,Name,Value)` specifies additional options using one or more name-value arguments. For example, you can define the initial values or the initial transformed values of model quantities, the lower and upper bounds or the transformed lower and upper bounds for parameter estimation, and the groups to have separate estimated parameters.

Input Arguments

`transformedNames` — Names of estimated model quantities

character vector | string | string vector | cell array of character vectors

Names of estimated model quantities, specified as a character vector, string, string vector, or cell array of character vectors. To name a species unambiguously, use the qualified name, which includes the name of the compartment that the species is in. To name a reaction-scoped parameter, use the reaction name to qualify the parameter. Each character vector (or string) must be in one of these formats:

- Name or qualified name of a model quantity, such as `'Cl'`, `'Reaction1.k'`,`'[c 1].[r 1]'`
- Name of a supported parameter transform (`log`, `logit`, or `probit`) followed by a quantity name in parentheses, such as `'log(Cl)'`, `'logit(Reaction1.k)'`, `'probit([c 1].[r 1])'`

For details, see “Parameter Transformations”.

Name-Value Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `estimated = estimatedInfo('log(Central)','InitialValue', 1,'Bounds',[0 10])`

`InitialTransformedValue` — Initial transformed values of model quantities
vector | cell array

Initial transformed values of model quantities, specified as a vector or cell array. It must have the same length as `transformedNames`. If it is a cell array, each element of the cell must be a scalar or the empty matrix `[]`.

You cannot specify this name-value argument along with the `'InitialValue'` name-value argument.

`InitialValue` — Initial values of model quantities
vector | cell array

Initial values of model quantities, specified as a vector or cell array. It must have the same length as `transformedNames`. If it is a cell array, each element of the cell must be a scalar or the empty matrix `[]`.

You cannot specify this name-value argument along with the `'InitialTransformedValue'` name-value argument.

Bounds — Lower and upper bounds for estimated parameters
`[]` (default) | matrix | cell array

Lower and upper bounds for estimated parameters (`boundValues`), specified as a matrix or cell array. If `boundValues` is a matrix, it is an *N*-by-2 matrix of numbers, where *N* is either 1 or the length of `transformedNames`. If it is a cell array, each element must be a vector of size 1-by-2 or empty `[]`.

Each row of `boundValues` corresponds to the lower (the first number) and upper (the second number) bounds of each element (such as a parameter) of `estimInfo`. The lower bound must be less than the upper bound. If you specify a single row, these bounds are applied to all elements of `estimInfoArray`.

All methods support parameter bounds in `sbiofit` (that is, `fminsearch`, `nlinfit`, `fminunc`, `fmincon`, `lsqcurvefit`, `lsqnonlin`, `patternsearch`, `ga`, `particleswarm`, and scattersearch on page 1-98). When using `fminsearch`, `nlinfit`, or `fminunc` with bounds, the objective function returns `Inf` if bounds are exceeded. When you turn on options such as `FunValCheck`, the optimization may error if bounds are exceeded during estimation. If using `nlinfit`, it may report warnings about the Jacobian being ill-conditioned or not being able to estimate if the final result is too close to the bounds. `sbiofitmixed` does not support parameter bounds.

You cannot specify this name-value argument along with the `'TransformedBounds'` name-value argument.

`TransformedBounds` — Transformed lower and upper bounds for estimated parameters
`[]` (default) | matrix | cell array

Transformed lower and upper bounds for estimated parameters (`tBoundValues`), specified as a matrix or cell array. `tBoundValues` is a *N*-by-2 matrix of numbers, where *N* is either 1 or the length of `transformedNames`. If it is a cell array, each element must be a vector of size 1-by-2 or empty `[]`.

Each row of `tBoundValues` corresponds to the lower (the first number) and upper (the second number) bounds of each element (such as a parameter) of `estimInfo`. The lower bound must be less than the upper bound. If you specify a single row, the bounds are applied to all elements of `estimInfoArray`.

You cannot specify this name-value argument along with the `'Bounds'` name-value argument.

`CategoryVariableName` — Group names for estimated parameters
character vector | string | string vector | cell array of character vectors

Group names for estimated parameters, specified as a character vector, string, string vector, or cell array of character vectors. Each character vector (or string) must be one of the following.

- Name of a variable in the data used for fitting
- `'<GroupVariableName>'` (default)
- `'<None>'`

`'<GroupVariableName>'` indicates that each group in the data uses a separate parameter estimate. `'<None>'` indicates that all groups in the data use the same parameter estimate.

If the data you plan to use for fitting contains variables that group data into different categories, you can specify the names of those variables. For instance, if you have a variable called `Sex` which indicates male and female individuals, you can specify `'Sex'` as the `'CategoryVariableName'`. This means that all male individuals have one set of parameter estimates and all females have a separate set.

Output Arguments

`estimInfo` — Estimated model quantity
`estimatedInfo` object

Estimated model quantity, returned as an `estimatedInfo` object.

`estimInfoArray` — Estimated model quantities
`estimatedInfo` object | vector

Estimated model quantities, returned as an `estimatedInfo` object or vector of `estimatedInfo` objects. If `transformedNames` is a single character vector, `estimInfoArray` is a scalar `estimatedInfo` object. Otherwise, `estimInfoArray` is a vector of `estimatedInfo` objects with the same length as the input argument `transformedNames`.

Properties

`Name` — Name of an estimated model quantity
character vector

Name of an estimated model quantity, specified as a character vector. Changing this property also updates the `TransformedName` property.

`Transform` — Applied transformation for the quantity value during estimation
`''` | `'log'` | `'logit''probit'`

Applied transformation for the quantity value during estimation, specified as `''`, `'log'`, `'logit'`, or `'probit'`. An empty character vector `''` indicates that no transform is applied.

A log transform ensures that the component value is always positive during estimation. The `logit` and `probit` transforms constrain component values to lie between 0 and 1.

The `probit` function is the inverse cumulative distribution function associated with the standard normal distribution. For the `probit` transform, SimBiology uses the `norminv` function. Hence Statistics and Machine Learning Toolbox is required for the transform.

The logit function, which is the inverse of sigmoid function, is defined as `logit(x) = log(x) − log(1 − x)`.

`TransformedName` — Combined transform name and quantity name
character vector

This property is read-only.

Combined transform name (such as `'log'`) and quantity name (such as `'Central'`), specified as a character vector (such as `'log(Central)'`).

`InitialValue` — Initial values of model quantities used for estimation
empty matrix | scalar

Initial values of model quantities used for estimation, specified as an empty matrix `[]` or a real, finite, scalar value. The empty matrix indicates that the initial values for estimation are obtained from the relevant quantity property (`Value` for parameters, `InitialAmount` for species, and `Capacity` for compartments).

Changing this property automatically updates the `InitialTransformedValue` property of corresponding model quantities.

`InitialTransformedValue` — Initial transformed values of model quantities used for estimation
empty matrix | scalar

Initial transformed values of model quantities used for estimation, specified as an empty matrix `[]` or a scalar value. The empty matrix indicates that the initial transformed values for estimation are obtained by transforming the relevant quantity property (`Value` for parameters, `InitialAmount` for species, and `Capacity` for compartments).

Changing this property automatically updates the `InitialValue` property of corresponding model quantities.

`Bounds` — Lower and upper bounds for an estimated parameter
empty matrix | 1-by-2 vector

Lower and upper bounds for an estimated parameter, specified as an empty matrix `[]` or a 1-by-2 vector of real, finite values. The empty matrix `[]` indicates that the only bound constraints are those

introduced by the value of `Transform`. For example, setting `Transform` to `'log'` constrains the parameter to the range `[0,inf]`. Changing this property also updates `TransformedBounds`.

The lower bound must be less than the upper bound.

`TransformedBounds` — Transformed lower and upper bound for an estimated parameter
empty matrix | 1-by-2 vector

Transformed lower and upper bound for an estimated parameter, specified as an empty matrix `[]` or a 1-by-2 vector of real, finite values. The empty matrix `[]` indicates that the value of the parameter in transformed space is not constrained. Changing this property also updates `Bounds`.

The lower bound must be less than the upper bound.

`CategoryVariableName` — Data groups to have separate estimated parameters
character vector | cell array of character vectors

Data groups to have separate estimated parameters, specified as a character vector or a cell array of character vectors. The character vector can be the name of a variable in the data used for fitting or one of the keywords: `'<GroupVariableName>'` or `'<None>'`.

`'<GroupVariableName>'` indicates that each group in the data uses a separate parameter estimate. `'<None>'` indicates that all groups in the data use the same parameter estimate.

If you specify `'Pooled'` name-value argument (to either `true` or `false`) when you run `sbiofit`, then the function ignores this variable. `sbiofitmixed` always ignores this property.

Examples

Specify Estimated Parameters Using an EstimatedInfo Object

Create a one-compartment PK model with bolus dosing and linear clearance.

```
pkmd                    = PKModelDesign;
pkc1                    = addCompartment(pkmd,'Central');
pkc1.DosingType         = 'Bolus';
pkc1.EliminationType    = 'linear-clearance';
pkc1.HasResponseVariable = true;
```

Suppose you want to estimate the volume of the central compartment (`Central`). You can specify such estimated model quantity as well as appropriate parameter transform (`log` transform in this example), initial value, and parameter bound using the `estimatedInfo` object.

```
estimated = estimatedInfo('log(Central)','InitialValue', 1,'Bounds',[0 10])
```

```
estimated =
  estimatedInfo with properties:

                      Name: 'Central'
                 Transform: 'log'
             TransformedName: 'log(Central)'
                InitialValue: 1
    InitialTransformedValue: 0
                    Bounds: [0 10]
          TransformedBounds: [-Inf 2.3026]
```

```
CategoryVariableName: '<GroupVariableName>'
```

Fit One-Compartment Model to Individual PK Profile

Background

This example shows how to fit an individual's PK profile data to one-compartment model and estimate pharmacokinetic parameters.

Suppose you have drug plasma concentration data from an individual and want to estimate the volume of the central compartment and the clearance. Assume the drug concentration versus the time profile follows the monoexponential decline $C_t = C_0 e^{-k_e t}$, where C_t is the drug concentration at time t, C_0 is the initial concentration, and k_e is the elimination rate constant that depends on the clearance and volume of the central compartment $k_e = Cl/V$.

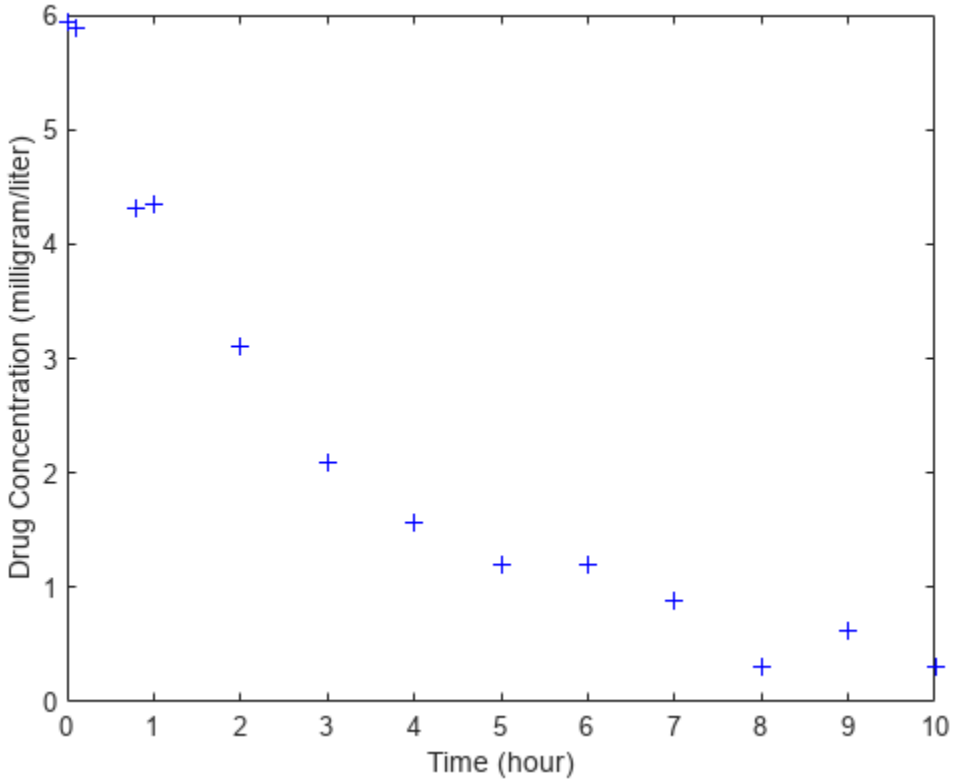
The synthetic data in this example was generated using the following model, parameters, and dose:

- One-compartment model with bolus dosing and first-order elimination
- Volume of the central compartment (`Central`) = 1.70 liter
- Clearance parameter (`Cl_Central`) = 0.55 liter/hour
- Constant error model
- Bolus dose of 10 mg

Load Data and Visualize

The data is stored as a table with variables `Time` and `Conc` that represent the time course of the plasma concentration of an individual after an intravenous bolus administration measured at 13 different time points. The variable units for `Time` and `Conc` are hour and milligram/liter, respectively.

```
load('data15.mat')
plot(data.Time,data.Conc,'b+')
xlabel('Time (hour)');
ylabel('Drug Concentration (milligram/liter)');
```



Convert to groupedData Format

Convert the data set to a `groupedData` object, which is the required data format for the fitting function `sbiofit` for later use. A `groupedData` object also lets you set independent variable and group variable names (if they exist). Set the units of the `Time` and `Conc` variables. The units are optional and only required for the `UnitConversion` feature, which automatically converts matching physical quantities to one consistent unit system.

```
gData = groupedData(data);
gData.Properties.VariableUnits = {'hour','milligram/liter'};
gData.Properties
```

```
ans = struct with fields:
                Description: ''
                   UserData: []
             DimensionNames: {'Row'  'Variables'}
              VariableNames: {'Time'  'Conc'}
       VariableDescriptions: {}
              VariableUnits: {'hour'  'milligram/liter'}
         VariableContinuity: []
                   RowNames: {}
           CustomProperties: [1x1 matlab.tabular.CustomProperties]
          GroupVariableName: ''
    IndependentVariableName: 'Time'
```

`groupedData` automatically set the name of the `IndependentVariableName` property to the `Time` variable of the data.

Construct a One-Compartment Model

Use the built-in PK library to construct a one-compartment model with bolus dosing and first-order elimination where the elimination rate depends on the clearance and volume of the central compartment. Use the `configset` object to turn on unit conversion.

```
pkmd                    = PKModelDesign;
pkc1                    = addCompartment(pkmd,'Central');
pkc1.DosingType         = 'Bolus';
pkc1.EliminationType    = 'linear-clearance';
pkc1.HasResponseVariable = true;
model                   = construct(pkmd);
configset               = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
```

For details on creating compartmental PK models using the SimBiology® built-in library, see “Create Pharmacokinetic Models”.

Define Dosing

Define a single bolus dose of 10 milligram given at time = 0. For details on setting up different dosing schedules, see “Doses in SimBiology Models”.

```
dose                = sbiodose('dose');
dose.TargetName     = 'Drug_Central';
dose.StartTime      = 0;
dose.Amount         = 10;
dose.AmountUnits    = 'milligram';
dose.TimeUnits      = 'hour';
```

Map Response Data to the Corresponding Model Component

The data contains drug concentration data stored in the `Conc` variable. This data corresponds to the `Drug_Central` species in the model. Therefore, map the data to `Drug_Central` as follows.

```
responseMap = {'Drug_Central = Conc'};
```

Specify Parameters to Estimate

The parameters to fit in this model are the volume of the central compartment (Central) and the clearance rate (Cl_Central). In this case, specify log-transformation for these biological parameters since they are constrained to be positive. The `estimatedInfo` object lets you specify parameter transforms, initial values, and parameter bounds if needed.

```
paramsToEstimate    = {'log(Central)','log(Cl_Central)'};
estimatedParams     = estimatedInfo(paramsToEstimate,'InitialValue',[1 1],'Bounds',[1 5;0.5 2]);
```

Estimate Parameters

Now that you have defined one-compartment model, data to fit, mapped response data, parameters to estimate, and dosing, use `sbiofit` to estimate parameters. The default estimation function that `sbiofit` uses will change depending on which toolboxes are available. To see which function was used during fitting, check the `EstimationFunction` property of the corresponding results object.

```
fitConst = sbiofit(model,gData,responseMap,estimatedParams,dose);
```

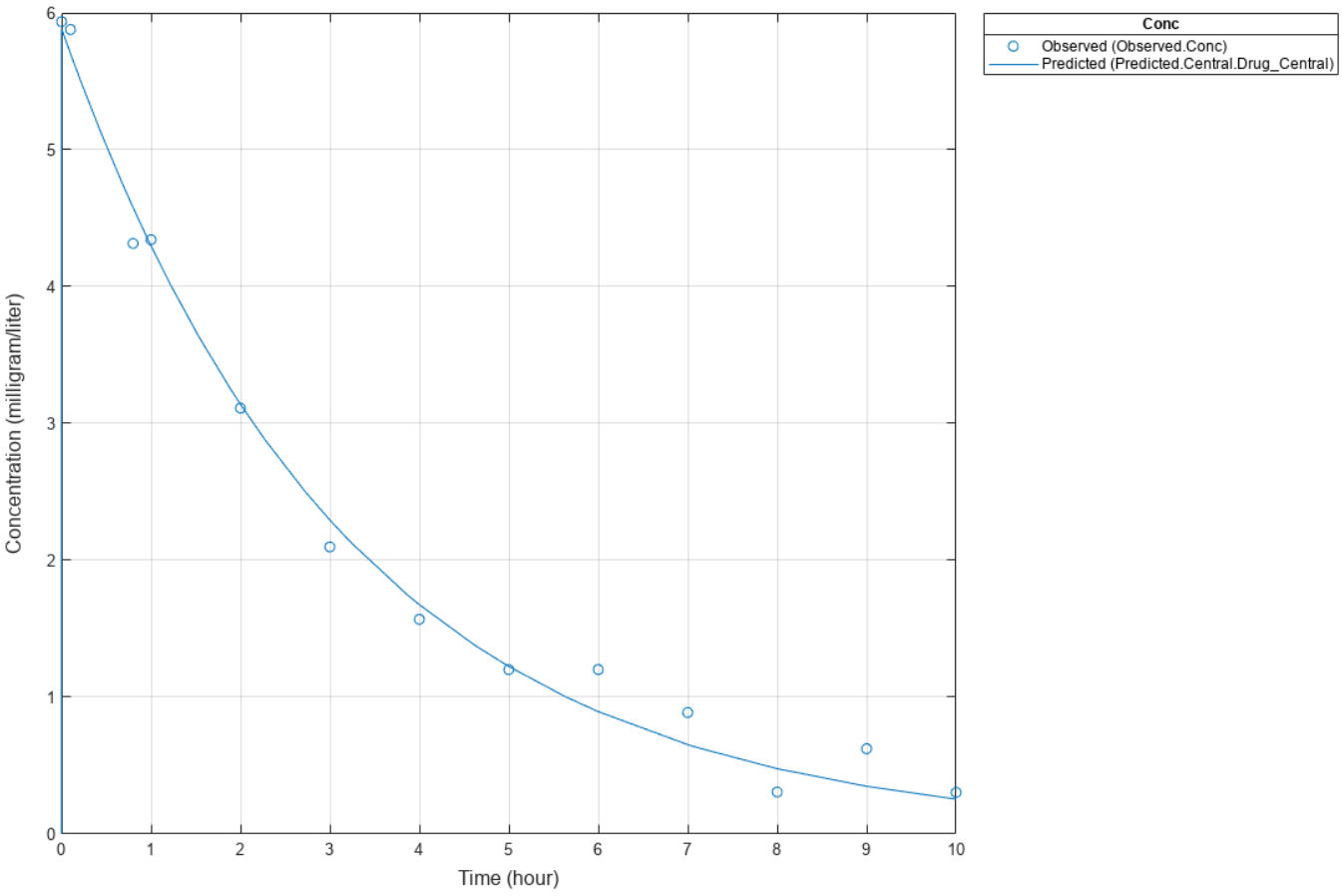
Display Estimated Parameters and Plot Results

Notice the parameter estimates were not far off from the true values (1.70 and 0.55) that were used to generate the data. You may also try different error models to see if they could further improve the parameter estimates.

```
fitConst.ParameterEstimates
```

```
ans=2×4 table
        Name          Estimate    StandardError      Bounds
    ______________    ________    _____________    __________

    {'Central'   }     1.6993       0.034821          1      5
    {'Cl_Central'}    0.53358        0.01968        0.5      2
```

```
s.Labels.XLabel     = 'Time (hour)';
s.Labels.YLabel     = 'Concentration (milligram/liter)';
plot(fitConst,'AxesStyle',s);
```



Use Different Error Models

Try three other supported error models (proportional, combination of constant and proportional error models, and exponential).

```
fitProp = sbiofit(model,gData,responseMap,estimatedParams,dose,...
                        'ErrorModel','proportional');
fitExp  = sbiofit(model,gData,responseMap,estimatedParams,dose,...
                        'ErrorModel','exponential');
fitComb = sbiofit(model,gData,responseMap,estimatedParams,dose,...
                        'ErrorModel','combined');
```

Use Weights Instead of an Error Model

You can specify weights as a numeric matrix, where the number of columns corresponds to the number of responses. Setting all weights to 1 is equivalent to the constant error model.

```
weightsNumeric = ones(size(gData.Conc));
fitWeightsNumeric = sbiofit(model,gData,responseMap,estimatedParams,dose,'Weights',weightsNumeric
```

Alternatively, you can use a function handle that accepts a vector of predicted response values and returns a vector of weights. In this example, use a function handle that is equivalent to the proportional error model.

```
weightsFunction = @(y) 1./y.^2;
fitWeightsFunction = sbiofit(model,gData,responseMap,estimatedParams,dose,'Weights',weightsFunct
```

Compare Information Criteria for Model Selection

Compare the loglikelihood, AIC, and BIC values of each model to see which error model best fits the data. A larger likelihood value indicates the corresponding model fits the model better. For AIC and BIC, the smaller values are better.

```
allResults = [fitConst,fitWeightsNumeric,fitWeightsFunction,fitProp,fitExp,fitComb];
errorModelNames = {'constant error model','equal weights','proportional weights', ...
                   'proportional error model','exponential error model',...
                   'combined error model'};
LogLikelihood = [allResults.LogLikelihood]';
AIC = [allResults.AIC]';
BIC = [allResults.BIC]';
t = table(LogLikelihood,AIC,BIC);
t.Properties.RowNames = errorModelNames;
t
```

```
t=6×3 table
                               LogLikelihood      AIC        BIC
                               _____________    _______    _______

    constant error model           3.9866       -3.9732    -2.8433
    equal weights                  3.9866       -3.9732    -2.8433
    proportional weights          -3.8472        11.694     12.824
    proportional error model      -3.8257        11.651     12.781
    exponential error model        1.1984        1.6032     2.7331
    combined error model           3.9163       -3.8326    -2.7027
```

Based on the information criteria, the constant error model (or equal weights) fits the data best since it has the largest loglikelihood value and the smallest AIC and BIC.

Display Estimated Parameter Values

Show the estimated parameter values of each model.

```
Estimated_Central       = zeros(6,1);
Estimated_Cl_Central    = zeros(6,1);
t2 = table(Estimated_Central,Estimated_Cl_Central);
t2.Properties.RowNames = errorModelNames;
for i = 1:height(t2)
    t2{i,1} = allResults(i).ParameterEstimates.Estimate(1);
    t2{i,2} = allResults(i).ParameterEstimates.Estimate(2);
end
t2
```

```
t2=6×2 table
                              Estimated_Central    Estimated_Cl_Central
                              _________________    ____________________

    constant error model            1.6993               0.53358
    equal weights                   1.6993               0.53358
    proportional weights            1.9045               0.51734
    proportional error model        1.8777               0.51147
    exponential error model         1.7872               0.51701
    combined error model            1.7008               0.53271
```

Conclusion

This example showed how to estimate PK parameters, namely the volume of the central compartment and clearance parameter of an individual, by fitting the PK profile data to one-compartment model. You compared the information criteria of each model and estimated parameter values of different error models to see which model best explained the data. Final fitted results suggested both the constant and combined error models provided the closest estimates to the parameter values used to generate the data. However, the constant error model is a better model as indicated by the loglikelihood, AIC, and BIC information criteria.

Estimate Category-Specific PK Parameters for Multiple Individuals

This example shows how to estimate category-specific (such as young versus old, male versus female), individual-specific, and population-wide parameters using PK profile data from multiple individuals.

Background

Suppose you have drug plasma concentration data from 30 individuals and want to estimate pharmacokinetic parameters, namely the volumes of central and peripheral compartment, the clearance, and intercompartmental clearance. Assume the drug concentration versus the time profile follows the biexponential decline $C_t = Ae^{-at} + Be^{-bt}$, where C_t is the drug concentration at time t, and a and b are slopes for corresponding exponential declines.

Load Data

This synthetic data contains the time course of plasma concentrations of 30 individuals after a bolus dose (100 mg) measured at different times for both central and peripheral compartments. It also contains categorical variables, namely Sex and Age.

```
clear
load('sd5_302RAgeSex.mat')
```

Convert to groupedData Format

Convert the data set to a `groupedData` object, which is the required data format for the fitting function `sbiofit`. A `groupedData` object also allows you set independent variable and group variable names (if they exist). Set the units of the `ID`, `Time`, `CentralConc`, `PeripheralConc`, `Age`, and `Sex` variables. The units are optional and only required for the `UnitConversion` feature, which automatically converts matching physical quantities to one consistent unit system.

```
gData = groupedData(data);
gData.Properties.VariableUnits = {'','hour','milligram/liter','milligram/liter','',''};
gData.Properties
```

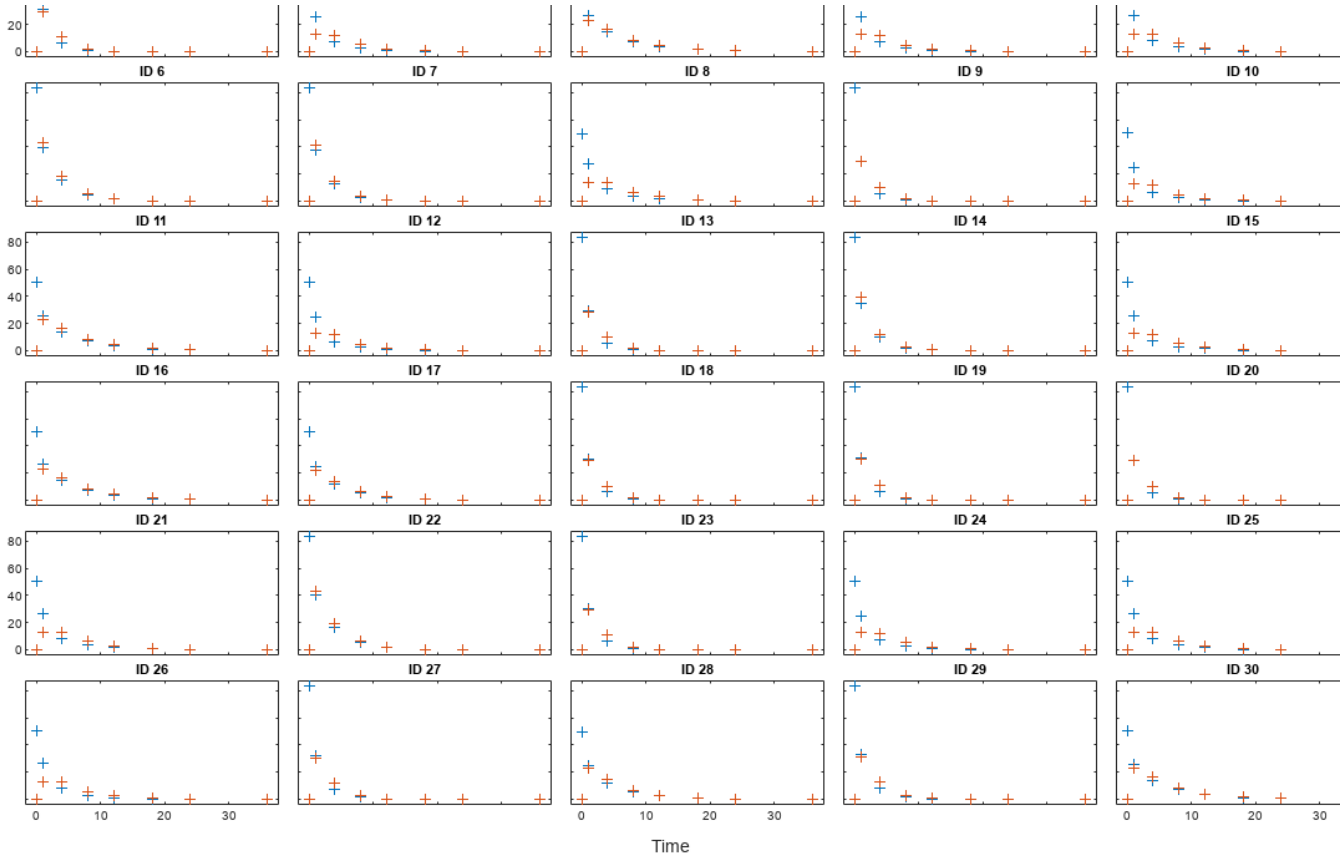
```
ans = struct with fields:
                Description: ''
                   UserData: []
              DimensionNames: {'Row'  'Variables'}
               VariableNames: {'ID'  'Time'  'CentralConc'  'PeripheralConc'  'Sex'  'Age'}
       VariableDescriptions: {}
              VariableUnits: {''  'hour'  'milligram/liter'  'milligram/liter'  ''  ''}
         VariableContinuity: []
                   RowNames: {}
             CustomProperties: [1x1 matlab.tabular.CustomProperties]
          GroupVariableName: 'ID'
    IndependentVariableName: 'Time'
```

The `IndependentVariableName` and `GroupVariableName` properties have been automatically set to the `Time` and `ID` variables of the data.

Visualize Data

Display the response data for each individual.

```
t = sbiotrellis(gData,'ID','Time',{'CentralConc','PeripheralConc'},...
                'Marker','+','LineStyle','none');
% Resize the figure.
t.hFig.Position(:) = [100 100 1280 800];
```



Set Up a Two-Compartment Model

Use the built-in PK library to construct a two-compartment model with infusion dosing and first-order elimination where the elimination rate depends on the clearance and volume of the central compartment. Use the `configset` object to turn on unit conversion.

```
pkmd                                    = PKModelDesign;
pkc1                                    = addCompartment(pkmd,'Central');
pkc1.DosingType                         = 'Bolus';
pkc1.EliminationType                    = 'linear-clearance';
pkc1.HasResponseVariable                = true;
pkc2                                    = addCompartment(pkmd,'Peripheral');
model                                   = construct(pkmd);
configset                               = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
```

For details on creating compartmental PK models using the SimBiology® built-in library, see “Create Pharmacokinetic Models”.

Define Dosing

Assume every individual receives a bolus dose of 100 mg at time = 0. For details on setting up different dosing strategies, see “Doses in SimBiology Models”.

```
dose             = sbiodose('dose','TargetName','Drug_Central');
dose.StartTime   = 0;
dose.Amount      = 100;
```

```
dose.AmountUnits = 'milligram';
dose.TimeUnits   = 'hour';
```

Map the Response Data to Corresponding Model Components

The data contains measured plasma concentration in the central and peripheral compartments. Map these variables to the appropriate model components, which are `Drug_Central` and `Drug_Peripheral`.

```
responseMap = {'Drug_Central = CentralConc','Drug_Peripheral = PeripheralConc'};
```

Specify Parameters to Estimate

Specify the volumes of central and peripheral compartments `Central` and `Peripheral`, intercompartmental clearance `Q12`, and clearance `Cl_Central` as parameters to estimate. The `estimatedInfo` object lets you optionally specify parameter transforms, initial values, and parameter bounds. Since both `Central` and `Peripheral` are constrained to be positive, specify a log-transform for each parameter.

```
paramsToEstimate    = {'log(Central)', 'log(Peripheral)', 'Q12', 'Cl_Central'};
estimatedParam      = estimatedInfo(paramsToEstimate,'InitialValue',[1 1 1 1]);
```

Estimate Individual-Specific Parameters

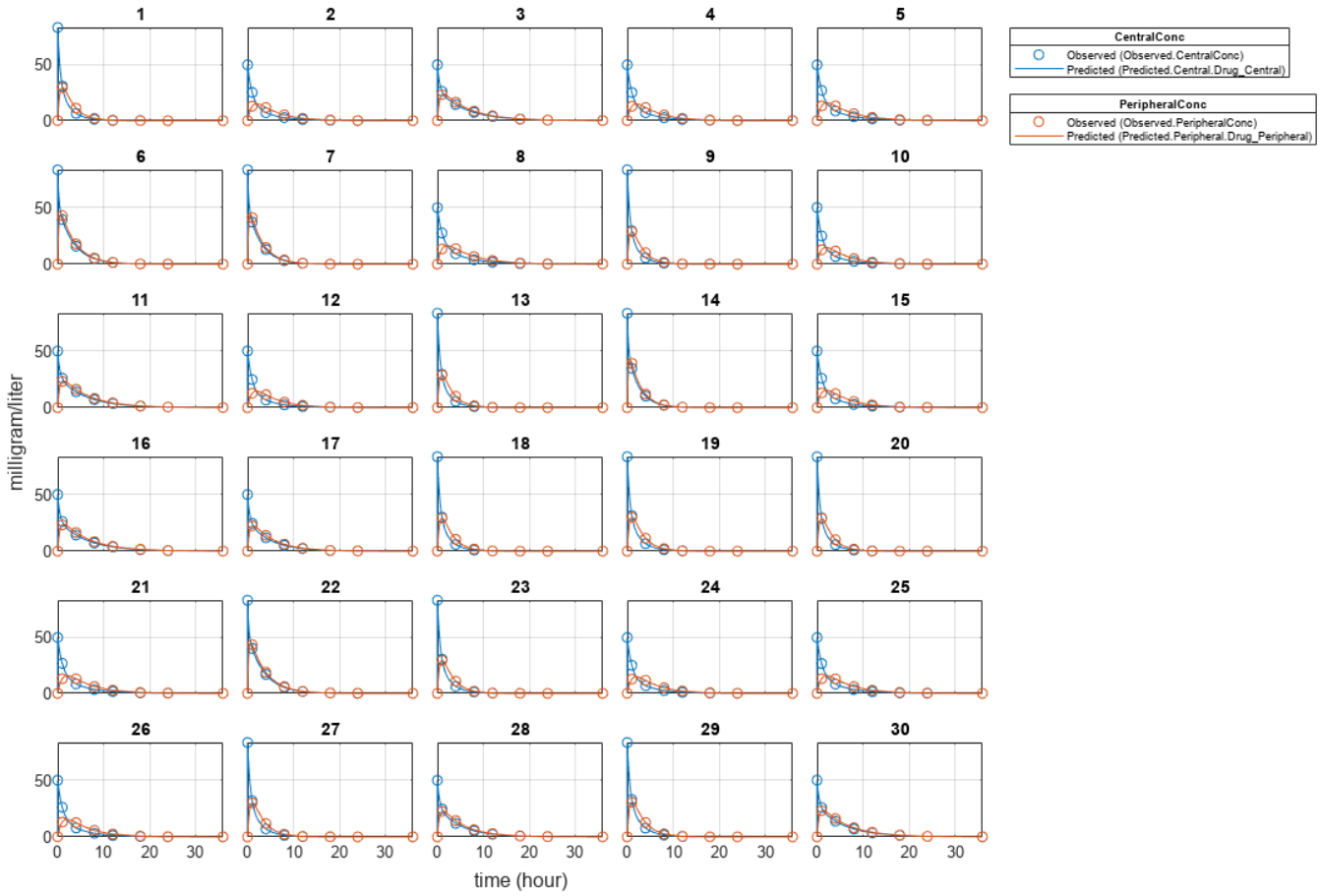
Estimate one set of parameters for each individual by setting the `'Pooled'` name-value pair argument to `false`.

```
unpooledFit =  sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',false);
```

Display Results

Plot the fitted results versus the original data for each individual (group).

```
plot(unpooledFit);
```



For an unpooled fit, `sbiofit` always returns one results object for each individual.

Examine Parameter Estimates for Category Dependencies

Explore the unpooled estimates to see if there is any category-specific parameters, that is, if some parameters are related to one or more categories. If there are any category dependencies, it might be possible to reduce the number of degrees of freedom by estimating just category-specific values for those parameters.

First extract the ID and category values for each ID

```
catParamValues = unique(gData(:,{'ID','Sex','Age'}));
```

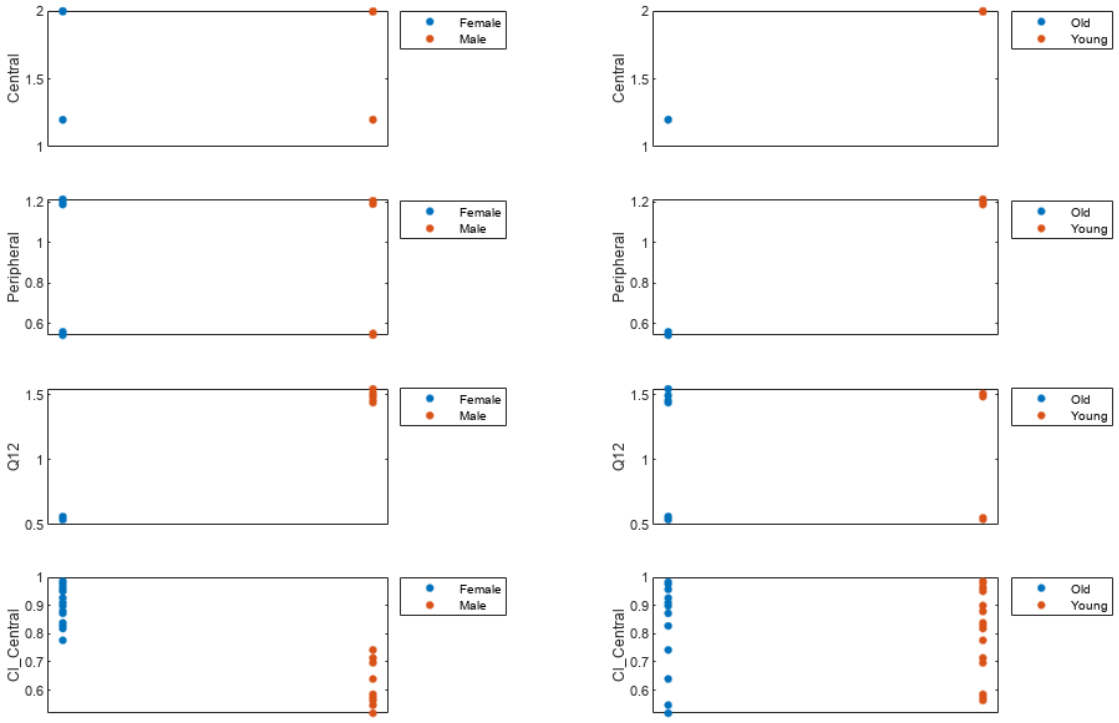
Add variables to the table containing each parameter's estimate.

```
allParamValues            = vertcat(unpooledFit.ParameterEstimates);
catParamValues.Central    = allParamValues.Estimate(strcmp(allParamValues.Name, 'Central'));
catParamValues.Peripheral = allParamValues.Estimate(strcmp(allParamValues.Name, 'Peripheral'));
catParamValues.Q12        = allParamValues.Estimate(strcmp(allParamValues.Name, 'Q12'));
catParamValues.Cl_Central = allParamValues.Estimate(strcmp(allParamValues.Name, 'Cl_Central'));
```

Plot estimates of each parameter for each category. `gscatter` requires Statistics and Machine Learning Toolbox™. If you do not have it, use other alternative plotting functions such as `plot`.

```
h           = figure;
ylabels     = ["Central","Peripheral","Q12","Cl\_Central"];
```

```
plotNumber  = 1;
for i = 1:4
    thisParam = estimatedParam(i).Name;

    % Plot for Sex category
    subplot(4,2,plotNumber);
    plotNumber  = plotNumber + 1;
    gscatter(double(catParamValues.Sex), catParamValues.(thisParam), catParamValues.Sex);
    ax          = gca;
    ax.XTick    = [];
    ylabel(ylabels(i));
    legend('Location','bestoutside')
    % Plot for Age category
    subplot(4,2,plotNumber);
    plotNumber  = plotNumber + 1;
    gscatter(double(catParamValues.Age), catParamValues.(thisParam), catParamValues.Age);
    ax          = gca;
    ax.XTick    = [];
    ylabel(ylabels(i));
    legend('Location','bestoutside')
end
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```



Based on the plot, it seems that young individuals tend to have higher volumes of central and peripheral compartments (`Central`, `Peripheral`) than old individuals (that is, the volumes seem to

be age-specific). In addition, males tend to have lower clearance rates (`Cl_Central`) than females but the opposite for the Q12 parameter (that is, the clearance and Q12 seem to be sex-specific).

Estimate Category-Specific Parameters

Use the `'CategoryVariableName'` property of the `estimatedInfo` object to specify which category to use during fitting. Use `'Sex'` as the group to fit for the clearance `Cl_Central` and `Q12` parameters. Use `'Age'` as the group to fit for the `Central` and `Peripheral` parameters.

```
estimatedParam(1).CategoryVariableName = 'Age';
estimatedParam(2).CategoryVariableName = 'Age';
estimatedParam(3).CategoryVariableName = 'Sex';
estimatedParam(4).CategoryVariableName = 'Sex';
categoryFit = sbiofit(model,gData,responseMap,estimatedParam,dose)
```

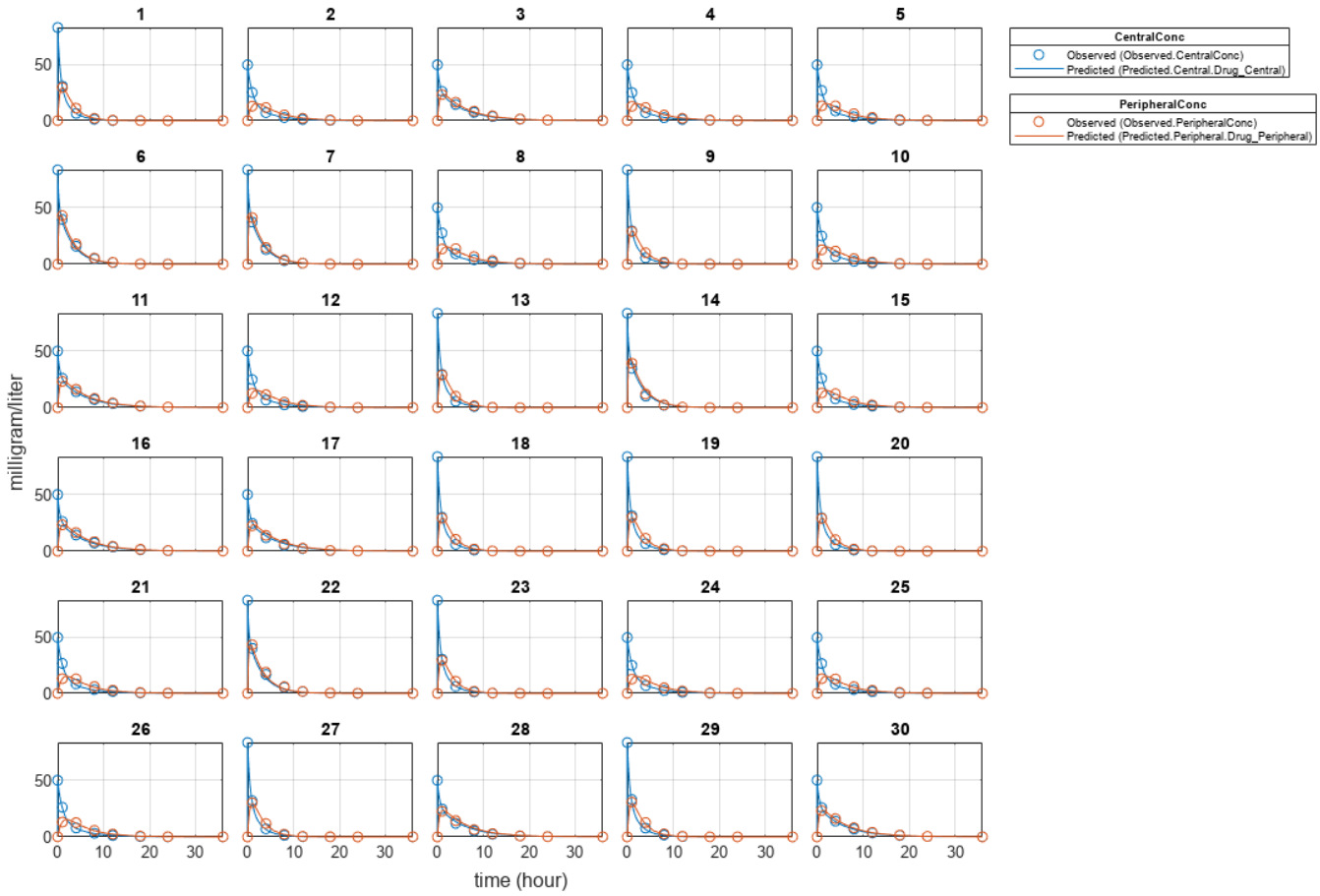
```
categoryFit =
  OptimResults with properties:

                  ExitFlag: 3
                    Output: [1x1 struct]
                 GroupName: []
                      Beta: [8x5 table]
        ParameterEstimates: [120x6 table]
                         J: [240x8x2 double]
                      COVB: [8x8 double]
          CovarianceMatrix: [8x8 double]
                         R: [240x2 double]
                       MSE: 0.4362
                       SSE: 205.8690
                   Weights: []
              LogLikelihood: -477.9195
                       AIC: 971.8390
                       BIC: 1.0052e+03
                       DFE: 472
            DependentFiles: {1x3 cell}
                      Data: [240x6 groupedData]
   EstimatedParameterNames: {'Central'  'Peripheral'  'Q12'  'Cl_Central'}
            ErrorModelInfo: [1x3 table]
        EstimationFunction: 'lsqnonlin'
```

When fitting by category (or group), `sbiofit` always returns one results object, not one for each category level. This is because both male and female individuals are considered to be part of the same optimization using the same error model and error parameters, similarly for the young and old individuals.

Plot Results

Plot the category-specific estimated results.

```
plot(categoryFit);
```



For the `Cl_Central` and `Q12` parameters, all males had the same estimates, and similarly for the females. For the `Central` and `Peripheral` parameters, all young individuals had the same estimates, and similarly for the old individuals.

Estimate Population-Wide Parameters

To better compare the results, fit the model to all of the data pooled together, that is, estimate one set of parameters for all individuals by setting the `'Pooled'` name-value pair argument to `true`. The warning message tells you that this option will ignore any category-specific information (if they exist).

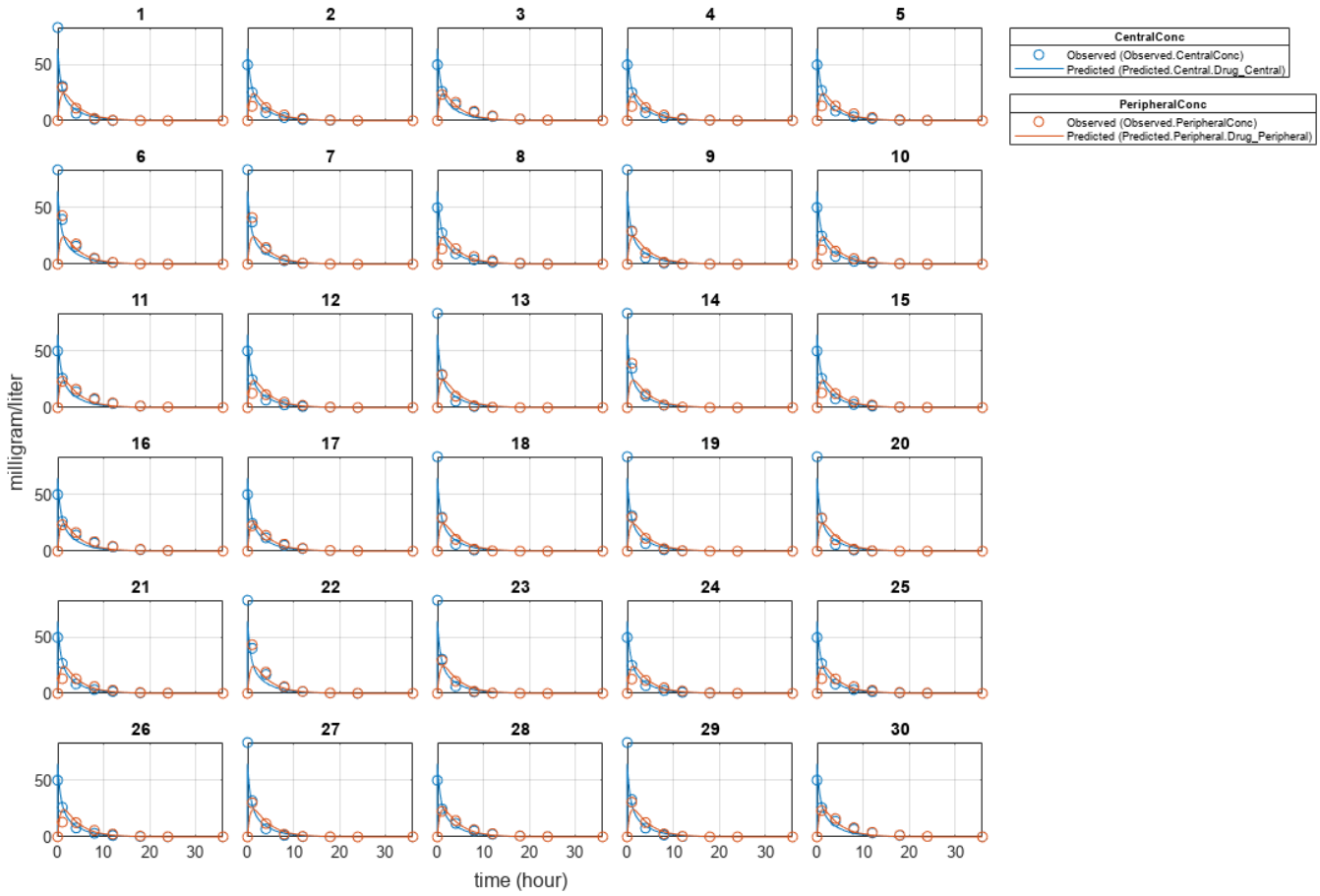
```
pooledFit = sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',true);
```

```
Warning: CategoryVariableName property of the estimatedInfo object is ignored when using the 'Poo
```

Plot Results

Plot the fitted results versus the original data. Although a separate plot was generated for each individual, the data was fitted using the same set of parameters (that is, all individuals had the same fitted line).

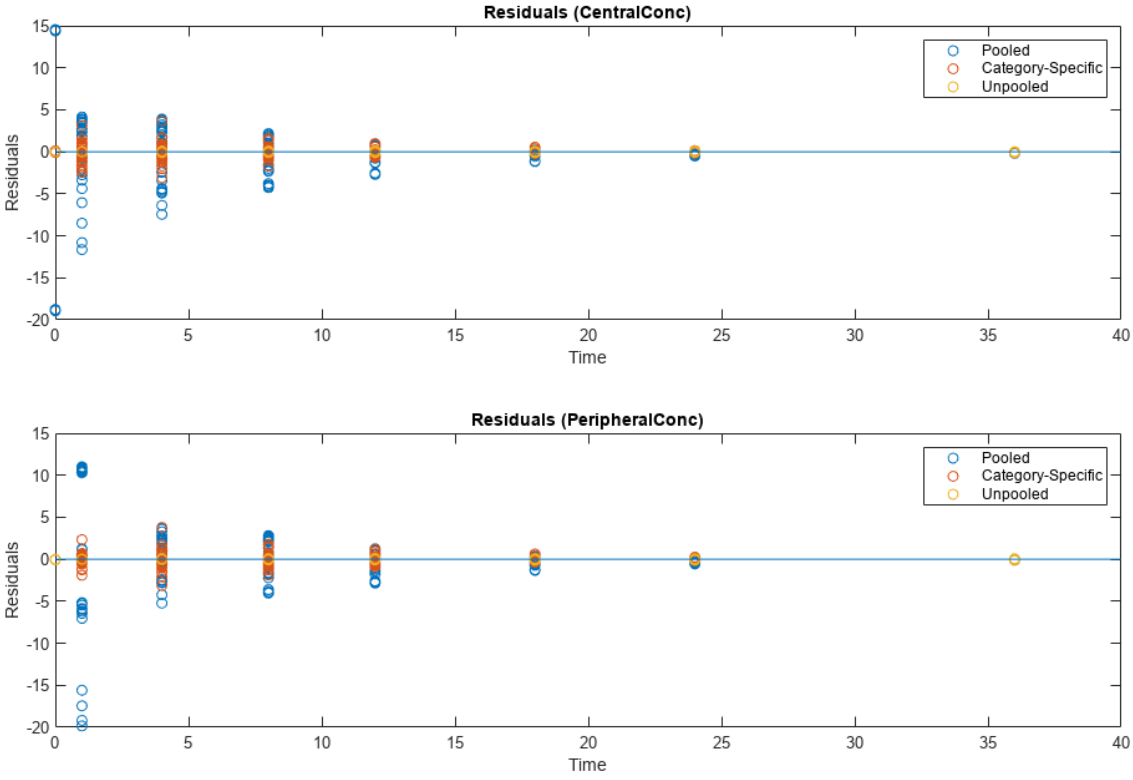
```
plot(pooledFit);
```



Compare Residuals

Compare residuals of `CentralConc` and `PeripheralConc` responses for each fit.

```
t = gData.Time;
allResid(:,:,1) = pooledFit.R;
allResid(:,:,2) = categoryFit.R;
allResid(:,:,3) = vertcat(unpooledFit.R);

h = figure;
responseList = {'CentralConc', 'PeripheralConc'};
for i = 1:2
    subplot(2,1,i);
    oneResid = squeeze(allResid(:,i,:));
    plot(t,oneResid,'o');
    refline(0,0); % A reference line representing a zero residual
    title(sprintf('Residuals (%s)', responseList{i}));
    xlabel('Time');
    ylabel('Residuals');
    legend({'Pooled','Category-Specific','Unpooled'});
end
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```



As shown in the plot, the unpooled fit produced the best fit to the data as it fit the data to each individual. This was expected since it used the most number of degrees of freedom. The category-fit reduced the number of degrees of freedom by fitting the data to two categories (sex and age). As a result, the residuals were larger than the unpooled fit, but still smaller than the population-fit, which estimated just one set of parameters for all individuals. The category-fit might be a good compromise between the unpooled and pooled fitting provided that any hierarchical model exists within your data.

Version History

Introduced in R2014a

See Also

`sbiofit` | `sbiofitmixed` | `groupedData` | `CovariateModel`

Topics

“Fit Two-Compartment Model to PK Profiles of Multiple Individuals” on page 1-67
“Estimate Yeast G Protein Model Parameter” on page 1-82
“Parameter Transformations”
“Nonlinear Regression”

Event object

Store event information

Description

Events are used to describe sudden changes in model behavior. An event lets you specify discrete transitions in model component values that occur when a user-specified condition become true. You can specify that the event occurs at a particular time, or specify a time-independent condition.

For details on how events are handled during a simulation, see “Events in SimBiology Models”.

See “Property Summary” on page 2-280 for links to event property reference pages.

Properties define the characteristics of an object. For example, an event object includes properties that allow you to specify the conditions to trigger an event (`Trigger`), and what to do after the event is triggered (`EventFcn`). Use the `get` and `set` commands to list object properties and change their values at the command line. You can graphically change object properties in the SimBiology desktop.

Tip If UnitConversion is on and your model has any event, follow the recommendation below.

Non-dimensionalize any parameters used in the event `Trigger` if they are not already dimensionless. For example, suppose you have a trigger `x > 1`, where *x* is the species concentration in mole/liter. Non-dimensionalize *x* by scaling (dividing) it with a constant such as `x/x0 > 1`, where *x0* is a parameter defined as 1.0 mole/liter. Note that *x* does not have to have the same unit as the constant *x0*, but must be dimensionally consistent with it. For example, the unit of *x* can be picomole/liter instead of mole/liter.

Constructor Summary

addevent (model)	Add event object to model object

Method Summary

copyobj	Copy SimBiology object and its children
delete	Delete SimBiology object
display	Display summary of SimBiology object
get	Get SimBiology object properties
rename	Rename object and update expressions
set	Set SimBiology object properties

Property Summary

Active	Indicate object in use during simulation
EventFcns	Event expression
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Tag	Specify label for SimBiology object
Trigger	Event trigger
Type	Display SimBiology object type
UserData	Specify data to associate with object

See Also

`AbstractKineticLaw object`, `Configset object`, `KineticLaw object`, `Model object`, `Parameter object`, `Reaction object`, `Root object`, `Rule object`, `Species object`

Version History

Introduced in R2007b

export (model)

Export SimBiology models for deployment and standalone applications

Syntax

```
exportedModel = export(model)
exportedModel = export(model,editobjs)
exportedModel = export(model,editobjs,modifiers)
exportedModel = export(model,editobjs,editdoses,variants)
```

Description

`exportedModel = export(model)` returns a `SimBiology.export.Model` object, `exportedModel`, from a SimBiology `model object`, `model` including all doses which are editable in the exported model. In addition, if the `model` has any active variants, they are automatically applied to determine the default initial values in the exported model. By default, all species, parameters, compartments, and doses are editable in the exported model. When you simulate the exported model, you can specify different initial values or different dose conditions.

`exportedModel = export(model,editobjs)` specifies `editobjs`, which is a species, parameter, compartment, or vector of these objects that are editable in the exported model. All doses are exported and are editable in the exported model. If the `model` has any active variants, they are automatically applied to determine the default initial values in the exported model. When you simulate the exported model, you can specify different initial values for `editobjs` or different dose conditions.

`exportedModel = export(model,editobjs,modifiers)` additionally specifies `modifiers` which is a dose, variant, vector of these objects or an empty array `[]`.

`exportedModel = export(model,editobjs,editdoses,variants)` additionally specifies `editdoses`, a dose object or vector of dose objects and `variants`, a variant object or vector of variant objects.

Method Summary

Methods for exported model objects

accelerate	Prepare exported SimBiology model for acceleration
getIndex	Get indices into ValueInfo and InitialValues properties
getdose	Return exported SimBiology model dose object
isAccelerated	Determine whether an exported SimBiology model is accelerated
simulate	Simulate exported SimBiology model

Input Arguments

`model` — SimBiology model

SimBiology model object

SimBiology model, specified as a SimBiology `model object`.

`editobjs` — Editable model quantities in the exported model
species object | parameter object | compartment object | vector of objects

Editable model quantities in the exported model, specified as a species, parameter, or compartment object or a vector of these objects.

`modifiers` — Model modifiers
dose object | variant object | vector of objects | `[]`

Model modifiers, specified as a dose or variant object, a vector of these objects, or an empty array `[]`.

If `modifiers` is a vector of dose objects, then only these doses are editable in the exported model.

If `modifiers` is an empty array `[]`, then no doses are editable in the exported model, and all active variants are applied to determine the default initial values of model quantities in the exported model.

If `modifiers` is a vector of variant objects, then specified variants are applied to determine the default initial values. All doses in the model are exported.

When you simulate the exported model, you can specify different initial values for `editobjs` or different dose conditions for editable doses.

`editdoses` — Editable doses
dose object | vector of objects

Editable doses, specified as a dose object or vector of dose objects. The specified dose objects are editable in the exported model.

`variants` — Variants
variant object | vector of objects

Variants, specified as a variant object or a vector of objects. The specified variant objects are applied to determine the default initial values in the exported model.

Output Arguments

`exportedModel` — Exported model
`SimBiology.export.Model`

Exported model, specified as a `SimBiology.export.Model` object.

Examples

Export a SimBiology Model

Export a SimBiology model object.

```
modelObj = sbmlimport('lotka');
exportedModel = export(modelObj)
```

```
exportedModel =
  Model with properties:

           Name: 'lotka'
```

```
     ExportTime: '03-Mar-2023 08:42:23'
    ExportNotes: ''
```

Display the editable values (compartments, species, and parameters) information for the exported model object.

```
{exportedModel.ValueInfo.Name}
```

```
ans = 1x8 cell
    {'unnamed'}    {'x'}    {'y1'}    {'y2'}    {'z'}    {'c1'}    {'c2'}    {'c3'}
```

There are 8 editable values in the exported model. Export the model again, allowing only the parameters (`c1`, `c2`, and `c3`) to be editable.

```
parameters = sbioselect(modelObj,'Type','parameter');
exportedModelParam = export(modelObj,parameters);
{exportedModelParam.ValueInfo.Name}
```

```
ans = 1x3 cell
    {'c1'}    {'c2'}    {'c3'}
```

Export the model a third time, allowing the parameters and species to be editable.

```
PS = sbioselect(modelObj,'Type',{'species','parameter'});
exportedModelPS = export(modelObj,PS);
{exportedModelPS.ValueInfo.Name}
```

```
ans = 1x7 cell
    {'x'}    {'y1'}    {'y2'}    {'z'}    {'c1'}    {'c2'}    {'c3'}
```

Exported SimBiology Model Dose Objects

Open a sample SimBiology model project, and export the included model object.

```
sbioloadproject('AntibacterialPKPD')
em = export(m1);
```

Get the editable doses from the exported model object.

```
doses = getdose(em)
```

```
doses=1×4 object
  1x4 RepeatDose array with properties:

    Interval
    RepeatCount
    StartTime
    TimeUnits
    Amount
    AmountUnits
    DurationParameterName
    LagParameterName
```

```
    Name
    Notes
    Parent
    Rate
    RateUnits
    TargetName
```

The exported model has 4 repeated dose objects.

Display the 3rd dose object from the exported model object.

```
doses(3)
```

```
ans =
  RepeatDose with properties:

                Interval: 12
             RepeatCount: 27
               StartTime: 0
               TimeUnits: 'hour'
                  Amount: 500
             AmountUnits: 'milligram'
   DurationParameterName: 'TDose'
        LagParameterName: ''
                    Name: '500 mg bid'
                   Notes: ''
                  Parent: 'Antibacterial'
                    Rate: 0
                RateUnits: ''
              TargetName: 'Central.Drug'
```

Change the dosing amount for this dose object.

```
doses(3).Amount = 600;
```

```
doses(3)
```

```
ans =
  RepeatDose with properties:

                Interval: 12
             RepeatCount: 27
               StartTime: 0
               TimeUnits: 'hour'
                  Amount: 600
             AmountUnits: 'milligram'
   DurationParameterName: 'TDose'
        LagParameterName: ''
                    Name: '500 mg bid'
                   Notes: ''
                  Parent: 'Antibacterial'
                    Rate: 0
                RateUnits: ''
              TargetName: 'Central.Drug'
```

Version History

Introduced in R2012b

See Also

`SimBiology.export.Model` | `Model object` | `Parameter object` | `Species object` | `Compartment object`

Topics

“Perform PK/PD Modeling and Simulation to Guide Dosing Strategy for Antibiotics”
“Deploy a SimBiology Exported Model”

findUnusedComponents (model)

Find unused species, parameters, and compartments in a model

Syntax

```
unused = findUnusedComponents(model)
unused = findUnusedComponents(model,dose)
unused = findUnusedComponents(model,dose,variant)
```

Description

`unused = findUnusedComponents(model)` returns a vector of species, compartments, and parameters that are not used in `model`, which is a SimBiology `Model object`. For details of what SimBiology checks to decide whether a component is used, see “Component Usage”.

`unused = findUnusedComponents(model,dose)` also searches for unused components in `dose`, which is a `RepeatDose object`, `ScheduleDose object`, or a vector of dose objects.

`unused = findUnusedComponents(model,dose,variant)` also searches for unused components in `variant`, which is a `Variant object` or a vector of variant objects.

Input Arguments

`model` — SimBiology model
SimBiology model object

SimBiology model, specified as a SimBiology `Model object`.

`dose` — Dose object
ScheduleDose object | RepeatDose object | vector

Dose object, specified as a `ScheduleDose object`, `RepeatDose object`, or vector of dose objects.

`variant` — Variant
variant object | vector

Variant, specified as a `Variant object` or vector of variant objects.

Output Arguments

`unused` — Unused components
vector

Unused components, returned as a vector of species, parameters, and compartments.

Examples

Find Unused Components in a Model

Load a sample project.

```
sbioloadproject gprotein.sbproj
```

Check if there is any unused species, compartments, or parameters.

```
unused = findUnusedComponents(m1)
```

```
unused =
  0x1 QuantityComponent array with properties:

    Constant
    Value
    Units
    BoundaryCondition
    Name
    Parent
    Notes
    Tag
    Type
    UserData
```

Add some parameters to the model that are not used.

```
p1 = addparameter(m1,'p1');
p2 = addparameter(m1,'p2');
```

Look for those unused parameters.

```
unused = findUnusedComponents(m1)
```

```
unused =
   SimBiology Parameter Array

   Index:    Name:    Value:    Units:
   1         p1       1
   2         p2       1
```

Version History

Introduced in R2016b

See Also

`findUsages` | `Model object`

Topics

“Component Usage”

findUsages

Find out how a species, parameter, or compartment is used in a model

Syntax

```
[componentList,usageTable] = findUsages(object)
[componentList,usageTable] = findUsages(object,dose)
[componentList,usageTable] = findUsages(object,dose,variant)
```

Description

`[componentList,usageTable] = findUsages(object)` returns a vector of components that use the `object` and a table providing details about the usages. The `object` can be a species, parameter, or compartment object. For details of what SimBiology checks to decide whether a component is used, see “Component Usage”.

`[componentList,usageTable] = findUsages(object,dose)` also searches for usages of the `object` in `dose`, which is a `RepeatDose object`, `ScheduleDose object`, or a vector of dose objects.

`[componentList,usageTable] = findUsages(object,dose,variant)` also searches for usages of the `object` in `variant`, which is a `Variant object` or a vector of variant objects.

Examples

Find Out How a Quantity is Used in a Model

Load a sample project.

```
sbioloadproject gprotein.sbproj
```

Check and see how the rate of G protein inactivation parameter `kGd` is used in the model.

```
kGd = sbioselect(m1,'Name','kGd');
[components,usages] = findUsages(kGd);
```

`components` is a vector of components that use the parameter `kGd`. Display these components.

```
for i = 1:length(components)
    components(i)
end
```

```
ans =
   SimBiology Reaction Array

   Index:    Reaction:
   1         Ga -> Gd


ans =
   SimBiology Kinetic Law Array
```

```
   Index:    KineticLawName:
   1         MassAction
```

Based on the information from the `usages` table, the parameter is being used as a reaction rate parameter.

```
usages
```

```
usages=2×3 table
              Component                       Property                 Usage
    ____________________________    ____________________________    _________

    1x1 SimBiology.ModelComponent    {'ReactionRate'          }    {'kGd*Ga'}
    1x1 SimBiology.ModelComponent    {'ParameterVariableNames'}    {'kGd'   }
```

Input Arguments

`object` — Species, parameter, compartment, unit, or unit prefix

species object | parameter object | compartment object

Species, parameter, compartment, unit, or unit prefix, specified as a `Species object`. `Parameter object`, and `Compartment object`.

`dose` — Dose object

ScheduleDose object | RepeatDose object | vector

Dose object, specified as a `ScheduleDose object`, `RepeatDose object`, or vector of dose objects.

`variant` — Variant

variant object | vector

Variant, specified as a `Variant object` or vector of variant objects.

Output Arguments

`componentList` — List of model components that use the input object

vector

List of model components that use the input `object`, returned as a vector.

`usageTable` — Usage Information

table

Usage information, returned as a table. Table variables are:

- *Component*– a vector of components that use the `object`
- *Property*– a cell array of character vectors listing the corresponding properties that refer to the object
- *Usage*– a cell array reporting the usages as follows:

- For rules, the value of the Rule property,
- For reactions, the value of the Reaction or ReactionRate property,
- For kinetic laws, the name stored in the SpeciesVariableNames or ParameterVariableNames,
- For events, the value of the Trigger property or the value of `EventFcns{i}`, where *i* the index of an event function that use the component.
- For variants, the value of `Content{i}`, where *i* is the index of the content entry that use the component.
- For doses, the value of the relevant property, that is, TargetName, `DurationParameterName`, or LagParameterName.
- For species making use of a compartment, the name of the compartment listed in the Parent property of the species.

Version History

Introduced in R2016b

See Also

`findUnusedComponents` | `Species object` | `Parameter object` | `Compartment object`

Topics

“Component Usage”

findUsages

Find out how an `AbstractKineticLaw` object is used

Syntax

```
rxnList= findUsages(aklObj,model)
```

Description

`rxnList= findUsages(aklObj,model)` returns a vector of reactions in `model` that use the `AbstractKineticLaw object` `aklObj`. For details of what SimBiology checks to decide whether an abstract kinetic law is used, see “Component Usage”.

Examples

Find Out How an Abstract Kinetic Law is Used in a Model

Load a sample project.

```
sbioloadproject gprotein.sbproj
```

List all reactions in the model that use the `MassAction` abstract kinetic law.

```
akl = sbioselect('Type','abstract_kinetic_law','Name','MassAction');
list = findUsages(akl,m1)
```

```
list =
   SimBiology Reaction Array

   Index:    Reaction:
   1         L + R <-> RL
   2         Gd + Gbg -> G
   3         G + RL -> Ga + Gbg + RL
   4         R <-> null
   5         RL -> null
   6         Ga -> Gd
```

Input Arguments

`aklObj` — Abstract kinetic law

AbstractKineticLaw object

Abstract kinetic law, specified as a `AbstractKineticLaw object`.

`model` — SimBiology model

model object | vector

SimBiology model, specified as a `model object`, or vector of model objects.

Output Arguments

`rxnList` — List of reactions that use `aklObj`
vector

List of reactions that use `aklObj`, returned as a vector of reaction objects.

Version History

Introduced in R2016b

See Also

`findUnusedComponents` | `abstractkineticlaw object` | `kineticlaw object` | `reaction object` | `findUsages(species,parameter,compartment)` | `findUsages(unit,unitprefix)`

Topics
“Component Usage”

findUsages

Find out how observable object is used in SimBiology model

Syntax

```
[componentList,usageTable] = findUsages(obsObj)
```

Description

`[componentList,usageTable] = findUsages(obsObj)` returns a vector of components that use the observable object `obsObj` and a table providing details about the usages. For information about how SimBiology determines whether a component is used, see “Component Usage”.

Examples

Find Usages of Observable Object

Load the “Target-Mediated Drug Disposition (TMDD) Model”.

```
sbioloadproject tmdd_with_TO.sbproj
```

Use the target occupancy (TO) as a response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'TO';
```

Add an observable that calculates the maximum of the `TO` profile.

```
obs1 = addobservable(m1,'Max_TO','max(TO)');
```

Add another observable that references the first observable.

```
obs2 = addobservable(m1,'Max_Square','Max_TO.^2');
```

Find usages of the first observable.

```
[c,t] = findUsages(obs1)
```

```
c =
   SimBiology Observable Array

   Index:    Name:         Expression:    Active:    Units:
   1         Max_Square    Max_TO.^2      true


t=1×3 table
            Component                Property           Usage
    _____________________________    _____________    ____________

    1x1 SimBiology.Observable    {'Expression'}    {'Max_TO.^2'}
```

Input Arguments

`obsObj` — Observable object
observable object

Observable object, specified as an `observable` object.

Output Arguments

`componentList` — List of model components that use the input object
vector of model components

List of model components that use the input object, returned as a vector of model components.

`usageTable` — Usage Information
table

Usage information, returned as a table. Table variables are:

- `Component` – Vector of components that use the object
- `Property` – Cell array of character vectors listing the corresponding properties that refer to the object
- `Usage` – Cell array of character vectors. Each character vector is the `Expression` property of another observable object that references the input object.

Version History

Introduced in R2020a

See Also

`Observable`

Topics
“Component Usage”

findUsages

Find out how a unit or unit prefix is used

Syntax

```
[componentList,usageTable] = findUsages(obj)
[componentList,usageTable] = findUsages(obj,model)
[componentList,usageTable] = findUsages(obj,model,dose)
```

Description

`[componentList,usageTable] = findUsages(obj)` returns a vector of components that use the unit or unit prefix object `obj` and a table providing details about how the `obj` is used in the `BuiltInLibrary` and `UserDefinedLibrary`. For details of what SimBiology checks to decide whether a unit or unit prefix is used by another component, see “Component Usage”.

`[componentList,usageTable] = findUsages(obj,model)` also searches for usages of the `obj` in `model`, which is a SimBiology model, or a vector of model objects.

`[componentList,usageTable] = findUsages(obj,model,dose)` also searches for usages of the `obj` in `dose`, which is a `ScheduleDose object`, `RepeatDose object`, or a vector of dose objects.

Examples

Find Out How a Unit is Used in a Library

Create the unit object.

```
gram = sbioselect('Type','Unit','Name','gram');
```

Check and see how the gram unit is used in the built-in library. If you have a custom library, the function also searches it.

```
gramUsage = findUsages(gram)
```

```
gramUsage =
   SimBiology Unit Array

   Index:    Library:    Name:      Composition:                          Multiplier:
   1         BuiltIn     gram       gram                                  1
   2         BuiltIn     joule      (meter^2*kilogram)/second^2           1
   3         BuiltIn     calorie    (meter^2*kilogram)/second^2           4.1868
   4         BuiltIn     pascal     kilogram/(meter*second^2)             1
   5         BuiltIn     watt       (kilogram*meter^2)/second^3           1
   6         BuiltIn     newton     (kilogram*meter)/second^2             1
   7         BuiltIn     dyne       (gram*centimeter)/second^2            1
   8         BuiltIn     volt       (kilogram*meter^2)/(ampere*second^3)  1
   9         BuiltIn     farad      (ampere^2*second^4)/(kilogram*meter^2)1
   10        BuiltIn     ohm        (kilogram*meter^2)/(ampere^2*second^3)1
```

```
11        BuiltIn     siemens    (ampere^2*second^3)/(kilogram*meter^2)    1
12        BuiltIn     weber      (kilogram*meter^2)/(ampere*second^2)      1
13        BuiltIn     tesla      kilogram/(second^2*ampere)                1
14        BuiltIn     henry      (kilogram*meter^2)/(ampere^2*second^2)    1
```

Input Arguments

`obj` — Unit or unit prefix

unit object | unit prefix object

Unit or unit prefix, specified as a `Unit object`, or `UnitPrefix object`

`model` — SimBiology model

model object | vector

SimBiology model, specified as a `Model object` or vector of model objects.

`dose` — Dose object

ScheduleDose object | RepeatDose object | vector

Dose object, specified as a `ScheduleDose object`, `RepeatDose object`, or vector of dose objects.

Output Arguments

`componentList` — List of model components that use the unit or unit prefix

vector

List of model components that use the unit or unit prefix, returned as a vector.

`usageTable` — Usage Information

table

Usage information, returned as a table. Table variables are:

- *Component*– a vector of components that use the `obj`
- *Property*– a cell array of character vectors listing the corresponding properties that use the `obj`, and
- *Usage*– a cell array of character vectors stored in the relevant properties, that is, InitialAmountUnits, CapacityUnits, ValueUnits, TimeUnits, AmountUnits, RateUnits, or Composition.

Version History

Introduced in R2016b

fit

Perform parameter estimation using SimBiology problem object

Syntax

```
fitResults = fit(problemObject)
[fitResults,simdataI] = fit(problemObject)
[fitResults,simdataI,simdataP] = fit(problemObject)
```

Description

`fitResults = fit(problemObject)` performs parameter estimation using the model, data, and options defined by `problemObject` and returns the fitted results.

`[fitResults,simdataI] = fit(problemObject)` also returns simulation data `simdataI` using the estimated parameter values. If `problemObject.FitFunction` is `"sbiofitmixed"`, simulations use the individual parameter estimates.

`[fitResults,simdataI,simdataP] = fit(problemObject)` also returns simulation results using population parameter estimates. This syntax is supported only when `problemObject.FitFunction` is `"sbiofitmixed"`.

Examples

Fit PK Parameters Using SimBiology Problem-Based Workflow

This example shows how to estimate PK parameters of a SimBiology model using a problem-based approach.

Load a synthetic data set. It contains drug plasma concentration data measured in both central and peripheral compartments.

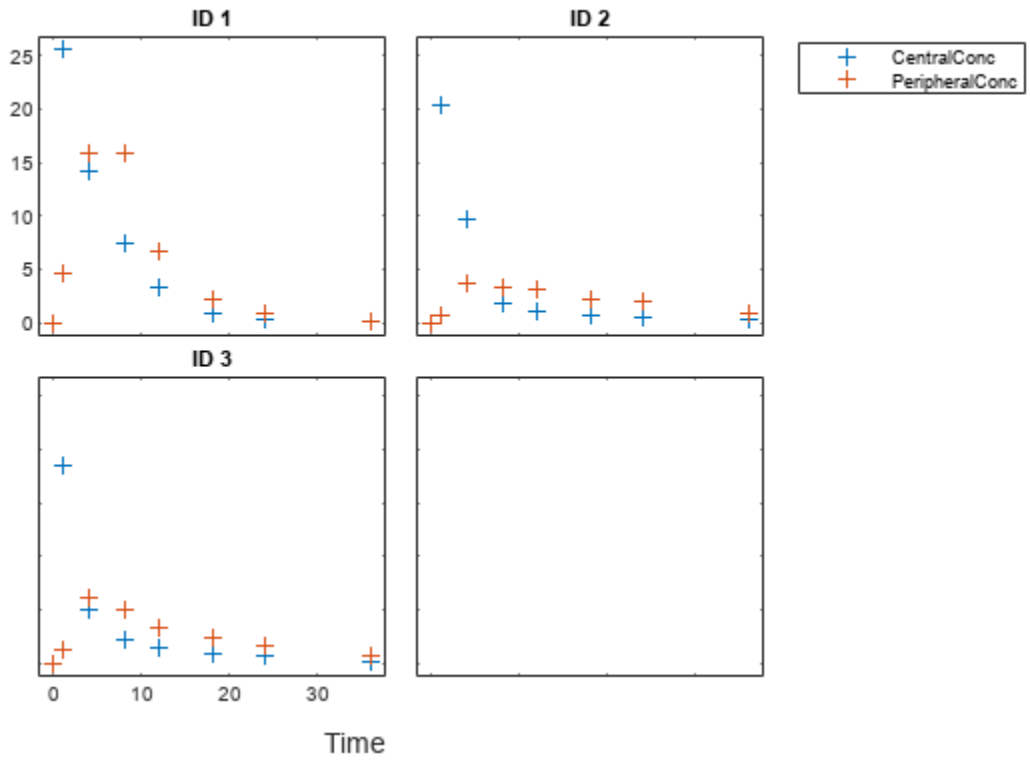
```
load('data10_32R.mat')
```

Convert the data set to a `groupedData` object.

```
gData = groupedData(data);
gData.Properties.VariableUnits = ["","hour","milligram/liter","milligram/liter"];
```

Display the data.

```
sbiotrellis(gData,"ID","Time",["CentralConc","PeripheralConc"],...
            Marker="+",LineStyle="none");
```



Use the built-in PK library to construct a two-compartment model with infusion dosing and first-order elimination. Use the configset object to turn on unit conversion.

```
pkmd                 = PKModelDesign;
pkc1                 = addCompartment(pkmd,"Central");
pkc1.DosingType      = "Infusion";
pkc1.EliminationType = "linear-clearance";
pkc1.HasResponseVariable = true;
pkc2                 = addCompartment(pkmd,"Peripheral");
model2cpt            = construct(pkmd);
configset            = getconfigset(model2cpt);
configset.CompileOptions.UnitConversion = true;
```

Assume every individual receives an infusion dose at time = 0, with a total infusion amount of 100 mg at a rate of 50 mg/hour. For details on setting up different dosing strategies, see “Doses in SimBiology Models”.

```
dose             = sbiodose("dose","TargetName","Drug_Central");
dose.StartTime   = 0;
dose.Amount      = 100;
dose.Rate        = 50;
dose.AmountUnits = "milligram";
dose.TimeUnits   = "hour";
dose.RateUnits   = "milligram/hour";
```

Create a problem object.

```
problem = fitproblem
```

```
problem =
  fitproblem with properties:

   Required:
                    Data: [0x0 groupedData]
               Estimated: [1x0 estimatedInfo]
             FitFunction: "sbiofit"
                   Model: [0x0 SimBiology.Model]
             ResponseMap: [1x0 string]

   Optional:
                   Doses: [0x0 SimBiology.Dose]
            FunctionName: "auto"
                 Options: []
            ProgressPlot: 0
             UseParallel: 0
                Variants: [0x0 SimBiology.Variant]

   sbiofit options:
              ErrorModel: "constant"
                  Pooled: "auto"
     SensitivityAnalysis: "auto"
                 Weights: []
```

Define the required properties of the object.

```
problem.Data        = gData;
problem.Estimated   = estimatedInfo(["log(Central)","log(Peripheral)","Q12","Cl_Central"],Initia
problem.Model       = model2cpt;
problem.ResponseMap = ["Drug_Central = CentralConc","Drug_Peripheral = PeripheralConc"];
```

Define the dose to be applied during fitting.

```
problem.Doses        = dose;
```

Show the progress of the estimation.

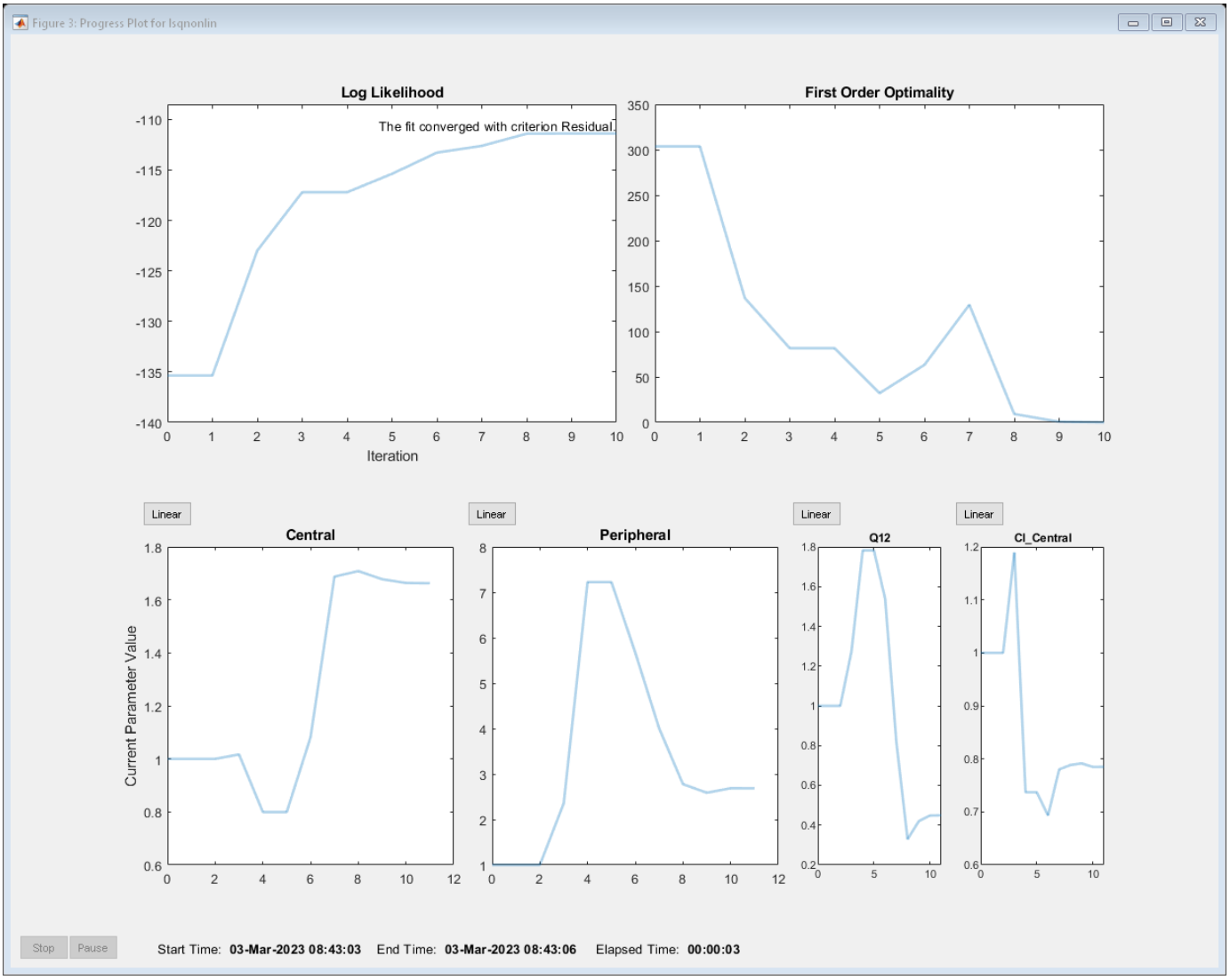
```
problem.ProgressPlot = true;
```

Fit the model to all of the data pooled together: that is, estimate one set of parameters for all individuals by setting the `Pooled` property to `true`.

```
problem.Pooled      = true;
```

Perform the estimation using the `fit` function of the object.

```
pooledFit = fit(problem);
```



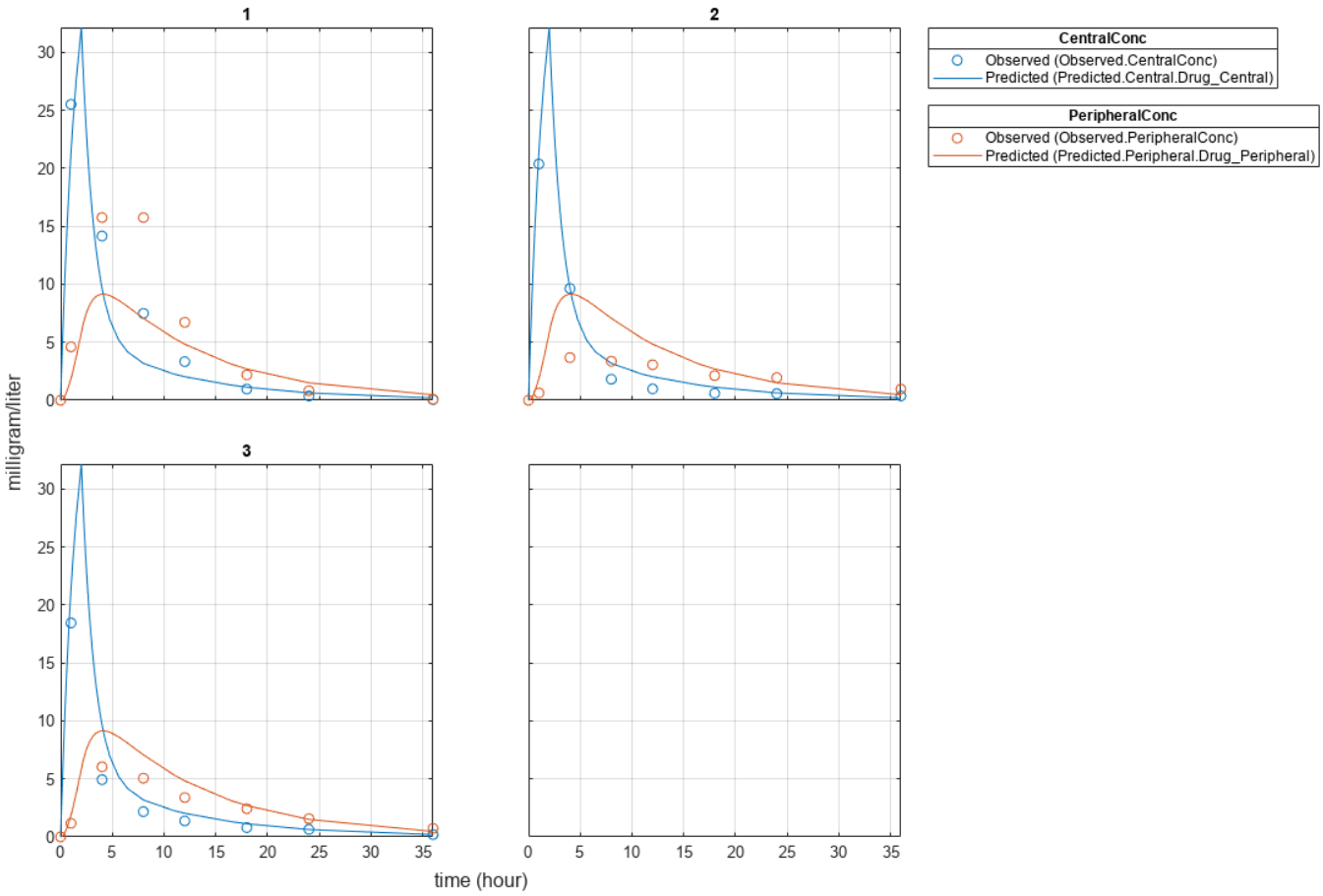
Display the estimated parameter values.

```
pooledFit.ParameterEstimates
```

```
ans=4×3 table
        Name         Estimate    StandardError
    _____________    ________    _____________

    {'Central'   }     1.6627        0.16569
    {'Peripheral'}     2.6864         1.0644
    {'Q12'       }    0.44945        0.19943
    {'Cl_Central'}    0.78497       0.095621
```

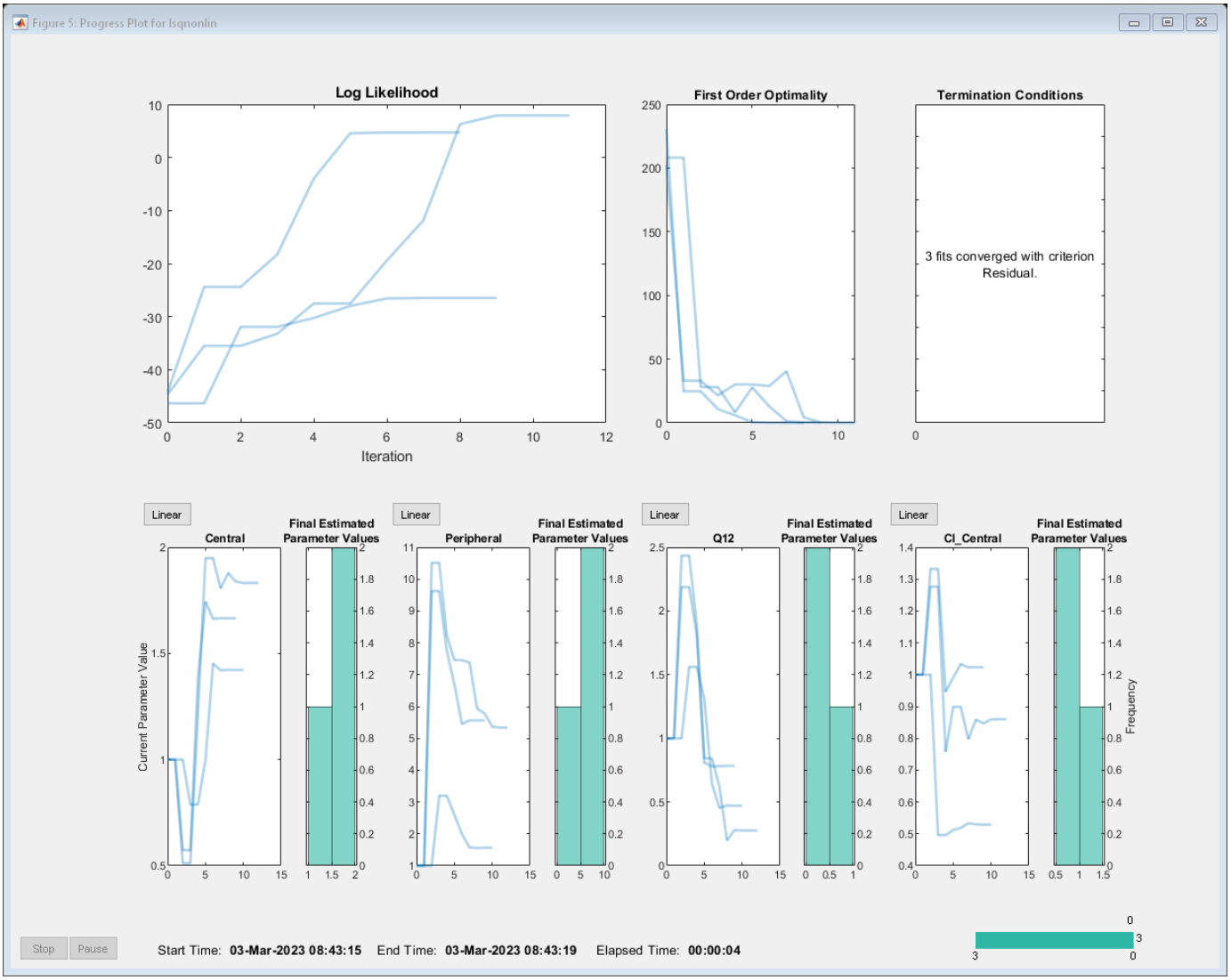
Plot the fitted results.

```
plot(pooledFit);
```



Estimate one set of parameters for each individual and see if the parameter estimates improve.

```
problem.Pooled  = false;
unpooledFit     = fit(problem);
```



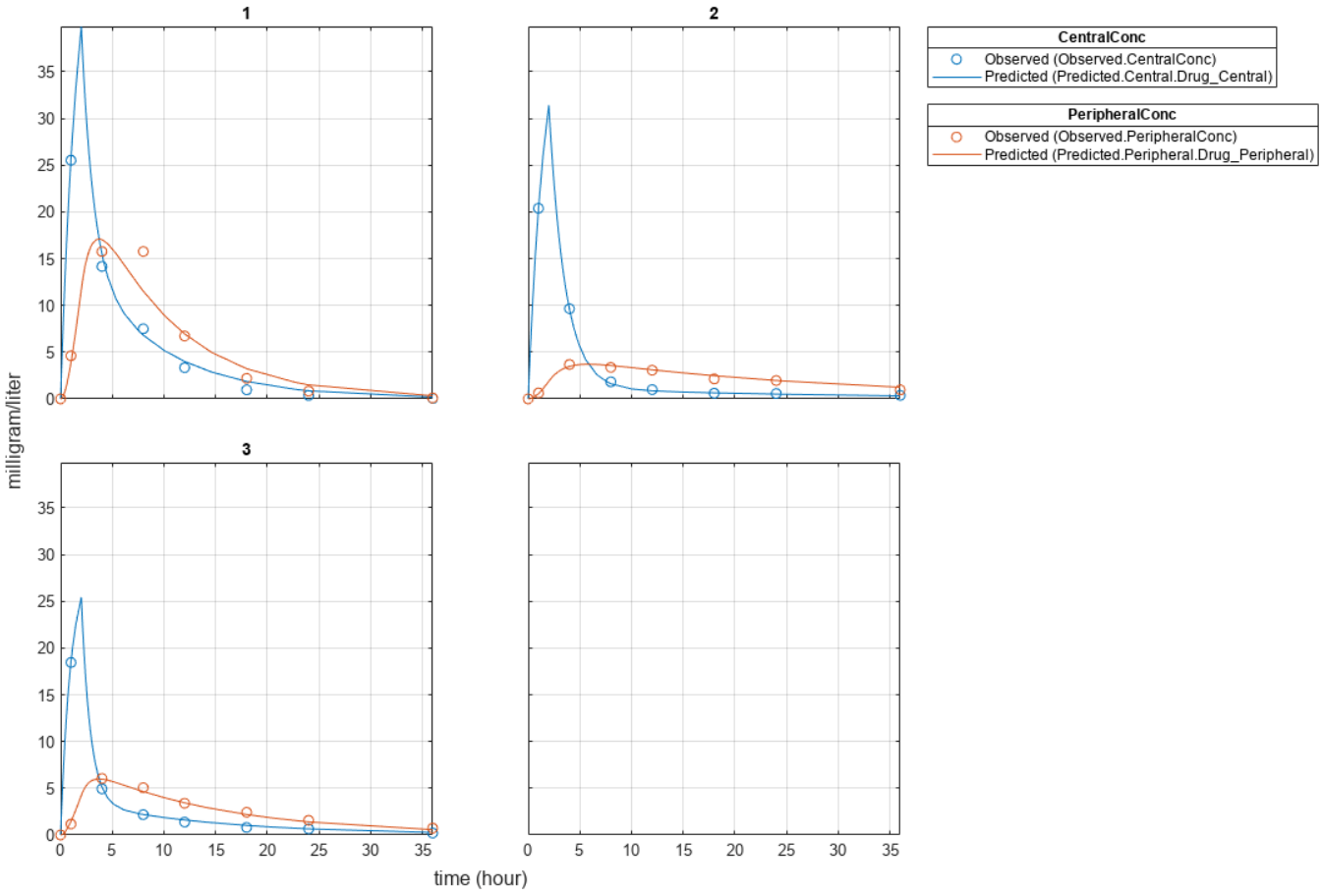
Display the estimated parameter values.

```
unpooledFit.ParameterEstimates
```

```
ans=4×3 table
        Name          Estimate    StandardError
    ______________    ________    _____________

    {'Central'   }      1.422       0.12334
    {'Peripheral'}     1.5619       0.36355
    {'Q12'       }    0.47163       0.15196
    {'Cl_Central'}     0.5291      0.036978


ans=4×3 table
        Name          Estimate    StandardError
    ______________    ________    _____________

    {'Central'   }     1.8322       0.019672
```

```
    {'Peripheral'}     5.3364        0.65327
    {'Q12'       }     0.2764       0.030799
    {'Cl_Central'}    0.86035       0.026257


ans=4×3 table
        Name          Estimate    StandardError
    ______________    ________    _____________

    {'Central'   }     1.6657       0.038529
    {'Peripheral'}     5.5632        0.37063
    {'Q12'       }    0.78361       0.058657
    {'Cl_Central'}     1.0233       0.027311
```

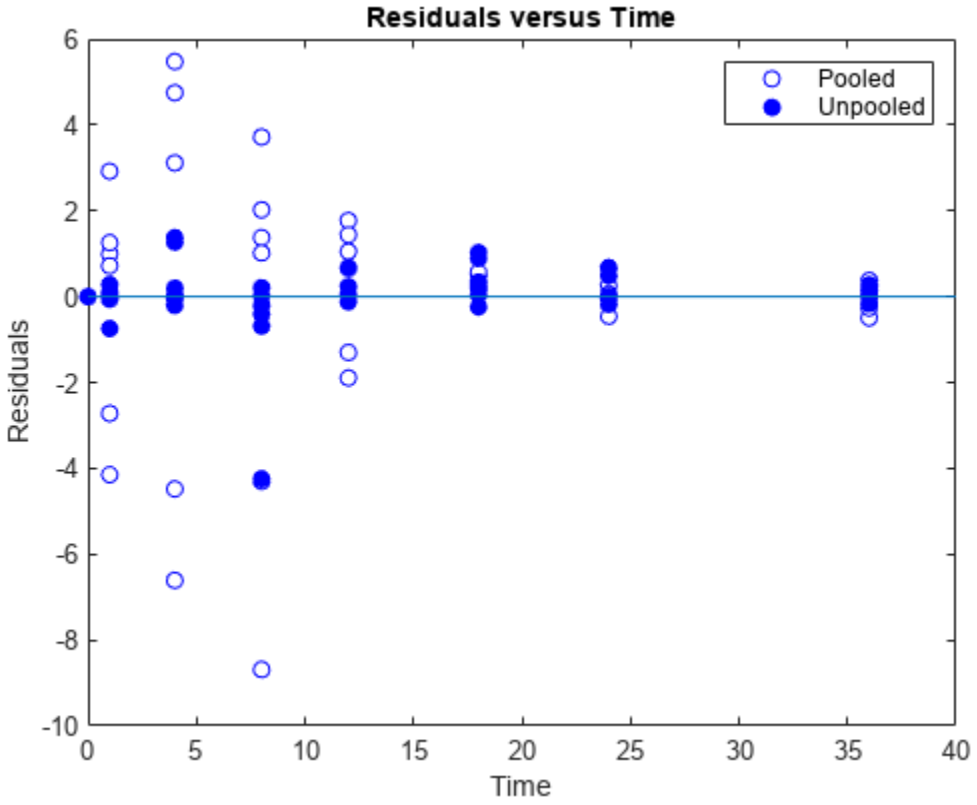
```
plot(unpooledFit);
```



Generate a plot of the residuals over time to compare the pooled and unpooled fit results. The figure indicates unpooled fit residuals are smaller than those of the pooled fit, as expected. In addition to comparing residuals, other rigorous criteria can be used to compare the fitted results.

```
t = [gData.Time;gData.Time];
res_pooled = vertcat(pooledFit.R);
res_pooled = res_pooled(:);
res_unpooled = vertcat(unpooledFit.R);
```

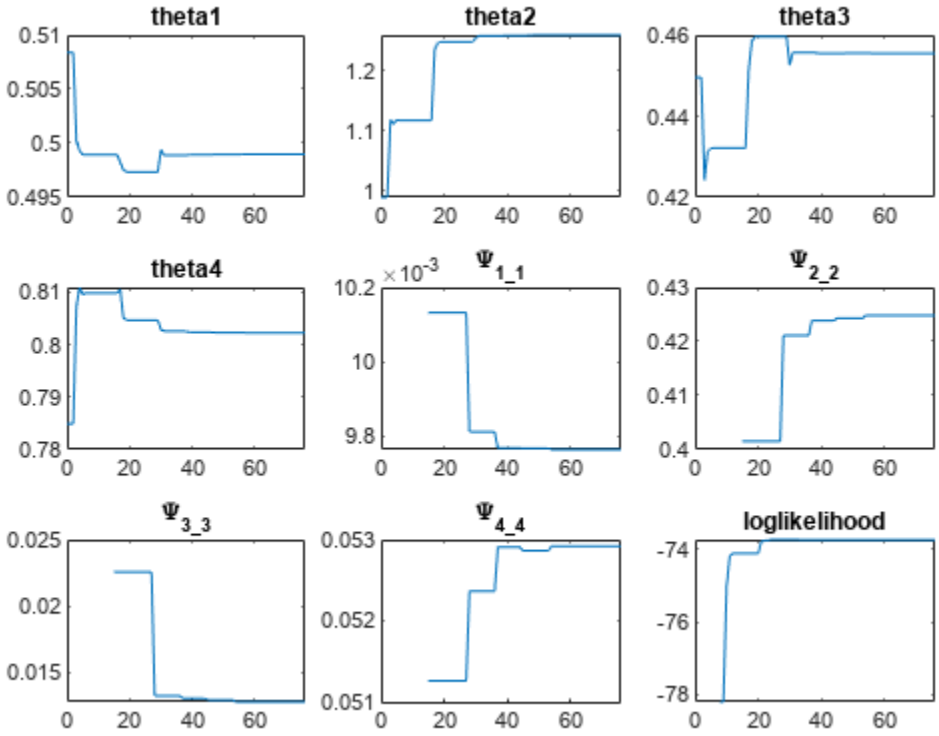
```
res_unpooled = res_unpooled(:);
figure;
plot(t,res_pooled,"o",MarkerFaceColor="w",markerEdgeColor="b")
hold on
plot(t,res_unpooled,"o",MarkerFaceColor="b",markerEdgeColor="b")
refl = refline(0,0); % A reference line representing a zero residual
title("Residuals versus Time");
xlabel("Time");
ylabel("Residuals");
legend(["Pooled","Unpooled"]);
```



As illustrated, the unpooled fit accounts for variations due to the specific subjects in the study, and, in this case, the model fits better to the data. However, the pooled fit returns population-wide parameters. As an alternative, if you want to estimate population-wide parameters while considering individual variations, you can perform nonlinear mixed-effects (NLME) estimation by setting `problem.FitFunction` to `sbiofitmixed`.

```
problem.FitFunction = "sbiofitmixed";
```

```
NLMEResults = fit(problem);
```



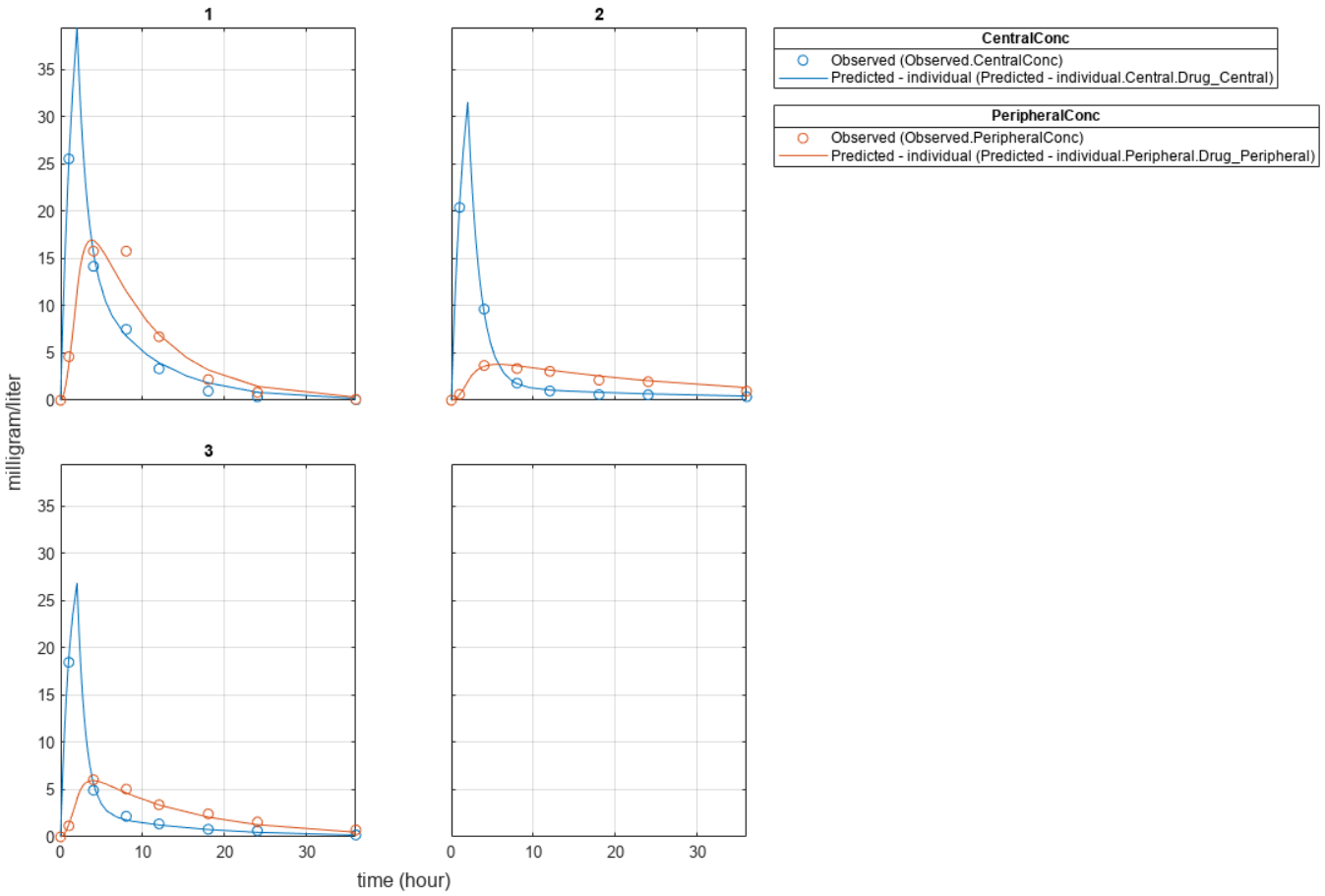
Display the estimated parameter values.

```
NLMEResults.IndividualParameterEstimates
```

```
ans=12×3 table
    Group          Name          Estimate
    _____    _______________    _________

      1      {'Central'   }      1.4623
      1      {'Peripheral'}      1.5306
      1      {'Q12'       }      0.4587
      1      {'Cl_Central'}     0.53208
      2      {'Central'   }       1.783
      2      {'Peripheral'}      6.6623
      2      {'Q12'       }      0.3589
      2      {'Cl_Central'}      0.8039
      3      {'Central'   }      1.7135
      3      {'Peripheral'}      4.2844
      3      {'Q12'       }     0.54895
      3      {'Cl_Central'}      1.0708
```

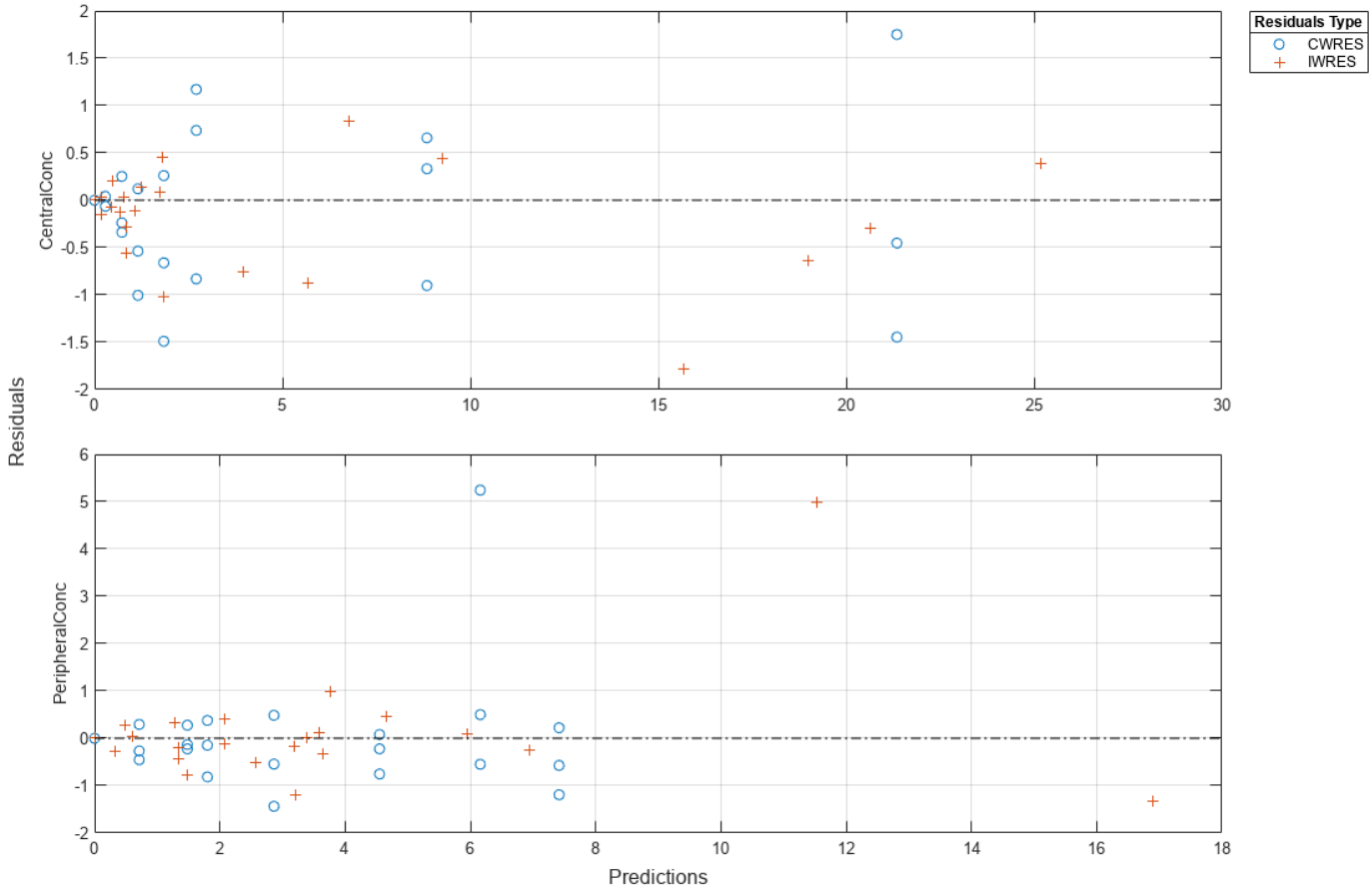
Plot the fitted results.

```
plot(NLMEResults);
```



Plot the conditional weighted residuals (CWRES) and individual weighted residuals (IWRES) of model predicted values.

```
plotResiduals(NLMEResults,'predictions')
```



Input Arguments

`problemObject` — SimBiology estimation problem

`fitproblem` object

SimBiology estimation problem, specified as a `fitproblem` object.

Output Arguments

`fitResults` — Estimation results

`OptimResults` object | `NLINResults` object | `NLMEResults` object | vector of results objects

Estimation results, returned as a scalar `OptimResults` on page 2-478 object, `NLINResults` on page 2-457 object, vector of `OptimResults` or `NLINResults` objects, or scalar `NLMEResults on page 2-461` object.

The returned results object type varies depending on if you used `problemObject.FitFunction="sbiofit"` or `problemObject.FitFunction="sbiofitmixed"`.

- If FitFunction="sbiofit" and FunctionName="nlinfit", the returned results object type is NLINResults on page 2-457. For other optimization functions, the returned object type is OptimResults on page 2-478 .
- If FitFunction="sbiofitmixed", the returned object type is always NLMEResults on page 2-461.

When you use FitFunction="sbiofit", the function returns either a scalar results object or vector of results objects as follows.

For an unpooled fit, the function fits each group separately using group-specific parameters, and fitResults is a vector of results objects with one results object for each group.

For a pooled fit, the function performs fitting for all individuals or groups simultaneously using the same parameter estimates, and fitResults is a scalar results object.

When the pooled option is not specified, and CategoryVariableName values of estimatedInfo objects are all <none>, fitResults is a single results object. This is the same behavior as a pooled fit.

When the pooled option is not specified, and CategoryVariableName values of estimatedInfo objects are all <GroupVariableName>, fitResults is a vector of results objects. This is the same behavior as an unpooled fit.

In all other cases, fitResults is a scalar object containing estimated parameter values for different groups or categories specified by CategoryVariableName.

See the “Pooled” on page 2-0 property for details on how to perform a pooled, unpooled, or category fit.

When you use FitFunction="sbiofitmixed", the function always returns a scalar NLMEResults object.

simdataI — Simulation results
vector of SimData objects

Simulation results, returned as a vector of SimData objects representing simulation results for each group (or individual) using individual-specific parameter estimates.

The states reported in simDataI are the states that are included in problemObject.ResponseMap as well as any other states listed in the StatesToLog property of the runtime options (RuntimeOptions) of the SimBiology model problemObject.Model.

simdataP — Simulation results
vector of SimData objects

Simulation results, returned as a vector of SimData objects representing simulation results for each group (or individual) using only fixed-effect estimates (population parameter estimates).

The states reported in simDataP are the states that are included in problemObject.ResponseMap as well as any other states listed in the StatesToLog property of the runtime options (RuntimeOptions) of the SimBiology model problemObject.Model.

Version History

Introduced in R2021b

See Also

`fitproblem` | `sbiofit` | `sbiofitmixed`

fitproblem

SimBiology problem object for parameter estimation

Description

Create a `fitproblem` object to estimate model parameters using nonlinear regression or nonlinear mixed-effects modeling.

Creation

Create the object using `fitproblem`.

Properties

Required properties

`Data` — Data to fit
`0`-by-`0` `groupedData` array (default) | `groupedData` object

Data to fit, specified as a `groupedData` on page 2-412 object.

The name of the time variable must be defined in the `IndependentVariableName` property of `Data`. For instance, if the time variable name is `'TIME'`, then specify it as follows.

```
prob = fitproblem;
prob.Data = groupedData;
prob.Data.TIME = [1:1:10];
prob.Data.Properties.IndependentVariableName = 'TIME';
```

If the data contains more than one group of measurements, the grouping variable name must be defined in the `GroupVariableName` property of `Data`. For example, if the grouping variable name is `'GROUP'`, then specify it as follows.

```
prob.Data.Properties.GroupVariableName = 'GROUP';
```

A group usually refers to a set of measurements that represent a single time course, often corresponding to a particular individual or experimental condition.

`Estimated` — Estimated parameters
`1`-by-`0` `estimatedInfo` array (default) | `estimatedInfo` object | vector of `estimatedInfo` objects | `CovariateModel` object

Estimated parameters, specified as an `estimatedInfo` on page 2-259 object, a vector of `estimatedInfo` objects, or a scalar `CovariateModel` object.

This property defines the estimated parameters in the model and other optional information such as their initial estimates, transformations, bound constraints, and categories. Supported transforms are `log`, `logit`, and `probit`. For details, see “Parameter Transformations”.

When you perform nonlinear regression by setting `object.FitFunction = "sbiofit"`, then:

- Using `scattersearch` as an optimization function on page 2-0 requires you to specify finite transformed bounds for each estimated parameter.
- If you do not specify the “Pooled” on page 2-0 property, the software uses the `CategoryVariableName` property of the `estimatedInfo` object to decide if parameters must be estimated for each individual, group, category, or all individuals as a whole. Set the `Pooled` property to override any `CategoryVariableName` values. For details about the `CategoryVariableName` property, see `EstimatedInfo object`.
- The software uses the `categorical` function to identify groups. If any group values are converted to the same value by `categorical`, then those observations are treated as belonging to the same group. For instance, if some observations have no group information (that is, an empty character vector `''`), then `categorical` converts empty character vectors to `<undefined>`, and these observations are treated as one group.

For nonlinear mixed-effects modeling with `object.FitFunction="sbiofitmixed"`, the `CategoryVariablename` property of `estimatedInfo` object is ignored.

`FitFunction` — Name of SimBiology estimation function
`"sbiofit"` (default) | `"sbiofitmixed"`

Name of a SimBiology estimation function to use, specified as `"sbiofit"` or `"sbiofitmixed"`. Use `sbiofit` for nonlinear regression problems and `sbiofitmixed` for nonlinear mixed-effects problems.

`Model` — SimBiology model
`0`-by-`0` `Model` array (default) | `Model` object

SimBiology model used to fit the data, specified as a `Model` on page 2-439 object.

`ResponseMap` — Mapping between model components and data variables
1-by-0 empty string array (default) | character vector | string | string vector | cell array of character vectors

Mapping between model components and data variables, specified as a character vector, string, string vector, or cell array of character vectors.

Each character vector or string is an equation-like expression, similar to assignment rules. It contains the name (or qualified name) of a quantity (species, compartment, or parameter) or an `observable` object in the model, followed by the character `'='` and the name of a variable in `Data`. For clarity, white spaces are allowed between names and `'='`.

For example, if you have the concentration data `'CONC'` in `Data` for a species `'Drug_Central'`, you can specify it as follows.

```
ResponseMap = 'Drug_Central = CONC';
```

To name a species unambiguously, use the qualified name, which includes the name of the compartment. To name a reaction-scoped parameter, use the reaction name to qualify the parameter.

If the model component name or `grpData` variable name is not a valid MATLAB variable name, surround it by square brackets, such as:

```
ResponseMap = '[Central 1].Drug = [Central 1 Conc]';
```

If a variable name itself contains square brackets, you cannot use it in the expression to define the mapping information.

If any (qualified) name matches two components of the same type, an error is issued when you run the `fit` function of the object. To resolve the error, you can use a (qualified) name that matches two components of different types, and the function first finds the species with the given name, followed by compartments and then parameters.

Data Types: `char` | `string` | `cell`

Optional properties

`Doses` — Doses applied during fitting

`0`-by-`0` `Dose` array (default) | `RepeatDose` | `ScheduleDose` object | object | 2-D matrix of dose objects | cell vector of dose objects

Doses applied during fitting, specified as an empty array or 2-D matrix of dose objects (`ScheduleDose` on page 2-802 object or `RepeatDose` on page 2-747 object). By default, the software applies no doses even if the model has active doses.

For a matrix of dose objects, it must have a single row or one row per group in the input data. If it has a single row, the same doses are applied to all groups during simulation. If it has multiple rows, each row is applied to a separate group, in the same order as the groups appear in the input data. Multiple columns are allowed so that you can apply multiple dose objects to each group.

For a cell vector of doses, it must have one element or one element per group in the input data. Each element must be `[]` or a vector of doses. Each element of the cell is applied to a separate group, in the same order as the groups appear in the input data.

In addition to manually constructing dose objects using `sbiodose`, if the input `groupedData` object has dosing information, you can use the `createDoses` method to construct doses.

`FunctionName` — Name of optimization function

`"auto"` (default) | character vector | string

Name of an optimization function that is called by `FitFunction` (`sbiofit` or `sbiofitmixed`), specified as a character vector or string.

If `FitFunction="sbiofit"`, valid choices are as follows.

- `"auto"`
- `"fminsearch"`
- `"nlinfit"` (Statistics and Machine Learning Toolbox is required.)
- `"fminunc"` (Optimization Toolbox is required.)
- `"fmincon"` (Optimization Toolbox is required.)
- `"lsqcurvefit"` (Optimization Toolbox is required.)
- `"lsqnonlin"` (Optimization Toolbox is required.)
- `"patternsearch"` (Global Optimization Toolbox is required.)
- `"ga"` (Global Optimization Toolbox is required.)
- `"particleswarm"` (Global Optimization Toolbox is required.)
- `"scattersearch"` on page 1-98

By default (that is, `FunctionName="auto"` and `FitFunction="sbiofit"`), the `fitproblem` object uses the first available estimation function among the following: `lsqnonlin`, `nlinfit`, or `fminsearch`. The same priority applies to the default local solver choice for `scattersearch`.

If `FitFunction="sbiofitmixed"`, the valid choices are:

- `"auto"`
- `"nlmefit"`
- `"nlmefitsa"`

When `FunctionName="auto"` and `FitFunction="sbiofitmixed"`, the object uses `"nlmefit"` as the optimization function.

Data Types: `char` | `string`

`Options` — Options for optimization function
`[]` (default) | struct | `optimoptions` object

Options for the optimization function, specified as a scalar struct, `optimoptions` object or empty array `[]`.

When `FitFunction="sbiofit"`, you can use the following options:

- `statset` struct for `nlinfit`
- `optimset` struct for `fminsearch`
- `optimoptions` object for `lsqcurvefit`, `lsqnonlin`, `fmincon`, `fminunc`, `particleswarm`, `ga`, and `patternsearch`
- `struct` for `scattersearch`

See “Default Options for Optimization Functions Called by sbiofit” on page 2-327 for more details and default options associated with each estimation function.

When `FitFunction="sbiofitmixed"`, define a structure as follows:

- The structure can contain fields and default values that are the name-value arguments accepted by `nlmefit` and `nlmefitsa`, except the following that are not supported.
  - `'FEConstDesign'`
  - `'FEGroupDesign'`
  - `'FEObsDesign'`
  - `'FEParamsSelect'`
  - `'ParamTransform'`
  - `'REConstDesign'`
  - `'REGroupDesign'`
  - `'REObsDesign'`
  - `'Vectorization'`

  `'REParamsSelect'` is only supported when you provide a vector of `estimatedInfo` objects when specifying the estimated parameters.
- Use the `statset` function only to set the `'Options'` field of the structure (`opt`), as follows.

  ```
  opt.Options = statset('Display','iter','TolX',1e-3,'TolFun',1e-3);
  ```
- For other supported name-value arguments (see `nlmefit` and `nlmefitsa`), set them as follows.

```
opt.ErrorModel = 'proportional';
opt.ApproximationType = 'LME';
```

`ProgressPlot` — Flag to show progress of parameter estimation
`false` or `0` (default) | `true` or `1`

Flag to show the progress of parameter estimation, specified as a numeric or logical `1` (`true`) or `0` (`false`). If the flag is `true`, a new figure opens containing plots during fitting.

When `FitFunction="sbiofit"`:

- Plots show the log-likelihood, termination criteria, and estimated parameters for each iteration. This option is not supported for `nlinfit`.
- If you are using the Optimization Toolbox functions (`fminunc`, `fmincon`, `lsqcurvefit`, `lsqnonlin`), the figure also shows the First Order Optimality (Optimization Toolbox) plot.
- For an unpooled fit, each line on the plots represents an individual. For a pooled fit, a single line represents all individuals. The line becomes faded when the fit is complete. The plots also keep track of the progress when you run `sbiofit` (for both pooled and unpooled fits) in parallel using remote clusters. For details, see “Progress Plot”.

When `FitFunction="sbiofitmixed"`, the plots show the values of fixed effects parameters (`theta`), the estimates of the variance parameters, that is, the diagonal elements of the covariance matrix of the random effects (Ψ), and the log-likelihood. For details, see “Progress Plot”.

Data Types: `double` | `logical`

`UseParallel` — Flag to enable parallelization
`false` or `0` (default) | `true` or `1`

Flag to enable parallelization, specified as a numeric or logical `1` (`true`) or `0` (`false`). If the flag is `true` and Parallel Computing Toolbox is available, the software enables the parallelization by doing the following:

1. Create `SimFunction` objects with `UseParallel=true`.
2. Pass the flag `UseParallel=true` to the optimization function, such as `lsqnonlin`. Note that some optimization functions do not support parallelization. See the reference page of the corresponding optimization function to find out about the parallelization support.
3. When `FitFunction="sbiofit"`, and you are performing an unpooled fit (`Pooled=false`) for multiple groups, each fit is run in parallel. For a pooled fit (`Pooled=true`), parallelization happens at the solver level. In other words, solver computations, such as objective function evaluations, are run in parallel.

Data Types: `double` | `logical`

`Variants` — Variants applied during fitting
`0`-by-`0` `Variant` array (default) | 2-D matrix of variants | cell vector of variants

Variants applied during fitting, specified as an empty array `[]` or a 2-D matrix or cell vector of variant objects. By default, the software applies no variants even if the model has active variants.

For a matrix of variant objects, the number of rows must be one or must match the number of groups in the input data. The *i*th row of variant objects is applied to the simulation of the *i*th group. The variants are applied in order from the first column to the last. If this matrix has only one row of variants, they are applied to all simulations.

For a cell vector of variant objects, the number of cells must be one or must match the number of groups in the input data. Each element must be `[]` or a vector of variants. If this cell vector has a single cell containing a vector of variants, they are applied to all simulations. If the cell vector has multiple cells, the variants in the *i*th cell are applied to the simulation of the *i*th group.

In addition to manually constructing variant objects using `sbiovariant`, if the input `groupedData` object has variant information, you can use `createVariants` to construct variants.

Optional properties for FitFunction="sbiofit" only

`ErrorModel` — Error model

`"constant"` (default) | character vector | string | string vector | cell array of character vector | categorical vector | table

Error models used for estimation, specified as a character vector, string, string vector, cell array of character vectors, categorical vector, or table.

If it is a table, it must contain a single variable that is a column vector of error model names. The names can be a cell array of character vectors, string vector, or a vector of categorical variables. If the table has more than one row, then the `RowNames` property must match the response variable names specified in the right hand side of `ResponseMap`. If the table does not use the `RowNames` property, the *n*th error is associated with the *n*th response.

If you specify only one error model, then `sbiofit` estimates one set of error parameters for all responses.

If you specify multiple error models using a categorical vector, string vector, or cell array of character vectors, the length of the vector or cell array must match the number of responses in `ResponseMap`.

You can specify multiple error models only if you are using these methods: `lsqnonlin`, `lsqcurvefit`, `fmincon`, `fminunc`, `fminsearch`, `patternsearch`, `ga`, and `particleswarm`.

Four built-in error models are available. Each model defines the error using a standard mean-zero and unit-variance (Gaussian) variable e, simulation results f, and one or two parameters a and b.

- `"constant"`: $y = f + ae$
- `"proportional"`: $y = f + b|f|e$
- `"combined"`: $y = f + (a + b|f|)e$
- `"exponential"`: $y = f * \exp(ae)$

Note

- If you specify an error model, you cannot specify weights except for the constant error model.
- If you use a proportional or combined error model during data fitting, avoid specifying data points at times where the solution (simulation result) is zero or the steady state is zero. Otherwise, you can run into division-by-zero problems. It is recommended that you remove those data points from the data set. For details on the error parameter estimation functions, see “Maximum Likelihood Estimation” on page 1-94.

Data Types: `double` | `char` | `string` | `table` | `cell`

`Pooled` — Fit option flag
`"auto"` (default) | `true` or `1` | `false` or `0`

Fit option flag to fit each individual or pool all individual data, specified as a numeric or logical `1` (`true`) or `0` (`false`), or `"auto"`.

If `Pooled` is set to `"auto"`, the software infers the value from the `Estimated` property as follows.

If `Estimated` is an `estimatedInfo` object with its `CategoryVariableName` property set to the default value `<GroupVariableName>`, then the `Pooled` property is set to `false`. Otherwise, the property is set to `true`.

- When the property is `false`, the `fit` function of the object estimates each group or individual separately using group- or individual-specific parameters, and the returned fit result is a vector of results objects with one result for each group.
- When the property is `true`, the `fit` function performs fitting for all individuals or groups simultaneously using the same parameter estimates, and the returned result is a scalar results object.

Note Use this option to override the `CategoryVariableName` value of an `estimatedInfo` object.

Data Types: `char` | `string` | `double` | `logical`

`SensitivityAnalysis` — Flag to use parameter sensitivities to determine gradients of the objective function
`"auto"` (default) | `true` or `1` | `false` or `0`

Flag to use parameter sensitivities to determine gradients of the objective function, specified as a numeric or logical `1` (`true`) or `0` (`false`), or `"auto"`.

The default behavior (`"auto"`) is as follows.

- The property is `true` for `fmincon`, `fminunc`, `lsqnonlin`, `lsqcurvefit`, and `scattersearch` methods.
- Otherwise, the property is `false`.

If it is `true`, the software always uses the `sundials` solver, regardless of what you have selected as the SolverType property in the `Configset` object.

The software uses the complex-step approximation method to calculate parameter sensitivities. Such calculated sensitivities can be used to determine gradients of the objective function during parameter estimation to improve fitting. The default behavior of `sbiofit` is to use such sensitivities to determine gradients whenever the algorithm is gradient-based and if the SimBiology model supports sensitivity analysis. For details about the model requirements and sensitivity analysis, see “Sensitivity Analysis in SimBiology”.

Data Types: `double` | `logical` | `char` | `string`

`Weights` — Weights used during fitting
`[]` (default) | matrix | function handle

Weights used for fitting, specified as an empty array `[]`, matrix of real positive weights where the number of columns corresponds to the number of responses, or a function handle that accepts a vector of predicted response values and returns a vector of real positive weights.

If you specify an error model, you cannot use weights except for the constant error model. If neither the `ErrorModel` or `Weights` is specified, by default, the software uses the constant error model with equal weights.

Data Types: `double` | `function_handle`

Object Functions

fit	Perform parameter estimation using SimBiology problem object
resetoptions	Reset optional SimBiology fit problem properties

Examples

Fit PK Parameters Using SimBiology Problem-Based Workflow

This example shows how to estimate PK parameters of a SimBiology model using a problem-based approach.

Load a synthetic data set. It contains drug plasma concentration data measured in both central and peripheral compartments.

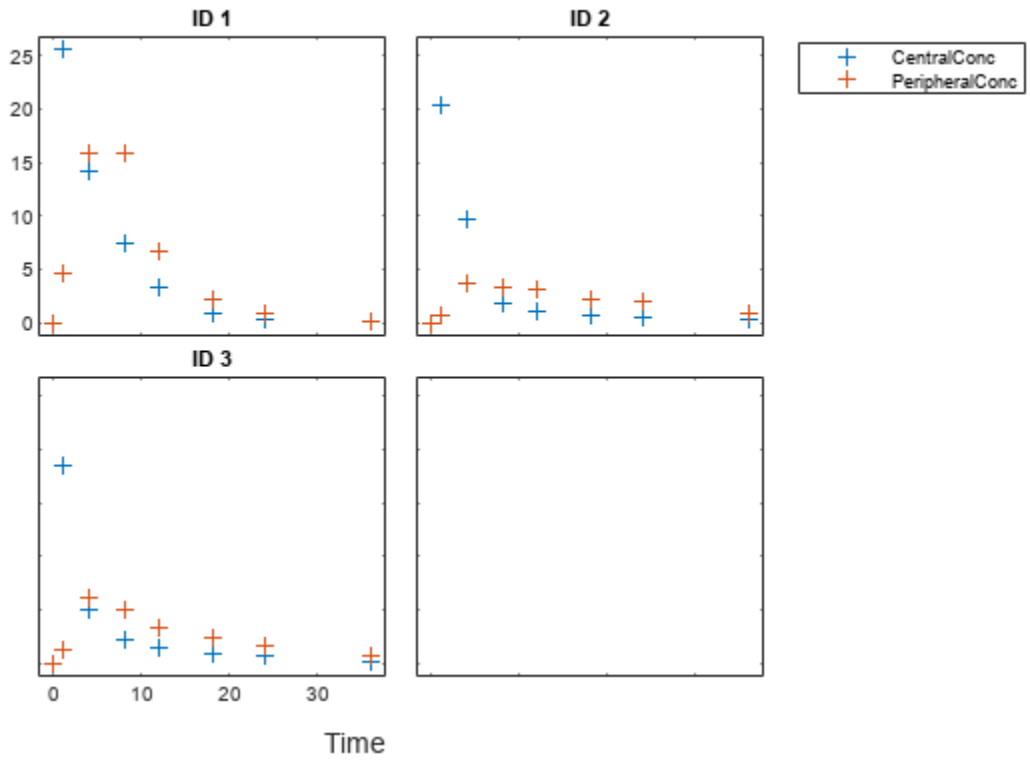
```
load('data10_32R.mat')
```

Convert the data set to a `groupedData` object.

```
gData = groupedData(data);
gData.Properties.VariableUnits = ["","hour","milligram/liter","milligram/liter"];
```

Display the data.

```
sbiotrellis(gData,"ID","Time",["CentralConc","PeripheralConc"],...
            Marker="+",LineStyle="none");
```



Use the built-in PK library to construct a two-compartment model with infusion dosing and first-order elimination. Use the configset object to turn on unit conversion.

```
pkmd                 = PKModelDesign;
pkc1                 = addCompartment(pkmd,"Central");
pkc1.DosingType      = "Infusion";
pkc1.EliminationType = "linear-clearance";
pkc1.HasResponseVariable = true;
pkc2                 = addCompartment(pkmd,"Peripheral");
model2cpt            = construct(pkmd);
configset            = getconfigset(model2cpt);
configset.CompileOptions.UnitConversion = true;
```

Assume every individual receives an infusion dose at time = 0, with a total infusion amount of 100 mg at a rate of 50 mg/hour. For details on setting up different dosing strategies, see “Doses in SimBiology Models”.

```
dose             = sbiodose("dose","TargetName","Drug_Central");
dose.StartTime   = 0;
dose.Amount      = 100;
dose.Rate        = 50;
dose.AmountUnits = "milligram";
dose.TimeUnits   = "hour";
dose.RateUnits   = "milligram/hour";
```

Create a problem object.

```
problem = fitproblem
```

```
problem =
  fitproblem with properties:

   Required:
                    Data: [0x0 groupedData]
               Estimated: [1x0 estimatedInfo]
             FitFunction: "sbiofit"
                   Model: [0x0 SimBiology.Model]
             ResponseMap: [1x0 string]

   Optional:
                   Doses: [0x0 SimBiology.Dose]
            FunctionName: "auto"
                 Options: []
            ProgressPlot: 0
             UseParallel: 0
                Variants: [0x0 SimBiology.Variant]

   sbiofit options:
              ErrorModel: "constant"
                  Pooled: "auto"
    SensitivityAnalysis: "auto"
                 Weights: []
```

Define the required properties of the object.

```
problem.Data        = gData;
problem.Estimated   = estimatedInfo(["log(Central)","log(Peripheral)","Q12","Cl_Central"],Initia
problem.Model       = model2cpt;
problem.ResponseMap = ["Drug_Central = CentralConc","Drug_Peripheral = PeripheralConc"];
```

Define the dose to be applied during fitting.

```
problem.Doses        = dose;
```

Show the progress of the estimation.

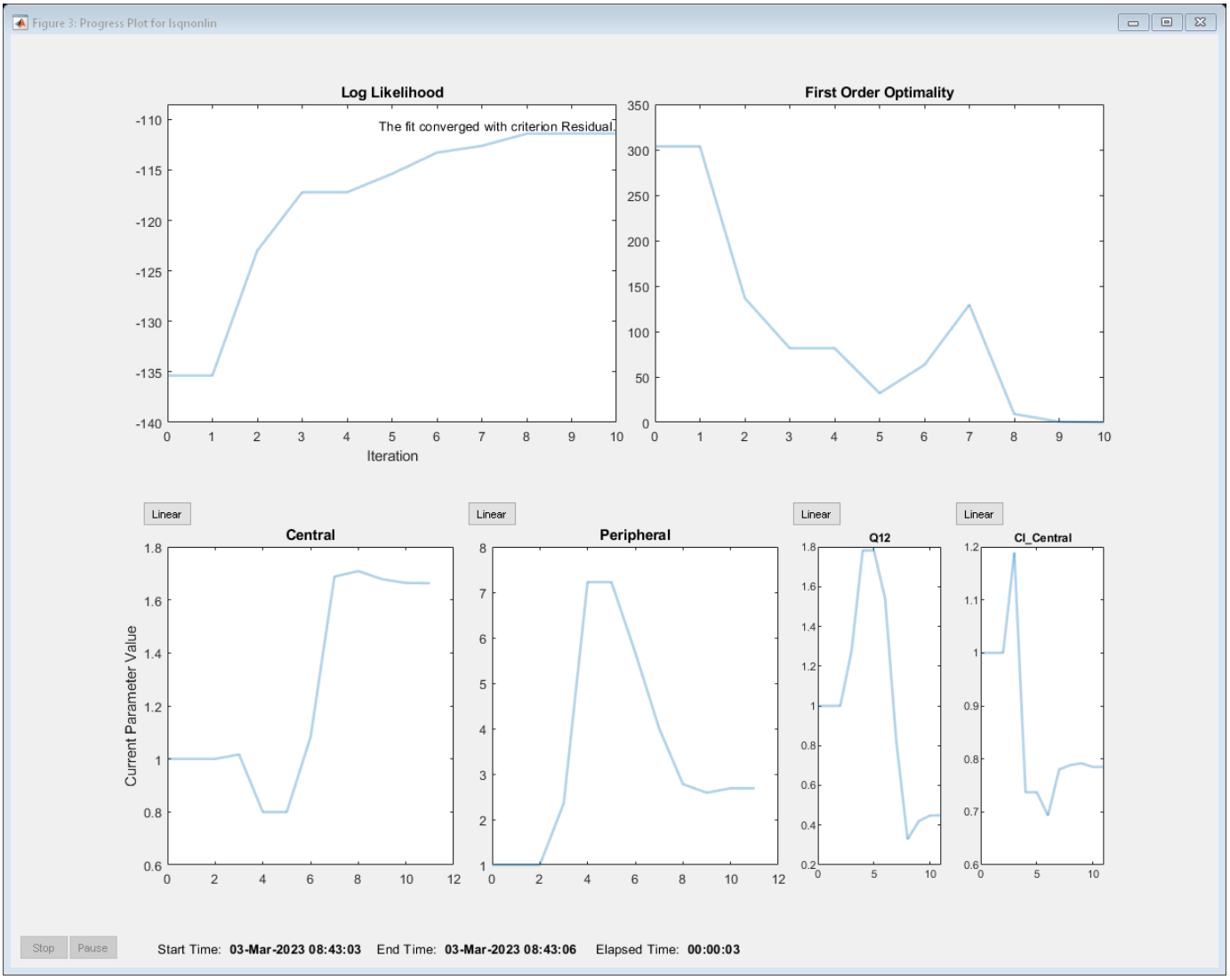
```
problem.ProgressPlot = true;
```

Fit the model to all of the data pooled together: that is, estimate one set of parameters for all individuals by setting the `Pooled` property to `true`.

```
problem.Pooled      = true;
```

Perform the estimation using the `fit` function of the object.

```
pooledFit = fit(problem);
```



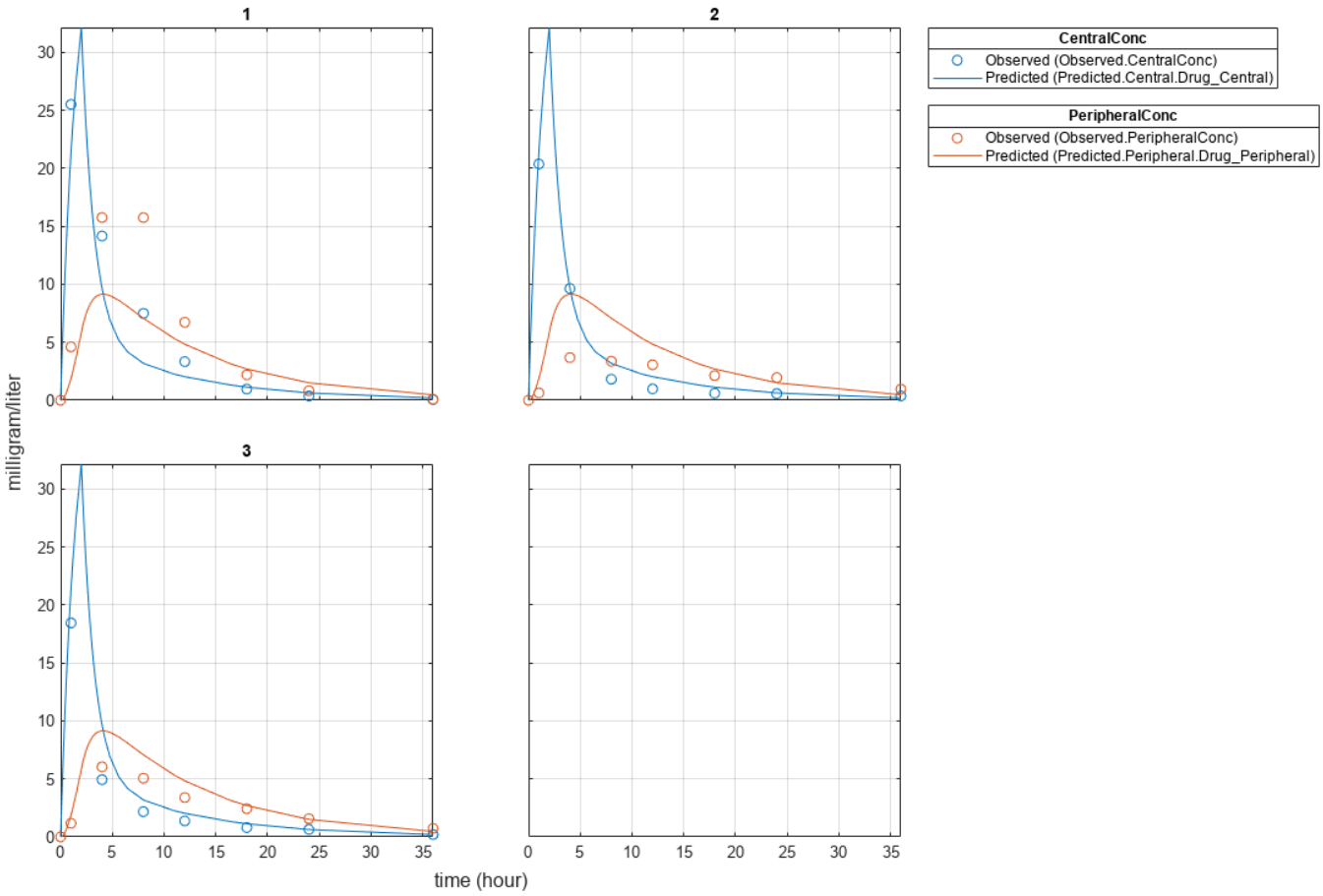
Display the estimated parameter values.

```
pooledFit.ParameterEstimates
```

```
ans=4×3 table
        Name         Estimate    StandardError
    _____________    ________    _____________

    {'Central'   }     1.6627        0.16569
    {'Peripheral'}     2.6864         1.0644
    {'Q12'       }    0.44945        0.19943
    {'Cl_Central'}    0.78497       0.095621
```

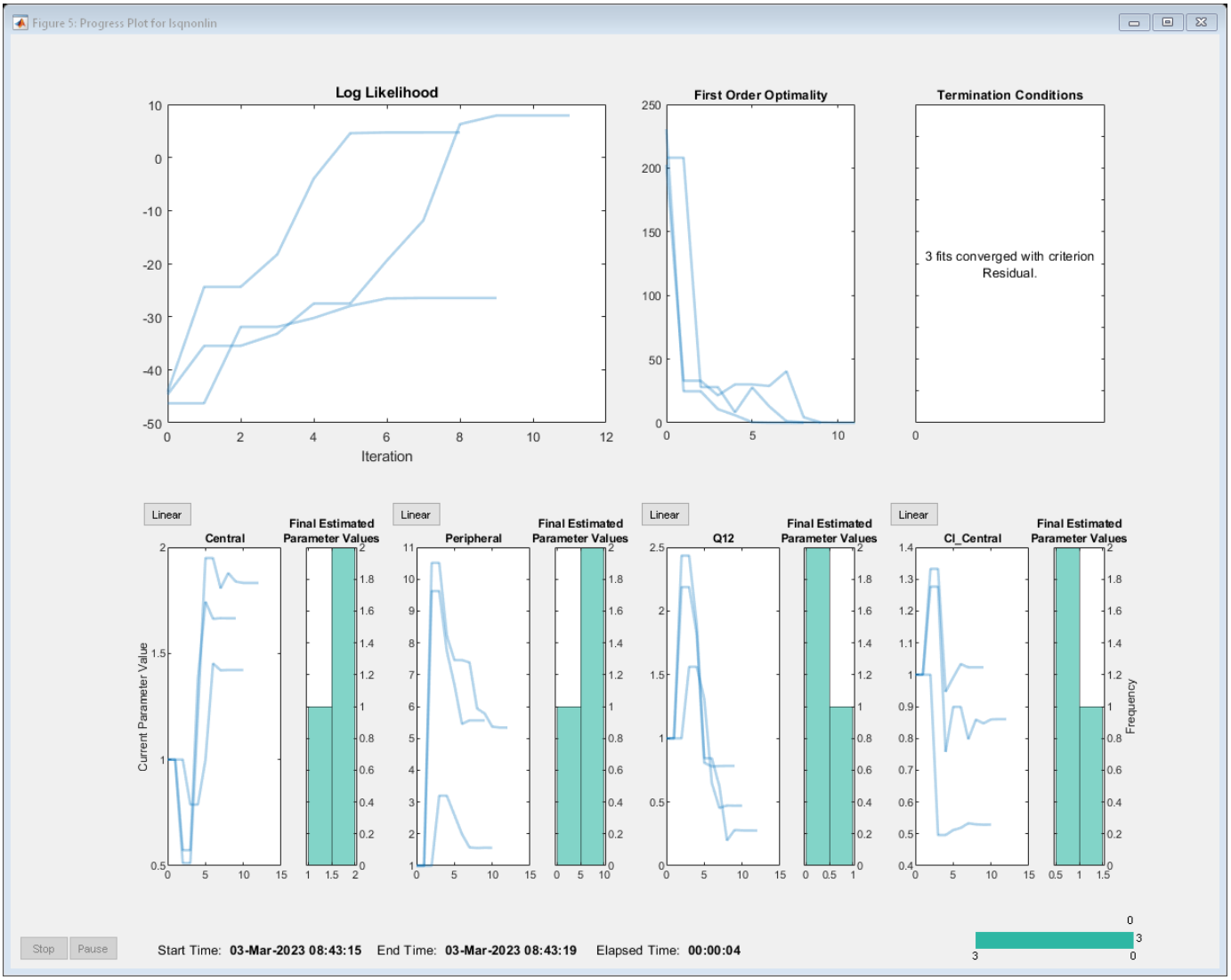
Plot the fitted results.

```
plot(pooledFit);
```



Estimate one set of parameters for each individual and see if the parameter estimates improve.

```
problem.Pooled  = false;
unpooledFit     = fit(problem);
```



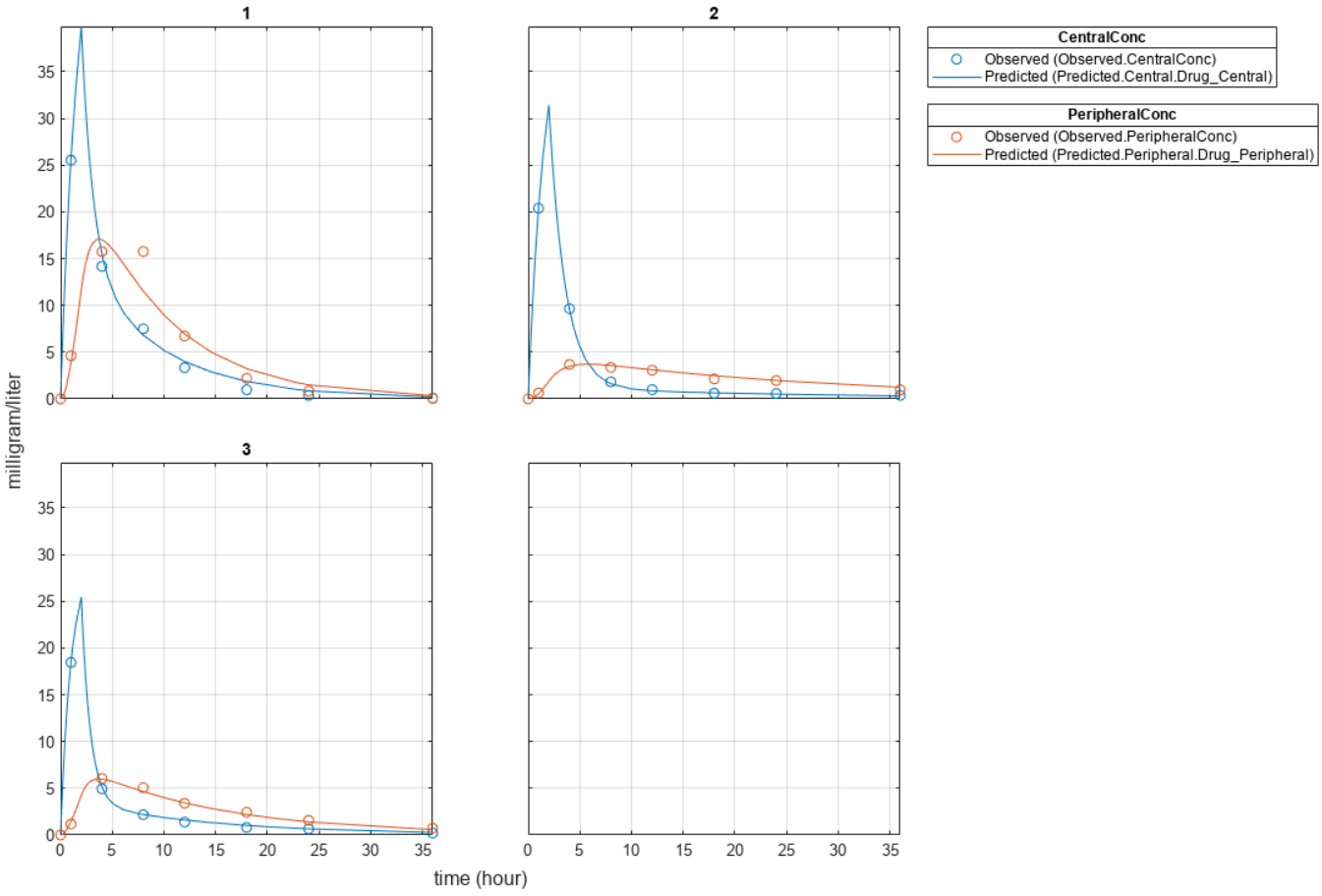
Display the estimated parameter values.

```
unpooledFit.ParameterEstimates
```

```
ans=4×3 table
        Name          Estimate    StandardError
    ______________    ________    _____________

    {'Central'   }      1.422       0.12334
    {'Peripheral'}     1.5619       0.36355
    {'Q12'       }    0.47163       0.15196
    {'Cl_Central'}     0.5291      0.036978


ans=4×3 table
        Name          Estimate    StandardError
    ______________    ________    _____________

    {'Central'   }     1.8322       0.019672
```

```
    {'Peripheral'}     5.3364        0.65327
    {'Q12'       }     0.2764       0.030799
    {'Cl_Central'}    0.86035       0.026257


ans=4×3 table
        Name          Estimate    StandardError
    ______________    ________    _____________

    {'Central'   }     1.6657       0.038529
    {'Peripheral'}     5.5632        0.37063
    {'Q12'       }    0.78361       0.058657
    {'Cl_Central'}     1.0233       0.027311
```

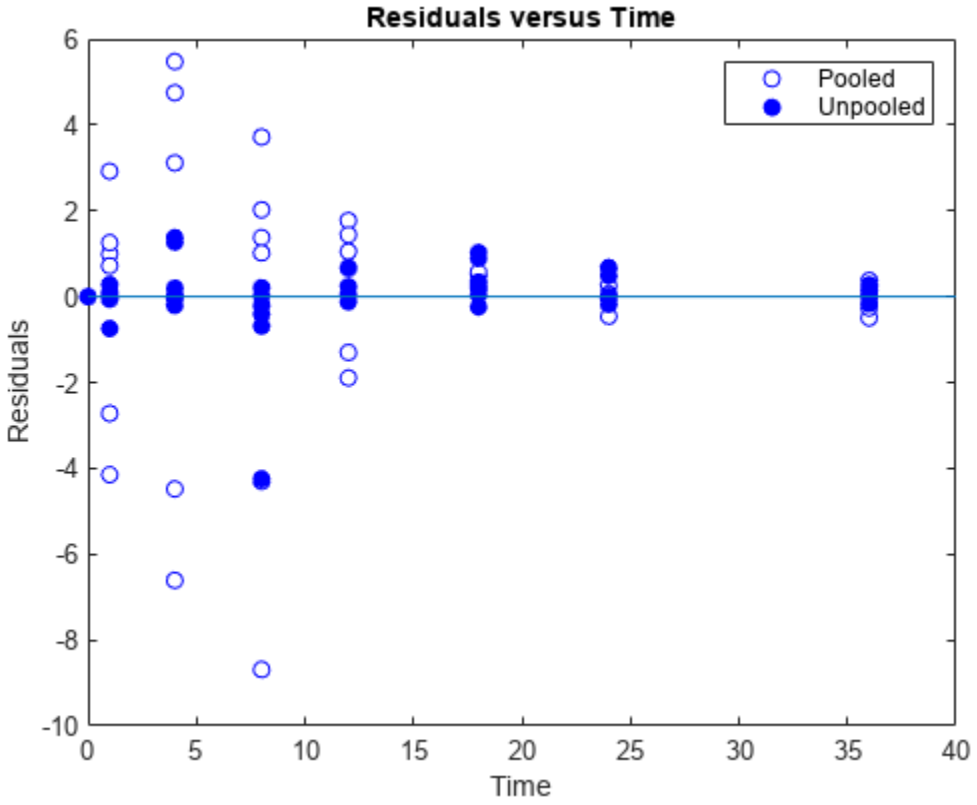
```
plot(unpooledFit);
```



Generate a plot of the residuals over time to compare the pooled and unpooled fit results. The figure indicates unpooled fit residuals are smaller than those of the pooled fit, as expected. In addition to comparing residuals, other rigorous criteria can be used to compare the fitted results.

```
t = [gData.Time;gData.Time];
res_pooled = vertcat(pooledFit.R);
res_pooled = res_pooled(:);
res_unpooled = vertcat(unpooledFit.R);
```

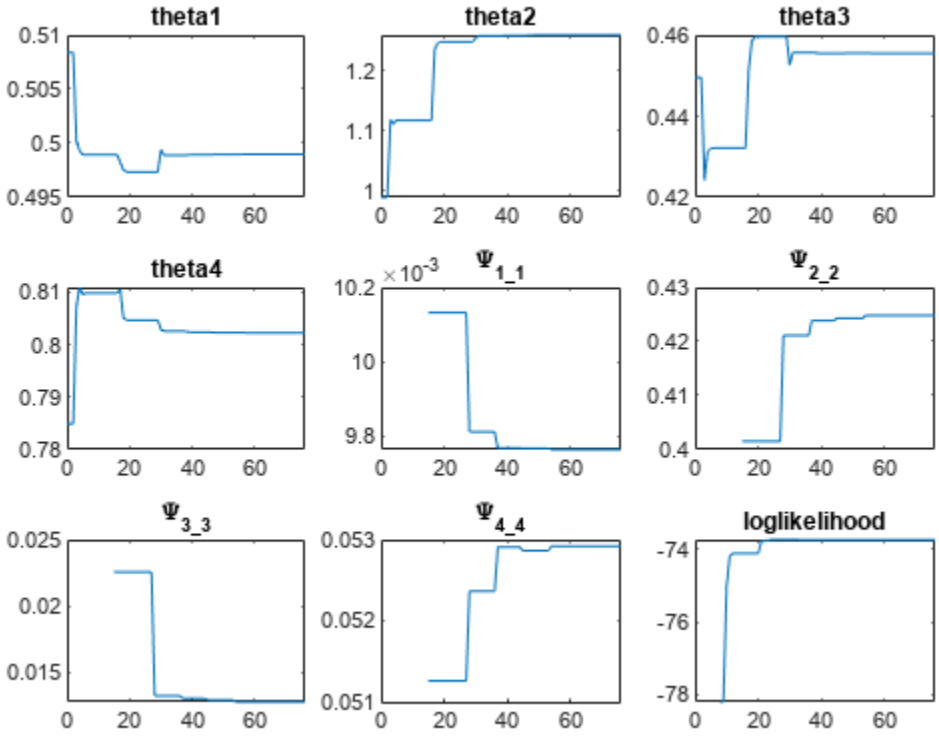
```
res_unpooled = res_unpooled(:);
figure;
plot(t,res_pooled,"o",MarkerFaceColor="w",markerEdgeColor="b")
hold on
plot(t,res_unpooled,"o",MarkerFaceColor="b",markerEdgeColor="b")
refl = refline(0,0); % A reference line representing a zero residual
title("Residuals versus Time");
xlabel("Time");
ylabel("Residuals");
legend(["Pooled","Unpooled"]);
```



As illustrated, the unpooled fit accounts for variations due to the specific subjects in the study, and, in this case, the model fits better to the data. However, the pooled fit returns population-wide parameters. As an alternative, if you want to estimate population-wide parameters while considering individual variations, you can perform nonlinear mixed-effects (NLME) estimation by setting `problem.FitFunction` to `sbiofitmixed`.

```
problem.FitFunction = "sbiofitmixed";
```

```
NLMEResults = fit(problem);
```



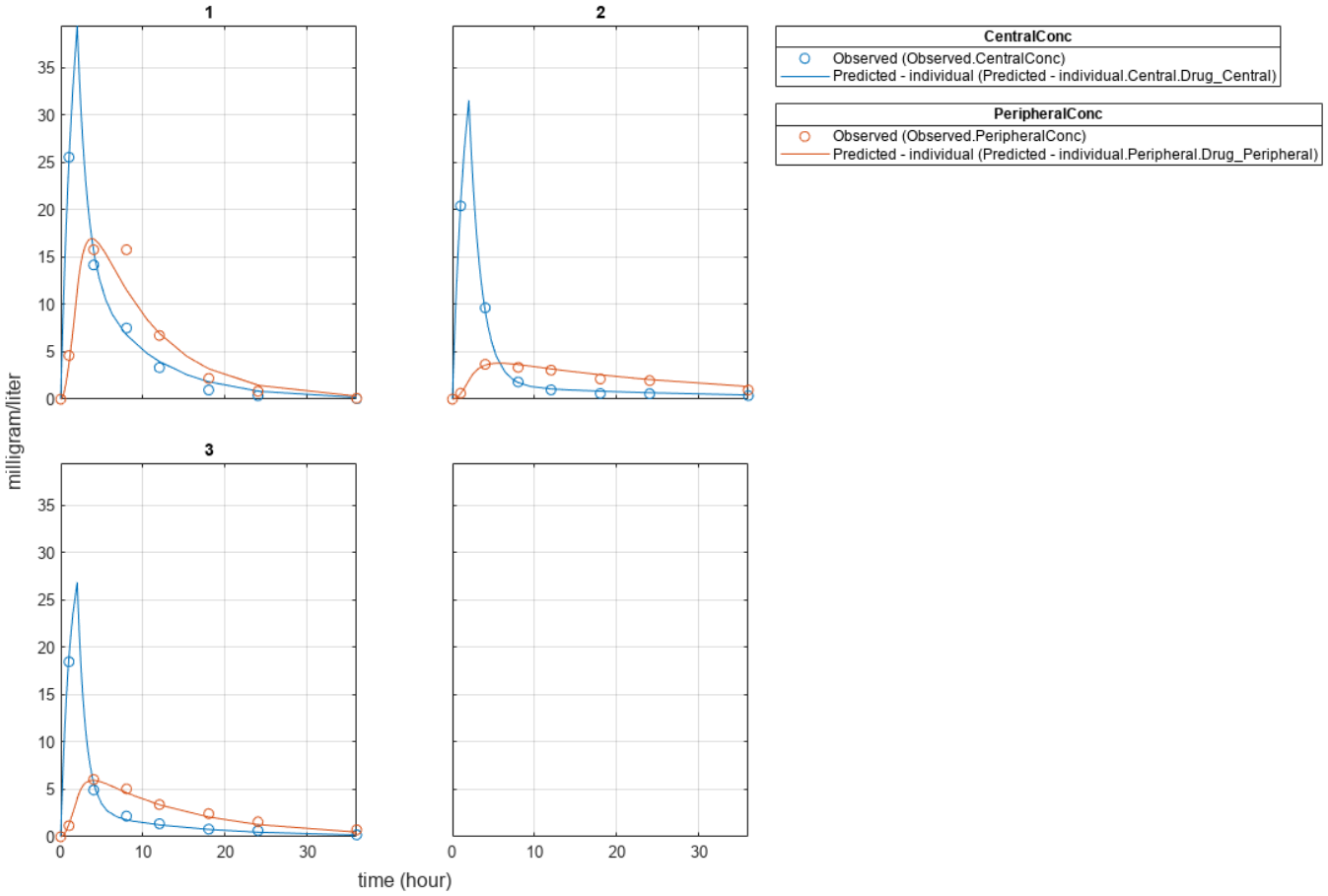
Display the estimated parameter values.

```
NLMEResults.IndividualParameterEstimates
```

```
ans=12×3 table
    Group          Name          Estimate
    _____    _______________    ________

      1      {'Central'   }      1.4623
      1      {'Peripheral'}      1.5306
      1      {'Q12'       }      0.4587
      1      {'Cl_Central'}     0.53208
      2      {'Central'   }       1.783
      2      {'Peripheral'}      6.6623
      2      {'Q12'       }      0.3589
      2      {'Cl_Central'}      0.8039
      3      {'Central'   }      1.7135
      3      {'Peripheral'}      4.2844
      3      {'Q12'       }     0.54895
      3      {'Cl_Central'}      1.0708
```

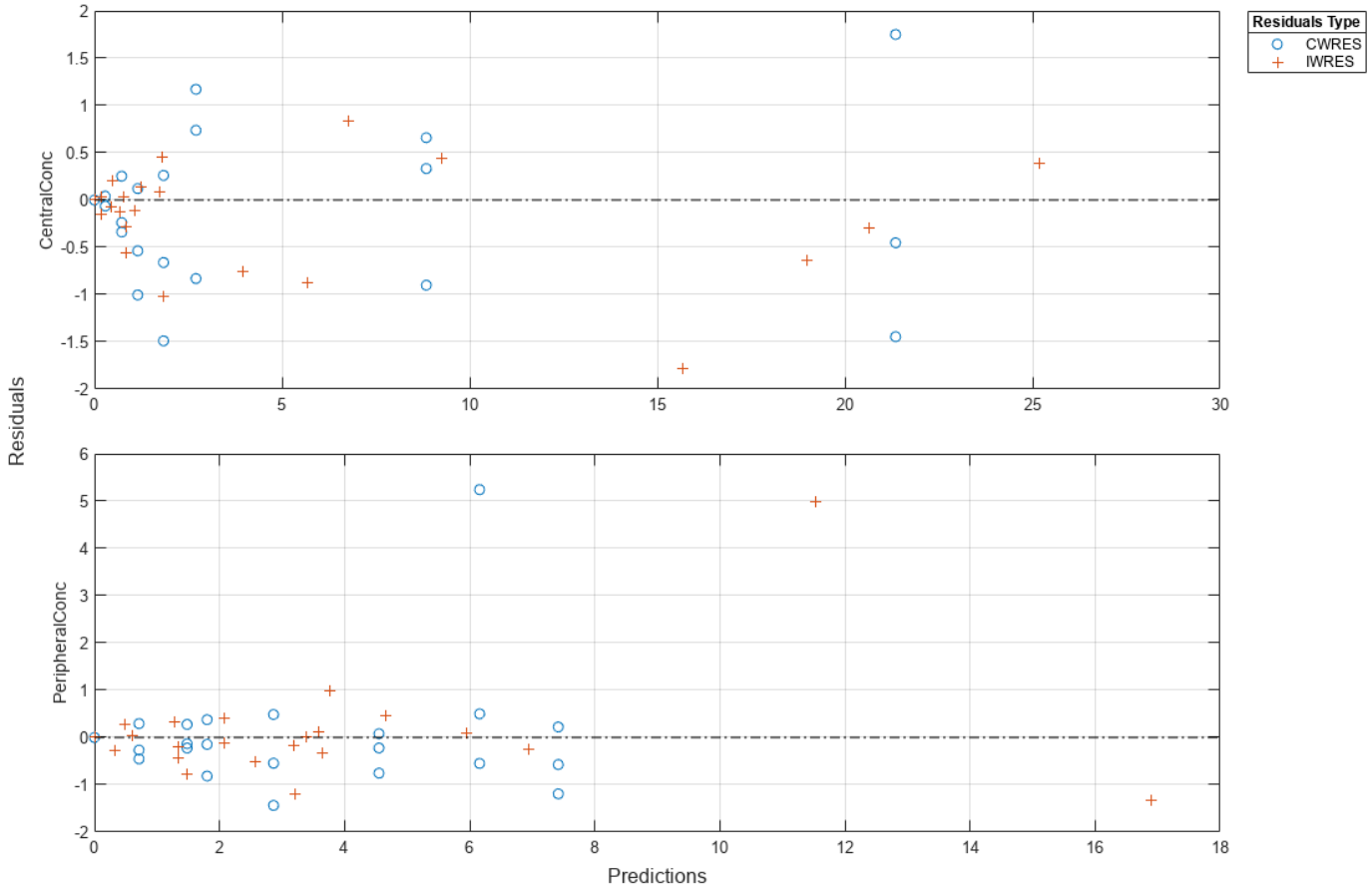
Plot the fitted results.

```
plot(NLMEResults);
```



Plot the conditional weighted residuals (CWRES) and individual weighted residuals (IWRES) of model predicted values.

```
plotResiduals(NLMEResults,'predictions')
```



More About

Default Options for Optimization Functions Called by sbiofit

The following table summarizes the default options for various estimation functions.

Function	Default Options
`nlinfit`	`sbiofit` uses the default options structure associated with `nlinfit`, except for: `FunValCheck = 'off'` `DerivStep = max(eps^(1/3), min(1e-4,SolverOptions.RelativeTolerance))`, where the `SolverOptions` property corresponds to the model's active `configset object`.

Function	Default Options
`fmincon`	`sbiofit` uses the default options structure associated with `fmincon`, except for: `Display = 'off'` `FunctionTolerance = 1e-6*abs(f0)`, where `f0` is the initial value of the objective function. `OptimalityTolerance = 1e-6*abs(f0)`, where `f0` is the initial value of the objective function. `Algorithm = 'trust-region-reflective'` when `'SensitivityAnalysis'` is true, or `'interior-point'` when `'SensitivityAnalysis'` is false. `FiniteDifferenceStepSize = max(eps^(1/3),min(1e-4,SolverOptions.RelativeTolerance))`, where the `SolverOptions` property corresponds to the model active `configset object`. `TypicalX = 1e-6*x0`, where `x0` is an array of transformed initial estimates.
`fminunc`	`sbiofit` uses the default options structure associated with `fminunc`, except for: `Display = 'off'` `FunctionTolerance = 1e-6*abs(f0)`, where `f0` is the initial value of the objective function. `OptimalityTolerance = 1e-6*abs(f0)`, where `f0` is the initial value of the objective function. `Algorithm = 'trust-region'` when `'SensitivityAnalysis'` is true, or `'quasi-newton'` when `'SensitivityAnalysis'` is false. `FiniteDifferenceStepSize = max(eps^(1/3),min(1e-4,SolverOptions.RelativeTolerance))`, where the `SolverOptions` property corresponds to the model active `configset object`. `TypicalX = 1e-6*x0`, where `x0` is an array of transformed initial estimates.
`fminsearch`	`sbiofit` uses the default options structure associated with `fminsearch`, except for: `Display = 'off'` `TolFun = 1e-6*abs(f0)`, where `f0` is the initial value of the objective function.

Function	Default Options
`lsqcurvefit`, `lsqnonlin`	Requires Optimization Toolbox. `sbiofit` uses the default options structure associated with `lsqcurvefit` and `lsqnonlin`, except for: `Display = 'off'` `FunctionTolerance = 1e-6*norm(f0)`, where `f0` is the initial value of the objective function. `OptimalityTolerance = 1e-6*norm(f0)`, where `f0` is the initial value of the objective function. `FiniteDifferenceStepSize = max(eps^(1/3),min(1e-4,SolverOptions.RelativeTolerance))`, where the `SolverOptions` property corresponds to the model active `configset object`. `TypicalX = 1e-6*x0`, where `x0` is an array of transformed initial estimates.

`patternsearch`	Requires Global Optimization Toolbox.
	
	`sbiofit` uses the default options object (`optimoptions`) associated with `patternsearch`, except for:
	`Display = 'off'`
	`FunctionTolerance = 1e-6*abs(f0)`, where `f0` is the initial value of the objective function.
	`MeshTolerance = 1.0e-3`
	`AccelerateMesh = true`

`ga`	Requires Global Optimization Toolbox.
	
	`sbiofit` uses the default options object (`optimoptions`) associated with `ga`, except for:
	`Display = 'off'`
	`FunctionTolerance = 1e-6*abs(f0)`, where `f0` is the initial value of the objective function.
	`MutationFcn = @mutationadaptfeasible`

`particleswarm`	Requires Global Optimization Toolbox. `sbiofit` uses the following default options for the `particleswarm` algorithm, except for: `Display = 'off'` `FunctionTolerance = 1e-6*abs(f0)`, where `f0` is the initial value of the objective function. `InitialSwarmSpan = 2000 or 8`; `2000` for estimated parameters with no transform; `8` for estimated parameters with `log`, `logit`, or `probit` transforms.
`scattersearch`	See “Scatter Search Algorithm” on page 1-98.

Version History

Introduced in R2021b

See Also

`sbiofit` | `sbiofitmixed` | `EstimatedInfo object` | `groupedData object` | `LeastSquaresResults object` | `NLINResults object` | `OptimResults object` | `sbiofitmixed` | `nlinfit` | `fmincon` | `fminunc` | `fminsearch` | `lsqcurvefit` | `lsqnonlin` | `patternsearch` | `ga` | `particleswarm`

Topics

“What is Nonlinear Regression?”
“What Is a Nonlinear Mixed-Effects Model?”
“Parameter Transformations”
“Maximum Likelihood Estimation”
“Supported Methods for Parameter Estimation in SimBiology”
“Sensitivity Analysis in SimBiology”
“Create Data File with SimBiology Definitions”

fitted

Return simulation results of SimBiology model fitted using least-squares regression

Syntax

```
[yfit,parameterEstimates] = fitted(resultsObj)
```

Description

`[yfit,parameterEstimates] = fitted(resultsObj)` returns simulation results `yfit` and parameter estimates `parameterEstimates` from a fitted SimBiology model.

Tip Use this method to retrieve simulation results from the fitted model if you did not specify the second optional output argument that corresponds to simulation results when you first ran `sbiofit`.

Examples

Estimate Yeast G Protein Model Parameter

This example uses the yeast heterotrimeric G protein model and experimental data reported by [1]. For details about the model, see the **Background** section in “Parameter Scanning, Parameter Estimation, and Sensitivity Analysis in the Yeast Heterotrimeric G Protein Cycle”.

Load the G protein model.

```
sbioloadproject gprotein
```

Store the experimental data containing the time course for the fraction of active G protein.

```
time = [0 10 30 60 110 210 300 450 600]';
GaFracExpt = [0 0.35 0.4 0.36 0.39 0.33 0.24 0.17 0.2]';
```

Create a `groupedData` object based on the experimental data.

```
tbl = table(time,GaFracExpt);
grpData = groupedData(tbl);
```

Map the appropriate model component to the experimental data. In other words, indicate which species in the model corresponds to which response variable in the data. In this example, map the model parameter `GaFrac` to the experimental data variable `GaFracExpt` from `grpData`.

```
responseMap = 'GaFrac = GaFracExpt';
```

Use an `estimatedInfo` object to define the model parameter `kGd` as a parameter to be estimated.

```
estimatedParam = estimatedInfo('kGd');
```

Perform the parameter estimation.

```
fitResult = sbiofit(m1,grpData,responseMap,estimatedParam);
```

View the estimated parameter value of `kGd`.

```
fitResult.ParameterEstimates
```

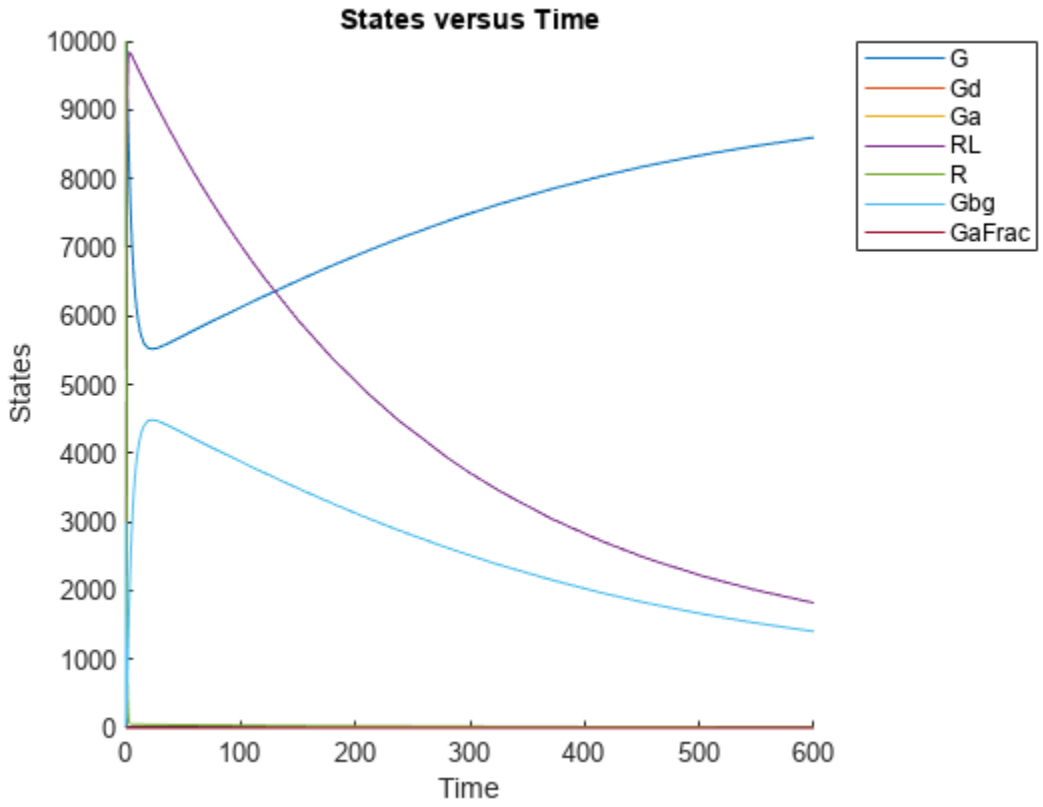
```
ans=1×3 table
     Name      Estimate    StandardError
    _______    ________    _____________

    {'kGd'}    0.11307      3.4439e-05
```

Suppose you want to plot the model simulation results using the estimated parameter value. You can either rerun the `sbiofit` function and specify to return the optional second output argument, which contains simulation results, or use the `fitted` method to retrieve the results without rerunning `sbiofit`.

```
[yfit,paramEstim] = fitted(fitResult);
```

Plot the simulation results.

```
sbioplot(yfit);
```



Input Arguments

`resultsObj` — Estimation results

`OptimResults` object | `NLINResults` object | vector of results objects

Estimation results, specified as an `OptimResults object`, `NLINResults object`, or vector of results objects which contains estimation results from running `sbiofit`.

Output Arguments

`yfit` — Simulation results

vector of `SimData` objects

Simulation results, returned as a vector of `SimData` objects. The states reported in `yfit` are the states that were included in the `responseMap` input argument of `sbiofit` as well as any other states listed in the `StatesToLog` property of the runtime options (`RuntimeOptions`) of the SimBiology model.

`parameterEstimates` — Estimated parameter values

table

Estimated parameter values, returned as a table. This argument is identical to the `resultsObj.ParameterEstimates` property.

Version History

Introduced in R2014a

References

[1] Yi, T-M., Kitano, H., and Simon, M. (2003). A quantitative characterization of the yeast heterotrimeric G protein cycle. PNAS. 100, 10764–10769.

See Also

`NLINResults object` | `OptimResults object` | `sbiofit`

fitted

Return the simulation results of a fitted nonlinear mixed-effects model

Syntax

```
[yfit,parameterEstimates]= fitted(resultsObj)
[yfit,parameterEstimates]= fitted(resultsObj,'ParameterType',value)
```

Description

`[yfit,parameterEstimates]= fitted(resultsObj)` returns simulation results `yfit` and parameter estimates `parameterEstimates` from a fitted nonlinear mixed-effect model.

`[yfit,parameterEstimates]= fitted(resultsObj,'ParameterType',value)` returns simulation results that are simulated using either individual or population parameter estimates. The two choices for `value` are `'population'` or `'individual'` (default).

Tip Use this method to retrieve simulation results from the fitted model if you did not specify the second or third optional output argument that corresponds to simulation results when you first ran `sbiofitmixed`.

Input Arguments

`resultsObj` — Estimation results

`NLMEResults` object

Estimation results, specified as an `NLMEResults object`, which contains estimation results returned by `sbiofitmixed`.

`value` — Parameter type

character vector | string

Parameter type, specified as `'population'` or `'individual'` (default). If `'population'`, the method returns the model simulation results using the population parameter estimates. If `'individual'`, it returns simulation results using the individual-specific parameter estimates.

Output Arguments

`yfit` — Simulation results

vector of `SimData` objects

Simulation results, returned as a vector of `SimData` objects. The states reported in `yfit` are the states that were included in the `responseMap` input argument of `sbiofitmixed` as well as any other states listed in the `StatesToLog` property of the runtime options (`RuntimeOptions`) of the SimBiology model.

`parameterEstimates` — Estimated parameter values

table

Estimated parameter values, returned as a table. This is identical to `resultsObj.IndividualParameterEstimates` property when the `value` argument is `'individual'` or `resultsObj.PopulationParameterEstimates` property when the `value` is `'population'`.

Version History

Introduced in R2014a

See Also

`NLMEResults object` | `sbiofitmixed`

generate

Generate scenarios from `SimBiology.Scenarios` object and return table

Syntax

```
scenariosTable = generate(sObj)
scenariosTable = generate(sObj,n)
scenariosTable = generate( ___ ,'StandardizedOutput',tf)
```

Description

`scenariosTable = generate(sObj)` generates scenarios from the `SimBiology.Scenarios` object `sObj` and returns a table, where each row represents a scenario and each column represents an entry.

`scenariosTable = generate(sObj,n)` returns only the specified n^{th} row (scenario) of the scenarios table.

`scenariosTable = generate( ___ ,'StandardizedOutput',tf)` enables standardization of doses in the output table.

Examples

Generate Different Simulation Scenarios for Glucose-Insulin Response

Load the model of glucose-insulin response. For details about the model, see the **Background** section in “Simulate the Glucose-Insulin Response”.

```
sbioloadproject('insulindemo','m1');
```

The model contains different parameter values and initial conditions that represents different insulin impairments (such as Type 2 diabetes, low insulin sensitivity, and so on) stored in five variants.

```
variants = getvariant(m1)
```

```
variants =
   SimBiology Variant Array

   Index:  Name:             Active:
   1       Type 2 diabetic   false
   2       Low insulin se... false
   3       High beta cell... false
   4       Low beta cell ... false
   5       High insulin s... false
```

Suppress an informational warning that is issued during simulations.

```
warnSettings = warning('off','SimBiology:DimAnalysisNotDone_MatlabFcn_Dimensionless');
```

Select a dose that represents a single meal of 78 grams of glucose.

```
singleMeal = sbioselect(m1,'Name','Single Meal');
```

Create a `Scenarios` object to represent different initial conditions combined with the dose. That is, create a `scenario` object where each variant is paired (or combined) with the dose, for a total of five simulation scenarios.

```
sObj = SimBiology.Scenarios;
add(sObj,'cartesian','variants',variants);
add(sObj,'cartesian','dose',singleMeal)
```

```
ans =
  Scenarios (5 scenarios)

                  Name            Content           Number
                ________    ____________________    ______

    Entry 1     variants    SimBiology variants      5
    x Entry 2   dose        SimBiology dose          1

  See also Expression property.
```

`sObj` contains two entries. Use the `generate` function to combine the entries and generate five scenarios. The function returns a scenarios table, where each row represents a scenario and each column represents an entry of the `Scenarios` object.

```
scenariosTbl = generate(sObj)
```

```
scenariosTbl=5×2 table
           variants                    dose
    ____________________    ____________________________

    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
```

Change the entry name of the first entry.

```
rename(sObj,1,'Insulin Impairements')
```

```
ans =
  Scenarios (5 scenarios)

                        Name                  Content           Number
                ____________________    ____________________    ______

    Entry 1     Insulin Impairements    SimBiology variants      5
    x Entry 2   dose                    SimBiology dose          1

  See also Expression property.
```

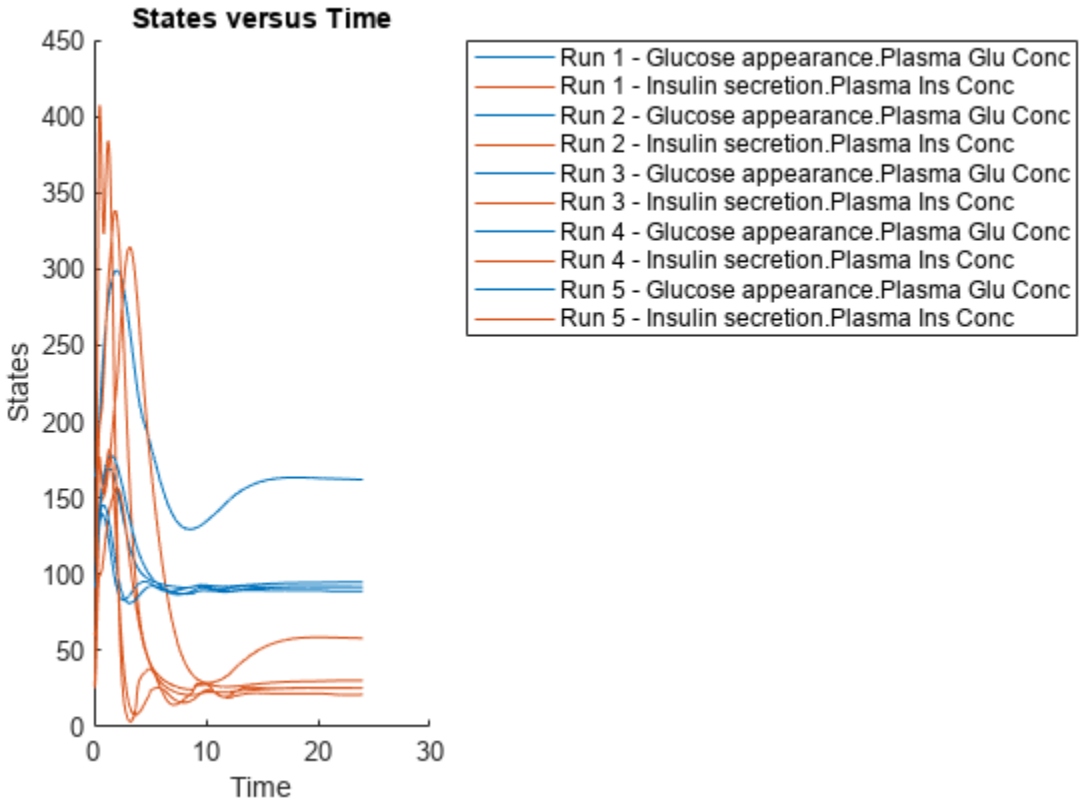
Create a `SimFunction` object to simulate the generated scenarios. Use the `Scenarios` object as the input and specify the plasma glucose and insulin concentrations as reponses (outputs of the function to be plotted). Specify `[]` for the dose input argument since the `Scenarios` object already has the dosing information.

```
f = createSimFunction(m1,sObj,{'[Plasma Glu Conc]','[Plasma Ins Conc]'},[])

f = 
SimFunction

Parameters:

              Name                 Value          Type                            Units                
    _________________________    ______    ______________    ____________________________________

    {'Plasma Volume (Glu)'   }      1.88    {'parameter'}    {'deciliter'                        
    {'k1'                    }     0.065    {'parameter'}    {'1/minute'                         
    {'k2'                    }     0.079    {'parameter'}    {'1/minute'                         
    {'Plasma Volume (Ins)'   }      0.05    {'parameter'}    {'liter'                            
    {'m1'                    }      0.19    {'parameter'}    {'1/minute'                         
    {'m2'                    }     0.484    {'parameter'}    {'1/minute'                         
    {'m4'                    }    0.1936    {'parameter'}    {'1/minute'                         
    {'m5'                    }    0.0304    {'parameter'}    {'minute/picomole'                  
    {'m6'                    }    0.6469    {'parameter'}    {'dimensionless'                    
    {'Hepatic Extraction'    }       0.6    {'parameter'}    {'dimensionless'                    
    {'kmax'                  }    0.0558    {'parameter'}    {'1/minute'                         
    {'kmin'                  }     0.008    {'parameter'}    {'1/minute'                         
    {'kabs'                  }    0.0568    {'parameter'}    {'1/minute'                         
    {'kgri'                  }         0    {'parameter'}    {'1/minute'                         
    {'f'                     }       0.9    {'parameter'}    {'dimensionless'                    
    {'a'                     }         0    {'parameter'}    {'1/milligram'                      
    {'b'                     }      0.82    {'parameter'}    {'dimensionless'                    
    {'c'                     }         0    {'parameter'}    {'1/milligram'                      
    {'d'                     }      0.01    {'parameter'}    {'dimensionless'                    
    {'kp1'                   }       2.7    {'parameter'}    {'milligram/minute'                 
    {'kp2'                   }    0.0021    {'parameter'}    {'1/minute'                         
    {'kp3'                   }     0.009    {'parameter'}    {'(milligram/minute)/(picomole/liter
    {'kp4'                   }    0.0618    {'parameter'}    {'(milligram/minute)/picomole'      
    {'ki'                    }    0.0079    {'parameter'}    {'1/minute'                         
    {'[Ins Ind Glu Util]'    }         1    {'parameter'}    {'milligram/minute'                 
    {'Vm0'                   }    2.5129    {'parameter'}    {'milligram/minute'                 
    {'Vmx'                   }     0.047    {'parameter'}    {'(milligram/minute)/(picomole/liter
    {'Km'                    }    225.59    {'parameter'}    {'milligram'                        
    {'p2U'                   }    0.0331    {'parameter'}    {'1/minute'                         
    {'K'                     }      2.28    {'parameter'}    {'picomole/(milligram/deciliter)'   
    {'alpha'                 }      0.05    {'parameter'}    {'1/minute'                         
    {'beta'                  }      0.11    {'parameter'}    {'(picomole/minute)/(milligram/decil
    {'gamma'                 }       0.5    {'parameter'}    {'1/minute'                         
    {'ke1'                   }    0.0005    {'parameter'}    {'1/minute'                         
    {'ke2'                   }       339    {'parameter'}    {'milligram'                        
    {'Basal Plasma Glu Conc'}     91.76    {'parameter'}    {'milligram/deciliter'              
    {'Basal Plasma Ins Conc'}     25.49    {'parameter'}    {'picomole/liter'                   

Observables: 

            Name                Type                 Units          
    _____________________    ___________    _______________________

    {'[Plasma Glu Conc]'}    {'species'}    {'milligram/deciliter'}
    {'[Plasma Ins Conc]'}    {'species'}    {'picomole/liter'     }

Dosed:
```

```
    TargetName       TargetDimension
    __________    ______________________

     {'Dose'}     {'Mass (e.g., gram)'}

TimeUnits: hour
```

Simulate the model for 24 hours and plot the simulation data. The data contains five runs, where each run represents a scenario in the Scenarios object.

```
sd = f(sObj,24);
sbioplot(sd)
```




```
ans =
  Axes (SbioPlot) with properties:

            XLim: [0 30]
            YLim: [0 450]
          XScale: 'linear'
          YScale: 'linear'
    GridLineStyle: '-'
        Position: [0.0920 0.1100 0.2956 0.8150]
           Units: 'normalized'

  Show all properties
```

If you have Statistics and Machine Learning Toolbox™, you can also draw sample values for model quantities from various probability distributions. For instance, suppose that the parameters `Vmx` and `kp3`, which are known for the low and high insulin sensitivity, follow the lognormal distribution. You can generate sample values for these parameters from such a distribution, and perform a scan to explore model behavior.

Define the lognormal probability distribution object for `Vmx`.

```
pd_Vmx = makedist('lognormal')
```

```
pd_Vmx =
  LognormalDistribution

  Lognormal distribution
       mu = 0
    sigma = 1
```

By definition, the parameter `mu` is the mean of logarithmic values. To vary the parameter value around the base (model) value of the parameter, set `mu` to `log(`*`model_value`*`)`. Set the standard deviation (*sigma*) to 0.2. For a small *sigma* value, the mean of a lognormal distribtion is approximately equal to `log(`*`model_value`*`)`. For details, see “Lognormal Distribution” (Statistics and Machine Learning Toolbox).

```
Vmx = sbioselect(m1,'Name','Vmx');
pd_Vmx.mu = log(Vmx.Value);
pd_Vmx.sigma = 0.2
```

```
pd_Vmx =
  LognormalDistribution

  Lognormal distribution
       mu = -3.05761
    sigma =      0.2
```

Similarly define the probability distribution for kp3.

```
pd_kp3 = makedist('lognormal');
kp3 = sbioselect(m1,'Name','kp3');
pd_kp3.mu = log(kp3.Value);
pd_kp3.sigma = 0.2
```

```
pd_kp3 =
  LognormalDistribution

  Lognormal distribution
       mu = -4.71053
    sigma =      0.2
```

Now define a joint probability distribution to draw sample values for Vmx and kp3, with a rank correlation to specify some correlation between these two parameters. Note that this correlation assumption is for the illustration purposes of this example only and may not be biologically relevant.

First remove the variants entry (entry 1) from `sObj`.

```
remove(sObj,1)
```

```
ans =
  Scenarios (1 scenarios)

              Name        Content        Number
              ____    _______________    ______

    Entry 1    dose    SimBiology dose      1

  See also Expression property.
```

Add an entry that defines the joint probability distribution with a rank correlation matrix.

```
add(sObj,'cartesian',["Vmx","kp3"],[pd_Vmx, pd_kp3],'RankCorrelation',[1,0.5;0.5,1])
```

```
ans =
  Scenarios (2 scenarios)

                   Name           Content              Number
                   ____    ________________________    ___________

    Entry 1         dose    SimBiology dose           1
    x (Entry 2.1    Vmx     Lognormal distribution    2 (default)
    + Entry 2.2)    kp3     Lognormal distribution    2 (default)

  See also Expression property.
```

By default, the number of samples to draw from the joint distribution is set to 2. Increase the number of samples.

```
updateEntry(sObj,2,'Number',50)
```

```
ans =
  Scenarios (50 scenarios)

                   Name           Content             Number
                   ____    ________________________    ______

    Entry 1         dose    SimBiology dose             1
    x (Entry 2.1    Vmx     Lognormal distribution      50
    + Entry 2.2)    kp3     Lognormal distribution      50

  See also Expression property.
```

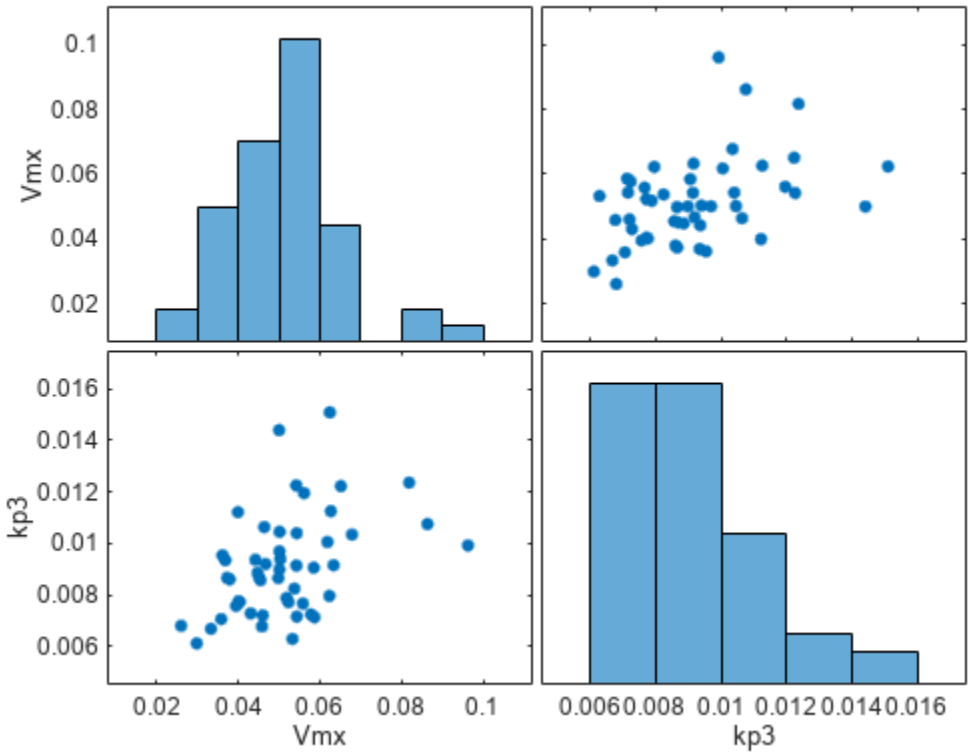
Verify that the `Scenarios` object can be simulated with the model. The `verify` function throws an error if any entry does not resolve uniquely to an object in the model or the entry contents have inconsistent lengths (sample sizes). The function throws a warning if multiple entries resolve to the same object in the model.

```
verify(sObj,m1)
```

Generate the simulation scenarios. Plot the sample values using `plotmatrix`. You can see the value of `Vmx` is varied around its model value 0.047 and that of `kp3` around 0.009.

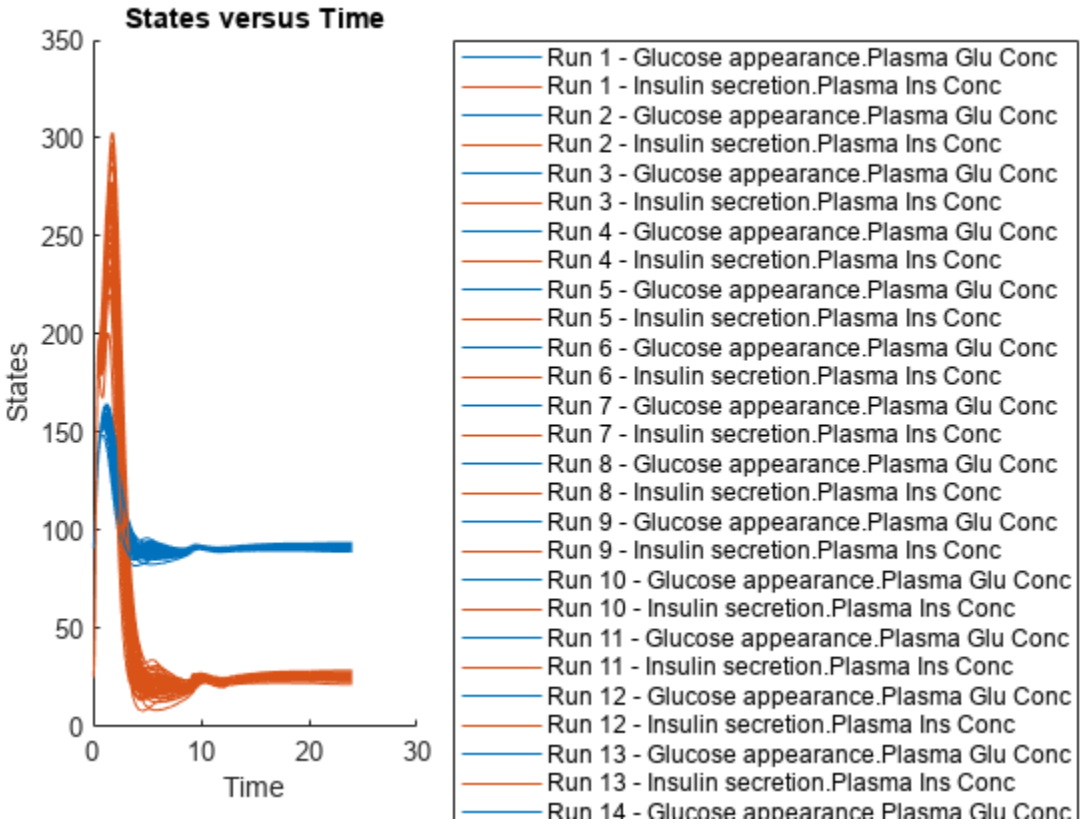
```
sTbl = generate(sObj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl.Vmx,sTbl.kp3]);
```

```
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
ax(2,1).XLabel.String = "Vmx";
ax(2,2).XLabel.String = "kp3";
```



Simulate the scenarios using the same SimFunction you created previously. You do not need to create a new SimFunction object even though the Scenarios object has been updated.

```
sd2 = f(sObj,24);
sbioplot(sd2);
```



By default, SimBiology uses the random sampling method. You can change it to the Latin hypercube sampling (or sobol or halton) for a more systematic space-filling approach.

```
entry2struct = getEntry(sObj,2)
```

```
entry2struct = struct with fields:
                Name: {'Vmx'  'kp3'}
             Content: [2x1 prob.LognormalDistribution]
              Number: 50
    RankCorrelation: [2x2 double]
          Covariance: []
      SamplingMethod: 'random'
    SamplingOptions: [0x0 struct]
```

```
entry2struct.SamplingMethod = 'lhs'
```

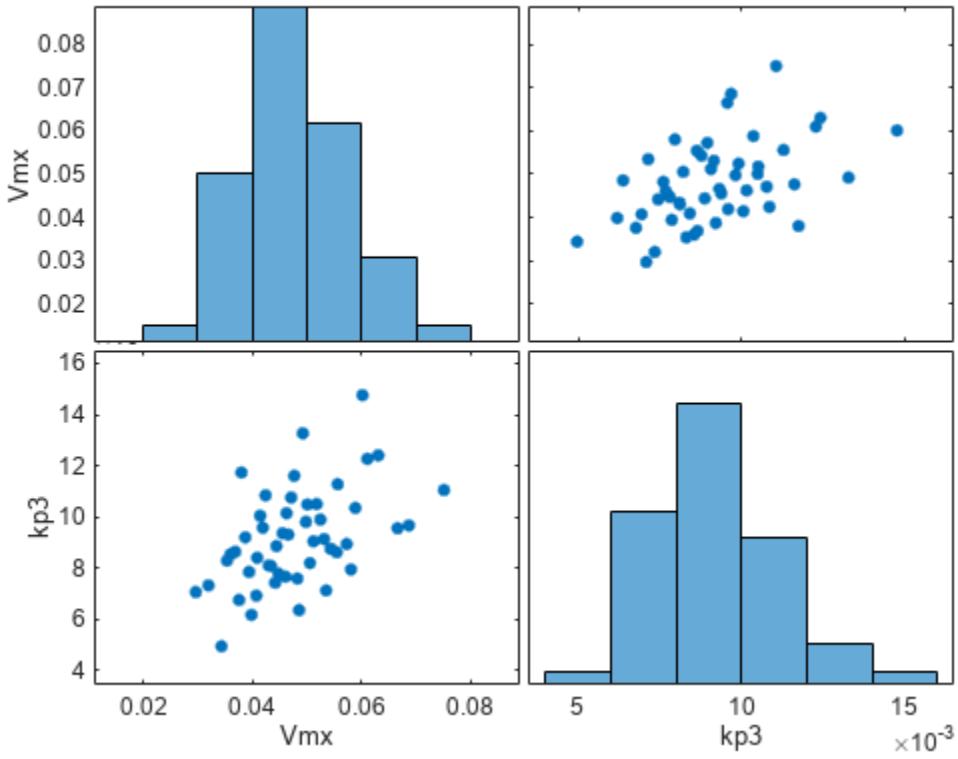
```
entry2struct = struct with fields:
                Name: {'Vmx'  'kp3'}
             Content: [2x1 prob.LognormalDistribution]
              Number: 50
    RankCorrelation: [2x2 double]
          Covariance: []
      SamplingMethod: 'lhs'
    SamplingOptions: [0x0 struct]
```

You can now use the updated structure to modify entry 2.

```
updateEntry(sObj,2,entry2struct)

ans =
  Scenarios (50 scenarios)

                    Name           Content             Number
                    ____    _____________________     ______

    Entry 1         dose    SimBiology dose             1
    x (Entry 2.1    Vmx     Lognormal distribution      50
    + Entry 2.2)    kp3     Lognormal distribution      50

  See also Expression property.
```

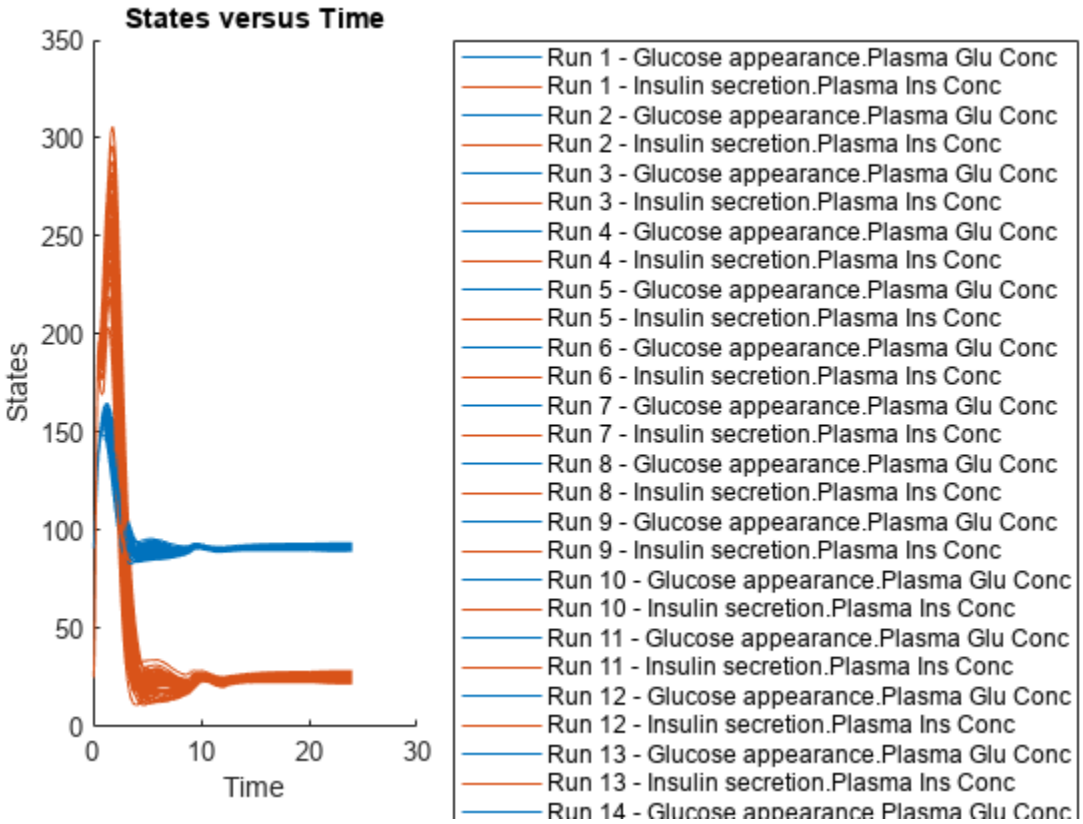
Visualize the sample values.

```
sTbl2 = generate(sObj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl2.Vmx,sTbl2.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
ax(2,1).XLabel.String = "Vmx";
ax(2,2).XLabel.String = "kp3";
```



Simulate the scenarios.

```
sd3 = f(sObj,24);
sbioplot(sd3);
```



Restore warning settings.

```
warning(warnSettings);
```

Input Arguments

`sObj` — Simulation scenarios

`SimBiology.Scenarios` object

Simulation scenarios, specified as a `SimBiology.Scenarios` object.

`n` — Index of scenario

positive integer

Index of a scenario to return as the output, specified as a positive integer. `n` must be less than or equal to the total number of scenarios (rows) in the scenarios table.

Example: 4

Data Types: `double`

`tf` — Flag to enable standardization of doses

`false` (default) | `true`

Flag to enable standardization of doses in the output, specified as `true` or `false`.

Set `tf` to true if you plan to pass in a dose table as an input on page 2-0 to a `SimFunction object`. The standardization procedure expands the dose samples to a cell array of dose tables with consistent target names within each column. For example, let `d1` and `d2` have different dose targets. The doses get standardized to:

```
{getTable(d1),[];[],getTable(d2)}
```

Example: `true`

Data Types: `logical`

Output Arguments

`scenariosTable` — Table of simulation scenarios
`table`

Table of simulation scenarios, returned as a table. Each row represents a scenario and each column represents an entry.

Version History

Introduced in R2019b

See Also

`SimBiology.Scenarios` | `SimFunction object` | `createSimFunction (model)`

Topics

“SimBiology.Scenarios Terminology” on page 2-799
“Combine Simulation Scenarios in SimBiology”

get

Get SimBiology object properties

Syntax

```
S = get(sobj)
propertyValues = get(sobj,propertyNames)
```

Description

`S = get(sobj)` returns a structure containing a field for each property of `sobj`, a SimBiology object.

`propertyValues = get(sobj,propertyNames)` returns the values of the properties specified by `propertyNames`.

Examples

Get Model Dosing Information

Load the bioavailability model.

```
sbioloadproject('Bioavailability.sbproj');
```

Retrieve the name of the model.

```
modelName = get(m1,'Name')
```

```
modelName =
'Bioavailability Model'
```

Check the dosing information.

```
m1.Doses
```

```
ans =
   SimBiology Dose Array

   Index:    Name:        Type:
   1         Oral dose    schedule
   2         IV Dose      schedule
```

Retrieve the `TimeUnits` and `AmountUnits` properties of the first dose (Oral).

```
propValues = get(m1.Doses(1),{'TimeUnits','AmountUnits'})
```

```
propValues = 1x2 cell
    {'hour'}    {'milligram'}
```

Retrieve the properties of both the Oral and IV doses.

```
propValues = get(m1.Doses,{'TimeUnits','AmountUnits'})

propValues = 2x2 cell
    {'hour'}    {'milligram'}
    {'hour'}    {'milligram'}
```

Input Arguments

`sobj` — Object

SimBiology object | array of SimBiology objects

Object, specified as a SimBiology object or array of SimBiology objects.

`propertyNames` — Names of object properties

character vector | string | string vector | cell array of character vectors

Names of the object properties, specified as a character vector, string, string vector, or cell array of character vectors.

Example: `{'Name','Type'}`

Output Arguments

`S` — Object property data

structure | structure array

Object property data, returned as a structure or structure array containing a field for each property of the object in `sobj`.

`propertyValues` — Property values

property value | cell array

Property values, returned as a property value or cell array of property values. If `propertyNames` is a cell array, `propertyValues` is an *m*-by-*n* cell array, where *m* is the number of objects in `sobj` and *n* is the number of names in `propertyNames`.

Version History

Introduced in R2008b

See Also

`set` | `SimData`

getadjacencymatrix (model)

Get adjacency matrix from model object

Note The order of species in the output arguments (`M` and `Headings`) matches the order of species returned by `modelObj.Species`.

Syntax

```
M = getadjacencymatrix(modelObj)
[M, Headings] = getadjacencymatrix(modelObj)
[M, Headings, Mask] = getadjacencymatrix(modelObj)
```

Arguments

`M`	Adjacency matrix for `modelObj`.
`modelObj`	Specify the `model object`.
`Headings`	Return row and column headings. If species are in multiple compartments, species names are qualified with the compartment name in the form `compartmentName.speciesName`. For example, `nucleus.DNA`, `cytoplasm.mRNA`.
`Mask`	Return `1` for the species object and `0` for the reaction object to `Mask`.

Description

`M = getadjacencymatrix(modelObj)` returns an adjacency matrix (`M`) for the model object (`modelObj`).

An adjacency matrix is defined by listing all species contained by `modelObj` and all reactions contained by `modelObj` column-wise and row-wise in a matrix. The reactants of the reactions are represented in the matrix with a 1 at the location of [row of species, column of reaction]. The products of the reactions are represented in the matrix with a 1 at the location of [row of reaction, column of species]. All other locations in the matrix are 0.

`[M, Headings] = getadjacencymatrix(modelObj)` returns the adjacency matrix to `M` and the row and column headings to `Headings`. `Headings` is defined by listing all `Name` property values of species contained by `modelObj` and all `Name` property values of reactions contained by `modelObj`.

`[M, Headings, Mask] = getadjacencymatrix(modelObj)` returns an array of 1s and 0s to `Mask`, where a 1 represents a species object and a 0 represents a reaction object.

Examples

1 Read in`m1`, a model object, using `sbmlimport`:

```
m1 = sbmlimport('lotka.xml');
```

2 Get the adjacency matrix for `m1`:

```
[M, Headings] = getadjacencymatrix(m1)
```

See Also

`getstoichmatrix`, `model object`

Version History

Introduced in R2006a

R2019b: The function returns species in a new order
Behavior changed in R2019b

The order of species in the output arguments (`M` and `Headings`) matches the order of species returned by `modelObj.Species`.

getComponents

Get model components associated with SimBiology model comparison results

Syntax

```
tbl = getComponents(diffResults)
tbl = getComponents(diffResults,rowIdx)
```

Description

`tbl = getComponents(diffResults)` returns a table of model components associated with the comparison results `diffResults`, a `SimBiology.DiffResults` object. Specifically, the function returns the model components listed in the `diffResults.Comparisons` table.

`tbl = getComponents(diffResults,rowIdx)` specifies a vector of row indices `rowIdx` to return the model components associated with the requested rows from the `diffResults.Comparisons` table.

Examples

Compare SimBiology Models

Load a source model.

```
model1      = sbmlimport("lotka");
y1          = sbioselect(model1, "Type", "species", "Name", "y1");
y1.Value    = 880;
```

Load a target model to compare against the source model.

```
model2      = sbmlimport("lotka");
y1          = sbioselect(model2, "Type", "species", "Name", "y1");
y1.Value    = 920;
```

Compare the models using `sbiodiff` and display the comparison table.

```
diffResults = sbiodiff(model1,model2);
diffTable   = diffResults.Comparisons
```

```
diffTable=1×6 table
          Class      Source    Target    Property    SourceValue    TargetValue
        _________    ______    ______    ________    ___________    ___________

    1    "Species"     "y1"      "y1"     "Value"       {[880]}        {[920]}
```

You can also view the comparison results graphically in the Comparison tool.

```
visdiff(diffResults);
```

Get a table of model components associated with the changes reported in the comparison table.

```
tbl = getComponents(diffResults)

tbl=1×2 table
                  Source                          Target
          ____________________________    ____________________________

    1     {1x1 SimBiology.Species}        {1x1 SimBiology.Species}
```

Input Arguments

`diffResults` — Model comparison results

`SimBiology.DiffResults` object

Model comparison results, specified as a `SimBiology.DiffResults` object. Use `sbiodiff` to generate this object.

`rowIdx` — Row indices for `diffResults.Comparisons` table

`1:height(diffResults.Comparisons)` (default) | vector of positive integers

Row indices for the `diffResults.Comparisons` table, specified as a vector of positive integers.

Example: `[2 5 10]`

Data Types: `double`

Output Arguments

`tbl` — Model components from comparison results

table

Model components from the comparison results, returned as a table.

The table has two columns *Source* and *Target*. Each column is a cell array and contains the model components that were changed between the source and target models. If a component was inserted or deleted, then the value of the corresponding entry in the *Source* or *Target* column is `<missing>`. Changes made to the components in this table do not affect the components reported in the `diffResults.Comparisons` table.

Version History

Introduced in R2022a

See Also

`sbiodiff` | `SimBiology.DiffResults` | `visdiff`

Topics

“Compare SimBiology Models”
“SimBiology Model Matching Policy”

getconfigset (model)

Get configuration set object from model object

Syntax

```
configsetObj = getconfigset(modelObj, 'NameValue')
configsetObj = getconfigset(modelObj)
configsetObj = getconfigset(modelObj,'active')
```

Arguments

modelObj	`Model object`. Enter a variable name for a model object.
NameValue	Name of the `configset` object.
configsetObj	Object holding the simulation-specific information.

Description

configsetObj = `getconfigset(`*modelObj*`, '`*NameValue*`')` returns the configuration set attached to `modelObj` that is named *NameValue*, to *configsetObj*.

configsetObj = `getconfigset(`*modelObj*`)` returns a vector of all attached configuration sets, to *configsetObj*.

configsetObj = `getconfigset(`*modelObj*`,'active')` retrieves the active configuration set.

A configuration set object stores simulation-specific information. A SimBiology model can contain multiple `configsets` with one being active at any given time. The active configuration set contains the settings that are used during the simulation.

Use the `setactiveconfigset` function to define the active `configset`. *modelObj* always contains at least one `configset` object with the name configured to `'default'`. Additional `configset` objects can be added to *modelObj* with the method `addconfigset`.

Examples

1 Retrieve the default `configset` object from the `modelObj`.

```
modelObj  = sbiomodel('cell');
configsetObj = getconfigset(modelObj)

   Configuration Settings - default (active)
     SolverType:                  ode15s
     StopTime:                    10

   SolverOptions:
     AbsoluteTolerance:           1.000000e-06
     RelativeTolerance:           1.000000e-03
     SensitivityAnalysis:         false
```

```
  RuntimeOptions:
    StatesToLog:                all

  CompileOptions:
    UnitConversion:             false
    DimensionalAnalysis:        true

  SensitivityAnalysisOptions:
    Inputs:                     0
    Outputs:                    0
```

2 Configure the `SolverType` to `ssa`.

```
set(configsetObj, 'SolverType', 'ssa')
get(configsetObj)
```

```
                        Active: 1
                 CompileOptions: [1x1 SimBiology.CompileOptions]
                           Name: 'default'
                          Notes: ''
                 RuntimeOptions: [1x1 SimBiology.RuntimeOptions]
     SensitivityAnalysisOptions: [1x1 SimBiology.SensitivityAnalysisOptions]
                  SolverOptions: [1x1 SimBiology.SSASolverOptions]
                     SolverType: 'ssa'
                       StopTime: 10
           MaximumNumberOfLogs: Inf
              MaximumWallClock: Inf
                     TimeUnits: 'second'
                          Type: 'configset'
```

See Also

`model object`, `addconfigset`, `removeconfigset`, `setactiveconfigset`

Version History

Introduced in R2006a

getCovariateData

Create design matrix needed for fit

Syntax

```
CovData = getCovariateData(PKDataObj)
```

Description

`CovData = getCovariateData(PKDataObj)` creates `CovData`, a dataset (Statistics and Machine Learning Toolbox) array containing only the covariate data from the data set in `PKDataObj`, a `PKData` object. `CovData` contains one row for each individual and one column for each covariate.

Use this function to view the covariate data when writing equations for the "Expression" on page 2-0 property of a `CovariateModel` object.

Input Arguments

`PKDataObj` — Data used for fitting

`PKData` object

Data used for fitting, specified as a `PKData` object.

Output Arguments

`CovData` — Covariate data

`dataset`

Covariate data, returned as a `dataset`.

Version History

Introduced in R2011b

See Also

`CovariateModel` | `PKData` on page 2-491

Topics

"Model the Population Pharmacokinetics of Phenobarbital in Neonates"
"Specify a Covariate Model"

getdata

Get simulation data from `SimData` object

Syntax

```
[t,x,names] = getdata(simdata)
sdOut = getdata(simdata)
___ = getdata(simdata,format)
```

Description

`[t,x,names] = getdata(simdata)` returns the simulation time points `t`, the simulation data `x`, and corresponding `names` for the data columns.

`sdOut = getdata(simdata)` returns the simulation results as a `SimData` object `sdOut`.

`___ = getdata(simdata,format)` returns the simulation data in the specified `format`.

Examples

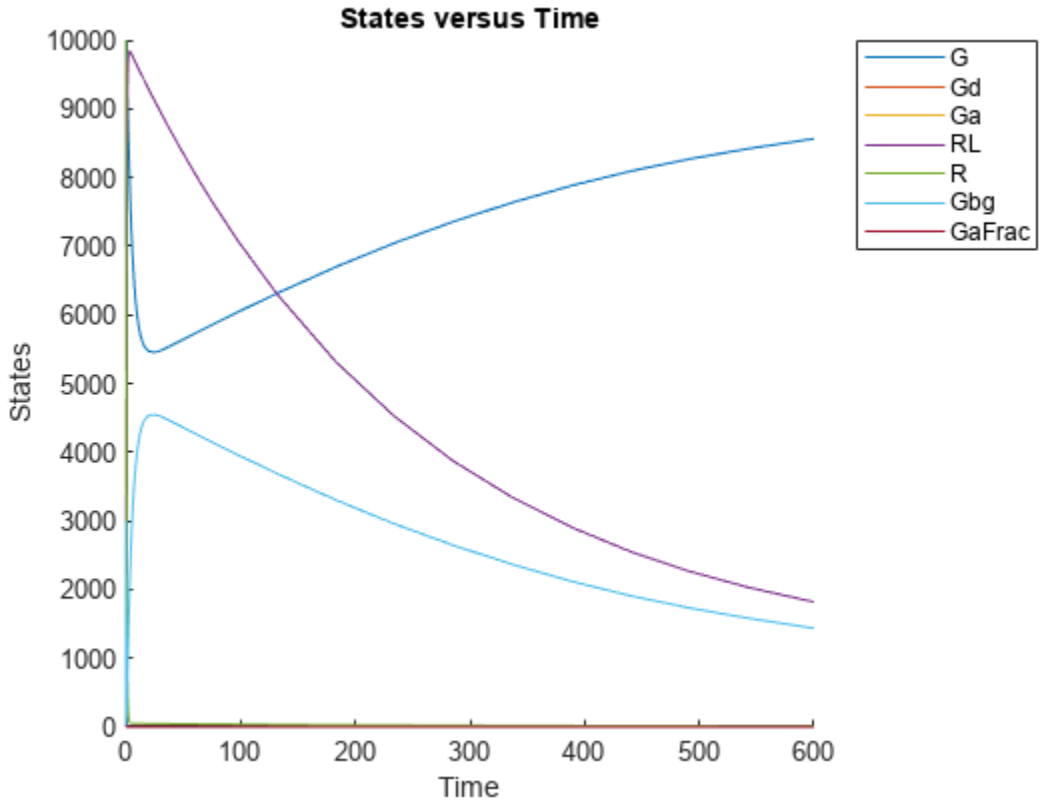
Extract Data from SimData Object

Load the G-protein model.

```
sbioloadproject('gprotein.sbproj');
```

Simulate the model.

```
sdObj = sbiosimulate(m1);
sbioplot(sdObj);
```



The plot shows all the states together. Plot each state separately on its own axes in a subplot.

First, extract the simulation data from the `SimData` object.

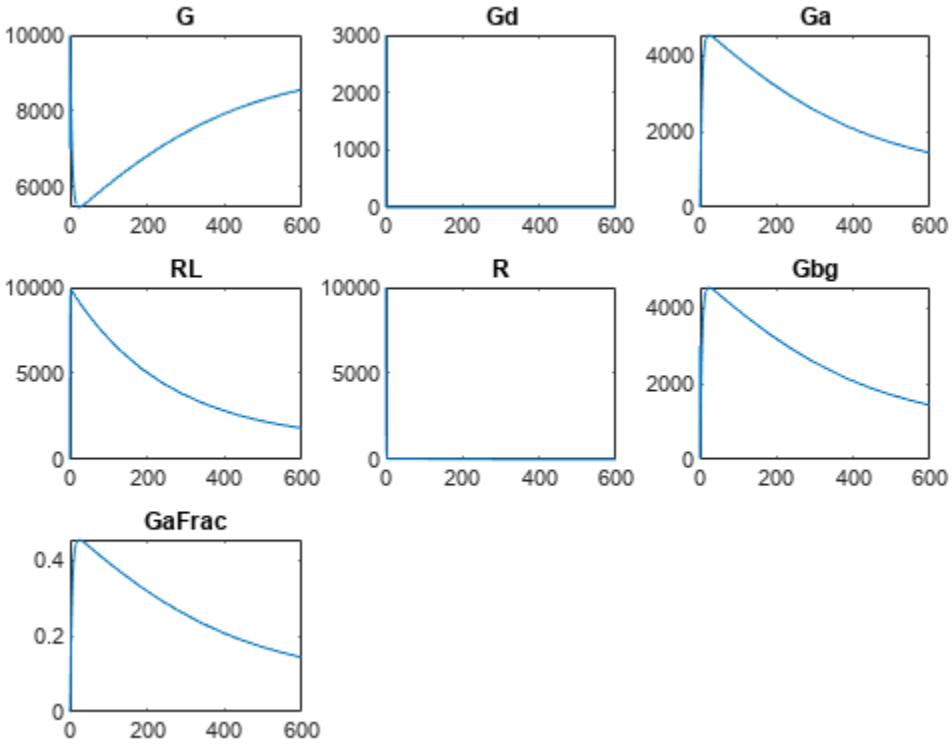
```
[time,data,names] = getdata(sdObj);
```

Calculate the number of rows and columns needed for the subplot.

```
sqrtnames = sqrt(numel(names));
nrows = round(sqrtnames);
ncolumns = ceil(sqrtnames);
```

Create a subplot and plot each state on its own axes.

```
figure
for(i = 1:numel(names))
    subplot(nrows,ncolumns,i)
    plot(time,data(:,i));
    title(names(i));
end
```



Input Arguments

`simdata` — Simulation data

`SimData` object | array of `SimData` objects

Simulation data, specified as a `SimData` object or array of `SimData` objects.

`format` — Simulation data format

character vector | string

Simulation data format, specified as a character vector or string. Some formats require you to specify only one output argument. The valid formats follow.

- `'num'` — This format returns simulation time points and simulation data in numeric arrays and the names of quantities and sensitivities as a cell array. This format is the default when you run `getdata` with multiple output arguments.
- `'nummetadata'` — This format returns a cell array of metadata structures instead of the names of quantities and sensitivities as the third output argument.
- `'numqualnames'` — This format returns qualified names in the third output argument to resolve ambiguities.

You must specify only one output argument for the following formats.

- `'simdata'` — This format returns data in a new `SimData` object or an array of `SimData` objects. This format is the default when you specify a single output argument.
- `'struct'` — This format returns a structure or structure array that contains both data and metadata.
- `'ts'` — This format returns data as a cell array.
  - If `simdata` is scalar, the cell array is an *m*-by-1 array, where each element is a `timeseries` object. *m* is the number of quantities and sensitivities logged during the simulation.
  - If `simdata` is not scalar, the cell array is *k*-by-1, where each element of the cell array is an *m*-by-1 cell array of `timeseries` objects. *k* is the size of `simdata`, and *m* is the number of quantities or sensitivities in each `SimData` object in `simdata`. In other words, the function returns an individual time series for each state or column and for each `SimData` object in `simdata`.
- `'tslumped'` — This format returns the data as a cell array of `timeseries` objects, combining data from each `SimData` object into a single time series.

Output Arguments

`t` — Simulation time points
numeric vector | cell array

Simulation time points, returned as a numeric vector or cell array. If `simdata` is scalar, `t` is an *n*-by-1 vector, where *n* is the number of time points. If `simdata` is an array of objects, `t` is a *k*-by-1 cell array, where *k* is the size of `simdata`.

`x` — Simulation data
numeric matrix | cell array

Simulation data, returned as a numeric matrix or cell array. If `simdata` is scalar, `x` is an *n*-by-*m* matrix, where *n* is the number of time points and *m* is the number of quantities and sensitivities logged during the simulation. If `simdata` is an array of objects, `x` is a *k*-by-1 cell array, where *k* is the size of `simdata`.

`names` — Names of quantities and sensitivities
cell array

Names of quantities and sensitivities logged during the simulation, returned as a cell array. If `simdata` is scalar, `names` is an *m*-by-1 cell array. If `simdata` is an array of objects, `names` is a *k*-by-1 cell array, where *k* is the size of `simdata`.

`sdOut` — Simulation results
`SimData` object

Simulation results, returned as a `SimData` object.

Version History

Introduced in R2008b

See Also

get | set | SimData

getdose

Return exported SimBiology model dose object

Syntax

```
doses = getdose(model)
doses = getdose(model,doseName)
```

Description

`doses = getdose(model)` returns all the `SimBiology.export.Dose` objects associated with the exported model.

`doses = getdose(model,doseName)` returns the export dose object with the `Name` property matching `doseName`.

Examples

Retrieve SimBiology Model Dose Objects

Open a sample SimBiology model project, and export the included model object.

```
sbioloadproject('AntibacterialPKPD')
em = export(m1);
```

Display the editable doses in the exported model object.

```
doses = getdose(em)
```

```
doses =

  1x4 RepeatDose array with properties:

    Interval
    RepeatCount
    StartTime
    TimeUnits
    Amount
    AmountUnits
    DurationParameterName
    LagParameterName
    Name
    Notes
    Parent
    Rate
    RateUnits
    TargetName
```

The exported model has 4 repeated dose objects. Display the dose names.

```
{doses.Name}
```

```
ans =

    '250 mg bid'    '250 mg tid'    '500 mg bid'    '500 mg tid'
```

Extract only the 3rd dose object from the exported model object.

```
dose3 = getdose(em,'500 mg bid')
```

```
dose3 =

  RepeatDose with properties:

                Interval: 12
             RepeatCount: 27
               StartTime: 0
               TimeUnits: 'hour'
                  Amount: 500
             AmountUnits: 'milligram'
   DurationParameterName: 'TDose'
        LagParameterName: ''
                    Name: '500 mg bid'
                   Notes: ''
                  Parent: 'Antibacterial'
                    Rate: 0
               RateUnits: ''
              TargetName: 'Central.Drug'
```

Input Arguments

`model` — Input model

`SimBiology.export.Model` object

Input model, specified as a `SimBiology.export.Model` object.

`doseName` — Dose name

character vector | string scalar

Dose name, specified as a character vector or string scalar. The `doseName` input must contain a name to match against the `Name` property of the export dose objects in `model`. If you do not specify `doseName`, then `getdose` returns all dose objects.

Output Arguments

`doses` — Output doses

export dose objects

Output doses, returned as export dose objects in `model`, or the export dose object with `Name` property `doseName`.

Version History

Introduced in R2012b

See Also

`SimBiology.export.Model` | `SimBiology.export.Dose` | `export`

Topics

“Perform PK/PD Modeling and Simulation to Guide Dosing Strategy for Antibiotics”
“Deploy a SimBiology Exported Model”

getdose (model)

Return SimBiology dose object

Syntax

```
doseObj = getdose(modelObj)
doseObj = getdose(modelObj, 'DoseName')
```

Arguments

modelObj	Selects a `model object` that contains a dose object.
DoseName	Name of a dose object contained in a model object. *DoseName* is from the dose object property, `Name`.

Outputs

doseObj	`ScheduleDose` or `RepeatDose` object retrieved from a model object. A `RepeatDose` or `ScheduleDose` object defines an increase (dose) to a species amount during a simulation.

Description

doseObj = `getdose(`*modelObj*`)` returns a Simbiology dose object (*doseObj*) contained in a Simbiology model object (*modelObj*).

doseObj = `getdose(`*modelObj*`, '`*DoseName*`')` returns a SimBiology dose object (*modelObj*) with the name *DoseName*.

Examples

Get a dose object from a model object.

1. Create a model object, and then add a dose object to the model object.

```
modelObj = sbiomodel('mymodel');
dose1Obj = adddose(modelObj, 'dose1');
```

2. Get the `dose` object from a model object.

```
myModelDose = getdose(modelObj);
```

See Also

`Model` methods:

- `adddose` — add a dose object to a model object
- `getdose` — get dose information from a model object

- `removedose` — remove a dose object from a model object

Dose object constructor `sbiodose`.

`ScheduleDose object` and `RepeatDose object` methods:

- `copyobj` — copy a dose object from one model object to another model object
- `get` — view properties for a dose object
- `set` — define or modify properties for a dose object

Version History

Introduced in R2012b

getEntry

Get entry contents from `SimBiology.Scenarios` object

Syntax

```
entryStruct = getEntry(sObj,entryNameOrIndex)
entryStruct = getEntry(sObj,entryIndex,subIndex)
```

Description

`entryStruct = getEntry(sObj,entryNameOrIndex)` returns a structure containing the contents of the entry (or subentry on page 2-799) specified by `entryNameOrIndex`.

`entryStruct = getEntry(sObj,entryIndex,subIndex)` returns a structure containing the contents of a subentry specified by `entryIndex` and `subIndex`.

Examples

Generate Different Simulation Scenarios for Glucose-Insulin Response

Load the model of glucose-insulin response. For details about the model, see the **Background** section in “Simulate the Glucose-Insulin Response”.

```
sbioloadproject('insulindemo','m1');
```

The model contains different parameter values and initial conditions that represents different insulin impairments (such as Type 2 diabetes, low insulin sensitivity, and so on) stored in five variants.

```
variants = getvariant(m1)
```

```
variants =
   SimBiology Variant Array

   Index:  Name:             Active:
   1       Type 2 diabetic   false
   2       Low insulin se... false
   3       High beta cell... false
   4       Low beta cell ... false
   5       High insulin s... false
```

Suppress an informational warning that is issued during simulations.

```
warnSettings = warning('off','SimBiology:DimAnalysisNotDone_MatlabFcn_Dimensionless');
```

Select a dose that represents a single meal of 78 grams of glucose.

```
singleMeal = sbioselect(m1,'Name','Single Meal');
```

Create a `Scenarios` object to represent different initial conditions combined with the dose. That is, create a `scenario` object where each variant is paired (or combined) with the dose, for a total of five simulation scenarios.

```
sObj = SimBiology.Scenarios;
add(sObj,'cartesian','variants',variants);
add(sObj,'cartesian','dose',singleMeal)
```

```
ans =
  Scenarios (5 scenarios)

                  Name            Content          Number
                ________    ____________________    ______

    Entry 1     variants    SimBiology variants      5
    x Entry 2   dose        SimBiology dose          1

  See also Expression property.
```

`sObj` contains two entries. Use the `generate` function to combine the entries and generate five scenarios. The function returns a scenarios table, where each row represents a scenario and each column represents an entry of the `Scenarios` object.

```
scenariosTbl = generate(sObj)
```

```
scenariosTbl=5×2 table
           variants                    dose
    ___________________________    ____________________________

    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
```

Change the entry name of the first entry.

```
rename(sObj,1,'Insulin Impairements')
```

```
ans =
  Scenarios (5 scenarios)

                       Name                Content          Number
                ____________________    ____________________    ______

    Entry 1     Insulin Impairements    SimBiology variants      5
    x Entry 2   dose                    SimBiology dose          1

  See also Expression property.
```

Create a `SimFunction` object to simulate the generated scenarios. Use the `Scenarios` object as the input and specify the plasma glucose and insulin concentrations as reponses (outputs of the function to be plotted). Specify `[]` for the dose input argument since the `Scenarios` object already has the dosing information.

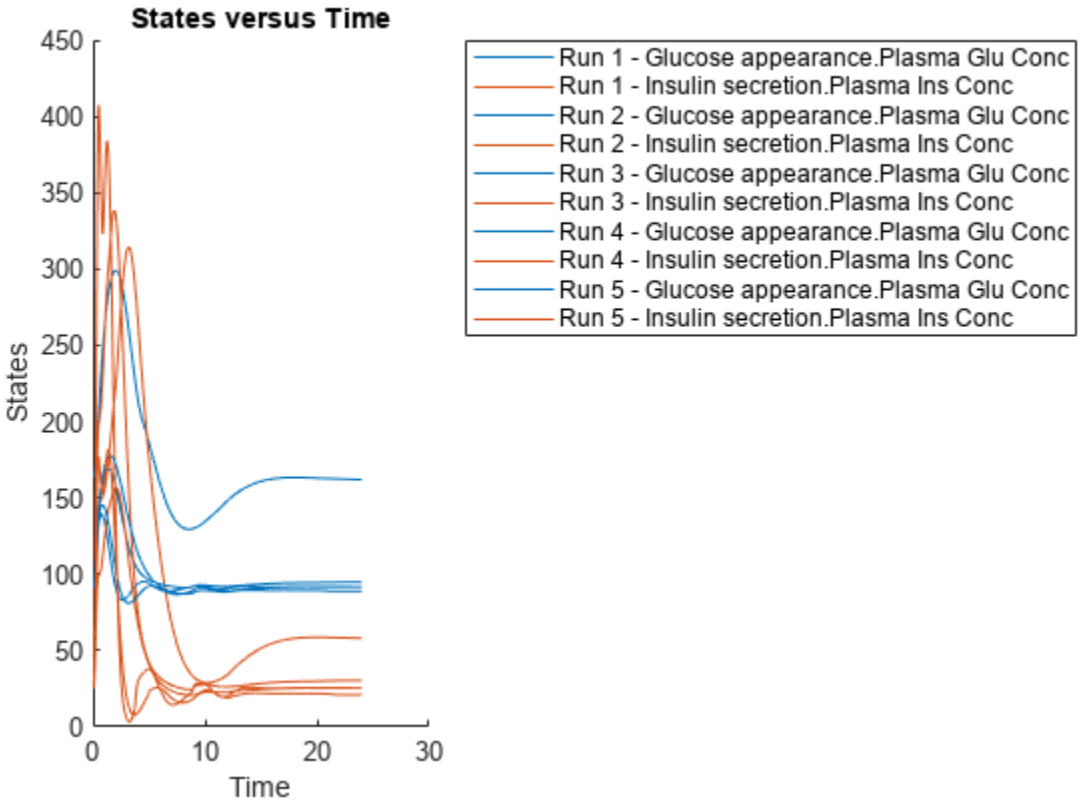
```
f = createSimFunction(m1,sObj,{'[Plasma Glu Conc]','[Plasma Ins Conc]'},[])
```

```
f =
SimFunction

Parameters:

              Name               Value        Type                        Units
    _____________________________    ______    _____________    ____________________________________

    {'Plasma Volume (Glu)'  }      1.88    {'parameter'}    {'deciliter'
    {'k1'                   }     0.065    {'parameter'}    {'1/minute'
    {'k2'                   }     0.079    {'parameter'}    {'1/minute'
    {'Plasma Volume (Ins)'  }      0.05    {'parameter'}    {'liter'
    {'m1'                   }      0.19    {'parameter'}    {'1/minute'
    {'m2'                   }     0.484    {'parameter'}    {'1/minute'
    {'m4'                   }    0.1936    {'parameter'}    {'1/minute'
    {'m5'                   }    0.0304    {'parameter'}    {'minute/picomole'
    {'m6'                   }    0.6469    {'parameter'}    {'dimensionless'
    {'Hepatic Extraction'   }       0.6    {'parameter'}    {'dimensionless'
    {'kmax'                 }    0.0558    {'parameter'}    {'1/minute'
    {'kmin'                 }     0.008    {'parameter'}    {'1/minute'
    {'kabs'                 }    0.0568    {'parameter'}    {'1/minute'
    {'kgri'                 }         0    {'parameter'}    {'1/minute'
    {'f'                    }       0.9    {'parameter'}    {'dimensionless'
    {'a'                    }         0    {'parameter'}    {'1/milligram'
    {'b'                    }      0.82    {'parameter'}    {'dimensionless'
    {'c'                    }         0    {'parameter'}    {'1/milligram'
    {'d'                    }      0.01    {'parameter'}    {'dimensionless'
    {'kp1'                  }       2.7    {'parameter'}    {'milligram/minute'
    {'kp2'                  }    0.0021    {'parameter'}    {'1/minute'
    {'kp3'                  }     0.009    {'parameter'}    {'(milligram/minute)/(picomole/liter)
    {'kp4'                  }    0.0618    {'parameter'}    {'(milligram/minute)/picomole'
    {'ki'                   }    0.0079    {'parameter'}    {'1/minute'
    {'[Ins Ind Glu Util]'   }         1    {'parameter'}    {'milligram/minute'
    {'Vm0'                  }    2.5129    {'parameter'}    {'milligram/minute'
    {'Vmx'                  }     0.047    {'parameter'}    {'(milligram/minute)/(picomole/liter)
    {'Km'                   }    225.59    {'parameter'}    {'milligram'
    {'p2U'                  }    0.0331    {'parameter'}    {'1/minute'
    {'K'                    }      2.28    {'parameter'}    {'picomole/(milligram/deciliter)'
    {'alpha'                }      0.05    {'parameter'}    {'1/minute'
    {'beta'                 }      0.11    {'parameter'}    {'(picomole/minute)/(milligram/decili
    {'gamma'                }       0.5    {'parameter'}    {'1/minute'
    {'ke1'                  }    0.0005    {'parameter'}    {'1/minute'
    {'ke2'                  }       339    {'parameter'}    {'milligram'
    {'Basal Plasma Glu Conc'}     91.76    {'parameter'}    {'milligram/deciliter'
    {'Basal Plasma Ins Conc'}     25.49    {'parameter'}    {'picomole/liter'

Observables:

          Name              Type              Units
    ____________________    __________    ____________________

    {'[Plasma Glu Conc]'}    {'species'}    {'milligram/deciliter'}
    {'[Plasma Ins Conc]'}    {'species'}    {'picomole/liter'     }

Dosed:

    TargetName       TargetDimension
    __________    ____________________
```

```
    {'Dose'}    {'Mass (e.g., gram)'}

TimeUnits: hour
```

Simulate the model for 24 hours and plot the simulation data. The data contains five runs, where each run represents a scenario in the Scenarios object.

```
sd = f(sObj,24);
sbioplot(sd)
```




```
ans =
  Axes (SbioPlot) with properties:

            XLim: [0 30]
            YLim: [0 450]
          XScale: 'linear'
          YScale: 'linear'
    GridLineStyle: '-'
         Position: [0.0920 0.1100 0.2956 0.8150]
            Units: 'normalized'

  Show all properties
```

If you have Statistics and Machine Learning Toolbox™, you can also draw sample values for model quantities from various probability distributions. For instance, suppose that the parameters `Vmx` and

kp3, which are known for the low and high insulin sensitivity, follow the lognormal distribution. You can generate sample values for these parameters from such a distribution, and perform a scan to explore model behavior.

Define the lognormal probability distribution object for Vmx.

```
pd_Vmx = makedist('lognormal')
```

```
pd_Vmx =
  LognormalDistribution

  Lognormal distribution
       mu = 0
    sigma = 1
```

By definition, the parameter mu is the mean of logarithmic values. To vary the parameter value around the base (model) value of the parameter, set mu to log(*model_value*). Set the standard deviation (*sigma*) to 0.2. For a small *sigma* value, the mean of a lognormal distribtion is approximately equal to log(*model_value*). For details, see “Lognormal Distribution” (Statistics and Machine Learning Toolbox).

```
Vmx = sbioselect(m1,'Name','Vmx');
pd_Vmx.mu = log(Vmx.Value);
pd_Vmx.sigma = 0.2
```

```
pd_Vmx =
  LognormalDistribution

  Lognormal distribution
       mu = -3.05761
    sigma =      0.2
```

Similarly define the probability distribution for kp3.

```
pd_kp3 = makedist('lognormal');
kp3 = sbioselect(m1,'Name','kp3');
pd_kp3.mu = log(kp3.Value);
pd_kp3.sigma = 0.2
```

```
pd_kp3 =
  LognormalDistribution

  Lognormal distribution
       mu = -4.71053
    sigma =      0.2
```

Now define a joint probability distribution to draw sample values for Vmx and kp3, with a rank correlation to specify some correlation between these two parameters. Note that this correlation assumption is for the illustration purposes of this example only and may not be biologically relevant.

First remove the variants entry (entry 1) from sObj.

```
remove(sObj,1)
```

```
ans =
  Scenarios (1 scenarios)
```

```
                Name        Content        Number
                ____    _______________    ______

    Entry 1     dose    SimBiology dose      1

  See also Expression property.
```

Add an entry that defines the joint probability distribution with a rank correlation matrix.

```
add(sObj,'cartesian',["Vmx","kp3"],[pd_Vmx, pd_kp3],'RankCorrelation',[1,0.5;0.5,1])
```

```
ans =
  Scenarios (2 scenarios)

                    Name           Content              Number
                    ____    ________________________    ___________

    Entry 1         dose    SimBiology dose             1
    x (Entry 2.1    Vmx     Lognormal distribution      2 (default)
    + Entry 2.2)    kp3     Lognormal distribution      2 (default)

  See also Expression property.
```

By default, the number of samples to draw from the joint distribution is set to 2. Increase the number of samples.

```
updateEntry(sObj,2,'Number',50)
```

```
ans =
  Scenarios (50 scenarios)

                    Name           Content             Number
                    ____    ________________________    ______

    Entry 1         dose    SimBiology dose               1
    x (Entry 2.1    Vmx     Lognormal distribution       50
    + Entry 2.2)    kp3     Lognormal distribution       50

  See also Expression property.
```

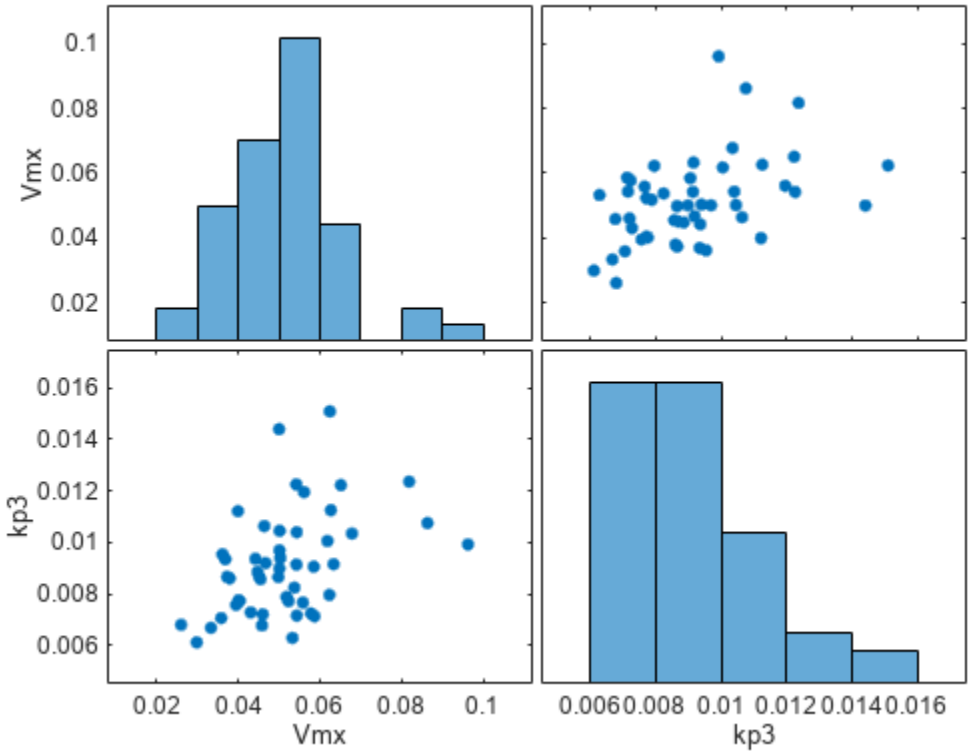
Verify that the `Scenarios` object can be simulated with the model. The `verify` function throws an error if any entry does not resolve uniquely to an object in the model or the entry contents have inconsistent lengths (sample sizes). The function throws a warning if multiple entries resolve to the same object in the model.

```
verify(sObj,m1)
```

Generate the simulation scenarios. Plot the sample values using `plotmatrix`. You can see the value of `Vmx` is varied around its model value 0.047 and that of `kp3` around 0.009.

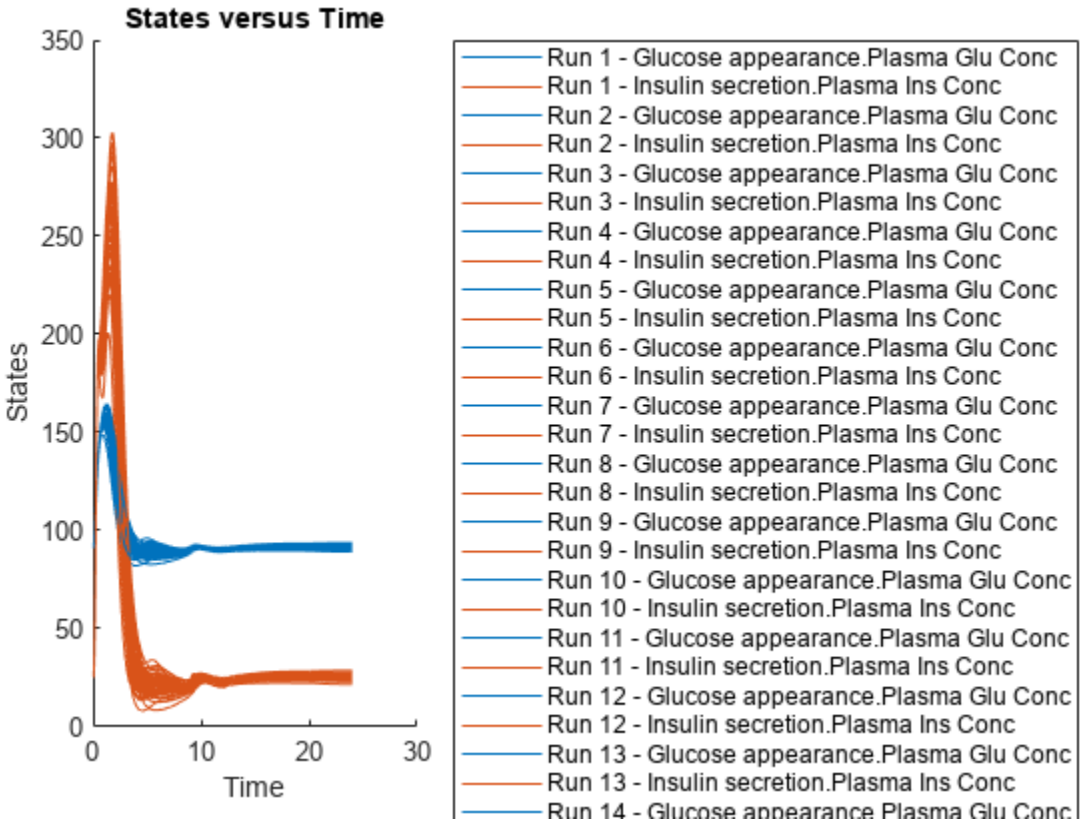
```
sTbl = generate(sObj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl.Vmx,sTbl.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
```

```
ax(2,1).XLabel.String = "Vmx";
ax(2,2).XLabel.String = "kp3";
```



Simulate the scenarios using the same SimFunction you created previously. You do not need to create a new SimFunction object even though the Scenarios object has been updated.

```
sd2 = f(sObj,24);
sbioplot(sd2);
```



By default, SimBiology uses the random sampling method. You can change it to the Latin hypercube sampling (or sobol or halton) for a more systematic space-filling approach.

```
entry2struct = getEntry(sObj,2)
```

```
entry2struct = struct with fields:
                Name: {'Vmx'  'kp3'}
             Content: [2x1 prob.LognormalDistribution]
              Number: 50
    RankCorrelation: [2x2 double]
          Covariance: []
      SamplingMethod: 'random'
    SamplingOptions: [0x0 struct]
```

```
entry2struct.SamplingMethod = 'lhs'
```

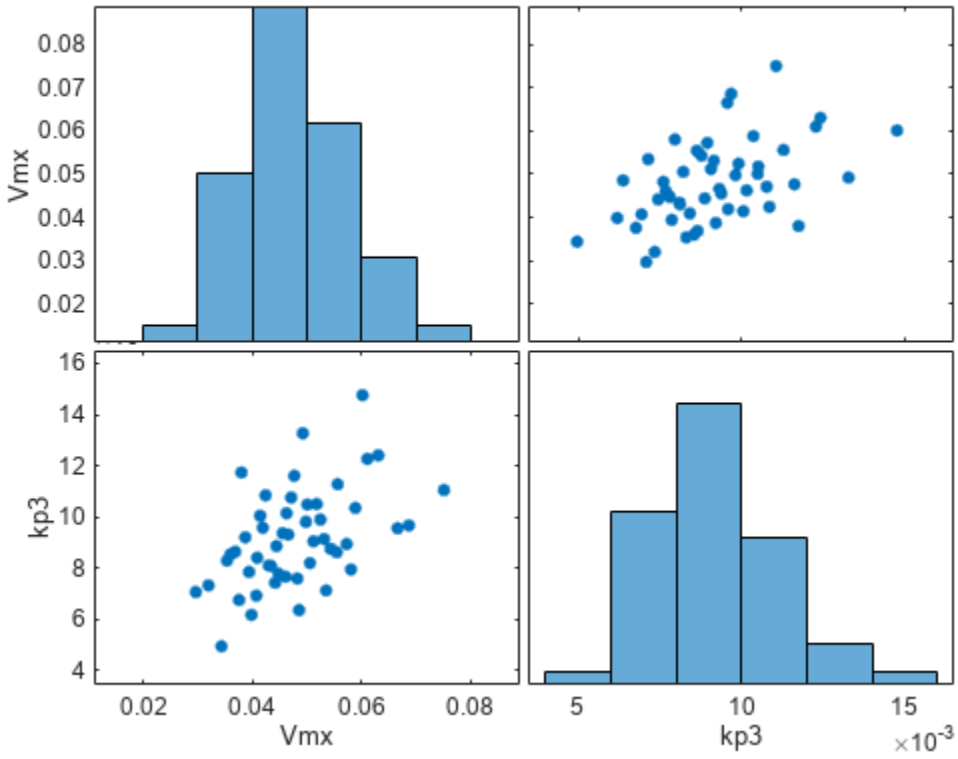
```
entry2struct = struct with fields:
                Name: {'Vmx'  'kp3'}
             Content: [2x1 prob.LognormalDistribution]
              Number: 50
    RankCorrelation: [2x2 double]
          Covariance: []
      SamplingMethod: 'lhs'
    SamplingOptions: [0x0 struct]
```

You can now use the updated structure to modify entry 2.

```
updateEntry(sObj,2,entry2struct)

ans =
  Scenarios (50 scenarios)

                    Name           Content             Number
                    ____    ____________________      ______

    Entry 1         dose    SimBiology dose             1
    x (Entry 2.1    Vmx     Lognormal distribution      50
    + Entry 2.2)    kp3     Lognormal distribution      50

  See also Expression property.
```

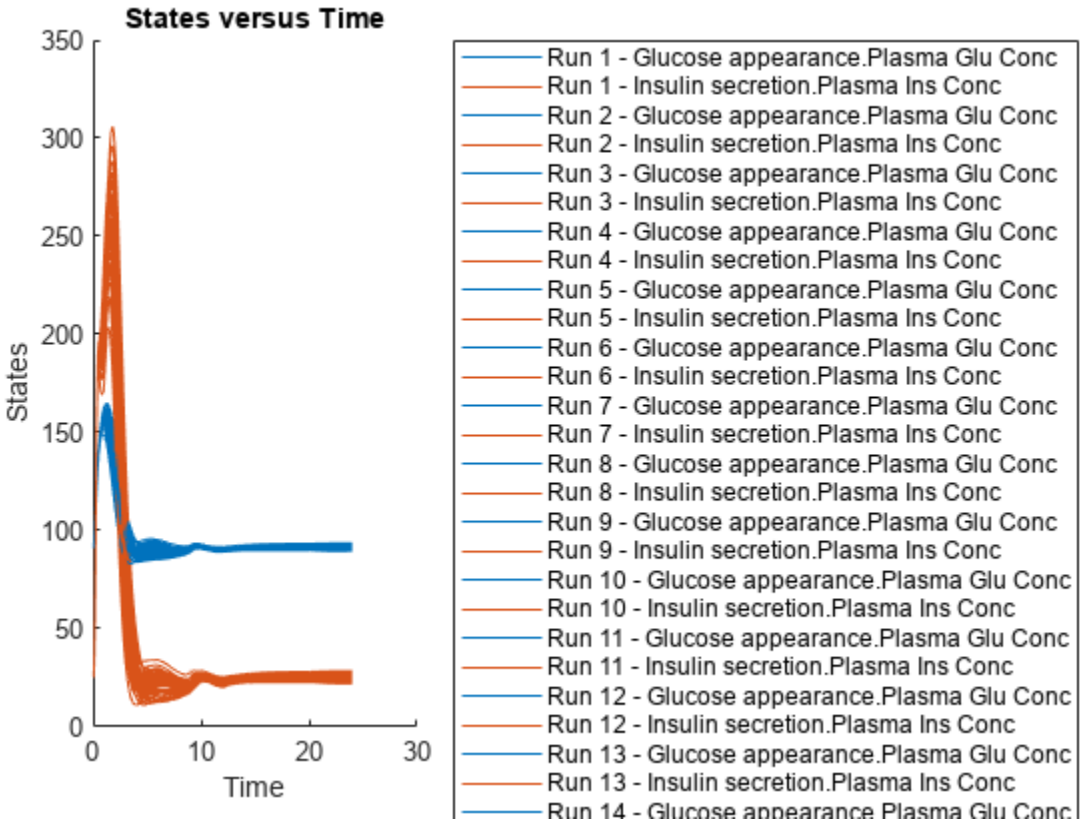
Visualize the sample values.

```
sTbl2 = generate(sObj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl2.Vmx,sTbl2.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
ax(2,1).XLabel.String = "Vmx";
ax(2,2).XLabel.String = "kp3";
```



Simulate the scenarios.

```
sd3 = f(sObj,24);
sbioplot(sd3);
```



Restore warning settings.

```
warning(warnSettings);
```

Input Arguments

`sObj` — Simulation scenarios

`SimBiology.Scenarios` object

Simulation scenarios, specified as a `SimBiology.Scenarios` object.

`entryNameOrIndex` — Entry name or index

character vector | string | scalar positive integer

Entry name or index, specified as a character vector, string, or scalar positive integer. You can also specify the name of a subentry.

If you are specifying an index, it must be smaller than or equal to the number of entries in the object.

Data Types: `double` | `char` | `string`

`entryIndex` — Entry index

scalar positive integer

Entry index, specified as a scalar positive integer. The entry index must be smaller than or equal to the number of entries in the object.

Data Types: `double`

`subIndex` — Entry subindex
scalar positive integer

Entry subindex, specified as a scalar positive integer. The subindex must be smaller than or equal to the number of subentries in the entry.

Data Types: `double`

Output Arguments

`entryStruct` — Entry content
structure

Entry content, returned as a structure.

`entryStruct` has the following fields:

- `Name` – Character vector or cell array of character vectors specifying the names of entries.
- `Content` – Vector of numeric values, dose objects, variant objects, or probability distribution objects.

If you query a random sampling entry without specifying a subentry, or if the random sampling entry references only one model component, `entryStruct` has the following additional fields:

- `Number` – Number of samples drawn from the distribution. If this field is empty `[]`, the number of samples is inferred from other entries. The default value is 2.
- `RankCorrelation` – Rank correlation matrix. This field is empty `[]` if no correlation matrix is specified.
- `Covariance` – Covariance matrix. This field is empty `[]` if no covariance matrix is specified.
- `SamplingMethod` – Character vector specifying the sampling method. Values are:
  - `'random'` – Random sampling (default).
  - `'lhs'` – Latin hypercube sampling.
  - `'copula'` – Multivariate sample using a copula.
  - `'sobol'` – Sobol quasirandom sample set.
  - `'halton'` – Halton quasirandom sample set.

  For details, see Sampling Methods on page 2-0 .

Version History

Introduced in R2019b

See Also

`SimBiology.Scenarios` | `SimFunction object` | `createSimFunction (model)`

Topics

“SimBiology.Scenarios Terminology” on page 2-799

“Combine Simulation Scenarios in SimBiology”

getequations

Return system of equations for model object

Syntax

```
equations = getequations(modelobj)
equations = getequations(modelobj,configsetobj,variantobj,doseobj)
```

Description

`equations = getequations(modelobj)` returns `equations`, a character vector containing the system of equations that represent `modelobj`, a `model object`. The function uses any active configset, active variants, and active doses, if any, and generates the system of equations. You must specify a deterministic solver.

`equations = getequations(modelobj,configsetobj,variantobj,doseobj)` returns the system of equations that represent the model specified by a `Model` object, `Variant` objects, and dose objects (`RepeatDose` or `ScheduleDose`). The function uses only the specified configset, doses, and variants to generate the equations. Any other configset, doses, and variants are ignored. You must specify a deterministic solver.

If you set `csObj` to `[]`, then the function uses the active configset object.

If you set `variantObj` to `[]`, then the function uses no variants.

If you set `doseObj` to `[]`, then the function uses no doses.

Input Arguments

`modelobj`

Object of the `Model` on page 2-439 class.

Note If using `modelobj` as the only input argument, the active `Configset` object must specify a deterministic solver.

Default:

`configsetobj`

Object of the `Configset` on page 2-170 class. This object must specify a deterministic solver.

Default: `[]` (Empty, which specifies the active `Configset` object for `modelobj`)

`variantobj`

Object or array of objects of the `Variant` on page 2-913 class.

Default: `[]` (Empty, which specifies no variant object)

`doseobj`

Object or array of objects of the `RepeatDose` on page 2-747 or `ScheduleDose` on page 2-802 class.

Default: `[]` (Empty, which specifies no dose object)

Output Arguments

`equations`

Character vector containing the system of equations that represent a model. Equations for reactions, rules, events, variants, and doses are included.

Examples

View System of Equations for Simple Model

View system of equations that represent a simple model, containing only reactions.

Import the lotka model, included with SimBiology, into a variable named `model1`:

```
model1 = sbmlimport('lotka');
```

View all equations that represent the `model1` model and its active configset:

```
m1equations = getequations(model1)
```

```
m1equations =

ODEs:
d(y1)/dt = 1/unnamed*(ReactionFlux1 - ReactionFlux2)
d(y2)/dt = 1/unnamed*(ReactionFlux2 - ReactionFlux3)
d(z)/dt = 1/unnamed*(ReactionFlux3)

Fluxes:
ReactionFlux1 = c1*y1*x
ReactionFlux2 = c2*y1*y2
ReactionFlux3 = c3*y2

Parameter Values:
c1 = 10
c2 = 0.01
c3 = 10
unnamed = 1

Initial Conditions:
x = 1
y1 = 900
y2 = 900
z = 0
```

MATLAB displays the ODEs, fluxes, parameter values, and initial conditions for the reactions in `model1`.

View System of Equations for Model and Dose

View system of equations that represent a model, containing only reactions, and a repeated dose.

Import the lotka model, included with SimBiology, into a variable named `model1`:

```
model1 = sbmlimport('lotka');
```

Add a repeated dose to the model:

```
doseObj1 =  adddose(model1,'dose1','repeat');
```

Set the properties of the dose to administer 3 mg, at a rate of 10 mg/hour, 6 times, at an interval of every 24 hours, to species `y1`:

```
doseObj1.Amount = 0.003;
doseObj1.AmountUnits = 'gram';
doseObj1.Rate = 0.010;
doseObj1.RateUnits = 'gram/hour';
doseObj1.Repeat = 6;
doseObj1.Interval = 24;
doseObj1.TimeUnits = 'hour';
doseObj1.TargetName = 'y1';
```

View all equations that represent the `model1` model, its active configset, and the repeated dose:

```
m1_with_dose_equations = getequations (model1,[],[],doseObj1)
```

```
m1_with_dose_equations =

ODEs:
d(y1)/dt = 1/unnamed*(ReactionFlux1 - ReactionFlux2) + dose1
d(y2)/dt = 1/unnamed*(ReactionFlux2 - ReactionFlux3)
d(z)/dt = 1/unnamed*(ReactionFlux3)

Fluxes:
ReactionFlux1 = c1*y1*x
ReactionFlux2 = c2*y1*y2
ReactionFlux3 = c3*y2

Parameter Values:
c1 = 10
c2 = 0.01
c3 = 10
unnamed = 1

Initial Conditions:
y1 = 900
y2 = 900
z = 0
x = 1

Doses:
Variable                    Type                Units
dose1                       repeatdose          gram
```

MATLAB displays the ODEs, fluxes, parameter values, and initial conditions for the reactions and the dose in `model1`.

Tips

Use `getequations` to see the system of equations that represent a model for:

- Publishing purposes
- Model debugging

See Also

`Model object` | `Configset object` | `Variant object` | `RepeatDose object` | `ScheduleDose object`

Topics

“Show Model Equations and Initial Conditions”

getIndex

Get indices into `ValueInfo` and `InitialValues` properties

Syntax

```
indices = getIndex(model,name)
indices = getIndex(model,name,type)
```

Description

`indices = getIndex(model,name)` returns the indices of all `ValueInfo` objects in a `SimBiology.export.Model` object that have a `QualifiedName` or `Name` property that match the specified `name` input argument.

- `getIndex` first tries to match the `QualifiedName` property. If there are matches, then `getIndex` returns their indices.
- If there are no matches based on `QualifiedName`, then `getIndex` tries to match the `Name` property. If there are matches, then `getIndex` returns their indices.
- If there are no matches based on `QualifiedName` or `Name`, then `getIndex` returns `[]`.

`indices = getIndex(model,name,type)` returns indices for only the `ValueInfo` objects with a `Type` property that matches the `type` input argument.

Examples

Index Exported SimBiology Editable Values

Load a sample SimBiology model object, and export.

```
modelObj = sbmlimport('lotka');
em = export(modelObj);
```

Get the index of the editable value with name `y1`.

```
ix = getIndex(em,'y1')
```

```
ix =

     3
```

Display the type of value.

```
em.ValueInfo(ix).Type
```

```
ans =

species
```

The name `y1` corresponds to an editable species.

Input Arguments

`model` — Input model

`SimBiology.export.Model` object

Input model, specified as a `SimBiology.export.Model` object.

`name` — Name of species, compartment, or parameter

character vector | string scalar

Name of a species, compartment, or parameter, specified as a character vector or string scalar. The `name` input must contain a name to match against the `QualifiedName`, then `Name` properties of the `ValueInfo` objects in `model`.

`type` — Type of value

`"species"` | `"compartment"` | `"parameter"`

Type of value, specified as `"species"`, `"compartment"`, or `"parameter"`, to match against the `Type` property of the `ValueInfo` objects in `model`. If you do not specify `type`, then `getIndex` returns the indices for all three types.

Output Arguments

`indices` — Matching indices

vector of integers

Matching indices, returned as a vector of integers indicating which `ValueInfo` objects in a `SimBiology.export.Model` object match on the specified `name` and `type`.

Version History

Introduced in R2012b

See Also

`SimBiology.export.Model` | `SimBiology.export.ValueInfo` | `export`

Topics

“Perform PK/PD Modeling and Simulation to Guide Dosing Strategy for Antibiotics”
“Deploy a SimBiology Exported Model”

getNumberScenarios

Return number of scenarios from `SimBiology.Scenarios` object

Syntax

```
numScenarios = getNumberScenarios(sObj)
```

Description

`numScenarios = getNumberScenarios(sObj)` returns the number of scenarios from the `SimBiology.Scenarios` object `sObj`.

Examples

Get Number of Simulation Scenarios

Create a SimBiology.Scenarios object for a parameter (k1) with sample values of 1.3 and 1.4.

```
sObj = SimBiology.Scenarios('k1',[1.3;1.4]);
```

Add a species (s1) with initial sample amounts of 2.7, 3.1, and 3.4. Use the cartesian combination method to combine entries.

```
add(sObj,'cartesian','s1',[2.7; 3.1; 3.4]);
```

Get the number of simulation sceanarios that the object has after combining the entries.

```
n = getNumberScenarios(sObj)
```

```
n = 6
```

Input Arguments

`sObj` — Simulation scenarios

`SimBiology.Scenarios` object

Simulation scenarios, specified as a `SimBiology.Scenarios` object.

Output Arguments

`numScenarios` — Number of scenarios

nonnegative integer

Total number of scenarios, returned as a nonnegative integer.

Version History

Introduced in R2019b

See Also

`SimBiology.Scenarios` | `SimFunction object` | `createSimFunction (model)`

Topics

“SimBiology.Scenarios Terminology” on page 2-799
“Combine Simulation Scenarios in SimBiology”

getparameters (kineticlaw)

Get specific parameters in kinetic law object

Syntax

```
parameterObj = getparameters(kineticlawObj)
parameterObj = getparameters(kineticlawObj, ParameterVariablesValue)
```

Arguments

kineticlawObj	Retrieve parameters used by the kinetic law object.
ParameterVariablesValue	Retrieve parameters used by the kinetic law object corresponding to the specified parameter in the `ParameterVariables` property of the kinetic law object. Specify a character vector, string scalar, string vector, or cell array of character vectors.

Description

parameterObj = `getparameters(`*kineticlawObj*`)` returns the parameters used by the kinetic law object `kineticlawObj` to `parameterObj`.

parameterObj = `getparameters(`*kineticlawObj*`, `*ParameterVariablesValue*`)` returns the parameter in the `ParameterVariableNames` property that corresponds to the parameter specified in the `ParameterVariables` property of `kineticlawObj`, to `parameterObj`. `ParameterVariablesValue` is the name of the parameter as it appears in the `ParameterVariables` property of `kineticlawObj`. `ParameterVariablesValue` can be a character vector, string scalar, string vector, or cell array of character vectors.

If you change the name of a parameter, you must configure all applicable elements such as rules that use the parameter, any user-specified `ReactionRate`, or the kinetic law object property `ParameterVariableNames`. Use the method `setparameter` to configure `ParameterVariableNames`.

Examples

Create a model, add a reaction, and assign the `ParameterVariableNames` for the reaction rate equation.

1. Create the model object, and then add a reaction object.

   ```
   modelObj = sbiomodel('my_model');
   reactionObj = addreaction(modelObj, 'a -> c + d');
   ```

2. Create a kinetic law object for the reaction object, of the type `'Henri-Michaelis-Menten'`.

   ```
   kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
   ```

3. Add two parameter objects.

```
parameterObj1 = addparameter(kineticlawObj,'Va');
parameterObj2 = addparameter(kineticlawObj,'Ka');
```

4 The `'Henri-Michaelis-Menten'` kinetic law has two parameter variables (`Vm` and `Km`) that should to be set. To set these variables:

```
setparameter(kineticlawObj,'Vm', 'Va');
setparameter(kineticlawObj,'Km', 'Ka');
```

5 To retrieve a parameter variable:

```
parameterObj3 = getparameters(kineticlawObj, 'Vm')
```

MATLAB returns:

```
SimBiology Parameter Array

Index:    Name:    Value:    ValueUnits:
  1         Va       1

parameterObj4 = getparameters (kineticlawObj, 'Km')
```

See Also

`addparameter`, `getspecies`, `setparameter`

Version History

Introduced in R2006a

getsensmatrix

Get 3-D sensitivity matrix from `SimData` object

Syntax

```
[t,r,outputFactors,inputFactors] = getsensmatrix(simdata)
[t,r,outputFactors,inputFactors] = getsensmatrix(simdata,outputFactorNames,
inputFactorNames)
```

Description

`[t,r,outputFactors,inputFactors] = getsensmatrix(simdata)` returns the time `t` and sensitivity data `r` as well as all the `outputFactors` and `inputFactors` (sensitivity outputs and inputs) from the `SimData` object `simdata`.

`[t,r,outputFactors,inputFactors] = getsensmatrix(simdata,outputFactorNames, inputFactorNames)` returns the sensitivity data for only the outputs and inputs specified by `outputFactorNames` and `inputFactorNames`, respectively.

Examples

Calculate Local Sensitivities Using SimFunctionSensitivity Object

This example shows how to calculate the local sensitivities of some species in the Lotka-Volterra model using the `SimFunctionSensitivity` object.

Load the sample project.

```
sbioloadproject lotka;
```

Define the input parameters.

```
params = {'Reaction1.c1', 'Reaction2.c2'};
```

Define the observed species, which are the outputs of simulation.

```
observables  = {'y1', 'y2'};
```

Create a `SimFunctionSensitivity` object. Set the sensitivity output factors to all species (`y1` and `y2`) specified in the `observables` argument and input factors to those in the `params` argument (`c1` and `c2`) by setting the name-value pair argument to `'all'`.

```
f = createSimFunction(m1,params,observables,[],'SensitivityOutputs','all','SensitivityInputs','a
```

```
f =
SimFunction

Parameters:

          Name          Value        Type
    ________________    _____    _____________
```

```
    {'Reaction1.c1'}      10     {'parameter'}
    {'Reaction2.c2'}    0.01     {'parameter'}

Observables:

     Name        Type
    ______    ___________

    {'y1'}    {'species'}
    {'y2'}    {'species'}

Dosed: None

Sensitivity Input Factors:

           Name              Type
    _________________    _____________

    {'Reaction1.c1'}    {'parameter'}
    {'Reaction2.c2'}    {'parameter'}

Sensitivity Output Factors:

     Name        Type
    ______    ___________

    {'y1'}    {'species'}
    {'y2'}    {'species'}

Sensitivity Normalization:

Full
```

Calculate sensitivities by executing the object with `c1` and `c2` set to 10 and 0.1, respectively. Set the output times from 1 to 10. `t` contains time points, `y` contains simulation data, and `sensMatrix` is the sensitivity matrix containing sensitivities of `y1` and `y2` with respect to `c1` and `c2`.

```
[t,y,sensMatrix] = f([10,0.1],[],[],1:10);
```

Retrieve the sensitivity information at time point 5.

```
temp = sensMatrix{:};
sensMatrix2 = temp(t{:}==5,:,:);
sensMatrix2 = squeeze(sensMatrix2)

sensMatrix2 = 2×2

   37.6987   -6.8447
  -40.2791    5.8225
```

The rows of `sensMatrix2` represent the output factors (`y1` and `y2`). The columns represent the input factors (`c1` and `c2`).

$$sensMatrix2 = \begin{bmatrix} \frac{\partial y1}{\partial c1} & \frac{\partial y1}{\partial c2} \\ \frac{\partial y2}{\partial c1} & \frac{\partial y2}{\partial c2} \end{bmatrix}$$

Set the stop time to 15, without specifying the output times. In this case, the output times are the solver time points by default.

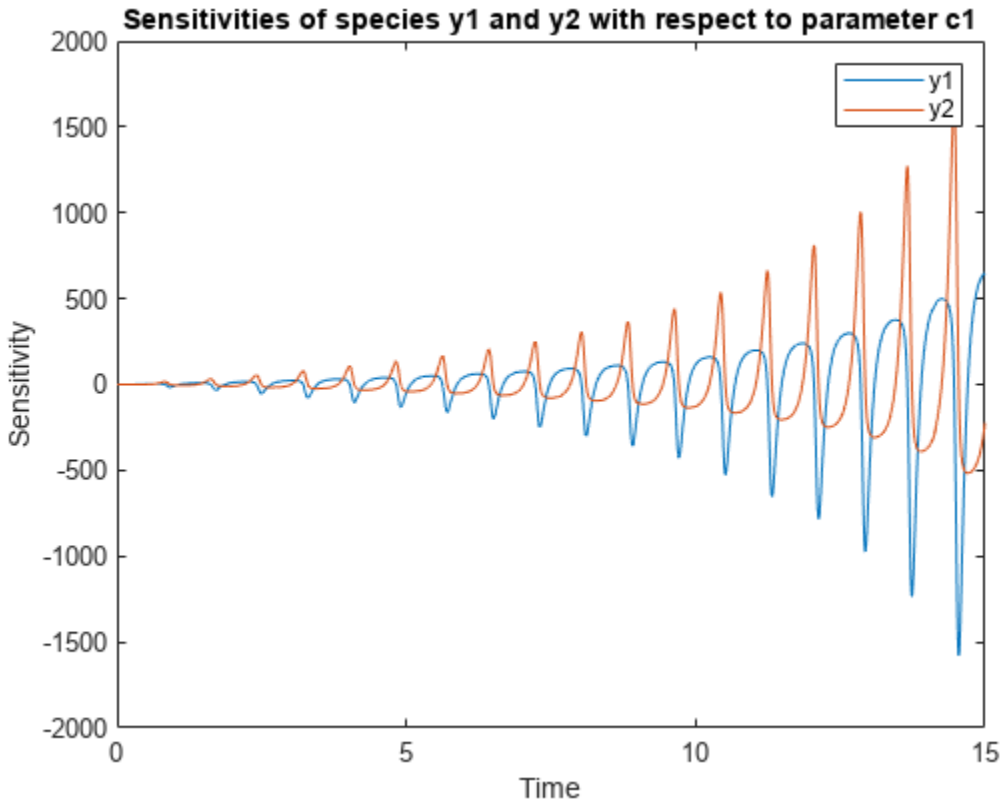
```
sd = f([10,0.1],15);
```

Retrieve the calculated sensitivities from the `SimData` object `sd`.

```
[t,y,outputs,inputs] = getsensmatrix(sd);
```

Plot the sensitivities of species `y1` and `y2` with respect to `c1`.

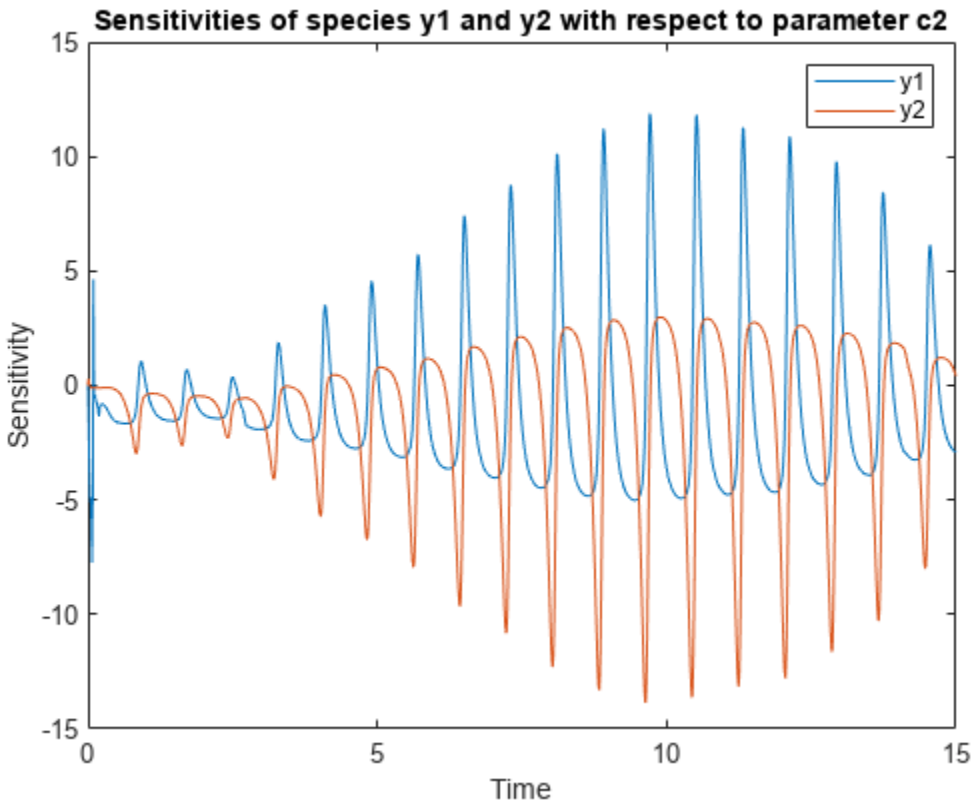
```
figure;
plot(t,y(:,:,1));
legend(outputs);
title('Sensitivities of species y1 and y2 with respect to parameter c1');
xlabel('Time');
ylabel('Sensitivity');
```



Plot the sensitivities of species `y1` and `y2` with respect to `c2`.

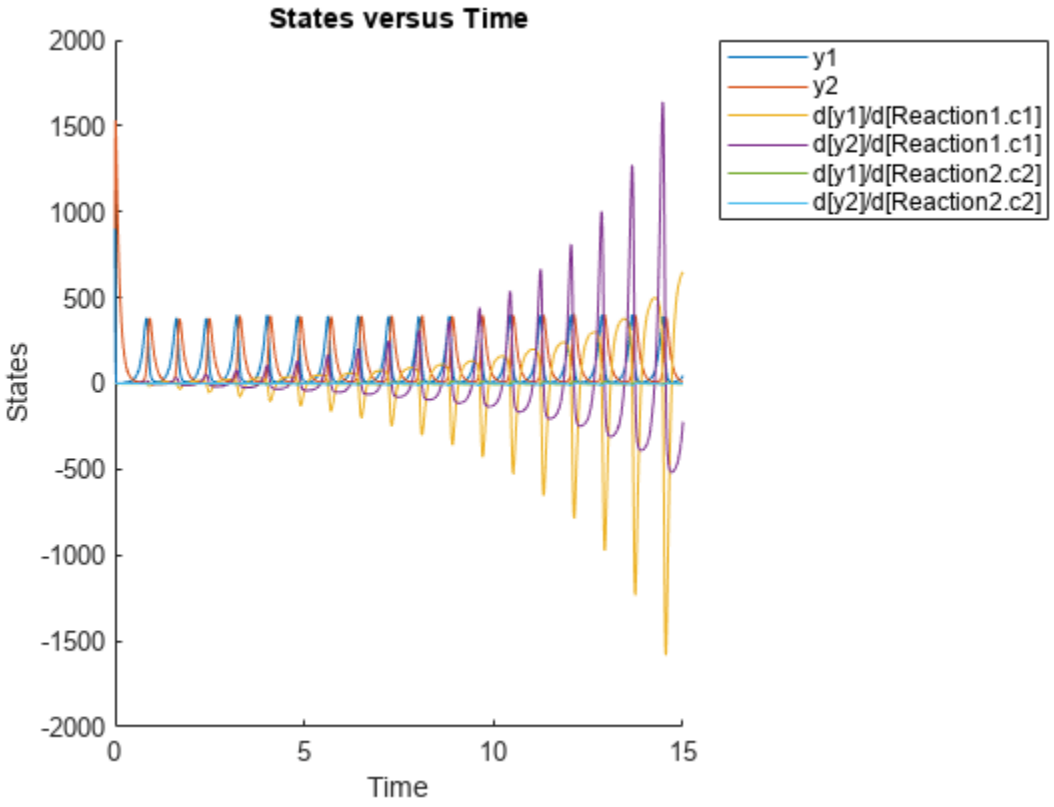
```
figure;
plot(t,y(:,:,2));
```

```
legend(outputs);
title('Sensitivities of species y1 and y2 with respect to parameter c2');
xlabel('Time');
ylabel('Sensitivity');
```



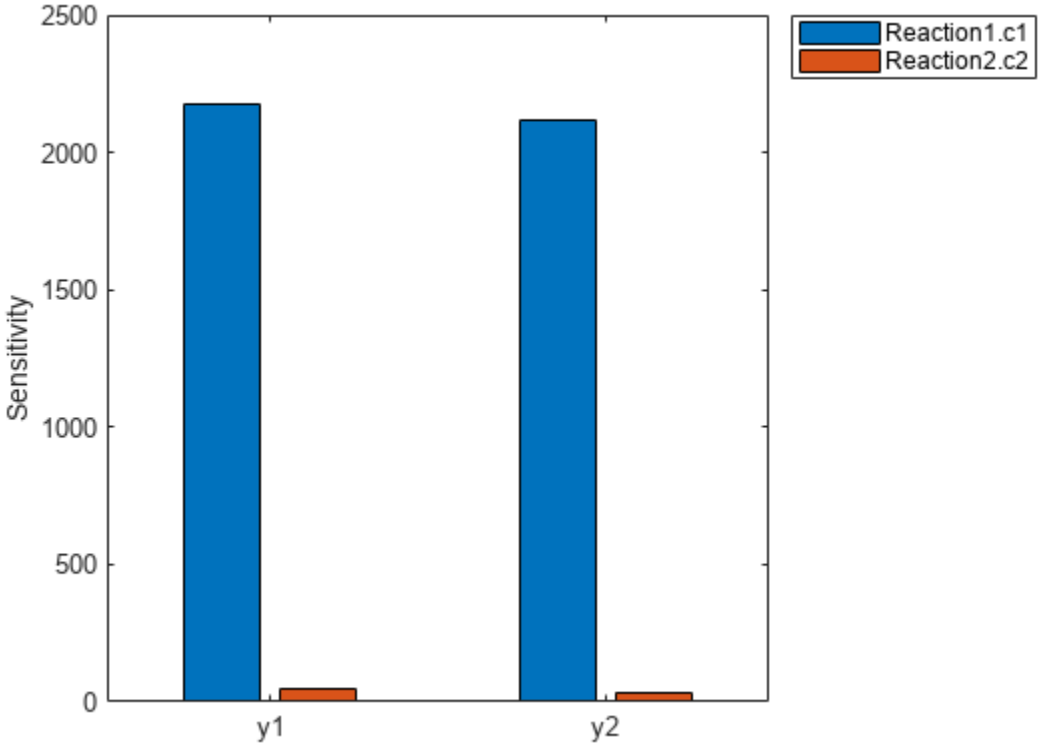
Alternatively, you can use `sbioplot`.

```
sbioplot(sd);
```



You can also plot the sensitivity matrix using the time integral for the calculated sensitivities of `y1` and `y2`. The plot indicates `y1` and `y2` are more sensitive to `c1` than `c2`.

```
[~, in, out] = size(y);
result = zeros(in, out);
for i = 1:in
    for j = 1:out
        result(i,j) = trapz(t(:),abs(y(:,i,j)));
    end
end
figure;
hbar = bar(result);
haxes = hbar(1).Parent;
haxes.XTick = 1:length(outputs);
haxes.XTickLabel = outputs;
legend(inputs,'Location','NorthEastOutside');
ylabel('Sensitivity');
```



Input Arguments

`simdata` — Simulation data

`SimData` object | array of `SimData` objects

Simulation data, specified as a `SimData` object or array of `SimData` objects. If `simdata` is an array of objects, the outputs are cell arrays in which each cell contains data for the corresponding object in the `SimData` array.

`outputFactorNames` — Names of sensitivity outputs

`[]` (default) | character vector | string | string vector | cell array of character vectors

Names of sensitivity outputs, specified as an empty array `[]`, character vector, string, string vector, or cell array of character vectors.

By default, the function uses an empty array `[]` to return sensitivity data for all output factors in `simdata`.

`inputFactorNames` — Names of sensitivity inputs

`[]` (default) | character vector | string | string vector | cell array of character vectors

Names of sensitivity inputs, specified as an empty array `[]`, character vector, string, string vector, or cell array of character vectors.

By default, the function uses an empty array `[]` to return sensitivity data on all input factors in `simdata`.

Output Arguments

`t` — Simulation time points

m-by-1 numeric vector | cell array

Simulation time points for the sensitivity data, returned as an *m*-by-1 numeric vector or cell array. *m* is the number of time points.

`r` — Sensitivity data

m-by-*n*-by-*p* array | cell array

Sensitivity data, returned as an *m*-by-*n*-by-*p* array or cell array. *m* is the number of time points, *n* is the number of sensitivity outputs, and *p* is the number of sensitivity inputs.

The `outputFactors` output argument labels the second dimension of `r` and `inputFactors` labels the third dimension of `r`. For example, `r(:,i,j)` is the time course for the sensitivity of the state `outputFactors{i}` to the input `inputFactor{j}`.

The function returns only the sensitivity data already in the `SimData` object. It does not calculate the sensitivities. For details on setting up and performing a sensitivity calculation, see “Local Sensitivity Analysis (LSA)”. During setup, you can also specify how to normalize the sensitivity data.

`outputFactors` — Names of sensitivity outputs

n-by-1 cell array

Names of sensitivity outputs, returned as an *n*-by-1 cell array. *n* is the number of sensitivity outputs.

The output factors are the states for which you calculated the sensitivities. In other words, the sensitivity outputs are the numerators. For more information, see “Local Sensitivity Analysis (LSA)”.

`inputFactors` — Names of sensitivity inputs

p-by-1 cell array

Names of sensitivity inputs, returned as an *p*-by-1 cell array. *p* is the number of input factors.

The input factors are the states with respect to which you calculated the sensitivities. In other words, the sensivity inputs are the denominators as explained in “Local Sensitivity Analysis (LSA)”.

Version History

Introduced in R2008b

See Also

`SimData` | `sbiosimulate` | `SimFunctionSensitivity object`

Topics

“Local Sensitivity Analysis (LSA)”
“Calculate Local Sensitivities Using sbiosimulate”
“Calculate Local Sensitivities Using SimFunctionSensitivity object”

getSimulationResults

Retrieve model simulation results and sample values used for computing Sobol indices

Syntax

```
[samplesTable,simdata,validRuns] = getSimulationResults(sobolObj,idx)
```

Description

`[samplesTable,simdata,validRuns] = getSimulationResults(sobolObj,idx)` returns the simulation results and sample values in the `SimBiology.gsa.Sobol` object `sobolObj` for the specified index `idx`. The index represents the *i*th column in `sobolObj.SimulationInfo.SimData` on page 2-0 . This function is useful when you want to troubleshoot or find out which parameter samples generated the simulation data that resulted in failed model simulations.

Examples

Perform Global Sensitivity Analysis by Computing First- and Total-Order Sobol Indices

Load the “Tumor Growth Model”.

```
sbioloadproject tumor_growth_vpop_sa.sbproj
```

Get a variant with the estimated parameters and the dose to apply to the model.

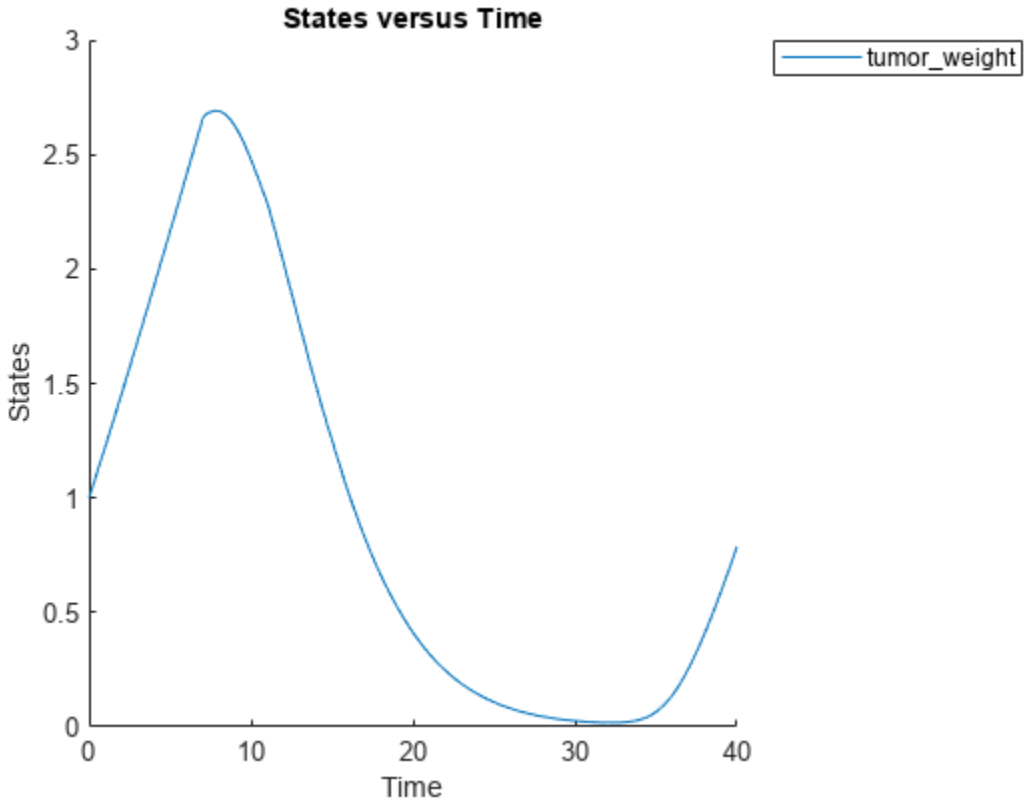
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

Get the active configset and set the tumor weight as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'tumor_weight';
```

Simulate the model and plot the tumor growth profile.

```
sbioplot(sbiosimulate(m1,cs,v,d));
```



Perform global sensitivity analysis (GSA) on the model to find the model parameters that the tumor growth is sensitive to.

First, retrieve model parameters of interest that are involved in the pharmacodynamics of the tumor growth. Define the model response as the tumor weight.

```
modelParamNames = {'L0','L1','w0','k1','k2'};
outputName = 'tumor_weight';
```

Then perform GSA by computing the first- and total-order Sobol indices using `sbiosobol`. Set `'ShowWaitBar'` to `true` to show the simulation progress. By default, the function uses 1000 parameter samples to compute the Sobol indices [1].

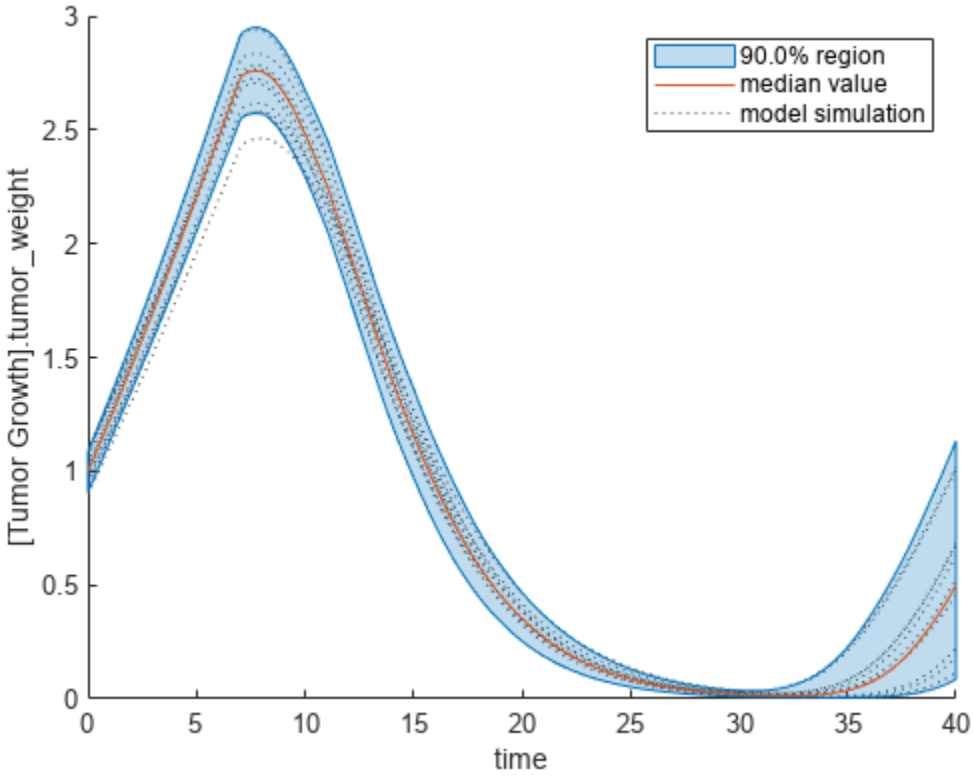
```
rng('default');
sobolResults = sbiosobol(m1,modelParamNames,outputName,Variants=v,Doses=d,ShowWaitBar=true)
```

```
sobolResults =
  Sobol with properties:

                Time: [444x1 double]
        SobolIndices: [5x1 struct]
            Variance: [444x1 table]
    ParameterSamples: [1000x5 table]
         Observables: {'[Tumor Growth].tumor_weight'}
      SimulationInfo: [1x1 struct]
```

You can change the number of samples by specifying the `'NumberSamples'` name-value pair argument. The function requires a total of `(number of input parameters + 2) * NumberSamples` model simulations.

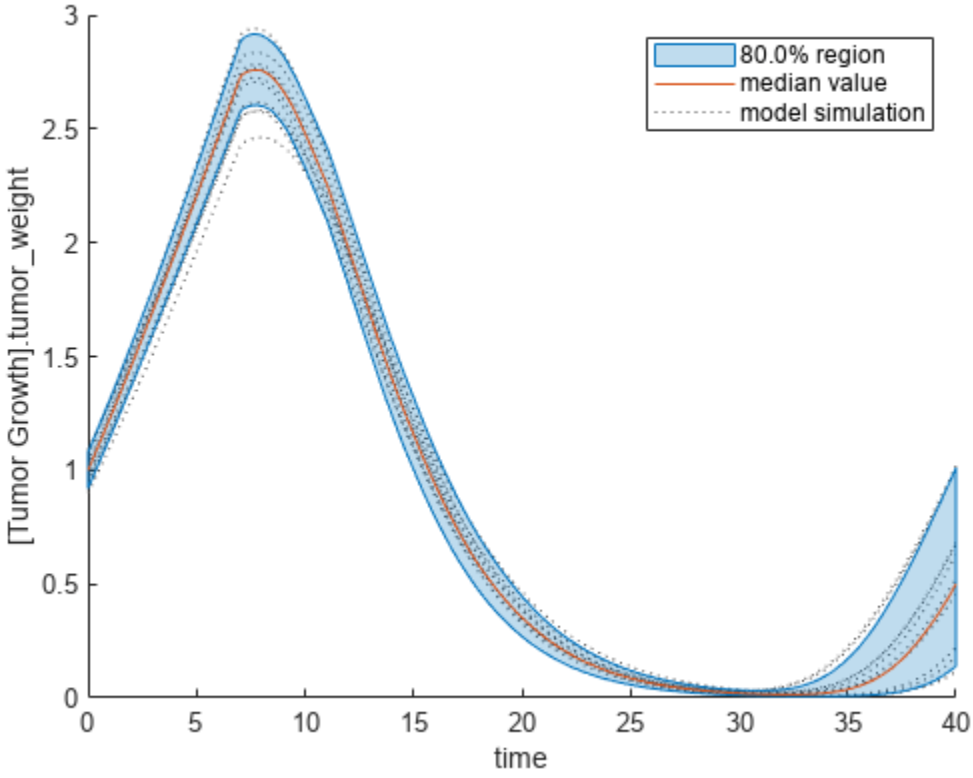
Show the mean model response, the simulation results, and a shaded region covering 90% of the simulation results.

```
plotData(sobolResults,ShowMedian=true,ShowMean=false);
```



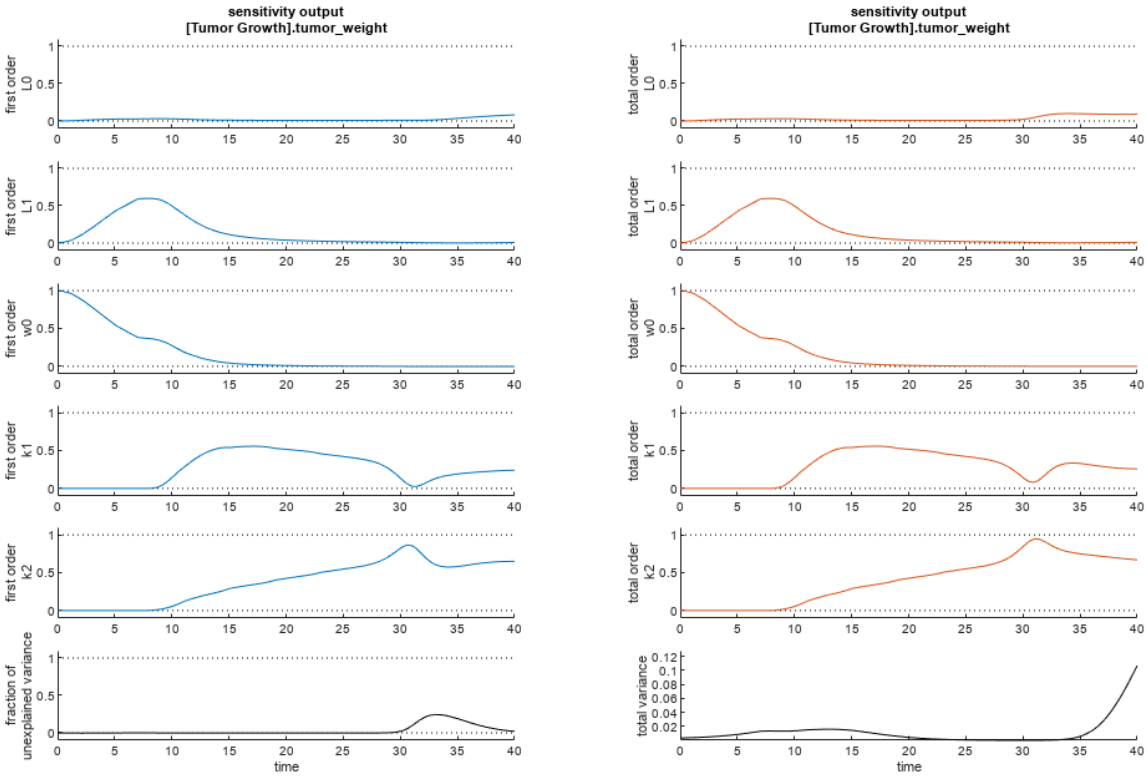
You can adjust the quantile region to a different percentage by specifying `'Alphas'` for the lower and upper quantiles of all model responses. For instance, an alpha value of 0.1 plots a shaded region between the `100 * alpha` and `100 * (1 - alpha)` quantiles of all simulated model responses.

```
plotData(sobolResults,Alphas=0.1,ShowMedian=true,ShowMean=false);
```



Plot the time course of the first- and total-order Sobol indices.

```
h = plot(sobolResults);
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```

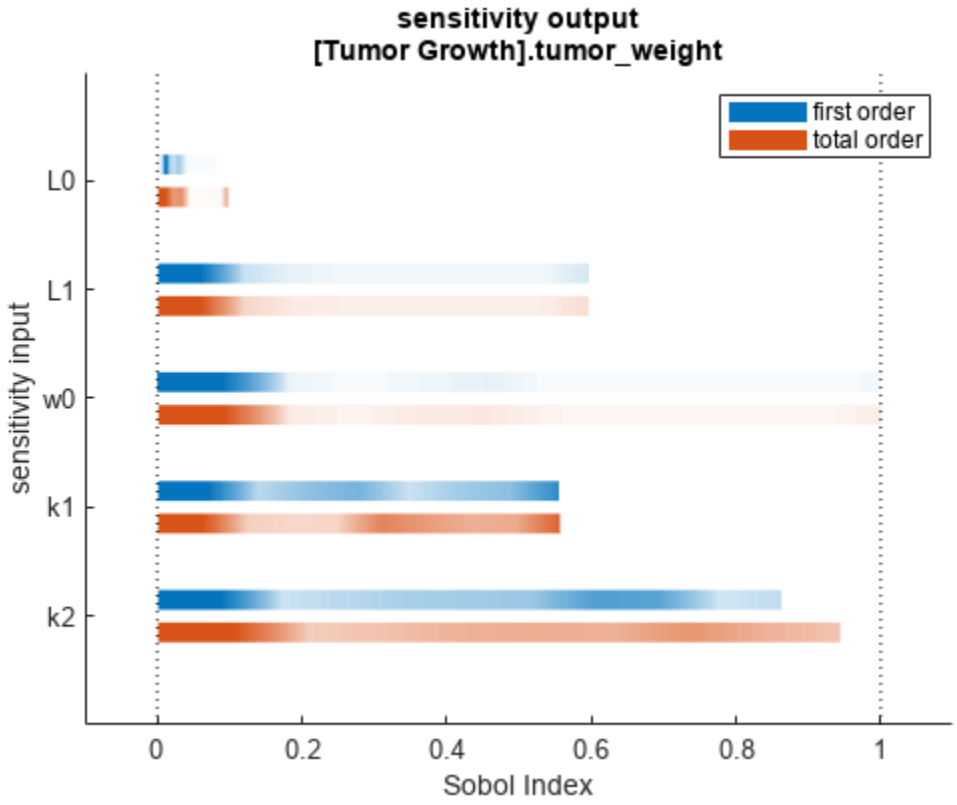


The first-order Sobol index of an input parameter gives the fraction of the overall response variance that can be attributed to variations in the input parameter alone. The total-order index gives the fraction of the overall response variance that can be attributed to any joint parameter variations that include variations of the input parameter.

From the Sobol indices plots, parameters `L1` and `w0` seem to be the most sensitive parameters to the tumor weight before the dose was applied at t = 7. But after the dose is applied, `k1` and `k2` become more sensitive parameters and contribute most to the after-dosing stage of the tumor weight. The total variance plot also shows a larger variance for the after-dose stage at t > 35 than for the before-dose stage of the tumor growth, indicating that `k1` and `k2` might be more important parameters to investigate further. The fraction of unexplained variance shows some variance at around t = 33, but the total variance plot shows little variance at t = 33, meaning the unexplained variance could be insignificant. The fraction of unexplained variance is calculated as 1 - (sum of all the first-order Sobol indices), and the total variance is calculated using `var(response)`, where `response` is the model response at every time point.

You can also display the magnitudes of the sensitivities in a bar plot. Darker colors mean that those values occur more often over the whole time course.

```
bar(sobolResults);
```



You can specify more samples to increase the accuracy of the Sobol indices, but the simulation can take longer to finish. Use `addsamples` to add more samples. For example, if you specify 1500 samples, the function performs `1500 * (2 + number of input parameters)` simulations.

```
gsaMoreSamples = addsamples(gsaResults,1500)
```

The “SimulationInfo” on page 2-0 property of the result object contains various information for computing the Sobol indices. For instance, the model simulation data (SimData) for each simulation using a set of parameter samples is stored in the `SimData` field of the property. This field is an array of `SimData` objects.

```
sobolResults.SimulationInfo.SimData
```

```
SimBiology SimData Array : 1000-by-7

Index:    Name:         ModelName:         DataCount:
1           -           Tumor Growth Model 1
2           -           Tumor Growth Model 1
3           -           Tumor Growth Model 1
...
7000        -           Tumor Growth Model 1
```

You can find out if any model simulation failed during the computation by checking the `ValidSample` field of `SimulationInfo`. In this example, the field shows no failed simulation runs.

```
all(sobolResults.SimulationInfo.ValidSample)
```

```
ans = 1x7 logical array

   1   1   1   1   1   1   1
```

`SimulationInfo.ValidSample` is a table of logical values. It has the same size as `SimulationInfo.SimData`. If `ValidSample` indicates that any simulations failed, you can get more information about those simulation runs and the samples used for those runs by extracting information from the corresponding column of `SimulationInfo.SimData`. Suppose that the fourth column contains one or more failed simulation runs. Get the simulation data and sample values used for that simulation using `getSimulationResults`.

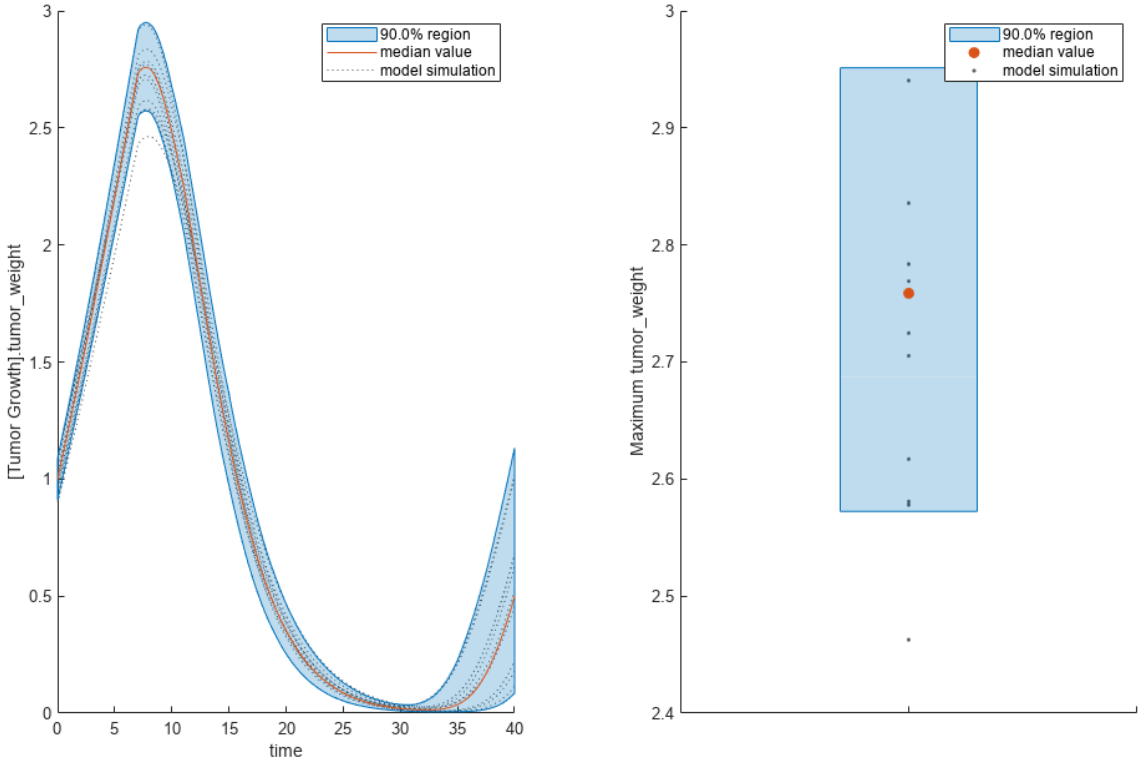
```
[samplesUsed,sd,validruns] = getSimulationResults(sobolResults,4);
```

You can add custom expressions as observables and compute Sobol indices for the added observables. For example, you can compute the Sobol indices for the maximum tumor weight by defining a custom expression as follows.

```
% Suppress an information warning that is issued during simulation.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
% Add the observable expression.
sobolObs = addobservable(sobolResults,'Maximum tumor_weight','max(tumor_weight)','Units','gram');
```

Plot the computed simulation results showing the 90% quantile region.

```
h2 = plotData(sobolObs,ShowMedian=true,ShowMean=false);
h2.Position(:) = [100 100 1280 800];
```



You can also remove the observable by specifying its name.

```
gsaNoObs = removeobservable(sobolObs,'Maximum tumor_weight');
```

Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

`sobolObj` — Results containing Sobol indices

`SimBiology.gsa.Sobol` object

Results containing the first- and total-order Sobol indices, specified as a `SimBiology.gsa.Sobol` object.

`idx` — Index

positive integer

Index to extract the simulation results in `sobolObj.SimulationInfo.SimData` on page 2-0 , specified as a positive integer. The index must be smaller than *“params” on page 1-0 + 2*, where *params* is the number of input parameters. For more information, see “Retrieve Simulation Results and Sample Values Using getSimulationResults” on page 2-402.

Data Types: `double`

Output Arguments

`samplesTable` — Table containing parameter sample values

table

Table containing parameter sample values, returned as a table.

`simdata` — Simulation results

vector of `SimData` objects

Simulation results obtained using the samples in `samplesTable`, returned as a vector of `SimData` objects.

`validRuns` — Indicators of run success or failure

logical vector

Indicators of run success or failure, returned as a logical vector. Each element indicates the success or failure of the corresponding simulation run in `simdata`.

More About

Retrieve Simulation Results and Sample Values Using `getSimulationResults`

`getSimulationResults` returns the *i*th column from the SimData array `sobolObj.SimulationInfo.SimData` on page 2-0 , which is one of the object properties.

As explained in “Saltelli Method to Compute Sobol Indices” on page 1-279, A and B are sample matrices. A_B^i is a matrix where all columns are from A except the ith column, which is from B for i = 1, 2,...,*“params” on page 1-0* . *params* is the number of input parameters.

The simulation data used to compute Sobol indices is stored in `sobolObj.SimulationInfo.SimData`. The array size is *`NumberSamples`*`-by-`*`params`*` + 2`, where *NumberSamples on page 1-0* is the number of samples. The number of columns is `2 + params` because the first two columns correspond to simulation results from A and B. The rest of the columns correspond to A_B^1, A_B^2, ..., A_B^{params} . In other words, you can consider the following:

sobolObj.SimulationInfo.SimData = $\left[SimData(A), SimData(B), SimData\left(A_B^1\right), SimData\left(A_B^2\right), ..., SimData\left(A_B^{params}\right)\right]$

Here, the first column corresponds to simulation data using the sample matrix A, the second column corresponds to simulation data using the sample matrix B, the third column corresponds to simulation data using the matrix A_B^1, and so on.

For instance, `getSimulationResults(sobolObj,3)` returns:

- `samplesTable` (first output), which is A_B^1.
- `simdata` (second output), which contains simulation results using the samples from A_B^1. This is the third column of `sobolObj.SimulationInfo.SimData`.
- `validRuns` (third output), which contains logical values that indicate the success or failure of each simulation run in `simdata` (second output). `validRuns` corresponds to the ith column of `sobolObj.SimulationInfo.ValidSample` on page 2-0 .

Version History

Introduced in R2020a

References

[1] Saltelli, Andrea, Paola Annoni, Ivano Azzini, Francesca Campolongo, Marco Ratto, and Stefano Tarantola. “Variance Based Sensitivity Analysis of Model Output. Design and Estimator for the Total Sensitivity Index.” *Computer Physics Communications* 181, no. 2 (February 2010): 259–70. https://doi.org/10.1016/j.cpc.2009.09.018.

See Also

`SimBiology.gsa.Sobol` | `sbiosobol` | `plot` | `plotData` | `bar`

getspecies (kineticlaw)

Get specific species in kinetic law object

Syntax

```
speciesObj = getspecies(kineticlawObj)
speciesObj = getspecies(kineticlawObj, SpeciesVariablesValue)
```

Arguments

kineticlawObj	Retrieve species used by the kinetic law object.
SpeciesVariablesValue	Retrieve species used by the kinetic law object corresponding to the specified species in the `SpeciesVariables` property of the kinetic law object. Specify a character vector, string scalar, string vector, or cell array of character vectors.

Description

speciesObj = `getspecies(`*kineticlawObj*`)` returns the species used by the kinetic law object `kineticlawObj` to `speciesObj`.

speciesObj = `getspecies(`*kineticlawObj*`, `*SpeciesVariablesValue*`)` returns the species in the `SpeciesVariableNames` property to `speciesObj`.

`SpeciesVariablesValue` is the name of the species as it appears in the `SpeciesVariables` property of `kineticlawObj`. `SpeciesVariablesValue` can be a character vector, string scalar, string vector, or cell array of character vectors.

Species names are referenced by reaction objects, kinetic law objects, and model objects. If you change the name of a species, the reaction updates to use the new name. You must, however, configure all other applicable elements such as rules that use the species, and the kinetic law object `SpeciesVariableNames`. Use the method `setspecies` to configure `SpeciesVariableNames`.

Examples

Create a model, add a reaction, and then assign the `SpeciesVariableNames` for the reaction rate equation.

1. Create a model object, and then add a reaction object.

   ```
   modelObj = sbiomodel('my_model');
   reactionObj = addreaction(modelObj, 'a -> c + d');
   ```

2. Create a kinetic law object for the reaction object, of the type `'Henri-Michaelis-Menten'`.

   ```
   kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
   ```

   `reactionObj` `KineticLaw` property is configured to `kineticlawObj`.

3 The `'Henri-Michaelis-Menten'` kinetic law has one species variable (`S`) that should to be set. To set this variable:

```
setspecies(kineticlawObj,'S', 'a');
```

4 Retrieve the species variable using `getspecies`.

```
speciesObj = getspecies (kineticlawObj, 'S')
```

MATLAB returns:

```
SimBiology Species Array

Index:  Compartment: Name: InitialAmount: InitialAmountUnits:
   1      unnamed     a        0
```

See Also

`addspecies`, `getparameters`, `setparameter`, `setspecies`

Version History

Introduced in R2006a

getstoichmatrix (model)

Get stoichiometry matrix from model object

Note The order of species in the output arguments (`M` and `objSpecies`) matches the order of species returned by `modelObj.Species`.

Syntax

```
M = getstoichmatrix(modelObj)
[M,objSpecies] = getstoichmatrix(modelObj)
[M,objSpecies,objReactions] = getstoichmatrix(modelObj)
```

Arguments

M	Stoichiometry matrix for *modelObj*.
modelObj	Specify the `model object`.
objSpecies	Return the list of *modelObj* species by `Name` property of the species. If the species are in multiple compartments, species names are qualified with the compartment name in the form `compartmentName.speciesName`. For example, `nucleus.DNA`, `cytoplasm.mRNA`.
objReactions	Return the list of *modelObj* reactions by the `Name` property of reactions.

Description

`getstoichmatrix` returns a stoichiometry matrix for a model object.

M = `getstoichmatrix(`*modelObj*`)` returns a stoichiometry matrix for a SimBiology model object (*modelObj*) to *M*.

A stoichiometry matrix is defined by listing all reactions contained by *modelObj* column-wise and all species contained by *modelObj* row-wise in a matrix. The species of the reaction are represented in the matrix with the stoichiometric value at the location of [row of species, column of reaction]. Reactants have negative values. Products have positive values. All other locations in the matrix are 0.

For example, if *modelObj* is a model object with two reactions with names `R1` and `R2` and Reaction values of `2 A + B -> 3 C` and `B + 3 D -> 4 A`, the stoichiometry matrix would be defined as:

```
      R1   R2
A     -2    4
B     -1   -1
C      3    0
D      0   -3
```

`[M,objSpecies] = getstoichmatrix(modelObj)` returns the stoichiometry matrix to *`M`* and the species to *`objSpecies`*. *`objSpecies`* is defined by listing all `Name` property values of species contained by *`Obj`*. In the above example, *`objSpecies`* would be `{'A', 'B', 'C', 'D'}`;.

`[M,objSpecies,objReactions] = getstoichmatrix(modelObj)` returns the stoichiometry matrix to *`M`* and the reactions to *`objReactions`*. *`objReactions`* is defined by listing all `Name` property values of reactions contained by *`modelObj`*. In the above example, *`objReactions`* would be `{'R1', 'R2'}`.

Examples

1. Read in `m1`, a model object, using `sbmlimport`:

   ```
   m1 = sbmlimport('lotka.xml');
   ```

2. Get the stoichiometry matrix for the `m1`:

   ```
   [M,objSpecies,objReactions] = getstoichmatrix(m1)
   ```

See Also

`model object`, `getadjacencymatrix`, “Determining the Stoichiometry Matrix for a Model”

Version History

Introduced in R2006a

R2019b: The function returns species in a new order
Behavior changed in R2019b

The order of species in the output arguments (`M` and `objSpecies`) matches the order of species returned by `modelObj.Species`.

getTable(ScheduleDose,RepeatDose)

Return data from SimBiology dose object as table

Syntax

```
tbl = getTable(doseObj)
```

Description

`tbl = getTable(doseObj)` returns dosing data from the dose object `doseObj` as a table `tbl`.

Input Arguments

`doseObj` — Dose object

`ScheduleDose` object | `RepeatDose` object | array of dose objects

Dose object, specified as a `ScheduleDose object` or `RepeatDose object` or array of these objects.

Output Arguments

`tbl` — Dosing data

table | cell array of tables

Dosing data, returned as a table or cell array of tables. If `doseObj` is an array of dose objects, then `tbl` is a cell array of tables with the same size as `doseObj`.

If `doseObj` is a `RepeatDose` object and any of the `StartTime`, `Amount`, `Rate`, `Interval`, and `RepeatCount` properties are parameterized, the table shows the name of the parameter in the corresponding column instead.

Examples

Retrieve a Table of Dosing Information from a RepeatDose Object

Create a RepeatDose object with some dosing information.

```
rdose = sbiodose('rd','repeat');
rdose.TargetName = 'x';
rdose.StartTime = 5;
rdose.TimeUnits = 'second';
rdose.Amount = 300;
rdose.AmountUnits = 'molecule';
rdose.Rate = 1;
rdose.RateUnits = 'molecule/second';
rdose.Interval = 100;
rdose.RepeatCount = 2;
```

Get a table of such dosing information.

```
tbl = getTable(rdose)

tbl =

    StartTime    Amount    Rate    Interval    RepeatCount
    _________    ______    ____    ________    ___________

    5            300       1       100         2
```

Note that the units are also copied over and assigned to `tbl.Properties.VariableUnits` property.

```
tbl.Properties

ans =

              Description: ''
    VariableDescriptions: {}
           VariableUnits: {'second'  'molecule'  'molecule/second'  'second'  ''}
          DimensionNames: {'Row'  'Variable'}
                UserData: []
                RowNames: {}
           VariableNames: {'StartTime'  'Amount'  'Rate'  'Interval'  'RepeatCount'}
```

Retrieve a Table of Dosing Information from a Schedule Object

Create a ScheduleDose object with some dosing information.

```
sdose = sbiodose('sdose','schedule');
sdose.Amount = [100 200 300];
sdose.Time = [5 10 15];
```

Get a table of such dosing information.

```
tbl = getTable(sdose)

tbl =

    Time    Amount
    ____    ______

     5      100
    10      200
    15      300
```

Version History

Introduced in R2014a

See Also

`setTable` | `ScheduleDose object` | `RepeatDose object`

getvariant (model)

Get variant from model

Syntax

```
variantObj = getvariant(modelObj)

variantObj = getvariant(modelObj, 'NameValue')
```

Arguments

variantObj	`Variant object` returned by the `getvariant` method.
modelObj	`Model object` from which to get the variant.
'NameValue'	Name of the variant to get from the model object *modelObj*.

Description

variantObj = `getvariant(`*modelObj*`)` returns SimBiology variant objects contained by the SimBiology `model object` *modelObj* to *variantObj*.

A SimBiology variant object stores alternate values for properties on a SimBiology model. For more information on variants, see `Variant object`.

variantObj = `getvariant(`*modelObj*`, '`*NameValue*`')` returns the SimBiology variant object with the name *NameValue*, contained by the SimBiology model object, *modelObj*.

View properties for a variant object with the `get` command, and modify properties for a variant object with the `set` command.

Note Remember to use the `addcontent` method instead of using the `set` method on the `Content` property, because the `set` method replaces the data in the `Content` property whereas `addcontent` appends the data.

To copy a variant object to another model, use `copyobj`. To remove a variant object from a SimBiology model, use the `delete` method.

Examples

1. Create a model containing several variants.

```
modelObj = sbiomodel('mymodel');
variantObj1 = addvariant(modelObj, 'v1');
variantObj2 = addvariant(modelObj, 'v2');
```

2. Get all variants in the model.

```
vObjs = getvariant(modelObj)
```

```
SimBiology Variant Array

   Index:  Name:             Active:
   1       v1                false
   2       v2                false
```

3 Get the variant object named `'v2'` from the model.

```
vObjv2 = getvariant(modelObj, 'v2');
```

See Also

`Model object`, `Variant object`, `addvariant`, `removevariant`

Version History

Introduced in R2007b

groupedData

Table-like collection of data and metadata for fitting in SimBiology

Description

The `groupedData` object is the required data format to store data needed for fitting using `fitproblem`, `sbiofit`, and `sbiofitmixed`. It is a `table`-like object with a few differences.

- The `groupedData` object has two additional properties to identify the independent variable and an optional grouping variable.
- The `groupedData` object has additional methods that let you create doses and variants from data set and convert a `groupedData` object to a table.
- `groupedData.Properties` is a structure.

Creation

Syntax

```
grpData = groupedData
grpData = groupedData(tbl)
grpData = groupedData(tbl,groupVarName)
grpData = groupedData(tbl,groupVarName,independentVarName)
```

Description

`grpData = groupedData` creates an empty `groupedData` object.

`grpData = groupedData(tbl)` creates a `groupedData` object by copying a table or dataset object `tbl`. The `GroupVariableName` and `IndependentVariableName` properties of the `grpData` object are implicitly determined by looking for the first case-insensitive match to a list of variable names of `tbl` (`tbl.Properties.VariableNames`). For the grouping variable, the list of names is `ID`, `Group`, `I`, and `Run`. For the independent variable, the list of names is `Time`, `T`, and `IDV`. If there are no matches, `GroupVariableName` and `IndependentVariableName` are set to empty character vectors `''`.

`grpData = groupedData(tbl,groupVarName)` sets the `GroupVariableName` property of the `grpData` object to `groupVarName`. The `IndependentVariableName` property is implicitly set as in the previous syntax.

`grpData = groupedData(tbl,groupVarName,independentVarName)` additionally sets the `IndependentVariableName` property of the `grpData` object to `independentVarName`.

Input Arguments

`tbl` — Data
table | dataset

Data, specified as a `table` or `dataset`.

`groupVarName` — Grouping variable name
character vector | string

Grouping variable name, specified as a character vector or string. An empty character vector `''` or string `""` indicates that there is no group variable.

`independentVarName` — Independent variable name
character vector | string

Independent variable name, specified as a character vector or string. An empty character vector `''` or string `""` indicates that there is no independent variable.

Output Arguments

`grpData` — Grouped data
`groupedData` object

Grouped data, returned as a `groupedData` object.

Properties

The `groupedData` object supports all properties of `table` and provides the following additional properties.

`GroupVariableName` — Name of grouping variable
character vector

Name of the grouping variable that indicates the groups in the data, specified as a character vector. To indicate that there are no groups (or just one group), set the property to the empty character vector `''`.

Example: `'ID'`

`IndependentVariableName` — Name of independent variable
`''` (default) | character vector

Name of the independent variable in the data such as time, specified as a character vector.

Example: `'TIME'`

Object Functions

The `groupedData` object supports many functions of `table`. However, it does not support the math operations that the table supports, such as `+`, `-`, `/` , `min`, `max`, `mean`, and so on. To see a list of math operations that the table supports, see here. The `groupedData` object has the following additional functions.

createDoses	Create dose objects from groupedData object
createVariants	Create variant objects from groupedData object
groupedData2table	Convert groupedData object to table

Examples

Create groupedData from Existing Data Set

Load the sample data set.

```
load pheno.mat ds
```

Create a `groupedData` object from the data set `ds`.

```
grpData = groupedData(ds);
```

Display the object properties.

```
grpData.Properties
```

```
ans = struct with fields:
                Description: ''
                   UserData: []
             DimensionNames: {'Observations'  'Variables'}
              VariableNames: {'ID'  'TIME'  'DOSE'  'WEIGHT'  'APGAR'  'CONC'}
       VariableDescriptions: {}
              VariableUnits: {}
         VariableContinuity: []
                   RowNames: {}
           CustomProperties: [1x1 matlab.tabular.CustomProperties]
          GroupVariableName: 'ID'
    IndependentVariableName: 'TIME'
```

`GroupVariableName` and `IndpendentVariableName` have been automatically assigned to 'ID' and 'Time', respectively.

Version History

Introduced in R2014a

See Also

`sbiofit` | `sbiofitmixed` | `table`

Topics

“Import Tabular Data from Files”
“Supported Files and Data Types”
“Create Data File with SimBiology Definitions”

groupedData2table

Convert groupedData object to table

Syntax

```
tbl = groupedData2table(grpData)
```

Description

`tbl = groupedData2table(grpData)` converts a `groupedData` object `grpData` to a table.

Examples

Convert groupedData to Table

Load the sample data set.

```
load pheno.mat ds
```

Create a groupedData object from the data set `ds`.

```
grpData = groupedData(ds);
```

Display the object properties.

```
grpData.Properties
```

```
ans = struct with fields:
                Description: ''
                   UserData: []
              DimensionNames: {'Observations'  'Variables'}
               VariableNames: {'ID'  'TIME'  'DOSE'  'WEIGHT'  'APGAR'  'CONC'}
       VariableDescriptions: {}
              VariableUnits: {}
         VariableContinuity: []
                   RowNames: {}
           CustomProperties: [1x1 matlab.tabular.CustomProperties]
          GroupVariableName: 'ID'
    IndependentVariableName: 'TIME'
```

`GroupVariableName` and `IndpendentVariableName` have been automatically assigned to 'ID' and 'Time', respectively.

Convert the groupedData to a table.

```
tbl = groupedData2table(grpData);
```

Display the first 5 rows of the table.

```
tbl(1:5,:)
```

```
ans=5×6 table
    ID    TIME    DOSE    WEIGHT    APGAR    CONC
    __    ____    ____    ______    _____    ____

    1        0     25       1.4        7       NaN
    1        2    NaN       1.4        7      17.3
    1     12.5    3.5       1.4        7       NaN
    1     24.5    3.5       1.4        7       NaN
    1       37    3.5       1.4        7       NaN
```

Input Arguments

`grpData` — Grouped data

`groupedData` object

Grouped data, specified as a `groupedData` object.

Output Arguments

`tbl` — Data table

table

Data table, returned as a `table`.

Version History

Introduced in R2014a

See Also

`table` | `groupedData` | `sbiofit` | `sbiofitmixed`

histogram

Plot histogram of multiparametric global sensitivity analysis results

Syntax

```
h = histogram(mpgsaObj)
h = histogram(mpgsaObj,Name,Value)
```

Description

`h = histogram(mpgsaObj)` plots a histogram of multiparametric global sensitivity analysis (MPGSA) results and returns the figure handle `h`.

`h = histogram(mpgsaObj,Name,Value)` uses additional options specified by one or more name-value pair arguments.

Examples

Perform Multiparametric Global Sensitivity Analysis (MPGSA)

Load the “Target-Mediated Drug Disposition (TMDD) Model”.

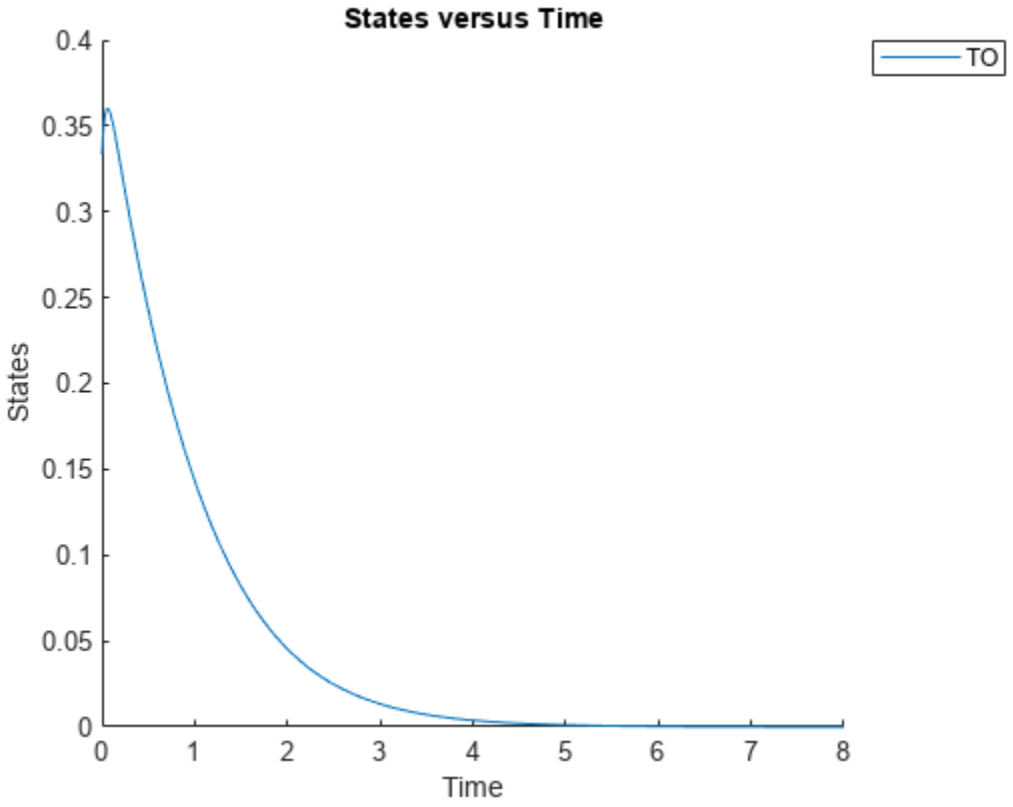
```
sbioloadproject tmdd_with_TO.sbproj
```

Get the active configset and set the target occupancy (`TO`) as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'TO';
```

Simulate the model and plot the `TO` profile.

```
sbioplot(sbiosimulate(m1,cs));
```



Define an exposure (area under the curve of the TO profile) threshold for the target occupancy.

```
classifier = 'trapz(time,TO) <= 0.1';
```

Perform MPGSA to find sensitive parameters with respect to the TO. Vary the parameter values between predefined bounds to generate 10,000 parameter samples.

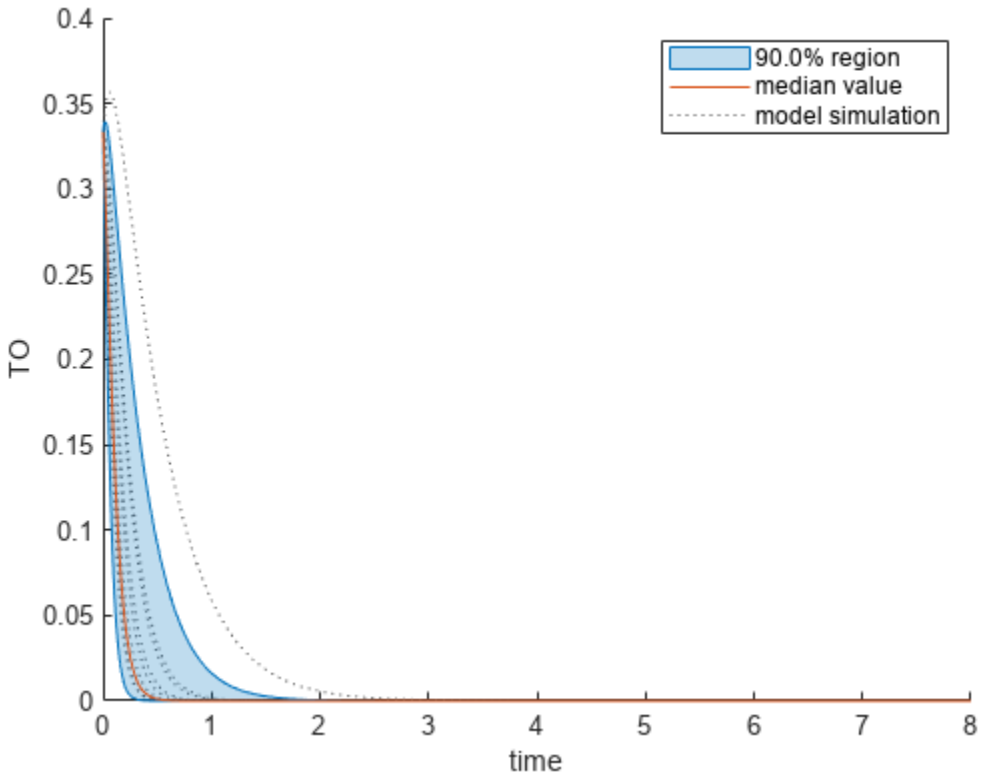
```
% Suppress an information warning that is issued during simulation.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
rng(0,'twister'); % For reproducibility
params = {'kel','ksyn','kdeg','km'};
bounds = [0.1, 1;
          0.1, 1;
          0.1, 1;
          0.1, 1];
mpgsaResults = sbiompgsa(m1,params,classifier,Bounds=bounds,NumberSamples=10000)
```

```
mpgsaResults =
  MPGSA with properties:

                  Classifiers: {'trapz(time,TO) <= 0.1'}
    KolmogorovSmirnovStatistics: [4x1 table]
                    ECDFData: {4x4 cell}
             SignificanceLevel: 0.0500
                      PValues: [4x1 table]
             SupportHypothesis: [10000x1 table]
              ParameterSamples: [10000x4 table]
                   Observables: {'TO'}
```

```
                SimulationInfo: [1x1 struct]
```

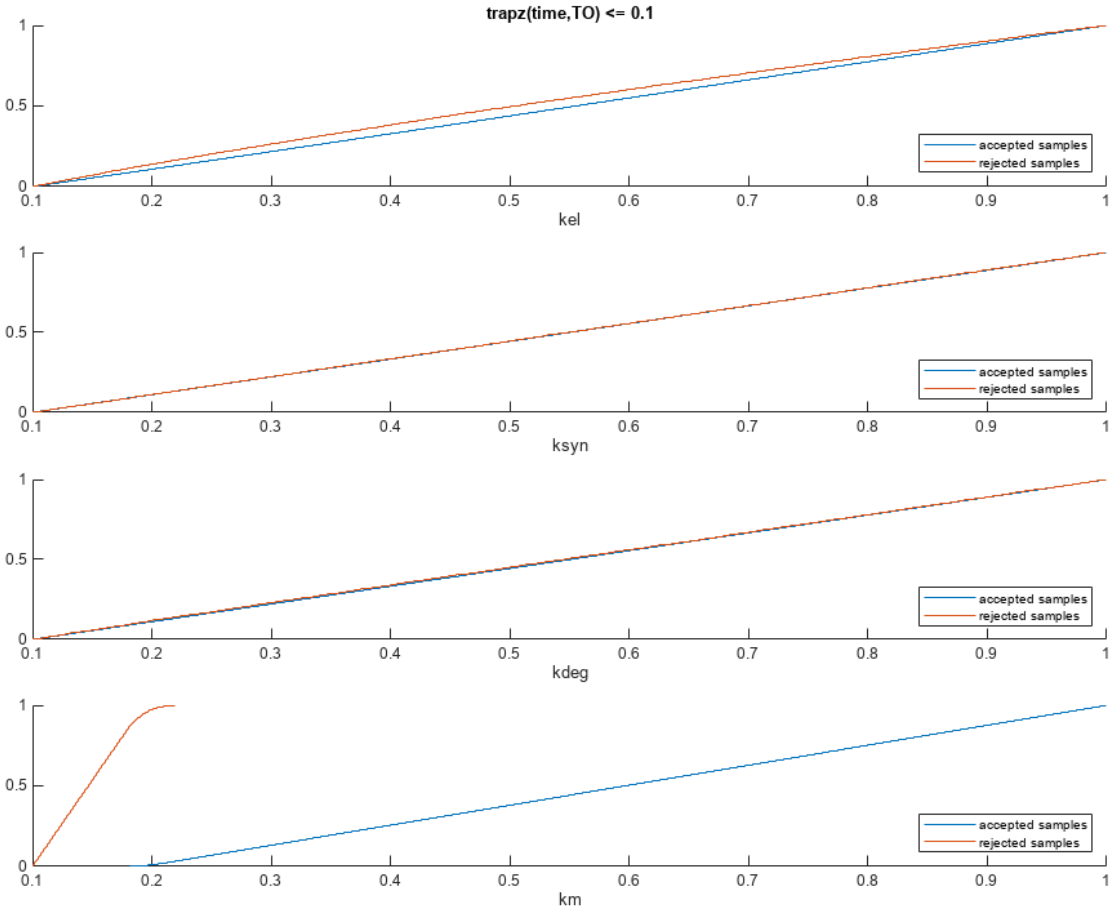
Plot the quantiles of the simulated model response.

```
plotData(mpgsaResults,ShowMedian=true,ShowMean=false);
```



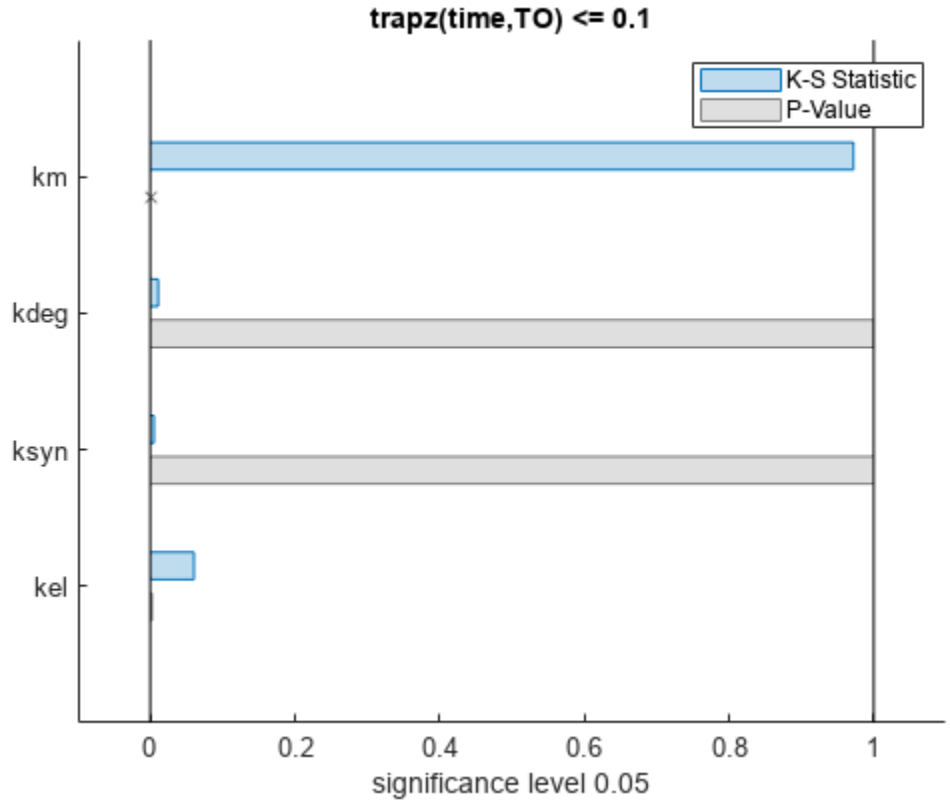
Plot the empirical cumulative distribution functions (eCDFs) of the accepted and rejected samples. Except for `km`, none of the parameters shows a significant difference in the eCDFs for the accepted and rejected samples. The `km` plot shows a large Kolmogorov-Smirnov (K-S) distance between the eCDFs of the accepted and rejected samples. The K-S distance is the maximum absolute distance between two eCDFs curves.

```
h = plot(mpgsaResults);
% Resize the figure.
pos = h.Position(:);
h.Position(:) = [pos(1) pos(2) pos(3)*2 pos(4)*2];
```



To compute the K-S distance between the two eCDFs, SimBiology uses a two-sided test based on the null hypothesis that the two distributions of accepted and rejected samples are equal. See `kstest2` (Statistics and Machine Learning Toolbox) for details. If the K-S distance is large, then the two distributions are different, meaning that the classification of the samples is sensitive to variations in the input parameter. On the other hand, if the K-S distance is small, then variations in the input parameter do not affect the classification of samples. The results suggest that the classification is insensitive to the input parameter. To assess the significance of the K-S statistic rejecting the null-hypothesis, you can examine the p-values.

```
bar(mpgsaResults)
```



The bar plot shows two bars for each parameter: one for the K-S distance (K-S statistic) and another for the corresponding p-value. You reject the null hypothesis if the p-value is less than the significance level. A cross (`x`) is shown for any p-value that is almost 0. You can see the exact p-value corresponding to each parameter.

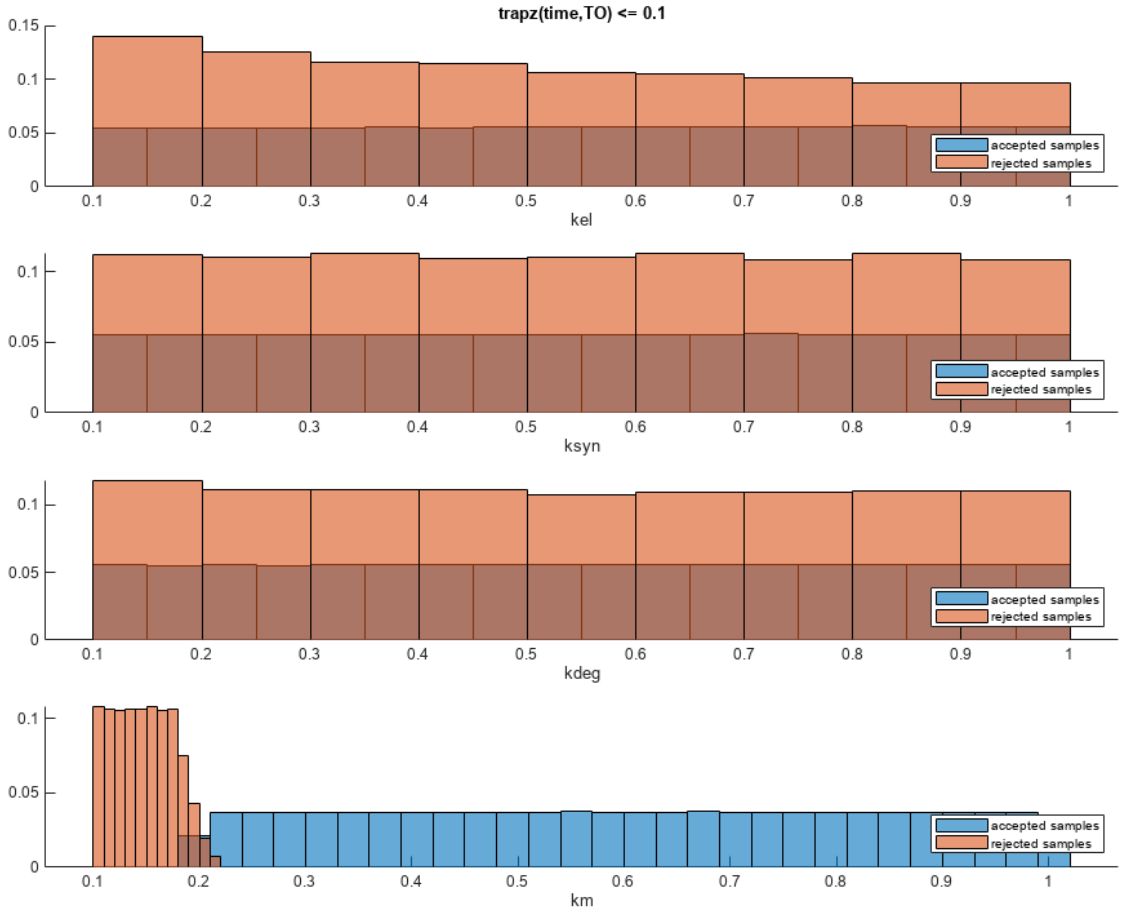
```
[mpgsaResults.ParameterSamples.Properties.VariableNames',mpgsaResults.PValues]
```

```
ans=4×2 table
      Var1      trapz(time,TO) <= 0.1
    ________    _____________________

    {'kel' }          0.0021877
    {'ksyn'}                  1
    {'kdeg'}            0.99983
    {'km'  }                  0
```

The p-values of `km` and `kel` are less than the significance level (0.05), supporting the alternative hypothesis that the accepted and rejected samples come from different distributions. In other words, the classification of the samples is sensitive to `km` and `kel` but not to other parameters (`kdeg` and `ksyn`).

You can also plot the histograms of accepted and rejected samples. The historgrams let you see trends in the accepted and rejected samples. In this example, the histogram of `km` shows that there are more accepted samples for larger `km` values, while the `kel` histogram shows that there are fewer rejected samples as `kel` increases.

```
h2 = histogram(mpgsaResults);
% Resize the figure.
pos = h2.Position(:);
h2.Position(:) = [pos(1) pos(2) pos(3)*2 pos(4)*2];
```



Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

`mpgsaObj` — Multiparametric global sensitivity analysis results

`SimBiology.gsa.MPGSA` object

Multiparametric global sensitivity analysis results, specified as a `SimBiology.gsa.MPGSA` object.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `h = histogram(results,'Classifier',1)` specifies to plot histograms of MPGSA results of the first classifier.

`Parameters` — Input model quantities to plot

character vector | string | string vector | cell array of character vectors | vector of positive integers

Input model quantities, namely parameters, species, or compartments, to plot, specified as a character vector, string, string vector, cell array of character vectors, or a vector of positive integers indexing into the columns of the `mpgsaObj.ParameterSamples` table.

Example: `'Parameters','k1'`

Data Types: `double` | `char` | `string` | `cell`

`Classifiers` — Classifiers to plot

character vector | string | string vector | cell array of character vectors | vector of positive integers

Classifiers to plot, specified as a character vector, string, string vector, cell array of character vectors, or a vector of positive integers.

Specify the expressions of classifiers to plot as a character vector, string, string vector, cell array of character vectors. Alternatively, you can specify a vector of positive integers indexing into `mpgsaObj.Classifiers`.

Example: `'Classifiers',[1 3]`

Data Types: `double` | `char` | `string` | `cell`

`AcceptedSamplesColor` — Color of accepted samples

three-element row vector | hexadecimal color code | color name

Color of accepted samples, specified as a three-element row vector, hexadecimal color code, color name, or a short name. By default, the function uses the first MATLAB default color. To view the default color order, enter `get(groot,'defaultAxesColorOrder')` or see the “ColorOrder” property.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see “Specify Plot Colors”.

Example: `'AcceptedSamplesColor',[0.4,0.3,0.2]`

Data Types: `double`

`RejectedSamplesColor` — Color of rejected samples

three-element row vector | hexadecimal color code | color name

Color of rejected samples, specified as a three-element row vector, hexadecimal color code, color name, or a short name. By default, the function uses the second MATLAB default color. To view the default color order, enter `get(groot,'defaultAxesColorOrder')` or see the “ColorOrder” property.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see “Specify Plot Colors”.

Example: `'RejectedSamplesColor',[0.9,0.5,0.2]`

Data Types: `double`

Output Arguments

h — Handle

figure handle

Handle to the figure, specified as a figure handle.

Version History

Introduced in R2020a

References

[1] Tiemann, Christian A., Joep Vanlier, Maaike H. Oosterveer, Albert K. Groen, Peter A. J. Hilbers, and Natal A. W. van Riel. “Parameter Trajectory Analysis to Identify Treatment Effects of Pharmacological Interventions.” Edited by Scott Markel. *PLoS Computational Biology* 9, no. 8 (August 1, 2013): e1003166. https://doi.org/10.1371/journal.pcbi.1003166.

See Also

`SimBiology.gsa.MPGSA` | `sbiompgsa` | `plotData` | `bar` | `kstest2` | `ecdf`

isAccelerated(SimFunction)

Determine if SimFunction object is accelerated

Syntax

```
tf = isaccelerated(F)
tf = isaccelerated(F,computerType)
```

Arguments

`F`	`SimFunction object` created by the `createSimFunction` method of a SimBiology model.
`computerType`	Character vector specifying a computer type. You can specify any valid `archstr` supported by the function `computer`.

Description

`tf = isaccelerated(F)` returns true if `SimFunction object` `F` is accelerated for the current type of computer or `false` otherwise.

`tf = isaccelerated(F,computerType)` returns `true` if `F` is accelerated for the specified type of computer or `false` otherwise.

Note `F` is automatically accelerated at the first function execution. However, manually accelerate the object if you want it accelerated in your deployment applications.

Examples

Simulate SimFunction Object

This example uses the Lotka-Volterra (predator-prey) model described by Gillespie [1].

Load the sample project containing the lotka model.

```
sbioloadproject lotka;
```

Create a SimFunction object `f` with `c1` and `c2` as input parameters to be scanned, and `y1` and `y2` as the output of the function with no dose.

```
f = createSimFunction(m1,{'Reaction1.c1', 'Reaction2.c2'},{'y1', 'y2'}, [])
```

```
f =

SimFunction

Parameters:
```

```
          Name          Value       Type
    ________________    _____    ___________

    'Reaction1.c1'        10     'parameter'
    'Reaction2.c2'      0.01     'parameter'

Observables:

    Name      Type
    ____    _________

    'y1'    'species'
    'y2'    'species'

Dosed: None
```

The `SimFunction` object `f` is not set for acceleration at the time of creation. But it will be automatically accelerated when executed.

```
f.isAccelerated
```

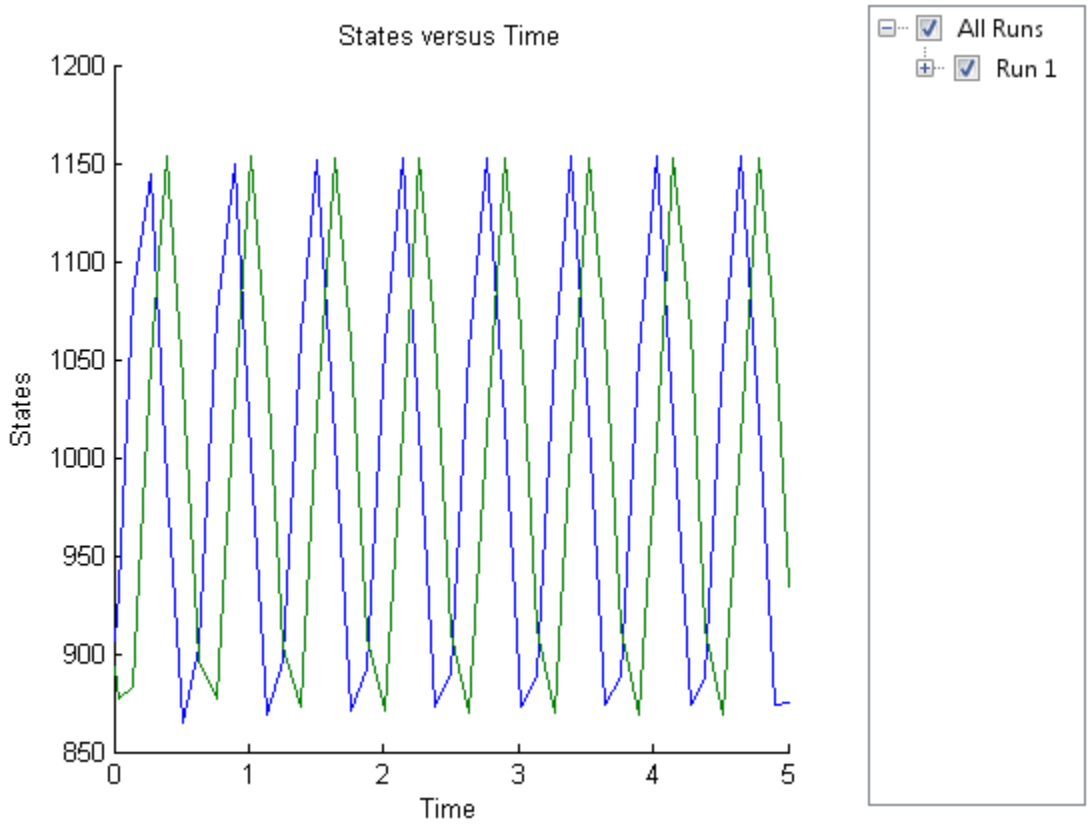
```
ans =

     0
```

Define an input matrix that contains parameter values for `c1` and `c2`.

```
phi = [10 0.01];
```

Run simulations until the stop time is 5 and plot the simulation results.

```
sbioplot(f(phi,5))
```



Confirm the `SimFunction` object `f` was accelerated during execution.

```
f.isAccelerated
```

```
ans =

     1
```

See Also

`createSimFunction`, `SimFunction object`

Version History

Introduced in R2012b

References

[1] Gillespie D.T. "Exact Stochatic Simulation of Coupled Chemical Reactions," (1977) The Journal of Physical Chemistry, 81(25), 2340-2361.

isAccelerated

Determine whether an exported SimBiology model is accelerated

Syntax

```
tf = isAccelerated(model)
tf = isAccelerated(model,computerType)
```

Description

`tf = isAccelerated(model)` returns `true` if `model` is accelerated for the current type of computer, and `false` otherwise.

`tf = isAccelerated(model,computerType)` returns `true` if `model` is accelerated for the specified computer type.

Examples

Accelerate Exported SimBiology Model

Load a sample SimBiology model object, and export.

```
modelObj = sbmlimport('lotka');
em = export(modelObj)
```

```
em =

  Model with properties:

          Name: 'lotka'
    ExportTime: '12-Dec-2012 15:20:13'
   ExportNotes: ''
```

Accelerate the exported model.

```
accelerate(em);
em.isAccelerated
```

```
ans =

     1
```

The logical value 1 indicates that the exported model is accelerated.

Input Arguments

`model` — Input model

`SimBiology.export.Model` object

Input model, specified as a `SimBiology.export.Model` object.

`computerType` — Computer type
character vector | string scalar

Computer type, specified as a character vector or string scalar. You can specify any valid system architecture supported by the function `computer`.

Output Arguments

`tf` — Output indicating if model is accelerated
logical value

Output indicating if model is accelerated, returned as a logical value. `tf` is `true` if `model` is accelerated for the current computer type, or computer type specified by `computerType`. `tf` is `false` if the exported model is not accelerated for the specified computer type.

Version History

Introduced in R2012b

See Also

`SimBiology.export.Model` | `accelerate` | `computer`

Topics
“Perform PK/PD Modeling and Simulation to Guide Dosing Strategy for Antibiotics”
“Deploy a SimBiology Exported Model”

KineticLaw object

Kinetic law information for reaction

Description

The kinetic law object holds information about the abstract kinetic law applied to a reaction and provides a template for the reaction rate. In the model, the SimBiology software uses the information you provide in a fully defined kinetic law object to determine the `ReactionRate` property in the reaction object.

When you first create a kinetic law object, you must specify the name of the abstract kinetic law to use. The SimBiology software fills in the `KineticLawName` property and the `Expression` property in the kinetic law object with the name of the abstract kinetic law you specified and the mathematical expression respectively. The software also fills in the `ParameterVariables` property and the `SpeciesVariables` property of the kinetic law object with the values found in the corresponding properties of the abstract kinetic law object.

To obtain the reaction rate, you must fully define the kinetic law object:

1. In the ParameterVariableNames property, specify the parameters from the model that you want to substitute in the expression (`Expression` on page 3-58 property).
2. In the SpeciesVariableNames property, specify the species from the model that you want to substitute in the expression.

   The SimBiology software substitutes in the expression, the names of parameter variables and species variables in the order specified in the `ParameterVariables` and `SpeciesVariables` properties respectively.

   The software then shows the substituted expression as the reaction rate in the ReactionRate property of the reaction object. If the kinetic law object is not fully defined, the `ReactionRate` property remains `''` (empty).

For links to kinetic law object property reference pages, see “Property Summary” on page 2-433.

Properties define the characteristics of an object. Use the `get` and `set` commands to list object properties and change their values at the command line. You can interactively change object properties in the **SimBiology Model Builder** app.

For an explanation of how relevant properties relate to one another, see “Command Line” on page 2-431.

The following sections use a kinetic law example to show how you can fully define your kinetic law object to obtain the reaction rate in the **SimBiology Model Builder** app and at the command line.

The Henri-Michaelis-Menten kinetic law is expressed as follows:

$$V_m * S/(K_m + S)$$

In the SimBiology software `Henri-Michaelis-Menten` is a built-in abstract kinetic law, where V_m and K_m are defined in the ParameterVariables property of the abstract kinetic law object, and S is defined in the SpeciesVariables property of the abstract kinetic law object.

SimBiology Model Builder app

To fully define a kinetic law in the app, define the names of the species variables and parameter variables that participate in the reaction rate. For an example, see “Add and Configure Reactions”.

Command Line

To fully define the kinetic law object at the command line, define the names of the parameters in the ParameterVariableNames property of the kinetic law object, and define the species names in the SpeciesVariableNames property of the kinetic law object. For example, to apply the `Henri-Michaelis-Menten` abstract kinetic law to a reaction

```
A -> B
where Vm = Va, Km = Ka
and S = A
```

Define `Va` and `Ka` in the `ParameterVariableNames` property to substitute the variables that are in the `ParameterVariables` property (`Vm` and `Km`). Define `A` in the `SpeciesVariableName` property to be used to substitute the species variable in the `SpeciesVariables` property (`S`). Specify the order of the model parameters to be used for substitution in the same order that the parameter variables are listed in the `ParameterVariables` property. Similarly, specify species order if more than one species variable is represented.

```
% Find the order of the parameter variables
% in the kinetic law expression.

get(kineticlawObj, 'ParameterVariables')

ans =

    'Vm'    'Km'

% Find the species variable in the
% kinetic law expression

get(kineticlawObj, 'SpeciesVariables')
ans =

    'S'

% Specify the parameters and species variables
% to be used in the substitution.
% Remember to specify order, for example Vm = Va
% Vm is listed first in 'ParameterVariables',
% therefore list Va first in 'ParameterVariableNames'.

set(kineticlawObj,'ParameterVariableNames', {'Va' 'Ka'});
set(kineticlawObj,'SpeciesVariableNames', {'A'});
```

The rate equation is assigned in the reaction object as follows:

Va*A/(Ka + A)

For a detailed procedure, see “Examples” on page 2-433.

The following table summarizes the relationships between the properties in the abstract kinetic law object and the kinetic law object in the context of the above example.

Property	Property Purpose	Abstract Kinetic Law Object	Kinetic Law Object
`Name` (abstract kinetic law object) `KineticLawName` (kinetic law object)	Name of abstract kinetic law applied to a reaction. For example: `Henri-Michaelis -Menten`	Read-only for built-in abstract kinetic law. User-determined for user-defined abstract kinetic law.	Read-only
`Expression`	Mathematical expression used to determine the reaction rate equation. For example: $V_m*S/(K_m+S)$	Read-only for built-in abstract kinetic law. User-determined for user-defined abstract kinetic law.	Read-only; depends on abstract kinetic law applied to reaction.
`ParameterVariables`	Variables in `Expression` that are parameters. For example: `Vm and Km`	Read-only for built-in abstract kinetic law. User-determined for user-defined abstract kinetic law.	Read-only; depends on abstract kinetic law applied to reaction.
`SpeciesVariables`	Variables in `Expression` that are species. For example: `S`	Read-only for built-in abstract kinetic law. User-determined for user-defined abstract kinetic law.	Read-only; depends on abstract kinetic law applied to reaction.
`ParameterVariableNames`	Variables in `ReactionRate` that are parameters. For example: `Va and Ka`	Not applicable	Define these variables corresponding to `ParameterVariables`.
`SpeciesVariablesNames`	Variables in `ReactionRate` that are species. For example: `A`	Not applicable	Define these variables corresponding to `SpeciesVariables`.

Constructor Summary

addkineticlaw (reaction)	Create kinetic law object and add to reaction object

Method Summary

addparameter (model, kineticlaw)	Create parameter object and add to model or kinetic law object
copyobj	Copy SimBiology object and its children
delete	Delete SimBiology object
display	Display summary of SimBiology object
get	Get SimBiology object properties
getparameters (kineticlaw)	Get specific parameters in kinetic law object
getspecies (kineticlaw)	Get specific species in kinetic law object
rename	Rename object and update expressions
reorder (model, compartment, kinetic law)	Reorder component lists
set	Set SimBiology object properties
setparameter (kineticlaw)	Specify specific parameters in kinetic law object
setspecies (kineticlaw)	Specify species in kinetic law object

Property Summary

Expression	Expression to determine reaction rate equation or expression of observable object
KineticLawName	Name of kinetic law applied to reaction
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parameters	Array of parameter objects
ParameterVariableNames	Cell array of reaction rate parameters
ParameterVariables	Parameters in kinetic law definition
Parent	Indicate parent object
SpeciesVariableNames	Cell array of species in reaction rate equation
SpeciesVariables	Species in abstract kinetic law
Tag	Specify label for SimBiology object
Type	Display SimBiology object type
UserData	Specify data to associate with object

Examples

This example shows how to define the reaction rate for a reaction.

1 Create a model object, and add a reaction object to the model.

```
modelObj = sbiomodel ('my_model');
reactionObj = addreaction (modelObj, 'A -> B');
```

2 Define a kinetic law for the reaction object.

```
kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
```

3 Query the parameters and species variables defined in the kinetic law.

```
get(kineticlawObj, 'ParameterVariables')

ans =

    'Vm'    'Km'

get(kineticlawObj, 'SpeciesVariables')
ans =

    'S'
```

4 Define `Va` and `Ka` as `ParameterVariableNames`, which correspond to the `ParameterVariables` `Vm` and `Km`. To set these variables, first create the parameter variables as parameter objects (`parameterObj1, parameterObj2`) with the names `Va` and `Ka`, and then add them to `kineticlawObj`. The species object with `Name` `A` is created when `reactionObj` is created and need not be redefined.

```
parameterObj1 = addparameter(kineticlawObj, 'Va');
parameterObj2 = addparameter(kineticlawObj, 'Ka');
```

5 Set the variable names for the kinetic law object.

```
set(kineticlawObj,'ParameterVariableNames', {'Va' 'Ka'});
set(kineticlawObj,'SpeciesVariableNames', {'A'});
```

6 Verify that the reaction rate is expressed correctly in the reaction object `ReactionRate` property.

```
get (reactionObj, 'ReactionRate')
```

MATLAB returns:

```
ans =

Va*A/(Ka+A)
```

See Also

`AbstractKineticLaw object`, `Configset object`, `Model object`, `Parameter object`, `Reaction object`, `Root object`, `Rule object`, `Species object`

SimBiology property Expression(AbstractKineticLaw, KineticLaw)

Version History

Introduced in R2006b

LeastSquaresResults

Results object containing estimation results from least-squares regression

Description

The `LeastSquaresResults` contains estimation results from fitting a SimBiology model to data using `sbiofit` with any supported algorithm.

Creation

Use the `sbiofit` function to create a `LeastSquaresResults` object that is a superclass of two results objects: `NLINResults object` and `OptimResults object`.

If `sbiofit` uses the `nlinfit` estimation algorithm, the results object is the `NLINResults` object. If `sbiofit` uses any other supporting algorithm, then the results object is an `OptimResults` object. See the `sbiofit` function for the list of supported algorithms.

Properties

`GroupName` — Name of the group associated with the results
categorical | empty array

Name of the group associated with the results, specified as a categorical. If the `'Pooled'` name-value pair argument was set to `true` when you ran `sbiofit`, then `GroupName` is returned as an empty array or `[]`.

`Beta` — Table of estimated parameters
table

Table of estimated parameters, specified as a table. The *j*th row of the table represents the *j*th estimated parameter β_j. It contains transformed values of parameter estimates if any parameter transform is specified. Standard errors of these parameter estimates (`StandardError`) are calculated as: `sqrt(diag(COVB))`.

It can also contain the following variables:

- `Bounds` — the values of transformed parameter bounds that you specified during fitting
- `CategoryVariableName` — the names of categories or groups that you specified during fitting
- `CategoryValue` — the values of category variables specified by `CategoryVariableName`

This table contains one row per distinct parameter value.

`ParameterEstimates` — Table of estimated parameters
table

Table of estimated parameters, specified as a table. The *j*th row of the table represents the *j*th estimated parameter β_j. This table contains untransformed values of parameter estimates. Standard

errors of these parameter estimates (`StandardError`) are calculated as: `sqrt(diag(CovarianceMatrix))`.

It can also contain the following variables:

- `Bounds` — the values of transformed parameter bounds that you specified during fitting
- `CategoryVariableName` — the names of categories or groups that you specified during fitting
- `CategoryValue` — the values of category variables specified by `CategoryVariableName`

This table contains sets of parameter values that are identified for each individual or group.

`J` — Jacobian matrix of the model
array

Jacobian matrix of the model, specified as an array. The Jacobian matrix with respect to an estimated parameter is

$$J(i,j,k) = \left.\frac{\partial y_k}{\partial \beta_j}\right|_{t_i}$$

where t_i is the ith time point, β_j is the jth estimated parameter in the transformed space, and y_k is the kth response in the group of data.

`COVB` — Estimated covariance matrix for `Beta`
matrix

Estimated covariance matrix for `Beta`, specified as a matrix. This matrix is calculated as: `COVB = inv(J'*J)*MSE`.

`CovarianceMatrix` — Estimated covariance matrix for `ParameterEstimates`
matrix

Estimated covariance matrix for `ParameterEstimates`, specified as a matrix. This matrix is calculated as: `CovarianceMatrix = T'*COVB*T`, where `T = diag(JInvT(Beta))`. `JInvT(Beta)` returns a Jacobian matrix of `Beta` which is inverse transformed accordingly if you specified any transform to estimated parameters.

For instance, suppose you specified the log-transform for an estimated parameter `x` when you ran `sbiofit`. The inverse transform is: `InvT = exp(x)`, and its Jacobian is: `JInvT = exp(x)` since the derivative of `exp` is also `exp`.

`R` — Residuals matrix
matrix

Residuals matrix, specified as a matrix. R_{ij} is the residual for the ith time point and the jth response in the group of data.

`LogLikelihood` — Maximized loglikelihood for the fitted model
scalar

Maximized loglikelihood for the fitted model, specified as a scalar.

`AIC` — Akaike Information Criterion (AIC)
scalar

Akaike Information Criterion (AIC), specified as a scalar. The AIC is calculated as `AIC = 2*(-LogLikelihood + P)`, where *P* is the number of parameters.

`BIC` — Bayes Information Criterion (BIC)
scalar

Bayes Information Criterion (BIC), specified as a scalar. The BIC is calculated as `BIC = -2*LogLikelihood + P*log(N)`, where *N* is the number of observations, and *P* is the number of parameters.

`DFE` — Degrees of freedom for error
scalar

Degrees of freedom for error (DFE), specified as a scalar. The DFE is calculated as `DFE = N-P`, where *N* is the number of observations and *P* is the number of parameters.

`MSE` — Mean squared error
scalar

Mean squared error, specified as a scalar.

`SSE` — Sum of squared (weighted) errors or residuals
scalar

Sum of squared (weighted) errors or residuals, specified as a scalar.

`Weights` — Matrix of weights
matrix

Matrix of weights, specified as a matrix with one column per response and one row per observation.

`Data` — Data used for fitting
`groupedData` object

Data used for fitting, specified as a `groupedData` object.

In most cases, this `Data` property contains a copy of `groupedData` specified as the input data in the `sbiofit on page 1-0` call or the Data property of a `fitproblem` object. One exception is that the `Data` property of unpooled fit results objects contain only the subset of data for the individual group used for fitting.

`EstimatedParameterNames` — Estimated parameter names
cell array of character vectors

Estimated parameter names, specified as a cell array of character vectors.

`ErrorModelInfo` — Error models and estimated error model parameters
table

Error models and estimated error model parameters, specified as a table.

- The table has one row per error model.
- The `ErrorModelInfo.Properties.RowsNames` property identifies which responses the row applies to.

- The table contains three variables: `ErrorModel`, `a`, and `b`. The `ErrorModel` variable is categorical. The variables `a` and `b` can be `NaN` when they do not apply to a particular error model.

There are four built-in error models. Each model defines the error using a standard mean-zero and unit-variance (Gaussian) variable e, the function value f, and one or two parameters a and b. In SimBiology, the function f represents simulation results from a SimBiology model.

- `'constant'`: $y = f + ae$
- `'proportional'`: $y = f + b|f|e$
- `'combined'`: $y = f + (a + b|f|)e$
- `'exponential'`: $y = f * \exp(ae)$

`EstimationFunction` — Name of the estimation function
character vector

Name of the estimation function, specified as a character vector.

`DependentFiles` — File names to include for deployment
cell array of character vectors

File names to include for deployment, specified as a cell array of character vectors.

Note `Loglikelihood`, `AIC`, and `BIC` properties are empty for `LeastSquaresResults` objects that were obtained before R2016a.

Object Functions

boxplot	Create box plot showing the variation of estimated SimBiology model parameters
fitted	Return simulation results of SimBiology model fitted using least-squares regression
plot	Compare simulation results to the training data, creating a time-course subplot for each group
plotActualVersusPredicted	Compare predictions to actual data, creating a subplot for each response
plotResidualDistribution	Plot the distribution of the residuals
plotResiduals	Plot residuals for each response, using time, group, or prediction as x-axis
predict	Simulate and evaluate fitted SimBiology model
random	Simulate SimBiology model, adding variations by sampling error model
summary	Return structure array that contains estimated values and fit quality statistics

Version History

Introduced in R2014a

See Also

`NLINResults object` | `OptimResults object` | `sbiofit` | `sbiofitmixed`

Model object

Model and component information

Description

The SimBiology model object represents a *model*, which is a collection of interrelated reactions and rules that transform, transport, and bind species. The model includes model components such as compartments, reactions, parameters, rules, and events. Each of the components is represented as a property of the model object. A model object also has a default configuration set object to define simulation settings. You can also add more configuration set objects to a model object.

See “Property Summary” on page 2-441 for links to model property reference pages.

Properties define the characteristics of an object. Use the `get` and `set` commands to list object properties and change their values at the command line. You can graphically change object properties in the SimBiology desktop.

You can retrieve SimBiology model objects from the SimBiology root object. A SimBiology model object has its `Parent` property set to the SimBiology root object. The root object contains a list of model objects that are accessible from the MATLAB command line and from the SimBiology desktop. Because both the command line and the desktop point to the same model object in the `Root object`, any changes you make to the model at the command line are reflected in the desktop, and vice versa.

Constructor Summary

sbiomodel	Construct model object

Method Summary

addcompartment (model, compartment)	Create compartment object
addconfigset (model)	Create configuration set object and add to model object
adddose (model)	Add dose object to model
addevent (model)	Add event object to model object
addobservable	Add observable object to SimBiology model
addparameter (model, kineticlaw)	Create parameter object and add to model or kinetic law object
addreaction (model)	Create reaction object and add to model object
addrule (model)	Create rule object and add to model object
addspecies (model, compartment)	Create species object and add to compartment object within model object
addvariant (model)	Add variant to model
copyobj	Copy SimBiology object and its children
createSimFunction (model)	Create SimFunction object
delete	Delete SimBiology object
display	Display summary of SimBiology object
export (model)	Export SimBiology models for deployment and standalone applications
findUnusedComponents (model)	Find unused species, parameters, and compartments in a model
get	Get SimBiology object properties
getadjacencymatrix (model)	Get adjacency matrix from model object
getconfigset (model)	Get configuration set object from model object
getdose (model)	Return SimBiology dose object
getequations	Return system of equations for model object
getstoichmatrix (model)	Get stoichiometry matrix from model object
getvariant (model)	Get variant from model
removeconfigset (model)	Remove configuration set from model
removedose (model)	Remove dose object from model
removevariant (model)	Remove variant from model
rename	Rename object and update expressions
reorder (model, compartment, kinetic law)	Reorder component lists
set	Set SimBiology object properties
setactiveconfigset (model)	Set active configuration set for model object
verify (model, variant)	Validate and verify SimBiology model

Property Summary

Compartments	Array of compartments in model or compartment
Events	Contain all event objects
Name	Specify name of object
Notes	HTML text describing SimBiology object
Observables	Array of observable objects
Parameters	Array of parameter objects
Parent	Indicate parent object
Reactions	Array of reaction objects
Rules	Array of rules in model object
Tag	Specify label for SimBiology object
Type	Display SimBiology object type
UserData	Specify data to associate with object

See Also

`AbstractKineticLaw object`, `Configset object`, `KineticLaw object`, `Parameter object`, `Reaction object`, `Root object`, `Rule object`, `Species object`

Version History

Introduced in R2006b

move

Move SimBiology species or parameter object to new parent

Syntax

```
spObj = move(spObj,parentObj)
spObj = move(spObj,parentObj,conflictOption)
```

Description

`spObj = move(spObj,parentObj)` moves a SimBiology species or parameter object `spObj` to a new parent SimBiology object `parentObj`. The function automatically updates the corresponding expressions, observables, variants, and parameterized dose properties that reference `spObj`. Expressions include reactions, kinetic laws, rules, and events.

`spObj = move(spObj,parentObj,conflictOption)` specifies how to handle naming conflicts if `parentObj` is already the parent of another object with the same name as `spObj`.

Examples

Move SimBiology Species or Parameter Object to New Parent

Create a model with two compartments.

```
m = sbiomodel('cell');
c1 = addcompartment(m,'c1');
c2 = addcompartment(m,'c2');
B_c1 = addspecies(c1,'B');
B_c2 = addspecies(c2,'B');
p = addparameter(m,'k1',5);
r = addreaction(m,'c1.A + c1.B -> c2.B');
k = addkineticlaw(r,'MassAction');
k.ParameterVariableNames = 'k1';
```

The parameter is scoped to the model, which is the parent.

```
p.Parent
```

```
ans =
   SimBiology Model - cell

   Model Components:
     Compartments:      2
     Events:            0
     Parameters:        1
     Reactions:         1
     Rules:             0
     Species:           3
     Observables:       0
```

Move the model-scoped parameter to the kinetic law.

```
p = move(p,k);
```

The parent is now the kinetic law object instead of the model object.

```
p.Parent
```

```
ans =
   SimBiology Kinetic Law Array

   Index:    KineticLawName:
   1         MassAction
```

Move species `B` from compartment `c1` to `c2`. *c2* already has another species with the same name, so use the `'force'` option to resolve the naming conflict. The `move` function renames `B` to `B_1`.

```
B = move(B_c1,c2,'force')
```

```
B =
   SimBiology Species Array

   Index:    Compartment:    Name:    Value:    Units:
   1         c2              B_1      0
```

Input Arguments

`spObj` — SimBiology species or parameter

species object | parameter object

SimBiology species or parameter, specified as a species object or parameter object.

If `spObj` is a:

- Parameter object, `parentObj` must be a model, reaction, or kinetic law object.
- Species object, `parentObj` must be a compartment object.

If you move a parameter to a reaction, the reaction kinetic law is the new parent of the parameter. The function creates an `unknown` kinetic law if the reaction does not already have a kinetic law.

`parentObj` — Parent object

model object | reaction object | kinetic law object | compartment object

Parent object, specified as a model object, reaction object, kinetic law object, or compartment object.

`conflictOption` — Method to resolve naming conflicts

`'strict'` (default) | `'force'`

Method to resolve naming conflicts, specified as a character vector or string. Valid options are:

- `'strict'` — The function throws an error if `parentObj` is already the parent of another object with the same name as `spObj`.
- `'force'` — The function changes the name of `spObj` by appending `'_N'`, where `N` is the smallest number such that the new name of `spObj` is unique among all objects parented to `parentObj`.

Version History

Introduced in R2020b

See Also

`move` | `copyobj` | `Compartment` | `Species` | `Parameter` | `Model` | `Reaction` | `KineticLaw` | `Observable`

move

Move SimBiology compartment object to new owner

Syntax

```
compObj = move(compObj,newOwner)
```

Description

`compObj = move(compObj,newOwner)` moves a SimBiology compartment object `compObj` to a new owner `newOwner`.

Examples

Move SimBiology Compartment to New Owner

Create a model with two compartments.

```
m = sbiomodel('cell');
c1 = addcompartment(m,'c1');
c2 = addcompartment(m,'c2');
p = addparameter(m,'k1',5);
r = addreaction(m,'c1.A + c1.B -> c2.B');
k = addkineticlaw(r,'MassAction');
k.ParameterVariableNames = 'k1';
```

Move compartment `c1` to `c2`.

```
c1 = move(c1,c2);
```

The owner of `c1` is now `c2`.

```
c1.Owner
```

```
ans =
   SimBiology Compartment - c2

   Compartment Components:
     Value:             1
     Units:
     Compartments:      1
     Constant:          true
     Owner:
     Species:           1
```

Input Arguments

compObj — SimBiology compartment

compartment object

SimBiology compartment, specified as a compartment object.

`newOwner` — New owner object
model object | compartment object

New owner object, specified as a model object or compartment object.

Version History

Introduced in R2020b

See Also

`copyobj` | `move` | `Compartment` | `Species` | `Parameter` | `Model` | `Reaction` | `KineticLaw` | `Observable`

SimBiology.gsa.MPGSA

Object containing multiparametric global sensitivity analysis (MPGSA) results

Description

The `SimBiology.gsa.MPGSA` object contains multiparametric global sensitivity analysis [1] results returned by `sbiompgsa`.

Creation

Create a `SimBiology.gsa.MPGSA` object using `sbiompgsa`.

Properties

`Classifiers` — Expressions of model responses

cell array of character vectors

This property is read-only.

Expressions of model responses, specified as a cell array of character vectors.

Data Types: `cell`

`KolmogorovSmirnovStatistics` — Kolmogorov-Smirnov statistics

table

This property is read-only.

Kolmogorov-Smirnov statistics, specified as a table. The table size is [*params*,*classifiers*], where *params* is the number of input parameters and *classifiers* is the number of classifiers. Entry `[i,j]` contains the Kolmogorov-Smirnov statistic returned by `kstest2` comparing the two eCDFs of the *i*th parameter accepted and rejected by the *j*th classifier. If all samples are accepted or rejected by the classifier, entry `[i,j]` is set to `NaN`.

The `VariableNames` property contains the classifier expressions specified as the input to `sbiompgsa`. Long expressions are truncated with the addition of `'(classifier i)'`, where *i* is the classifier index. The `VariableDescriptions` property contains the untruncated classifier expressions.

Data Types: `table`

`ECDFData` — Computed eCDF data

cell array of numeric vectors

This property is read-only.

Computed eCDF data, specified as a cell array of numeric vectors. The size of the array is `[params,4,classifiers]`, where *params* is the number of input parameters and *classifiers* is the number of classifiers.

Cells `[i,1:2,j]` contain the “f” (Statistics and Machine Learning Toolbox) and “x” (Statistics and Machine Learning Toolbox) outputs from the `ecdf` function for the samples of parameter *i* accepted by the classifier *j*.

Cells `[i,3:4,j]` contain the corresponding outputs for the samples of parameter *i* rejected by the classifier *j*.

If the classifier accepts all samples or rejects all samples, the corresponding eCDF data is empty.

Data Types: `cell`

`SignificanceLevel` — Significance level of two-sided Kolmogorov-Smirnov test
`0.05` (default) | scalar value in the range (0,1)

This property is read-only.

Significance level of the two-sided Kolmogorov-Smirnov test, specified as a scalar value in the range (0,1). For details, see `kstest2` .

Data Types: `double`

`PValues` — Asymptotic *p*-values
table

This property is read-only.

Asymptotic *p*-values for the Kolmogorov-Smirnov tests, specified as a table. The table size is [*params*,*classifiers*], where *params* is the number of input parameters and *classifiers* is the number of classifiers.

Entry `[i,j]` contains the p-values returned by `kstest2` comparing the two eCDFs of the *i*th parameter being accepted and rejected by the *j*th classifier. If all samples are accepted or rejected by the classifier, entry `[i,j]` is set to `NaN`.

The `VariableNames` property contains the classifier expressions specified as the input to `sbiompgsa`. Long expressions are truncated with the addition of `'(classifier i)'`, where *i* is the classifier index. The `VariableDescriptions` property contains the untruncated classifier expressions.

Data Types: `table`

`SupportHypothesis` — Flags indicating if samples are accepted by classifiers
table

This property is read-only.

Flags indicating if the samples are accepted by the classifiers, specified as a table. The table size is [*NumberSamples*,*classifiers*], where *NumberSamples* is the number of parameter samples and *classifiers* is the number of classifiers.

The `VariableNames` property contains the classifier expressions specified as the input to `sbiompgsa`. Long expressions are truncated with the addition of `'(classifier i)'`, where *i* is the classifier index. The `VariableDescriptions` property contains the untruncated classifier expressions.

Data Types: `table`

`Observables` — Names of model responses or observables

cell array of character vectors

This property is read-only.

Names of model responses or observables, specified as a cell array of character vectors.

Data Types: `char`

`ParameterSamples` — Sampled parameter values

table

This property is read-only.

Sampled parameter values, specified as a table. Each row represents one parameter set and each column represents one input parameter. For details, see “Multiparametric Global Sensitivity Analysis (MPGSA)” on page 2-455.

Data Types: `table`

`SimulationInfo` — Simulation information used for multiparametric global sensitivity analysis

structure

This property is read-only.

Simulation information, such as simulation data and parameter samples, used for multiparametric global sensitivity analysis, specified as a structure. The structure contains the following fields.

- `SimFunction` — `SimFunction` object used for simulating model responses or observables.
- `SimData` — `SimData` array of size `[`*`NumberSamples`*`,1]`, where *“NumberSamples” on page 1-0* is the number of samples. The array contains simulation results from `ParameterSamples`.
- `OutputTimes` — Numeric column vector containing the common time vector of all `SimData` objects.
- `Bounds` — Numeric matrix of size `[`*`params`*`,2]`. *params* is the number of input parameters. The first column contains the lower bounds and the second column contains the upper bounds for sensitivity inputs.

  This field is set to `[]` if you provided parameter sample values as input when you called `sbiompgsa`.
- `DoseTables` — Cell array of dose tables used for the `SimFunction` evaluation. `DoseTables` is the output of `getTable(doseInput)`, where *doseInput* is the value specified for the `'Doses'` name-value pair argument in the call to `sbiosobol`, `sbiompgsa`, or `sbioelementaryeffects`. If no doses are applied, this field is set to `[]`.
- `ValidSample` — Logical vector of size `[`*`NumberSamples`*`,1]` indicating whether a simulation for a particular sample failed. Resampling of the simulation data (SimData) can result in `NaN` values if the data is extrapolated. Such SimData are indicated as invalid.
- `InterpolationMethod` — Name of the interpolation method for `SimData`.
- `SamplingMethod` — Name of the sampling method used to draw `ParameterSamples`. When you call `sbiompgsa` with `samples` (sampled model quantities) as the input, this field of the corresponding results object is set to `'unknown'`.

- `RandomState` — Structure containing the state of `rng` before drawing `ParameterSamples`. When you call `sbiompgsa` with `samples` (parameter sample values) as an input, this property of the corresponding results object is `[]`.

Data Types: `struct`

Object Functions

plotData	Plot quantile summary of model simulations from global sensitivity analysis (requires Statistics and Machine Learning Toolbox)
plot	Plot empirical CDF of multiparametric global sensitivity analysis
bar	Create bar plot of multiparametric global sensitivity analysis statistics
histogram	Plot histogram of multiparametric global sensitivity analysis results

Examples

Perform Multiparametric Global Sensitivity Analysis (MPGSA)

Load the "Target-Mediated Drug Disposition (TMDD) Model".

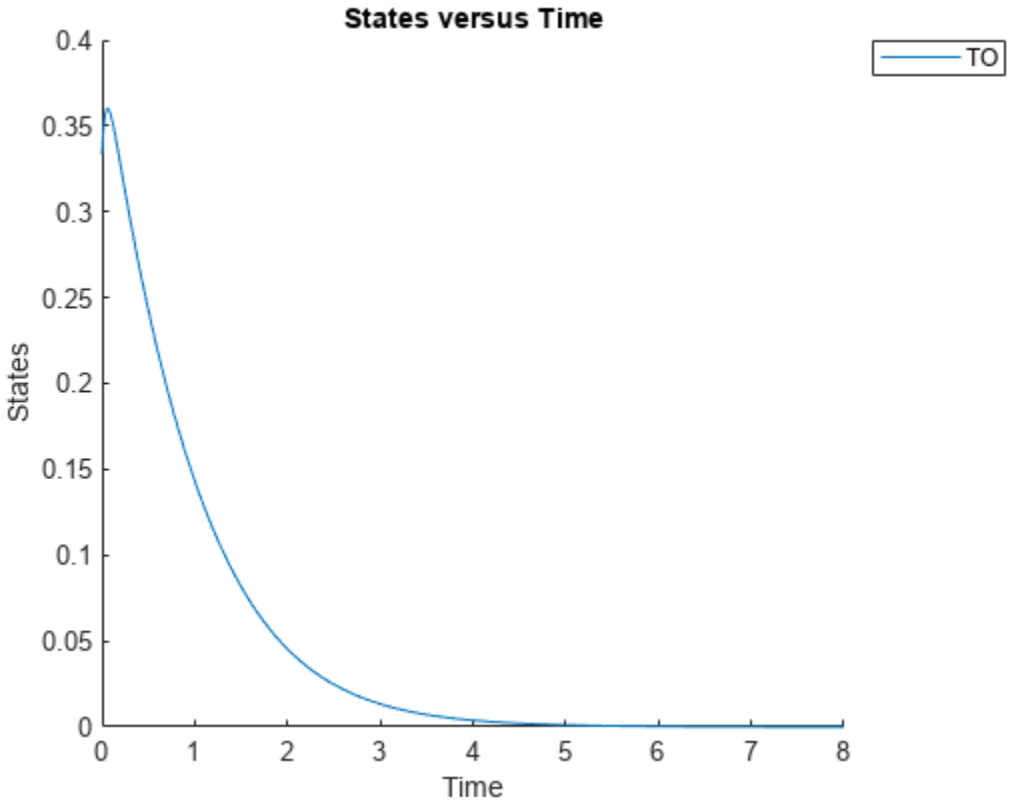
```
sbioloadproject tmdd_with_T0.sbproj
```

Get the active configset and set the target occupancy (`T0`) as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'T0';
```

Simulate the model and plot the `T0` profile.

```
sbioplot(sbiosimulate(m1,cs));
```



Define an exposure (area under the curve of the TO profile) threshold for the target occupancy.

```
classifier = 'trapz(time,TO) <= 0.1';
```

Perform MPGSA to find sensitive parameters with respect to the TO. Vary the parameter values between predefined bounds to generate 10,000 parameter samples.

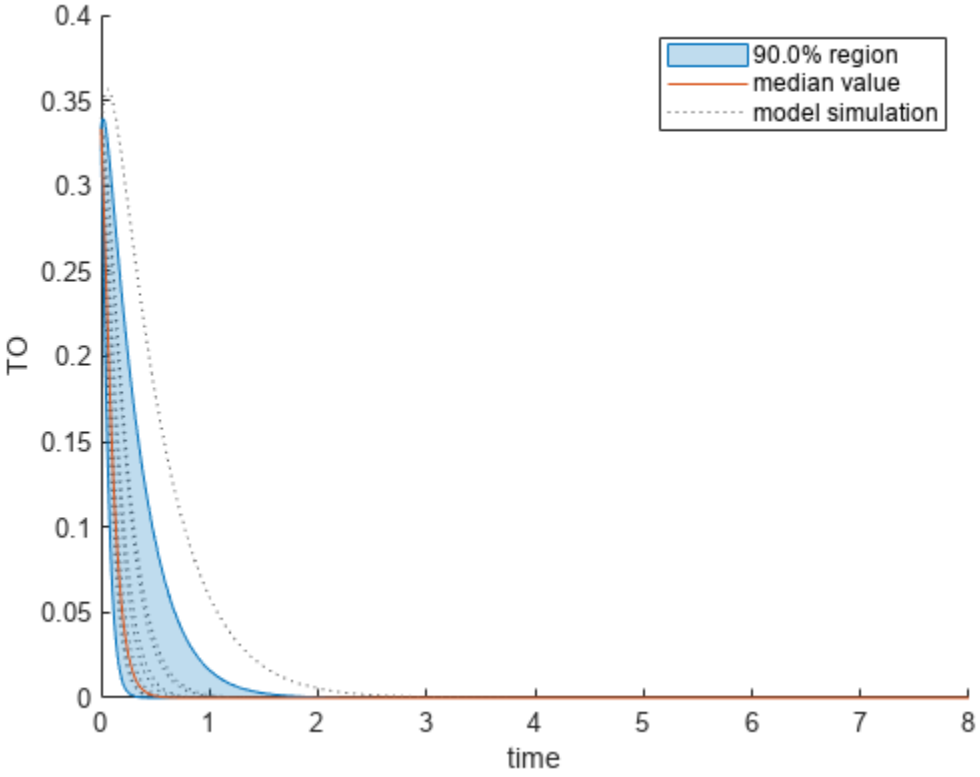
```
% Suppress an information warning that is issued during simulation.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
rng(0,'twister'); % For reproducibility
params = {'kel','ksyn','kdeg','km'};
bounds = [0.1, 1;
          0.1, 1;
          0.1, 1;
          0.1, 1];
mpgsaResults = sbiompgsa(m1,params,classifier,Bounds=bounds,NumberSamples=10000)
```

```
mpgsaResults =
  MPGSA with properties:

                   Classifiers: {'trapz(time,TO) <= 0.1'}
    KolmogorovSmirnovStatistics: [4x1 table]
                       ECDFData: {4x4 cell}
             SignificanceLevel: 0.0500
                       PValues: [4x1 table]
             SupportHypothesis: [10000x1 table]
              ParameterSamples: [10000x4 table]
                   Observables: {'TO'}
```

```
    SimulationInfo: [1x1 struct]
```

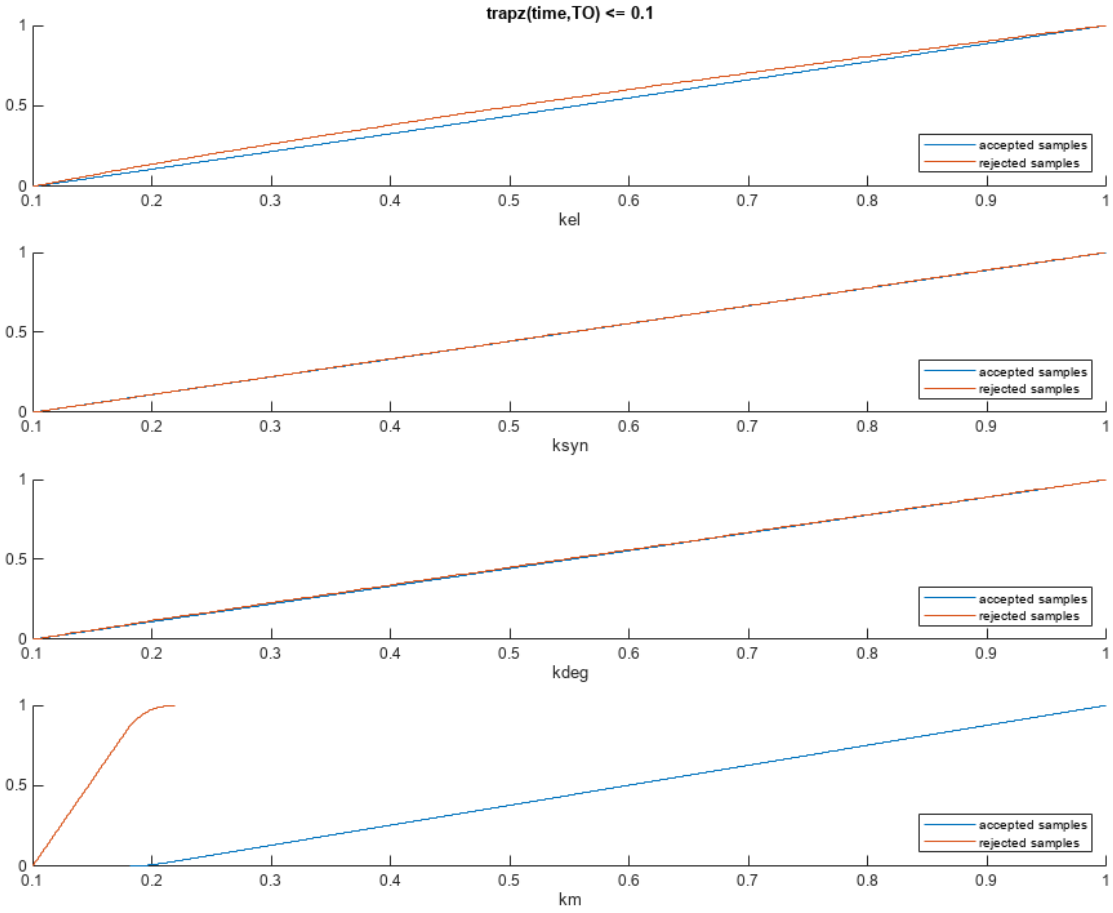
Plot the quantiles of the simulated model response.

```
plotData(mpgsaResults,ShowMedian=true,ShowMean=false);
```



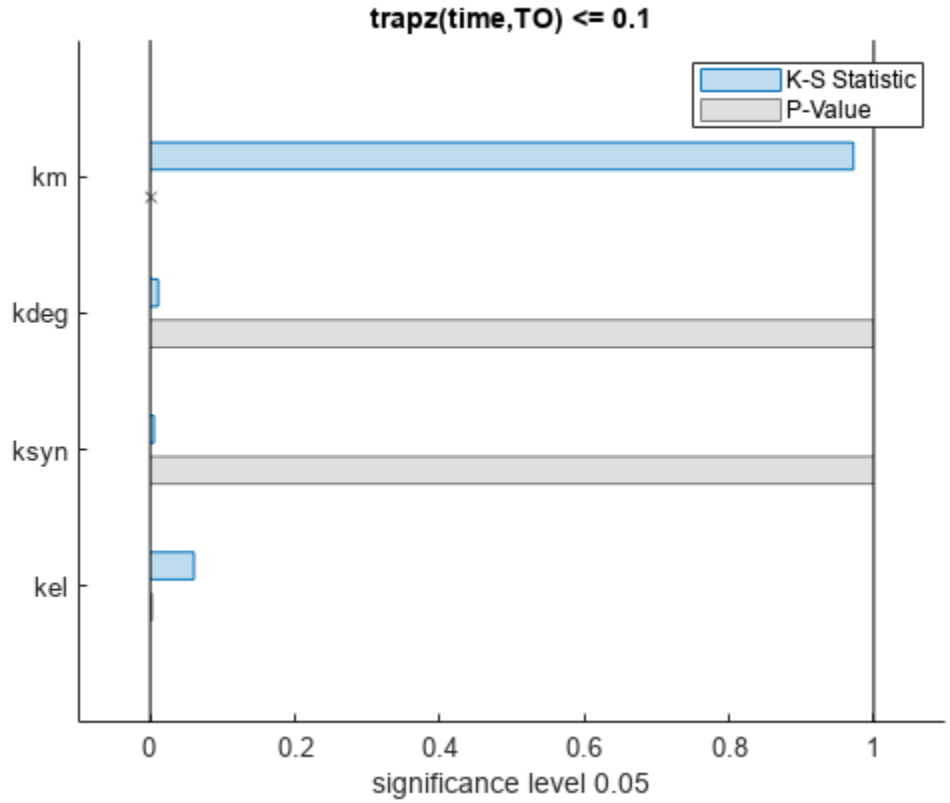
Plot the empirical cumulative distribution functions (eCDFs) of the accepted and rejected samples. Except for `km`, none of the parameters shows a significant difference in the eCDFs for the accepted and rejected samples. The `km` plot shows a large Kolmogorov-Smirnov (K-S) distance between the eCDFs of the accepted and rejected samples. The K-S distance is the maximum absolute distance between two eCDFs curves.

```
h = plot(mpgsaResults);
% Resize the figure.
pos = h.Position(:);
h.Position(:) = [pos(1) pos(2) pos(3)*2 pos(4)*2];
```



To compute the K-S distance between the two eCDFs, SimBiology uses a two-sided test based on the null hypothesis that the two distributions of accepted and rejected samples are equal. See `kstest2` (Statistics and Machine Learning Toolbox) for details. If the K-S distance is large, then the two distributions are different, meaning that the classification of the samples is sensitive to variations in the input parameter. On the other hand, if the K-S distance is small, then variations in the input parameter do not affect the classification of samples. The results suggest that the classification is insensitive to the input parameter. To assess the significance of the K-S statistic rejecting the null-hypothesis, you can examine the p-values.

```
bar(mpgsaResults)
```



The bar plot shows two bars for each parameter: one for the K-S distance (K-S statistic) and another for the corresponding p-value. You reject the null hypothesis if the p-value is less than the significance level. A cross (x) is shown for any p-value that is almost 0. You can see the exact p-value corresponding to each parameter.

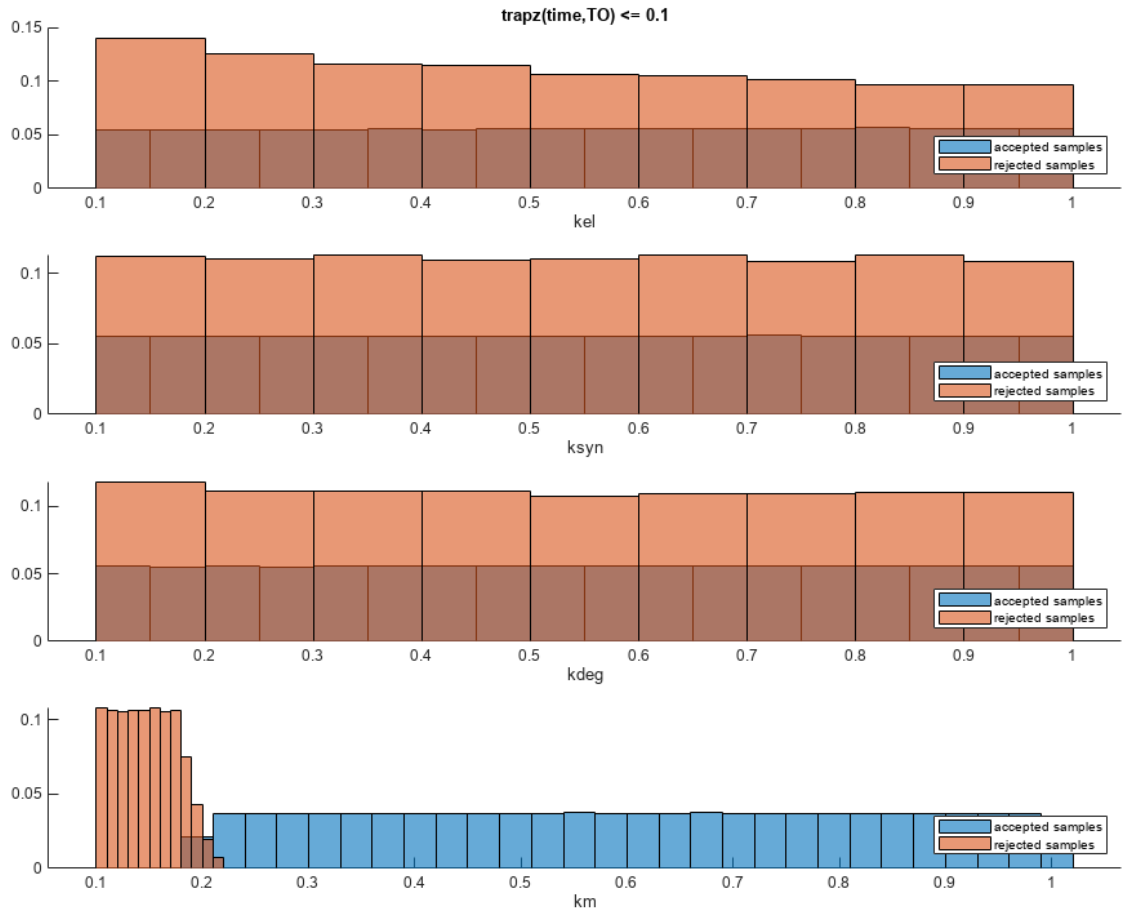
```
[mpgsaResults.ParameterSamples.Properties.VariableNames',mpgsaResults.PValues]
```

```
ans=4×2 table
      Var1      trapz(time,TO) <= 0.1
    ________    _____________________

    {'kel' }          0.0021877
    {'ksyn'}                  1
    {'kdeg'}            0.99983
    {'km'  }                  0
```

The p-values of `km` and `kel` are less than the significance level (0.05), supporting the alternative hypothesis that the accepted and rejected samples come from different distributions. In other words, the classification of the samples is sensitive to `km` and `kel` but not to other parameters (`kdeg` and `ksyn`).

You can also plot the histograms of accepted and rejected samples. The historgrams let you see trends in the accepted and rejected samples. In this example, the histogram of `km` shows that there are more accepted samples for larger `km` values, while the `kel` histogram shows that there are fewer rejected samples as `kel` increases.

```
h2 = histogram(mpgsaResults);
% Resize the figure.
pos = h2.Position(:);
h2.Position(:) = [pos(1) pos(2) pos(3)*2 pos(4)*2];
```



Restore the warning settings.

```
warning(warnSettings);
```

More About

Multiparametric Global Sensitivity Analysis (MPGSA)

Multiparametric global sensitivity analysis lets you study the relative importance of parameters with respect to a classifier defined by model responses. A classifier is an expression of model responses that evaluates to a logical vector. `sbiompgsa` implements the MPSA method described by Tiemann et. al. (see supporting information text S2) [1].

`sbiompgsa` performs the following steps.

1. Generate *N* parameter samples using a sampling method. `sbiompgsa` stores these samples as a table in a property, `mpgsaResults.ParameterSamples`, of the returned object. The number of rows is equal to the number of samples and the number of columns is equal to the number of input parameters.

   Tip You can specify *N* and the sampling method using the `'NumberSamples'` and `'SamplingMethod'` name-value pair arguments, respectively, when you call `sbiompgsa`.

2. Calculate the model response by simulating the model for each parameter set, which is a single realization of the model parameter values. In this case, a parameter set is equal to a row in the `ParameterSamples` table.
3. Evaluate the classifier. A classifier is an expression that evaluates to a logical vector. For instance, if your model response is the AUC of plasma drug concentration, you can define a classifier with a toxicity threshold of 0.8 where the AUC of the drug concentration above that threshold is considered toxic.
4. Parameter sets are then separated into two different groups, such as accepted (nontoxic) and rejected (toxic) groups.
5. For each input parameter, compute the empirical cumulative distribution functions (`ecdf`) of accepted and rejected sample values.
6. Compare the two eCDFs of accepted and rejected groups using the “Two-Sample Kolmogorov-Smirnov Test” (Statistics and Machine Learning Toolbox) to compute the Kolmogorov-Smirnov distance. The default significance level of the Kolmogorov-Smirnov test is `0.05`. If two eCDFs are similar, the distance is small, meaning the model response is not sensitive with respect to the input parameter. If two eCDFs are different, the distance is large, meaning the model response is sensitive to the parameter.

   Note The Kolmogorov-Smirnov test assumes that the samples follow a continuous distribution. Make sure that the eCDF plots are continuous as you increase the number of samples. If eCDFs are not continuous but step-like in the limit of infinite samples, then the results might not reflect the true sensitivities.

Version History

Introduced in R2020a

References

[1] Tiemann, Christian A., Joep Vanlier, Maaike H. Oosterveer, Albert K. Groen, Peter A. J. Hilbers, and Natal A. W. van Riel. “Parameter Trajectory Analysis to Identify Treatment Effects of Pharmacological Interventions.” Edited by Scott Markel. *PLoS Computational Biology* 9, no. 8 (August 1, 2013): e1003166. https://doi.org/10.1371/journal.pcbi.1003166.

See Also

`sbiosobol` | `sbiompgsa` | `kstest2` | `ecdf` | `Observable`

Topics

“Sensitivity Analysis in SimBiology”

NLINResults

Estimation results object for `nlinfit` algorithm

Description

The `NLINResults` object contains estimation results from fitting a SimBiology model to data using `sbiofit` with `nlinfit` as a choice of estimation algorithm. See the `sbiofit` function for a list of other supported algorithms.

Creation

Use `sbiofit` with `nlinfit` estimation algorithm to create an `NLINResults` object.

Properties

`GroupName` — Name of the group associated with the results

categorical | empty array

Name of the group associated with the results, specified as a categorical. If the `'Pooled'` name-value pair argument was set to `true` when you ran `sbiofit`, then `GroupName` is returned as an empty array or `[]`.

`Beta` — Table of estimated parameters

table

Table of estimated parameters, specified as a table. The *j*th row of the table represents the *j*th estimated parameter β_j. It contains transformed values of parameter estimates if any parameter transform is specified. Standard errors of these parameter estimates (`StandardError`) are calculated as: `sqrt(diag(COVB))`.

It can also contain the following variables:

- `Bounds` — the values of transformed parameter bounds that you specified during fitting
- `CategoryVariableName` — the names of categories or groups that you specified during fitting
- `CategoryValue` — the values of category variables specified by `CategoryVariableName`

This table contains one row per distinct parameter value.

`ParameterEstimates` — Table of estimated parameters

table

Table of estimated parameters, specified as a table. The *j*th row of the table represents the *j*th estimated parameter β_j. This table contains untransformed values of parameter estimates. Standard errors of these parameter estimates (`StandardError`) are calculated as: `sqrt(diag(CovarianceMatrix))`.

It can also contain the following variables:

- `Bounds` — the values of transformed parameter bounds that you specified during fitting
- `CategoryVariableName` — the names of categories or groups that you specified during fitting
- `CategoryValue` — the values of category variables specified by `CategoryVariableName`

This table contains sets of parameter values that are identified for each individual or group.

`J` — Jacobian matrix of the model
array

Jacobian matrix of the model, specified as an array. The Jacobian matrix with respect to an estimated parameter is

$$J(i,j,k) = \left.\frac{\partial y_k}{\partial \beta_j}\right|_{t_i}$$

where t_i is the ith time point, β_j is the jth estimated parameter in the transformed space, and y_k is the kth response in the group of data.

`COVB` — Estimated covariance matrix for `Beta`
matrix

Estimated covariance matrix for `Beta`, specified as a matrix. This matrix is calculated as: `COVB = inv(J'*J)*MSE`.

`CovarianceMatrix` — Estimated covariance matrix for `ParameterEstimates`
matrix

Estimated covariance matrix for `ParameterEstimates`, specified as a matrix. This matrix is calculated as: `CovarianceMatrix = T'*COVB*T`, where `T = diag(JInvT(Beta))`. `JInvT(Beta)` returns a Jacobian matrix of `Beta` which is inverse transformed accordingly if you specified any transform to estimated parameters.

For instance, suppose you specified the log-transform for an estimated parameter `x` when you ran `sbiofit`. The inverse transform is: `InvT = exp(x)`, and its Jacobian is: `JInvT = exp(x)` since the derivative of `exp` is also `exp`.

`R` — Residuals matrix
matrix

Residuals matrix, specified as a matrix. R_{ij} is the residual for the ith time point and the jth response in the group of data.

`LogLikelihood` — Maximized loglikelihood for the fitted model
scalar

Maximized loglikelihood for the fitted model, specified as a scalar.

`AIC` — Akaike Information Criterion (AIC)
scalar

Akaike Information Criterion (AIC), specified as a scalar. The AIC is calculated as `AIC = 2*(-LogLikelihood + P)`, where P is the number of parameters.

`BIC` — Bayes Information Criterion (BIC)
scalar

Bayes Information Criterion (BIC), specified as a scalar. The BIC is calculated as `BIC = -2*LogLikelihood + P*log(N)`, where *N* is the number of observations, and *P* is the number of parameters.

`DFE` — Degrees of freedom for error
scalar

Degrees of freedom for error (DFE), specified as a scalar. The DFE is calculated as `DFE = N-P`, where *N* is the number of observations and *P* is the number of parameters.

`MSE` — Mean squared error
scalar

Mean squared error, specified as a scalar.

`SSE` — Sum of squared (weighted) errors or residuals
scalar

Sum of squared (weighted) errors or residuals, specified as a scalar.

`Weights` — Matrix of weights
matrix

Matrix of weights, specified as a matrix with one column per response and one row per observation.

`Data` — Data used for fitting
`groupedData` object

Data used for fitting, specified as a `groupedData` object.

In most cases, this `Data` property contains a copy of `groupedData` specified as the input data in the `sbiofit on page 1-0` call or the Data property of a `fitproblem` object. One exception is that the `Data` property of unpooled fit results objects contain only the subset of data for the individual group used for fitting.

`EstimatedParameterNames` — Estimated parameter names
cell array of character vectors

Estimated parameter names, specified as a cell array of character vectors.

`ErrorModelInfo` — Error models and estimated error model parameters
table

Error models and estimated error model parameters, specified as a table.

- The table has one row per error model.
- The `ErrorModelInfo.Properties.RowsNames` property identifies which responses the row applies to.
- The table contains three variables: `ErrorModel`, `a`, and `b`. The `ErrorModel` variable is categorical. The variables `a` and `b` can be `NaN` when they do not apply to a particular error model.

There are four built-in error models. Each model defines the error using a standard mean-zero and unit-variance (Gaussian) variable *e*, the function value *f*, and one or two parameters *a* and *b*. In SimBiology, the function *f* represents simulation results from a SimBiology model.

- `'constant'`: $y = f + ae$
- `'proportional'`: $y = f + b|f|e$
- `'combined'`: $y = f + (a + b|f|)e$
- `'exponential'`: $y = f * \exp(ae)$

`EstimationFunction` — Name of the estimation function
character vector

Name of the estimation function, specified as a character vector.

`DependentFiles` — File names to include for deployment
cell array of character vectors

File names to include for deployment, specified as a cell array of character vectors.

Object Functions

boxplot	Create box plot showing the variation of estimated SimBiology model parameters
fitted	Return simulation results of SimBiology model fitted using least-squares regression
plot	Compare simulation results to the training data, creating a time-course subplot for each group
plotActualVersusPredicted	Compare predictions to actual data, creating a subplot for each response
plotResidualDistribution	Plot the distribution of the residuals
plotResiduals	Plot residuals for each response, using time, group, or prediction as x-axis
predict	Simulate and evaluate fitted SimBiology model
random	Simulate SimBiology model, adding variations by sampling error model
summary	Return structure array that contains estimated values and fit quality statistics

Version History

Introduced in R2014a

See Also

`LeastSquaresResults object` | `OptimResults object` | `sbiofit` | `sbiofitmixed`

NLMEResults

Results object containing estimation results from nonlinear mixed-effects modeling

Description

The `NLMEResults` object contains estimation results from fitting a nonlinear mixed-effects model using `sbiofitmixed`.

Creation

Use the `sbiofitmixed` function to create an `NLMEResults` object.

Properties

`FixedEffects` — Table of the estimated fixed effects and their standard errors
table

Table of the estimated fixed effects and their standard errors, specified as a table.

`RandomEffects` — Table of the estimated random effects for each group
table

Table of the estimated random effects for each group, specified as a table.

`IndividualParameterEstimates` — Table of estimated parameter values, including fixed and random effects
table

Table of estimated parameter values, including fixed and random effects, specified as a table.

`PopulationParameterEstimates` — Table of estimated parameter values, including only fixed effects
table

Table of estimated parameter values, including only fixed effects, specified as a table.

`RandomEffectCovarianceMatrix` — Table of the covariance matrix of the random effects
table

Table of the covariance matrix of the random effects, specified as a table.

`stats` — Statistics returned by the `nlmefit` and `nlmefitsa` algorithm
structure array

Statistics returned by the `nlmefit` and `nlmefitsa` algorithm, specified as a structure array.

`CovariateNames` — Covariate names
cell array of character vectors

Covariate names, specified as a cell array of character vectors.

`Data` — Data used for fitting
`groupedData` object

Data used for fitting, specified as a `groupedData` object.

This `Data` property contains a copy of `groupedData` specified as the input data in the `sbiofitmixed on page 1-0` call or the Data property of a `fitproblem` object.

`EstimatedParameterNames` — Estimated parameter names
cell array of character vectors

Estimated parameter names, specified as a cell array of character vectors.

`ErrorModelInfo` — Table describing the error models and estimated error model parameters
table

Table describing the error models and estimated error model parameters, specified as a table.

The table has one row with three variables: `ErrorModel`, `a`, and `b`. The `ErrorModel` variable is categorical. The variables `a` and `b` can be `NaN` when they do not apply to a particular error model.

There are four built-in error models. Each model defines the error using a standard mean-zero and unit-variance (Gaussian) variable e, the function value f, and one or two parameters a and b. In SimBiology, the function f represents simulation results from a SimBiology model.

- `'constant'`: $y = f + ae$
- `'proportional'`: $y = f + b|f|e$
- `'combined'`: $y = f + (a + b|f|)e$
- `'exponential'`: $y = f * \exp(ae)$

`EstimationFunction` — Name of the estimation function
`'nlmefit'` | `'nlmefitsa'`

Name of the estimation function, specified as `'nlmefit'` or `'nlmefitsa'`.

`LogLikelihood` — Maximized loglikelihood for the fitted model
scalar

Maximized loglikelihood for the fitted model, specified as a scalar.

`AIC` — Akaike Information Criterion (AIC)
scalar

Akaike Information Criterion (AIC), specified as a scalar. The AIC is calculated as `AIC = 2*(-LogLikelihood + P)`, where P is the number of parameters. For details, see `nlmefit`.

`BIC` — Bayes Information Criterion (BIC)
scalar

Bayes Information Criterion (BIC), specified as a scalar. The BIC is calculated as `BIC = -2*LogLikelihood + P*log(N)`, where N is the number of observations or groups, and P is the number of parameters. For details, see `nlmefit`.

`DFE` — Degrees of freedom for error

scalar

Degrees of freedom for error (DFE), specified as a scalar. The DFE is calculated as `DFE = N-P`, where N is the number of observations and P is the number of parameters.

Note If you are using the `nlmefitsa` method, `Loglikelihood`, `AIC`, and `BIC` properties are empty by default. To calculate these values, specify the `'LogLikMethod'` option of `nlmefitsa` when you run `sbiofitmixed` as follows.

```
opt.LogLikMethod = 'is';
fitResults = sbiofitmixed(...,'nlmefitsa',opt);
```

Object Functions

boxplot	Create box plot showing the variation of estimated SimBiology model parameters
covariateModel	Return a copy of the covariate model that was used for the nonlinear mixed-effects estimation using sbiofitmixed
fitted	Return the simulation results of a fitted nonlinear mixed-effects model
plot	Compare simulation results to the training data, creating a time-course subplot for each group
plotActualVersusPredicted	Compare predictions to actual data, creating a subplot for each response
plotResidualDistribution	Plot the distribution of the residuals
plotResiduals	Plot the residuals for each response, using the time, group, or prediction as the x-axis
predict	Simulate and evaluate fitted SimBiology model
random	Simulate a SimBiology model, adding variations by sampling the error model

Examples

Fit a One-Compartment PK Model to the Phenobarbital Data

This example uses data collected on 59 preterm infants given phenobarbital during the first 16 days after birth [1]. Each infant received an initial dose followed by one or more sustaining doses by intravenous bolus administration. A total of between 1 and 6 concentration measurements were obtained from each infant at times other than dose times, for a total of 155 measurements. Infant weights and APGAR scores (a measure of newborn health) were also recorded.

Load the data.

```
load pheno.mat ds
```

Convert the dataset to a `groupedData object`, a container for holding tabular data that is divided into groups. It can automatically identify commonly used variable names as the grouping variable or independent (time) variable. Display the properties of the data and confirm that `GroupVariableName` and `IndependentVariableName` are correctly identified as `'ID'` and `'TIME'`, respectively.

```
data = groupedData(ds);
data.Properties
```

```
ans = struct with fields:
                Description: ''
                   UserData: []
             DimensionNames: {'Observations'  'Variables'}
              VariableNames: {'ID'  'TIME'  'DOSE'  'WEIGHT'  'APGAR'  'CONC'}
       VariableDescriptions: {}
              VariableUnits: {}
         VariableContinuity: []
                   RowNames: {}
           CustomProperties: [1×1 matlab.tabular.CustomProperties]
          GroupVariableName: 'ID'
    IndependentVariableName: 'TIME'
```

Create a simple one-compartment PK model with bolus dosing and linear clearance to fit such data. Use the `PKModelDesign` object to construct the model. Each compartment is defined by a name, dosing type, a clearance type, and whether or not the dosing requires a lag parameter. After constructing the model, you can also get a `PKModelMap` object `map` that lists the names of species and parameters in the model that are most relevant for fitting.

```
pkmd = PKModelDesign;
addCompartment(pkmd,'Central','DosingType','Bolus',...
                    'EliminationType','linear-clearance',...
                    'HasResponseVariable',true,'HasLag',false);
[onecomp, map] = pkmd.construct;
```

Describe the experimentally measured response by mapping the appropriate model component to the response variable. In other words, indicate which species in the model corresponds to which response variable in the data. The `PKModelMap` property `Observed` indicates that the relevant species in the model is `Drug_Central`, which represents the drug concentration in the system. The relevant data variable is `CONC`, which you visualized previously.

```
map.Observed
```

```
ans = 1×1 cell array
    {'Drug_Central'}
```

Map the `Drug_Central` species to the `CONC` variable.

```
responseMap = 'Drug_Central = CONC';
```

The parameters to estimate in this model are the volume of the central compartment `Central` and the clearance rate `Cl_Central`. The `PKModelMap` property `Estimated` lists these relevant parameters. The underlying algorithm of `sbiofit` assumes parameters are normally distributed, but this assumption may not be true for biological parameters that are constrained to be positive, such as volume and clearance. Specify a log transform for the estimated parameters so that the transformed parameters follow a normal distribution. Use an `estimatedInfo` object to define such transforms and initial values (optional).

```
map.Estimated
```

```
ans = 2×1 cell
    {'Central'   }
    {'Cl_Central'}
```

Define such estimated parameters, appropriate transformations, and initial values.

```
estimatedParams = estimatedInfo({'log(Central)','log(Cl_Central)'},'InitialValue',[1 1]);
```

Each infant received a different schedule of dosing. The amount of drug is listed in the data variable `DOSE`. To specify these dosing during fitting, create dose objects from the data. These objects use the property `TargetName` to specify which species in the model receives the dose. In this example, the target species is `Drug_Central`, as listed by the `PKModelMap` property `Dosed`.

```
map.Dosed
```

```
ans = 1×1 cell array
    {'Drug_Central'}
```

Create a sample dose with this target name and then use the `createDoses` method of `groupedData` object `data` to generate doses for each infant based on the dosing data `DOSE`.

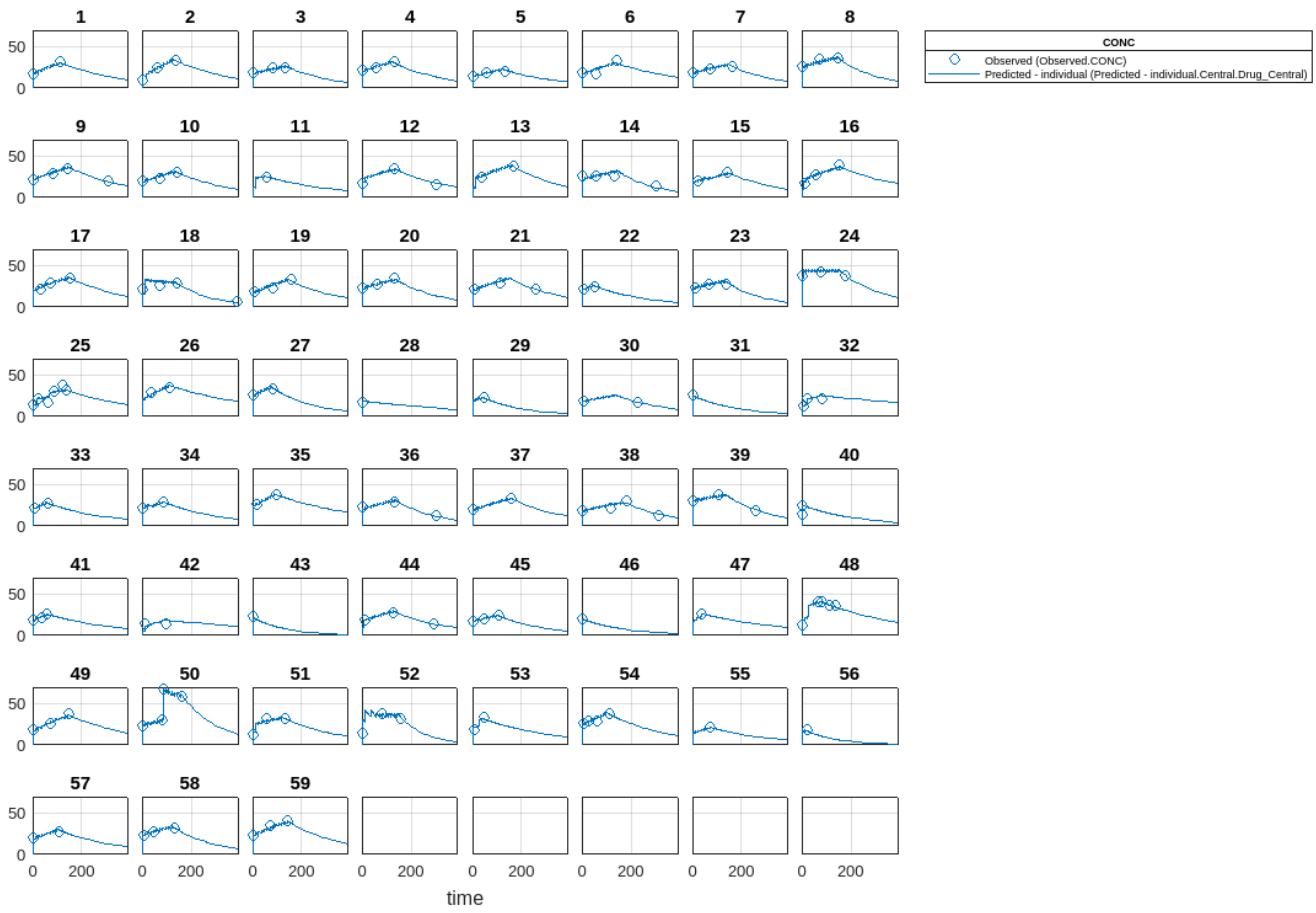
```
sampleDose = sbiodose('sample','TargetName','Drug_Central');
doses = createDoses(data,'DOSE','',sampleDose);
```

Fit the model.

```
[nlmeResults,simI,simP] = sbiofitmixed(onecomp,data,responseMap,estimatedParams,doses,'nlmefit')
```

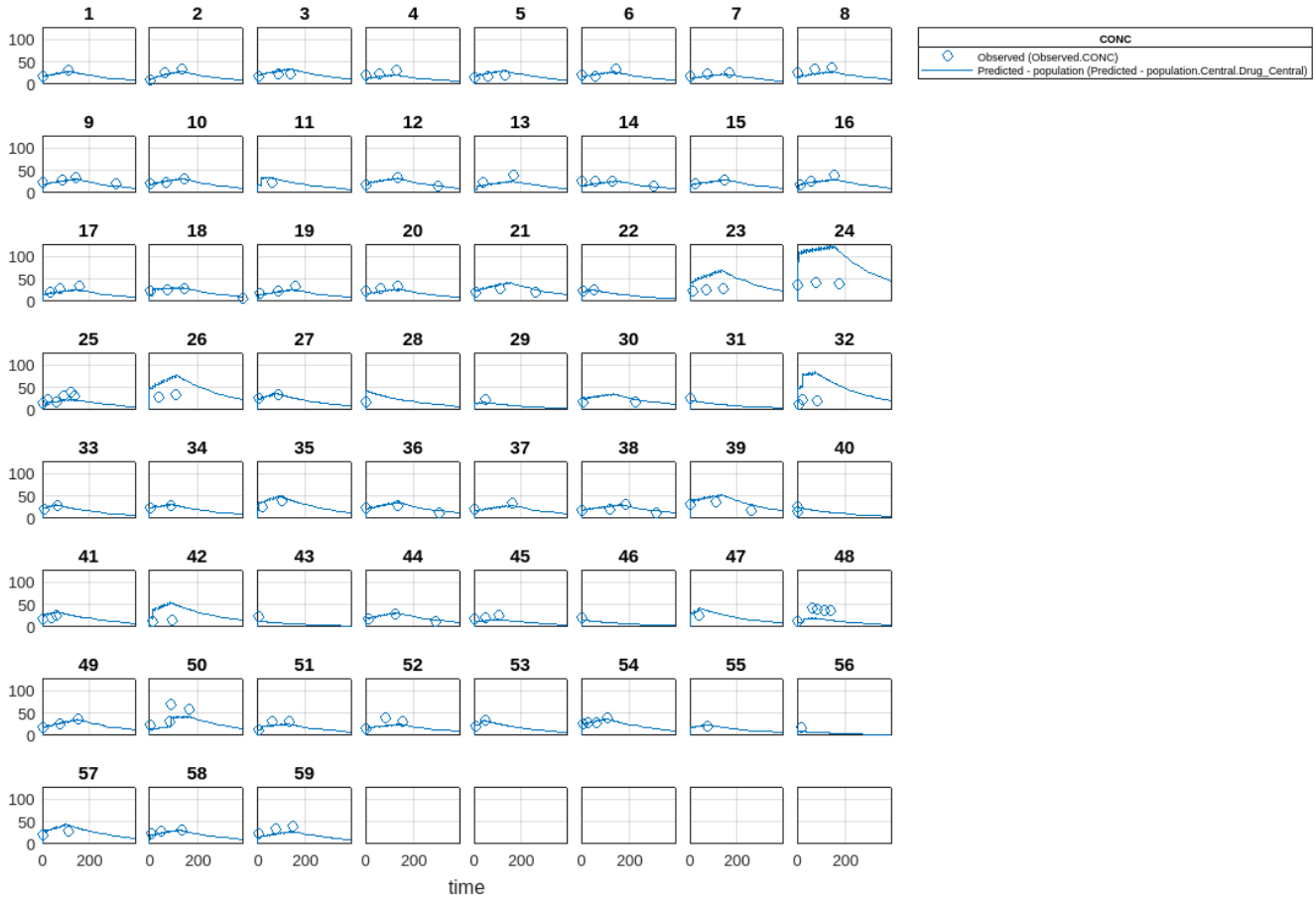
Visualize the fitted results using individual-specific parameter estimates.

```
plot(nlmeResults,'ParameterType','individual');
```



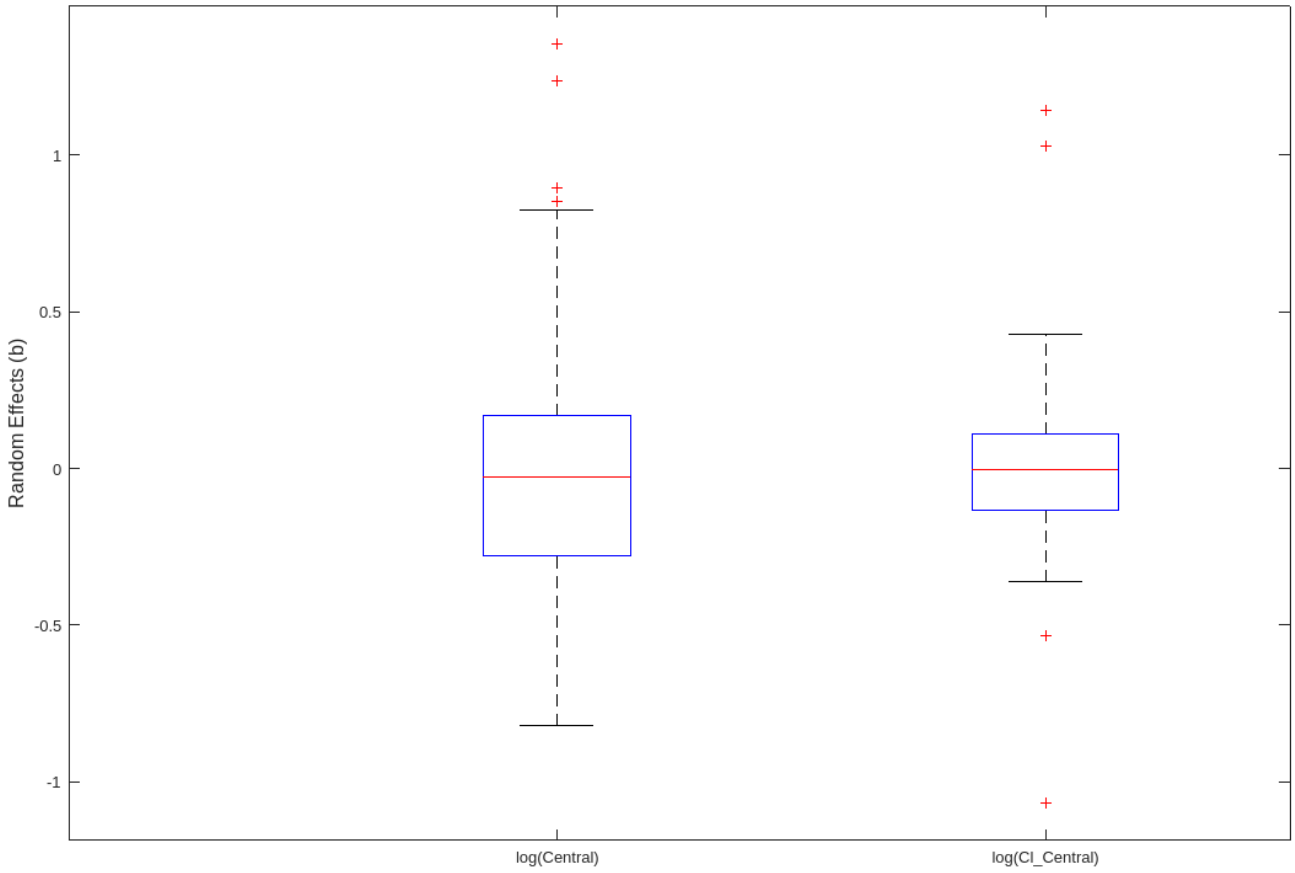
Visualize the fitted results using population parameter estimates.

```
plot(nlmeResults,'ParameterType','population');
```



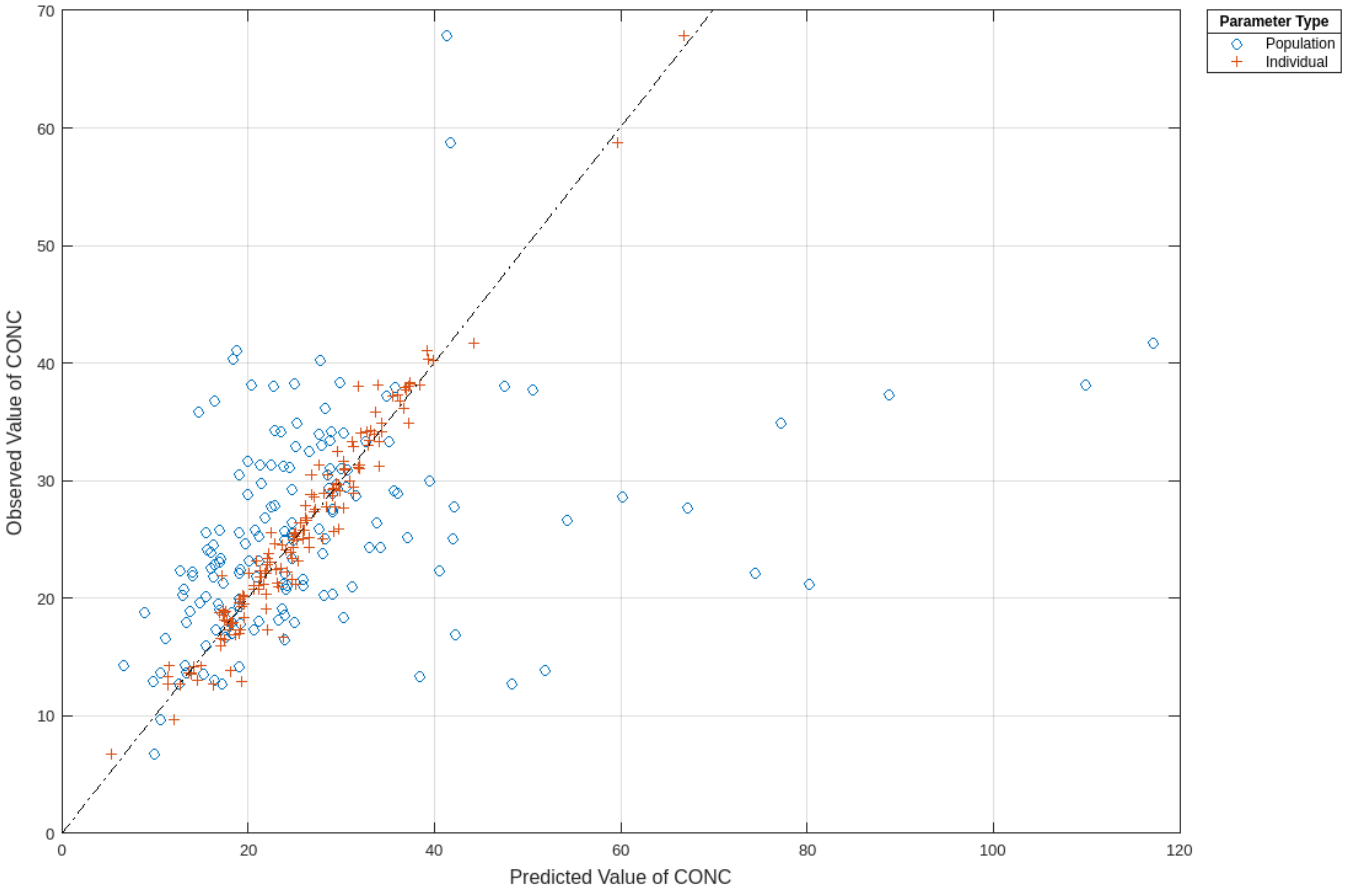
Display the variation of estimated parameters using boxplot.

```
boxplot(nlmeResults)
```



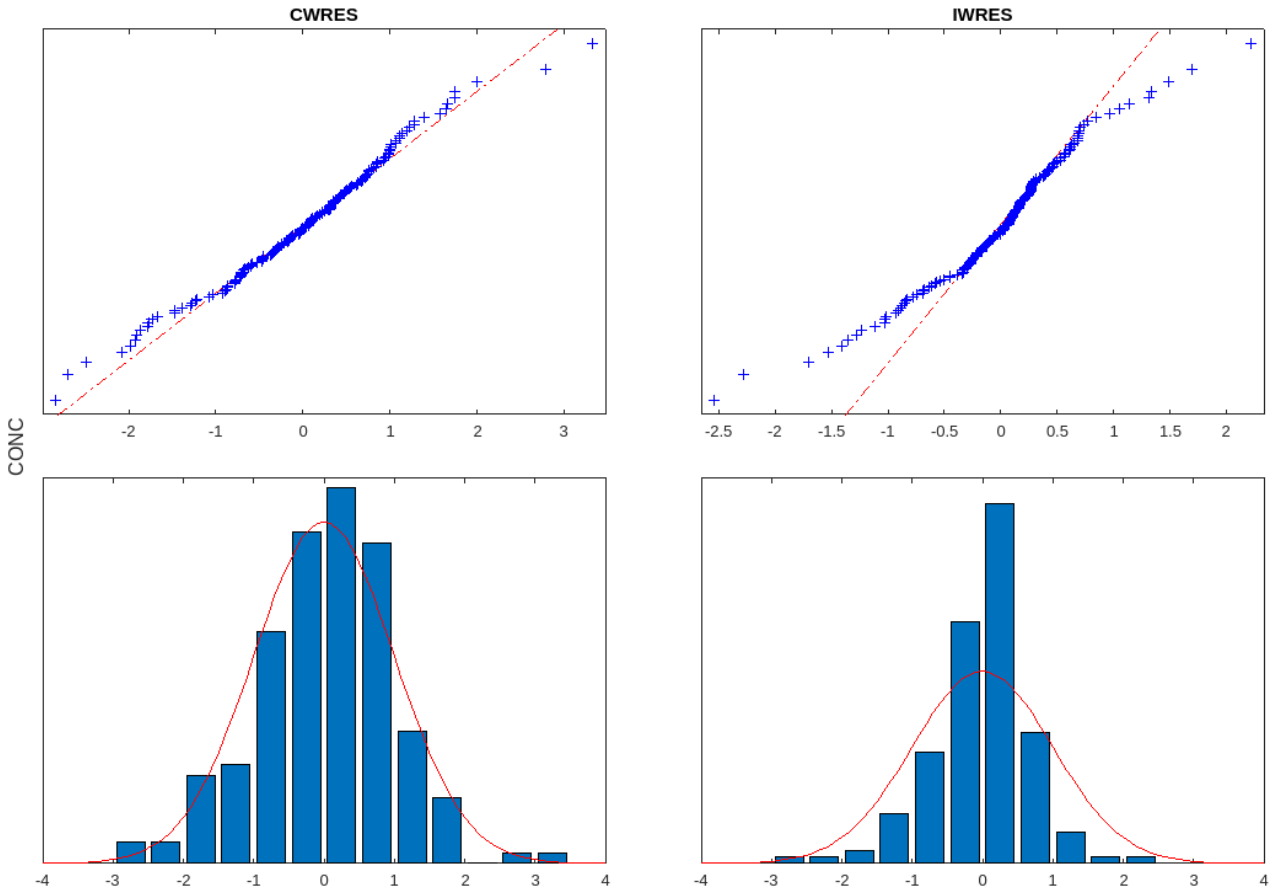
Compare the model predictions to the actual data.

```
plotActualVersusPredicted(nlmeResults)
```



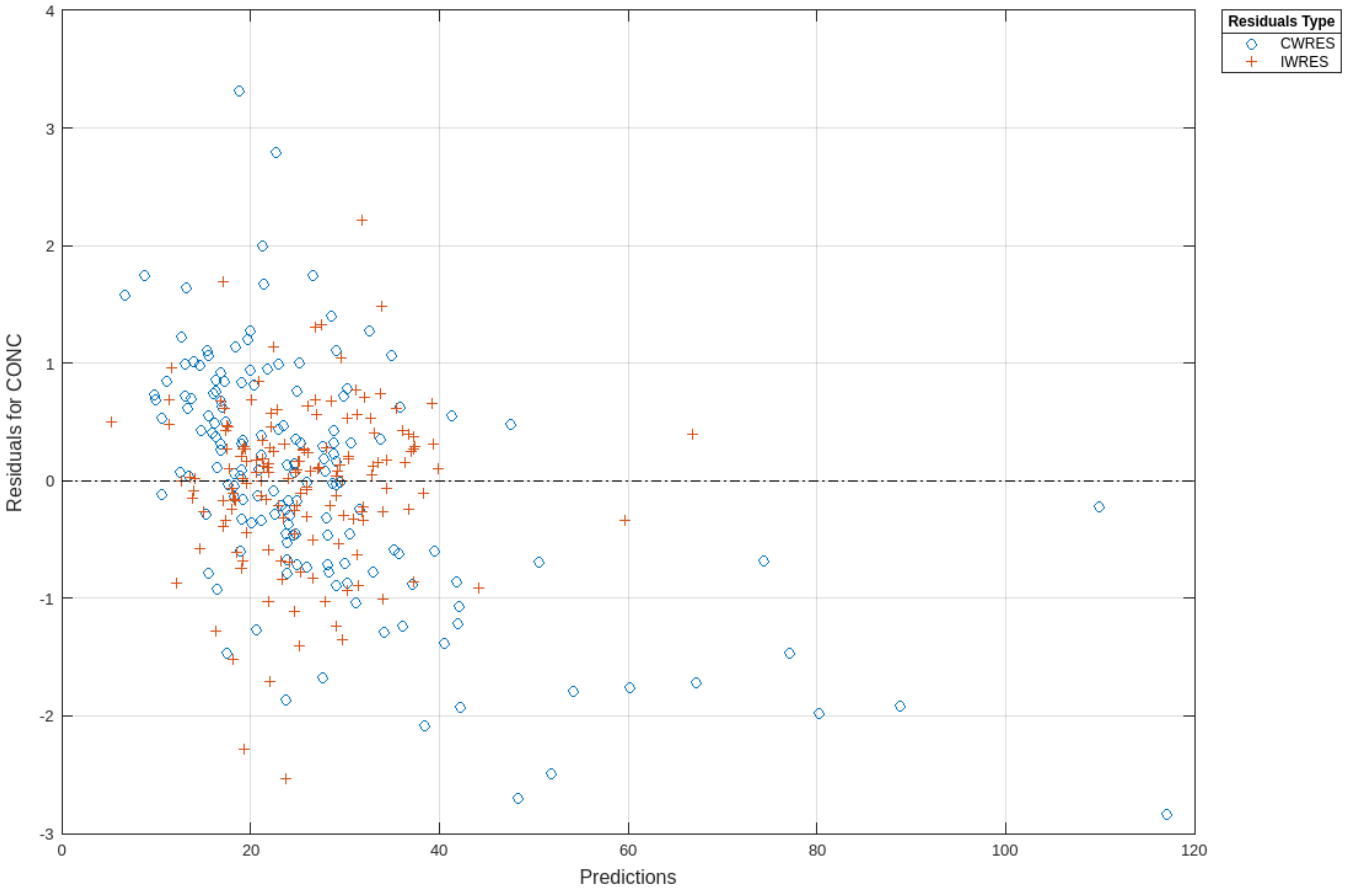
Plot the distribution of residuals.

```
plotResidualDistribution(nlmeResults)
```



Plot residuals for each response using the model predictions on *x*-axis.

```
plotResiduals(nlmeResults,'Predictions')
```



Version History

Introduced in R2014a

See Also

`sbiofitmixed` | `sbiofit` | `nlmefit` | `nlmefitsa`

Observable

Object containing expression for post-simulation calculations

Description

An observable object is a mathematical expression that lets you perform post-simulation calculations. For example, you can define an observable expression to compute the fraction of a ligand that is bound to a receptor at each time step, or compute some statistics such as area under the curve (AUC) of a drug concentration profile. You can also use an observable object as a response in simulation, data fitting, and global sensitivity analysis.

The name of each observable object in a SimBiology model must be unique, meaning no observable object can have the same name as another observable, species, compartment, parameter, reaction, variant, or dose in the model. An observable object can reference any model quantities that are logged (in `StatesToLog`). It can also reference other active observable objects provided that the expressions contain no algebraic loops. The object expression can reference simulation time using the variable *time*. Follow the recommended guidelines for expression evaluations. For instance, if a quantity name is not a valid MATLAB variable name, enclose the name in brackets `[]` when referring to it in an expression.

SimBiology evaluates the object expression using the entire time course of any referenced states or observables. The result of an observable expression must be a numeric scalar or vector. If it is a vector, it must be of the same length as the simulation time vector. The result is stored in the returned `SimData` object. Specifically, if the observable expression is scalar-valued, the result is stored in the `SimData.ScalarObservables` property. Otherwise, it is stored in `SimData.VectorObservables`.

Note

- Make sure to correctly vectorize the expressions. For example, use `A./(A+B)` instead of `A/(A+B)` if *A* and *B* are matrices.
- Avoid hardcoding expressions that expect any particular number of points or times. For example, instead of using `time(1:1000)`, use `time(1:min(1000,numel(time)))`.

Creation

Create an observable object using `addobservable`.

Properties

`Expression` — Mathematical expression
character vector

Mathematical expression of the observable object, specified as a character vector.

Example: `'x.^2'`

Data Types: `char`

`Units` — Units of observable results
`''` (default) | character vector

Units of the observable expression results, specified as a character vector.

Example: `'gram'`

Data Types: `char`

`Active` — Flag indicating whether to evaluate observable expression
`true` (default) | `false`

Flag indicating whether to evaluate the observable expression after model simulation, specified as `true` or `false`.

Example: `false`

Data Types: `logical`

`Name` — Object name
character vector

Object name, specified as a character vector.

Example: `'AUC'`

Data Types: `char`

`Parent` — Parent object
model object (default)

This property is read-only.

Parent object of the observable object, specified as a model object.

`Notes` — Description of object
`''` (default) | character vector

Description of the object, specified as a character vector.

Example: `'Drug AUC'`

Data Types: `char`

`Tag` — Object label
`''` (default) | character vector

Object label, specified as a character vector.

Example: `'area under the curve'`

Data Types: `char`

`Type` — Object type
`'observable'` (default)

This property is read-only.

Object type, specified as `'observable'`.

Data Types: `char`

`UserData` — Data to associate with object
`[]` (default) | any supported data type

Data to associate with the object, specified as any supported MATLAB data type.

Object Functions

copyobj	Copy SimBiology object and its children
findUsages	Find out how observable object is used in SimBiology model
get	Get SimBiology object properties
set	Set SimBiology object properties
delete	Delete SimBiology object
display	Display summary of SimBiology object
rename	Rename object and update expressions

Examples

Calculate Statistics After Model Simulation Using Observables

Load the "Target-Mediated Drug Disposition (TMDD) Model".

```
sbioloadproject tmdd_with_TO.sbproj
```

Set the target occupancy (`TO`) as a response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'TO';
```

Get the dosing information.

```
d = getdose(m1,'Daily Dose');
```

Scan over different dose amounts using a `SimBiology.Scenarios` object. To do so, first parameterize the `Amount` property of the dose. Then vary the corresponding parameter value using the `Scenarios` object.

```
amountParam = addparameter(m1,'AmountParam','Units',d.AmountUnits);
d.Amount = 'AmountParam';
d.Active = 1;
doseSamples = SimBiology.Scenarios('AmountParam',linspace(0,300,31));
```

Create a `SimFunction` to simulate the model. Set `TO` as the simulation output.

```
% Suppress informational warnings that are issued during simulation.
warning('off','SimBiology:SimFunction:DOSES_NOT_EMPTY');
f = createSimFunction(m1,doseSamples,'TO',d)
```

```
f =
SimFunction

Parameters:
```

```
        Name          Value        Type           Units
    ________________    _____    _____________    ___________

    {'AmountParam'}       1      {'parameter'}    {'nanomole'}

Observables:

     Name         Type              Units
    ______    _____________    _________________

    {'T0'}    {'parameter'}    {'dimensionless'}

Dosed:

      TargetName                TargetDimension                    Amount          AmountValue    A
    ________________    ____________________________________    _____________    ___________    -

    {'Plasma.Drug'}    {'Amount (e.g., mole or molecule)'}    {'AmountParam'}         1         -

TimeUnits: day
```

```
warning('on','SimBiology:SimFunction:DOSES_NOT_EMPTY');
```

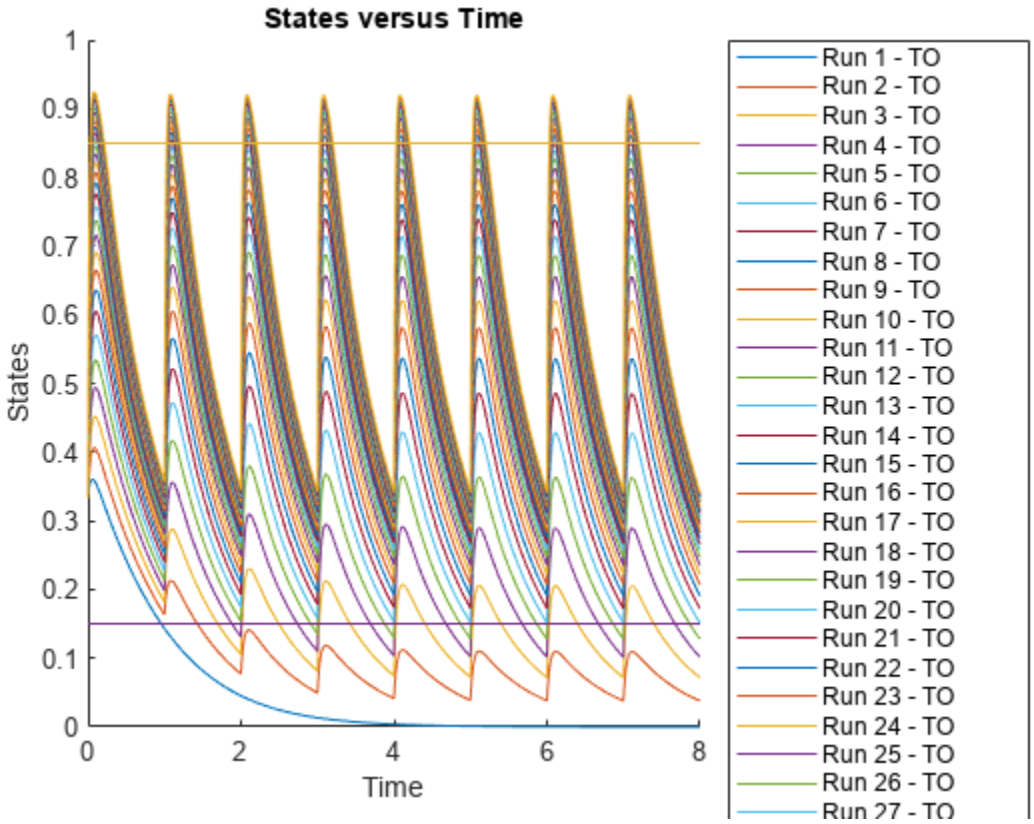
Simulate the model using the dose amounts generated by the `Scenarios` object. In this case, the object generates 31 different doses; hence the model is simulated 31 times and generates a `SimData` array.

```
doseTable = getTable(d);
sd = f(doseSamples,cs.StopTime,doseTable)
```

```
   SimBiology Simulation Data Array: 31-by-1

   ModelName:        TMDD
   Logged Data:
     Species:        0
     Compartment:    0
     Parameter:      1
     Sensitivity:    0
     Observable:     0
```

Plot the simulation results. Also add two reference lines that represent the safety and efficacy thresholds for `T0`. In this example, suppose that any `T0` value above 0.85 is unsafe, and any `T0` value below 0.15 has no efficacy.

```
h = sbioplot(sd);
time = sd(1).Time;
h.NextPlot = 'add';
safetyThreshold = plot(h,[min(time), max(time)],[0.85, 0.85],'DisplayName','Safety Threshold');
efficacyThreshold = plot(h,[min(time), max(time)],[0.15, 0.15],'DisplayName','Efficacy Threshold
```



Postprocess the simulation results. Find out which dose amounts are effective, corresponding to the `TO` responses within the safety and efficacy thresholds. To do so, add an observable expression to the simulation data.

```
% Suppress informational warnings that are issued during simulation.
warning('off','SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
newSD = addobservable(sd,'stat1','max(TO) < 0.85 & min(TO) > 0.15','Units','dimensionless')
```

```
SimBiology Simulation Data Array: 31-by-1

ModelName:        TMDD
Logged Data:
  Species:        0
  Compartment:    0
  Parameter:      1
  Sensitivity:    0
  Observable:     1
```

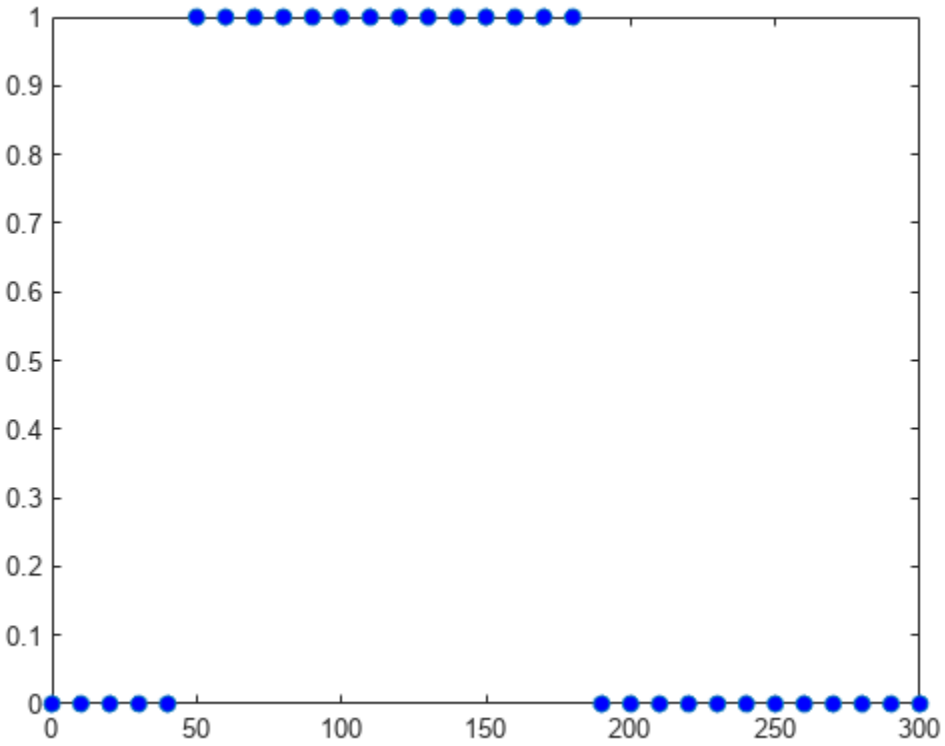
The addobservable function evaluates the new observable expression for each `SimData` in `sd` and returns the evaluated results as a new `SimData` array, `newSD`, which now has the added observable (`stat1`).

SimBiology stores the observable results in two different properties of a `SimData` object. If the results are scalar-valued, they are stored in `SimData.ScalarObservables`. Otherwise, they are

stored in `SimData.VectorObservables`. In this example, the `stat1` observable expression is scalar-valued.

Extract the scalar observable values and plot them against the dose amounts.

```
scalarObs = vertcat(newSD.ScalarObservables);
doseAmounts = generate(doseSamples);
figure
plot(doseAmounts.AmountParam,scalarObs.stat1,'o','MarkerFaceColor','b')
```



The plot shows that dose amounts ranging from 50 to 180 nanomoles provide `T0` responses that lie within the target efficacy and safety thresholds.

You can update the observable expression with different threshold amounts. The function recalculates the expression and returns the results in a new `SimData` object array.

```
newSD2 = updateobservable(newSD,'stat1','max(T0) < 0.75 & min(T0) > 0.30');
```

Rename the observable expression. The function renames the observable, updates any expressions that reference the renamed observable (if applicable), and returns the results in a new `SimData` object array.

```
newSD3 = renameobservable(newSD2,'stat1','EffectiveDose');
```

Restore the warning settings.

```
warning('on','SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
```

Version History

Introduced in R2020a

See Also

`addobservable(model)` | `addobservable(SimData)` | `updateobservable(SimData)` | `renameobservable(SimData)`

OptimResults

Estimation results object for any supported algorithm except `nlinfit`

Description

The `OptimResults` object contains estimation results from fitting a SimBiology model to data using the `sbiofit` function with any supported algorithm except `nlinfit`. See the `sbiofit` function for a list of supported algorithms.

Creation

Use `sbiofit` with any supported estimation algorithm except `nlinfit` to create an `OptimResults` object.

Properties

`GroupName` — Name of the group associated with the results
categorical | empty array

Name of the group associated with the results, specified as a categorical. If the `'Pooled'` name-value pair argument was set to `true` when you ran `sbiofit`, then `GroupName` is returned as an empty array or `[]`.

`Beta` — Table of estimated parameters
table

Table of estimated parameters, specified as a table. The *j*th row of the table represents the *j*th estimated parameter β_j. It contains transformed values of parameter estimates if any parameter transform is specified. Standard errors of these parameter estimates (`StandardError`) are calculated as: `sqrt(diag(COVB))`.

It can also contain the following variables:

- `Bounds` — the values of transformed parameter bounds that you specified during fitting
- `CategoryVariableName` — the names of categories or groups that you specified during fitting
- `CategoryValue` — the values of category variables specified by `CategoryVariableName`

This table contains one row per distinct parameter value.

`ParameterEstimates` — Table of estimated parameters
table

Table of estimated parameters, specified as a table. The *j*th row of the table represents the *j*th estimated parameter β_j. This table contains untransformed values of parameter estimates. Standard errors of these parameter estimates (`StandardError`) are calculated as: `sqrt(diag(CovarianceMatrix))`.

It can also contain the following variables:

- `Bounds` — the values of transformed parameter bounds that you specified during fitting
- `CategoryVariableName` — the names of categories or groups that you specified during fitting
- `CategoryValue` — the values of category variables specified by `CategoryVariableName`

This table contains sets of parameter values that are identified for each individual or group.

`J` — Jacobian matrix of the model
array

Jacobian matrix of the model, specified as an array. The Jacobian matrix with respect to an estimated parameter is

$$J(i,j,k) = \left.\frac{\partial y_k}{\partial \beta_j}\right|_{t_i}$$

where t_i is the ith time point, β_j is the jth estimated parameter in the transformed space, and y_k is the kth response in the group of data.

`COVB` — Estimated covariance matrix for `Beta`
matrix

Estimated covariance matrix for `Beta`, specified as a matrix. This matrix is calculated as: `COVB = inv(J'*J)*MSE`.

`CovarianceMatrix` — Estimated covariance matrix for `ParameterEstimates`
matrix

Estimated covariance matrix for `ParameterEstimates`, specified as a matrix. This matrix is calculated as: `CovarianceMatrix = T'*COVB*T`, where `T = diag(JInvT(Beta))`. `JInvT(Beta)` returns a Jacobian matrix of `Beta` which is inverse transformed accordingly if you specified any transform to estimated parameters.

For instance, suppose you specified the log-transform for an estimated parameter `x` when you ran `sbiofit`. The inverse transform is: `InvT = exp(x)`, and its Jacobian is: `JInvT = exp(x)` since the derivative of `exp` is also `exp`.

`R` — Residuals matrix
matrix

Residuals matrix, specified as a matrix. R_{ij} is the residual for the ith time point and the jth response in the group of data.

`LogLikelihood` — Maximized loglikelihood for the fitted model
scalar

Maximized loglikelihood for the fitted model, specified as a scalar.

`AIC` — Akaike Information Criterion (AIC)
scalar

Akaike Information Criterion (AIC), specified as a scalar. The AIC is calculated as `AIC = 2*(-LogLikelihood + P)`, where P is the number of parameters.

`BIC` — Bayes Information Criterion (BIC)
scalar

Bayes Information Criterion (BIC), specified as a scalar. The BIC is calculated as `BIC = -2*LogLikelihood + P*log(N)`, where *N* is the number of observations, and *P* is the number of parameters.

`DFE` — Degrees of freedom for error
scalar

Degrees of freedom for error (DFE), specified as a scalar. The DFE is calculated as `DFE = N-P`, where *N* is the number of observations and *P* is the number of parameters.

`MSE` — Mean squared error
scalar

Mean squared error, specified as a scalar.

`SSE` — Sum of squared (weighted) errors or residuals
scalar

Sum of squared (weighted) errors or residuals, specified as a scalar.

`Weights` — Matrix of weights
matrix

Matrix of weights, specified as a matrix with one column per response and one row per observation.

`Data` — Data used for fitting
`groupedData` object

Data used for fitting, specified as a `groupedData` object.

In most cases, this `Data` property contains a copy of `groupedData` specified as the input data in the `sbiofit on page 1-0` call or the Data property of a `fitproblem` object. One exception is that the `Data` property of unpooled fit results objects contain only the subset of data for the individual group used for fitting.

`EstimatedParameterNames` — Estimated parameter names
cell array of character vectors

Estimated parameter names, specified as a cell array of character vectors.

`ErrorModelInfo` — Error models and estimated error model parameters
table

Error models and estimated error model parameters, specified as a table.

- The table has one row per error model.
- The `ErrorModelInfo.Properties.RowsNames` property identifies which responses the row applies to.
- The table contains three variables: `ErrorModel`, `a`, and `b`. The `ErrorModel` variable is categorical. The variables `a` and `b` can be `NaN` when they do not apply to a particular error model.

There are four built-in error models. Each model defines the error using a standard mean-zero and unit-variance (Gaussian) variable *e*, the function value *f*, and one or two parameters *a* and *b*. In SimBiology, the function *f* represents simulation results from a SimBiology model.

- `'constant'`: $y = f + ae$
- `'proportional'`: $y = f + b|f|e$
- `'combined'`: $y = f + (a + b|f|)e$
- `'exponential'`: $y = f * \exp(ae)$

`EstimationFunction` — Name of the estimation function
character vector

Name of the estimation function, specified as a character vector.

`DependentFiles` — File names to include for deployment
cell array of character vectors

File names to include for deployment, specified as a cell array of character vectors.

`ExitFlag` — Exit flag specific to the estimation function
scalar

Exit flag specific to the estimation function, specified as a scalar. See the reference page of the specific algorithm to get more information on the value of `ExitFlag`.

`Output` — Additional outputs specific to the estimation function
structure array

Additional outputs specific to the estimation function, specified as a structure array. See the reference page of the specific algorithm to get more information on the values of the `Output` structure array.

Object Functions

boxplot	Create box plot showing the variation of estimated SimBiology model parameters
fitted	Return simulation results of SimBiology model fitted using least-squares regression
plot	Compare simulation results to the training data, creating a time-course subplot for each group
plotActualVersusPredicted	Compare predictions to actual data, creating a subplot for each response
plotResidualDistribution	Plot the distribution of the residuals
plotResiduals	Plot residuals for each response, using time, group, or prediction as x-axis
predict	Simulate and evaluate fitted SimBiology model
random	Simulate SimBiology model, adding variations by sampling error model
summary	Return structure array that contains estimated values and fit quality statistics

Examples

Fit One-Compartment Model to Individual PK Profile

Background

This example shows how to fit an individual's PK profile data to one-compartment model and estimate pharmacokinetic parameters.

Suppose you have drug plasma concentration data from an individual and want to estimate the volume of the central compartment and the clearance. Assume the drug concentration versus the time profile follows the monoexponential decline $C_t = C_0 e^{-k_e t}$, where C_t is the drug concentration at time t, C_0 is the initial concentration, and k_e is the elimination rate constant that depends on the clearance and volume of the central compartment $k_e = Cl/V$.

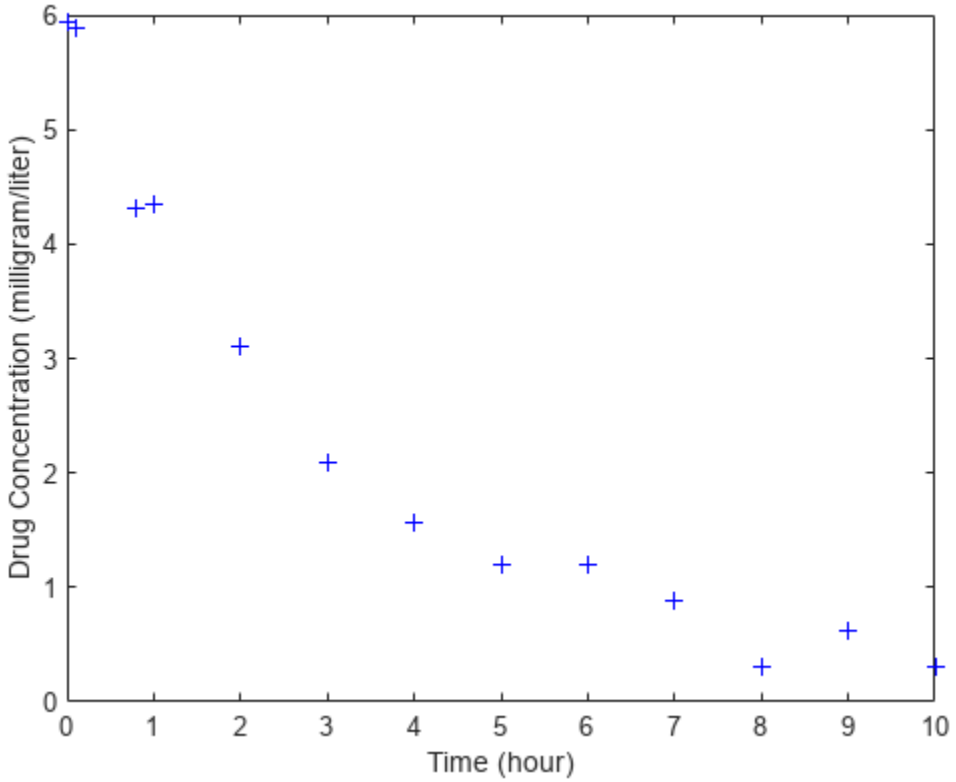
The synthetic data in this example was generated using the following model, parameters, and dose:

- One-compartment model with bolus dosing and first-order elimination
- Volume of the central compartment (`Central`) = 1.70 liter
- Clearance parameter (`Cl_Central`) = 0.55 liter/hour
- Constant error model
- Bolus dose of 10 mg

Load Data and Visualize

The data is stored as a table with variables `Time` and `Conc` that represent the time course of the plasma concentration of an individual after an intravenous bolus administration measured at 13 different time points. The variable units for `Time` and `Conc` are hour and milligram/liter, respectively.

```
load('data15.mat')
plot(data.Time,data.Conc,'b+')
xlabel('Time (hour)');
ylabel('Drug Concentration (milligram/liter)');
```



Convert to groupedData Format

Convert the data set to a `groupedData` object, which is the required data format for the fitting function `sbiofit` for later use. A `groupedData` object also lets you set independent variable and group variable names (if they exist). Set the units of the `Time` and `Conc` variables. The units are optional and only required for the `UnitConversion` feature, which automatically converts matching physical quantities to one consistent unit system.

```
gData = groupedData(data);
gData.Properties.VariableUnits = {'hour','milligram/liter'};
gData.Properties
```

```
ans = struct with fields:
                Description: ''
                   UserData: []
             DimensionNames: {'Row'  'Variables'}
              VariableNames: {'Time'  'Conc'}
       VariableDescriptions: {}
              VariableUnits: {'hour'  'milligram/liter'}
        VariableContinuity: []
                  RowNames: {}
          CustomProperties: [1x1 matlab.tabular.CustomProperties]
         GroupVariableName: ''
    IndependentVariableName: 'Time'
```

`groupedData` automatically set the name of the `IndependentVariableName` property to the `Time` variable of the data.

Construct a One-Compartment Model

Use the built-in PK library to construct a one-compartment model with bolus dosing and first-order elimination where the elimination rate depends on the clearance and volume of the central compartment. Use the `configset` object to turn on unit conversion.

```
pkmd                    = PKModelDesign;
pkc1                    = addCompartment(pkmd,'Central');
pkc1.DosingType         = 'Bolus';
pkc1.EliminationType    = 'linear-clearance';
pkc1.HasResponseVariable = true;
model                   = construct(pkmd);
configset               = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
```

For details on creating compartmental PK models using the SimBiology® built-in library, see “Create Pharmacokinetic Models”.

Define Dosing

Define a single bolus dose of 10 milligram given at time = 0. For details on setting up different dosing schedules, see “Doses in SimBiology Models”.

```
dose                = sbiodose('dose');
dose.TargetName     = 'Drug_Central';
dose.StartTime      = 0;
dose.Amount         = 10;
dose.AmountUnits    = 'milligram';
dose.TimeUnits      = 'hour';
```

Map Response Data to the Corresponding Model Component

The data contains drug concentration data stored in the `Conc` variable. This data corresponds to the `Drug_Central` species in the model. Therefore, map the data to `Drug_Central` as follows.

```
responseMap = {'Drug_Central = Conc'};
```

Specify Parameters to Estimate

The parameters to fit in this model are the volume of the central compartment (Central) and the clearance rate (Cl_Central). In this case, specify log-transformation for these biological parameters since they are constrained to be positive. The `estimatedInfo` object lets you specify parameter transforms, initial values, and parameter bounds if needed.

```
paramsToEstimate    = {'log(Central)','log(Cl_Central)'};
estimatedParams     = estimatedInfo(paramsToEstimate,'InitialValue',[1 1],'Bounds',[1 5;0.5 2]);
```

Estimate Parameters

Now that you have defined one-compartment model, data to fit, mapped response data, parameters to estimate, and dosing, use `sbiofit` to estimate parameters. The default estimation function that `sbiofit` uses will change depending on which toolboxes are available. To see which function was used during fitting, check the `EstimationFunction` property of the corresponding results object.

```
fitConst = sbiofit(model,gData,responseMap,estimatedParams,dose);
```

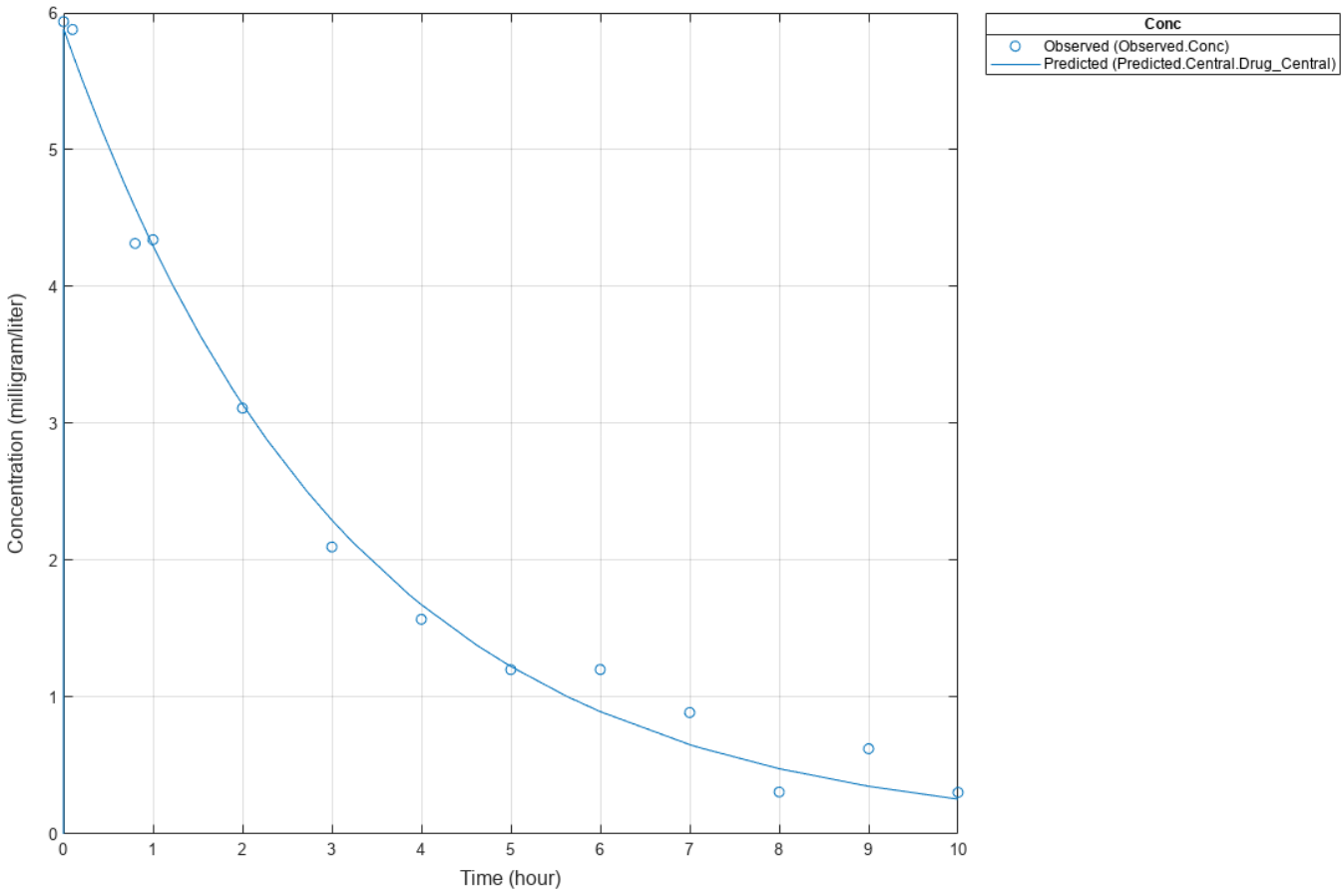
Display Estimated Parameters and Plot Results

Notice the parameter estimates were not far off from the true values (1.70 and 0.55) that were used to generate the data. You may also try different error models to see if they could further improve the parameter estimates.

```
fitConst.ParameterEstimates
```

```
ans=2×4 table
        Name          Estimate    StandardError      Bounds
    ______________    ________    _____________    __________

    {'Central'   }     1.6993       0.034821          1      5
    {'Cl_Central'}    0.53358        0.01968        0.5      2
```

```
s.Labels.XLabel     = 'Time (hour)';
s.Labels.YLabel     = 'Concentration (milligram/liter)';
plot(fitConst,'AxesStyle',s);
```



Use Different Error Models

Try three other supported error models (proportional, combination of constant and proportional error models, and exponential).

```
fitProp = sbiofit(model,gData,responseMap,estimatedParams,dose,...
                        'ErrorModel','proportional');
fitExp  = sbiofit(model,gData,responseMap,estimatedParams,dose,...
                        'ErrorModel','exponential');
fitComb = sbiofit(model,gData,responseMap,estimatedParams,dose,...
                        'ErrorModel','combined');
```

Use Weights Instead of an Error Model

You can specify weights as a numeric matrix, where the number of columns corresponds to the number of responses. Setting all weights to 1 is equivalent to the constant error model.

```
weightsNumeric = ones(size(gData.Conc));
fitWeightsNumeric = sbiofit(model,gData,responseMap,estimatedParams,dose,'Weights',weightsNumeric
```

Alternatively, you can use a function handle that accepts a vector of predicted response values and returns a vector of weights. In this example, use a function handle that is equivalent to the proportional error model.

```
weightsFunction = @(y) 1./y.^2;
fitWeightsFunction = sbiofit(model,gData,responseMap,estimatedParams,dose,'Weights',weightsFuncti
```

Compare Information Criteria for Model Selection

Compare the loglikelihood, AIC, and BIC values of each model to see which error model best fits the data. A larger likelihood value indicates the corresponding model fits the model better. For AIC and BIC, the smaller values are better.

```
allResults = [fitConst,fitWeightsNumeric,fitWeightsFunction,fitProp,fitExp,fitComb];
errorModelNames = {'constant error model','equal weights','proportional weights', ...
                   'proportional error model','exponential error model',...
                   'combined error model'};
LogLikelihood = [allResults.LogLikelihood]';
AIC = [allResults.AIC]';
BIC = [allResults.BIC]';
t = table(LogLikelihood,AIC,BIC);
t.Properties.RowNames = errorModelNames;
t
```

```
t=6×3 table
                               LogLikelihood      AIC        BIC
                               _____________    _______    _______

    constant error model           3.9866       -3.9732    -2.8433
    equal weights                  3.9866       -3.9732    -2.8433
    proportional weights          -3.8472        11.694     12.824
    proportional error model      -3.8257        11.651     12.781
    exponential error model        1.1984        1.6032     2.7331
    combined error model           3.9163       -3.8326    -2.7027
```

Based on the information criteria, the constant error model (or equal weights) fits the data best since it has the largest loglikelihood value and the smallest AIC and BIC.

Display Estimated Parameter Values

Show the estimated parameter values of each model.

```
Estimated_Central       = zeros(6,1);
Estimated_Cl_Central    = zeros(6,1);
t2 = table(Estimated_Central,Estimated_Cl_Central);
t2.Properties.RowNames = errorModelNames;
for i = 1:height(t2)
    t2{i,1} = allResults(i).ParameterEstimates.Estimate(1);
    t2{i,2} = allResults(i).ParameterEstimates.Estimate(2);
end
t2
```

```
t2=6×2 table
                                Estimated_Central    Estimated_Cl_Central
                                _________________    ____________________

    constant error model             1.6993               0.53358
    equal weights                    1.6993               0.53358
    proportional weights             1.9045               0.51734
    proportional error model         1.8777               0.51147
    exponential error model          1.7872               0.51701
    combined error model             1.7008               0.53271
```

Conclusion

This example showed how to estimate PK parameters, namely the volume of the central compartment and clearance parameter of an individual, by fitting the PK profile data to one-compartment model. You compared the information criteria of each model and estimated parameter values of different error models to see which model best explained the data. Final fitted results suggested both the constant and combined error models provided the closest estimates to the parameter values used to generate the data. However, the constant error model is a better model as indicated by the loglikelihood, AIC, and BIC information criteria.

Version History

Introduced in R2014a

See Also

`LeastSquaresResults object` | `NLINResults object` | `sbiofit` | `sbiofitmixed`

Parameter object

Parameter and scope information

Description

The parameter object represents a *parameter*, which is a quantity that can change or can be constant. SimBiology parameters are generally used to define rate constants. You can add parameter objects to a model object or a kinetic law object. The scope of a parameter depends on where you add the parameter object: If you add the parameter object to a model object, the parameter is available to all reactions in the model and the `Parent` property of the parameter object is `SimBiology.Model`. If you add the parameter object to a kinetic law object, the parameter is available only to the reaction for which you are using the kinetic law object and the `Parent` property of the parameter object is `SimBiology.KineticLaw`.

See “Property Summary” on page 2-489 for links to parameter object property reference pages.

Properties define the characteristics of an object. Use the `get` and `set` commands to list object properties and change their values at the command line. You can graphically change object properties in the graphical user interface.

Constructor Summary

addparameter (model, kineticlaw)	Create parameter object and add to model or kinetic law object

Method Summary

copyobj	Copy SimBiology object and its children
delete	Delete SimBiology object
display	Display summary of SimBiology object
findUsages	Find out how a species, parameter, or compartment is used in a model
get	Get SimBiology object properties
move	Move SimBiology species or parameter object to new parent
rename	Rename object and update expressions
set	Set SimBiology object properties

Property Summary

Constant	Specify variable or constant species amount, parameter value, or compartment capacity
ConstantValue	Specify variable or constant parameter value
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Tag	Specify label for SimBiology object
Type	Display SimBiology object type
Units	Units for species amount, parameter value, compartment capacity, observable expression
UserData	Specify data to associate with object
Value	Value of species, compartment, or parameter object
ValueUnits	Parameter value units

See Also

`AbstractKineticLaw object`, `Configset object`, `KineticLaw object`, `Model object`, `Reaction object`, `Root object`, `Rule object`, `Species object`

Version History

Introduced in R2006b

PKCompartment object

Used by `PKModelDesign` to create SimBiology model

Description

The `PKCompartment` object is used by the `PKModelDesign` object to construct a SimBiology model for pharmacokinetic modeling. `PKCompartment` holds the following information:

- Name of the compartment
- Dosing type
- Elimination type
- Whether the drug concentration in this compartment is reported

The `PKCompartment` class is a subclass of the `hgsetget` class which is a subclass of the `handle` class. For more information on the inherited methods, see `hgsetget`, and `handle`.

Construction

addCompartment (PKModelDesign)	Add compartment to `PKModelDesign` object

Method Summary

delete	Delete SimBiology object
display	Display summary of SimBiology object
get	Get SimBiology object properties
set	Set SimBiology object properties

Property Summary

DosingType	Drug dosing type in compartment
EliminationType	Drug elimination type from compartment
HasLag	Lag associated with dose targeting compartment
HasResponseVariable	Compartment drug concentration reported
Name	Specify name of object

See Also

“Create Pharmacokinetic Models” in the SimBiology User's Guide, `PKModelDesign object`

Version History

Introduced in R2009a

PKData object

Define roles of data set columns

Note `PKData object` will be removed in a future release. Use `groupedData object` instead.

Description

The properties of the `PKData` object specify what each column in the data represents. The `PKData` object specifies which columns in the data set represent the following:

- The grouping variable
- The independent and dependent variables
- The dose
- The rate (only if infusion is the dosing type)
- The covariates

This information is used by the fitting functions, `sbionlmefit` and `sbionlinfit`.

To create the `PKData` object specify:

```
pkDataObject = PKData(data);
```

Where `data` is the imported data set.

The `PKData` class is a subclass of the `hgsetget` class, which is a subclass of the `handle` class. For more information on the inherited methods, see `hgsetget` and `handle`.

Construction

`PKData`	Create `PKData` object

Method Summary

delete	Delete SimBiology object
display	Display summary of SimBiology object
get	Get SimBiology object properties
getCovariateData	Create design matrix needed for fit
set	Set SimBiology object properties

Property Summary

CovariateLabels	Identify covariate columns in data set
DataSet	`Dataset` object containing imported data
DependentVarLabel	Identify dependent variable column in data set
DependentVarUnits	Response units in PKData object
DoseLabel	Dose column in data set
DoseUnits	Dose units in PKData object
GroupID	Integer identifying each group in data set
GroupLabel	Identify group column in data set
GroupNames	Unique values from `GroupLabel` in data set
IndependentVarLabel	Identify independent variable column in data set
IndependentVarUnits	Time units in PKData object
RateUnits	Units for dose rate
RateLabel	Rate of infusion column in data set

See Also

`PKModelDesign object`

Version History

Introduced in R2009a

PKModelDesign object

Helper object to construct pharmacokinetic model

Description

Use the `PKModelDesign` object to construct a SimBiology model for PK modeling. The `PKModelDesign` object lets you specify the number of compartments, the type of dosing, and method of elimination which you then use to construct the SimBiology model object with the necessary compartments, species, reactions, rules, and events.

```
pkm = PKModelDesign;
```

Use the `addCompartment` method to add a compartment with a specified dosing and elimination. `addCompartment` adds each subsequent compartment and connects it to the previous compartment using a reversible reaction. This reaction models the flux between compartments in a PK model.

The `construct` method uses the `PKModelDesign` object to create a SimBiology model object.

The `PKModelDesign` class is a subclass of the `hgsetget` class, which is a subclass of the `handle` class. For more information on the inherited methods see `hgsetget` and `handle`.

Construction

`PKModelDesign`	Create `PKModelDesign` object

Method Summary

addCompartment (PKModelDesign)	Add compartment to `PKModelDesign` object
construct (PKModelDesign)	Construct SimBiology model from `PKModelDesign` object
delete	Delete SimBiology object
display	Display summary of SimBiology object
get	Get SimBiology object properties
set	Set SimBiology object properties

Property Summary

PKCompartments	Hold compartments in PK model

See Also

“Create Pharmacokinetic Models” in the SimBiology User's Guide, `PKCompartment object`

Version History

Introduced in R2009a

PKModelMap object

Define SimBiology model components' roles

Note `PKModelMap object` will be removed in a future release. Use a combination of `EstimatedInfo object`, `CovariateModel` object, cell array of character vectors, and `sbiodose`. See `sbiofit` and `sbiofitmixed` for illustrated examples.

Description

The `PKModelMap` object holds information about the dosing type, and defines which components of a SimBiology model represent the observed response, the dose, and the estimated parameters.

The `PKModelMap` class is a subclass of the `hgsetget` class which is a subclass of the `handle` class. For more information on the inherited methods see, `hgsetget`, and `handle`.

Construction

`PKModelMap`	Create `PKModelMap` object

Method Summary

delete	Delete SimBiology object
display	Display summary of SimBiology object
get	Get SimBiology object properties
set	Set SimBiology object properties

Property Summary

Dosed	Dosed object name
DosingType	Drug dosing type in compartment
Estimated	Names of parameters to estimate
LagParameter	Parameter specifying time lag for doses
Observed	Measured response object name
ZeroOrderDurationParameter	Zero-order dose absorption duration

See Also

`PKModelDesign object`

Version History

Introduced in R2009a

plot

Compare simulation results to the training data, creating a time-course subplot for each group

Syntax

```
plot(resultsObj)
plot(resultsObj,Name,Value)
```

Description

`plot(resultsObj)` displays a figure showing the comparison between simulation results to the training data, with a time-course subplot for each group.

`plot(resultsObj,Name,Value)` uses additional options specified by one or more name-value arguments.

Examples

Estimate Two-Compartment PK Parameters

Load the sample data set.

```
load data10_32R.mat
gData = groupedData(data);
gData.Properties.VariableUnits = ["","hour","milligram/liter","milligram/liter"];
```

Create a two-compartment PK model.

```
pkmd                 = PKModelDesign;
pkc1                 = addCompartment(pkmd,"Central");
pkc1.DosingType      = "Infusion";
pkc1.EliminationType = "linear-clearance";
pkc1.HasResponseVariable = true;
pkc2                 = addCompartment(pkmd,"Peripheral");
model                = construct(pkmd);
configset            = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
responseMap = ["Drug_Central = CentralConc","Drug_Peripheral = PeripheralConc"];
```

Provide model parameters to estimate.

```
paramsToEstimate   = ["log(Central)","log(Peripheral)","Q12","Cl_Central"];
estimatedParam     = estimatedInfo(paramsToEstimate,'InitialValue',[1 1 1 1]);
```

Assume every individual receives an infusion dose at time = 0, with a total infusion amount of 100 mg at a rate of 50 mg/hour.

```
dose             = sbiodose("dose","TargetName","Drug_Central");
dose.StartTime   = 0;
dose.Amount      = 100;
dose.Rate        = 50;
```

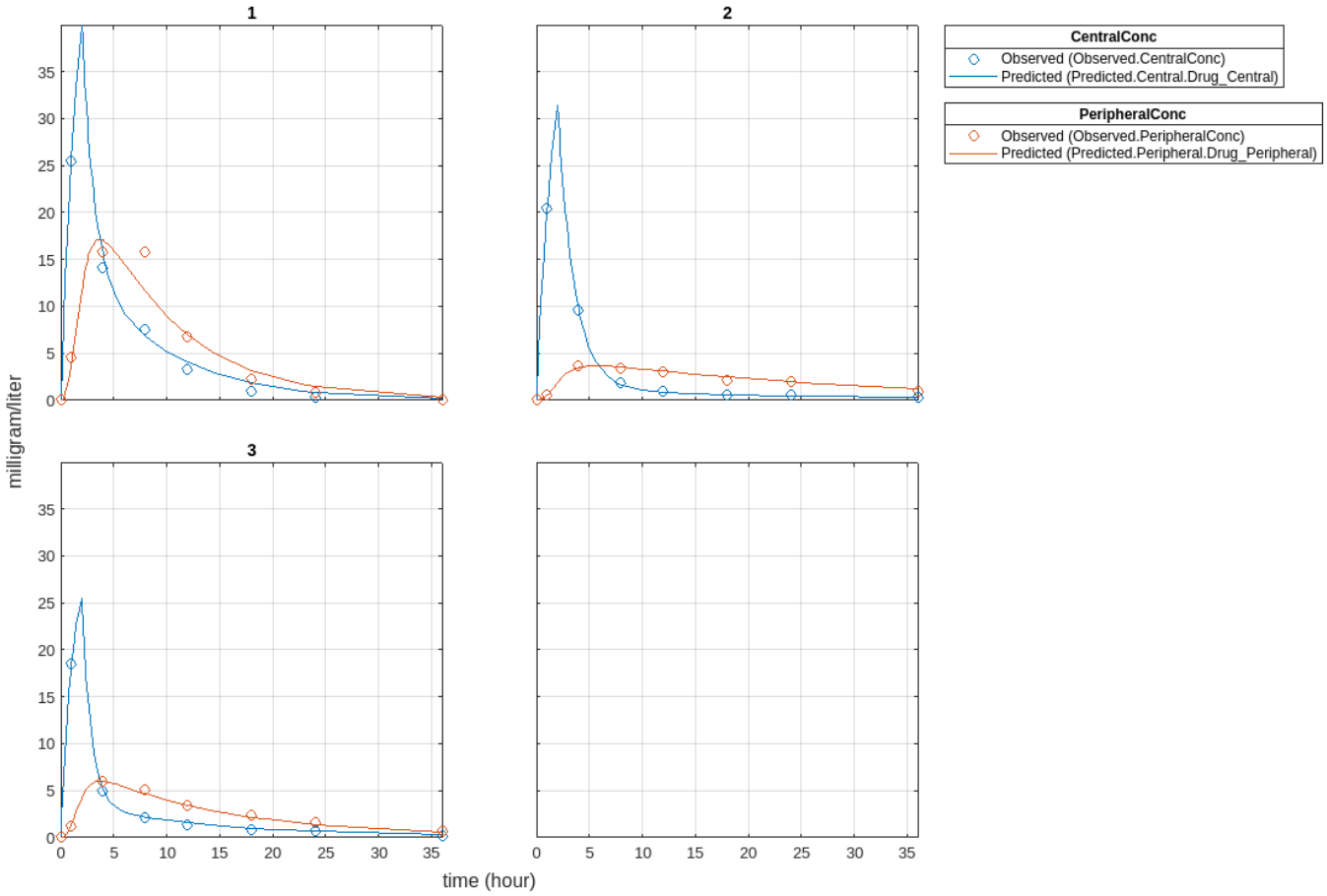
```
dose.AmountUnits = "milligram";
dose.TimeUnits   = "hour";
dose.RateUnits   = "milligram/hour";
```

Estimate model parameters. By default, the function estimates a set of parameter for each individual (unpooled fit).

```
fitResults =  sbiofit(model,gData,responseMap,estimatedParam,dose);
```

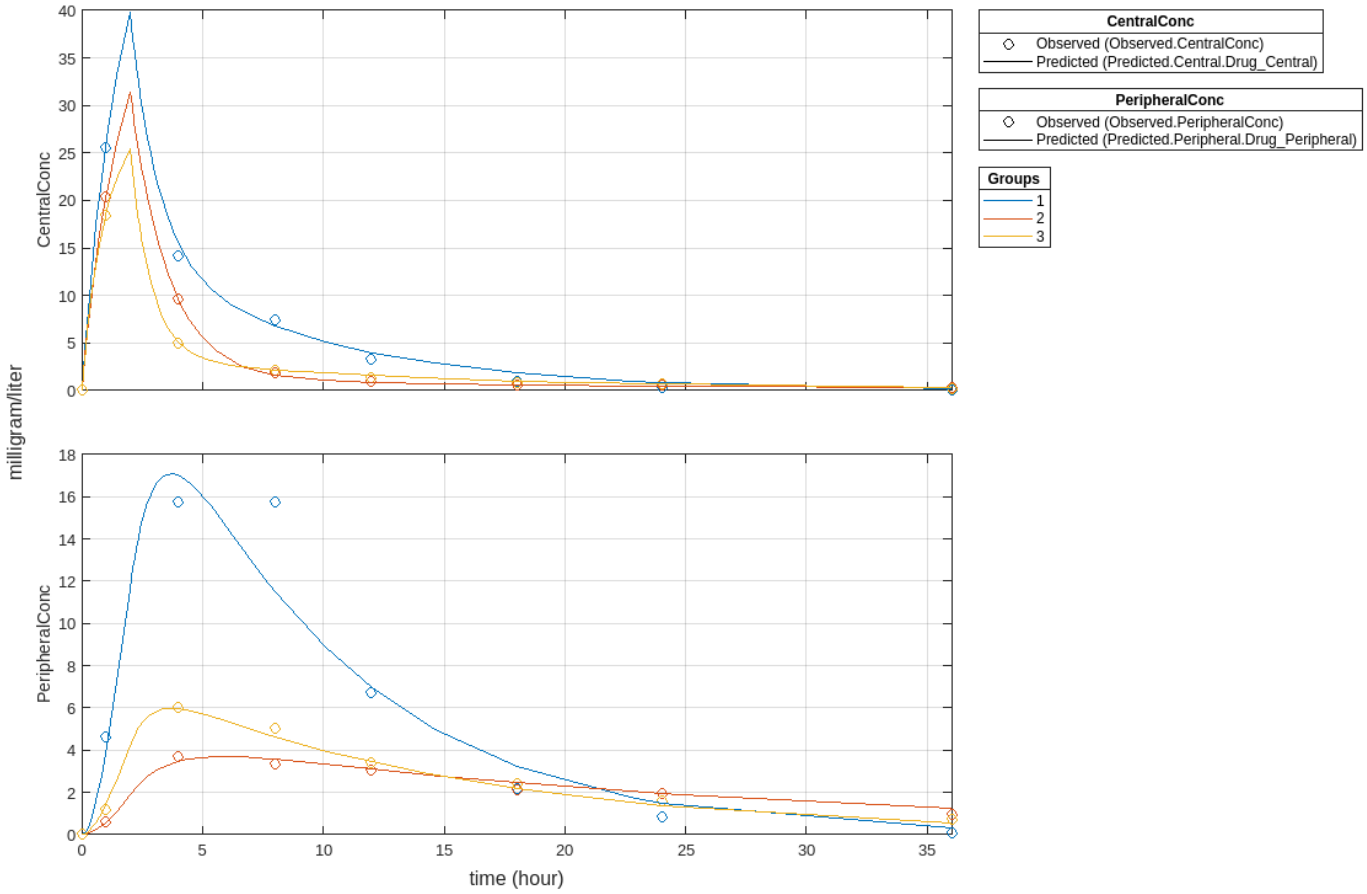
Plot the results.

```
plot(fitResults);
```



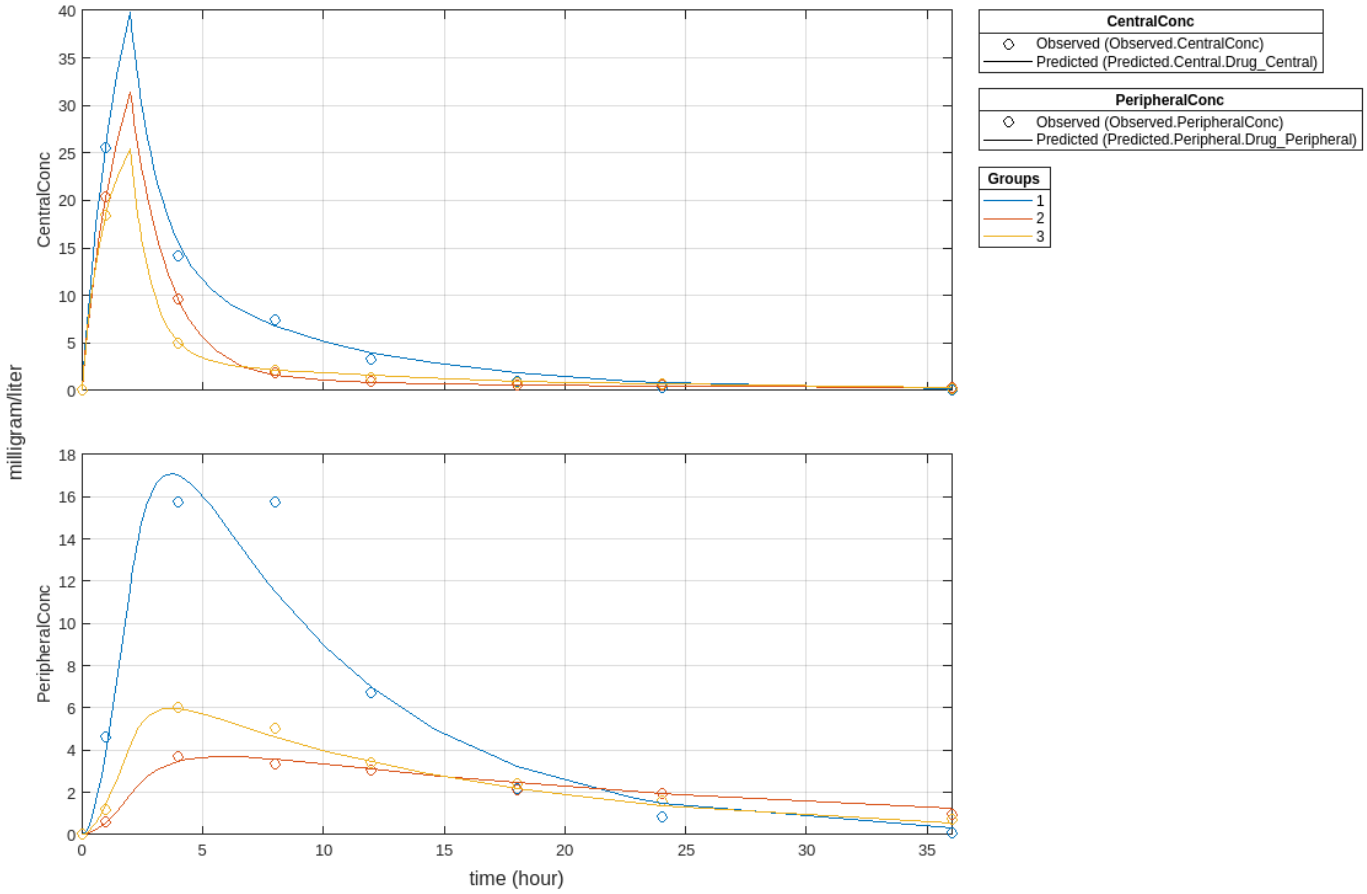
Plot all groups in one plot.

```
plot(fitResults,"PlotStyle","one axes");
```



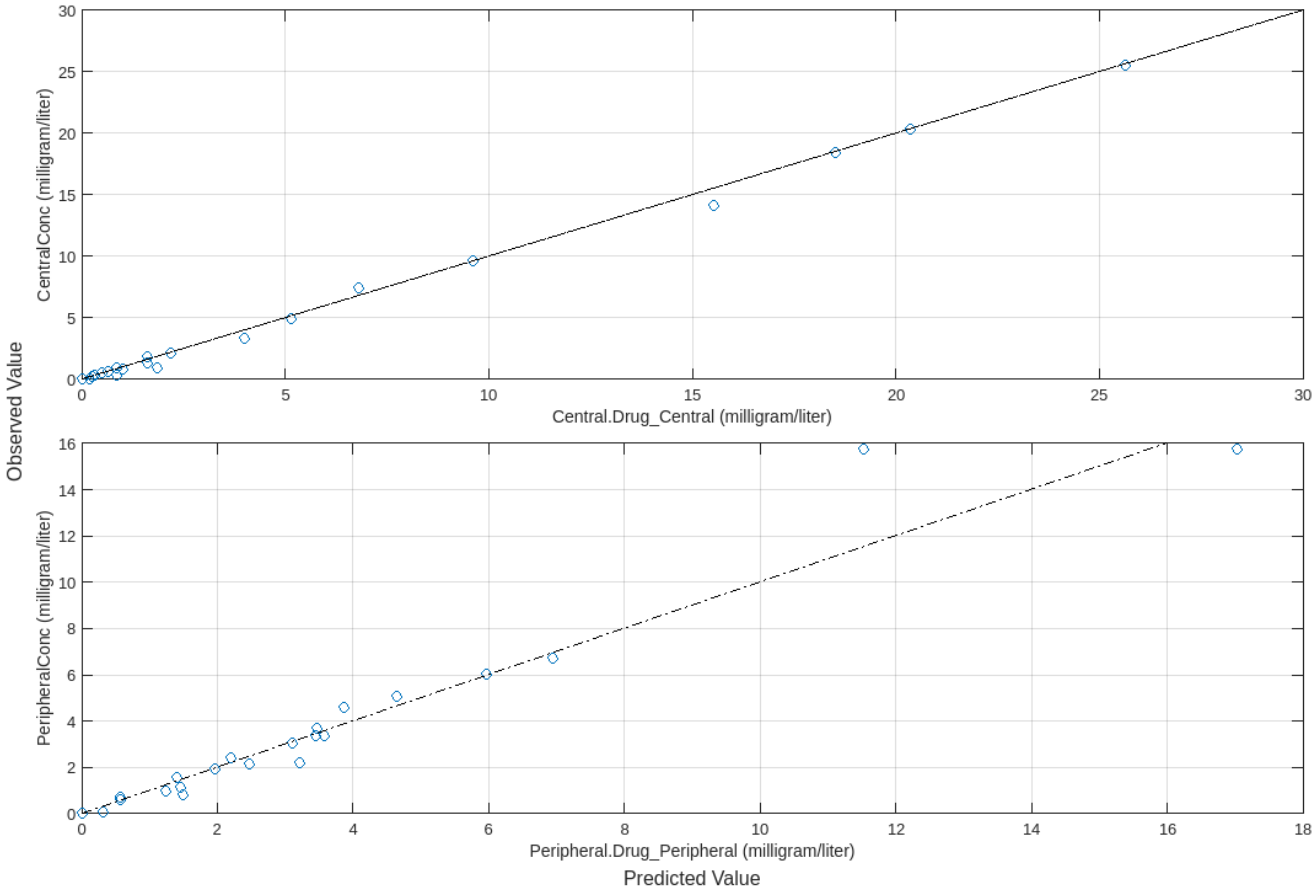
Change some axes properties.

```
s = struct;
s.Properties.XGrid = "on";
s.Properties.YGrid = "on";
plot(fitResults,"PlotStyle","one axes","AxesStyle",s);
```



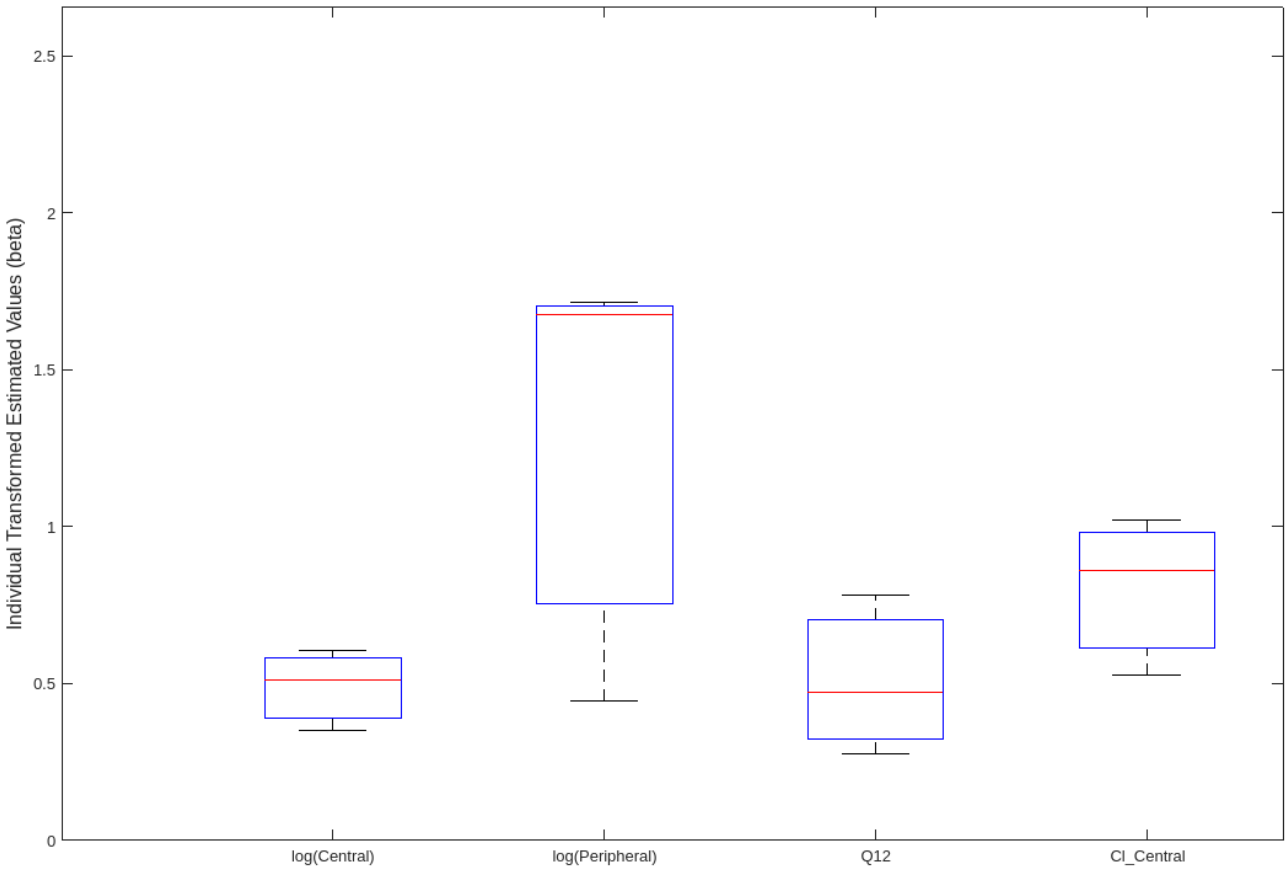
Compare the model predictions to the actual data.

```
plotActualVersusPredicted(fitResults)
```



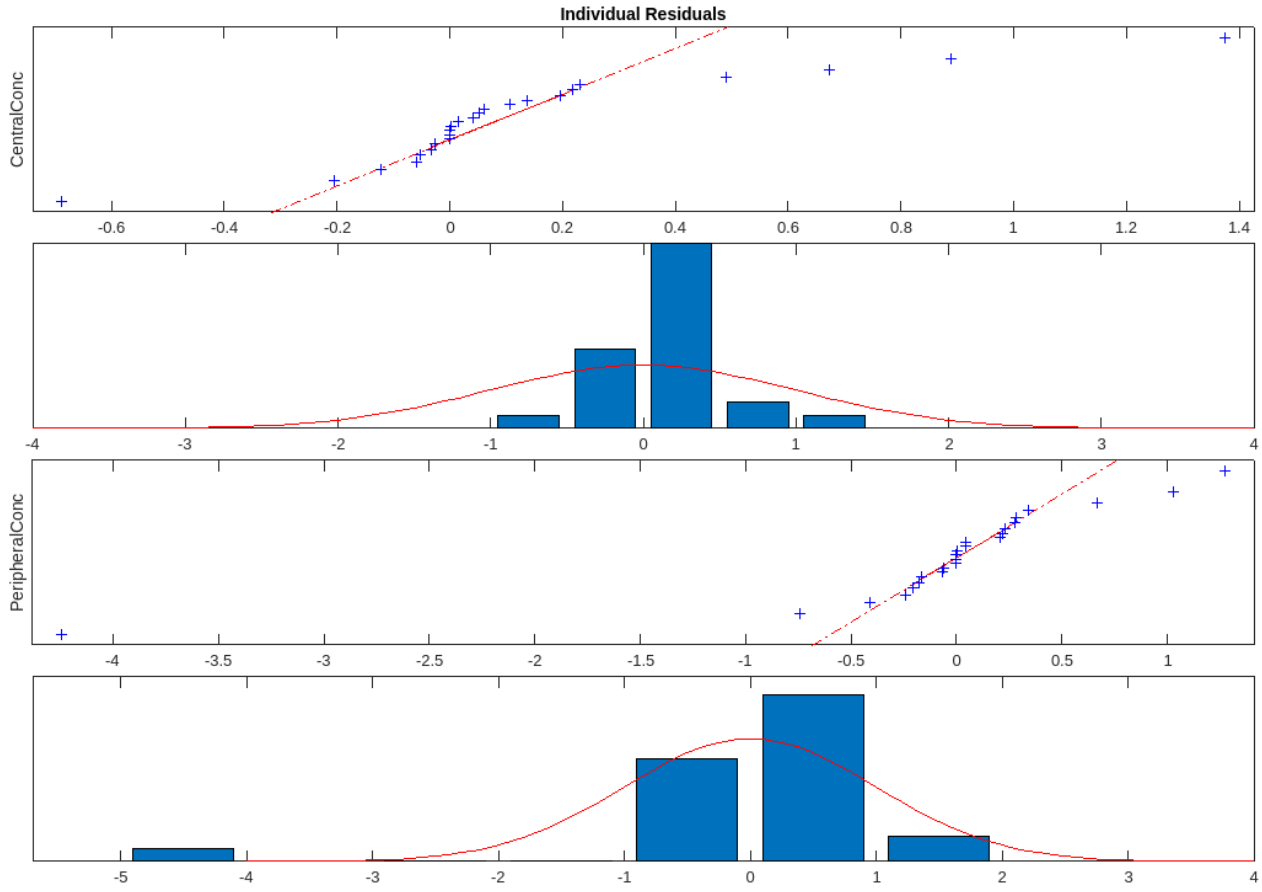
Use `boxplot` to show the variation of estimated model parameters.

```
boxplot(fitResults)
```



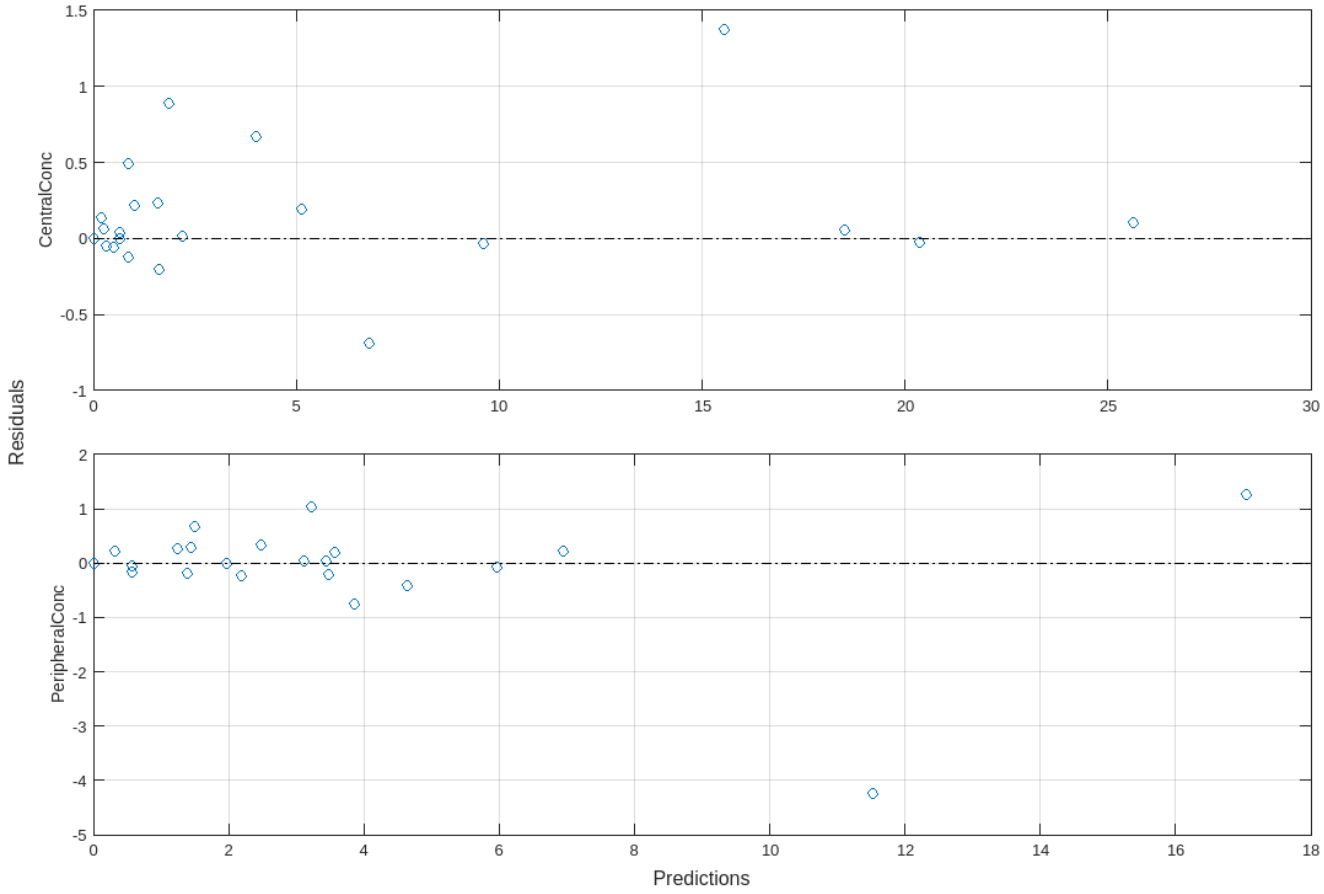
Plot the distribution of residuals. This normal probability plot shows the deviation from normality and the skewness on the right tail of the distribution of residuals. The default (constant) error model might not be the correct assumption for the data being fitted.

```
plotResidualDistribution(fitResults)
```



Plot residuals for each response using the model predictions on *x*-axis.

```
plotResiduals(fitResults,"Predictions")
```



Get the summary of the fit results. `stats.Name` contains the name for each table from `stats.Table`, which contains a list of tables with estimated parameter values and fit quality statistics.

```
stats = summary(fitResults);
stats.Name
```

```
ans =
'Unpooled Parameter Estimates'

ans =
'Statistics'

ans =
'Unpooled Beta'

ans =
'Residuals'

ans =
'Covariance Matrix'

ans =
'Error Model'
```

```
stats.Table
```

```
ans=3×9 table
    Group    Central Estimate    Central StandardError    Peripheral Estimate    Peripheral Stand
    _____    ________________    _____________________    ___________________    ________________

    {'1'}          1.422               0.12334                1.5619                0.36355
    {'2'}         1.8322              0.019672                5.3364                0.65327
    {'3'}         1.6657              0.038529                5.5632                0.37063

ans=3×7 table
    Group      AIC        BIC      LogLikelihood    DFE      MSE         SSE
    _____    _______    _______    _____________    ___    ________    _______

    {'1'}     60.961     64.051       -26.48        12        2.138     25.656
    {'2'}    -7.8379    -4.7475       7.9189        12     0.029012    0.34814
    {'3'}    -1.4336     1.6567       4.7168        12     0.043292     0.5195

ans=3×9 table
    Group    Central Estimate    Central StandardError    Peripheral Estimate    Peripheral Stand
    _____    ________________    _____________________    ___________________    ________________

    {'1'}        0.35208              0.086736               0.44589                0.23277
    {'2'}        0.60551              0.010737                1.6746                0.12242
    {'3'}        0.51027               0.02313                1.7162                0.06662

ans=24×4 table
    ID    Time    CentralConc    PeripheralConc
    __    ____    ___________    ______________

    1       0              0              0
    1       1        0.10646        -0.74394
    1       4         1.3745          1.2726
    1       8       -0.68825         -4.2435
    1      12        0.67383         0.21806
    1      18        0.88823          1.0269
    1      24        0.48941         0.66755
    1      36        0.13632         0.22948
    2       0              0              0
    2       1      -0.026731      -0.058311
    2       4      -0.033299       -0.20544
    2       8       -0.20466        0.20696
    2      12       -0.12223       0.045409
    2      18       0.041224        0.33883
    2      24      -0.059498      0.0036257
    2      36      -0.051645        0.27616
      ⋮

ans=12×6 table
    Group        Parameters         log(Central)    log(Peripheral)        Q12        Cl_Central
    _____    __________________    ____________    _______________    ___________    ___________

    {'1'}    {'log(Central)'   }       0.015213        -0.022539       -0.0086672       0.00115
    {'1'}    {'log(Peripheral)'}      -0.022539          0.13217         0.045746     -0.007313
    {'1'}    {'Q12'            }     -0.0086672         0.045746         0.023092     -0.002148
    {'1'}    {'Cl_Central'     }       0.001159       -0.0073135       -0.0021484      0.001367
    {'2'}    {'log(Central)'   }     0.00038701        -0.002161      -0.00010177     9.7448e-05
```

```
    {'2'}    {'log(Peripheral)'}      -0.002161          0.42676          0.019101      -0.01575
    {'2'}    {'Q12'            }    -0.00010177         0.019101         0.00094857    -0.0007332
    {'2'}    {'Cl_Central'     }     9.7448e-05        -0.015755        -0.00073328     0.0006894
    {'3'}    {'log(Central)'   }      0.0014845       -0.0054648         -0.0013216     0.0001663
    {'3'}    {'log(Peripheral)'}     -0.0054648          0.13737           0.016903     -0.007272
    {'3'}    {'Q12'            }     -0.0013216         0.016903          0.0034406    -0.0008253
    {'3'}    {'Cl_Central'     }     0.00016639       -0.0072722        -0.00082538     0.0007458
```

```
ans=3×5 table
    Group     Response      ErrorModel        a        b
    _____    __________    ____________    _______    ___

    {'1'}    {0×0 char}    {'constant'}     1.2663    NaN
    {'2'}    {0×0 char}    {'constant'}    0.14751    NaN
    {'3'}    {0×0 char}    {'constant'}    0.18019    NaN
```

Input Arguments

`resultsObj` — Estimation results

`OptimResults` object | `NLINResults` object | vector of results objects

Estimation results, specified as an `OptimResults object` or `NLINResults object`, or vector of results objects which contains estimation results from running `sbiofit`.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `plot(fitResults,'PlotStyle','one axes')` specifies to plot data from each run into one axes instead of plotting each run individually as a subplot.

`ParameterType` — Type of parameter estimates to plot

`'individual'` (default)

Type of parameter estimates to plot, specified as `'individual'`. For `LeastSquaresResults` objects, `'individual'` is the only option indicating to use the individual parameter estimates to plot the simulation results.

Data Types: `char` | `string`

`PlotStyle` — Plot style

`'trellis'` (default) | `'one axes'`

Plot style, specified as `'trellis'` or `'one axes'`. By default, the function plots the data from each run into its own subplot. To plot all data into one plot, use `'one axes'`.

Data Types: `char` | `string`

`AxesStyle` — Axes properties

structure

Axes properties, specified as a structure. The structure (`s`) has the following field names and values representing the axes properties.

Field Name	Value
`s.Labels.Title`	Character vector or string scalar.
`s.Labels.XLabel`	Character vector or string scalar.
`s.Labels.YLabel`	Character vector or string scalar.
`s.Properties.XGrid`	`'off'` (default) or `'on'`
`s.Properties.XScale`	`'linear'` (default) or `'log'`
`s.Properties.XDir`	`'normal'` (default) or `'reverse'`
`s.Properties.XLim`	Two-element vector of the form `[min max]`
`s.Properties.YGrid`	`'off'` (default) or `'on'`
`s.Properties.YScale`	`'linear'` (default) or `'log'`
`s.Properties.YDir`	`'normal'` (default) or `'reverse'`
`s.Properties.YLim`	Two-element vector of the form `[min max]`

Data Types: `structure`

Version History

Introduced in R2014a

See Also

`NLINResults object` | `OptimResults object` | `sbiofit`

plot

Compare simulation results to the training data, creating a time-course subplot for each group

Syntax

```
plot(resultsObj)
plot(resultsObj,'ParameterType',value)
```

Description

`plot(resultsObj)` compares simulation results to the training data, creating a time-course subplot for each group.

`plot(resultsObj,'ParameterType',value)` uses the individual or population parameter estimates as specified by `value`. The two choices for `value` are `'population'` or `'individual'` (default).

Input Arguments

`resultsObj` — Estimation results
`NLMEResults` object

Estimation results, specified as an `NLMEResults object`, which contains estimation results returned by `sbiofitmixed`.

`value` — Parameter type
character vector | string

Parameter type, specified as a character vector or string which must be one of the following: `'individual'` (default) or `'population'`.

Version History

Introduced in R2014a

See Also

`NLMEResults object` | `sbiofitmixed`

plot

Package: `SimBiology.fit`

Plot parameter confidence interval results

Syntax

```
fh = plot(paraCI)
fh = plot(paraCI,Name,Value)
```

Description

`fh = plot(paraCI)` plots confidence intervals from `paraCI`, a `ParameterConfidenceInterval` object or vector of objects.

- If the estimation status of a confidence interval (`paraCI.Results.Status` on page 2-0) is `success`, the `plot` function uses the first default color (blue) to plot a line and a centered dot for every parameter estimate. The function also plots a box to indicate the confidence intervals.
- If the status is `constrained` or `estimable`, the function uses the second default color (red) and plots a line, centered dot, and box to indicate the confidence intervals.
- If the status is `not estimable`, the function plots only a line and a centered cross in red.
- If there are any transformed parameters with estimated values that are 0 (for the `log` transform) and 0 or 1 (for the `probit` or `logit` transform), no confidence intervals are plotted for those parameter estimates.

`fh = plot(paraCI,Name,Value)` uses additional options specified by one or more `Name,Value` pair arguments.

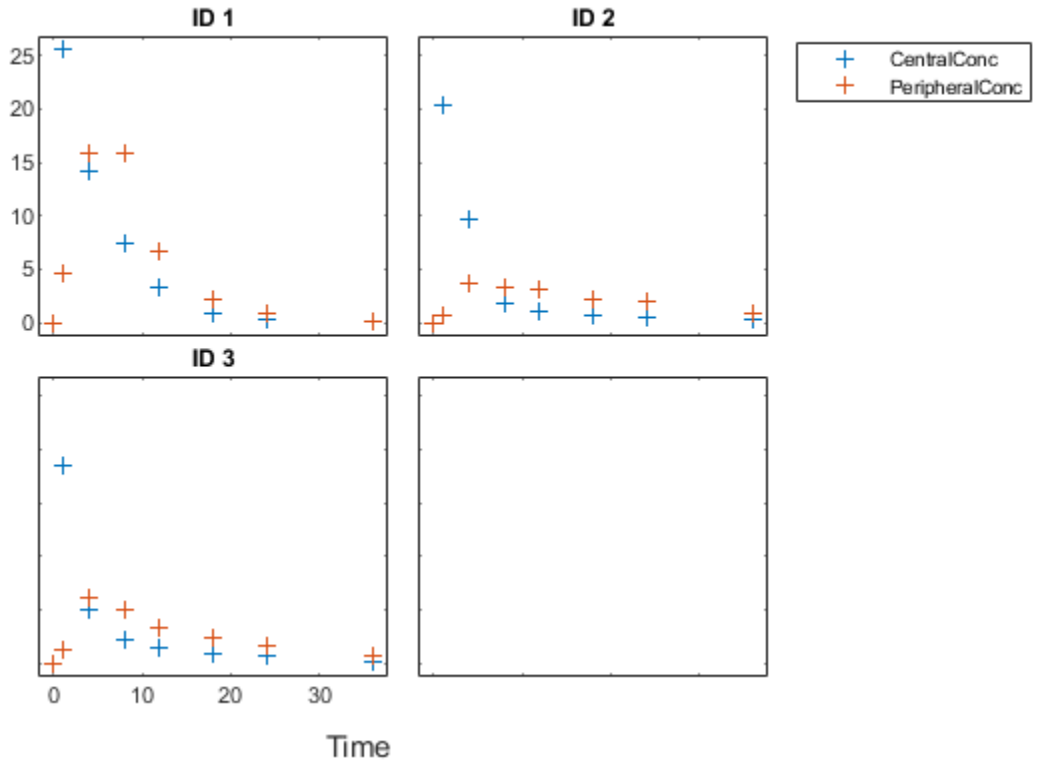
Examples

Plot Confidence Intervals of Estimated PK Parameters

Load Data

Load the sample data to fit.

```
load data10_32R.mat
gData = groupedData(data);
gData.Properties.VariableUnits = {'','hour','milligram/liter','milligram/liter'};
sbiotrellis(gData,'ID','Time',{'CentralConc','PeripheralConc'},'Marker','+',...
            'LineStyle','none');
```



Create Model

Create a two-compartment model.

```
pkmd                 = PKModelDesign;
pkc1                 = addCompartment(pkmd,'Central');
pkc1.DosingType      = 'Infusion';
pkc1.EliminationType = 'linear-clearance';
pkc1.HasResponseVariable = true;
pkc2                 = addCompartment(pkmd,'Peripheral');
model                = construct(pkmd);
configset            = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
```

Define Dosing

Define the infusion dose.

```
dose             = sbiodose('dose','TargetName','Drug_Central');
dose.StartTime   = 0;
dose.Amount      = 100;
dose.Rate        = 50;
dose.AmountUnits = 'milligram';
dose.TimeUnits   = 'hour';
dose.RateUnits   = 'milligram/hour';
```

Define Parameters

Define parameters to estimate.

```
responseMap = {'Drug_Central = CentralConc','Drug_Peripheral = PeripheralConc'};
paramsToEstimate   = {'log(Central)','log(Peripheral)','Q12','Cl_Central'};
estimatedParam     = estimatedInfo(paramsToEstimate,...
                                   'InitialValue',[1 1 1 1],...
                                   'Bounds',[0.1 3;0.1 10;0 10;0.1 2]);
```

Fit Model

Perform an unpooled fit, that is, one set of estimated parameters for each patient.

```
unpooledFit = sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',false);
```

Perform a pooled fit, that is, one set of estimated parameters for all patients.

```
pooledFit = sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',true);
```

Compute Confidence Intervals for Estimated Parameters

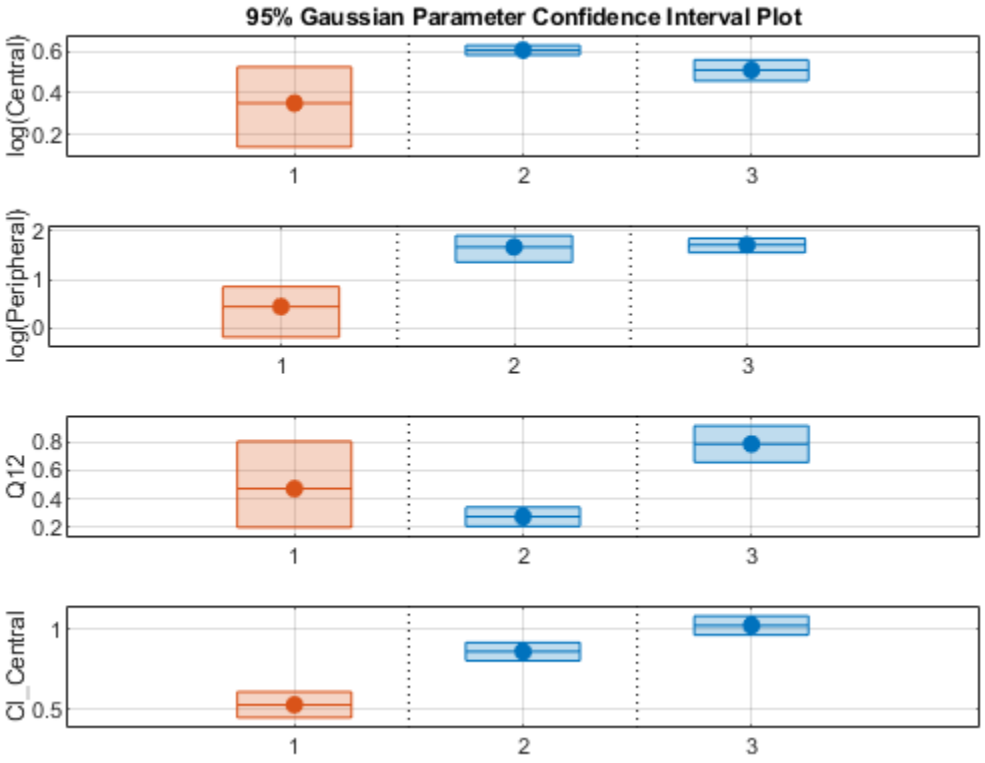
Compute 95% confidence intervals for each estimated parameter in the unpooled fit using the Gaussian approximation.

```
ciParamUnpooled = sbioparameterci(unpooledFit);
```

Plot the confidence intervals. If the estimation status of a confidence interval is `success`, it is plotted in blue (the first default color). Otherwise, it is plotted in red (the second default color), which indicates that further investigation into the fitted parameters might be required. If the confidence interval is `not estimable`, then the function plots a red line and centered cross. If there are any transformed parameters with estimated values that are 0 (for the log transform) and 1 or 0 (for the probit or logit transform), then no confidence intervals are plotted for those parameter estimates. To see the color order, type `get(groot,'defaultAxesColorOrder')`.

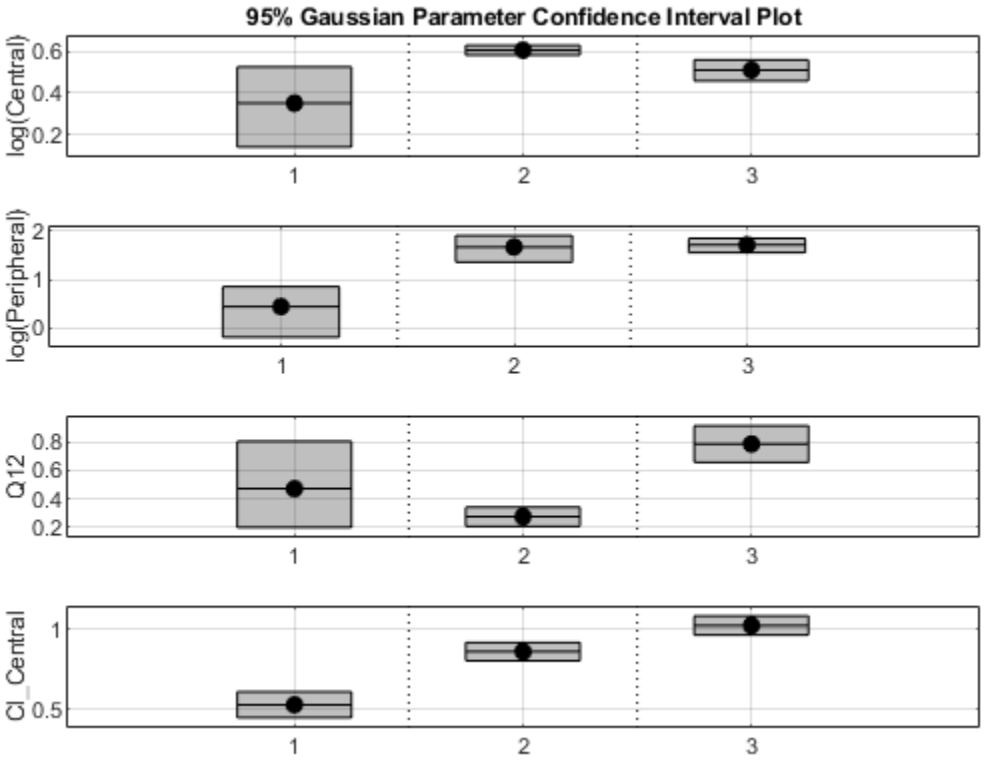
Groups are displayed from left to right in the same order that they appear in the `GroupNames` property of the object, which is used to label x-axis. The y-labels are the transformed parameter names.

```
plot(ciParamUnpooled)
```



Plot using a single color.

```
plot(ciParamUnpooled,'Color',[0 0 0])
```

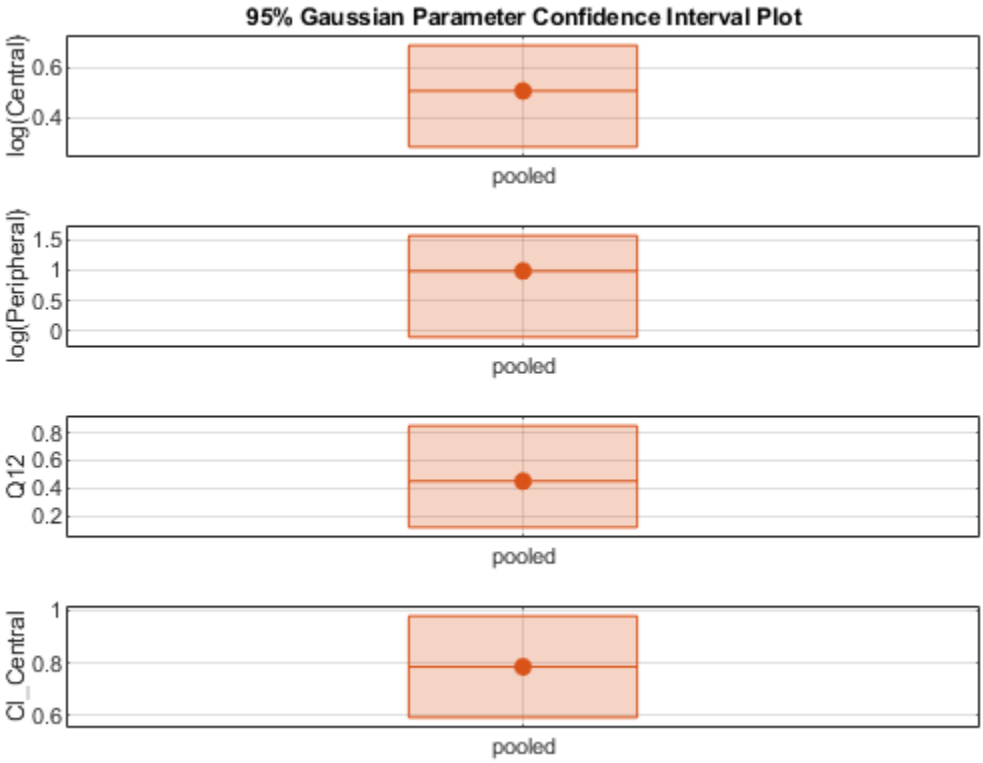


Compute the confidence intervals for the pooled fit.

```
ciParamPooled = sbioparameterci(pooledFit);
```

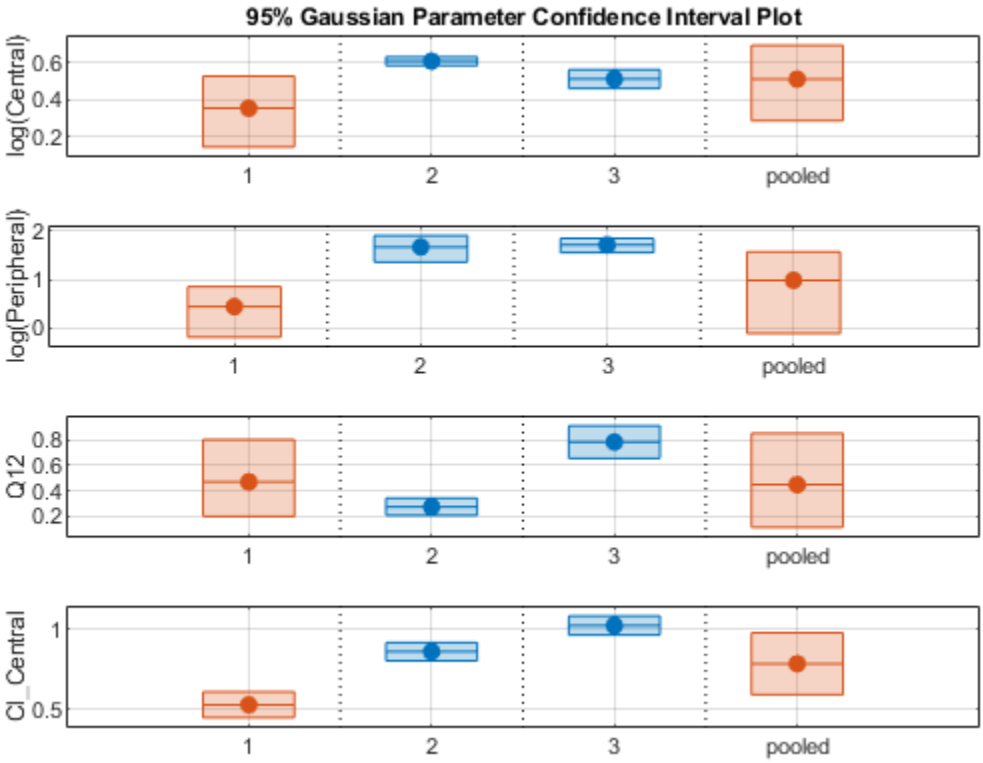
Plot the confidence intervals. The group name is labeled as "pooled" to indicate such fit.

```
plot(ciParamPooled)
```



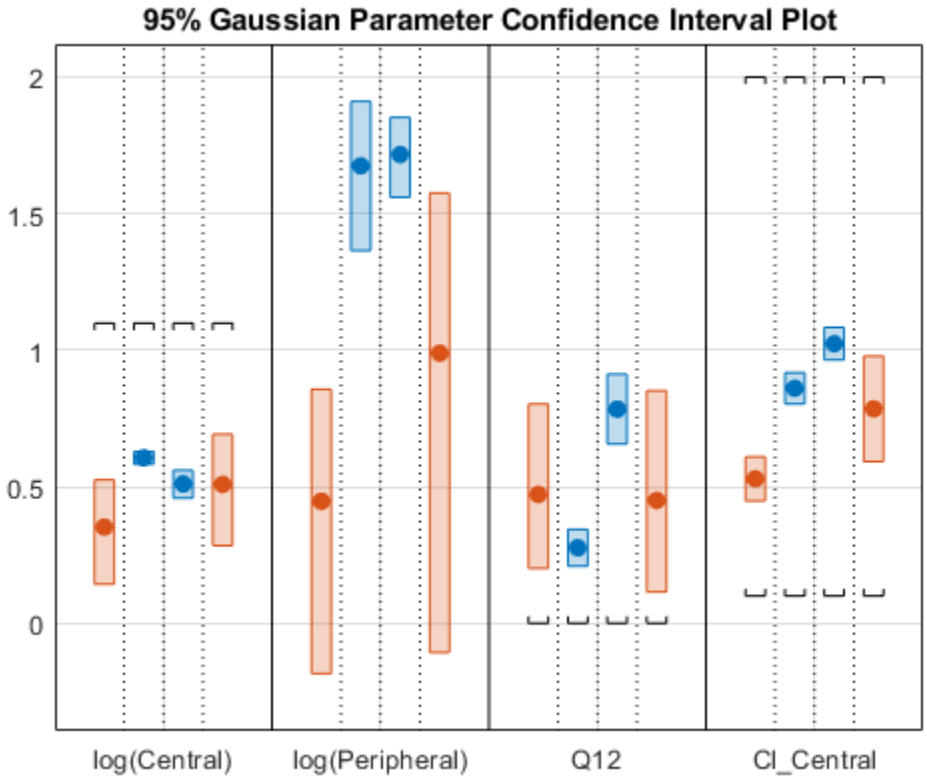
Plot all the confidence interval results together. By default, the confidence interval for each parameter estimate is plotted in a separate axes. Vertical dotted lines group confidence intervals of parameter estimates that were computed in a common fit. Parameter bounds defined in the original fit are marked by square brackets (if visible in the parameter range being plotted).

```
ciAll = [ciParamUnpooled;ciParamPooled];
plot(ciAll)
```



You can also plot all confidence intervals on one axes grouped by parameter estimates using the 'Grouped' layout.

```
plot(ciAll,'Layout','Grouped')
```



In this layout, you can point to the center marker of each confidence interval to see the group name. Each estimated parameter is separated by a vertical black line. Vertical dotted lines group confidence intervals of parameter estimates that were computed in a common fit. Parameter bounds defined in the original fit are marked by square brackets (if visible in the parameter range being plotted). Note the different scales on the y-axis due to parameter transformations. For instance, the y-axis of `Q12` is in the linear scale, but that of `Central` is in the log scale due to its log transform.

Compute Confidence Intervals Using Profile Likelihood

Compute 95% confidence intervals for each estimated parameter in the unpooled fit using the profile likelihood approach.

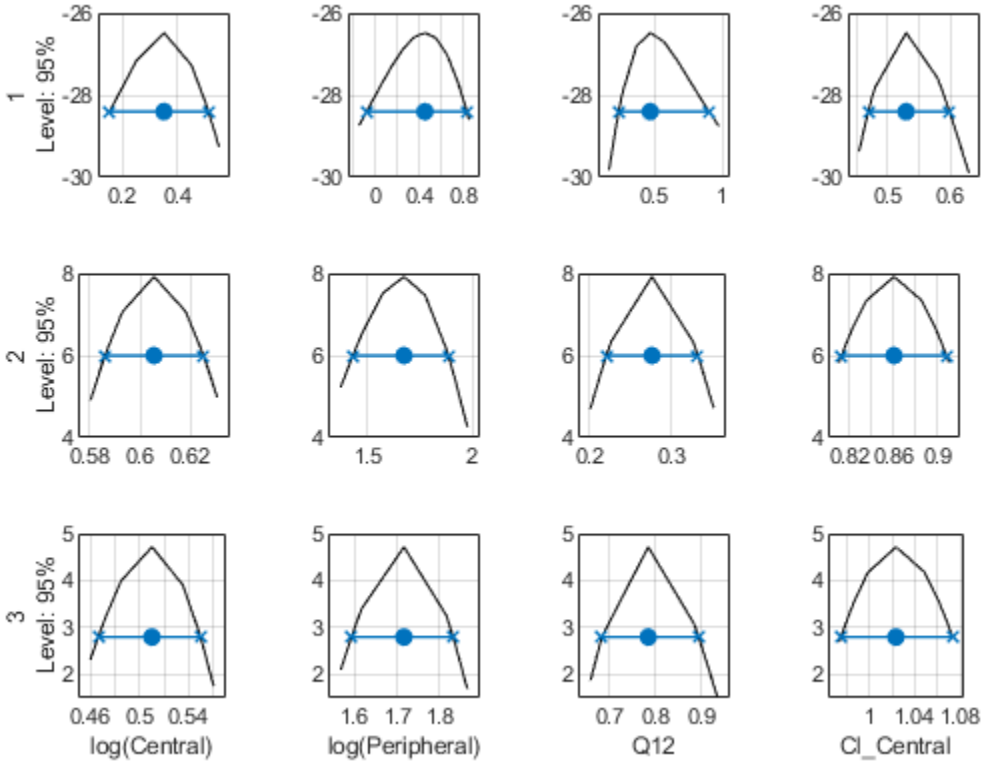
```
ciParamUnpooledProf = sbioparameterci(unpooledFit,'Type','profilelikelihood');
```

Compute the confidence intervals for the pooled fit.

```
ciParamPooledProf = sbioparameterci(pooledFit,'Type','profilelikelihood');
```

Plot the profile likelihood curves for the unpooled fit. The parameter bounds defined in the original fit are displayed by vertical dotted lines (if visible in the parameter range being plotted). The confidence interval is indicated by two crosses and a line in between them. The center dot denotes the parameter estimate. The profile likelihood is always plotted in the log scale. The x-axis scale depends on whether the parameter is transformed (log, probit, or logit scale) or not (linear scale).

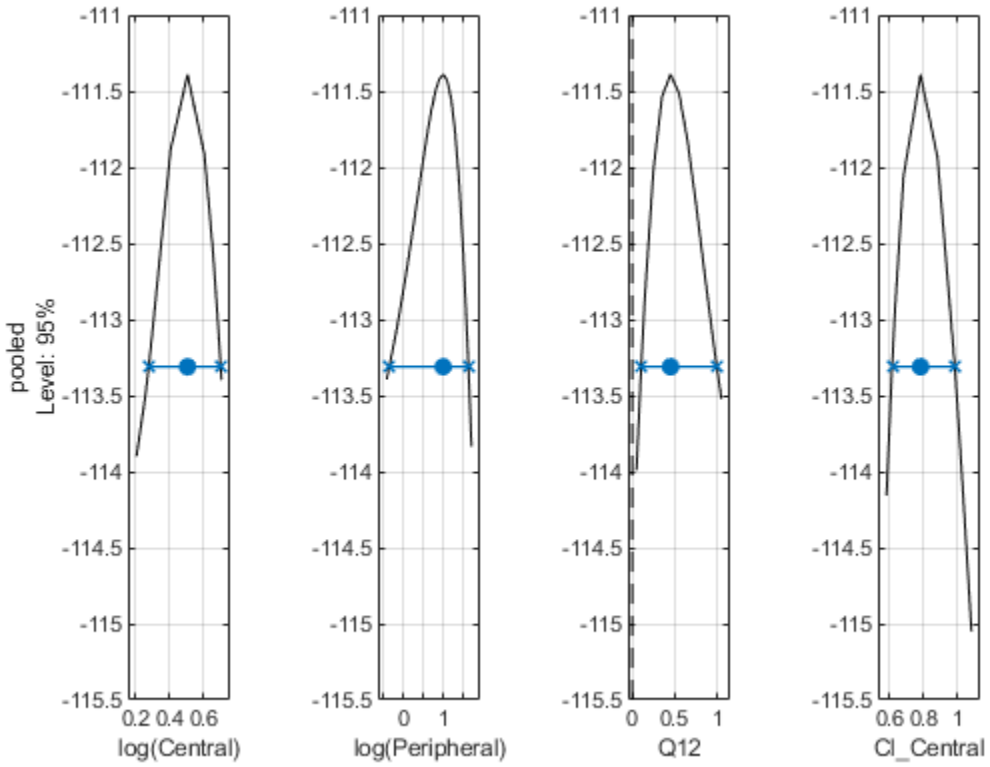
```
plot(ciParamUnpooledProf,'ProfileLikelihood',true);
```



Each group is plotted in a separate row, and each parameter is plotted in a separate column.

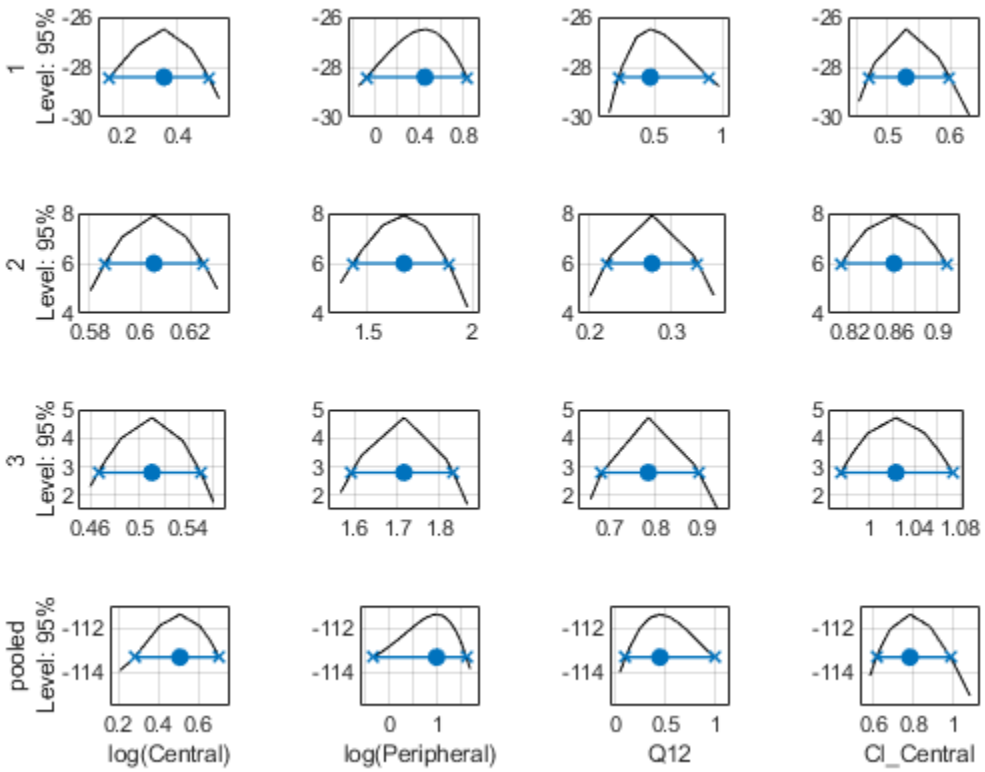
Plot the curves for the pooled fit.

```
plot(ciParamPooledProf,'ProfileLikelihood',true);
```



Plot all the confidence interval results together in the same figure.

```
plot([ciParamUnpooledProf;ciParamPooledProf],'ProfileLikelihood',true);
```



Input Arguments

`paraCI` — Parameter confidence interval results

`ParameterConfidenceInterval` object | vector

Parameter confidence interval results, specified as a `ParameterConfidenceInterval` object or a vector of objects.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `'ProfileLikelihood',true` specifies to plot the profile likelihood curves.

`Color` — Red-Green-Blue color triplet

three-element row vector

Red-Green-Blue color triplet, specified as the comma-separated pair consisting of `'Color'` and a three-element row vector. By default, confidence intervals that are not limited by the parameter bounds specified in the original fit are plotted using the first default color (blue), and those that are limited by the bounds are plotted using the second default color (red). If the confidence interval is not

estimable, it is also plotted in red. To see the default color order, enter `get(groot,'defaultAxesColorOrder')` or see the “ColorOrder” property.

Tip Use this name-value pair when you want to create plots with a single color, for instance, for publication purposes.

Example: `'Color',[0 0 0]`

`ProfileLikelihood` — Logical scalar to display profile likelihood curves
`false` (default) | `true`

Logical scalar to display profile likelihood curves for the `profileLikelihood` confidence intervals, specified as the comma-separated pair consisting of `'ProfileLikelihood'` and `true` or `false`.

The confidence interval is indicated by two crosses with a line in between them. A center dot denotes the parameter estimate. The `plot` function uses the first default color (blue) for successfully computed confidence intervals. Otherwise, the function uses the second default color (red). A vertical dotted line marks the parameter bounds defined in the original fit.

If there are multiple groups, each group is plotted in a separate row and each parameter is plotted in a separate column. The labels for the x-axis are the transformed parameter names (the `TransformedName` property of the `estimatedInfo` object used in the original fit). The labels for the y-axis are the group names (the `GroupNames` property of the confidence interval object) and the confidence level.

The profile likelihood curve is always plotted in the log scale. The x-axis scale depends on whether the parameter is transformed (log, probit, or logit scale) or not (linear scale).

Example: `'ProfileLikelihood',true`

`Layout` — Axes layout to display parameter confidence intervals
`'split'` (default) | `'grouped'`

Axes layout to display parameter confidence intervals, specified as the comma-separated pair consisting of `'Layout'` and a character vector `'split'` (default) or `'grouped'`.

The `'split'` layout displays the confidence interval for each parameter estimate on a separate axes.

The `'grouped'` layout displays all confidence intervals on one axes grouped by parameter estimates. Each estimated parameter is separated by a vertical black line.

In both cases, the parameter bounds defined in the original fit are marked by square brackets. The function uses vertical dotted lines to group confidence intervals of parameter estimates that have been computed in a common fit.

Example: `'Layout','grouped'`

Output Arguments

`fh` — Figure handle
handle

Figure handle of the plot, returned as a figure handle.

Version History

Introduced in R2017b

See Also

`ParameterConfidenceInterval` | `sbioparameterci`

plot

Package: `SimBiology.fit`

Plot confidence interval results for model predictions

Syntax

```
fh = plot(predCI)
fh = plot(predCI,Color=colorValue)
```

Description

`fh = plot(predCI)` plots confidence interval results from `predCI`, a `PredictionConfidenceInterval` object or vector of objects.

The function plots the observation data points as black plus signs and the model predictions as solid lines.

- If the status of confidence interval (`predCI`.Status on page 2-0) is `constrained` or `not estimable`, the function uses the second default color (red) to plot the confidence intervals.
- Otherwise, the function uses the first default color (blue) and plots the confidence intervals as shaded areas.

`fh = plot(predCI,Color=colorValue)` also specifies the color of confidence intervals.

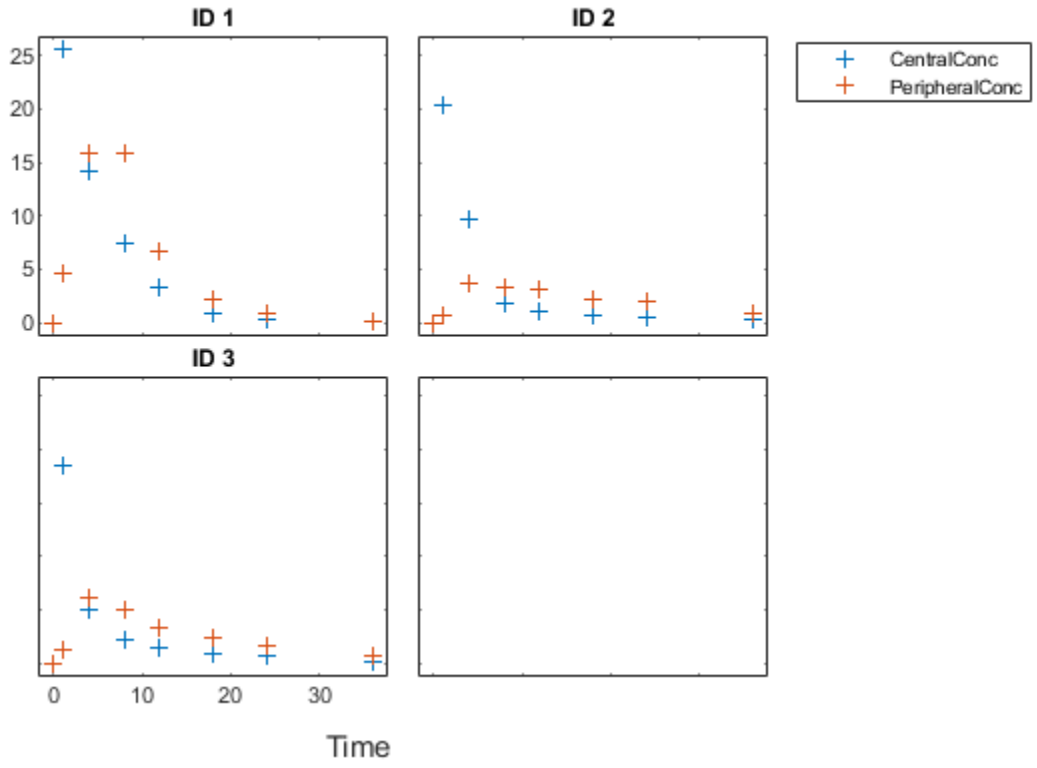
Examples

Plot Confidence Intervals of PK Model Predictions

Load Data

Load the sample data to fit.

```
load data10_32R.mat
gData = groupedData(data);
gData.Properties.VariableUnits = {'','hour','milligram/liter','milligram/liter'};
sbiotrellis(gData,'ID','Time',{'CentralConc','PeripheralConc'},'Marker','+',...
            'LineStyle','none');
```



Create Model

Create a two-compartment model.

```
pkmd                 = PKModelDesign;
pkc1                 = addCompartment(pkmd,'Central');
pkc1.DosingType      = 'Infusion';
pkc1.EliminationType = 'linear-clearance';
pkc1.HasResponseVariable = true;
pkc2                 = addCompartment(pkmd,'Peripheral');
model                = construct(pkmd);
configset            = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
```

Define Dosing

Define the infusion dose.

```
dose             = sbiodose('dose','TargetName','Drug_Central');
dose.StartTime   = 0;
dose.Amount      = 100;
dose.Rate        = 50;
dose.AmountUnits = 'milligram';
dose.TimeUnits   = 'hour';
dose.RateUnits   = 'milligram/hour';
```

Define Parameters

Define parameters to estimate.

```
responseMap = {'Drug_Central = CentralConc','Drug_Peripheral = PeripheralConc'};
paramsToEstimate   = {'log(Central)','log(Peripheral)','Q12','Cl_Central'};
estimatedParam     = estimatedInfo(paramsToEstimate,...
                                   'InitialValue',[1 1 1 1],...
                                   'Bounds',[0.1 3;0.1 10;0 10;0.1 2]);
```

Fit Model

Perform an unpooled fit, that is, one set of estimated parameters for each patient.

```
unpooledFit = sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',false);
```

Compute Confidence Intervals for Model Predictions

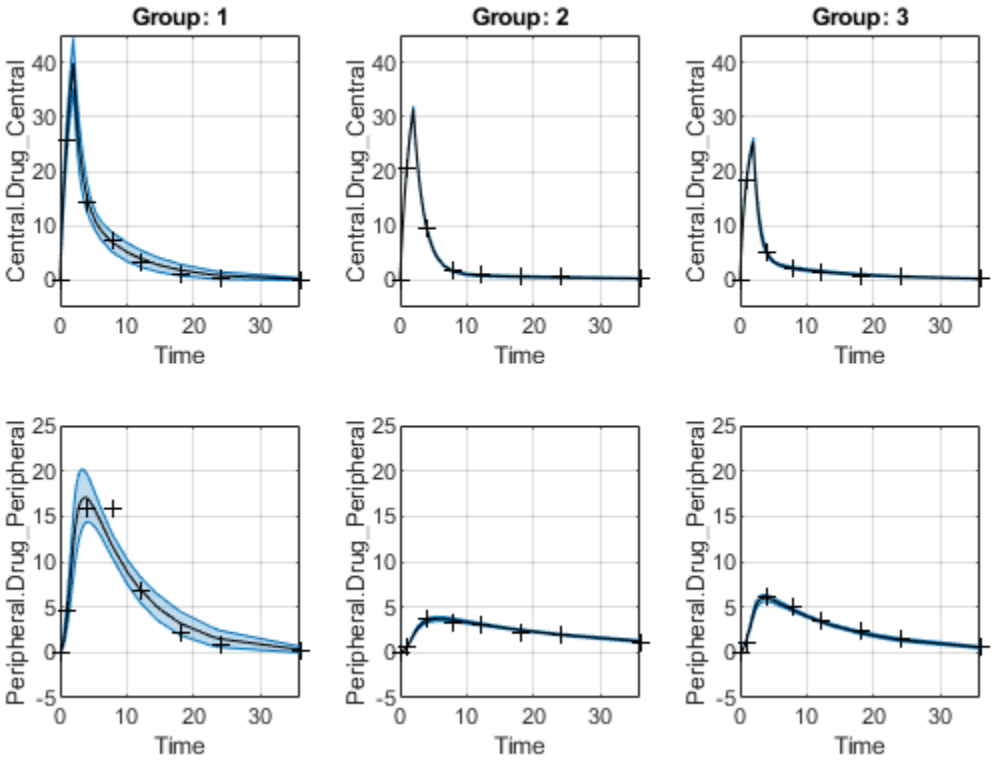
Compute 95% confidence intervals for predicted model responses in the unpooled fit using the Gaussian approximation.

```
ciPredUnpooled = sbiopredictionci(unpooledFit);
```

Plot the confidence intervals. If the estimation status of a confidence interval is `constrained` or `not estimable`, the function uses the second default color (red). Otherwise, the function uses the first default color (blue). To see the color order, type `get(groot,'defaultAxesColorOrder')`.

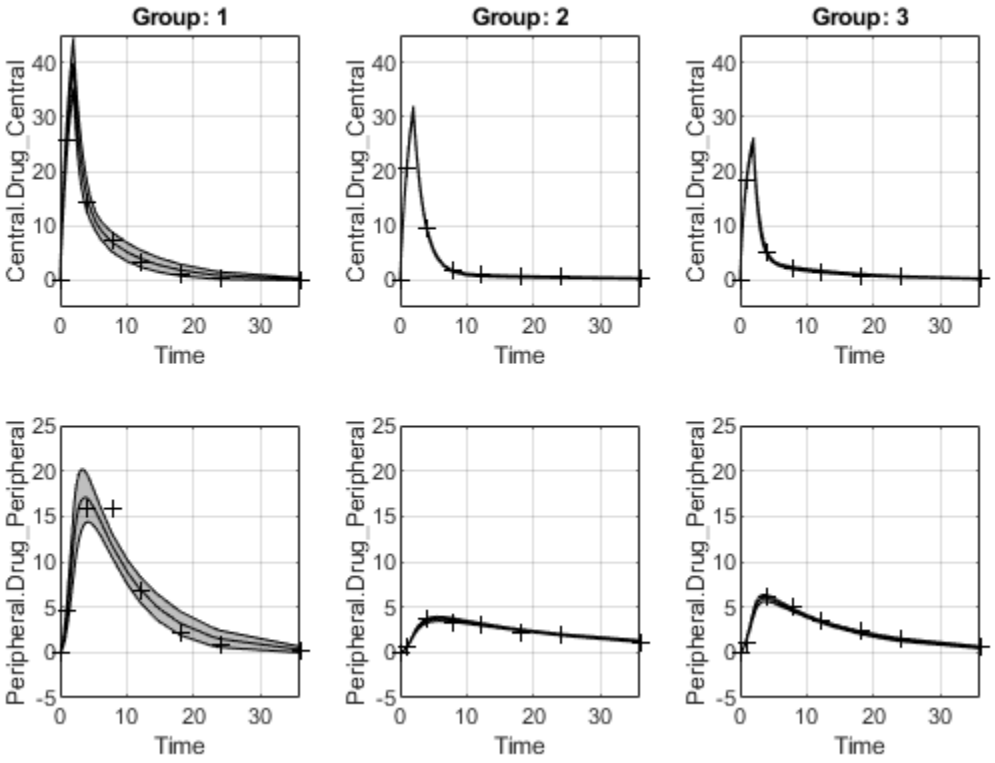
Each group is displayed in each column, from left to right, in the same order that they appear in the `GroupNames` property of the object, which is used to label each column.

```
plot(ciPredUnpooled)
```



Plot using a single color (black).

```
plot(ciPredUnpooled,'Color',[0 0 0])
```



Input Arguments

`predCI` — Confidence interval results for model predictions

`PredictionConfidenceInterval` object | vector

Confidence interval results for model predictions, specified as a `PredictionConfidenceInterval` object or a vector of objects.

If there are multiple groups, each group is displayed in each column, from left to right, in the same order that they appear in the `GroupNames` property of the object. Each row represents a model response.

`colorValue` — Color of confidence intervals

three-element row vector

Color of confidence intervals, specified as a three-element row vector. The vector represents the red-green-blue color triplet.

By default, confidence intervals that are not limited by parameter bounds specified in the original fit are plotted using the first default color (blue), and those that are limited by the bounds are plotted using the second default color (red). If the confidence interval is not estimable, it is also plotted in red. To see the default color order, enter `get(groot,'defaultAxesColorOrder')` or see the "ColorOrder" property.

Tip Use this name-value pair when you want to create plots with a single color, for instance, for publication purposes.

Example: `Color=[0 0 0]`

Data Types: `double`

Output Arguments

`fh` — Figure handle

handle

Figure handle of the plot, returned as a figure handle.

Version History

Introduced in R2017b

See Also

`PredictionConfidenceInterval` | `sbiopredictionci` | `ParameterConfidenceInterval` | `sbioparameterci`

plot

Plot empirical CDF of multiparametric global sensitivity analysis

Syntax

```
h = plot(mpgsaObj)
h = plot(mpgsaObj,Name,Value)
```

Description

`h = plot(mpgsaObj)` plots the empirical CDFs (`ecdf`) of multiparametric global sensitivity analysis (MPGSA) and returns the figure handle `h`.

`h = plot(mpgsaObj,Name,Value)` uses additional options specified by one or more name-value pair arguments.

Examples

Perform Multiparametric Global Sensitivity Analysis (MPGSA)

Load the “Target-Mediated Drug Disposition (TMDD) Model”.

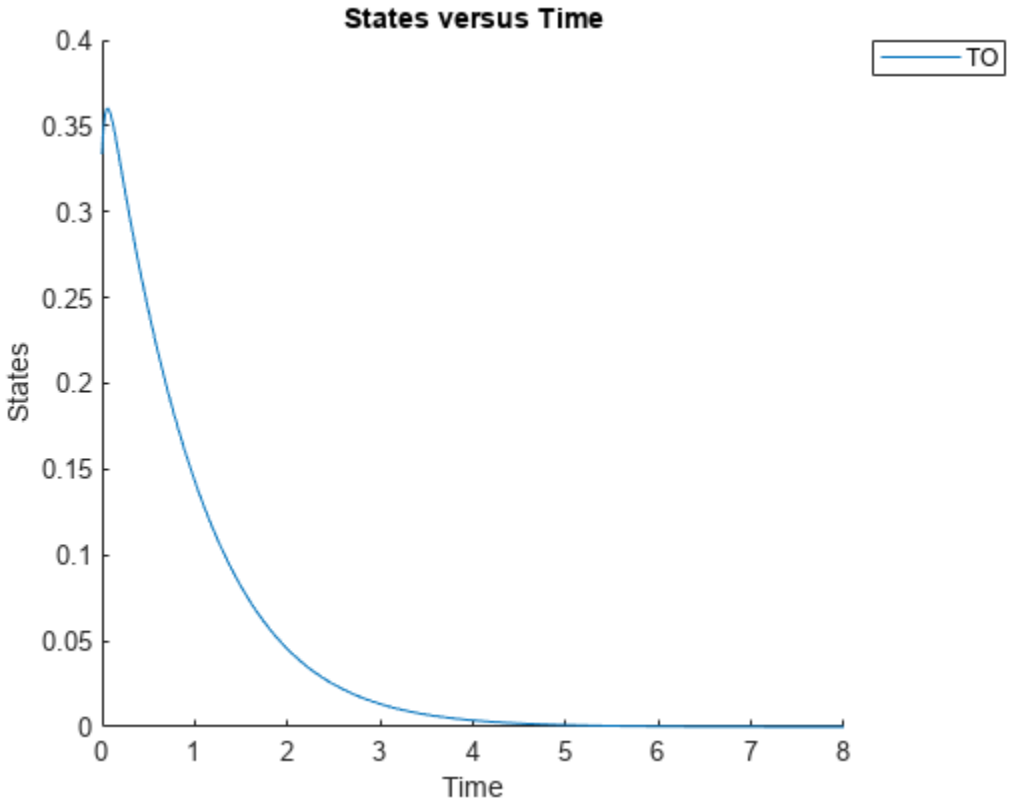
```
sbioloadproject tmdd_with_TO.sbproj
```

Get the active configset and set the target occupancy (`TO`) as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'TO';
```

Simulate the model and plot the `TO` profile.

```
sbioplot(sbiosimulate(m1,cs));
```



Define an exposure (area under the curve of the TO profile) threshold for the target occupancy.

```
classifier = 'trapz(time,TO) <= 0.1';
```

Perform MPGSA to find sensitive parameters with respect to the TO. Vary the parameter values between predefined bounds to generate 10,000 parameter samples.

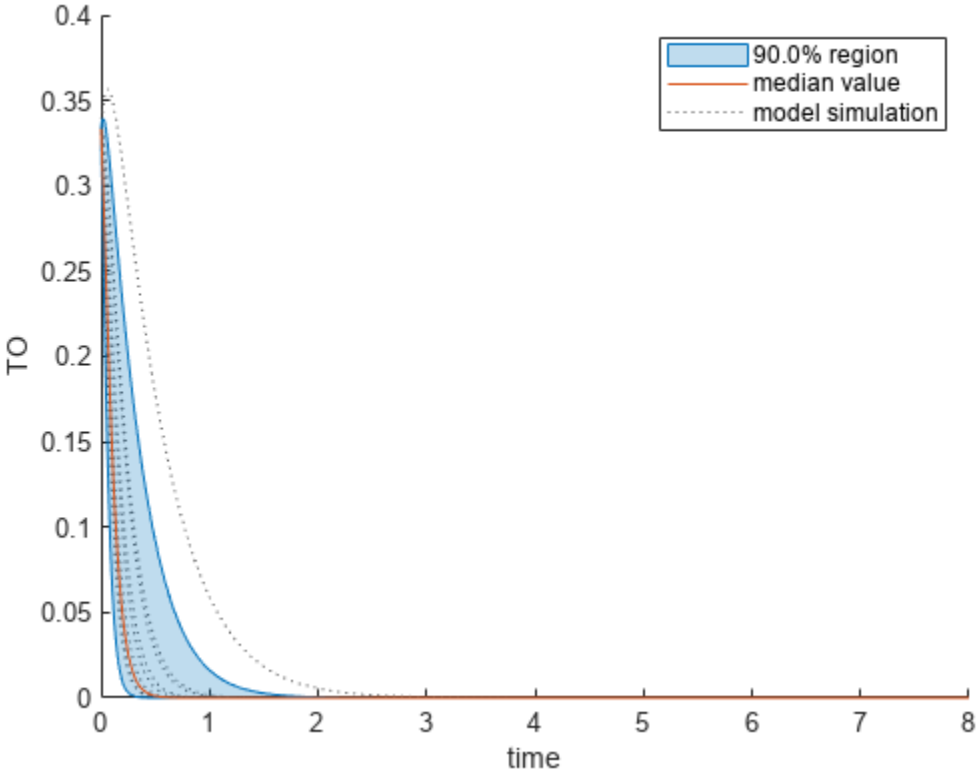
```
% Suppress an information warning that is issued during simulation.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
rng(0,'twister'); % For reproducibility
params = {'kel','ksyn','kdeg','km'};
bounds = [0.1, 1;
          0.1, 1;
          0.1, 1;
          0.1, 1];
mpgsaResults = sbiompgsa(m1,params,classifier,Bounds=bounds,NumberSamples=10000)
```

```
mpgsaResults =
  MPGSA with properties:

                   Classifiers: {'trapz(time,TO) <= 0.1'}
    KolmogorovSmirnovStatistics: [4x1 table]
                    ECDFData: {4x4 cell}
             SignificanceLevel: 0.0500
                      PValues: [4x1 table]
             SupportHypothesis: [10000x1 table]
              ParameterSamples: [10000x4 table]
                   Observables: {'TO'}
```

```
    SimulationInfo: [1x1 struct]
```

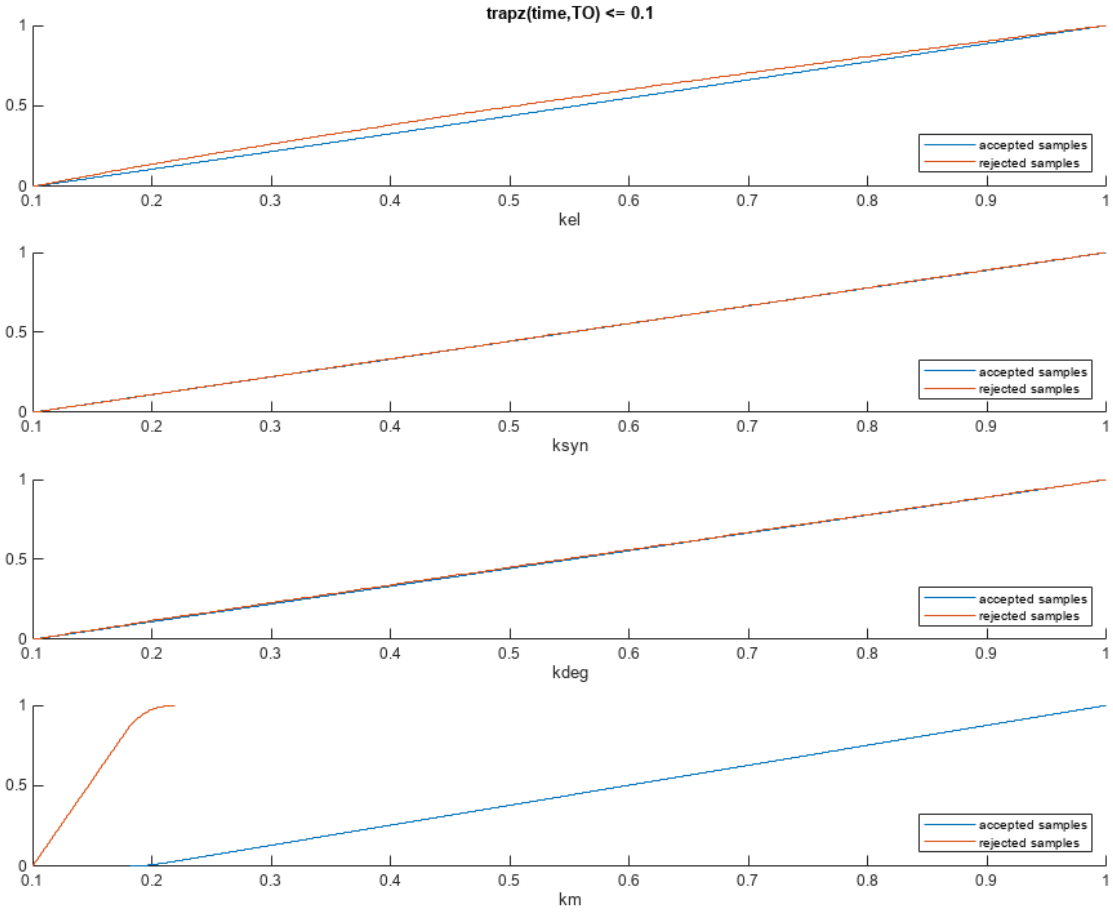
Plot the quantiles of the simulated model response.

```
plotData(mpgsaResults,ShowMedian=true,ShowMean=false);
```



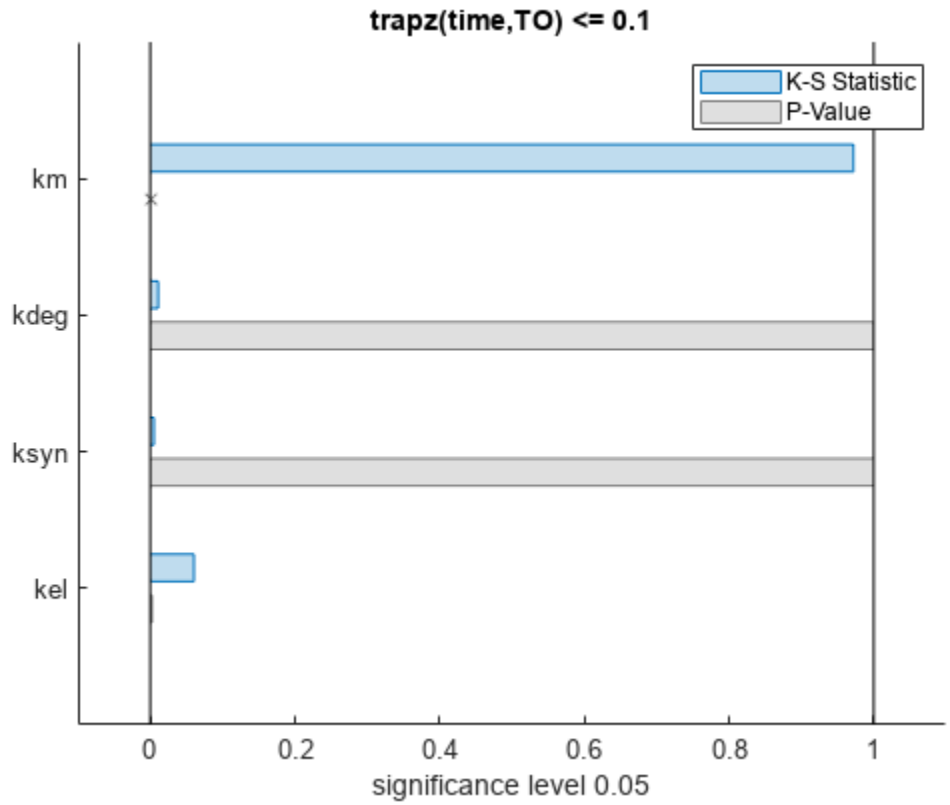
Plot the empirical cumulative distribution functions (eCDFs) of the accepted and rejected samples. Except for `km`, none of the parameters shows a significant difference in the eCDFs for the accepted and rejected samples. The `km` plot shows a large Kolmogorov-Smirnov (K-S) distance between the eCDFs of the accepted and rejected samples. The K-S distance is the maximum absolute distance between two eCDFs curves.

```
h = plot(mpgsaResults);
% Resize the figure.
pos = h.Position(:);
h.Position(:) = [pos(1) pos(2) pos(3)*2 pos(4)*2];
```



To compute the K-S distance between the two eCDFs, SimBiology uses a two-sided test based on the null hypothesis that the two distributions of accepted and rejected samples are equal. See `kstest2` (Statistics and Machine Learning Toolbox) for details. If the K-S distance is large, then the two distributions are different, meaning that the classification of the samples is sensitive to variations in the input parameter. On the other hand, if the K-S distance is small, then variations in the input parameter do not affect the classification of samples. The results suggest that the classification is insensitive to the input parameter. To assess the significance of the K-S statistic rejecting the null-hypothesis, you can examine the p-values.

```
bar(mpgsaResults)
```



The bar plot shows two bars for each parameter: one for the K-S distance (K-S statistic) and another for the corresponding p-value. You reject the null hypothesis if the p-value is less than the significance level. A cross (`x`) is shown for any p-value that is almost 0. You can see the exact p-value corresponding to each parameter.

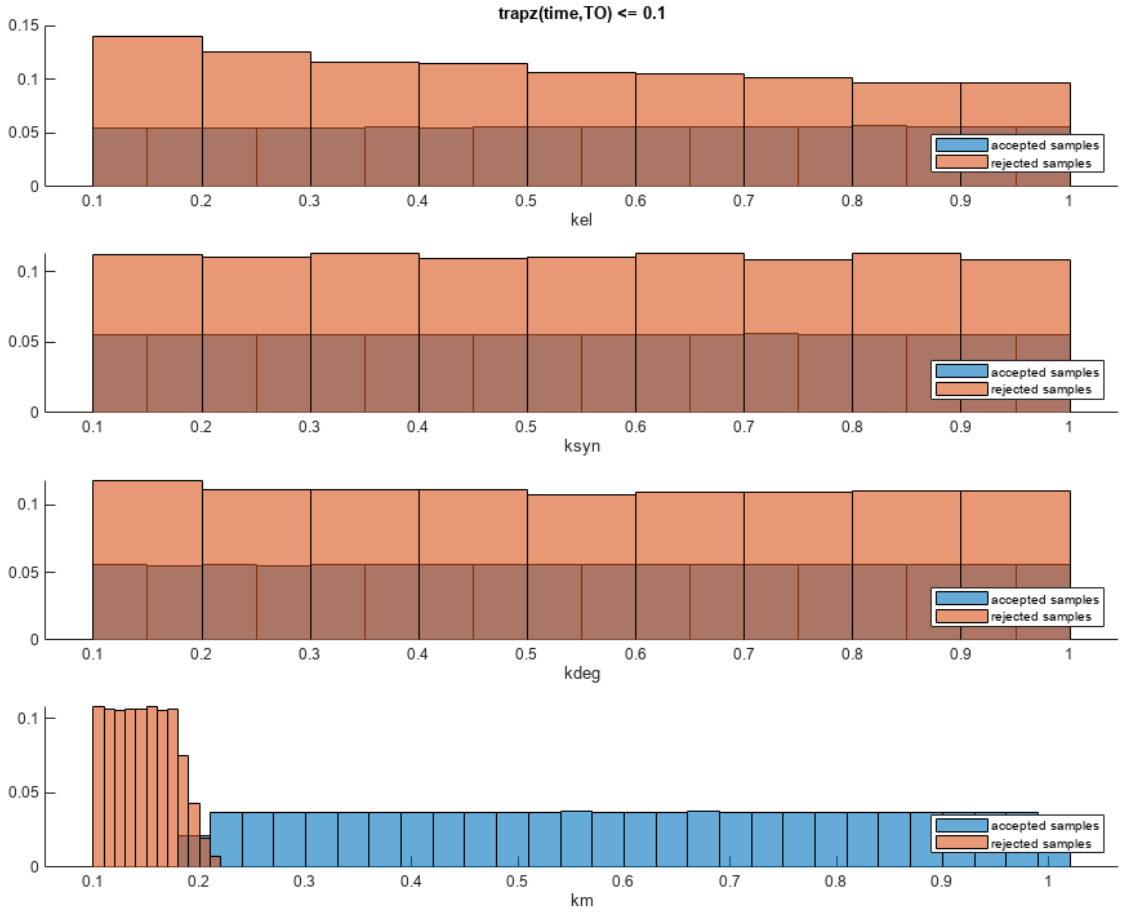
```
[mpgsaResults.ParameterSamples.Properties.VariableNames',mpgsaResults.PValues]
```

```
ans=4×2 table
      Var1      trapz(time,TO) <= 0.1
    ________    _____________________

    {'kel' }          0.0021877
    {'ksyn'}                  1
    {'kdeg'}            0.99983
    {'km'  }                  0
```

The p-values of `km` and `kel` are less than the significance level (0.05), supporting the alternative hypothesis that the accepted and rejected samples come from different distributions. In other words, the classification of the samples is sensitive to `km` and `kel` but not to other parameters (`kdeg` and `ksyn`).

You can also plot the histograms of accepted and rejected samples. The historgrams let you see trends in the accepted and rejected samples. In this example, the histogram of `km` shows that there are more accepted samples for larger `km` values, while the `kel` histogram shows that there are fewer rejected samples as `kel` increases.

```
h2 = histogram(mpgsaResults);
% Resize the figure.
pos = h2.Position(:);
h2.Position(:) = [pos(1) pos(2) pos(3)*2 pos(4)*2];
```



Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

`mpgsaObj` — Multiparametric global sensitivity analysis results

`SimBiology.gsa.MPGSA` object

Multiparametric global sensitivity analysis results, specified as a `SimBiology.gsa.MPGSA` object.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `h = plot(results,'Classifiers',1)` specifies to plot eCDFs of the first classifier.

`Parameters` — Input model quantities to plot

character vector | string | string vector | cell array of character vectors | vector of positive integers

Input model quantities, namely parameters, species, or compartments, to plot, specified as a character vector, string, string vector, cell array of character vectors, or a vector of positive integers indexing into the columns of the `mpgsaObj.ParameterSamples` table.

Example: `'Parameters','k1'`

Data Types: `double` | `char` | `string` | `cell`

`Classifiers` — Classifiers to plot

character vector | string | string vector | cell array of character vectors | vector of positive integers

Classifiers to plot, specified as a character vector, string, string vector, cell array of character vectors, or a vector of positive integers.

Specify the expressions of classifiers to plot as a character vector, string, string vector, cell array of character vectors. Alternatively, you can specify a vector of positive integers indexing into `mpgsaObj.Classifiers`.

Example: `'Classifiers',[1 3]`

Data Types: `double` | `char` | `string` | `cell`

`AcceptedSamplesColor` — Color of accepted samples

three-element row vector | hexadecimal color code | color name

Color of accepted samples, specified as a three-element row vector, hexadecimal color code, color name, or a short name. By default, the function uses the first MATLAB default color. To view the default color order, enter `get(groot,'defaultAxesColorOrder')` or see the “ColorOrder” property.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see “Specify Plot Colors”.

Example: `'AcceptedSamplesColor',[0.4,0.3,0.2]`

Data Types: `double`

`RejectedSamplesColor` — Color of rejected samples

three-element row vector | hexadecimal color code | color name

Color of rejected samples, specified as a three-element row vector, hexadecimal color code, color name, or a short name. By default, the function uses the second MATLAB default color. To view the default color order, enter `get(groot,'defaultAxesColorOrder')` or see the “ColorOrder” property.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see “Specify Plot Colors”.

Example: `'RejectedSamplesColor',[0.9,0.5,0.2]`

Data Types: `double`

Output Arguments

h — Handle
figure handle

Handle to the figure, specified as a figure handle.

Version History

Introduced in R2020a

References

[1] Tiemann, Christian A., Joep Vanlier, Maaike H. Oosterveer, Albert K. Groen, Peter A. J. Hilbers, and Natal A. W. van Riel. “Parameter Trajectory Analysis to Identify Treatment Effects of Pharmacological Interventions.” Edited by Scott Markel. *PLoS Computational Biology* 9, no. 8 (August 1, 2013): e1003166. https://doi.org/10.1371/journal.pcbi.1003166.

See Also

`SimBiology.gsa.MPGSA` | `sbiompgsa` | `plotData` | `bar` | `histogram` | `kstest2` | `ecdf`

plot

Plot means and standard deviations of elementary effects

Syntax

```
h = plot(eeObj)
h = plot(eeObj,Name=Value)
```

Description

`h = plot(eeObj)` plots the means and standard deviations of elementary effects and returns the figure handle `h`. When `eeObj` contains multiple sensitivity inputs and outputs, the function displays a subplot where the columns are the sensitivity outputs and rows are the sensitivity inputs.

`h = plot(eeObj,Name=Value)` uses additional options specified by one or more name-value arguments.

Examples

Perform GSA by Computing Elementary Effects

Load the “Tumor Growth Model”.

```
sbioloadproject tumor_growth_vpop_sa.sbproj
```

Get a variant with estimated parameters and the dose to apply to the model.

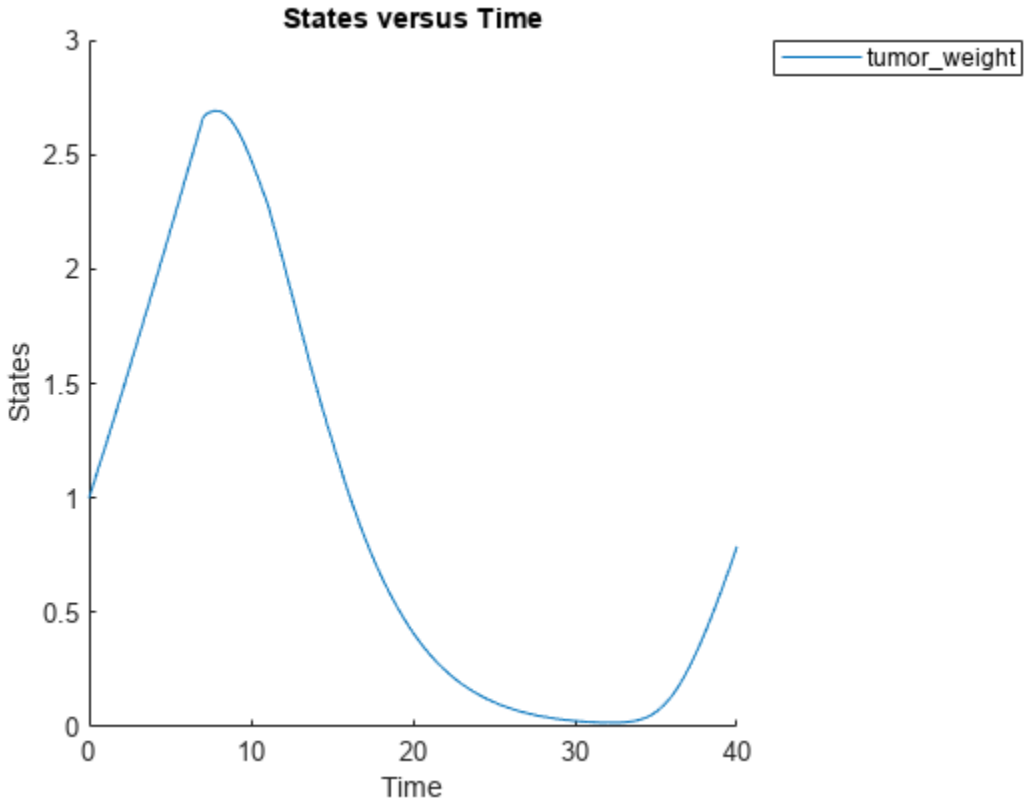
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

Get the active configset and set the tumor weight as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'tumor_weight';
```

Simulate the model and plot the tumor growth profile.

```
sbioplot(sbiosimulate(m1,cs,v,d));
```



Perform global sensitivity analysis (GSA) on the model to find the model parameters that the tumor growth is sensitive to.

First, define model parameters of interest, which are involved in the pharmacodynamics of the tumor growth. Define the model response as the tumor weight.

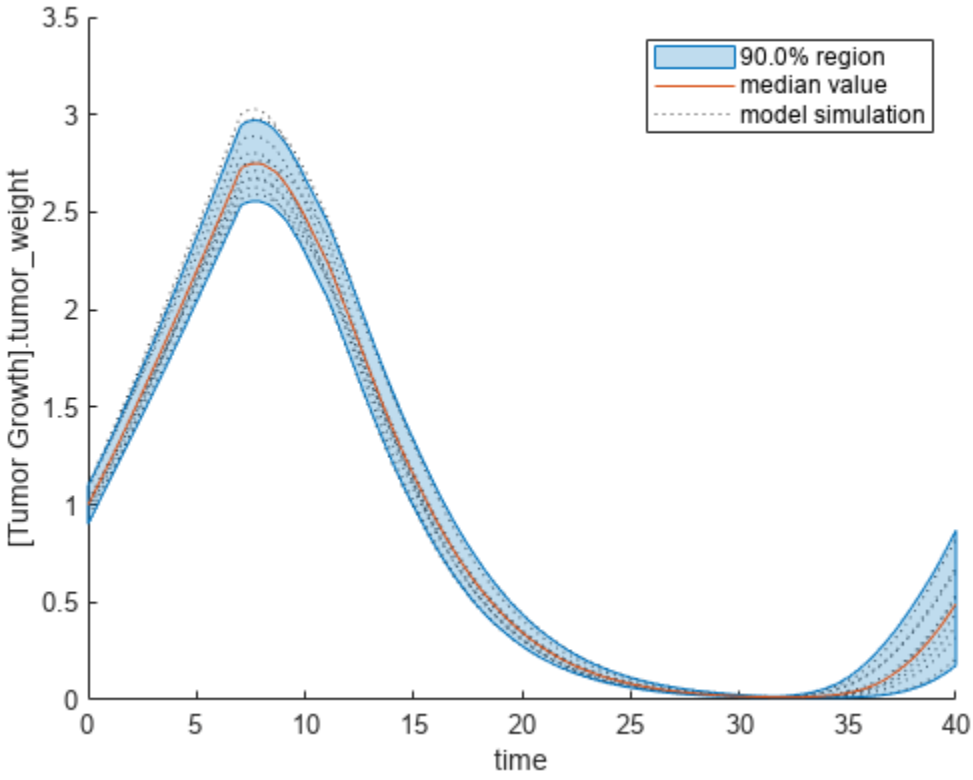
```
modelParamNames = {'L0','L1','w0','k1'};
outputName = 'tumor_weight';
```

Then perform GSA by computing the elementary effects using `sbioelementaryeffects`. Use `100` as the number of samples and set `ShowWaitBar` to `true` to show the simulation progress.

```
rng('default');
eeResults = sbioelementaryeffects(m1,modelParamNames,outputName,Variants=v,Doses=d,NumberSamples=
```

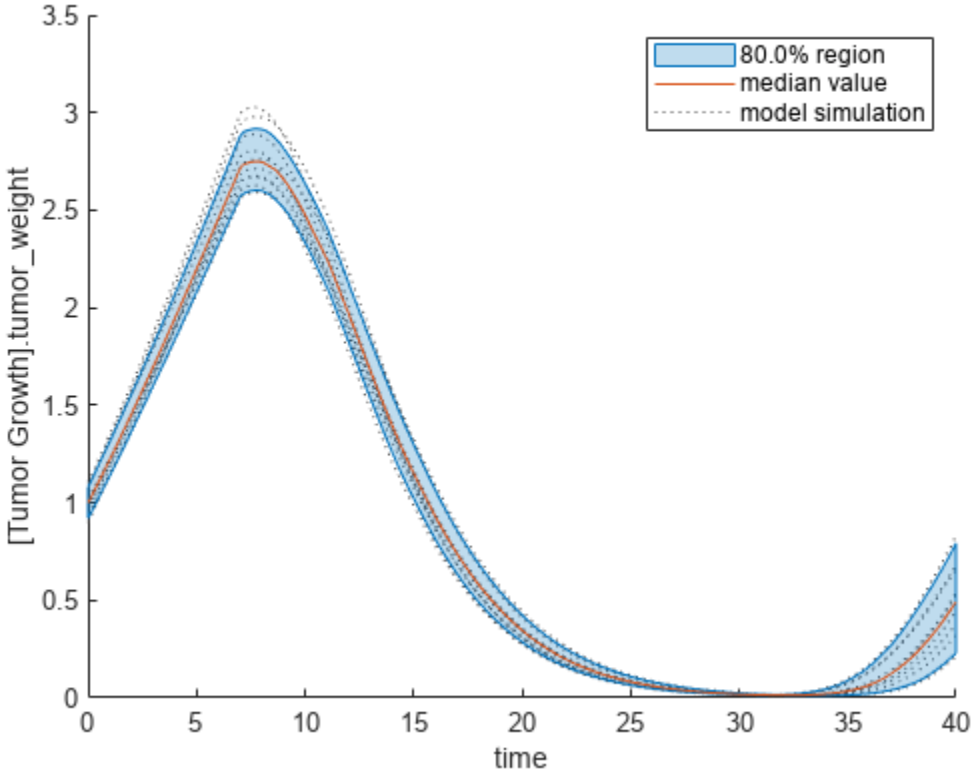
Show the median model response, the simulation results, and a shaded region covering 90% of the simulation results.

```
plotData(eeResults,ShowMedian=true,ShowMean=false);
```



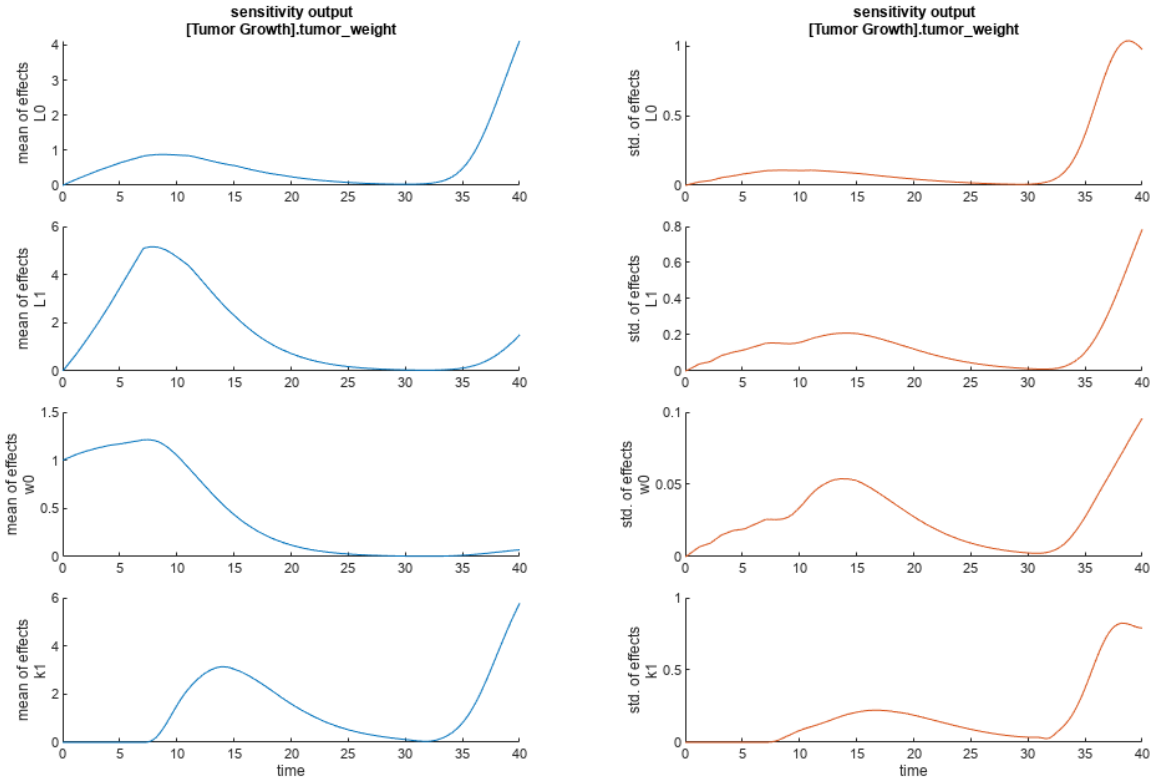
You can adjust the quantile region to a different percentage by specifying `Alphas` for the lower and upper quantiles of all model responses. For instance, an `alpha` value of 0.1 plots a shaded region between the `100*alpha` and `100*(1-alpha)` quantiles of all simulated model responses.

```
plotData(eeResults,Alphas=0.1,ShowMedian=true,ShowMean=false);
```



Plot the time course of the means and standard deviations of the elementary effects.

```
h = plot(eeResults);
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```

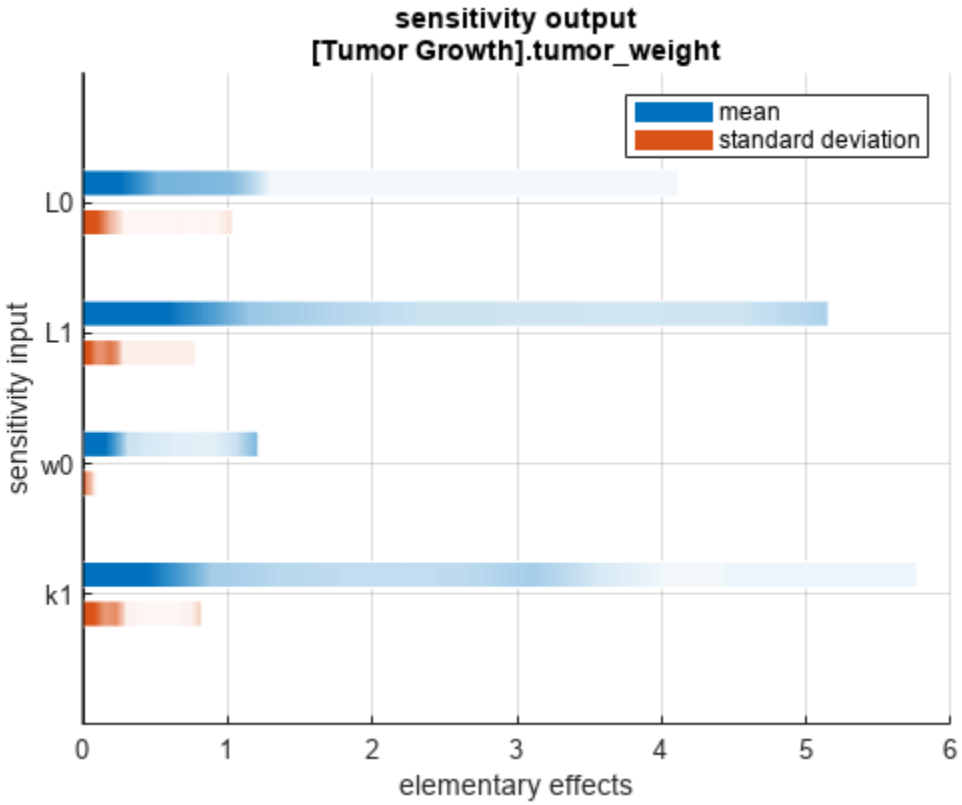


The mean of effects explains whether variations in input parameter values have any effect on the tumor weight response. The standard deviation of effects explains whether the sensitivity change is dependent on the location in the parameter domain.

From the mean of effects plots, parameters `L1` and `w0` seem to be the most sensitive parameters to the tumor weight before the dose is applied at t = 7. But, after the dose is applied, `k1` and `L0` become more sensitive parameters and contribute most to the after-dosing stage of the tumor weight. The plots of standard deviation of effects show more deviations for the larger parameter values in the later stage (t > 35) than for the before-dose stage of the tumor growth.

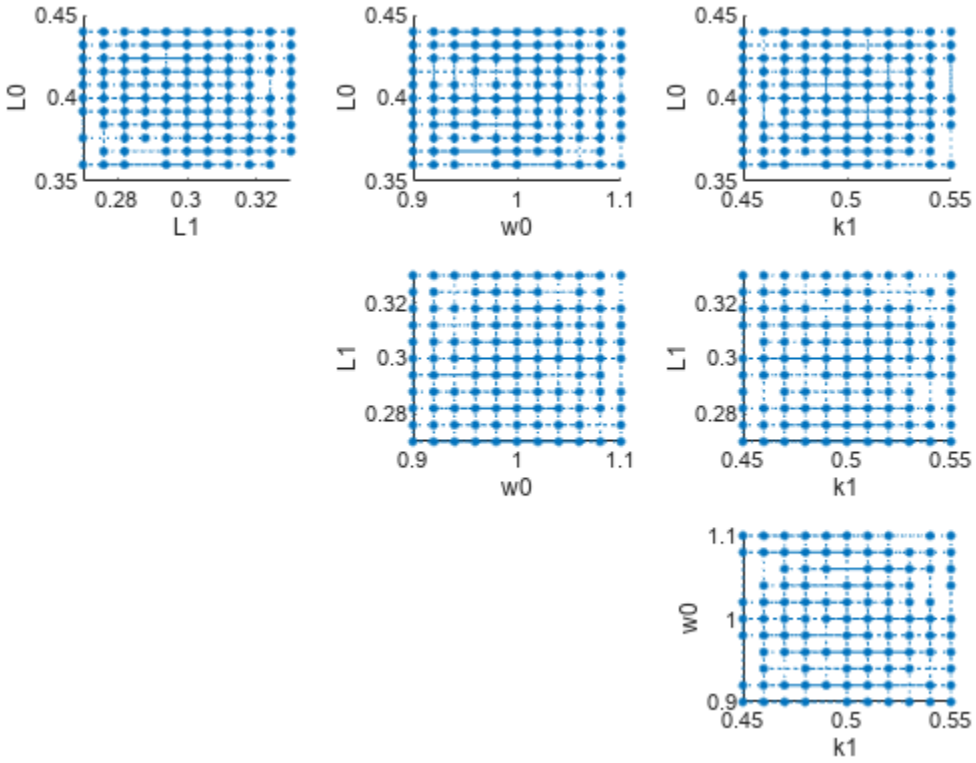
You can also display the magnitudes of the sensitivities in a bar plot. Each color shading represents a histogram representing values at different times. Darker colors mean that those values occur more often over the whole time course.

```
bar(eeResults);
```



You can also plot the parameter grids and samples used to compute the elementary effects.

```
plotGrid(eeResults)
```



You can specify more samples to increase the accuracy of the elementary effects, but the simulation can take longer to finish. Use `addsamples` to add more samples.

```
eeResults2 = addsamples(eeResults,200);
```

The `SimulationInfo` property of the result object contains various information for computing the elementary effects. For instance, the model simulation data (SimData) for each simulation using a set of parameter samples is stored in the `SimData` field of the property. This field is an array of `SimData` objects.

```
eeResults2.SimulationInfo.SimData
```

```
SimBiology SimData Array : 1500-by-1

Index:    Name:         ModelName:         DataCount:
1           -           Tumor Growth Model 1
2           -           Tumor Growth Model 1
3           -           Tumor Growth Model 1
...
1500        -           Tumor Growth Model 1
```

You can find out if any model simulation failed during the computation by checking the `ValidSample` field of `SimulationInfo`. In this example, the field shows no failed simulation runs.

```
all(eeResults2.SimulationInfo.ValidSample)
```

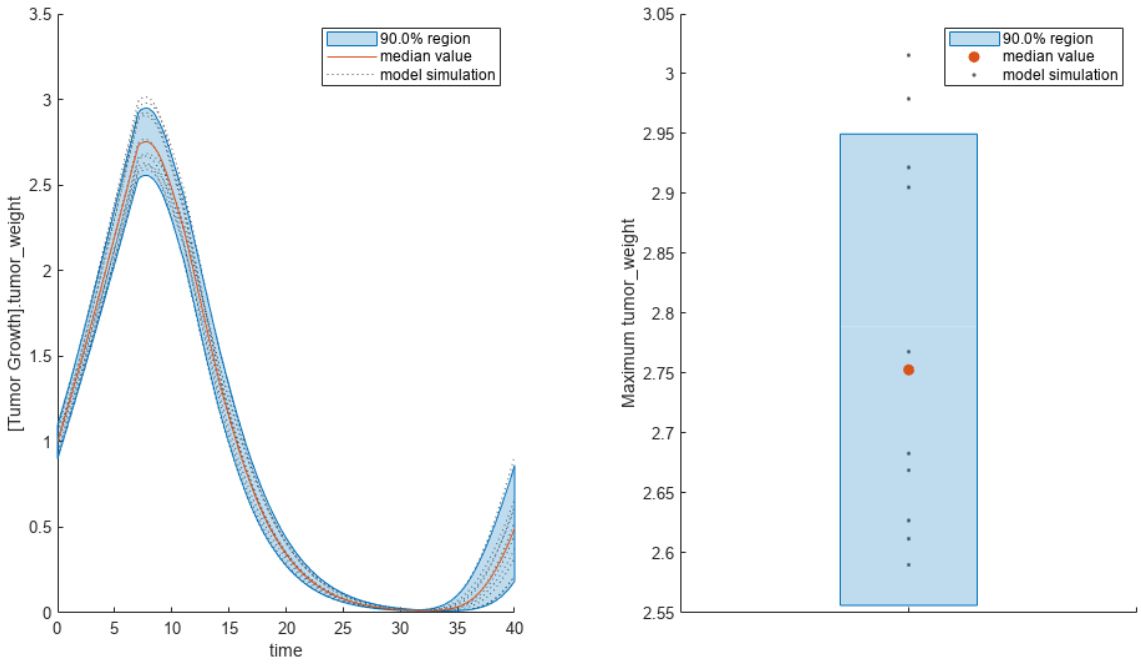
```
ans = logical
   1
```

You can add custom expressions as observables and compute the elementary effects of the added observables. For example, you can compute the effects for the maximum tumor weight by defining a custom expression as follows.

```
% Suppress an information warning that is issued.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
% Add the observable expression.
eeObs = addobservable(eeResults2,'Maximum tumor_weight','max(tumor_weight)','Units','gram');
```

Plot the computed simulation results showing the 90% quantile region.

```
h2 = plotData(eeObs,ShowMedian=true,ShowMean=false);
h2.Position(:) = [100 100 1500 800];
```



You can also remove the observable by specifying its name.

```
eeNoObs = removeobservable(eeObs,'Maximum tumor_weight');
```

Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

eeObj — Results containing means and standard deviations of elementary effects

`SimBiology.gsa.ElementaryEffects` object

Results containing the means and standard deviations of elementary effects, specified as a `SimBiology.gsa.ElementaryEffects` object.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Example: `h = plot(results,Observables='tumor_weight')` plots the mean and standard deviation of elementary effects corresponding to the tumor weight response.

`Parameters` — Input parameters to plot

character vector | string | string vector | cell array of character vectors | vector of positive integers

Input parameters to plot, specified as a character vector, string, string vector, cell array of character vectors, or vector of positive integers indexing into the columns of the `resultsObject.ParameterSamples` table. Use this name-value argument to select parameters and plot their corresponding GSA results. By default, all input parameters are included in the plot.

Data Types: `double` | `char` | `string` | `cell`

`Observables` — Model responses or observables to plot

character vector | string | string vector | cell array of character vectors | vector of positive integers

Model responses or observables to plot, specified as a character vector, string, string vector, cell array of character vectors, or vector of positive integers indexing into `resultsObject.Observables`. By default, the function plots GSA results for all model responses or observables.

Data Types: `double` | `char` | `string` | `cell`

`ShowMean` — Flag to plot means of elementary effects

`true` (default) | `false`

Flag to plot the means of elementary effects, specified as `true` or `false`.

Data Types: `logical`

`ShowStandardDeviation` — Flag to plot standard deviations of elementary effects

`true` (default) | `false`

Flag to plot the standard deviations of elementary effects, specified as `true` or `false`.

Data Types: `logical`

`MeanColor` — Color of means of elementary effects

three-element row vector | hexadecimal color code | color name

Color of the means of elementary effects, specified as a three-element row vector, hexadecimal color code, color name, or a short name. By default, the function uses the first MATLAB default color. To view the default color order, enter `get(groot,'defaultAxesColorOrder')` or see the "ColorOrder" property.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see "Specify Plot Colors".

Data Types: `double`

`StandardDeviationColor` — Color of standard deviation of elementary effects
three-element row vector | hexadecimal color code | color name

Color of the standard deviation of elementary effects, specified as a three-element row vector, hexadecimal color code, color name, or a short name. By default, the function uses the second MATLAB default color. To view the default color order, enter `get(groot,'defaultAxesColorOrder')` or see the “ColorOrder” property.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see “Specify Plot Colors”.

Data Types: `double`

Output Arguments

h — Handle
figure handle

Handle to the figure, specified as a figure handle.

Version History

Introduced in R2021b

See Also

`SimBiology.gsa.Sobol` | `SimBiology.gsa.ElementaryEffects` | `sbioelementaryeffects`

Topics
“Sensitivity Analysis in SimBiology”

plot

Plot first- and total-order Sobol indices and variances

Syntax

```
h = plot(sobolObj)
h = plot(sobolObj,Name,Value)
```

Description

`h = plot(sobolObj)` plots the variance decomposition in the form of the first- and total-order Sobol indices and returns the figure handle `h`.

`h = plot(sobolObj,Name,Value)` uses additional options specified by one or more name-value pair arguments.

Examples

Perform Global Sensitivity Analysis by Computing First- and Total-Order Sobol Indices

Load the “Tumor Growth Model”.

```
sbioloadproject tumor_growth_vpop_sa.sbproj
```

Get a variant with the estimated parameters and the dose to apply to the model.

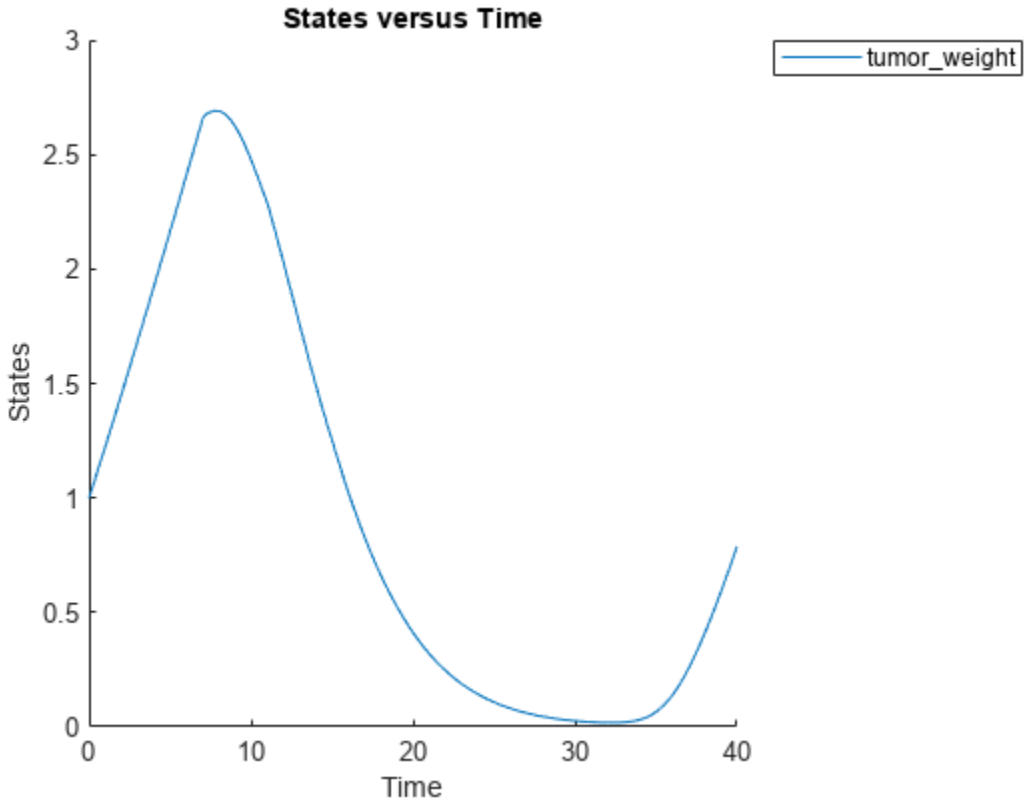
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

Get the active configset and set the tumor weight as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'tumor_weight';
```

Simulate the model and plot the tumor growth profile.

```
sbioplot(sbiosimulate(m1,cs,v,d));
```



Perform global sensitivity analysis (GSA) on the model to find the model parameters that the tumor growth is sensitive to.

First, retrieve model parameters of interest that are involved in the pharmacodynamics of the tumor growth. Define the model response as the tumor weight.

```
modelParamNames = {'L0','L1','w0','k1','k2'};
outputName = 'tumor_weight';
```

Then perform GSA by computing the first- and total-order Sobol indices using `sbiosobol`. Set `'ShowWaitBar'` to `true` to show the simulation progress. By default, the function uses 1000 parameter samples to compute the Sobol indices [1].

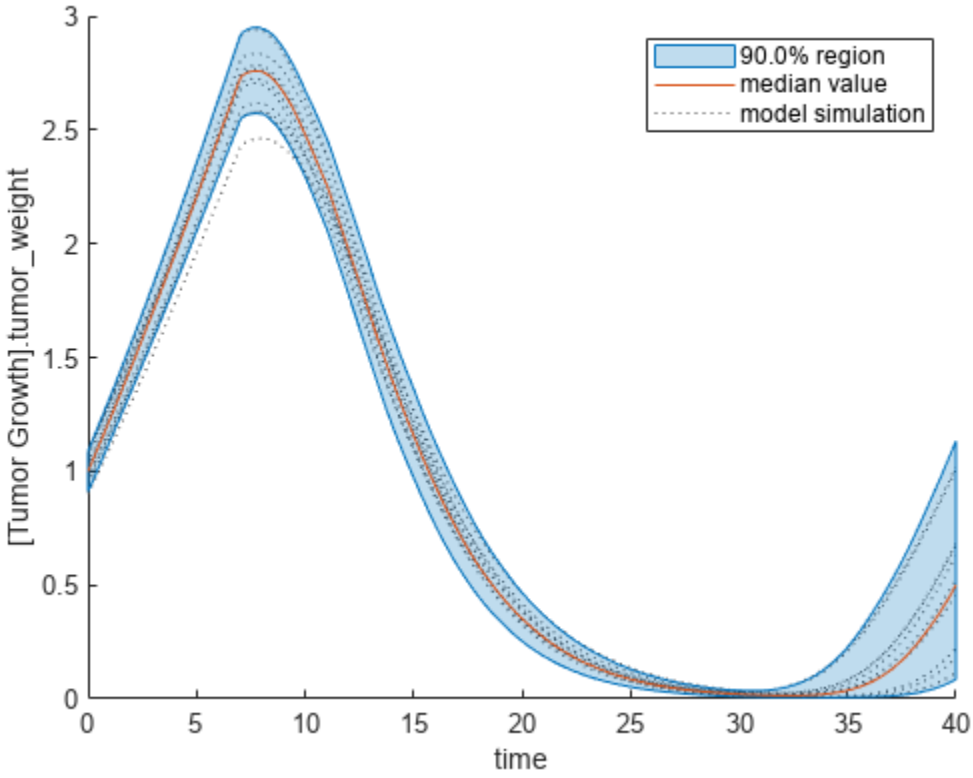
```
rng('default');
sobolResults = sbiosobol(m1,modelParamNames,outputName,Variants=v,Doses=d,ShowWaitBar=true)
```

```
sobolResults =
  Sobol with properties:

                Time: [444x1 double]
        SobolIndices: [5x1 struct]
            Variance: [444x1 table]
    ParameterSamples: [1000x5 table]
         Observables: {'[Tumor Growth].tumor_weight'}
      SimulationInfo: [1x1 struct]
```

You can change the number of samples by specifying the `'NumberSamples'` name-value pair argument. The function requires a total of `(number of input parameters + 2) * NumberSamples` model simulations.

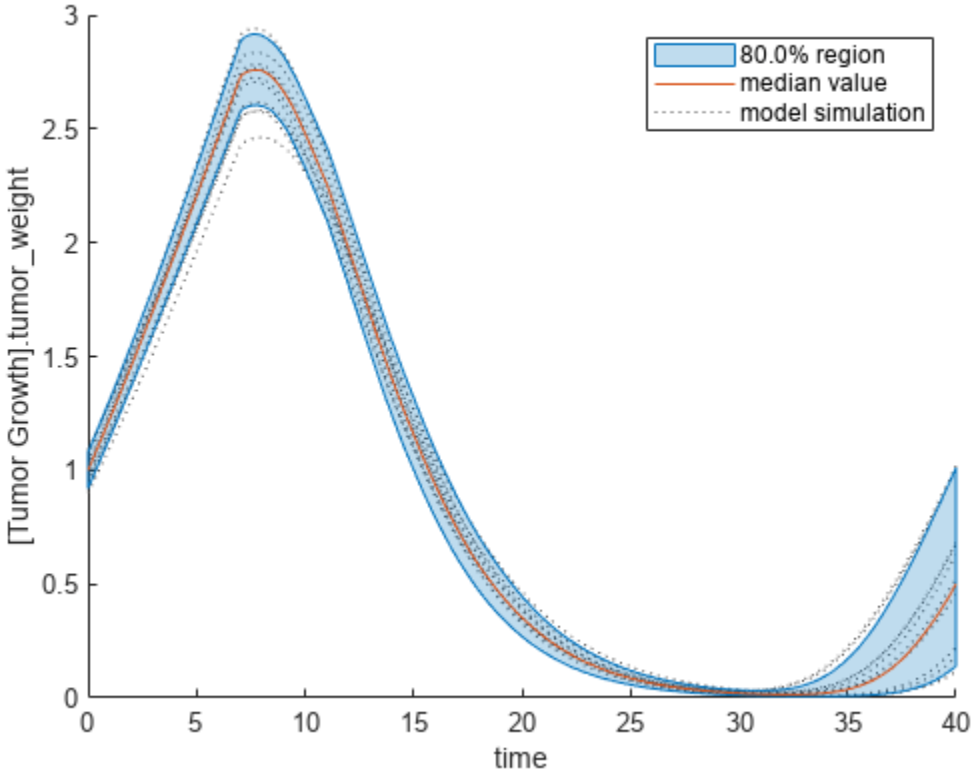
Show the mean model response, the simulation results, and a shaded region covering 90% of the simulation results.

```
plotData(sobolResults,ShowMedian=true,ShowMean=false);
```



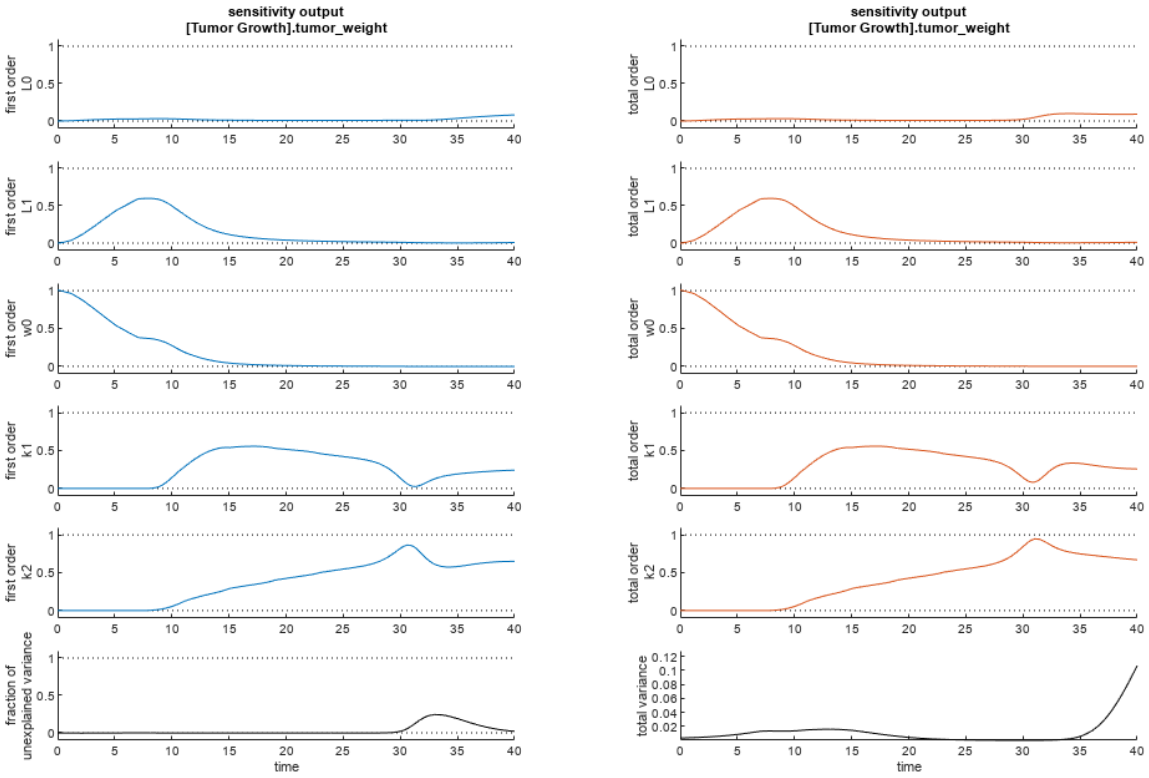
You can adjust the quantile region to a different percentage by specifying `'Alphas'` for the lower and upper quantiles of all model responses. For instance, an alpha value of 0.1 plots a shaded region between the `100 * alpha` and `100 * (1 - alpha)` quantiles of all simulated model responses.

```
plotData(sobolResults,Alphas=0.1,ShowMedian=true,ShowMean=false);
```



Plot the time course of the first- and total-order Sobol indices.

```
h = plot(sobolResults);
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```

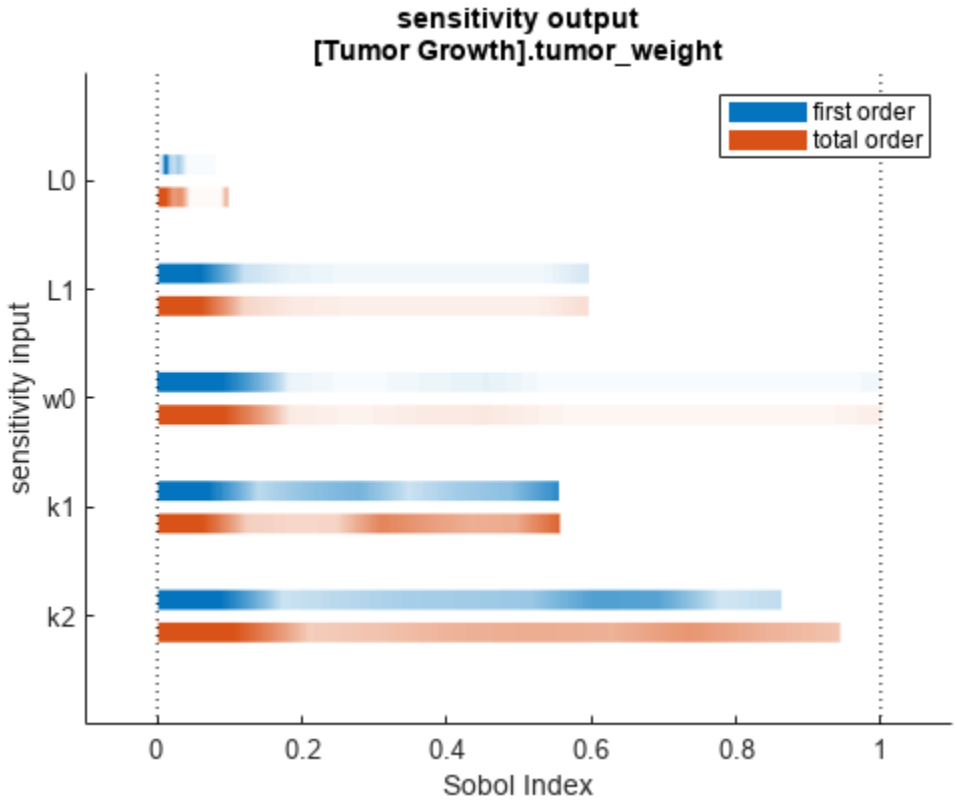


The first-order Sobol index of an input parameter gives the fraction of the overall response variance that can be attributed to variations in the input parameter alone. The total-order index gives the fraction of the overall response variance that can be attributed to any joint parameter variations that include variations of the input parameter.

From the Sobol indices plots, parameters `L1` and `w0` seem to be the most sensitive parameters to the tumor weight before the dose was applied at t = 7. But after the dose is applied, `k1` and `k2` become more sensitive parameters and contribute most to the after-dosing stage of the tumor weight. The total variance plot also shows a larger variance for the after-dose stage at t > 35 than for the before-dose stage of the tumor growth, indicating that `k1` and `k2` might be more important parameters to investigate further. The fraction of unexplained variance shows some variance at around t = 33, but the total variance plot shows little variance at t = 33, meaning the unexplained variance could be insignificant. The fraction of unexplained variance is calculated as 1 - (sum of all the first-order Sobol indices), and the total variance is calculated using `var(response)`, where `response` is the model response at every time point.

You can also display the magnitudes of the sensitivities in a bar plot. Darker colors mean that those values occur more often over the whole time course.

```
bar(sobolResults);
```



You can specify more samples to increase the accuracy of the Sobol indices, but the simulation can take longer to finish. Use `addsamples` to add more samples. For example, if you specify 1500 samples, the function performs `1500 * (2 + number of input parameters)` simulations.

```
gsaMoreSamples = addsamples(gsaResults,1500)
```

The “SimulationInfo” on page 2-0 property of the result object contains various information for computing the Sobol indices. For instance, the model simulation data (SimData) for each simulation using a set of parameter samples is stored in the `SimData` field of the property. This field is an array of `SimData` objects.

```
sobolResults.SimulationInfo.SimData
```

```
SimBiology SimData Array : 1000-by-7

Index:    Name:         ModelName:         DataCount:
1           -           Tumor Growth Model 1
2           -           Tumor Growth Model 1
3           -           Tumor Growth Model 1
...
7000        -           Tumor Growth Model 1
```

You can find out if any model simulation failed during the computation by checking the `ValidSample` field of `SimulationInfo`. In this example, the field shows no failed simulation runs.

```
all(sobolResults.SimulationInfo.ValidSample)
```

```
ans = 1x7 logical array

   1   1   1   1   1   1   1
```

`SimulationInfo.ValidSample` is a table of logical values. It has the same size as `SimulationInfo.SimData`. If `ValidSample` indicates that any simulations failed, you can get more information about those simulation runs and the samples used for those runs by extracting information from the corresponding column of `SimulationInfo.SimData`. Suppose that the fourth column contains one or more failed simulation runs. Get the simulation data and sample values used for that simulation using `getSimulationResults`.

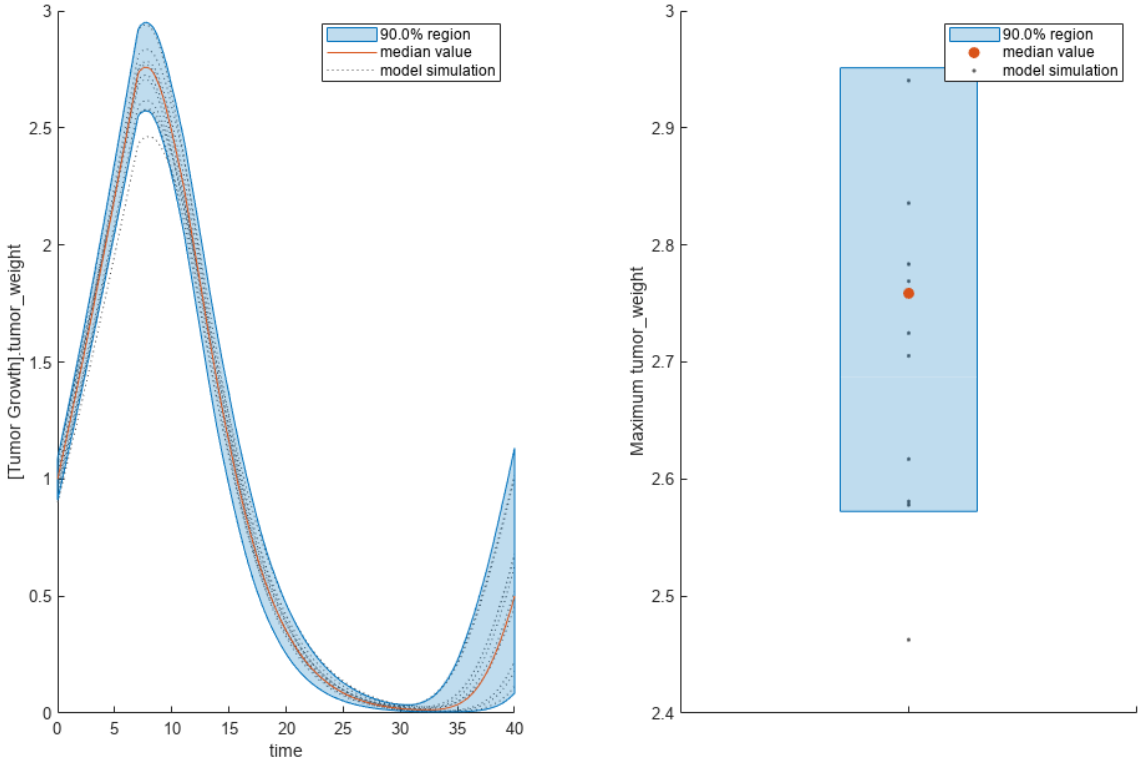
```
[samplesUsed,sd,validruns] = getSimulationResults(sobolResults,4);
```

You can add custom expressions as observables and compute Sobol indices for the added observables. For example, you can compute the Sobol indices for the maximum tumor weight by defining a custom expression as follows.

```
% Suppress an information warning that is issued during simulation.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
% Add the observable expression.
sobolObs = addobservable(sobolResults,'Maximum tumor_weight','max(tumor_weight)','Units','gram');
```

Plot the computed simulation results showing the 90% quantile region.

```
h2 = plotData(sobolObs,ShowMedian=true,ShowMean=false);
h2.Position(:) = [100 100 1280 800];
```



You can also remove the observable by specifying its name.

```
gsaNoObs = removeobservable(sobolObs,'Maximum tumor_weight');
```

Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

`sobolObj` — Results containing Sobol indices

`SimBiology.gsa.Sobol` object

Results containing the first- and total-order Sobol indices, specified as a `SimBiology.gsa.Sobol` object.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `h = plot(results,'Observables','tumor_weight')` specifies to plot Sobol indices corresponding to the tumor weight response.

`Parameters` — Input parameters to plot

character vector | string | string vector | cell array of character vectors | vector of positive integers

Input parameters to plot, specified as a character vector, string, string vector, cell array of character vectors, or vector of positive integers indexing into the columns of the `resultsObject.ParameterSamples` table. Use this name-value argument to select parameters and plot their corresponding GSA results. By default, all input parameters are included in the plot.

Data Types: `double` | `char` | `string` | `cell`

`Observables` — Model responses or observables to plot

character vector | string | string vector | cell array of character vectors | vector of positive integers

Model responses or observables to plot, specified as a character vector, string, string vector, cell array of character vectors, or vector of positive integers indexing into `resultsObject.Observables`. By default, the function plots GSA results for all model responses or observables.

Data Types: `double` | `char` | `string` | `cell`

`Color` — Color of first- and total-order Sobol indices

three-element row vector | hexadecimal color code | color name

Color of the first- and total-order Sobol indices, specified as a three-element row vector, hexadecimal color code, color name, or a short name. By default, the function uses the first MATLAB default color for the first order and the second default color for the total order. To view the default color order, enter `get(groot,'defaultAxesColorOrder')` or see the “ColorOrder” property.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see “Specify Plot Colors”.

Example: `'Color',[0.4,0.3,0.2]`

Data Types: `double`

`VarianceColor` — Color of total and unexplained variances
`[0,0,0]` (default) | three-element row vector | hexadecimal color code | color name

Color of the total and unexplained variances, specified as a three-element row vector, hexadecimal color code, color name, or a short name. By default, the function uses the color black `[0,0,0]`.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see “Specify Plot Colors”.

Example: `'VarianceColor',[0.2,0.5,0.8]`

Data Types: `double`

`DelimiterColor` — Color of delimiting lines
`[0,0,0]` (default) | three-element row vector | hexadecimal color code | color name

Color of the delimiting lines, specified as a three-element row vector, hexadecimal color code, color name, or a short name. By default, the function uses the color black `[0,0,0]`.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see “Specify Plot Colors”.

Example: `'DelimiterColor',[0.2,0.5,0.8]`

Data Types: `double`

Output Arguments

h — Handle
figure handle

Handle to the figure, specified as a figure handle.

Version History

Introduced in R2020a

References

[1] Saltelli, Andrea, Paola Annoni, Ivano Azzini, Francesca Campolongo, Marco Ratto, and Stefano Tarantola. “Variance Based Sensitivity Analysis of Model Output. Design and Estimator for the Total Sensitivity Index.” *Computer Physics Communications* 181, no. 2 (February 2010): 259–70. https://doi.org/10.1016/j.cpc.2009.09.018.

See Also

`SimBiology.gsa.Sobol` | `sbiosobol` | `plotData` | `bar`

plotActualVersusPredicted

Compare predictions to actual data, creating a subplot for each response

Syntax

```
plotActualVersusPredicted(resultsObj)
```

Description

`plotActualVersusPredicted(resultsObj)` shows the comparison between predictions to the actual data, with a subplot for each response.

Examples

Estimate Two-Compartment PK Parameters

Load the sample data set.

```
load data10_32R.mat
gData = groupedData(data);
gData.Properties.VariableUnits = ["","hour","milligram/liter","milligram/liter"];
```

Create a two-compartment PK model.

```
pkmd                 = PKModelDesign;
pkc1                 = addCompartment(pkmd,"Central");
pkc1.DosingType      = "Infusion";
pkc1.EliminationType = "linear-clearance";
pkc1.HasResponseVariable = true;
pkc2                 = addCompartment(pkmd,"Peripheral");
model                = construct(pkmd);
configset            = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
responseMap = ["Drug_Central = CentralConc","Drug_Peripheral = PeripheralConc"];
```

Provide model parameters to estimate.

```
paramsToEstimate   = ["log(Central)","log(Peripheral)","Q12","Cl_Central"];
estimatedParam     = estimatedInfo(paramsToEstimate,'InitialValue',[1 1 1 1]);
```

Assume every individual receives an infusion dose at time = 0, with a total infusion amount of 100 mg at a rate of 50 mg/hour.

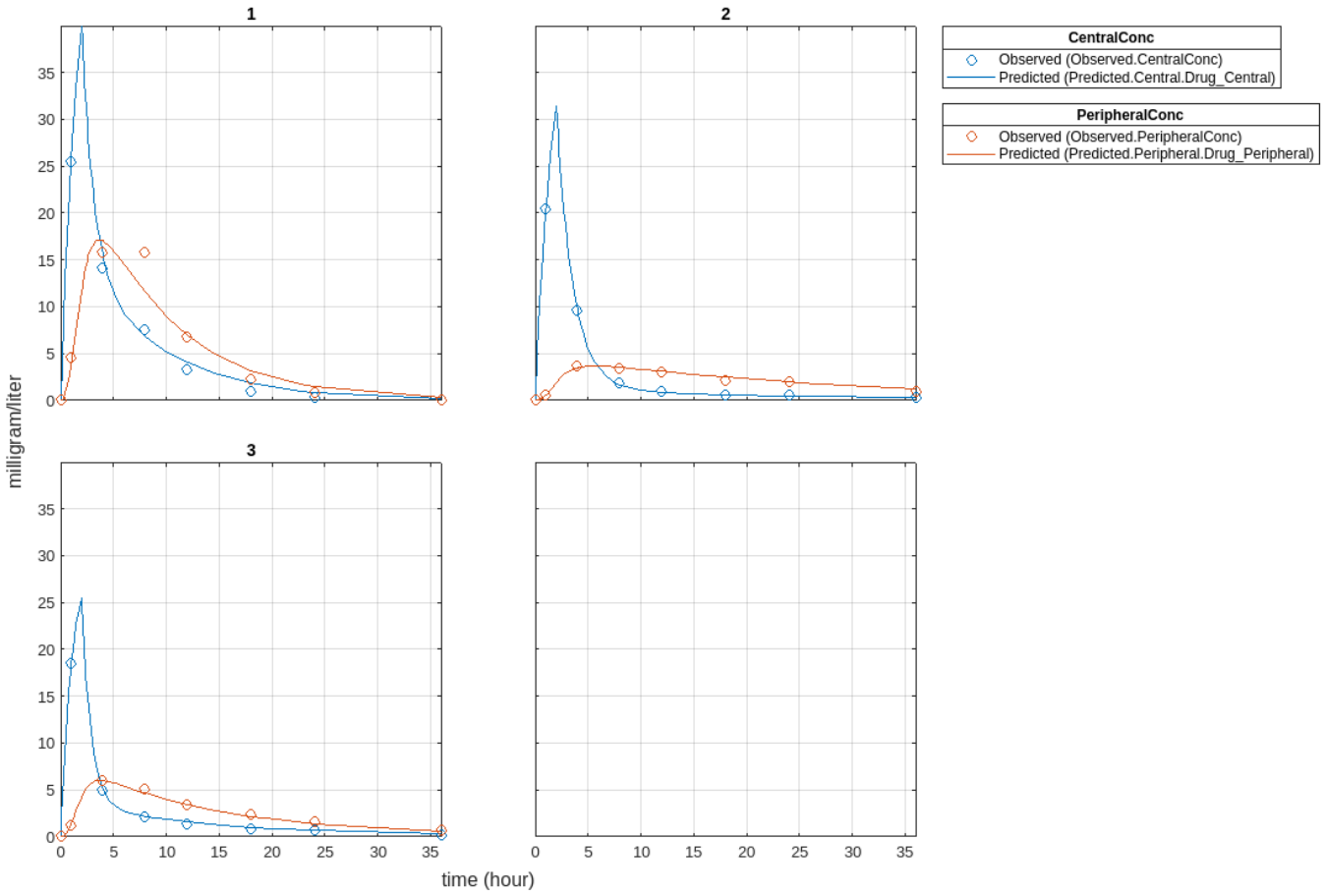
```
dose             = sbiodose("dose","TargetName","Drug_Central");
dose.StartTime   = 0;
dose.Amount      = 100;
dose.Rate        = 50;
dose.AmountUnits = "milligram";
dose.TimeUnits   = "hour";
dose.RateUnits   = "milligram/hour";
```

Estimate model parameters. By default, the function estimates a set of parameter for each individual (unpooled fit).

```
fitResults =  sbiofit(model,gData,responseMap,estimatedParam,dose);
```

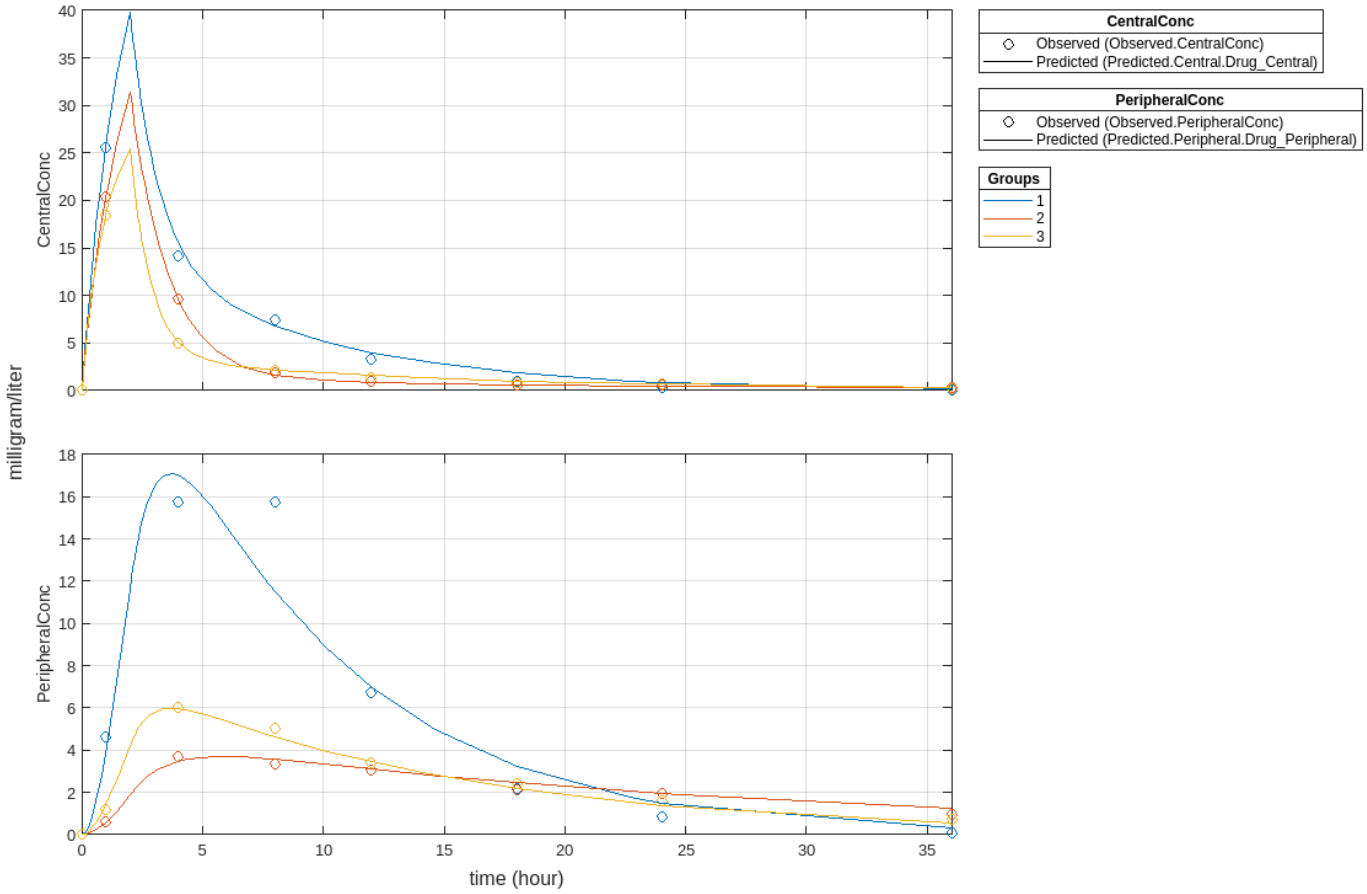
Plot the results.

```
plot(fitResults);
```



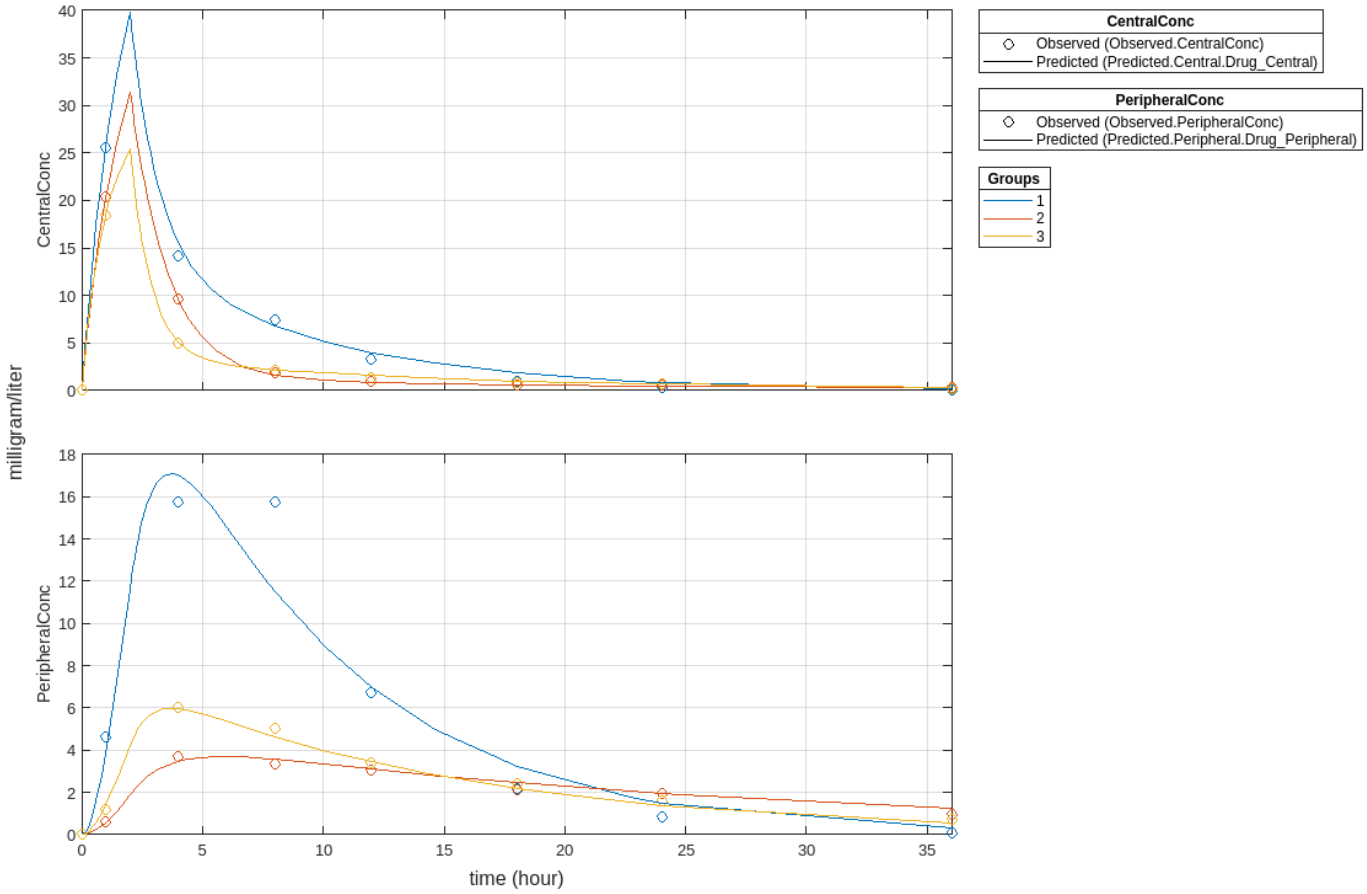
Plot all groups in one plot.

```
plot(fitResults,"PlotStyle","one axes");
```



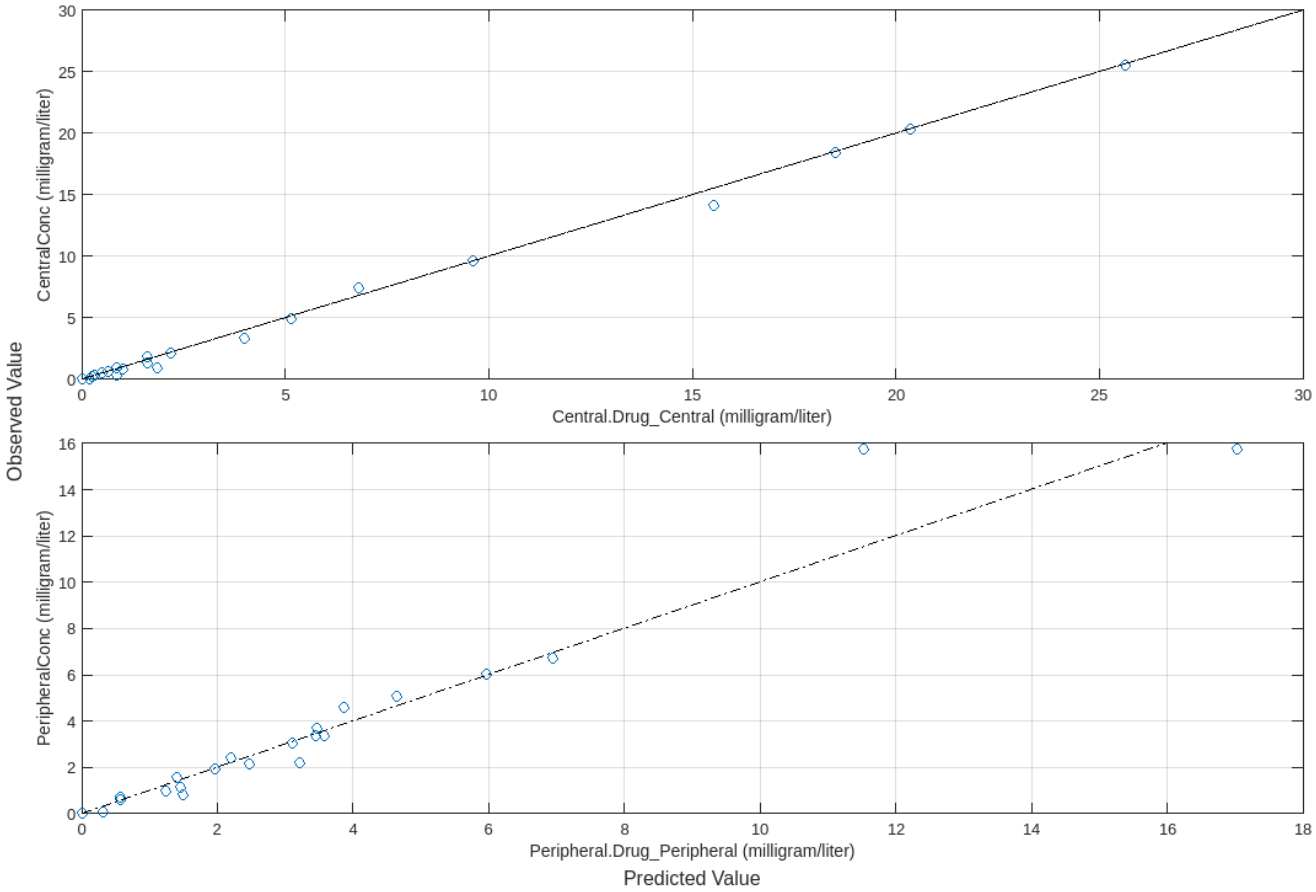
Change some axes properties.

```
s = struct;
s.Properties.XGrid = "on";
s.Properties.YGrid = "on";
plot(fitResults,"PlotStyle","one axes","AxesStyle",s);
```



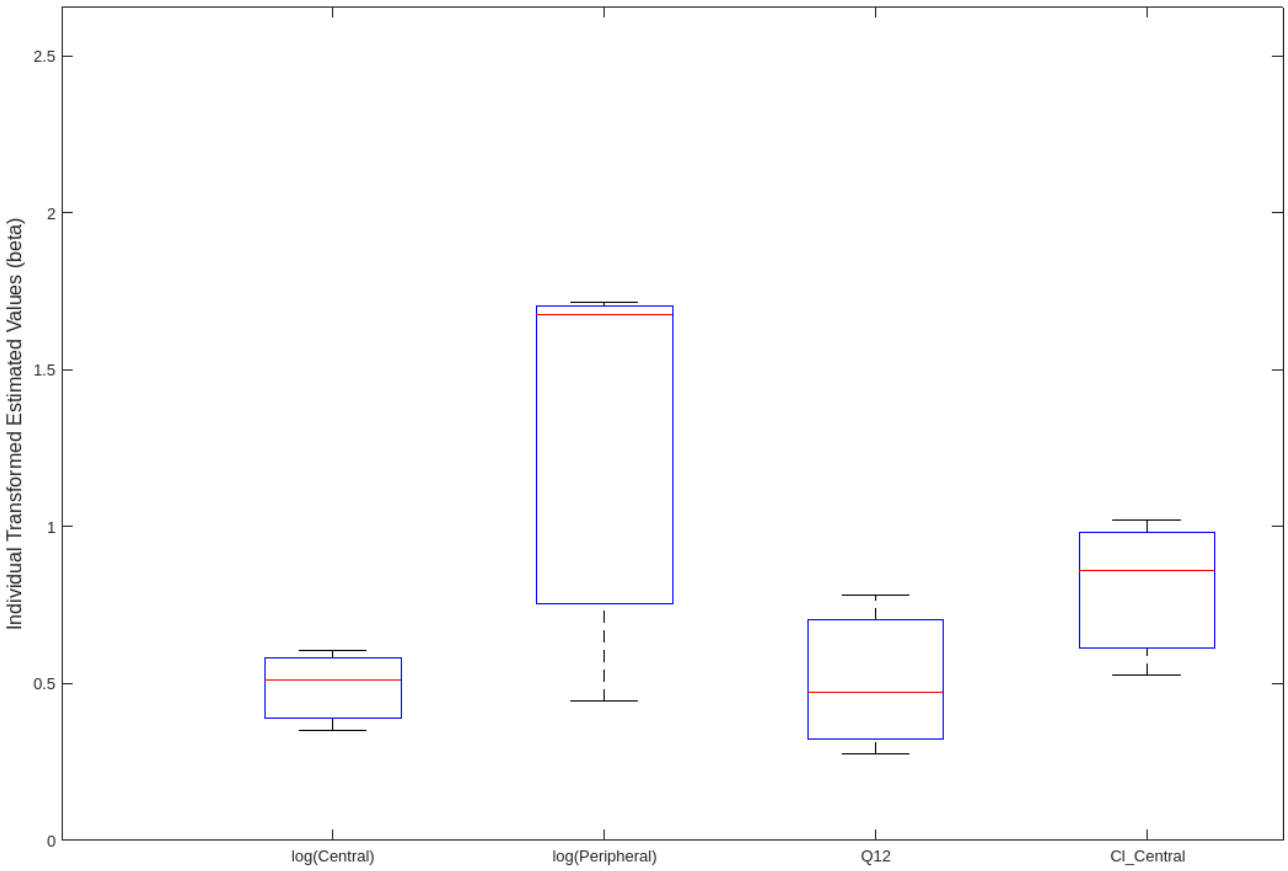
Compare the model predictions to the actual data.

```
plotActualVersusPredicted(fitResults)
```



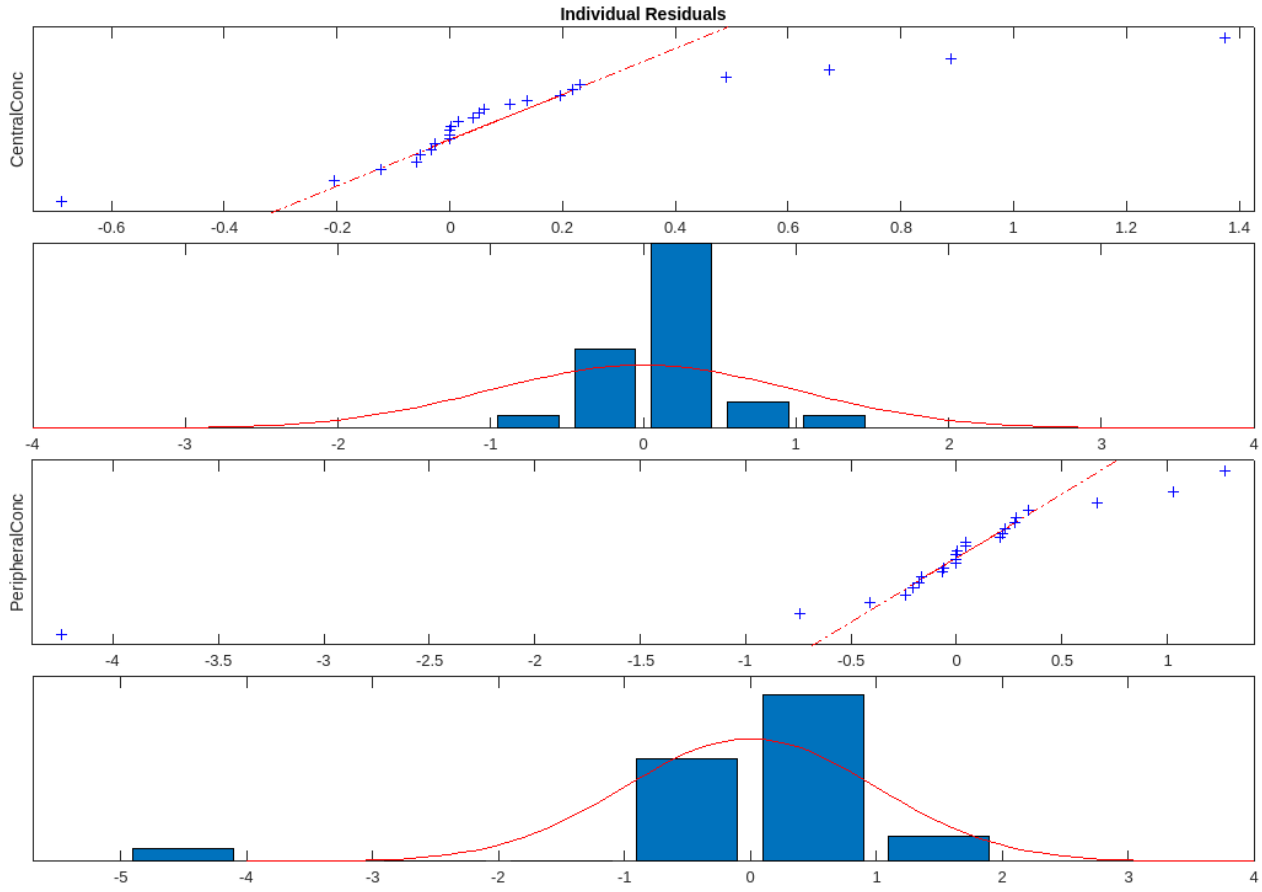
Use `boxplot` to show the variation of estimated model parameters.

```
boxplot(fitResults)
```



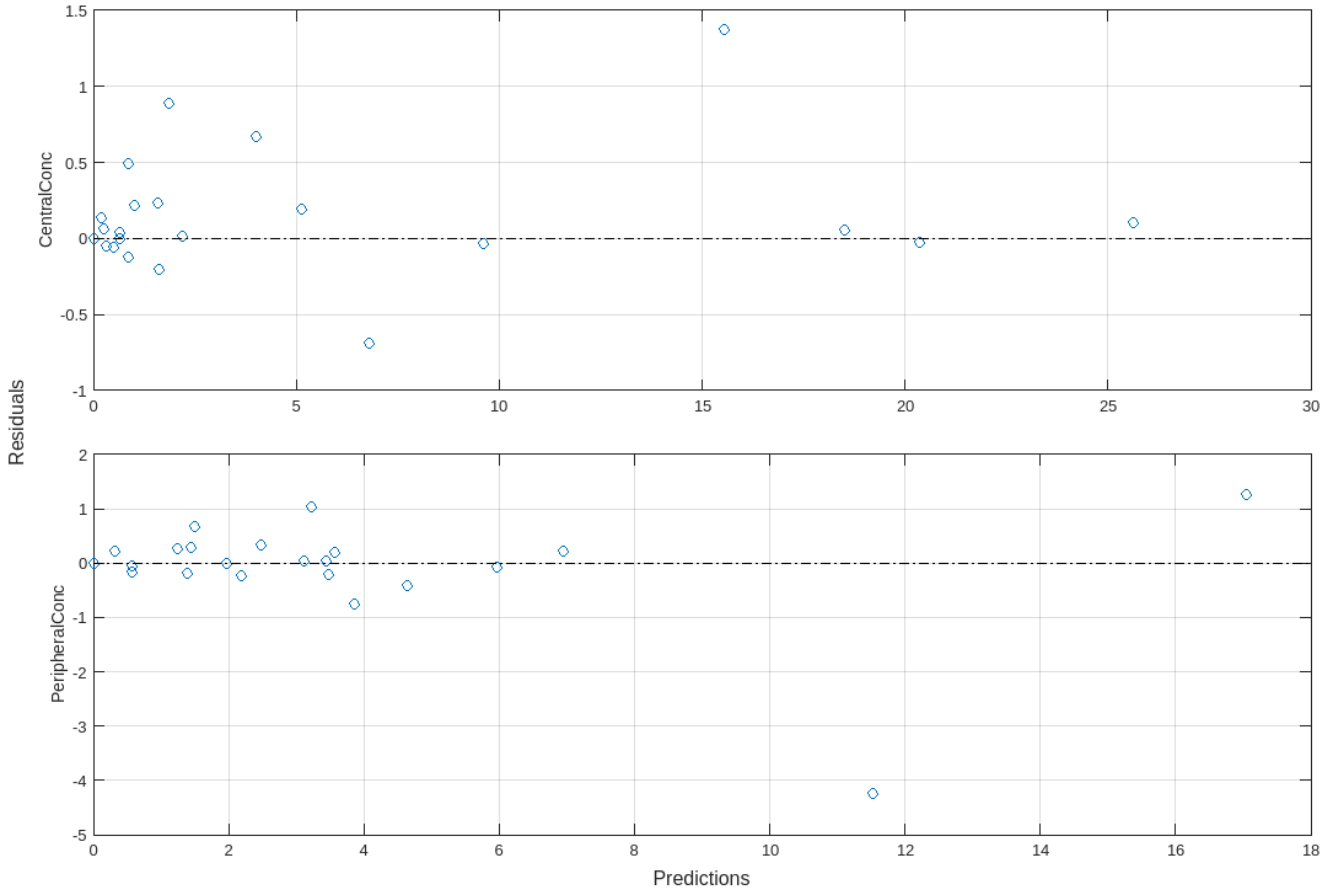
Plot the distribution of residuals. This normal probability plot shows the deviation from normality and the skewness on the right tail of the distribution of residuals. The default (constant) error model might not be the correct assumption for the data being fitted.

```
plotResidualDistribution(fitResults)
```



Plot residuals for each response using the model predictions on *x*-axis.

```
plotResiduals(fitResults,"Predictions")
```



Get the summary of the fit results. `stats.Name` contains the name for each table from `stats.Table`, which contains a list of tables with estimated parameter values and fit quality statistics.

```
stats = summary(fitResults);
stats.Name
```

```
ans =
'Unpooled Parameter Estimates'

ans =
'Statistics'

ans =
'Unpooled Beta'

ans =
'Residuals'

ans =
'Covariance Matrix'

ans =
'Error Model'
```

```
stats.Table
```

```
ans=3×9 table
    Group    Central Estimate    Central StandardError    Peripheral Estimate    Peripheral Stand
    _____    ________________    _____________________    ___________________    ________________

    {'1'}          1.422               0.12334                1.5619                0.36355
    {'2'}         1.8322              0.019672                5.3364                0.65327
    {'3'}         1.6657              0.038529                5.5632                0.37063

ans=3×7 table
    Group      AIC        BIC      LogLikelihood    DFE      MSE         SSE
    _____    _______    _______    _____________    ___    ________    _______

    {'1'}     60.961     64.051       -26.48        12        2.138     25.656
    {'2'}    -7.8379    -4.7475       7.9189        12     0.029012    0.34814
    {'3'}    -1.4336     1.6567       4.7168        12     0.043292     0.5195

ans=3×9 table
    Group    Central Estimate    Central StandardError    Peripheral Estimate    Peripheral Stand
    _____    ________________    _____________________    ___________________    ________________

    {'1'}        0.35208              0.086736               0.44589                0.23277
    {'2'}        0.60551              0.010737                1.6746                0.12242
    {'3'}        0.51027               0.02313                1.7162                0.06662

ans=24×4 table
    ID    Time    CentralConc    PeripheralConc
    __    ____    ___________    ______________

    1       0              0              0
    1       1        0.10646        -0.74394
    1       4         1.3745          1.2726
    1       8       -0.68825         -4.2435
    1      12        0.67383         0.21806
    1      18        0.88823          1.0269
    1      24        0.48941         0.66755
    1      36        0.13632         0.22948
    2       0              0              0
    2       1      -0.026731      -0.058311
    2       4      -0.033299       -0.20544
    2       8       -0.20466        0.20696
    2      12       -0.12223       0.045409
    2      18       0.041224        0.33883
    2      24      -0.059498      0.0036257
    2      36      -0.051645        0.27616
      ⋮

ans=12×6 table
    Group        Parameters         log(Central)    log(Peripheral)        Q12        Cl_Central
    _____    __________________    ____________    _______________    ___________    __________

    {'1'}    {'log(Central)'   }       0.015213        -0.022539       -0.0086672       0.00115
    {'1'}    {'log(Peripheral)'}      -0.022539          0.13217         0.045746     -0.007313
    {'1'}    {'Q12'            }     -0.0086672         0.045746         0.023092     -0.002148
    {'1'}    {'Cl_Central'     }       0.001159       -0.0073135       -0.0021484      0.001367
    {'2'}    {'log(Central)'   }     0.00038701        -0.002161      -0.00010177     9.7448e-0
```

```
    {'2'}    {'log(Peripheral)'}      -0.002161          0.42676          0.019101      -0.01575
    {'2'}    {'Q12'            }    -0.00010177         0.019101         0.00094857    -0.0007332
    {'2'}    {'Cl_Central'     }     9.7448e-05         -0.015755        -0.00073328     0.0006894
    {'3'}    {'log(Central)'   }      0.0014845        -0.0054648         -0.0013216     0.0001663
    {'3'}    {'log(Peripheral)'}     -0.0054648          0.13737           0.016903     -0.007272
    {'3'}    {'Q12'            }     -0.0013216         0.016903          0.0034406    -0.0008253
    {'3'}    {'Cl_Central'     }      0.00016639       -0.0072722        -0.00082538     0.0007458
```

```
ans=3×5 table
    Group     Response      ErrorModel        a        b
    _____    __________    ____________    _______    ___

    {'1'}    {0×0 char}    {'constant'}     1.2663    NaN
    {'2'}    {0×0 char}    {'constant'}    0.14751    NaN
    {'3'}    {0×0 char}    {'constant'}    0.18019    NaN
```

Input Arguments

`resultsObj` — Estimation results

`OptimResults` object | `NLINResults` object | vector of results objects

Estimation results, specified as an `OptimResults object` or `NLINResults object`, or vector of results objects which contains estimation results from running `sbiofit`.

Version History

Introduced in R2014a

See Also

`NLINResults object` | `OptimResults object` | `sbiofit`

plotActualVersusPredicted

Compare predictions to actual data, creating a subplot for each response

Syntax

```
plotActualVersusPredicted(resultsObj)
```

Description

`plotActualVersusPredicted(resultsObj)` returns a figure displaying the comparison between predictions to the actual data, with a subplot for each response.

Input Arguments

`resultsObj` — Estimation results
`NLMEResults` object

Estimation results, specified as an `NLMEResults object`, which contains estimation results returned by `sbiofitmixed`.

Version History

Introduced in R2014a

See Also

`NLMEResults object` | `sbiofitmixed`

plotData

Plot quantile summary of model simulations from global sensitivity analysis (requires Statistics and Machine Learning Toolbox)

Syntax

```
h = plotData(resultsObj)
h = plotData(resultsObj,Name,Value)
```

Description

`h = plotData(resultsObj)` plots quantiles and model responses of simulated samples and returns the figure handle `h`.

`h = plotData(resultsObj,Name,Value)` uses additional options specified by one or more name-value pair arguments.

Examples

Perform Global Sensitivity Analysis by Computing First- and Total-Order Sobol Indices

Load the “Tumor Growth Model”.

```
sbioloadproject tumor_growth_vpop_sa.sbproj
```

Get a variant with the estimated parameters and the dose to apply to the model.

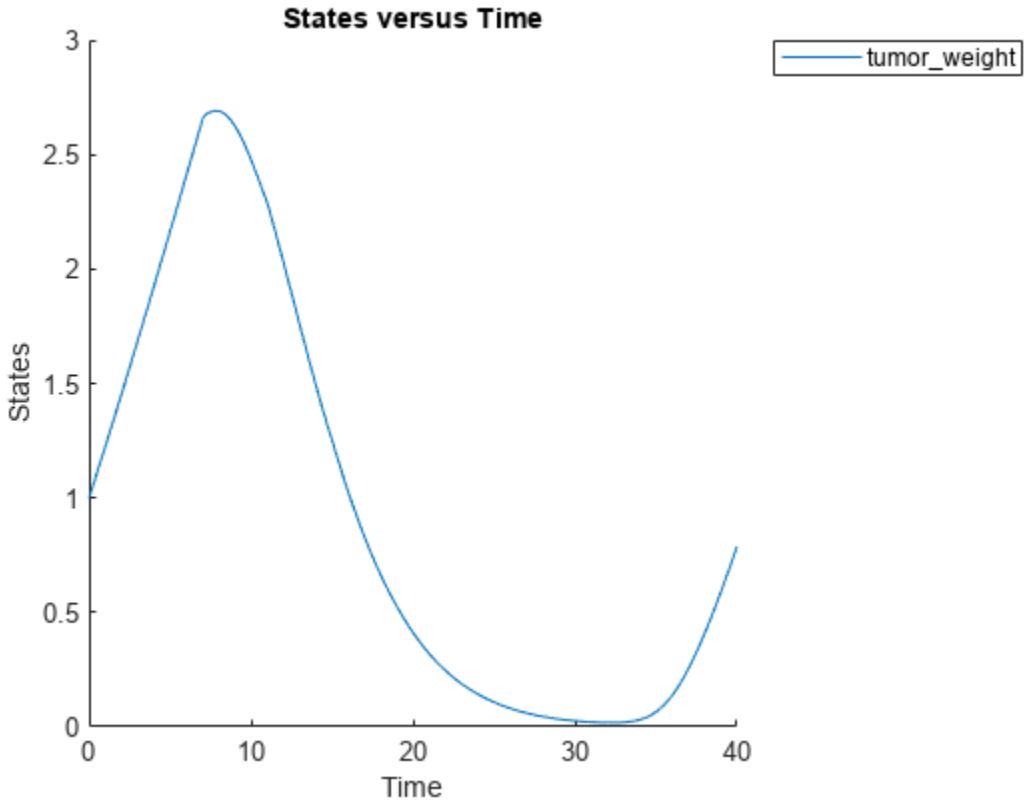
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

Get the active configset and set the tumor weight as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'tumor_weight';
```

Simulate the model and plot the tumor growth profile.

```
sbioplot(sbiosimulate(m1,cs,v,d));
```



Perform global sensitivity analysis (GSA) on the model to find the model parameters that the tumor growth is sensitive to.

First, retrieve model parameters of interest that are involved in the pharmacodynamics of the tumor growth. Define the model response as the tumor weight.

```
modelParamNames = {'L0','L1','w0','k1','k2'};
outputName = 'tumor_weight';
```

Then perform GSA by computing the first- and total-order Sobol indices using `sbiosobol`. Set `'ShowWaitBar'` to `true` to show the simulation progress. By default, the function uses 1000 parameter samples to compute the Sobol indices [1].

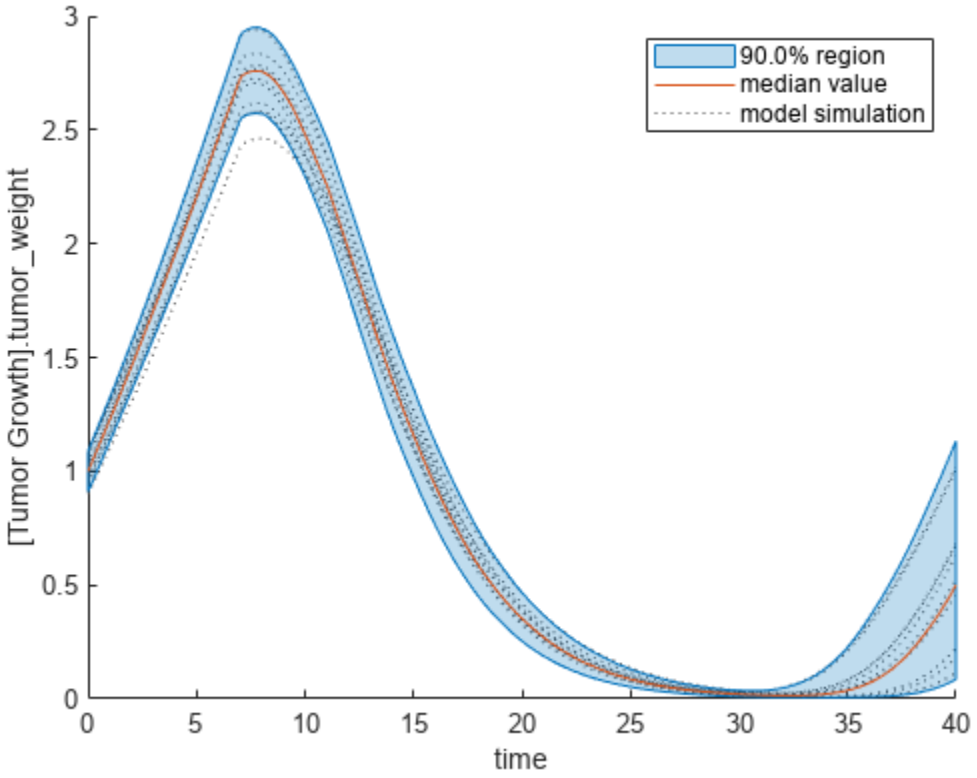
```
rng('default');
sobolResults = sbiosobol(m1,modelParamNames,outputName,Variants=v,Doses=d,ShowWaitBar=true)
```

```
sobolResults =
  Sobol with properties:

                Time: [444x1 double]
        SobolIndices: [5x1 struct]
            Variance: [444x1 table]
    ParameterSamples: [1000x5 table]
         Observables: {'[Tumor Growth].tumor_weight'}
      SimulationInfo: [1x1 struct]
```

You can change the number of samples by specifying the `'NumberSamples'` name-value pair argument. The function requires a total of `(number of input parameters + 2) * NumberSamples` model simulations.

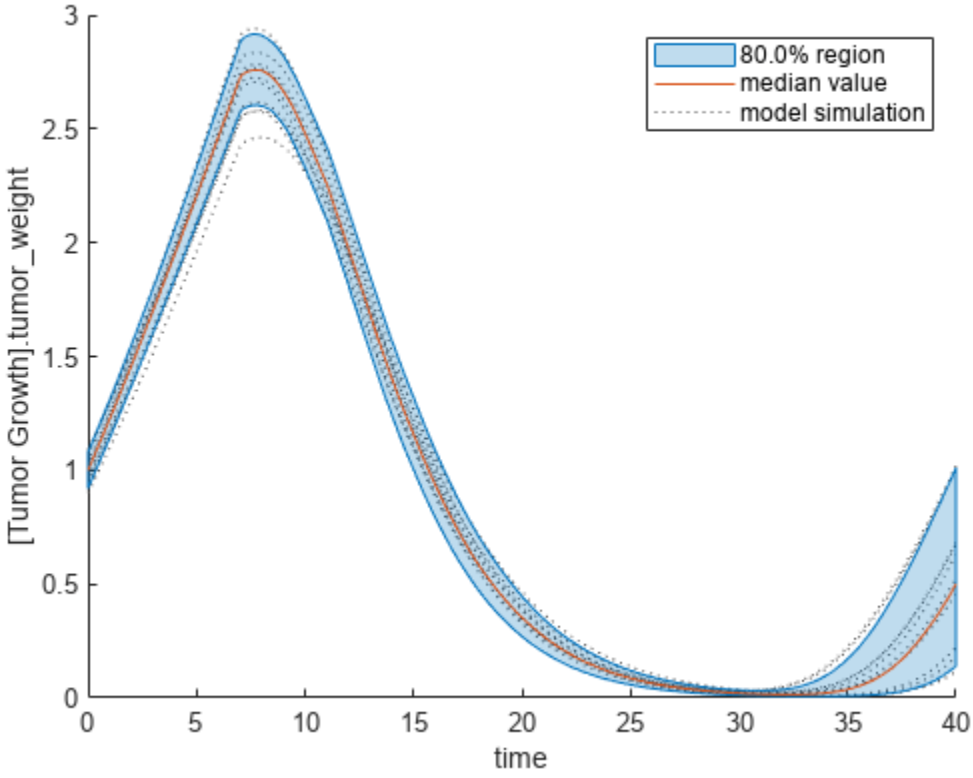
Show the mean model response, the simulation results, and a shaded region covering 90% of the simulation results.

```
plotData(sobolResults,ShowMedian=true,ShowMean=false);
```



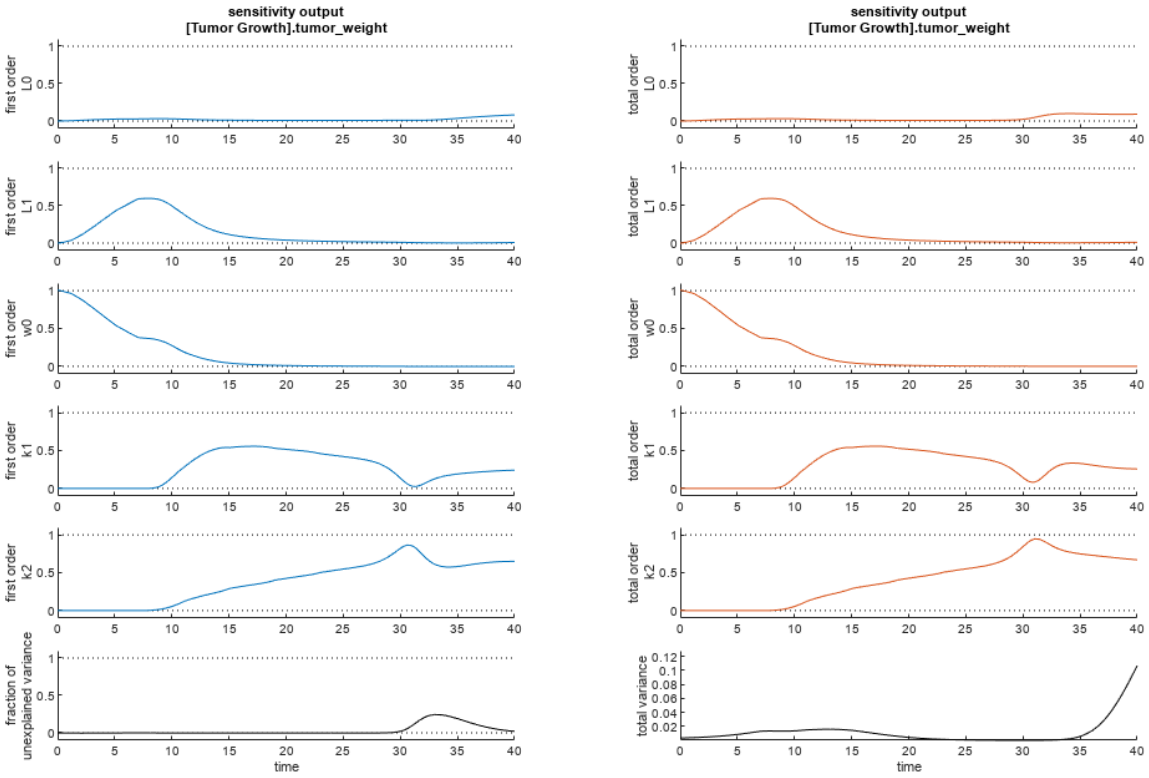
You can adjust the quantile region to a different percentage by specifying `'Alphas'` for the lower and upper quantiles of all model responses. For instance, an alpha value of 0.1 plots a shaded region between the `100 * alpha` and `100 * (1 - alpha)` quantiles of all simulated model responses.

```
plotData(sobolResults,Alphas=0.1,ShowMedian=true,ShowMean=false);
```



Plot the time course of the first- and total-order Sobol indices.

```
h = plot(sobolResults);
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```

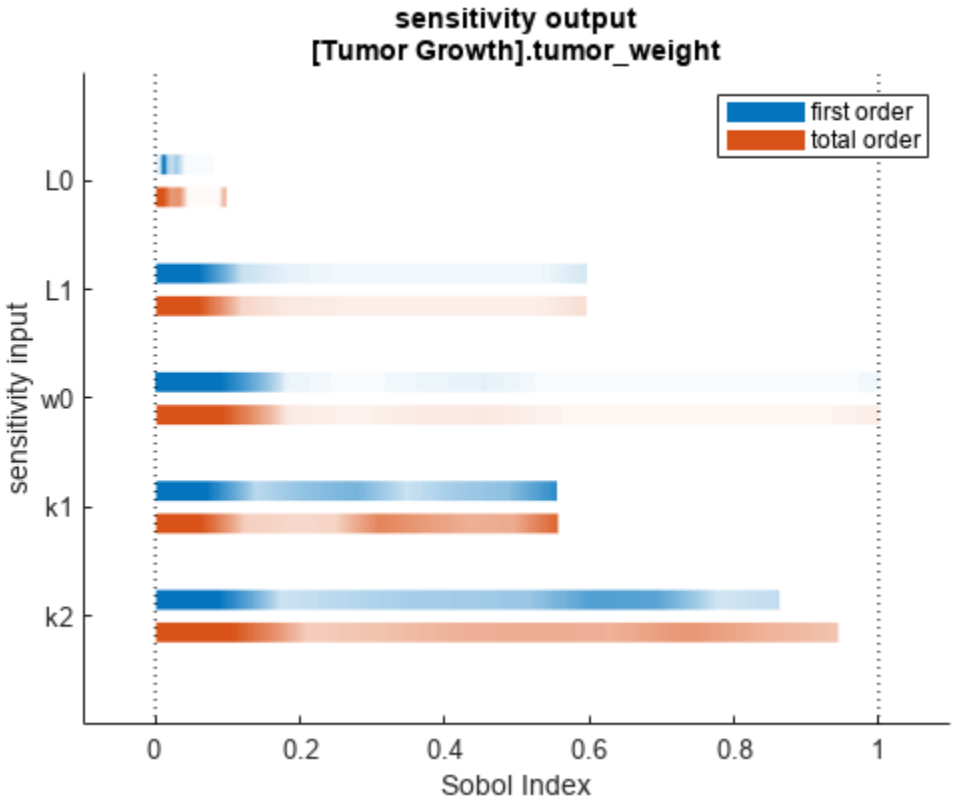


The first-order Sobol index of an input parameter gives the fraction of the overall response variance that can be attributed to variations in the input parameter alone. The total-order index gives the fraction of the overall response variance that can be attributed to any joint parameter variations that include variations of the input parameter.

From the Sobol indices plots, parameters `L1` and `w0` seem to be the most sensitive parameters to the tumor weight before the dose was applied at t = 7. But after the dose is applied, `k1` and `k2` become more sensitive parameters and contribute most to the after-dosing stage of the tumor weight. The total variance plot also shows a larger variance for the after-dose stage at t > 35 than for the before-dose stage of the tumor growth, indicating that `k1` and `k2` might be more important parameters to investigate further. The fraction of unexplained variance shows some variance at around t = 33, but the total variance plot shows little variance at t = 33, meaning the unexplained variance could be insignificant. The fraction of unexplained variance is calculated as 1 - (sum of all the first-order Sobol indices), and the total variance is calculated using `var(response)`, where `response` is the model response at every time point.

You can also display the magnitudes of the sensitivities in a bar plot. Darker colors mean that those values occur more often over the whole time course.

```
bar(sobolResults);
```



You can specify more samples to increase the accuracy of the Sobol indices, but the simulation can take longer to finish. Use `addsamples` to add more samples. For example, if you specify 1500 samples, the function performs `1500 * (2 + number of input parameters)` simulations.

```
gsaMoreSamples = addsamples(gsaResults,1500)
```

The “SimulationInfo” on page 2-0 property of the result object contains various information for computing the Sobol indices. For instance, the model simulation data (SimData) for each simulation using a set of parameter samples is stored in the `SimData` field of the property. This field is an array of `SimData` objects.

```
sobolResults.SimulationInfo.SimData
```

```
SimBiology SimData Array : 1000-by-7

Index:    Name:         ModelName:         DataCount:
1           -           Tumor Growth Model 1
2           -           Tumor Growth Model 1
3           -           Tumor Growth Model 1
...
7000        -           Tumor Growth Model 1
```

You can find out if any model simulation failed during the computation by checking the `ValidSample` field of `SimulationInfo`. In this example, the field shows no failed simulation runs.

```
all(sobolResults.SimulationInfo.ValidSample)
```

```
ans = 1x7 logical array

   1   1   1   1   1   1   1
```

`SimulationInfo.ValidSample` is a table of logical values. It has the same size as `SimulationInfo.SimData`. If `ValidSample` indicates that any simulations failed, you can get more information about those simulation runs and the samples used for those runs by extracting information from the corresponding column of `SimulationInfo.SimData`. Suppose that the fourth column contains one or more failed simulation runs. Get the simulation data and sample values used for that simulation using `getSimulationResults`.

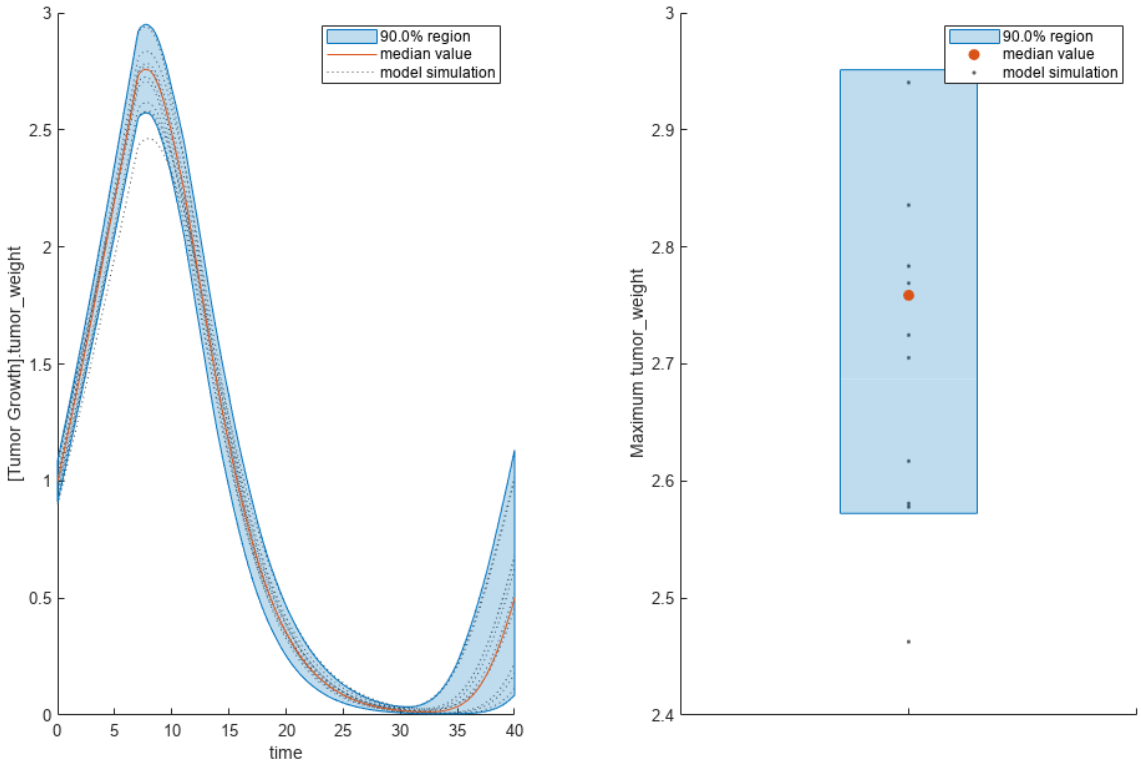
```
[samplesUsed,sd,validruns] = getSimulationResults(sobolResults,4);
```

You can add custom expressions as observables and compute Sobol indices for the added observables. For example, you can compute the Sobol indices for the maximum tumor weight by defining a custom expression as follows.

```
% Suppress an information warning that is issued during simulation.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
% Add the observable expression.
sobolObs = addobservable(sobolResults,'Maximum tumor_weight','max(tumor_weight)','Units','gram');
```

Plot the computed simulation results showing the 90% quantile region.

```
h2 = plotData(sobolObs,ShowMedian=true,ShowMean=false);
h2.Position(:) = [100 100 1280 800];
```



You can also remove the observable by specifying its name.

```
gsaNoObs = removeobservable(sobolObs,'Maximum tumor_weight');
```

Restore the warning settings.

```
warning(warnSettings);
```

Perform Multiparametric Global Sensitivity Analysis (MPGSA)

Load the "Target-Mediated Drug Disposition (TMDD) Model".

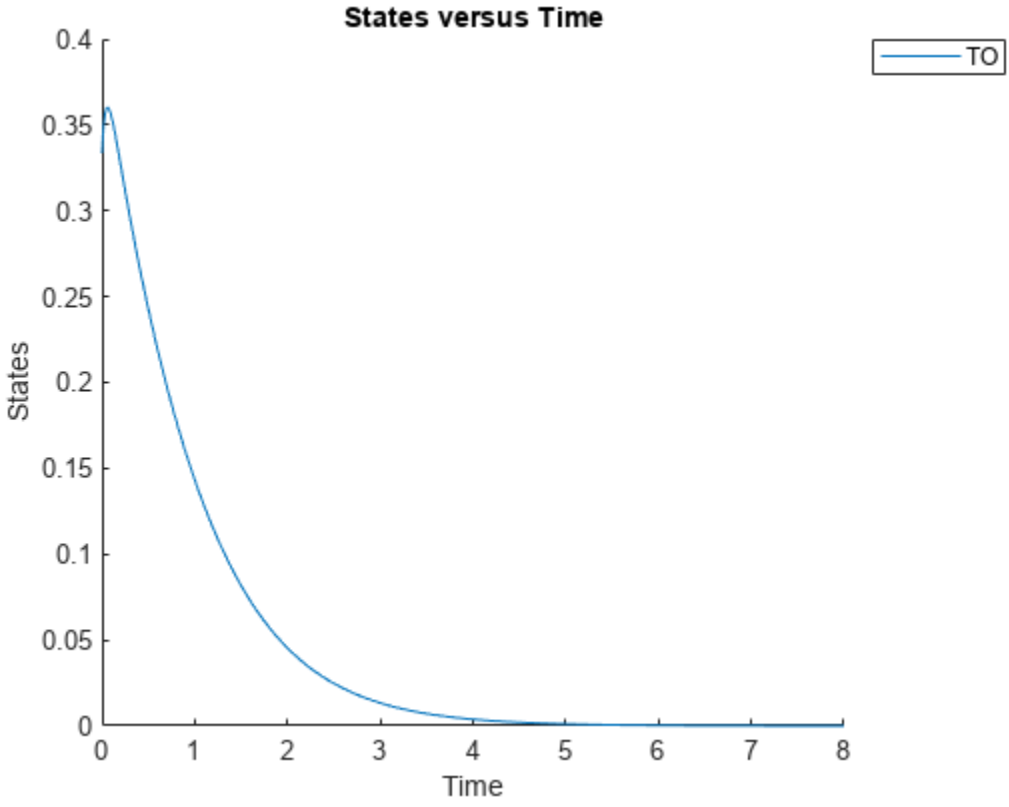
```
sbioloadproject tmdd_with_TO.sbproj
```

Get the active configset and set the target occupancy (TO) as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'TO';
```

Simulate the model and plot the TO profile.

```
sbioplot(sbiosimulate(m1,cs));
```



Define an exposure (area under the curve of the TO profile) threshold for the target occupancy.

```
classifier = 'trapz(time,TO) <= 0.1';
```

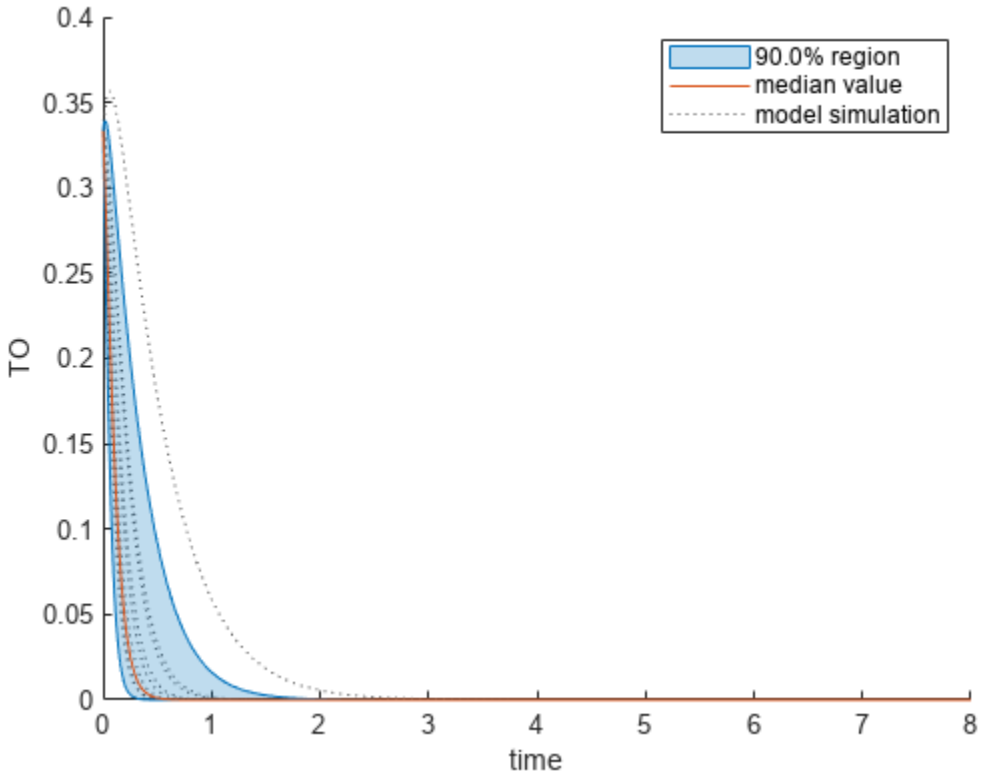
Perform MPGSA to find sensitive parameters with respect to the TO. Vary the parameter values between predefined bounds to generate 10,000 parameter samples.

```
% Suppress an information warning that is issued during simulation.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
rng(0,'twister'); % For reproducibility
params = {'kel','ksyn','kdeg','km'};
bounds = [0.1, 1;
          0.1, 1;
          0.1, 1;
          0.1, 1];
mpgsaResults = sbiompgsa(m1,params,classifier,Bounds=bounds,NumberSamples=10000)
```

```
mpgsaResults =
  MPGSA with properties:

                   Classifiers: {'trapz(time,TO) <= 0.1'}
    KolmogorovSmirnovStatistics: [4x1 table]
                       ECDFData: {4x4 cell}
             SignificanceLevel: 0.0500
                       PValues: [4x1 table]
             SupportHypothesis: [10000x1 table]
              ParameterSamples: [10000x4 table]
                   Observables: {'TO'}
                SimulationInfo: [1x1 struct]
```

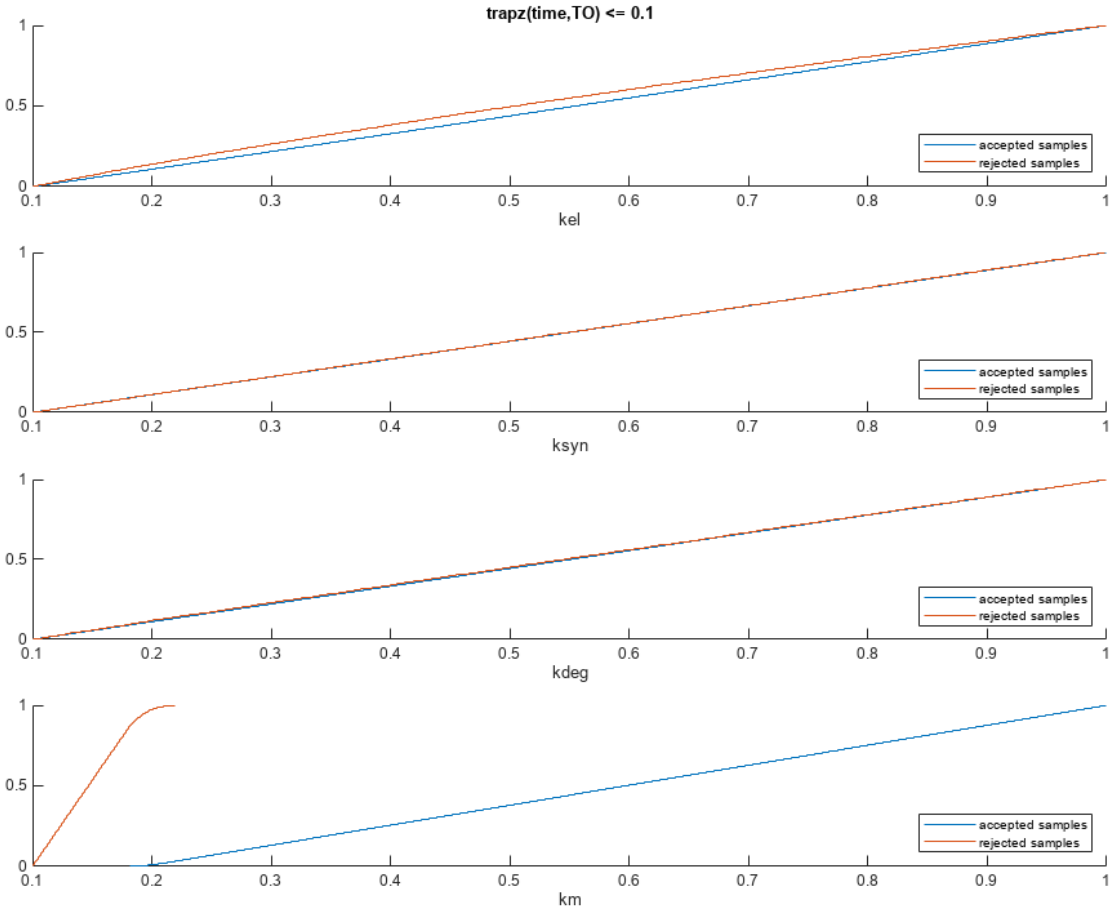
Plot the quantiles of the simulated model response.

```
plotData(mpgsaResults,ShowMedian=true,ShowMean=false);
```



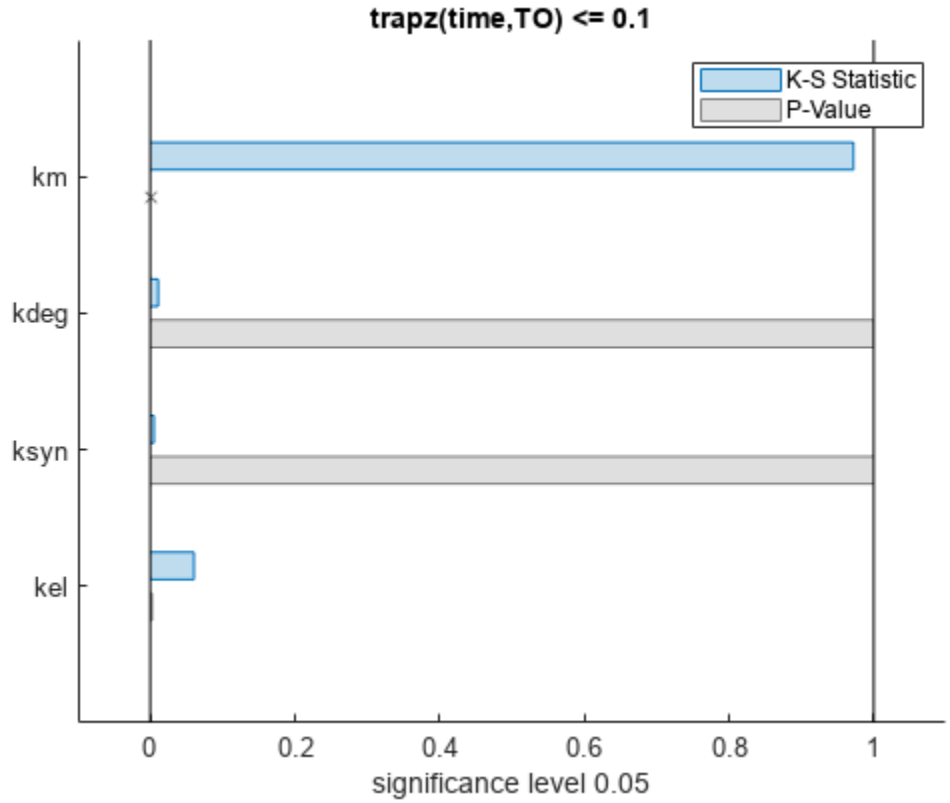
Plot the empirical cumulative distribution functions (eCDFs) of the accepted and rejected samples. Except for `km`, none of the parameters shows a significant difference in the eCDFs for the accepted and rejected samples. The `km` plot shows a large Kolmogorov-Smirnov (K-S) distance between the eCDFs of the accepted and rejected samples. The K-S distance is the maximum absolute distance between two eCDFs curves.

```
h = plot(mpgsaResults);
% Resize the figure.
pos = h.Position(:);
h.Position(:) = [pos(1) pos(2) pos(3)*2 pos(4)*2];
```



To compute the K-S distance between the two eCDFs, SimBiology uses a two-sided test based on the null hypothesis that the two distributions of accepted and rejected samples are equal. See `kstest2` (Statistics and Machine Learning Toolbox) for details. If the K-S distance is large, then the two distributions are different, meaning that the classification of the samples is sensitive to variations in the input parameter. On the other hand, if the K-S distance is small, then variations in the input parameter do not affect the classification of samples. The results suggest that the classification is insensitive to the input parameter. To assess the significance of the K-S statistic rejecting the null-hypothesis, you can examine the p-values.

```
bar(mpgsaResults)
```



The bar plot shows two bars for each parameter: one for the K-S distance (K-S statistic) and another for the corresponding p-value. You reject the null hypothesis if the p-value is less than the significance level. A cross (x) is shown for any p-value that is almost 0. You can see the exact p-value corresponding to each parameter.

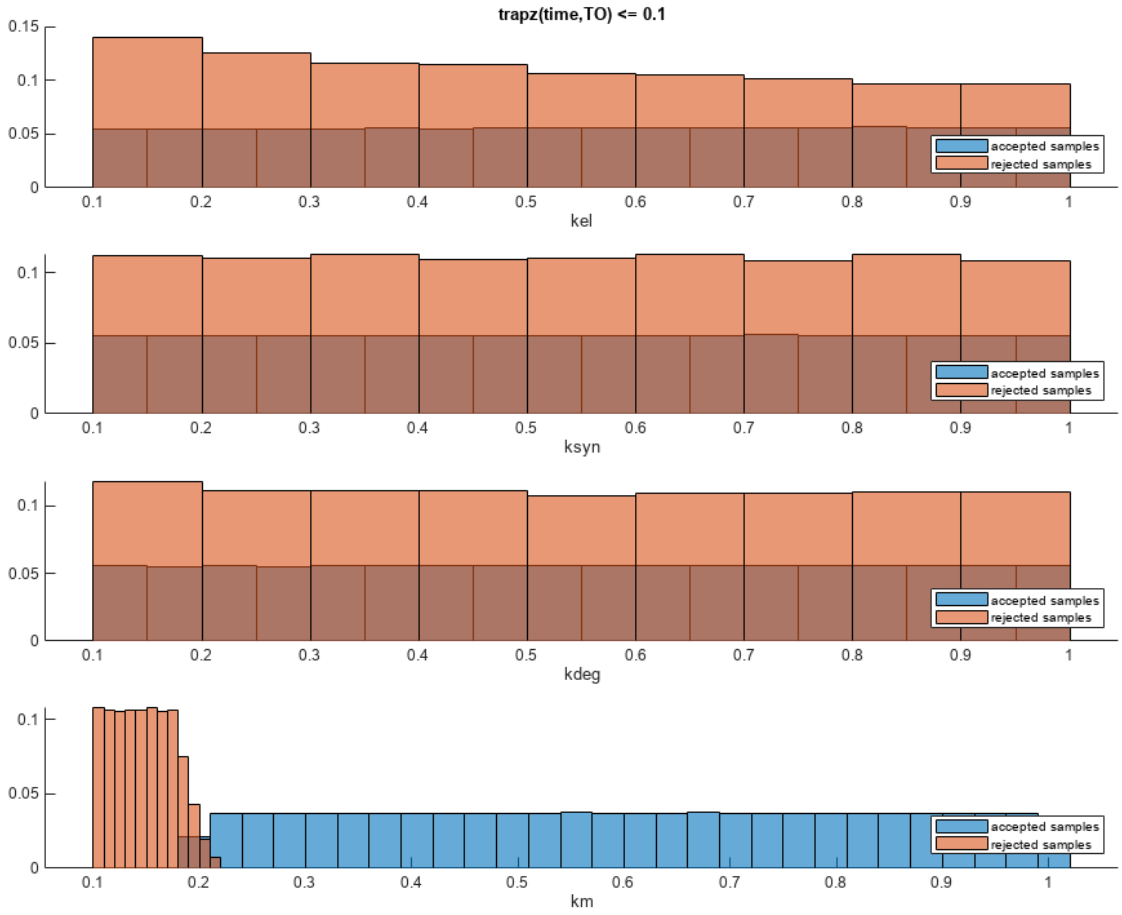
```
[mpgsaResults.ParameterSamples.Properties.VariableNames',mpgsaResults.PValues]
```

```
ans=4×2 table
      Var1      trapz(time,TO) <= 0.1
    ________    _____________________

    {'kel' }          0.0021877
    {'ksyn'}                  1
    {'kdeg'}            0.99983
    {'km'  }                  0
```

The p-values of `km` and `kel` are less than the significance level (0.05), supporting the alternative hypothesis that the accepted and rejected samples come from different distributions. In other words, the classification of the samples is sensitive to `km` and `kel` but not to other parameters (`kdeg` and `ksyn`).

You can also plot the histograms of accepted and rejected samples. The historgrams let you see trends in the accepted and rejected samples. In this example, the histogram of `km` shows that there are more accepted samples for larger `km` values, while the `kel` histogram shows that there are fewer rejected samples as `kel` increases.

```
h2 = histogram(mpgsaResults);
% Resize the figure.
pos = h2.Position(:);
h2.Position(:) = [pos(1) pos(2) pos(3)*2 pos(4)*2];
```



Restore the warning settings.

```
warning(warnSettings);
```

Perform GSA by Computing Elementary Effects

Load the “Tumor Growth Model”.

```
sbioloadproject tumor_growth_vpop_sa.sbproj
```

Get a variant with estimated parameters and the dose to apply to the model.

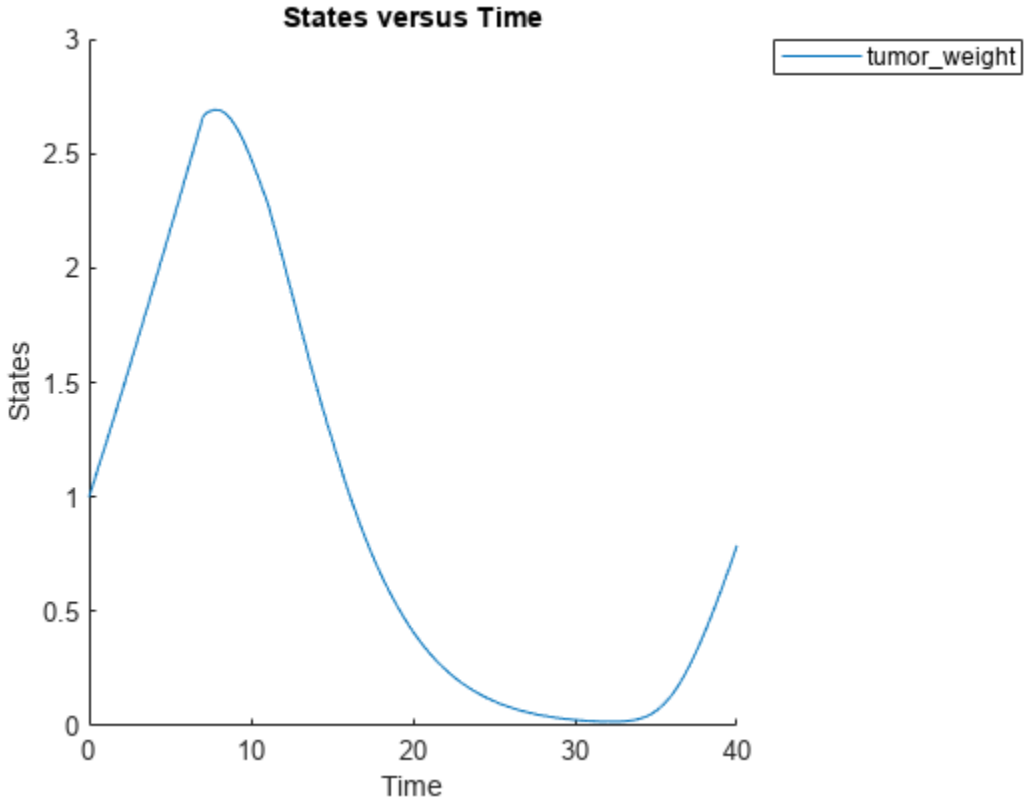
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

Get the active configset and set the tumor weight as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'tumor_weight';
```

Simulate the model and plot the tumor growth profile.

```
sbioplot(sbiosimulate(m1,cs,v,d));
```



Perform global sensitivity analysis (GSA) on the model to find the model parameters that the tumor growth is sensitive to.

First, define model parameters of interest, which are involved in the pharmacodynamics of the tumor growth. Define the model response as the tumor weight.

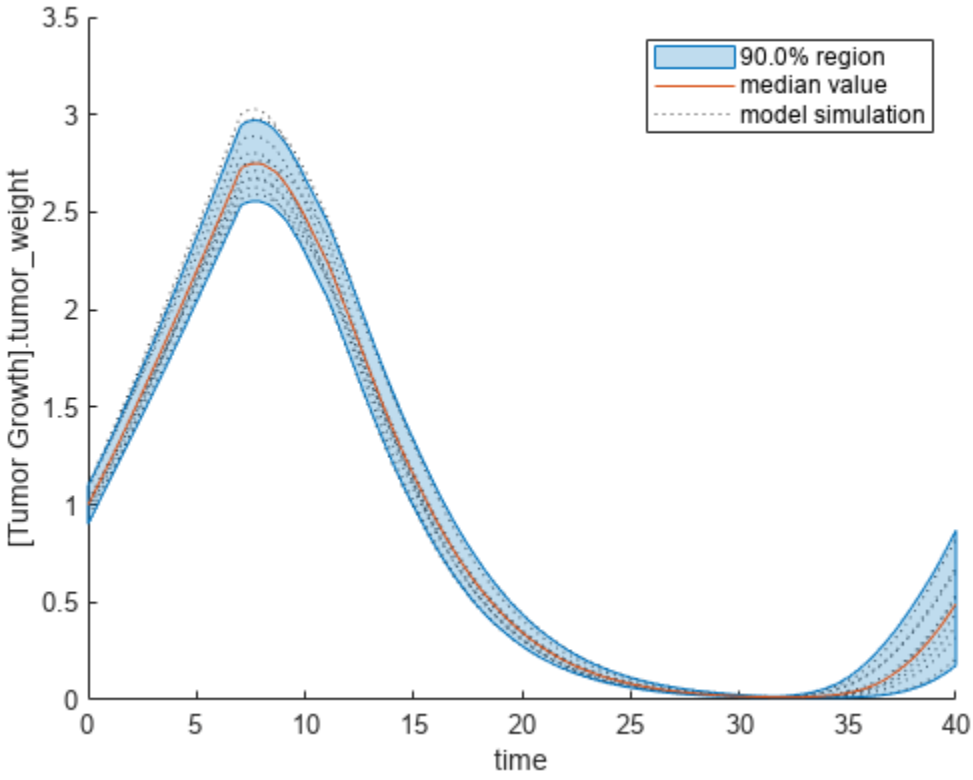
```
modelParamNames = {'L0','L1','w0','k1'};
outputName = 'tumor_weight';
```

Then perform GSA by computing the elementary effects using `sbioelementaryeffects`. Use `100` as the number of samples and set `ShowWaitBar` to `true` to show the simulation progress.

```
rng('default');
eeResults = sbioelementaryeffects(m1,modelParamNames,outputName,Variants=v,Doses=d,NumberSamples=
```

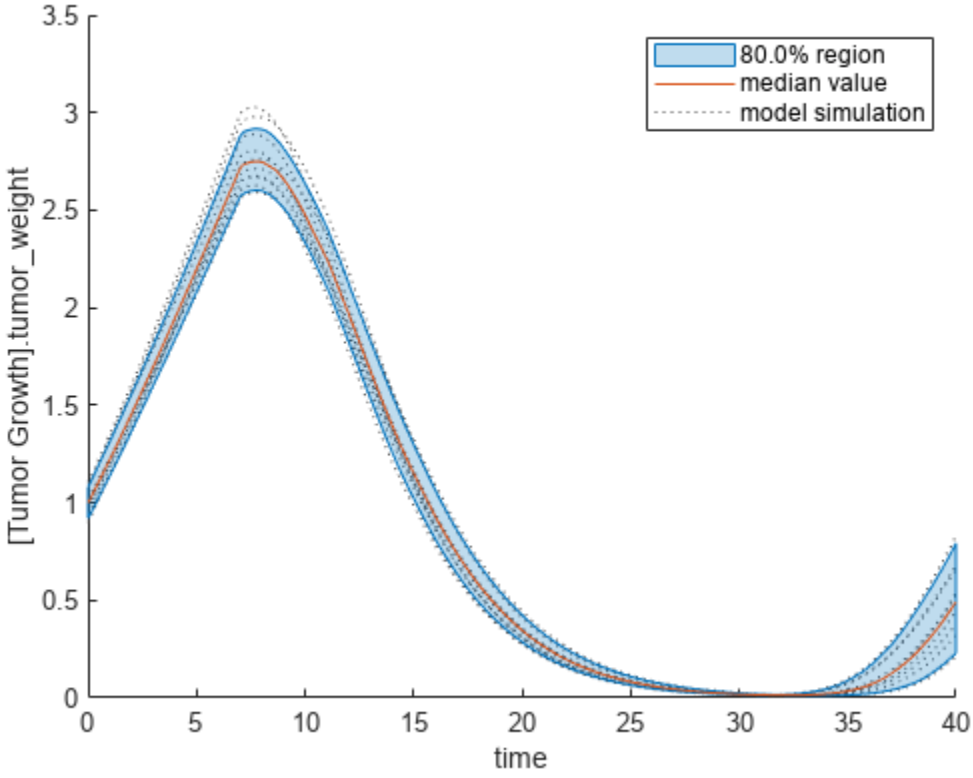
Show the median model response, the simulation results, and a shaded region covering 90% of the simulation results.

```
plotData(eeResults,ShowMedian=true,ShowMean=false);
```



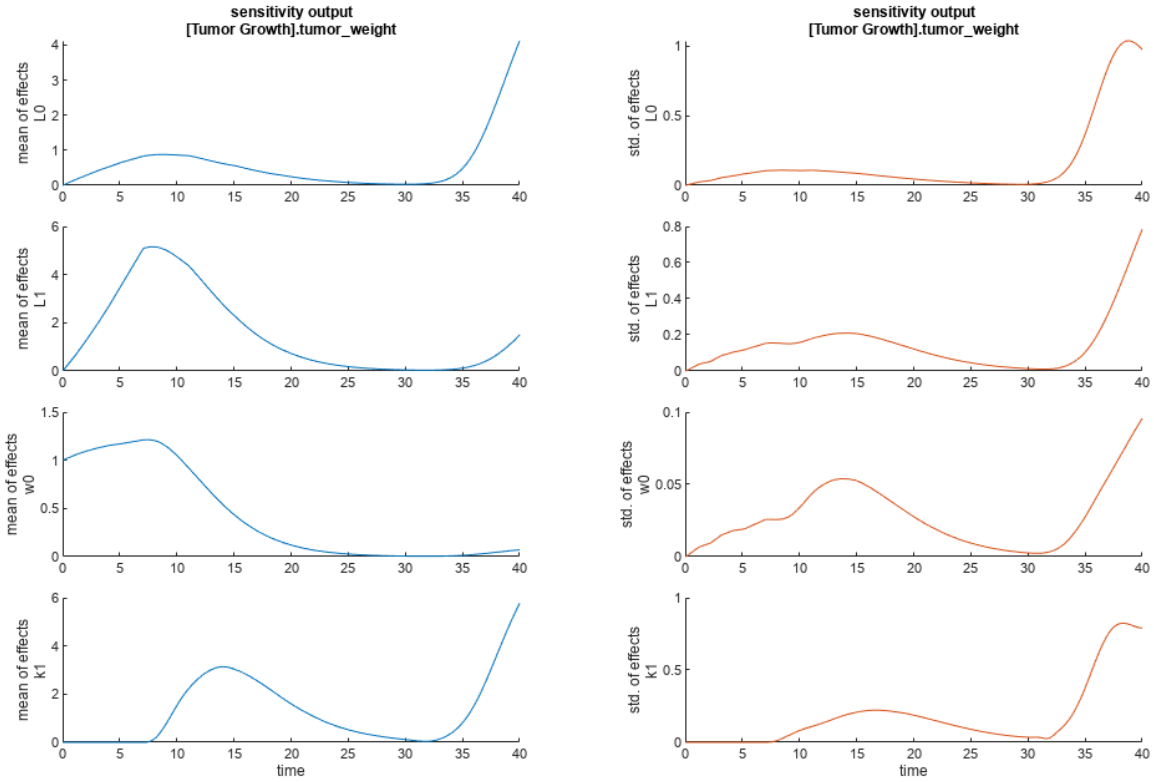
You can adjust the quantile region to a different percentage by specifying `Alphas` for the lower and upper quantiles of all model responses. For instance, an `alpha` value of 0.1 plots a shaded region between the `100*alpha` and `100*(1-alpha)` quantiles of all simulated model responses.

```
plotData(eeResults,Alphas=0.1,ShowMedian=true,ShowMean=false);
```



Plot the time course of the means and standard deviations of the elementary effects.

```
h = plot(eeResults);
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```

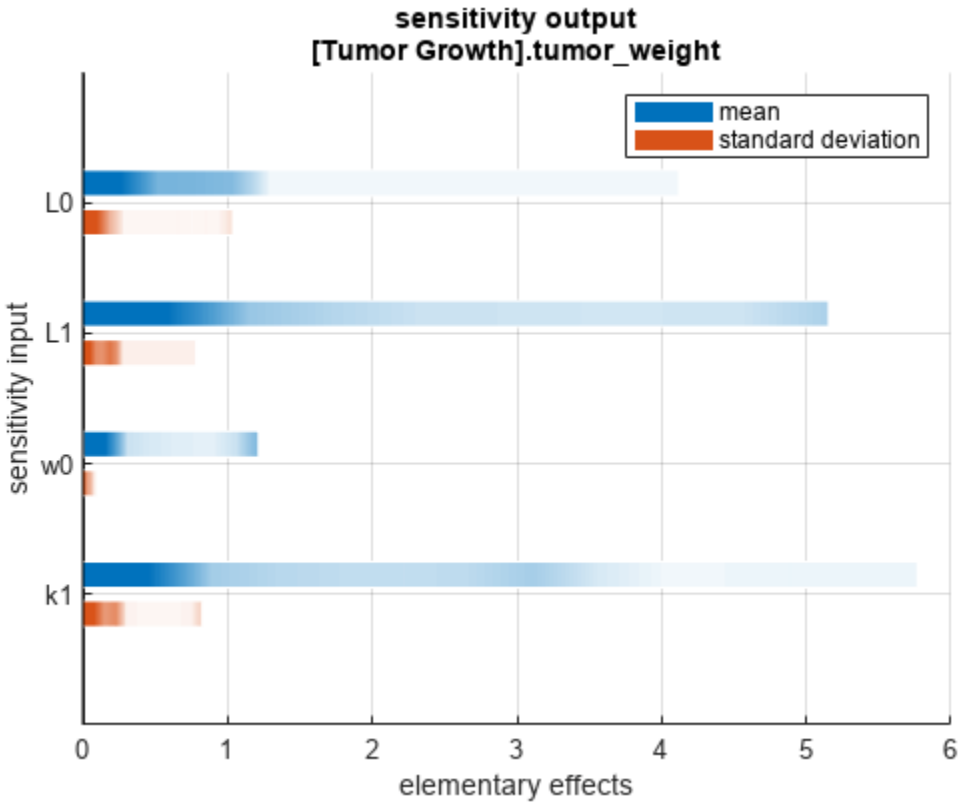


The mean of effects explains whether variations in input parameter values have any effect on the tumor weight response. The standard deviation of effects explains whether the sensitivity change is dependent on the location in the parameter domain.

From the mean of effects plots, parameters `L1` and `w0` seem to be the most sensitive parameters to the tumor weight before the dose is applied at t = 7. But, after the dose is applied, `k1` and `L0` become more sensitive parameters and contribute most to the after-dosing stage of the tumor weight. The plots of standard deviation of effects show more deviations for the larger parameter values in the later stage (t > 35) than for the before-dose stage of the tumor growth.

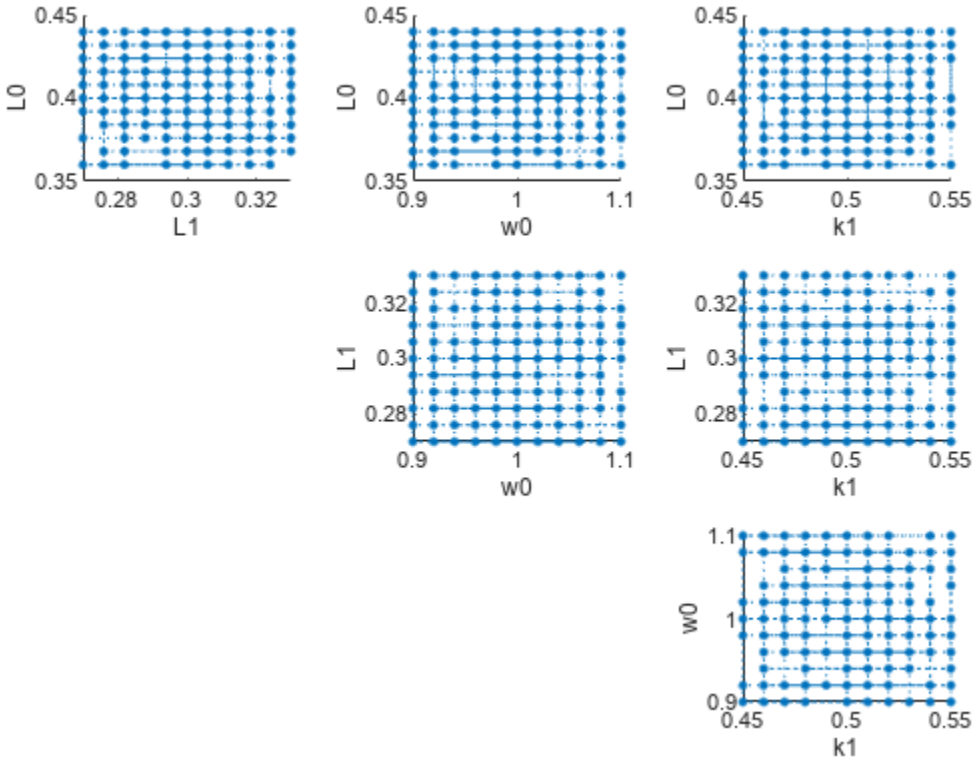
You can also display the magnitudes of the sensitivities in a bar plot. Each color shading represents a histogram representing values at different times. Darker colors mean that those values occur more often over the whole time course.

```
bar(eeResults);
```



You can also plot the parameter grids and samples used to compute the elementary effects.

```
plotGrid(eeResults)
```



You can specify more samples to increase the accuracy of the elementary effects, but the simulation can take longer to finish. Use `addsamples` to add more samples.

```
eeResults2 = addsamples(eeResults,200);
```

The `SimulationInfo` property of the result object contains various information for computing the elementary effects. For instance, the model simulation data (SimData) for each simulation using a set of parameter samples is stored in the `SimData` field of the property. This field is an array of `SimData` objects.

```
eeResults2.SimulationInfo.SimData
```

```
SimBiology SimData Array : 1500-by-1

Index:    Name:         ModelName:         DataCount:
1           -           Tumor Growth Model 1
2           -           Tumor Growth Model 1
3           -           Tumor Growth Model 1
...
1500        -           Tumor Growth Model 1
```

You can find out if any model simulation failed during the computation by checking the `ValidSample` field of `SimulationInfo`. In this example, the field shows no failed simulation runs.

```
all(eeResults2.SimulationInfo.ValidSample)
```

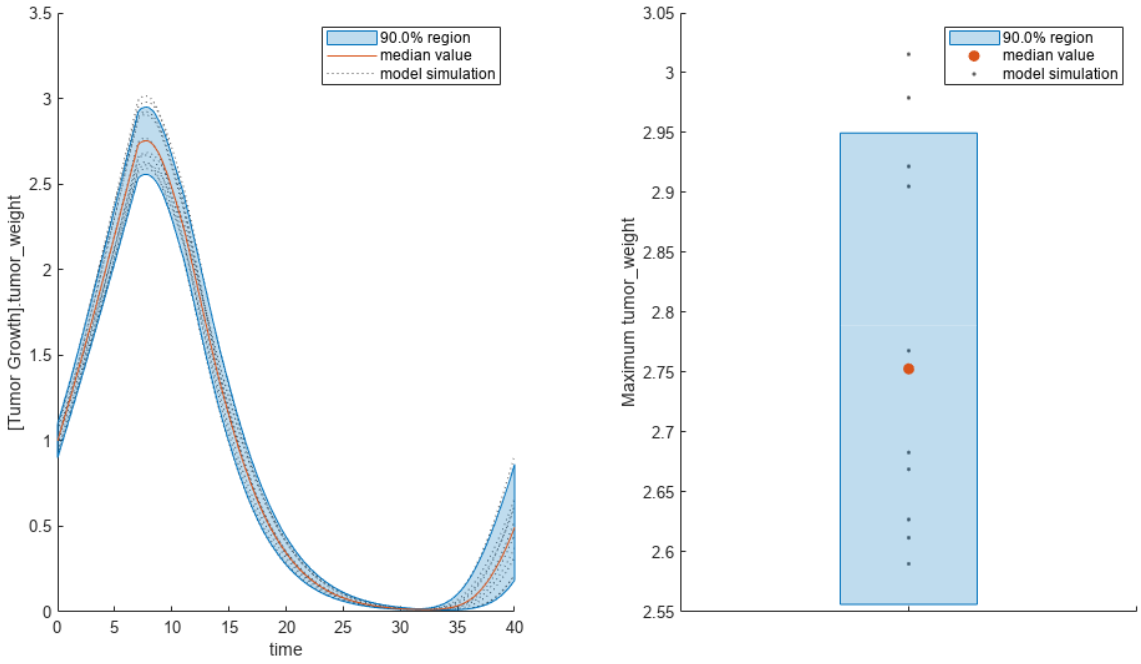
```
ans = logical
   1
```

You can add custom expressions as observables and compute the elementary effects of the added observables. For example, you can compute the effects for the maximum tumor weight by defining a custom expression as follows.

```
% Suppress an information warning that is issued.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
% Add the observable expression.
eeObs = addobservable(eeResults2,'Maximum tumor_weight','max(tumor_weight)','Units','gram');
```

Plot the computed simulation results showing the 90% quantile region.

```
h2 = plotData(eeObs,ShowMedian=true,ShowMean=false);
h2.Position(:) = [100 100 1500 800];
```



You can also remove the observable by specifying its name.

```
eeNoObs = removeobservable(eeObs,'Maximum tumor_weight');
```

Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

`resultsObj` — Global sensitivity analysis results

`SimBiology.gsa.Sobol` object | `SimBiology.gsa.MPGSA` object | `SimBiology.gsa.ElementaryEffects`

Global sensitivity analysis results, specified as a `SimBiology.gsa.Sobol`, `SimBiology.gsa.MPGSA`, or `SimBiology.gsa.ElementaryEffects` object.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Example: `h = plotData(results,MedianColor=green)` plots the median model response using the green color.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `h = plotData(results,'ResponseLeap',10)` plots every 10th model response.

`Observables` — Model responses or observables to plot

character vector | string | string vector | cell array of character vectors | vector of positive integers

Model responses or observables to plot, specified as a character vector, string, string vector, cell array of character vectors, or vector of positive integers indexing into `resultsObject.Observables`. By default, the function plots GSA results for all model responses or observables.

Data Types: `double` | `char` | `string` | `cell`

`Alphas` — Size of shaded region

0.05 (default) | positive scalar between 0 and 1 | numeric vector

Size of the quantile region in the plot, specified as a positive scalar between 0 and 1 or numeric vector. The percentage of a region is calculated as `100 * (1 - 2 * Alpha)`. Hence, the default alpha value of 0.05 corresponds to the 90% quantile region.

You can specify multiple values as a vector to plot multiple regions. For instance, `'Alphas',[0.05 0.1]` shows both 90% and 80% regions.

Data Types: `double`

`FaceColor` — Color of shaded regions

three-element row vector | hexadecimal color code | color name

Color of the shaded regions, specified as a three-element row vector, hexadecimal color code, color name, or a short name. By default, the function uses the first MATLAB default color. To view the default color order, enter `get(groot,'defaultAxesColorOrder')` or see the “ColorOrder” property.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see “Specify Plot Colors”.

Data Types: `double`

`MedianColor` — Color of median model response
three-element row vector | hexadecimal color code | color name

Color of the median model response, specified as a three-element row vector, hexadecimal color code, color name, or a short name. By default, the function uses the second MATLAB default color. To view the default color order, enter `get(groot,'defaultAxesColorOrder')` or see the “ColorOrder” property.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see “Specify Plot Colors”.

Data Types: `double`

`ShowMedian` — Flag to plot median model response
`false` (default) | `true`

Flag to plot the median model response, specified as `true` or `false`.

Data Types: `logical`

`MeanColor` — Color of mean model response
three-element row vector | hexadecimal color code | color name

Color of the mean model response, specified as a three-element row vector, hexadecimal color code, color name, or a short name. By default, the function uses the second MATLAB default color. To view the default color order, enter `get(groot,'defaultAxesColorOrder')` or see the “ColorOrder” property.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see “Specify Plot Colors”.

Data Types: `double`

`ShowMean` — Flag to plot mean model response
`true` (default) | `false`

Flag to plot the mean model response, specified as `true` or `false`.

Data Types: `logical`

`ResponseColor` — Color of model responses
`[0.3 0.3 0.3]` (default) | three-element row vector | hexadecimal color code | color name

Color of model responses or simulations, specified as a three-element row vector, hexadecimal color code, color name, or a short name. By default, the function uses the color gray `[0.3 0.3 0.3]`.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see “Specify Plot Colors”.

Data Types: `double`

`ResponseLeap` — Every *n*th response to plot
positive integer

Every *n*th response to plot, specified as a positive integer. By default, the function plots 10% of all model responses.

Data Types: `double`

Output Arguments

h — Handle
figure handle

Handle to the figure, specified as a figure handle.

Version History

Introduced in R2020a

R2022b: `plotData` shows median response instead of mean response
Behavior changed in R2022b

`plotData` shows the median model response instead of the mean model response by default. Use the name-value arguments `ShowMedian` or `ShowMean` to plot either the mean or median response. To preserve the behavior prior to R2022a, specify:

```
plotData(gsaResults,ShowMean=true,ShowMedian=false);
```

R2022a: `plotData` warns and shows median response
Warns starting in R2022a

`plotData` warns and shows the median model response instead of the mean model response.

References

[1] Saltelli, Andrea, Paola Annoni, Ivano Azzini, Francesca Campolongo, Marco Ratto, and Stefano Tarantola. “Variance Based Sensitivity Analysis of Model Output. Design and Estimator for the Total Sensitivity Index.” *Computer Physics Communications* 181, no. 2 (February 2010): 259–70. https://doi.org/10.1016/j.cpc.2009.09.018.

[2] Tiemann, Christian A., Joep Vanlier, Maaike H. Oosterveer, Albert K. Groen, Peter A. J. Hilbers, and Natal A. W. van Riel. “Parameter Trajectory Analysis to Identify Treatment Effects of Pharmacological Interventions.” Edited by Scott Markel. *PLoS Computational Biology* 9, no. 8 (August 1, 2013): e1003166. https://doi.org/10.1371/journal.pcbi.1003166.

[3] Morris, Max D. “Factorial Sampling Plans for Preliminary Computational Experiments.” *Technometrics* 33, no. 2 (May 1991): 161–74.

[4] Sohier, Henri, Jean-Loup Farges, and Helene Piet-Lahanier. “Improvement of the Representativity of the Morris Method for Air-Launch-to-Orbit Separation.” *IFAC Proceedings Volumes* 47, no. 3 (2014): 7954–59.

See Also

`SimBiology.gsa.Sobol` | `SimBiology.gsa.MPGSA` | `SimBiology.gsa.ElementaryEffects`

plotGrid

Plot parameter grid and points used to compute elementary effects

Syntax

```
h = plotGrid(eeObj)
h = plotGrid(eeObj,Name=Value)
```

Description

`h = plotGrid(eeObj)` plots the parameter grid and radial or chain points used to compute elementary effects. A dotted line between two points in the grid shows that an elementary effect between those two points was computed. For details, see “Elementary Effects for Global Sensitivity Analysis” on page 1-51.

`h = plotGrid(eeObj,Name=Value)` uses additional options specified by one or more name-value arguments.

Examples

Perform GSA by Computing Elementary Effects

Load the “Tumor Growth Model”.

```
sbioloadproject tumor_growth_vpop_sa.sbproj
```

Get a variant with estimated parameters and the dose to apply to the model.

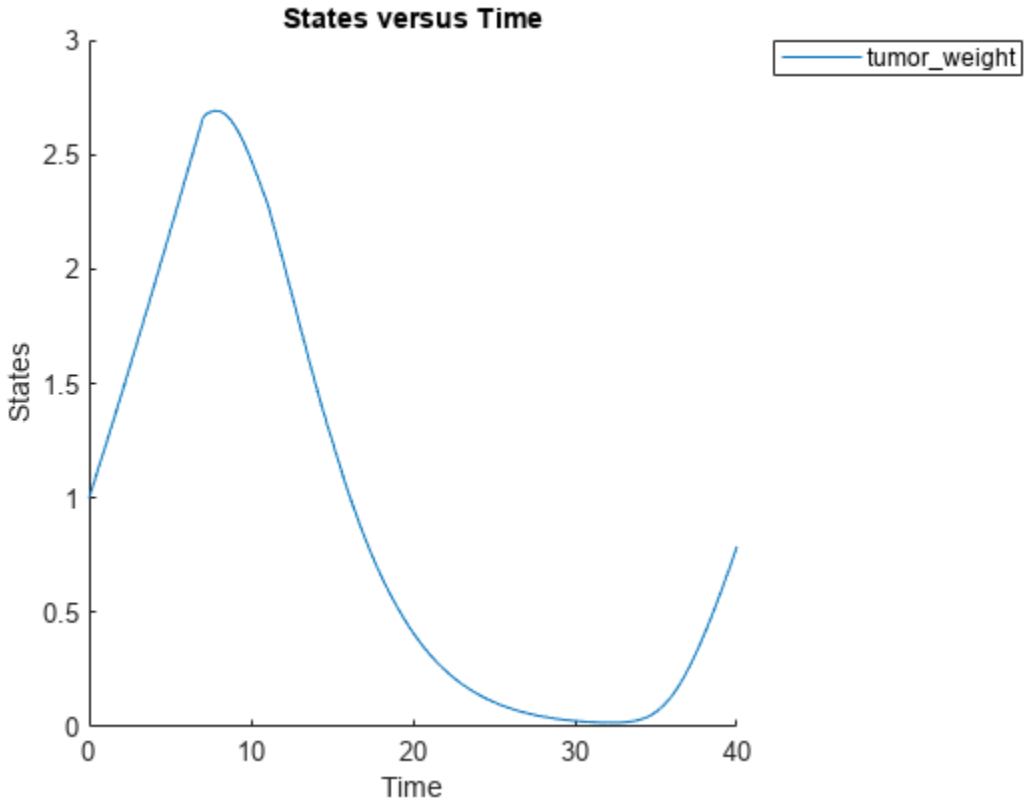
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

Get the active configset and set the tumor weight as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'tumor_weight';
```

Simulate the model and plot the tumor growth profile.

```
sbioplot(sbiosimulate(m1,cs,v,d));
```



Perform global sensitivity analysis (GSA) on the model to find the model parameters that the tumor growth is sensitive to.

First, define model parameters of interest, which are involved in the pharmacodynamics of the tumor growth. Define the model response as the tumor weight.

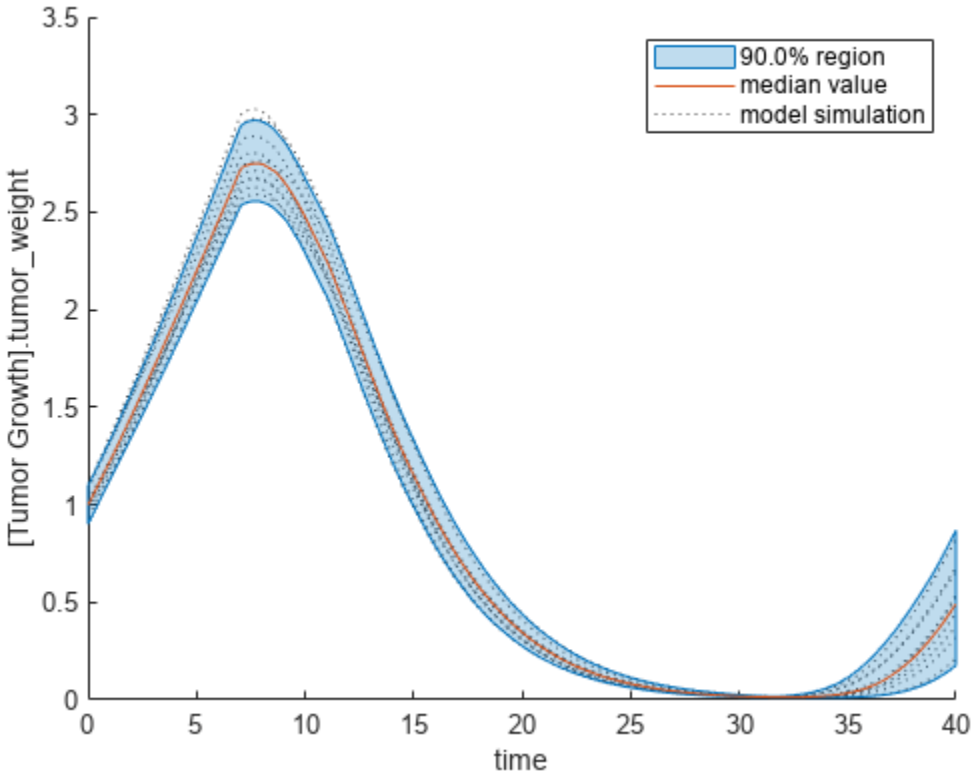
```
modelParamNames = {'L0','L1','w0','k1'};
outputName = 'tumor_weight';
```

Then perform GSA by computing the elementary effects using `sbioelementaryeffects`. Use `100` as the number of samples and set `ShowWaitBar` to `true` to show the simulation progress.

```
rng('default');
eeResults = sbioelementaryeffects(m1,modelParamNames,outputName,Variants=v,Doses=d,NumberSamples=
```

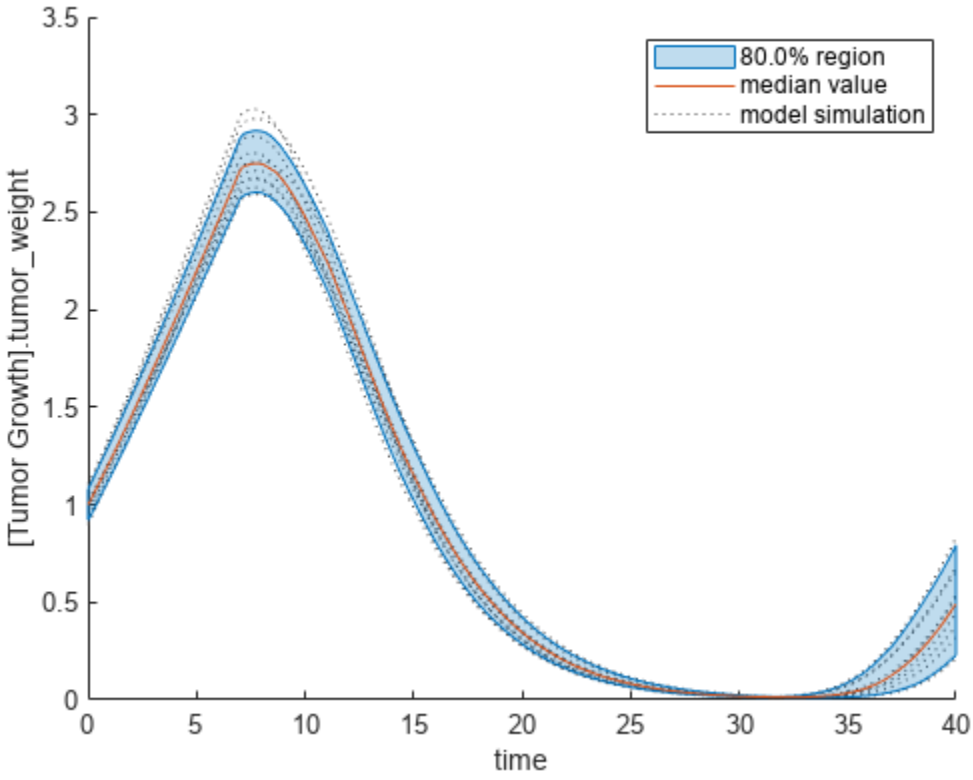
Show the median model response, the simulation results, and a shaded region covering 90% of the simulation results.

```
plotData(eeResults,ShowMedian=true,ShowMean=false);
```



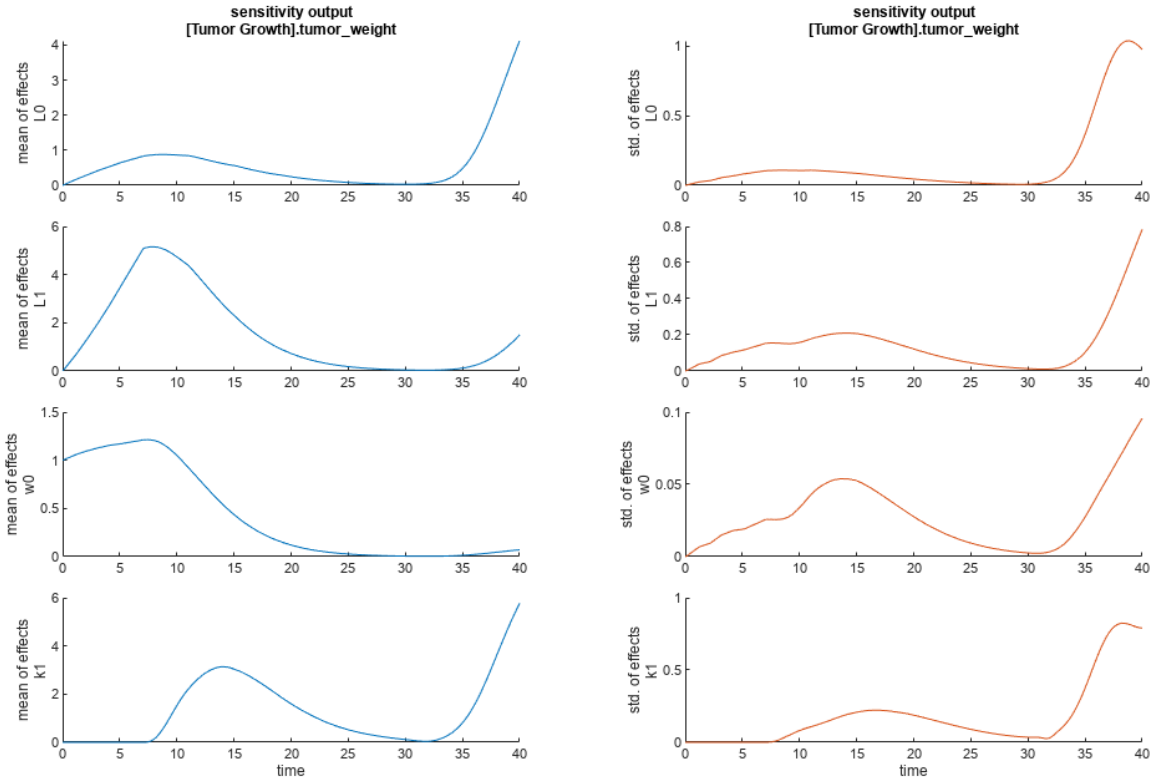
You can adjust the quantile region to a different percentage by specifying `Alphas` for the lower and upper quantiles of all model responses. For instance, an `alpha` value of 0.1 plots a shaded region between the `100*alpha` and `100*(1-alpha)` quantiles of all simulated model responses.

```
plotData(eeResults,Alphas=0.1,ShowMedian=true,ShowMean=false);
```



Plot the time course of the means and standard deviations of the elementary effects.

```
h = plot(eeResults);
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```

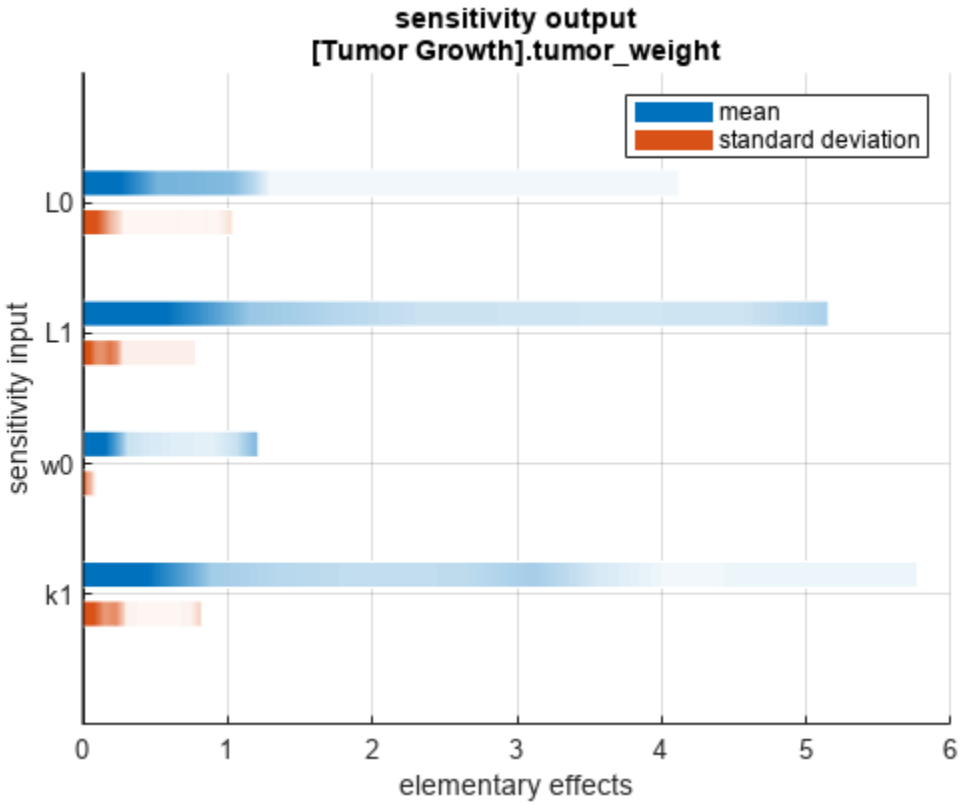


The mean of effects explains whether variations in input parameter values have any effect on the tumor weight response. The standard deviation of effects explains whether the sensitivity change is dependent on the location in the parameter domain.

From the mean of effects plots, parameters `L1` and `w0` seem to be the most sensitive parameters to the tumor weight before the dose is applied at t = 7. But, after the dose is applied, `k1` and `L0` become more sensitive parameters and contribute most to the after-dosing stage of the tumor weight. The plots of standard deviation of effects show more deviations for the larger parameter values in the later stage (t > 35) than for the before-dose stage of the tumor growth.

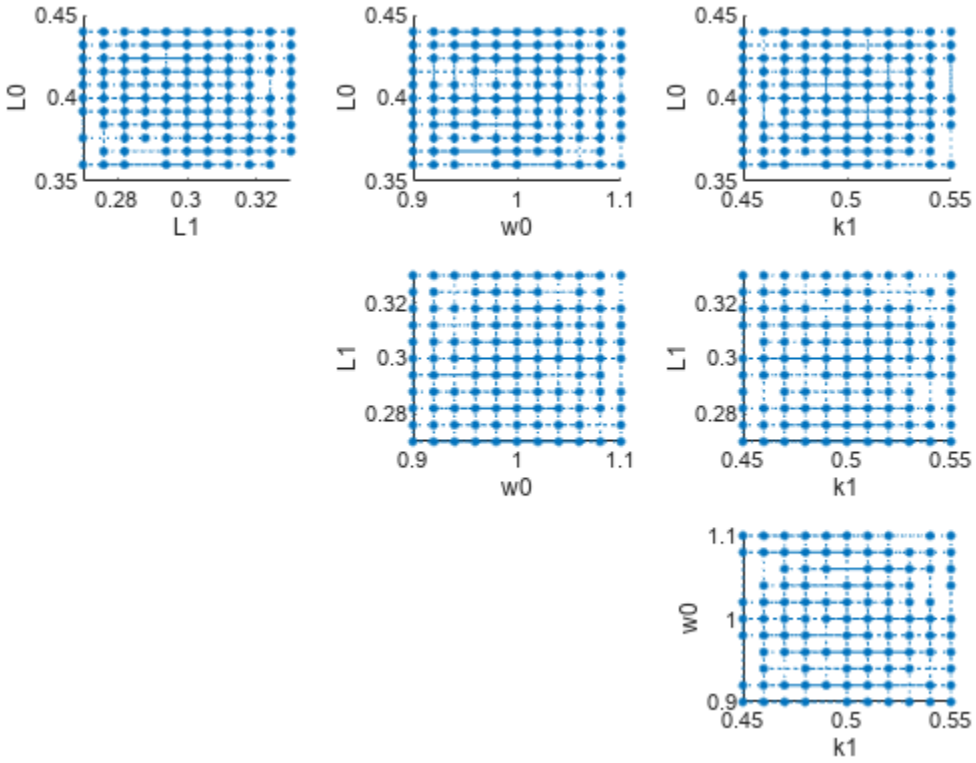
You can also display the magnitudes of the sensitivities in a bar plot. Each color shading represents a histogram representing values at different times. Darker colors mean that those values occur more often over the whole time course.

```
bar(eeResults);
```



You can also plot the parameter grids and samples used to compute the elementary effects.

```
plotGrid(eeResults)
```



You can specify more samples to increase the accuracy of the elementary effects, but the simulation can take longer to finish. Use `addsamples` to add more samples.

```
eeResults2 = addsamples(eeResults,200);
```

The `SimulationInfo` property of the result object contains various information for computing the elementary effects. For instance, the model simulation data (SimData) for each simulation using a set of parameter samples is stored in the `SimData` field of the property. This field is an array of `SimData` objects.

```
eeResults2.SimulationInfo.SimData
```

```
SimBiology SimData Array : 1500-by-1

Index:    Name:         ModelName:         DataCount:
1           -           Tumor Growth Model 1
2           -           Tumor Growth Model 1
3           -           Tumor Growth Model 1
...
1500        -           Tumor Growth Model 1
```

You can find out if any model simulation failed during the computation by checking the `ValidSample` field of `SimulationInfo`. In this example, the field shows no failed simulation runs.

```
all(eeResults2.SimulationInfo.ValidSample)
```

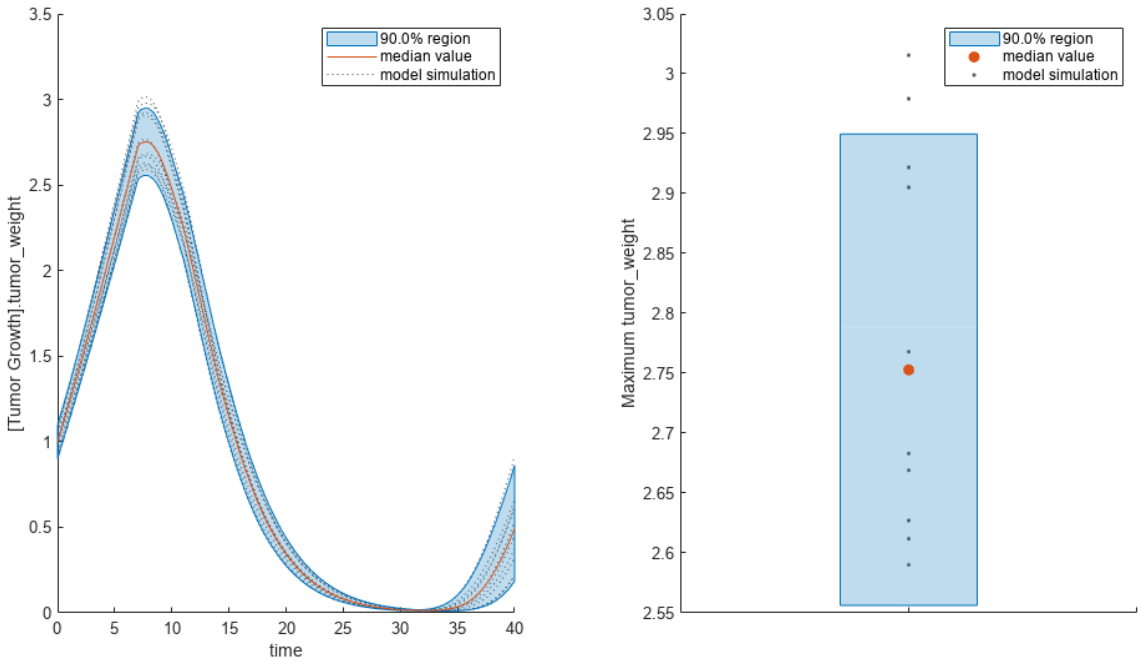
```
ans = logical
   1
```

You can add custom expressions as observables and compute the elementary effects of the added observables. For example, you can compute the effects for the maximum tumor weight by defining a custom expression as follows.

```
% Suppress an information warning that is issued.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
% Add the observable expression.
eeObs = addobservable(eeResults2,'Maximum tumor_weight','max(tumor_weight)','Units','gram');
```

Plot the computed simulation results showing the 90% quantile region.

```
h2 = plotData(eeObs,ShowMedian=true,ShowMean=false);
h2.Position(:) = [100 100 1500 800];
```



You can also remove the observable by specifying its name.

```
eeNoObs = removeobservable(eeObs,'Maximum tumor_weight');
```

Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

eeObj — Results containing means and standard deviations of elementary effects

`SimBiology.gsa.ElementaryEffects` object

Results containing the means and standard deviations of elementary effects, specified as a `SimBiology.gsa.ElementaryEffects` object.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Example: `h = plotGrid(results,'Parameters','k1')` specifies to plot the points for `k1`.

`Parameters` — Input parameters to plot

character vector | string | string vector | cell array of character vectors | vector of positive integers

Input parameters to plot, specified as a character vector, string, string vector, cell array of character vectors, or vector of positive integers indexing into the columns of the `resultsObject.ParameterSamples` table. Use this name-value argument to select parameters and plot their corresponding GSA results. By default, all input parameters are included in the plot.

Data Types: `double` | `char` | `string` | `cell`

`Color` — Color of radial or chain points in grid

three-element row vector | hexadecimal color code | color name

Color of the radial or chain points in the grid, specified as a three-element row vector, hexadecimal color code, color name, or a short name. By default, the function uses the first MATLAB default color. To view the default color order, enter `get(groot,'defaultAxesColorOrder')` or see the "ColorOrder" property.

For details on valid color names and corresponding RGB triplets and hexadecimal codes, see "Specify Plot Colors".

Data Types: `double`

Output Arguments

`h` — Handle

figure handle

Handle to the figure, specified as a figure handle.

Version History

Introduced in R2021b

See Also

`SimBiology.gsa.Sobol` | `SimBiology.gsa.ElementaryEffects` | `sbioelementaryeffects`

Topics

"Sensitivity Analysis in SimBiology"

plotResiduals

Plot residuals for each response, using time, group, or prediction as x-axis

Syntax

```
plotResiduals(resultsObj,type)
```

Description

`plotResiduals(resultsObj,type)` plots the residuals for each response, using the time, group, or model predictions as the x-axis as specified by the argument `type`.

Examples

Estimate Two-Compartment PK Parameters

Load the sample data set.

```
load data10_32R.mat
gData = groupedData(data);
gData.Properties.VariableUnits = ["","hour","milligram/liter","milligram/liter"];
```

Create a two-compartment PK model.

```
pkmd                 = PKModelDesign;
pkc1                 = addCompartment(pkmd,"Central");
pkc1.DosingType      = "Infusion";
pkc1.EliminationType = "linear-clearance";
pkc1.HasResponseVariable = true;
pkc2                 = addCompartment(pkmd,"Peripheral");
model                = construct(pkmd);
configset            = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
responseMap = ["Drug_Central = CentralConc","Drug_Peripheral = PeripheralConc"];
```

Provide model parameters to estimate.

```
paramsToEstimate   = ["log(Central)","log(Peripheral)","Q12","Cl_Central"];
estimatedParam     = estimatedInfo(paramsToEstimate,'InitialValue',[1 1 1 1]);
```

Assume every individual receives an infusion dose at time = 0, with a total infusion amount of 100 mg at a rate of 50 mg/hour.

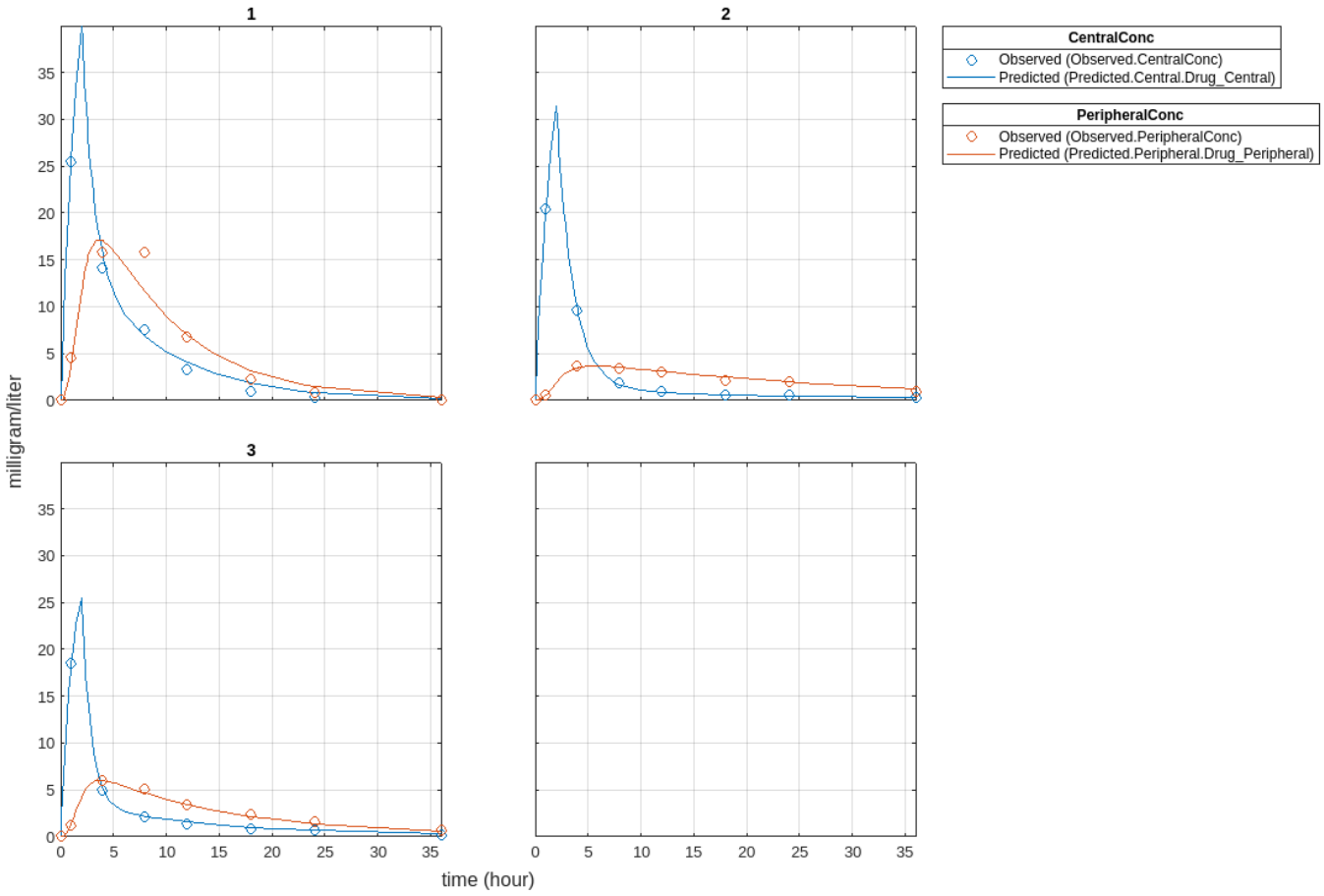
```
dose             = sbiodose("dose","TargetName","Drug_Central");
dose.StartTime   = 0;
dose.Amount      = 100;
dose.Rate        = 50;
dose.AmountUnits = "milligram";
dose.TimeUnits   = "hour";
dose.RateUnits   = "milligram/hour";
```

Estimate model parameters. By default, the function estimates a set of parameter for each individual (unpooled fit).

```
fitResults =  sbiofit(model,gData,responseMap,estimatedParam,dose);
```

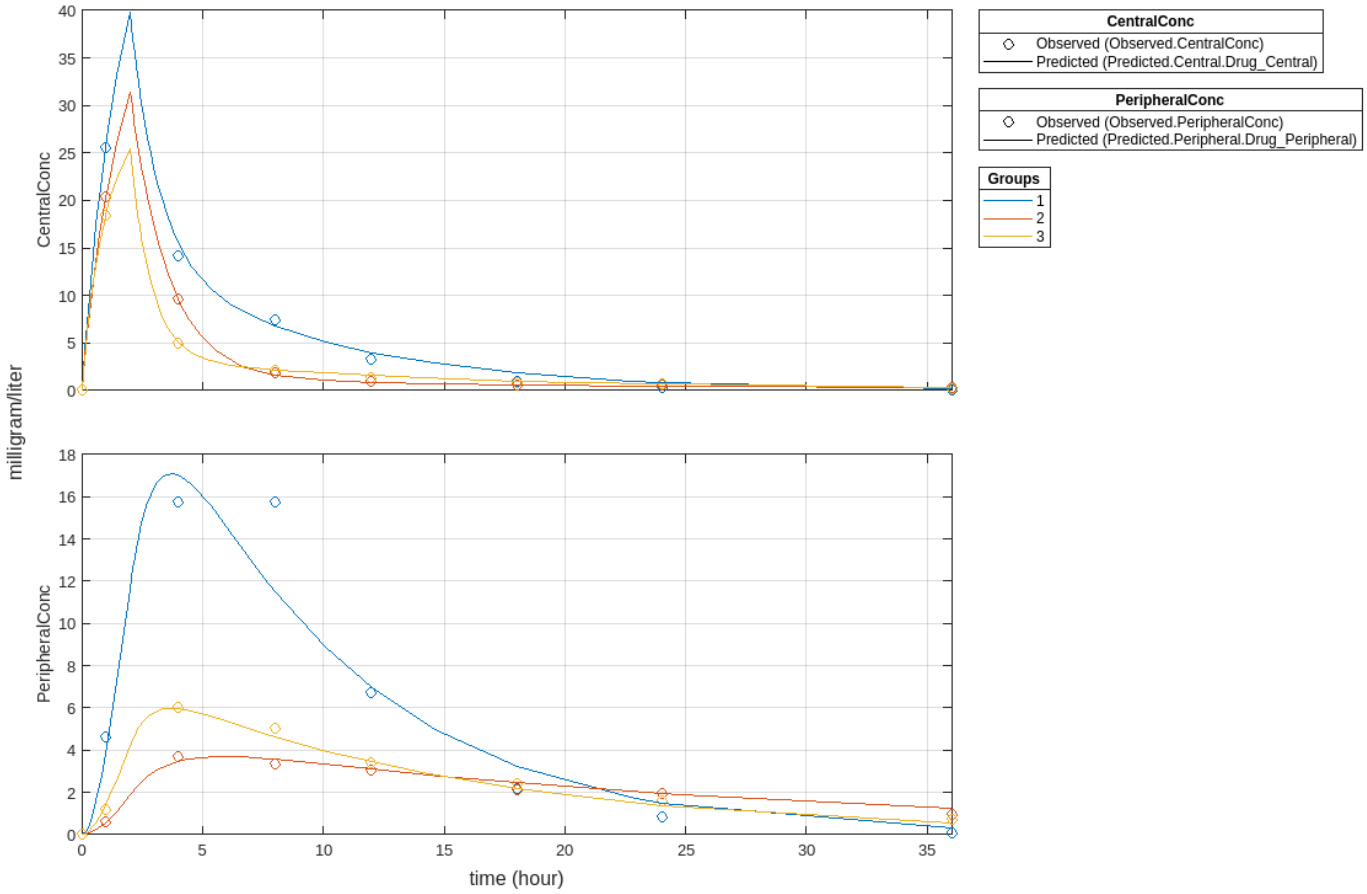
Plot the results.

```
plot(fitResults);
```



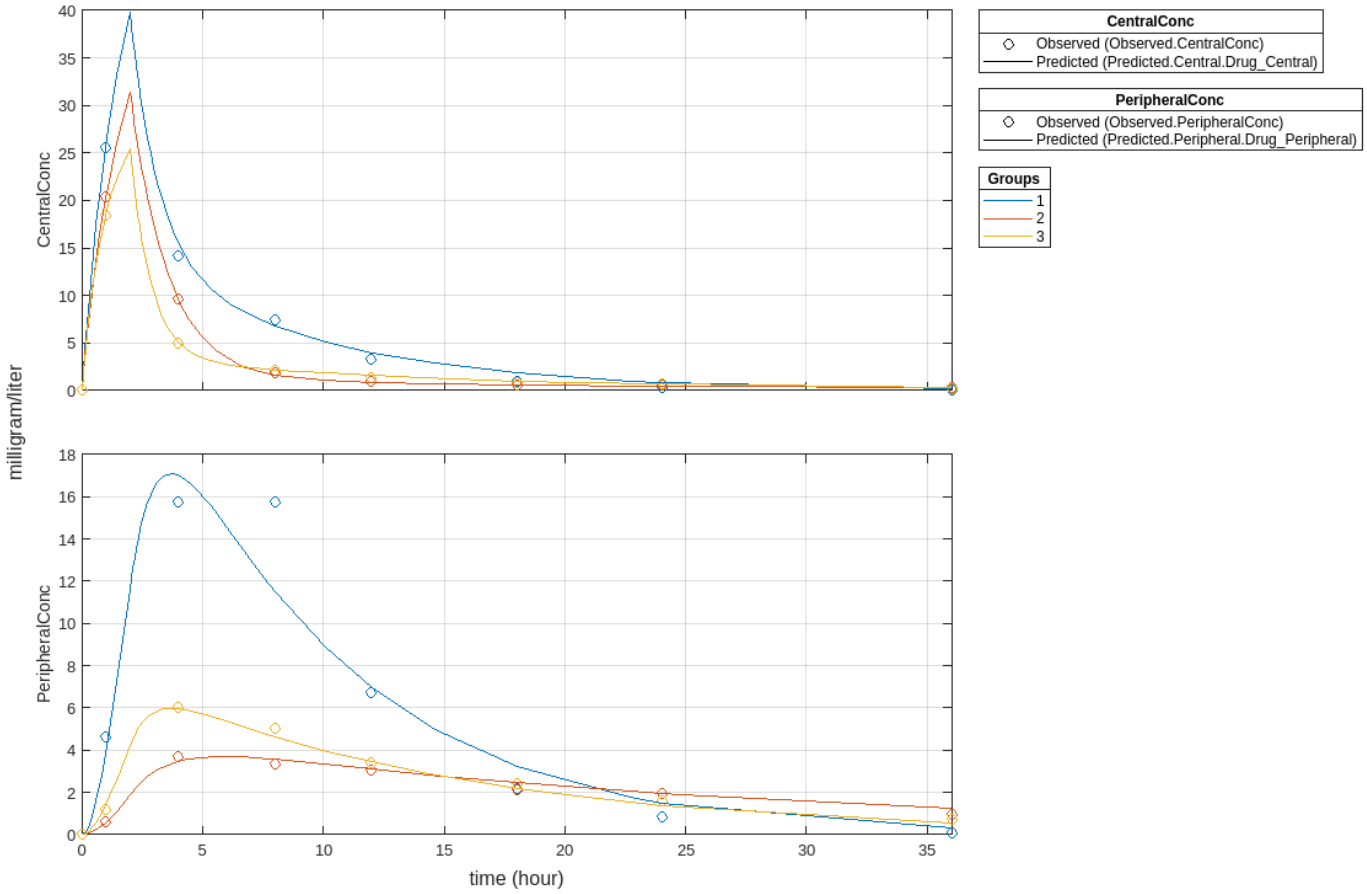
Plot all groups in one plot.

```
plot(fitResults,"PlotStyle","one axes");
```



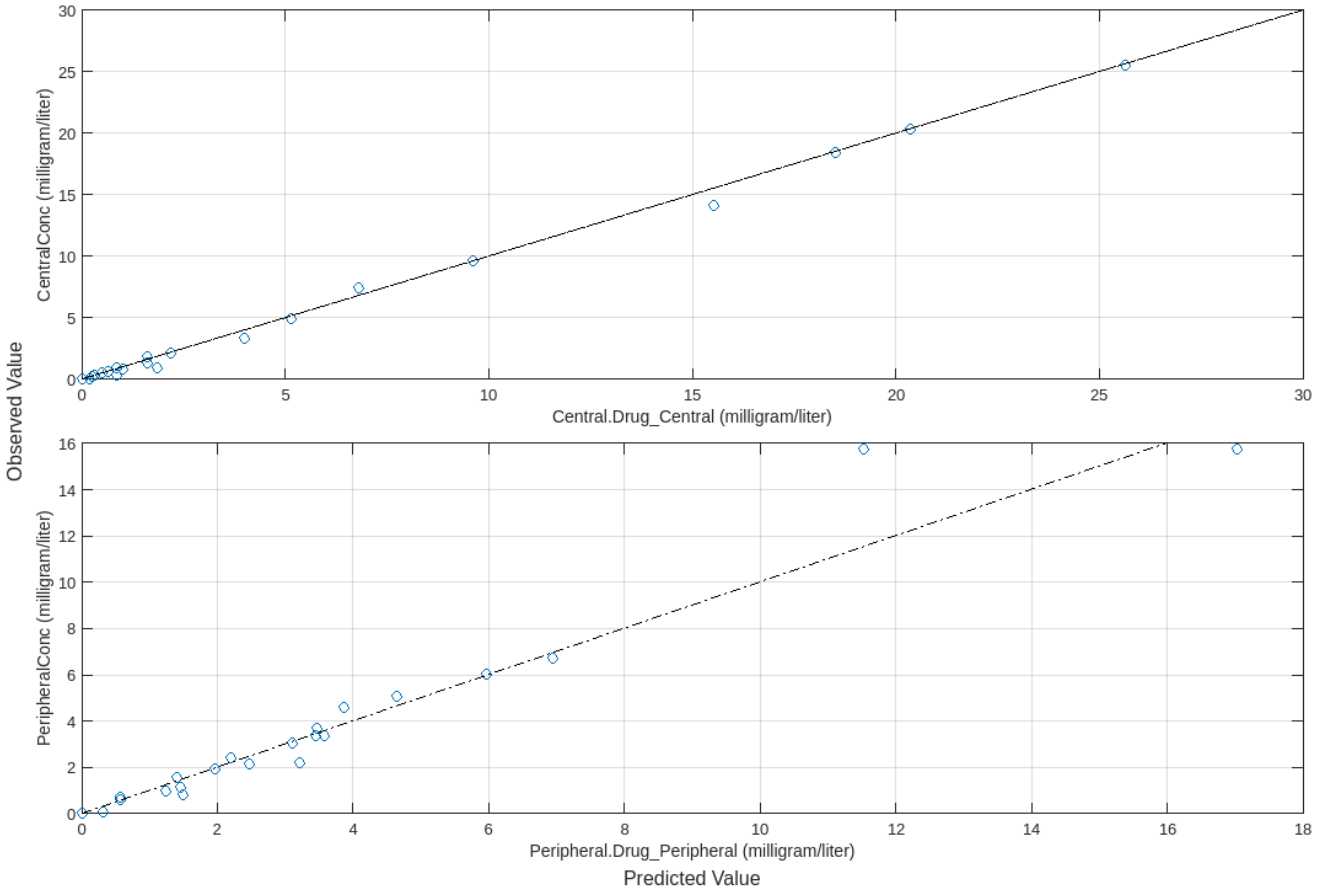
Change some axes properties.

```
s = struct;
s.Properties.XGrid = "on";
s.Properties.YGrid = "on";
plot(fitResults,"PlotStyle","one axes","AxesStyle",s);
```



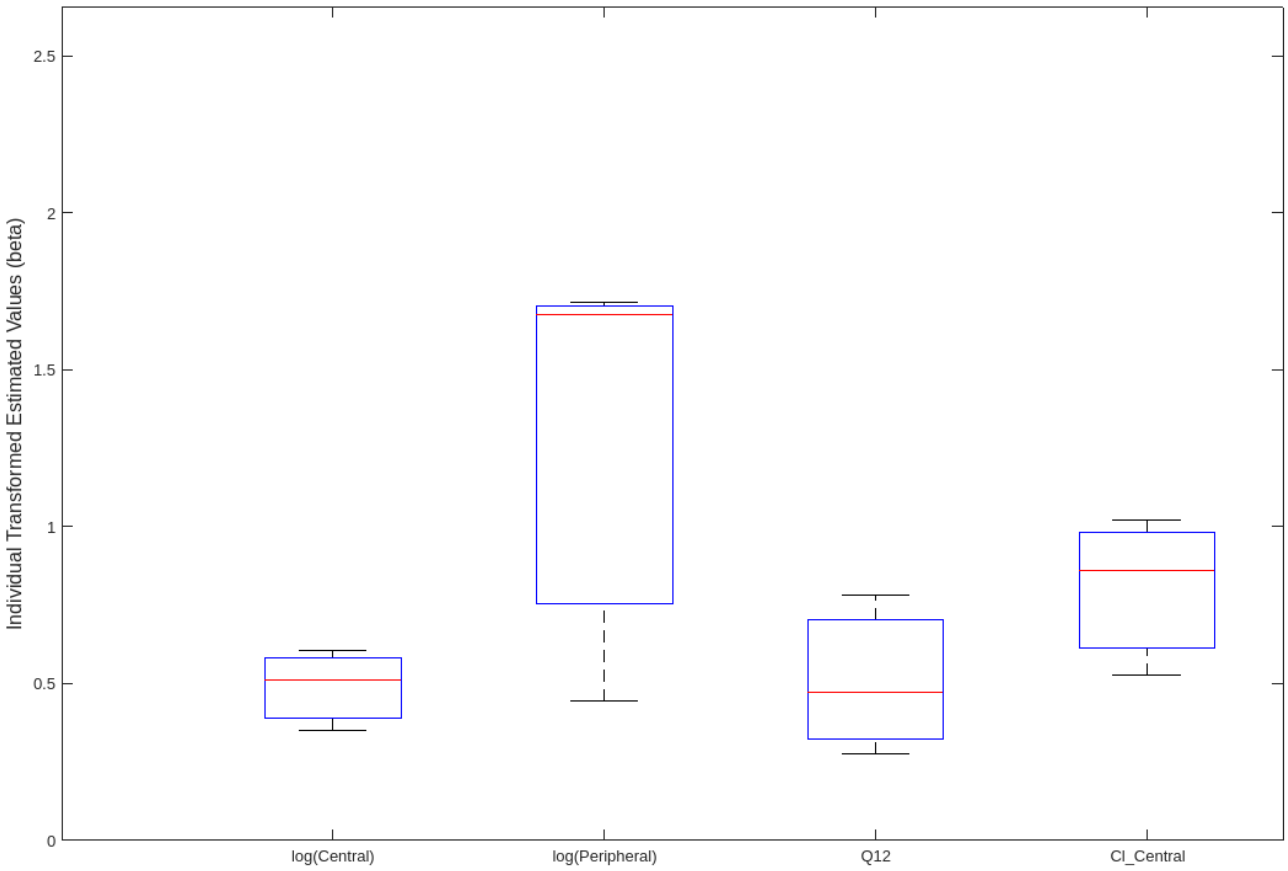
Compare the model predictions to the actual data.

```
plotActualVersusPredicted(fitResults)
```



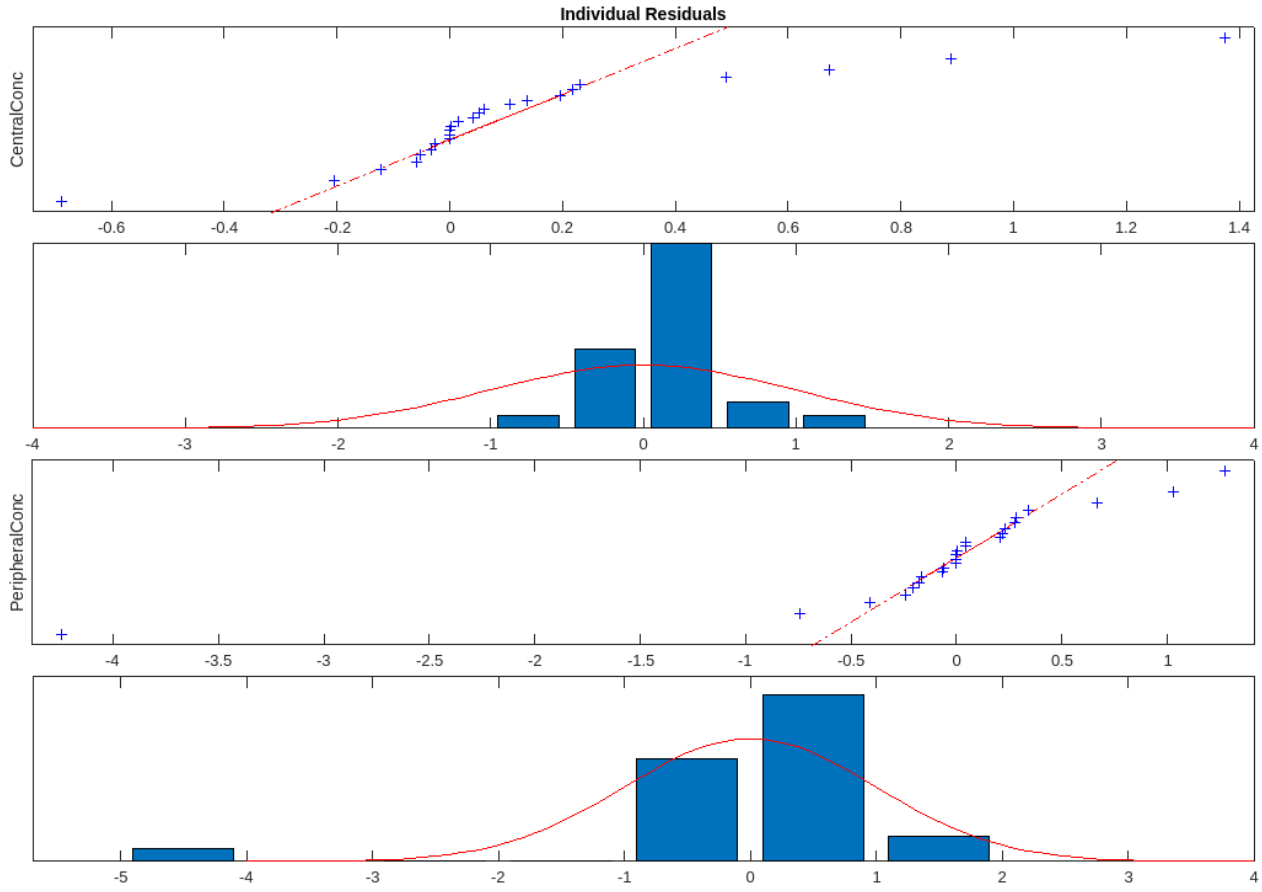
Use `boxplot` to show the variation of estimated model parameters.

```
boxplot(fitResults)
```



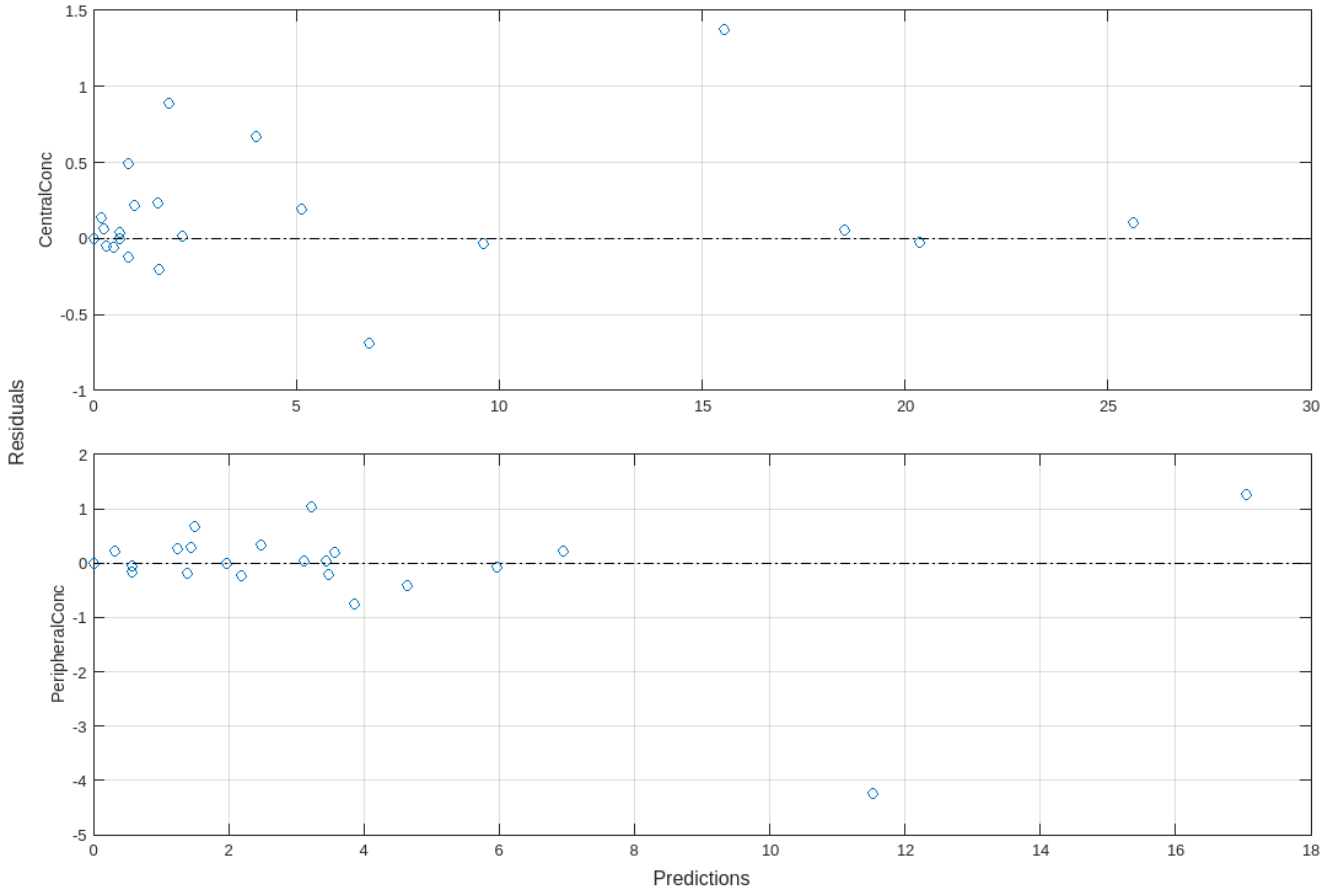
Plot the distribution of residuals. This normal probability plot shows the deviation from normality and the skewness on the right tail of the distribution of residuals. The default (constant) error model might not be the correct assumption for the data being fitted.

```
plotResidualDistribution(fitResults)
```



Plot residuals for each response using the model predictions on *x*-axis.

```
plotResiduals(fitResults,"Predictions")
```



Get the summary of the fit results. `stats.Name` contains the name for each table from `stats.Table`, which contains a list of tables with estimated parameter values and fit quality statistics.

```
stats = summary(fitResults);
stats.Name
```

```
ans =
'Unpooled Parameter Estimates'

ans =
'Statistics'

ans =
'Unpooled Beta'

ans =
'Residuals'

ans =
'Covariance Matrix'

ans =
'Error Model'
```

```
stats.Table
```

```
ans=3×9 table
    Group    Central Estimate    Central StandardError    Peripheral Estimate    Peripheral Stand
    _____    ________________    _____________________    ___________________    ________________

    {'1'}          1.422               0.12334                1.5619                0.36355
    {'2'}         1.8322              0.019672                5.3364                0.65327
    {'3'}         1.6657              0.038529                5.5632                0.37063

ans=3×7 table
    Group      AIC        BIC      LogLikelihood    DFE      MSE         SSE
    _____    _______    _______    _____________    ___    ________    _______

    {'1'}     60.961     64.051       -26.48        12        2.138     25.656
    {'2'}    -7.8379    -4.7475       7.9189        12     0.029012    0.34814
    {'3'}    -1.4336     1.6567       4.7168        12     0.043292     0.5195

ans=3×9 table
    Group    Central Estimate    Central StandardError    Peripheral Estimate    Peripheral Stand
    _____    ________________    _____________________    ___________________    ________________

    {'1'}         0.35208              0.086736               0.44589                0.23277
    {'2'}         0.60551              0.010737                1.6746                0.12242
    {'3'}         0.51027               0.02313                1.7162                0.06662

ans=24×4 table
    ID    Time    CentralConc    PeripheralConc
    __    ____    ___________    ______________

    1       0              0              0
    1       1        0.10646        -0.74394
    1       4         1.3745          1.2726
    1       8       -0.68825         -4.2435
    1      12        0.67383         0.21806
    1      18        0.88823          1.0269
    1      24        0.48941         0.66755
    1      36        0.13632         0.22948
    2       0              0              0
    2       1      -0.026731      -0.058311
    2       4      -0.033299       -0.20544
    2       8       -0.20466        0.20696
    2      12       -0.12223       0.045409
    2      18       0.041224        0.33883
    2      24      -0.059498      0.0036257
    2      36      -0.051645        0.27616
      ⋮

ans=12×6 table
    Group        Parameters          log(Central)    log(Peripheral)        Q12         Cl_Central
    _____    ___________________    ____________    _______________    ____________    ____________

    {'1'}    {'log(Central)'   }       0.015213        -0.022539        -0.0086672       0.001159
    {'1'}    {'log(Peripheral)'}      -0.022539          0.13217          0.045746     -0.0073135
    {'1'}    {'Q12'            }     -0.0086672         0.045746          0.023092     -0.0021484
    {'1'}    {'Cl_Central'     }       0.001159       -0.0073135        -0.0021484      0.0013674
    {'2'}    {'log(Central)'   }     0.00038701        -0.002161       -0.00010177     9.7448e-05
```

```
    {'2'}    {'log(Peripheral)'}      -0.002161          0.42676          0.019101      -0.01575
    {'2'}    {'Q12'            }    -0.00010177         0.019101         0.00094857    -0.0007332
    {'2'}    {'Cl_Central'     }     9.7448e-05        -0.015755        -0.00073328     0.0006894
    {'3'}    {'log(Central)'   }      0.0014845       -0.0054648         -0.0013216     0.0001663
    {'3'}    {'log(Peripheral)'}     -0.0054648          0.13737           0.016903     -0.007272
    {'3'}    {'Q12'            }     -0.0013216         0.016903          0.0034406    -0.0008253
    {'3'}    {'Cl_Central'     }     0.00016639       -0.0072722        -0.00082538     0.0007458
```

```
ans=3×5 table
    Group     Response      ErrorModel        a        b
    _____    __________    ____________    _______    ___

    {'1'}    {0×0 char}    {'constant'}     1.2663    NaN
    {'2'}    {0×0 char}    {'constant'}    0.14751    NaN
    {'3'}    {0×0 char}    {'constant'}    0.18019    NaN
```

Input Arguments

`resultsObj` — Estimation results

`OptimResults` object | `NLINResults` object | vector of results objects

Estimation results, specified as an `OptimResults object`, `NLINResults object`, or a vector of results object which contains estimation results returned by `sbiofit`.

`type` — x-axis option for residual plot

character vector | string

X-axis option for the residual plot, specified as a character vector or string that must be one of the following: `'Time'`, `'Group'`, or `'Predictions'`.

Version History

Introduced in R2014a

See Also

`NLINResults object` | `OptimResults object` | `sbiofit`

plotResiduals

Plot the residuals for each response, using the time, group, or prediction as the x-axis

Syntax

```
plotResiduals(resultsObj,type)
```

Description

`plotResiduals(resultsObj,type)` plots the residuals for each response, using the time, group, or predictions as the x-axis as specified by the argument `type`.

Input Arguments

`resultsObj` — Estimation results
`NLMEResults` object

Estimation results, specified as an `NLMEResults object`, which contains estimation results returned by `sbiofitmixed`.

`type` — X-axis option for residual plot
character vector | string

X-axis option for the residual plot, specified as a character vector or string which must be one of the following: `'Time'`, `'Group'`, or `'Predictions'`.

Version History

Introduced in R2014a

See Also

`NLMEResults object` | `sbiofitmixed`

plotResidualDistribution

Plot the distribution of the residuals

Syntax

```
plotResidualDistribution(resultsObj)
```

Description

`plotResidualDistribution(resultsObj)` shows the normal probability plot and the corresponding histogram of the residuals. Use the plot to check if the distribution of the residuals deviates from the normality.

Examples

Estimate Two-Compartment PK Parameters

Load the sample data set.

```
load data10_32R.mat
gData = groupedData(data);
gData.Properties.VariableUnits = ["","hour","milligram/liter","milligram/liter"];
```

Create a two-compartment PK model.

```
pkmd                 = PKModelDesign;
pkc1                 = addCompartment(pkmd,"Central");
pkc1.DosingType      = "Infusion";
pkc1.EliminationType = "linear-clearance";
pkc1.HasResponseVariable = true;
pkc2                 = addCompartment(pkmd,"Peripheral");
model                = construct(pkmd);
configset            = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
responseMap = ["Drug_Central = CentralConc","Drug_Peripheral = PeripheralConc"];
```

Provide model parameters to estimate.

```
paramsToEstimate   = ["log(Central)","log(Peripheral)","Q12","Cl_Central"];
estimatedParam     = estimatedInfo(paramsToEstimate,'InitialValue',[1 1 1 1]);
```

Assume every individual receives an infusion dose at time = 0, with a total infusion amount of 100 mg at a rate of 50 mg/hour.

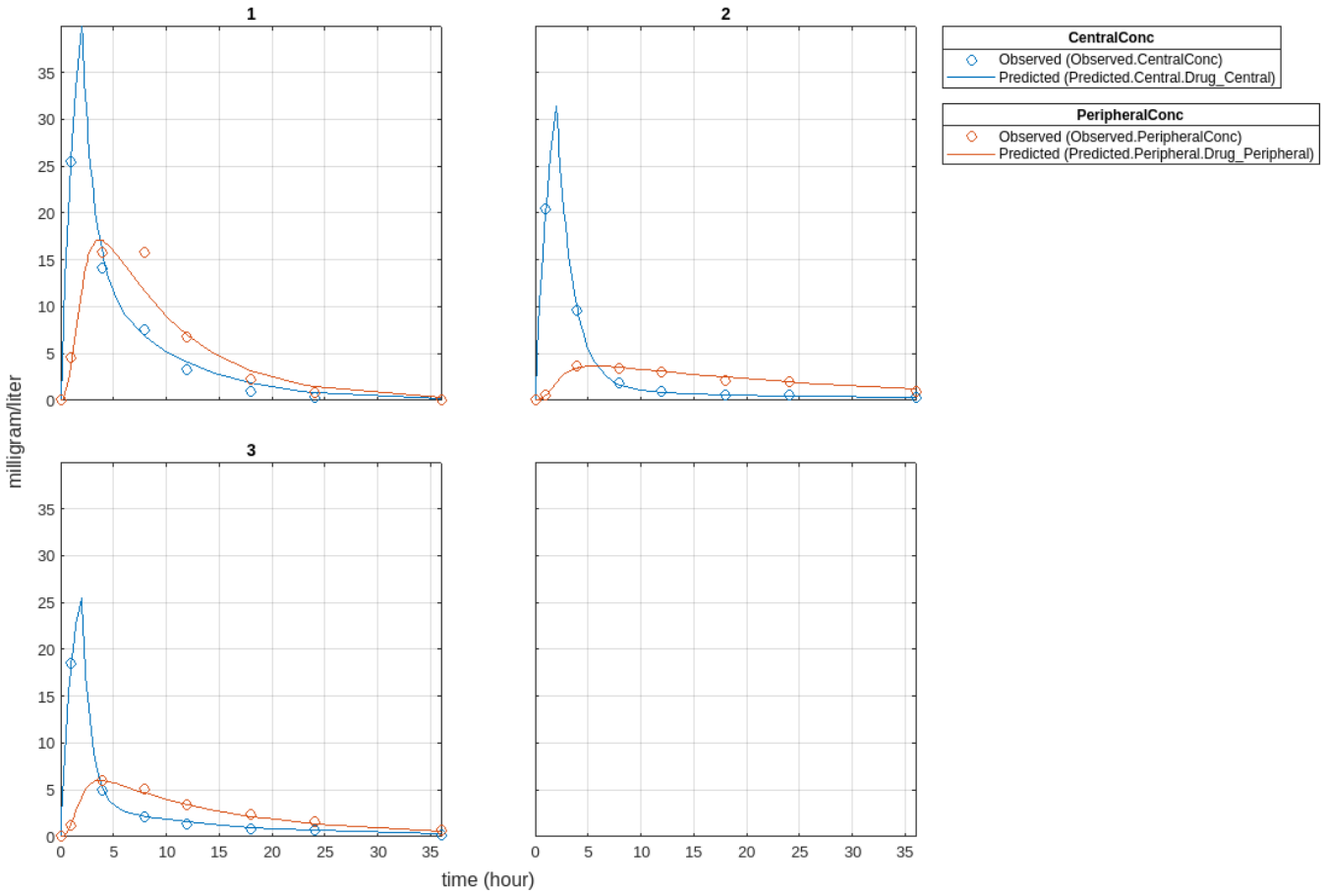
```
dose             = sbiodose("dose","TargetName","Drug_Central");
dose.StartTime   = 0;
dose.Amount      = 100;
dose.Rate        = 50;
dose.AmountUnits = "milligram";
dose.TimeUnits   = "hour";
dose.RateUnits   = "milligram/hour";
```

Estimate model parameters. By default, the function estimates a set of parameter for each individual (unpooled fit).

```
fitResults =  sbiofit(model,gData,responseMap,estimatedParam,dose);
```

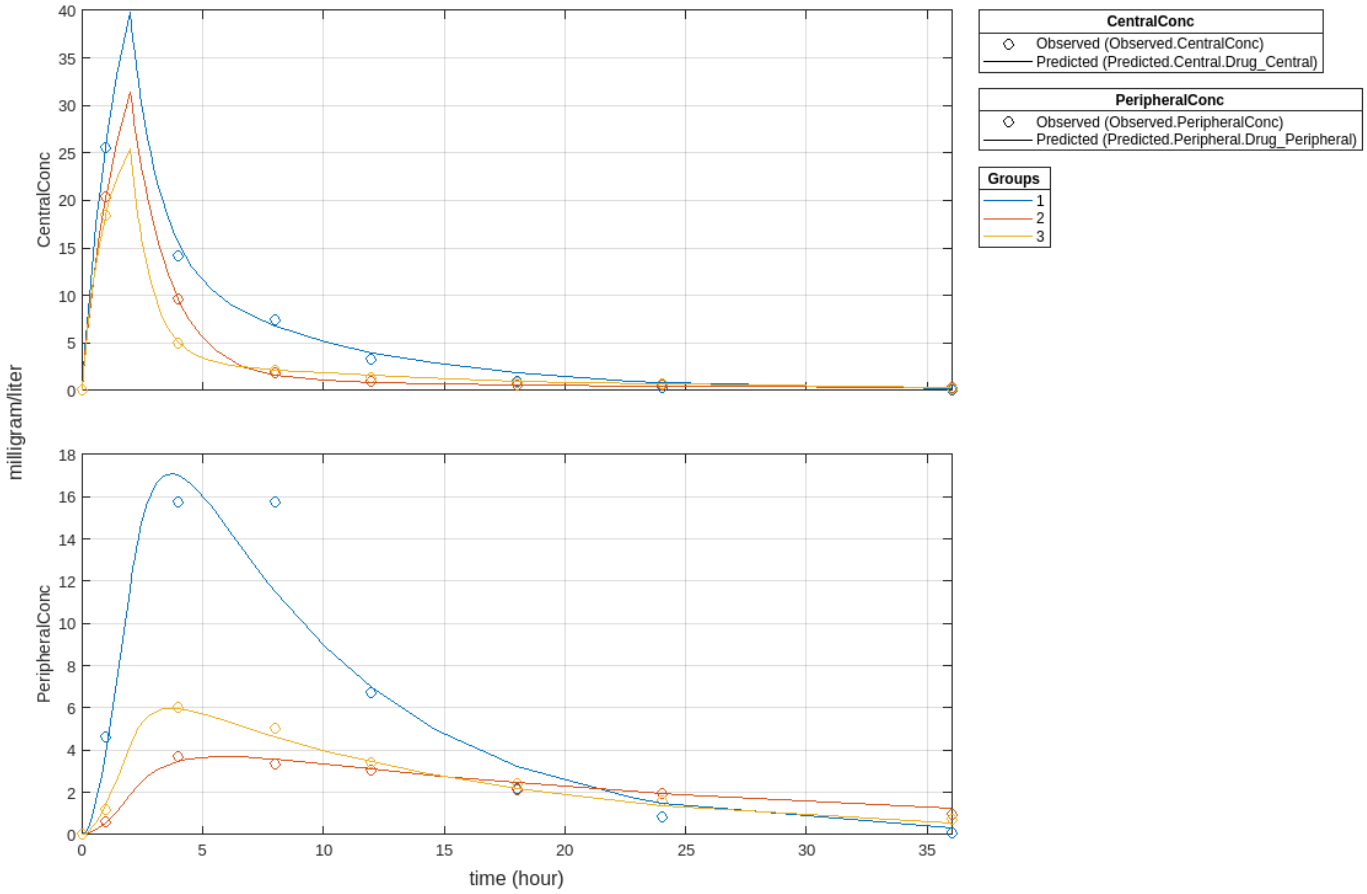
Plot the results.

```
plot(fitResults);
```



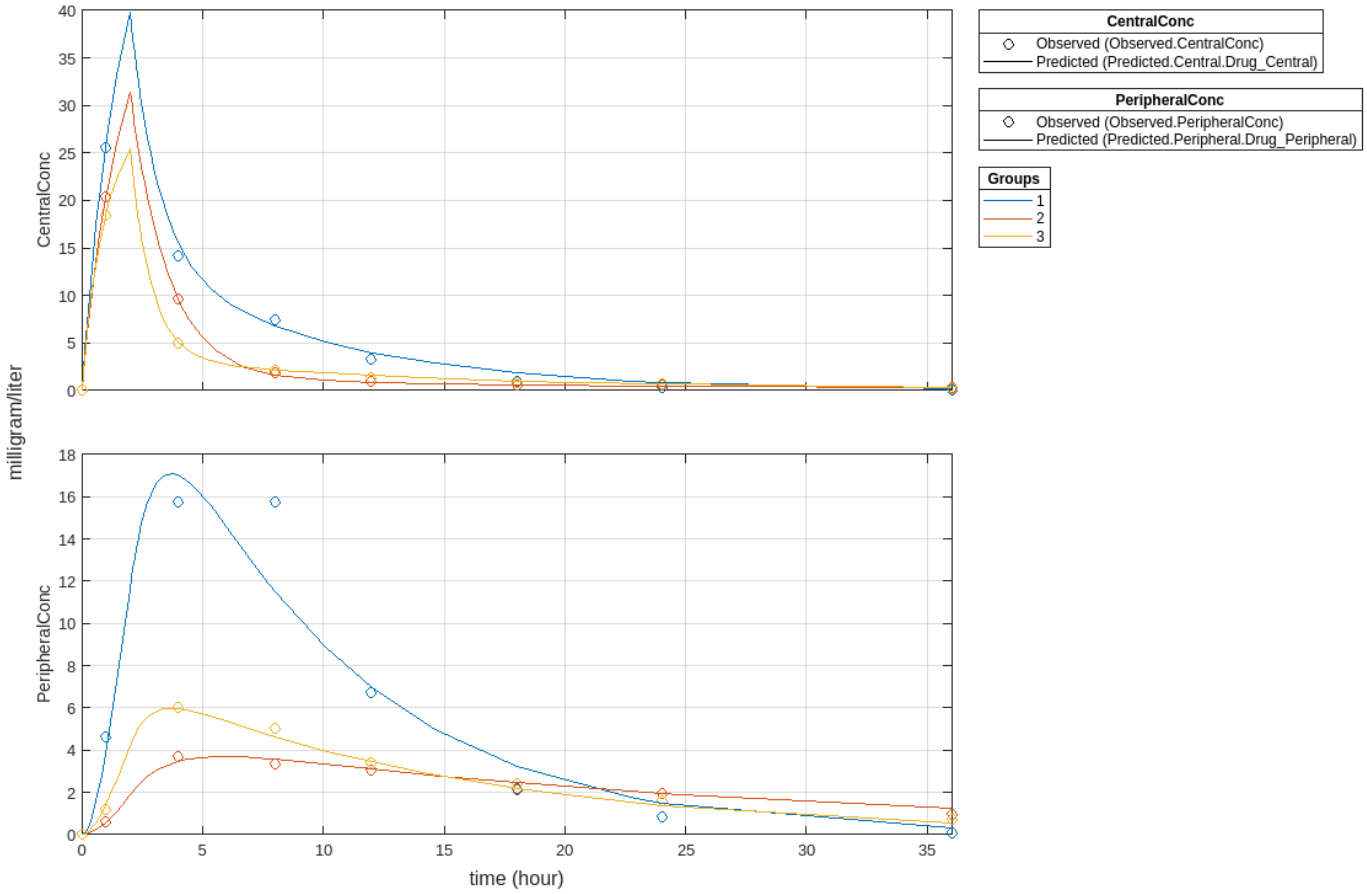
Plot all groups in one plot.

```
plot(fitResults,"PlotStyle","one axes");
```



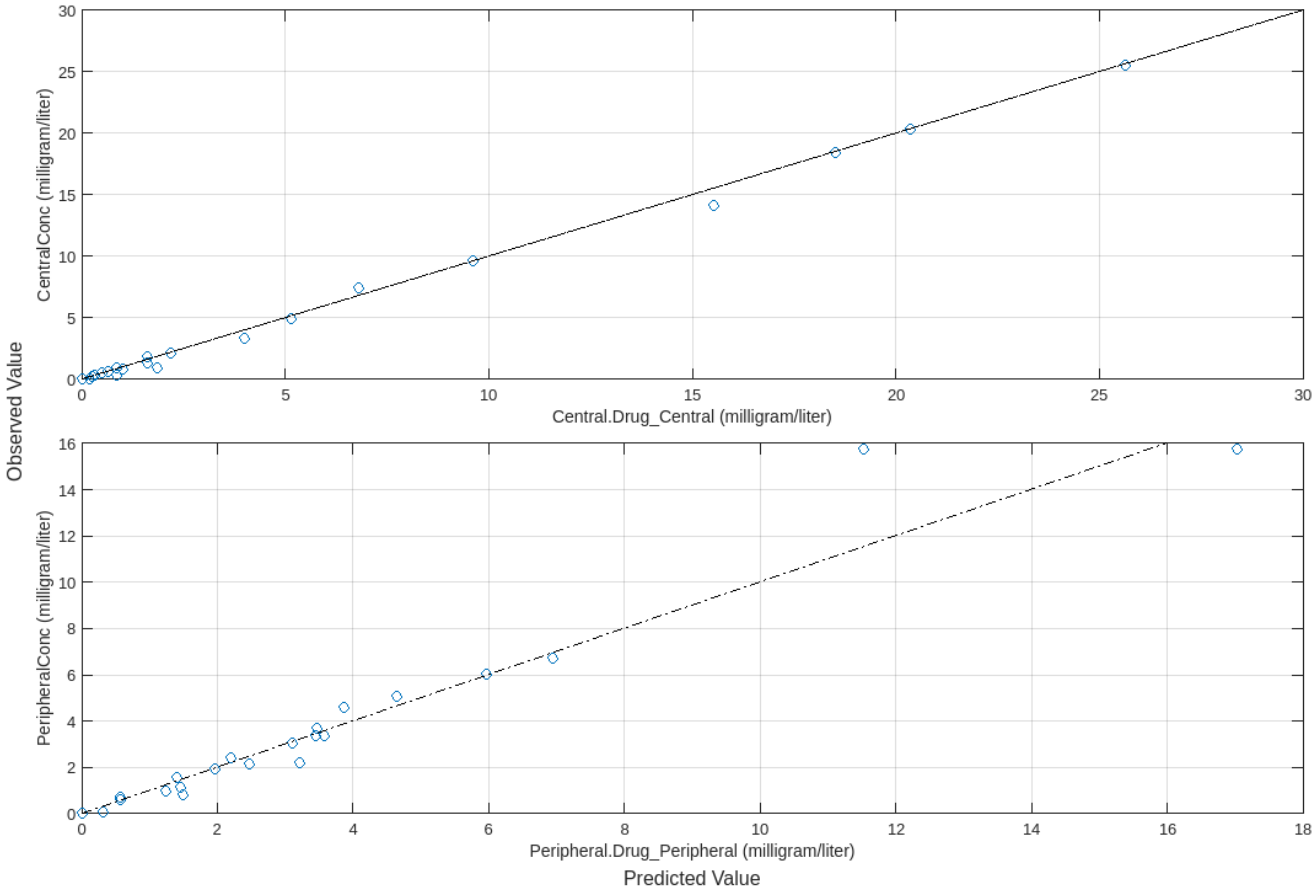
Change some axes properties.

```
s = struct;
s.Properties.XGrid = "on";
s.Properties.YGrid = "on";
plot(fitResults,"PlotStyle","one axes","AxesStyle",s);
```



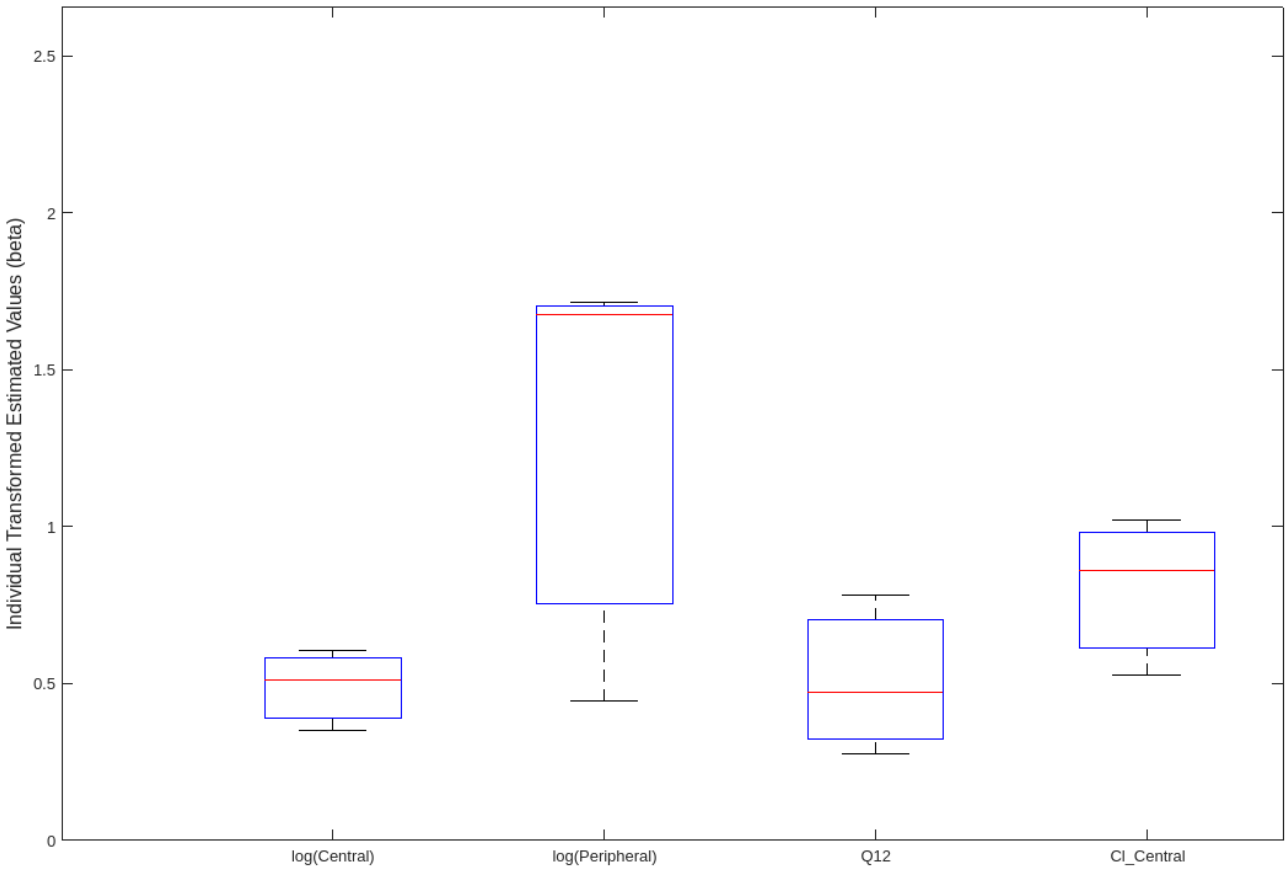
Compare the model predictions to the actual data.

```
plotActualVersusPredicted(fitResults)
```



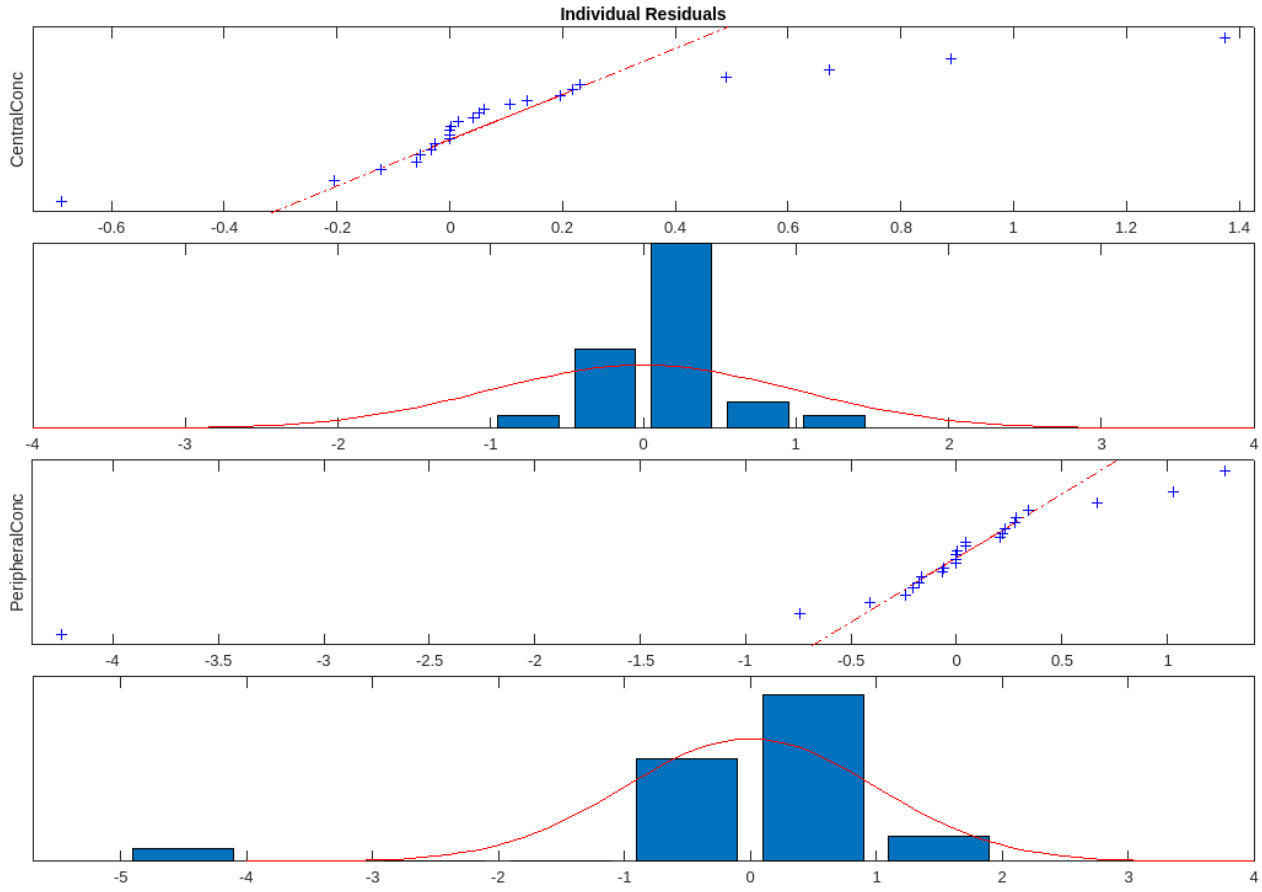
Use `boxplot` to show the variation of estimated model parameters.

```
boxplot(fitResults)
```



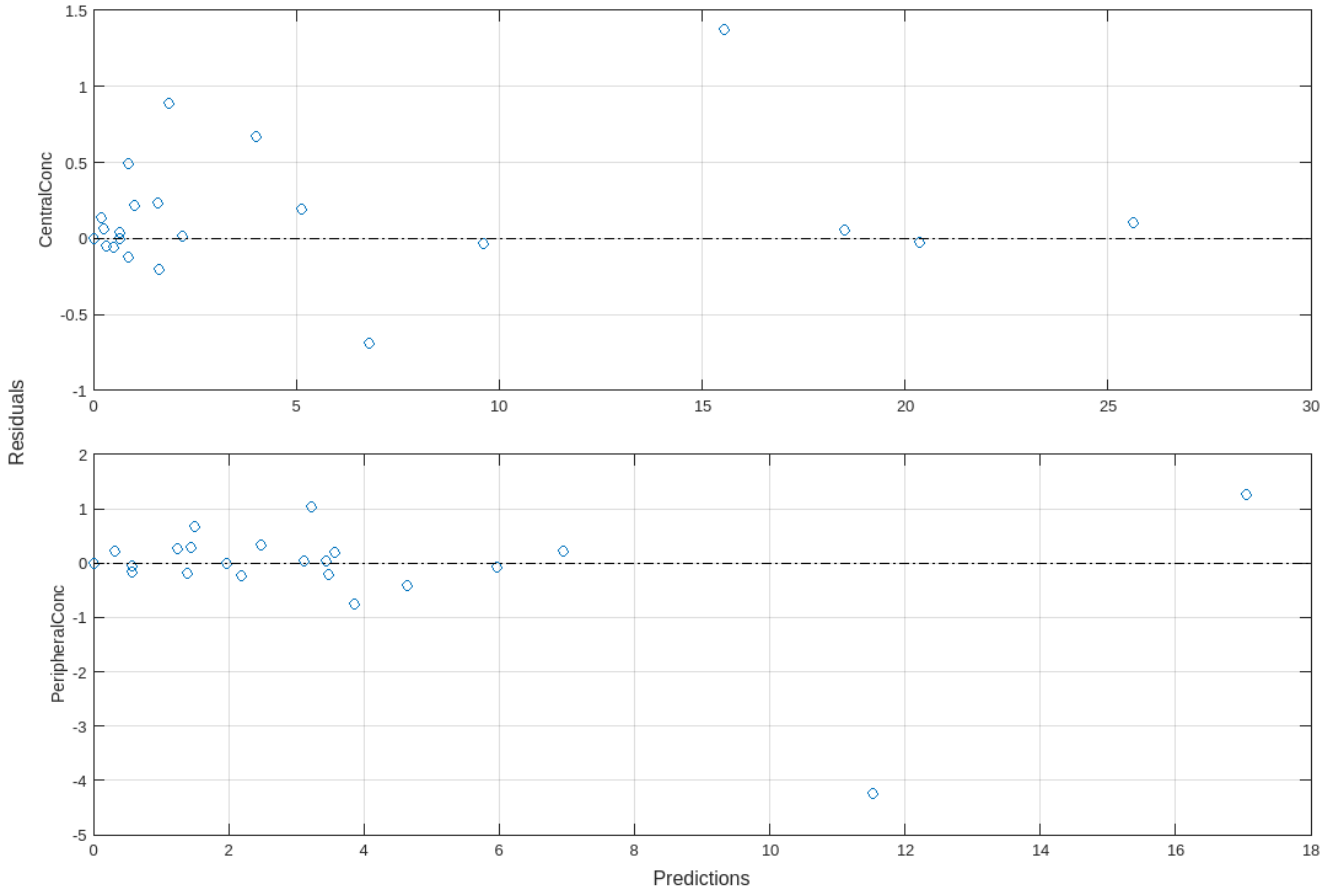
Plot the distribution of residuals. This normal probability plot shows the deviation from normality and the skewness on the right tail of the distribution of residuals. The default (constant) error model might not be the correct assumption for the data being fitted.

```
plotResidualDistribution(fitResults)
```



Plot residuals for each response using the model predictions on *x*-axis.

```
plotResiduals(fitResults,"Predictions")
```



Get the summary of the fit results. `stats.Name` contains the name for each table from `stats.Table`, which contains a list of tables with estimated parameter values and fit quality statistics.

```
stats = summary(fitResults);
stats.Name
```

```
ans =
'Unpooled Parameter Estimates'

ans =
'Statistics'

ans =
'Unpooled Beta'

ans =
'Residuals'

ans =
'Covariance Matrix'

ans =
'Error Model'
```

```
stats.Table
```

```
ans=3×9 table
    Group    Central Estimate    Central StandardError    Peripheral Estimate    Peripheral Stand
    _____    ________________    _____________________    ___________________    ________________

    {'1'}          1.422               0.12334                1.5619                0.36355
    {'2'}         1.8322              0.019672                5.3364                0.65327
    {'3'}         1.6657              0.038529                5.5632                0.37063

ans=3×7 table
    Group      AIC        BIC      LogLikelihood    DFE      MSE         SSE
    _____    _______    _______    _____________    ___    ________    _______

    {'1'}     60.961     64.051       -26.48        12        2.138     25.656
    {'2'}    -7.8379    -4.7475       7.9189        12     0.029012    0.34814
    {'3'}    -1.4336     1.6567       4.7168        12     0.043292     0.5195

ans=3×9 table
    Group    Central Estimate    Central StandardError    Peripheral Estimate    Peripheral Stand
    _____    ________________    _____________________    ___________________    ________________

    {'1'}        0.35208              0.086736               0.44589                0.23277
    {'2'}        0.60551              0.010737                1.6746                0.12242
    {'3'}        0.51027               0.02313                1.7162                0.06662

ans=24×4 table
    ID    Time    CentralConc    PeripheralConc
    __    ____    ___________    ______________

    1       0              0              0
    1       1        0.10646        -0.74394
    1       4         1.3745          1.2726
    1       8       -0.68825         -4.2435
    1      12        0.67383         0.21806
    1      18        0.88823          1.0269
    1      24        0.48941         0.66755
    1      36        0.13632         0.22948
    2       0              0              0
    2       1      -0.026731      -0.058311
    2       4      -0.033299       -0.20544
    2       8       -0.20466        0.20696
    2      12       -0.12223       0.045409
    2      18       0.041224        0.33883
    2      24      -0.059498      0.0036257
    2      36      -0.051645        0.27616
      ⋮

ans=12×6 table
    Group        Parameters          log(Central)    log(Peripheral)        Q12        Cl_Central
    _____    ___________________    ____________    _______________    ___________    __________

    {'1'}    {'log(Central)'   }       0.015213        -0.022539        -0.0086672       0.00115
    {'1'}    {'log(Peripheral)'}      -0.022539          0.13217          0.045746     -0.007313
    {'1'}    {'Q12'            }     -0.0086672         0.045746          0.023092     -0.002148
    {'1'}    {'Cl_Central'     }       0.001159       -0.0073135        -0.0021484      0.001367
    {'2'}    {'log(Central)'   }     0.00038701        -0.002161       -0.00010177     9.7448e-0
```

```
    {'2'}    {'log(Peripheral)'}      -0.002161          0.42676          0.019101      -0.01575
    {'2'}    {'Q12'            }    -0.00010177         0.019101         0.00094857    -0.0007332
    {'2'}    {'Cl_Central'     }     9.7448e-05         -0.015755        -0.00073328     0.0006894
    {'3'}    {'log(Central)'   }      0.0014845        -0.0054648         -0.0013216     0.0001663
    {'3'}    {'log(Peripheral)'}     -0.0054648          0.13737           0.016903     -0.007272
    {'3'}    {'Q12'            }     -0.0013216         0.016903          0.0034406    -0.0008253
    {'3'}    {'Cl_Central'     }      0.00016639       -0.0072722        -0.00082538     0.0007458
```

```
ans=3×5 table
    Group     Response      ErrorModel        a        b
    _____    __________    ____________    _______    ___

    {'1'}    {0×0 char}    {'constant'}     1.2663    NaN
    {'2'}    {0×0 char}    {'constant'}    0.14751    NaN
    {'3'}    {0×0 char}    {'constant'}    0.18019    NaN
```

Input Arguments

`resultsObj` — Estimation results

`OptimResults` object | `NLINResults` object | vector of results objects

Estimation results, specified as an `OptimResults object` or `NLINResults object`, or vector of results objects which contains estimation results from running `sbiofit`.

Version History

Introduced in R2014a

See Also

`NLINResults object` | `OptimResults object` | `sbiofit`

plotResidualDistribution

Plot the distribution of the residuals

Syntax

```
plotResidualDistribution(resultsObj)
```

Description

`plotResidualDistribution(resultsObj)` plots the distribution of the residuals.

Input Arguments

`resultsObj` — Estimation results
`NLMEResults` object

Estimation results, specified as an `NLMEResults object`, which contains estimation results from running `sbiofitmixed`.

Version History

Introduced in R2014a

See Also

`NLMEResults object` | `sbiofitmixed`

predict

Simulate and evaluate fitted SimBiology model

Syntax

```
[ynew,parameterEstimates]= predict(resultsObj)
[ynew,parameterEstimates]= predict(resultsObj,data,dosing)
[ynew,parameterEstimates]= predict(resultsObj,data,dosing,'Variants',v)
```

Description

`[ynew,parameterEstimates]= predict(resultsObj)` returns simulation results `ynew` and parameter estimates `parameterEstimates` of a fitted SimBiology model.

`[ynew,parameterEstimates]= predict(resultsObj,data,dosing)` returns simulation results `ynew` and estimated parameter values `parameterEstimates` from evaluating the fitted SimBiology model using the specified `data` and `dosing` information.

During simulations, `predict` uses the parameter values in the `resultsObj.ParameterEstimates` property. Use this method when you want to evaluate the fitted model and predict responses using new data and/or dosing information.

`[ynew,parameterEstimates]= predict(resultsObj,data,dosing,'Variants',v)` simulates the fitted model and applies the specified variants to each simulation.

Examples

Evaluate Fitted SimBiology Model

This example uses the yeast heterotrimeric G protein model and experimental data reported by [1]. For details about the model, see the **Background** section in “Parameter Scanning, Parameter Estimation, and Sensitivity Analysis in the Yeast Heterotrimeric G Protein Cycle”.

Load the G protein model.

```
sbioloadproject gprotein
```

Store the experimental data containing the time course for the fraction of active G protein.

```
time = [0 10 30 60 110 210 300 450 600]';
GaFracExpt = [0 0.35 0.4 0.36 0.39 0.33 0.24 0.17 0.2]';
```

Map the appropriate model component to the experimental data. In other words, indicate which species in the model corresponds to which response variable in the data. In this example, map the model parameter `GaFrac` to the experimental data variable `GaFracExpt` from `grpData`.

```
responseMap = 'GaFrac = GaFracExpt';
```

Create a `groupedData` object based on the experimental data.

```
tbl = table(time,GaFracExpt);
grpData = groupedData(tbl);
```

Use an `estimatedInfo` object to define the model parameter `kGd` as a parameter to be estimated.

```
estimatedParam = estimatedInfo('kGd');
```

Perform the parameter estimation.

```
fitResult = sbiofit(m1,grpData,responseMap,estimatedParam);
```

View the estimated parameter value of `kGd`.

```
fitResult.ParameterEstimates
```

```
ans=1×3 table
     Name      Estimate    StandardError
    _______    ________    _____________

    {'kGd'}    0.11307      3.4439e-05
```

Suppose you want to simulate the fitted model using different output times than those in the training data. You can use the `predict` method to do so.

Create a new variable `T` with different output times.

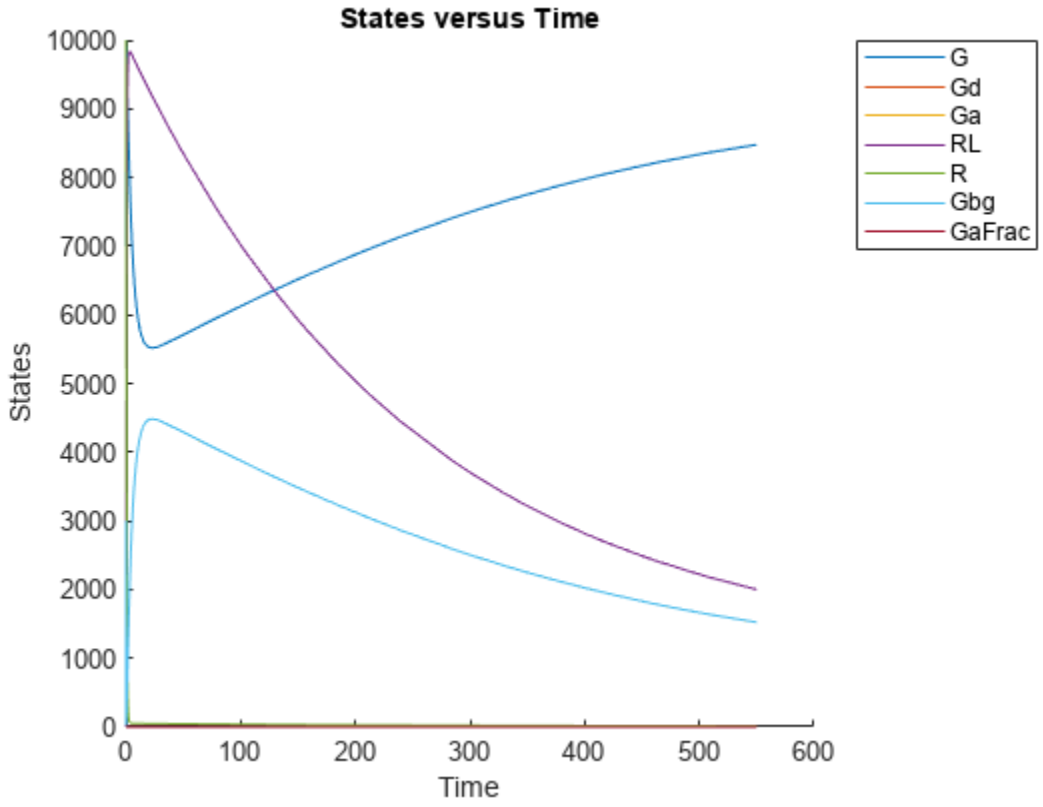
```
T = [0;10;50;80;100;150;300;350;400;450;500;550];
```

Use the `predict` method to simulate the fitted model on the new time points. No dosing was specified when you first ran `sbiofit`. Hence, you cannot use any dosing information with the `predict` method, and an empty array must be specified as the third input argument.

```
ynew = predict(fitResult,T,[]);
```

Plot the simulated data with the new output times.

```
sbioplot(ynew);
```



Estimate Category-Specific PK Parameters

This example shows how to estimate category-specific (such as young versus old, male versus female) PK parameters using the profile data from multiple individuals using a two-compartment model. The parameters to estimate are the volumes of central and peripheral compartment, the clearance, and intercompartmental clearance.

The synthetic data used in this example contains the time course of plasma concentrations of multiple individuals after a bolus dose (100 mg) measured at different times for both central and peripheral compartments. It also contains categorical variables, namely *Sex* and *Age*.

```
clear
load('sd5_302RAgeSex.mat');
```

Convert the data set to a groupedData object, which is the required data format for the fitting function sbiofit. A groupedData object allows you to set independent variable and group variable names (if they exist). Set the units of the ID, Time, CentralConc, PeripheralConc, Age, and Sex variables. The units are optional and only required for the UnitConversion feature, which automatically converts matching physical quantities to one consistent unit system.

```
gData = groupedData(data);
gData.Properties.VariableUnits = {'','hour','milligram/liter','milligram/liter','',''};
```

The IndependentVariableName and GroupVariableName properties have been automatically set to the Time and ID variables of the data.

```
gData.Properties
```

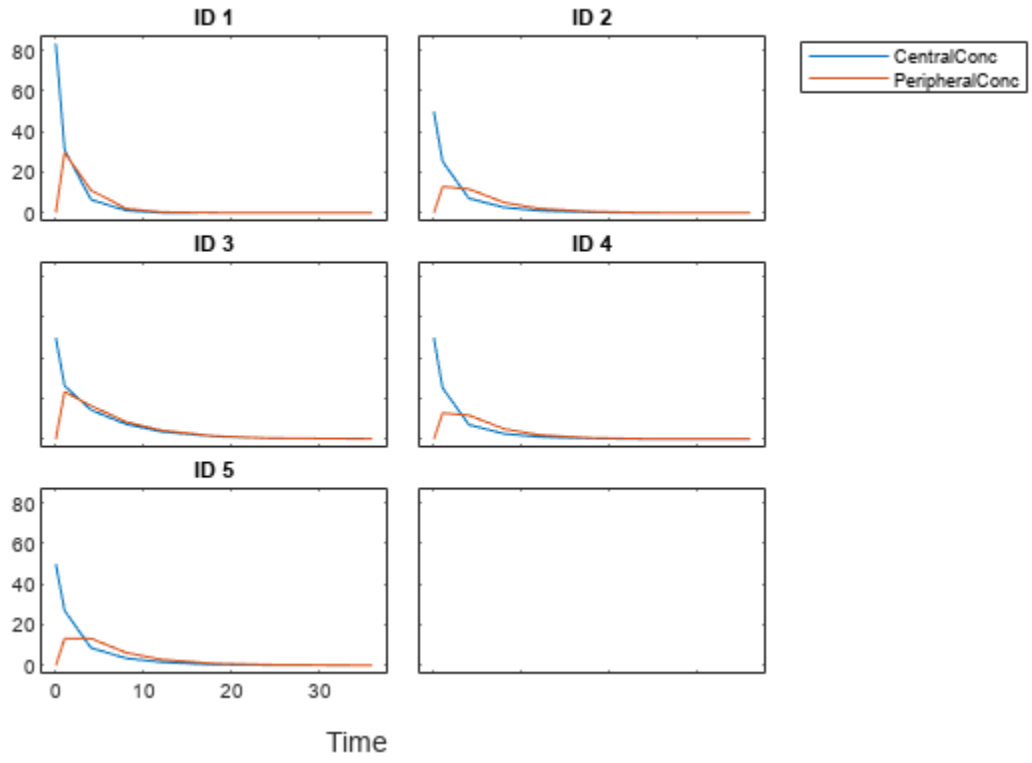
```
ans = struct with fields:
                Description: ''
                   UserData: []
             DimensionNames: {'Row'  'Variables'}
              VariableNames: {'ID'  'Time'  'CentralConc'  'PeripheralConc'  'Sex'  'Age'}
       VariableDescriptions: {}
              VariableUnits: {''  'hour'  'milligram/liter'  'milligram/liter'  ''  ''}
         VariableContinuity: []
                   RowNames: {}
          CustomProperties: [1x1 matlab.tabular.CustomProperties]
         GroupVariableName: 'ID'
    IndependentVariableName: 'Time'
```

For illustration purposes, use the first five individual data for training and the 6th individual data for testing.

```
trainData = gData([gData.ID < 6],:);
testData  = gData([gData.ID == 6],:);
```

Display the response data for each individual in the training set.

```
sbiotrellis(trainData,'ID','Time',{'CentralConc','PeripheralConc'});
```



Use the built-in PK library to construct a two-compartment model with infusion dosing and first-order elimination where the elimination rate depends on the clearance and volume of the central compartment. Use the configset object to turn on unit conversion.

```
pkmd                                    = PKModelDesign;
pkc1                                    = addCompartment(pkmd,'Central');
pkc1.DosingType                         = 'Bolus';
pkc1.EliminationType                    = 'linear-clearance';
pkc1.HasResponseVariable                = true;
pkc2                                    = addCompartment(pkmd,'Peripheral');
model                                   = construct(pkmd);
configset                               = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
```

Assume every individual receives a bolus dose of 100 mg at time = 0.

```
dose             = sbiodose('dose','TargetName','Drug_Central');
dose.StartTime   = 0;
dose.Amount      = 100;
dose.AmountUnits = 'milligram';
dose.TimeUnits   = 'hour';
```

The data contains measured plasma concentration in the central and peripheral compartments. Map these variables to the appropriate model components, which are Drug_Central and Drug_Peripheral.

```
responseMap = {'Drug_Central = CentralConc','Drug_Peripheral = PeripheralConc'};
```

Specify the volumes of central and peripheral compartments Central and Peripheral, intercompartmental clearance Q12, and clearance Cl_Central as parameters to estimate. The estimatedInfo object lets you optionally specify parameter transforms, initial values, and parameter bounds. Since both Central and Peripheral are constrained to be positive, specify a log-transform for each parameter.

```
paramsToEstimate    = {'log(Central)', 'log(Peripheral)', 'Q12', 'Cl_Central'};
estimatedParam      = estimatedInfo(paramsToEstimate,'InitialValue',[1 1 1 1]);
```

Use the 'CategoryVariableName' property of the estimatedInfo object to specify which category to use during fitting. Use 'Sex' as the group to fit for the clearance Cl_Central and Q12 parameters. Use 'Age' as the group to fit for the Central and Peripheral parameters.

```
estimatedParam(1).CategoryVariableName = 'Age';
estimatedParam(2).CategoryVariableName = 'Age';
estimatedParam(3).CategoryVariableName = 'Sex';
estimatedParam(4).CategoryVariableName = 'Sex';
categoryFit = sbiofit(model,trainData,responseMap,estimatedParam,dose)
```

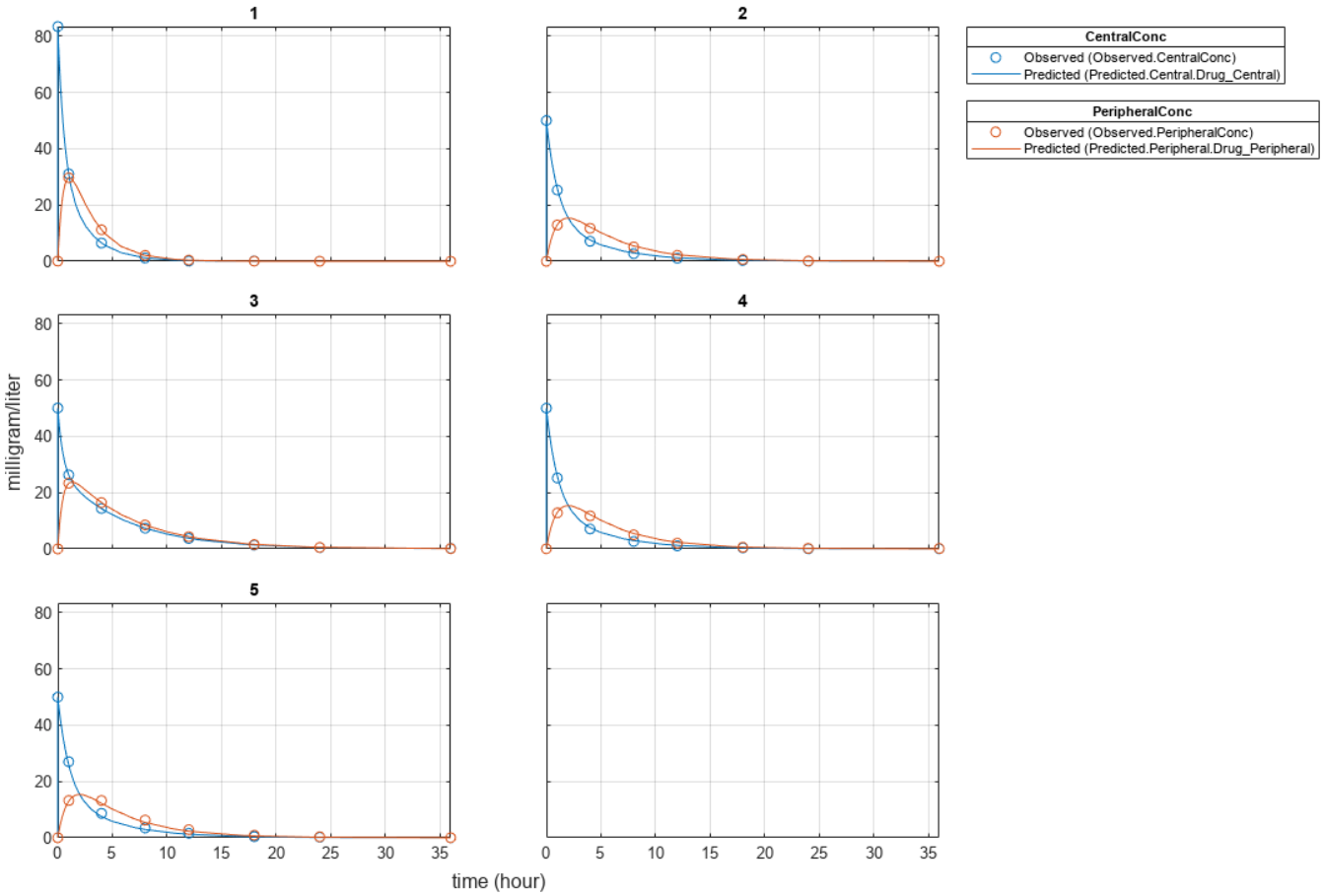
```
categoryFit =
  OptimResults with properties:

                  ExitFlag: 1
                    Output: [1x1 struct]
                 GroupName: []
                      Beta: [8x5 table]
        ParameterEstimates: [20x6 table]
                         J: [40x8x2 double]
                      COVB: [8x8 double]
          CovarianceMatrix: [8x8 double]
                         R: [40x2 double]
```

```
                    MSE: 0.1047
                    SSE: 7.5349
                Weights: []
          LogLikelihood: -19.0159
                    AIC: 54.0318
                    BIC: 73.0881
                    DFE: 72
          DependentFiles: {1x3 cell}
                   Data: [40x6 groupedData]
EstimatedParameterNames: {'Central'  'Peripheral'  'Q12'  'Cl_Central'}
          ErrorModelInfo: [1x3 table]
      EstimationFunction: 'lsqnonlin'
```

When fitting by category (or group), sbiofit always returns one results object, not one for each category level. This is because both male and female individuals are considered to be part of the same optimization using the same error model and error parameters, similarly for the young and old individuals.

Plot the category-specific estimated results. For the Cl_Central and Q12 parameters, all males had the same estimates, and similarly for the females. For the Central and Peripheral parameters, all young individuals had the same estimates, and similarly for the old individuals.

```
plot(categoryFit);
```



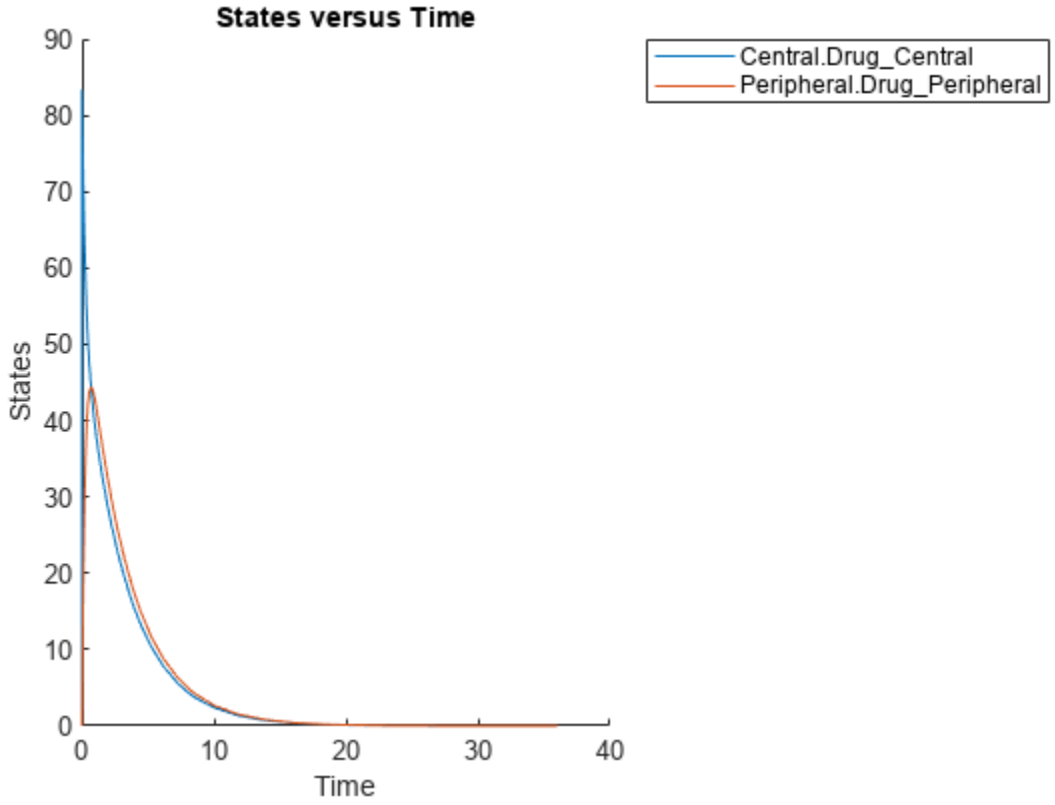
As for testing purposes, simulate the responses of the 6th individual who is an old male. Since you have estimated one set of parameters for the Age category (young versus old), and another set for Sex category (male versus female), you can simulate the responses of an old male even though there is no such individual in the training data.

Use the predict method to simulate the responses. ynew contains simulation data and paramestim contains parameter estimates used during simulation.

```
[ynew,paramestim] = predict(categoryFit,testData,dose);
```

Plot the simulated responses of the old male.

```
sbioplot(ynew);
```



The paramestim variable contains the estimated parameters used by the predict method. The parameter estimates for corresponding categories were obtained from the categoryFit.ParameterEstimates property. Specifically, Central and Peripheral parameter estimates are obtained from the Old group, and Q12 and Cl_Central parameter estimates are obtained from the Male group.

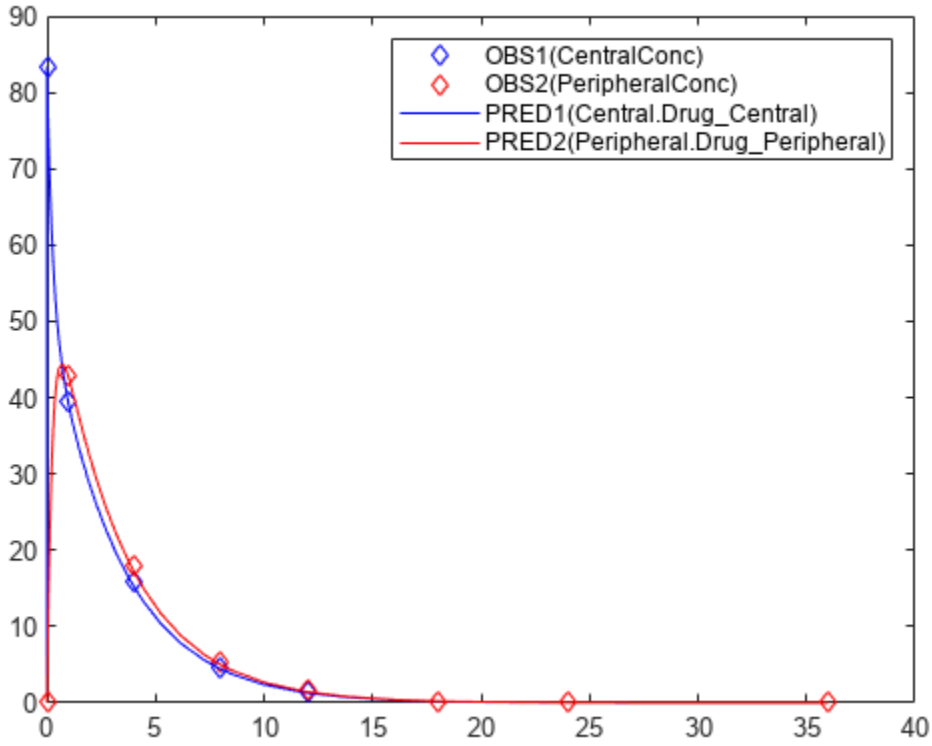
```
paramestim
```

```
paramestim=4×6 table
        Name          Estimate    StandardError    Group    CategoryVariableName    CategoryValue
    ______________    ________    _____________    _____    ____________________    _____________

    {'Central'   }     1.1993       0.0046483        6            {'Age'}               Old
```

```
    {'Peripheral'}    0.55195        0.015098        6            {'Age'}              Old
    {'Q12'       }     1.4969        0.074321        6            {'Sex'}              Male
    {'Cl_Central'}    0.56363       0.0072862        6            {'Sex'}              Male
```

Overlay the experimental results on the simulated data.

```
figure;
plot(testData.Time,testData.CentralConc,'LineStyle','none','Marker','d','MarkerEdgeColor','b');
hold on
plot(testData.Time,testData.PeripheralConc,'LineStyle','none','Marker','d','MarkerEdgeColor','r'
plot(ynew.Time,ynew.Data(:,1),'b');
plot(ynew.Time,ynew.Data(:,2),'r');
hold off
legend({'OBS1(CentralConc)','OBS2(PeripheralConc)',...
        'PRED1(Central.Drug\_Central)','PRED2(Peripheral.Drug\_Peripheral)'});
```



Input Arguments

`resultsObj` — Estimation results

`OptimResults` object | `NLINResults` object

Estimation results, specified as an `OptimResults object` or `NLINResults object`, which contains estimation results returned by `sbiofit`. It must be a scalar object.

data — Output times or grouped data
vector | cell array of vectors | groupedData object

Output times or grouped data, specified as a vector, or cell array of vectors of output times, or groupedData object.

If it is a vector of time points, predict simulates the model with new time points using the parameter estimates from the results object resultsObj.

If it is a cell array of vectors of time points, predict simulates the model *n* times using the output times from each time vector, where *n* is the length of data.

If it is a groupedData object, it must have an independent variable such as Time. It must also have a group variable if the training data used for fitting has such variable. You can use a groupedData object to query different combinations of categories if the resultsObj contains parameter estimates for each category. predict simulates the model for each group with the specified categories. For instance, suppose you have a set of parameter estimates for sex category (males versus females), and age category (young versus old) in your training data. You can use predict to simulate the responses of an old male (or any other combination) although such patient may not exist in the training data.

If the resultsObj is from estimating category-specific parameters, data must be a groupedData object.

Note If UnitConversion is turned on for the underlying SimBiology model that was used for fitting and data is a groupedData object, data must specify valid variable units via data.Properties.VariableUnits property. If it is a numeric vector or cell array of vectors of time points, predict uses the model's TimeUnits.

dosing — Dosing information
[] | {} | 2-D matrix of dose objects | cell vector of dose objects

Dosing information, specified as empty [] or {}, 2-D matrix or cell vector of SimBiology dose objects (ScheduleDose object or RepeatDose object).

If dosing is empty, no doses are applied during simulation, even if the model has active doses.

For a matrix of dose objects, it must have a single row or one row per group in the input data. If it has a single row, the same doses are applied to all groups during simulation. If it has multiple rows, each row is applied to a separate group, in the same order as the groups appear in the input data. Multiple columns are allowed so that you can apply multiple dose objects to each group.

For a cell vector of doses, it must have one element or one element per group in the input data. Each element must be [] or a vector of doses. Each element of the cell is applied to a separate group, in the same order as the groups appear in the input data.

In addition to manually constructing dose objects using sbiodose, if the input groupedData object has dosing information, you can use the createDoses method to construct doses.

Dose objects of the dosing input must be consistent with the original dosing data used with sbiofit. The objects must have the same values for dose properties (such as TargetName) or must be parameterized in the same way as the original dosing data. For instance, suppose that the original dosing matrix has two columns of doses, where the doses in the first column target species *x* and

those in the second column target species *y*. Then `dosing` must have doses in the first column targeting species *x* and those in the second column targeting species *y*. A parameterized dose example is as follows. Suppose that the `Amount` property of a dose used in the original `sbiofit` call is parameterized to a model-scoped parameter `'A'`. All doses for the corresponding group (column) in the `dosing` matrix input must have the `Amount` property parameterized to `'A'`.

The number of rows in the `dosing` matrix or number of elements in the `dosing` cell vector and the number of groups or output time vectors in `data` determine the total number of simulation results in the output `ynew`. For details, see the table in the `ynew` argument description.

Note If `UnitConversion` is turned on for the underlying SimBiology model that was used for fitting, `dosing` must specify valid amount and time units.

---

v — Variants to apply

`[]` | `{}` | 2-D matrix of variants | cell vector of variants

Variants to apply, specified as an empty array (`[]`, `{}`), 2-D matrix or cell vector of variant objects.

If you do not specify this argument, the function has the following behavior depending on whether the second input argument (`data`) is specified also or not.

- If `data` is not specified, the function applies the group-specific variants from the original call to `sbiofit`.
- If `data` is a vector or cell array of output times, the function does not apply the group-specific variants.
- If `data` is a `groupedData` object, the function applies variants only to groups whose group identifier matches a group identifier in the original training data that was used in the call to `sbiofit`.

Note

- The baseline variants that were specified by the “variants” on page 1-0 positional input argument in the original call to `sbiofit` are always applied to the model, and they are applied before any group-specific variants.
- If there are no baseline variants, that is, you did not specify the `variants` input when calling `sbiofit`, the `predict` function still applies the model active variants if there are any.

If the argument value is `[]` or `{}`, the function applies no group-specific variants.

If it is a matrix of variants, it must have either one row or one row per group. Each row is applied to a separate group, in the same order as the groups appear in `data` or `dosing`. If it has a single row, the same variants are applied to all groups during simulation. If there are multiple columns, the variants are applied in order from the first column to the last.

If it is a cell vector of variant objects, the number of cells must be one or must match the number of groups in the input data. Each element must be `[]` or a vector of variants. If there is a single cell containing a vector of variants, they are applied to all simulations. If there are multiple cells, the variants in the *i*th cell are applied to the simulation of the *i*th group.

The function defines the number of groups by examining the `data`, and `dosing` input arguments.

- `data` can have `1` or *N* groups.
- If `data` and `dosing` arguments are not specified, then the default data and dosing are determined as follows:
  - For unpooled fits, they are the data and dosing for the single group associated with that fit results.
  - For all other fits, they are the entire set of data and dosing associated with the call to `sbiofit`.

Output Arguments

`ynew` — Simulation results

vector of `SimData` objects

Simulation results, returned as a vector of `SimData` objects. The states reported in `ynew` are the states that were included in the `responseMap` input argument of `sbiofit` as well as any other states listed in the `StatesToLog` property of the runtime options (`RuntimeOptions`) of the SimBiology model.

The total number of simulation results in `ynew` depends on the number of groups or output time vectors in `data` and the number of rows in the `dosing` matrix.

Number of groups or output time vectors in `data`	Number of rows in the `dosing` matrix	Simulation results
`1`	`0`, that is, `dosing` is empty `[]`	The total number of `SimData` objects in `ynew` is 1. No doses are applied during simulation.
`1`	`1`	The total number of `SimData` objects in `ynew` is 1. The given row of doses is applied during the simulation.
`1`	*N*	The total number of `SimData` objects in `ynew` is *N*. Each row of `dosing` is applied to each simulation.
N	`0`, that is, `dosing` is empty `[]`	The total number of `SimData` objects in `ynew` is *N*. No doses are applied during simulation.
N	`1`	The total number of `SimData` objects in `ynew` is *N*. The same row of doses is applied to each simulation.

Number of groups or output time vectors in `data`	Number of rows in the `dosing` matrix	Simulation results
N	*N*	The total number of `SimData` objects in `ynew` is *N*. Each row of `dosing` is applied to a separate group, in the same order that groups appear in `data`.
M	*N*	The function throws an error when $M \neq N$.

`parameterEstimates` — Estimated parameter values
table

Estimated parameter values, returned as a table. This is identical to `resultsObj.ParameterEstimates` property. The `predict` method uses these parameter values during simulation.

Version History

Introduced in R2014a

References

[1] Yi, T-M., Kitano, H., and Simon, M. (2003). A quantitative characterization of the yeast heterotrimeric G protein cycle. PNAS. 100, 10764–10769.

See Also

`NLINResults object` | `OptimResults object` | `sbiofit`

predict

Simulate and evaluate fitted SimBiology model

Syntax

```
[ynew,parameterEstimates] = predict(resultsObj)
[ynew,parameterEstimates] = predict(resultsObj,data,dosing)
[ynew,parameterEstimates] = predict( ___ ,Name,Value)
```

Description

`[ynew,parameterEstimates] = predict(resultsObj)` returns simulation results `ynew` from evaluating the fitted SimBiology model. The estimated parameter values `parameterEstimates` used to compute `ynew` are from the original fit by `sbiofitmixed`.

`[ynew,parameterEstimates] = predict(resultsObj,data,dosing)` returns simulation results `ynew` from evaluating the fitted SimBiology model by using the specified `data` and `dosing` information.

`[ynew,parameterEstimates] = predict( ___ ,Name,Value)` uses additional options specified by one or more name-value arguments.

Tip Use this method to get model responses at specific time points or to predict model responses using different covariate data and dosing information.

Examples

Perform Nonlinear Mixed-Effects Estimation

Estimate nonlinear mixed-effects parameters using clinical pharmacokinetic data collected from 59 infants. Evaluate the fitted model given new data or dosing information.

Load Data

This example uses data collected on 59 preterm infants given phenobarbital during the first 16 days after birth [1]. `ds` is a table containing the concentration-time profile data and covariate information for each infant (or group).

```
load pheno.mat ds
```

Convert to groupedData

Convert the data to the groupedData format for parameter estimation.

```
data = groupedData(ds);
```

Display the first few rows of `data`.

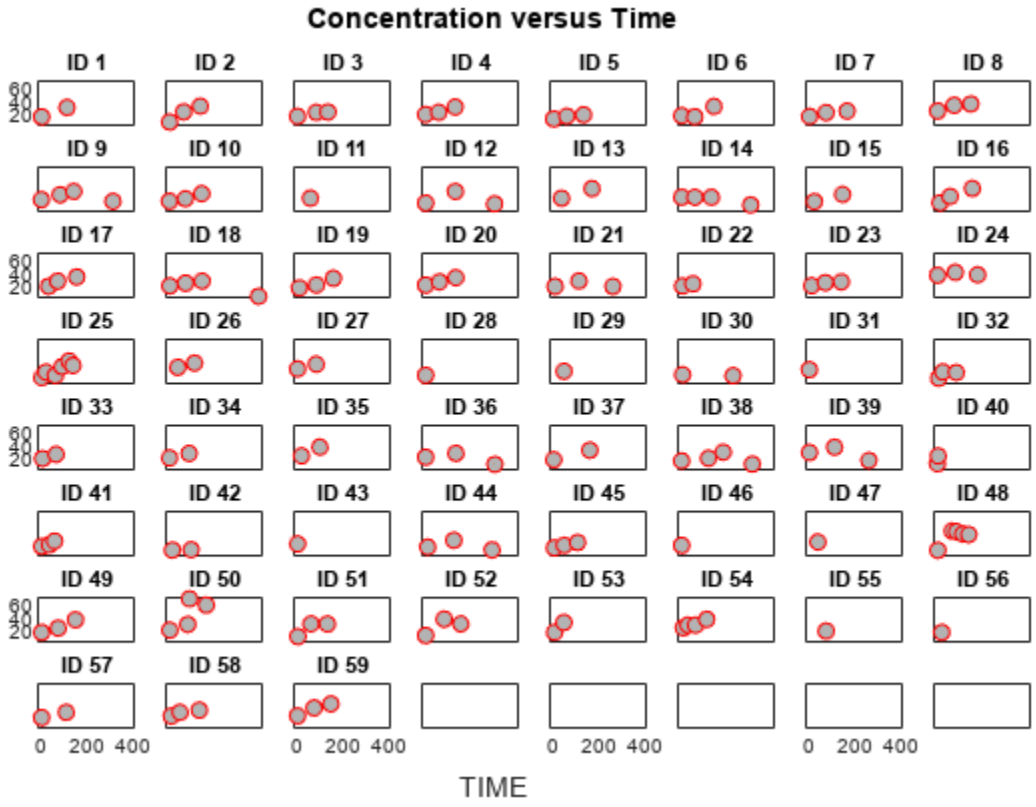
```
data(1:5,:)
```

```
ans =

  5x6 groupedData

    ID    TIME    DOSE    WEIGHT    APGAR    CONC
    __    ____    ____    ______    _____    ____

    1        0      25       1.4        7      NaN
    1        2     NaN       1.4        7     17.3
    1     12.5     3.5       1.4        7      NaN
    1     24.5     3.5       1.4        7      NaN
    1       37     3.5       1.4        7      NaN
```

Visualize Data

Display the data in a trellis plot.

```
t = sbiotrellis(data, 'ID', 'TIME', 'CONC', 'marker', 'o',...
       'markerfacecolor', [.7 .7 .7], 'markeredgecolor', 'r', ...
       'linestyle', 'none');
t.plottitle = 'Concentration versus Time';
```



Create a One-Compartment PK Model

Create a simple one-compartment PK model, with bolus dose administration and linear clearance elimination, to fit the data.

```
pkmd = PKModelDesign;
addCompartment(pkmd,'Central','DosingType','Bolus',...
                    'EliminationType','linear-clearance',...
                    'HasResponseVariable',true,'HasLag',false);
onecomp = pkmd.construct;
```

Map model species to response data.

```
responseMap = 'Drug_Central = CONC';
```

Define Estimated Parameters

The parameters to estimate in this model are the volume of the central compartment (`Central`) and the clearance rate (`Cl_Central`). `sbiofitmixed` calculates fixed and random effects for each parameter. The underlying algorithm computes normally distributed random effects, which might violate constraints for biological parameters that are always positive, such as volume and clearance. Therefore, specify a transform for the estimated parameters so that the transformed parameters follow a normal distribution. The resulting model is

$$log(V_i) = log(\phi_{V,i}) = \theta_V + \eta_{V,i}$$

and

$$log(Cl_i) = log(\phi_{Cl,i}) = \theta_{Cl} + \eta_{Cl,i},$$

where θ, *eta*, and ϕ are the fixed effects, random effects, and estimated parameter values respectively, calculated for each infant (group) i. Some arbitrary initial estimates for V (volume of central compartment) and Cl (clearance rate) are used here in the absence of better empirical data.

```
estimatedParams = estimatedInfo({'log(Central)','log(Cl_Central)'},'InitialValue',[1 1]);
```

Define Dosing

All infants were given the drug, represented by the `Drug_Central` species, where the dosing schedule varies among infants. The amount of drug is listed in the data variable DOSE. You can automatically generate dose objects from the data and use them during fitting. In this example, `Drug_Central` is the target species that receives the dose.

```
sampleDose = sbiodose('sample','TargetName','Drug_Central');
doses = createDoses(data,'DOSE','',sampleDose);
```

Fit the Model

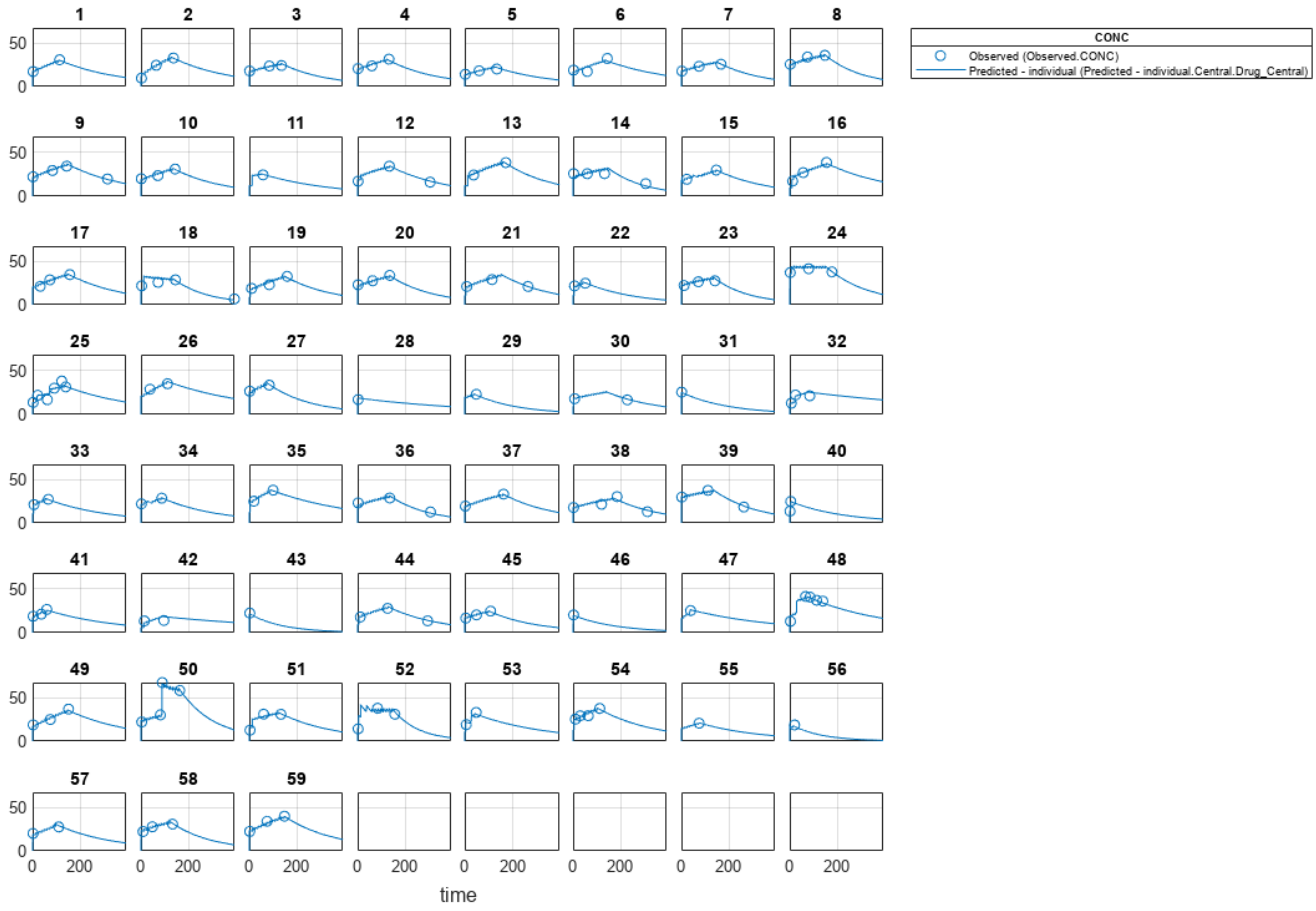
Use `sbiofitmixed` to fit the one-compartment model to the data.

```
nlmeResults = sbiofitmixed(onecomp,data,responseMap,estimatedParams,doses,'nlmefit');
```

Visualize Results

Visualize the fitted results using individual-specific parameter estimates.

```
plot(nlmeResults,'ParameterType','individual');
```



Use New Dosing Data to Simulate the Fitted Model

Suppose you want to predict how infants 1 and 2 would have responded under different dosing amounts. You can predict their responses as follows.

Create new dose objects with new dose amounts.

```
dose1 = doses(1);
dose1.Amount = dose1.Amount*2;
dose2 = doses(2);
dose2.Amount = dose2.Amount*1.5;
```

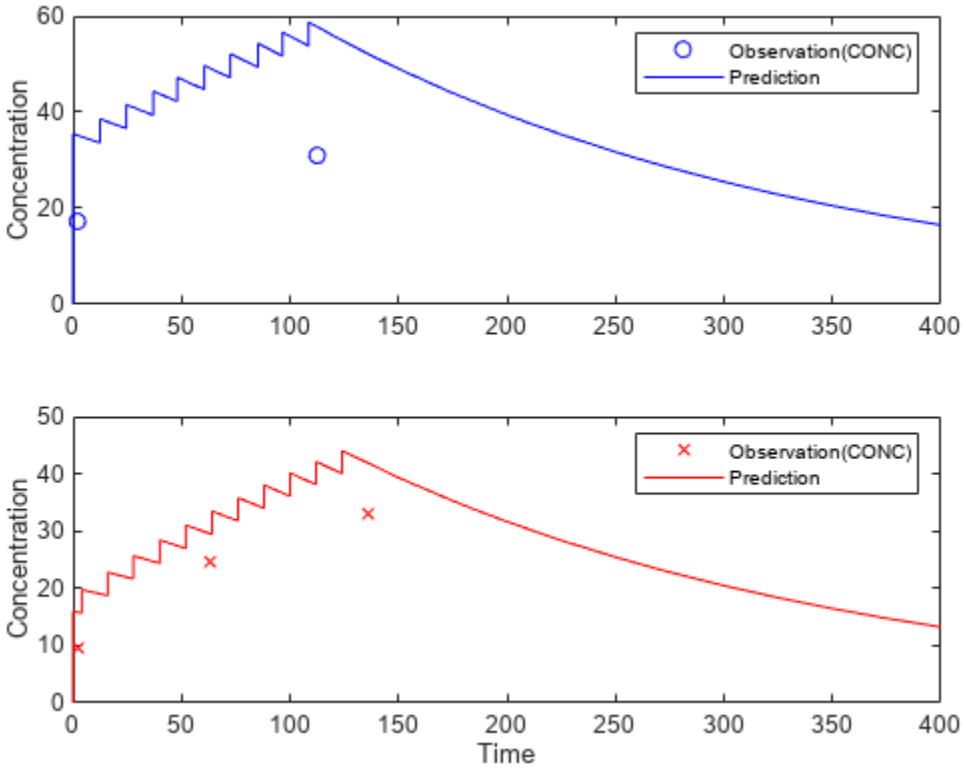
Use the `predict` function to evaluate the fitted model using the new dosing data. If you want response predictions at particular times, provide the new output time vector. Use the 'ParameterType' option to specify individual or population parameters to use. By default, `predict` uses the population parameters when you specify output times.

```
timeVec = [0:25:400];
newResults = predict(nlmeResults,timeVec,[dose1;dose2],'ParameterType','population');
```

Visualize the predicted responses while overlapping the experimental data for infants 1 and 2.

```
figure;
subplot(2,1,1)
plot(data.TIME(data.ID == 1),data.CONC(data.ID == 1),'bo')
```

```
hold on
plot(newResults(1).Time,newResults(1).Data,'b')
hold off
ylabel('Concentration')
legend('Observation(CONC)','Prediction')
subplot(2,1,2)
plot(data.TIME(data.ID == 2),data.CONC(data.ID == 2),'rx')
hold on
plot(newResults(2).Time,newResults(2).Data,'r')
hold off
legend('Observation(CONC)','Prediction')
ylabel('Concentration')
xlabel('Time')
```



Create a Covariate Model for the Covariate Dependencies

Suppose there is a correlation between volume and weight, and possibly volume and APGAR score. Consider the effect of weight by modeling two of these covariate dependencies: the volume of central (`Central`) and the clearance rate (`Cl_Central`) vary with weight. The model becomes

$$log(V_i) = log(\phi_{V,i}) = \theta_V + \theta_{V/weight} * weight_i + \eta_{V,i}$$

and

$$log(Cl_i) = log(\phi_{Cl,i}) = \theta_{Cl} + \theta_{Cl/weight} * weight_i + \eta_{Cl,i}$$

Use the `CovariateModel` object to define the covariate dependencies. For details, see “Specify a Covariate Model”.

```
covModel = CovariateModel;
covModel.Expression = ({'Central = exp(theta1 + theta2*WEIGHT + eta1)',...
                        'Cl_Central = exp(theta3 + theta4*WEIGHT + eta2)'});
```

Use `constructDefaultInitialEstimate` to create an `initialEstimates` struct.

```
initialEstimates = covModel.constructDefaultFixedEffectValues;
```

Use the `FixedEffectNames` property to display the thetas (fixed effects) defined in the model.

```
covModel.FixedEffectNames
```

```
ans = 4x1 cell
    {'theta1'}
    {'theta3'}
    {'theta2'}
    {'theta4'}
```

Use the `FixedEffectDescription` property to show the descriptions of corresponding fixed effects (thetas) used in the covariate expression. For example, `theta2` is the fixed effect for the weight covariate that correlates with the volume (`Central`), denoted as 'Central/WEIGHT'.

```
disp('Fixed Effects Description:');
```

```
Fixed Effects Description:
```

```
disp(covModel.FixedEffectDescription);
```

```
    {'Central'          }
    {'Cl_Central'       }
    {'Central/WEIGHT'   }
    {'Cl_Central/WEIGHT'}
```

Set the initial guesses for the fixed-effect parameter values for `Central` and `Cl_Central` using the values estimated from fitting the base model.

```
initialEstimates.theta1 = nlmeResults.FixedEffects.Estimate(1);
initialEstimates.theta3 = nlmeResults.FixedEffects.Estimate(2);
covModel.FixedEffectValues = initialEstimates;
```

Fit the Model

```
nlmeResults_cov = sbiofitmixed(onecomp,data,responseMap,covModel,doses,'nlmefit');
```

Display Fitted Parameters and Covariances

```
disp('Estimated Fixed Effects:');
```

```
Estimated Fixed Effects:
```

```
disp(nlmeResults_cov.FixedEffects);
```

```
       Name            Description          Estimate    StandardError
    ___________    ____________________    ________    _____________

    {'theta1'}    {'Central'          }    -0.45664      0.078933
```

```
    {'theta3'}    {'Cl_Central'       }     -5.9519        0.1177
    {'theta2'}    {'Central/WEIGHT'   }     0.52948      0.047342
    {'theta4'}    {'Cl_Central/WEIGHT'}     0.61954      0.071386
```

```
disp('Estimated Covariance Matrix:');
```

```
Estimated Covariance Matrix:
```

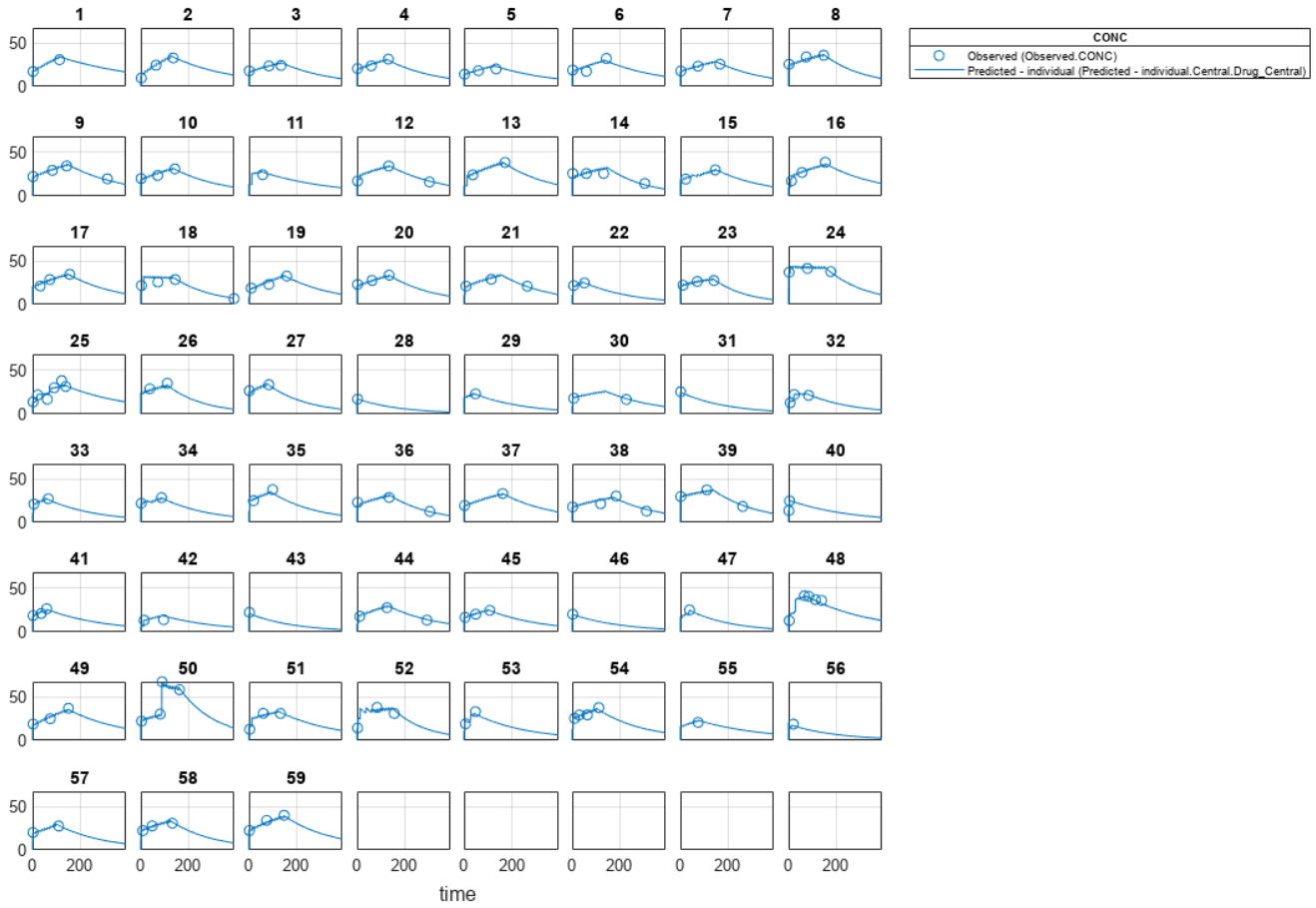
```
disp(nlmeResults_cov.RandomEffectCovarianceMatrix);
```

```
              eta1         eta2
            _______    ________

    eta1    0.046503           0
    eta2           0    0.041609
```

Visualize Results

Visualize the fitted results using individual-specific parameter estimates.

```
plot(nlmeResults_cov,'ParameterType','individual');
```



Use New Covariate Data to Evaluate the Fitted Model

Suppose you want to explore the responses of infants 1 and 2 using different covariate data, namely `WEIGHT`. You can do this by specifying the new `WEIGHT` data. The `ID` variable of the data corresponds to individual infants.

```
newData = data(data.ID == 1 | data.ID == 2,:);
newData.WEIGHT(newData.ID == 1) = 1.3;
newData.WEIGHT(newData.ID == 2) = 1.4;
```

Simulate the responses of infants 1 and 2 using the new covariate data.

```
[newResults_cov, newEstimates] = predict(nlmeResults_cov,newData,[dose1;dose2]);
```

`newEstimates` contains the updated parameter estimates for each individual (infants 1 and 2) after the model is reevaluated using the new covariate data.

```
newEstimates
```

```
newEstimates=4×3 table
    Group         Name         Estimate
    _____    _____________    _________

      1      {'Central'   }       2.5596
      1      {'Cl_Central'}    0.0065965
      2      {'Central'   }       1.7123
      2      {'Cl_Central'}    0.0064806
```

Compare to the estimated values from the original fit using the old covariate data.

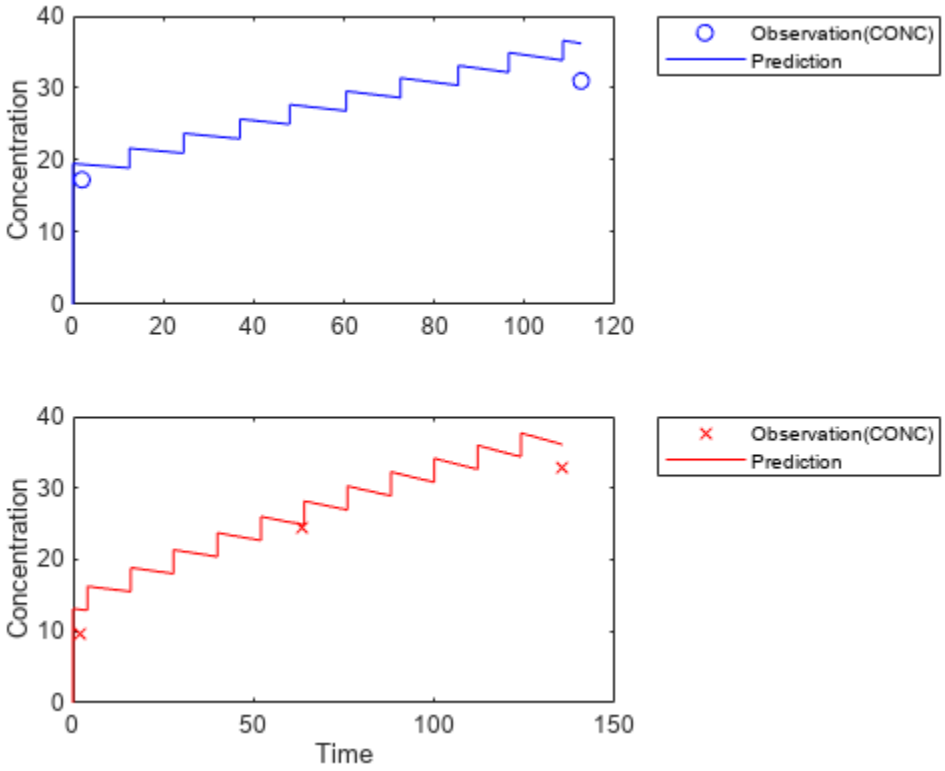
```
nlmeResults_cov.IndividualParameterEstimates( ...
            nlmeResults_cov.IndividualParameterEstimates.Group == '1' | ...
            nlmeResults_cov.IndividualParameterEstimates.Group == '2',:)
```

```
ans=4×3 table
    Group         Name         Estimate
    _____    _____________    _________

      1      {'Central'   }       2.6988
      1      {'Cl_Central'}    0.0070181
      2      {'Central'   }       1.8054
      2      {'Cl_Central'}    0.0068948
```

Visualize the new simulation results together with the experimental data for infant 1 and 2.

```
figure;
subplot(2,1,1);
plot(data.TIME(data.ID == 1),data.CONC(data.ID == 1),'bo')
hold on
plot(newResults_cov(1).Time,newResults_cov(1).Data,'b')
hold off
ylabel('Concentration')
legend('Observation(CONC)','Prediction','Location','NorthEastOutside')
subplot(2,1,2)
plot(data.TIME(data.ID == 2),data.CONC(data.ID == 2),'rx')
hold on
plot(newResults_cov(2).Time,newResults_cov(2).Data,'r')
```

```
hold off
legend('Observation(CONC)','Prediction','Location','NorthEastOutside')
ylabel('Concentration')
xlabel('Time')
```



References

[1] Grasela, T. H. Jr., and S. M. Donn. "Neonatal population pharmacokinetics of phenobarbital derived from routine clinical data." *Dev Pharmacol Ther* 1985:8(6). 374-83.

Input Arguments

`resultsObj` — Estimation results

scalar `NLMEResults` object

Estimation results, specified as a scalar `NLMEResults object`, which contains nonlinear mixed-effects estimation results returned by `sbiofitmixed`.

`data` — Grouped data or output times

`groupedData` object | vector | cell array of vectors

Grouped data or output times, specified as a `groupedData object`, vector, or cell array of vectors of output times.

If `data` is a `groupedData` object, it must have both group labels and output times specified. The group labels can refer to new groups or existing groups from the original fit. If the mixed-effects

model from the original fit (returned by `sbiofitmixed`) uses covariates, the `groupedData` object must also contain the covariate data with the same labels for the covariates (`CovariateLabels` property) specified in the original `CovariateModel` object.

By default, individual parameter estimates are used for simulating groups from the original fit, while population parameters are used for new groups, if any. See the `value` argument description for details.

The total number of simulation results in the output `ynew` depends on the number of groups or output time vectors in `data` and the number of rows in the `dosing` matrix. For details, see the table in the `ynew` argument description.

`dosing` — Dosing information

`[]` | `{}` | 2-D matrix of dose objects | cell vector of dose objects

Dosing information, specified as empty `[]` or `{}`, 2-D matrix or cell vector of SimBiology dose objects (`ScheduleDose object` or `RepeatDose object`).

If `dosing` is empty, no doses are applied during simulation, even if the model has active doses.

For a matrix of dose objects, it must have a single row or one row per group in the input data. If it has a single row, the same doses are applied to all groups during simulation. If it has multiple rows, each row is applied to a separate group, in the same order as the groups appear in the input data. Multiple columns are allowed so that you can apply multiple dose objects to each group.

For a cell vector of doses, it must have one element or one element per group in the input data. Each element must be `[]` or a vector of doses. Each element of the cell is applied to a separate group, in the same order as the groups appear in the input data.

In addition to manually constructing dose objects using `sbiodose`, if the input `groupedData` object has dosing information, you can use the `createDoses` method to construct doses.

Dose objects of the `dosing` input must be consistent with the original dosing data used with `sbiofitmixed`. The objects must have the same values for dose properties (such as `TargetName`) or must be parameterized in the same way as the original dosing data. For instance, suppose that the original dosing matrix has two columns of doses, where the doses in the first column target species *x* and those in the second column target species *y*. Then `dosing` must have doses in the first column targeting species *x* and those in the second column targeting species *y*. A parameterized dose example is as follows. Suppose that the `Amount` property of a dose used in the original `sbiofitmixed` call is parameterized to a model-scoped parameter `'A'`. All doses for the corresponding group (column) in the `dosing` matrix input must have the `Amount` property parameterized to `'A'`.

The number of rows in the `dosing` matrix or number of elements in the `dosing` cell vector and the number of groups or output time vectors in `data` determine the total number of simulation results in the output `ynew`. For details, see the table in the `ynew` argument description.

Note If `UnitConversion` is turned on for the underlying SimBiology model that was used for fitting, `dosing` must specify valid amount and time units.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `'ParameterType','population'` specifies to use population parameter estimates.

`ParameterType` — Parameter type

`'individual'` (default) | `'population'`

Parameter type, specified as `'individual'` (default) or `'population'`. If `value` is `'population'`, the `predict` method returns the simulation results using the population parameter estimates, that is, parameter values that are estimated using fixed effects (θs) only. The estimated parameter values used in simulation are identical to those in the `resultsObj.PopulationParameterEstimates` property, unless you specify a new `groupedData` object `data` with new covariate data. In this case, the method reevaluates the covariate model and the parameter estimates based on the new `groupedData` and covariate data.

If `value` is `'individual'`, the method returns the simulation results using the corresponding parameter values of the group in the `resultsObj.IndividualParameterEstimates` property. These values include both fixed- and random-effects estimates, that is, parameter values estimated using both fixed effects (θs) and random effects (ηs) . If `data` contains new groups, only fixed effects (population parameter estimates of the results object) are used for these groups.

By default, `predict` uses the individual parameter estimates of the results object when `data` is a `groupedData` object. If `data` is a vector of output times or cell array of vectors, `predict` uses the population parameter estimates of the results object instead.

Data Types: `char` | `string`

`Variants` — Variants to apply

`[]` | `{}` | 2-D matrix of variants | cell vector of variants

Variants to apply, specified as an empty array (`[]`, `{}`), 2-D matrix or cell vector of variant objects.

If you do not specify this argument, the function has the following behavior depending on whether the second input argument (`data`) is specified also or not.

- If `data` is not specified, the function applies the group-specific variants from the original call to `sbiofitmixed`.
- If `data` is a vector or cell array of output times, the function does not apply the group-specific variants.
- If `data` is a `groupedData` object, the function applies variants only to groups whose group identifier matches a group identifier in the original training data that was used in the call to `sbiofitmixed`.

Note

- The baseline variants that were specified by the “variants” on page 1-0 positional input argument in the original call to `sbiofitmixed` are always applied to the model, and they are applied before any group-specific variants.

- If there are no baseline variants, that is, you did not specify the `variants` input when calling `sbiofitmixed`, the function still applies the model active variants if there are any.

If the argument value is `[]` or `{}`, the function applies no group-specific variants.

If it is a matrix of variants, it must have either one row or one row per group. Each row is applied to a separate group, in the same order as the groups appear in `data` or `dosing`. If it has a single row, the same variants are applied to all groups during simulation. If there are multiple columns, the variants are applied in order from the first column to the last.

If it is a cell vector of variant objects, the number of cells must be one or must match the number of groups in the input data. Each element must be `[]` or a vector of variants. If there is a single cell containing a vector of variants, they are applied to all simulations. If there are multiple cells, the variants in the *i*th cell are applied to the simulation of the *i*th group.

The function defines the number of groups by examining the `data`, and `dosing` input arguments.

- `data` can have `1` or *N* groups.
- If `data` and `dosing` arguments are not specified, then the default data and dosing are determined as follows:
  - For unpooled fits, they are the data and dosing for the single group associated with that fit results.
  - For all other fits, they are the entire set of data and dosing associated with the call to `sbiofitmixed`.

Output Arguments

`ynew` — Simulation results

vector of `SimData` objects

Simulation results, returned as a vector of `SimData` objects. The states reported in `ynew` are the states included in the `responseMap` input argument of `sbiofitmixed` and any other states listed in the `StatesToLog` property of the runtime options (`RuntimeOptions`) of the SimBiology model.

The total number of simulation results in `ynew` depends on the number of groups or output time vectors in `data` and the number of rows in the `dosing` matrix.

Number of groups or output time vectors in `data`	Number of rows in the `dosing` matrix	Simulation results
`1`	`0`, that is, `dosing` is empty `[]`	The total number of `SimData` objects in `ynew` is 1. No doses are applied during simulation.
`1`	`1`	The total number of `SimData` objects in `ynew` is 1. The given row of doses is applied during the simulation.

Number of groups or output time vectors in `data`	Number of rows in the `dosing` matrix	Simulation results
1	*N*	The total number of `SimData` objects in `ynew` is *N*. Each row of `dosing` is applied to each simulation.
N	`0`, that is, `dosing` is empty `[]`	The total number of `SimData` objects in `ynew` is *N*. No doses are applied during simulation.
N	1	The total number of `SimData` objects in `ynew` is *N*. The same row of doses is applied to each simulation.
N	*N*	The total number of `SimData` objects in `ynew` is *N*. Each row of `dosing` is applied to a separate group, in the same order that groups appear in `data`.
M	*N*	The function throws an error when $M \neq N$.

`parameterEstimates` — Estimated parameter values
table

Estimated parameter values used for the predicted simulation results, returned as a table.

If `'ParameterType'` is `'individual'`, the reported parameter values are identical to the values in the `resultsObj.IndividualParameterEstimates` property. However, if `data` contains new groups, then only population parameter estimates (fixed effects) are used for these groups. The corresponding reported values in `parameterEstimates` for these groups are identical to the values in `resultsObj.PopulationParameterEstimates`.

If `'ParameterType'` is `'population'`, the reported parameter values are identical to the values in the `resultsObj.PopulationParameterEstimates` property unless you specify new covariate information in `data`. See the `value` argument description for details.

If `data` is a vector or a cell array of vectors of output times, the reported parameter values are identical to the values in `resultsObj.PopulationParameterEstimates`. Also, the groups reported represent the enumeration of simulations performed and are unrelated to group names in the original fit.

Version History

Introduced in R2014a

See Also

`NLMEResults object` | `sbiofitmixed` | `sbiosampleparameters` | `sbiosampleerror` | `CovariateModel`

Topics

“Model the Population Pharmacokinetics of Phenobarbital in Neonates”
“Nonlinear Mixed-Effects Modeling”

random

Simulate SimBiology model, adding variations by sampling error model

Syntax

```
[ynew,parameterEstimates] = random(resultsObj)
[ynew,parameterEstimates] = random(resultsObj,data,dosing)
[ynew,parameterEstimates]= random(resultsObj,data,dosing,'Variants',v)
```

Description

`[ynew,parameterEstimates] = random(resultsObj)` returns simulation results `ynew` with added noise using the error model information specified by the `resultsObj.ErrorModelInfo` property and estimated parameter values `parameterEstimates`.

`[ynew,parameterEstimates] = random(resultsObj,data,dosing)` uses the specified `data` and `dosing` information.

`[ynew,parameterEstimates]= random(resultsObj,data,dosing,'Variants',v)` also applies the specified variants to each simulation.

Note The noise is only added to states that are responses which are the states included in the `responseMap` input argument when you called `sbiofit` or the "ResponseMap" on page 2-0 property of `fitproblem`. If there is a separate error model for each response, the noise is added to each response separately using the corresponding error model.

Examples

Add Noise to Simulation Results of a Fitted SimBiology Model

This example uses the yeast heterotrimeric G protein model and experimental data reported by [1]. For details about the model, see the **Background** section in "Parameter Scanning, Parameter Estimation, and Sensitivity Analysis in the Yeast Heterotrimeric G Protein Cycle".

Load the G protein model.

```
sbioloadproject gprotein
```

Store the experimental data containing the time course for the fraction of active G protein.

```
time = [10 30 60 110 210 300 450 600]';
GaFracExpt = [0.35 0.4 0.36 0.39 0.33 0.24 0.17 0.2]';
```

Create a groupedData object based on the experimental data.

```
tbl = table(time,GaFracExpt);
grpData = groupedData(tbl);
```

Map the appropriate model component to the experimental data. In other words, indicate which species in the model corresponds to which response variable in the data. In this example, map the model parameter `GaFrac` to the experimental data variable `GaFracExpt` from `grpData`.

```
responseMap = 'GaFrac = GaFracExpt';
```

Use an `estimatedInfo` object to define the model parameter `kGd` as a parameter to be estimated.

```
estimatedParam = estimatedInfo('kGd');
```

Perform the parameter estimation. Use the name-value argument `ErrorModel` to specify the error model that adds error to simulation data.

```
fitResult = sbiofit(m1,grpData,responseMap,estimatedParam,ErrorModel="proportional");
```

View the estimated parameter value of `kGd`.

```
fitResult.ParameterEstimates
```

```
ans=1×3 table
     Name      Estimate    StandardError
    _______    ________    _____________

    {'kGd'}    0.10877       0.001397
```

Use the `random` method to retrieve the simulation data with added noise using the proportional error model which was specified by `sbiofit`. Note that the noise is added only to the response state, that is the `GaFrac` parameter.

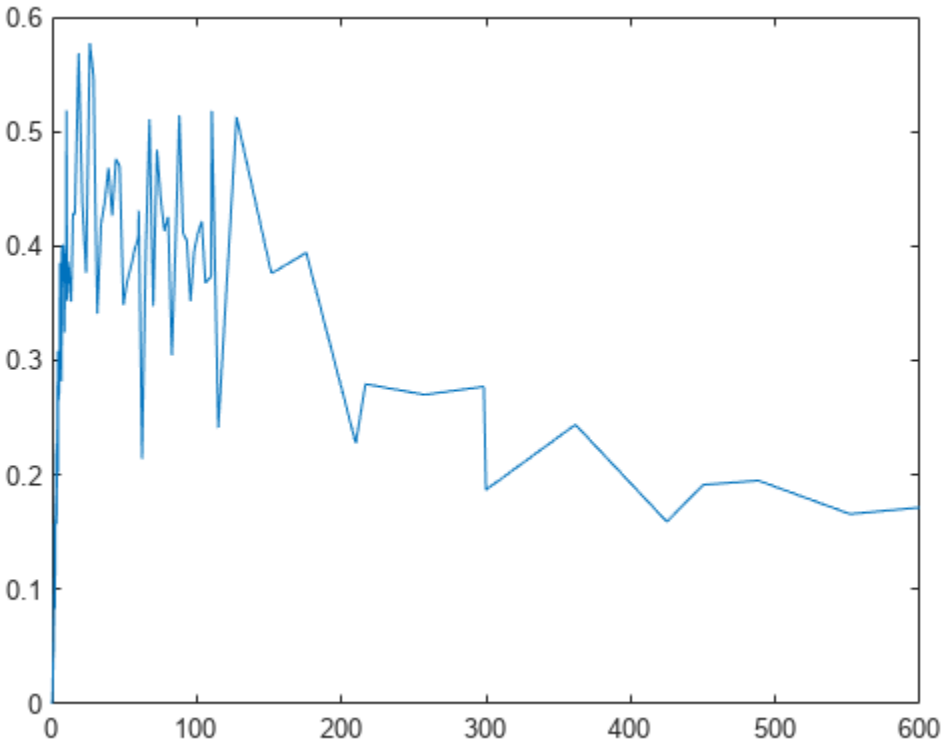
```
[ynew,paramEstim] = random(fitResult);
```

Select the simulation data for the `GaFrac` parameter.

```
GaFracNew = select(ynew,{'Name','GaFrac'});
```

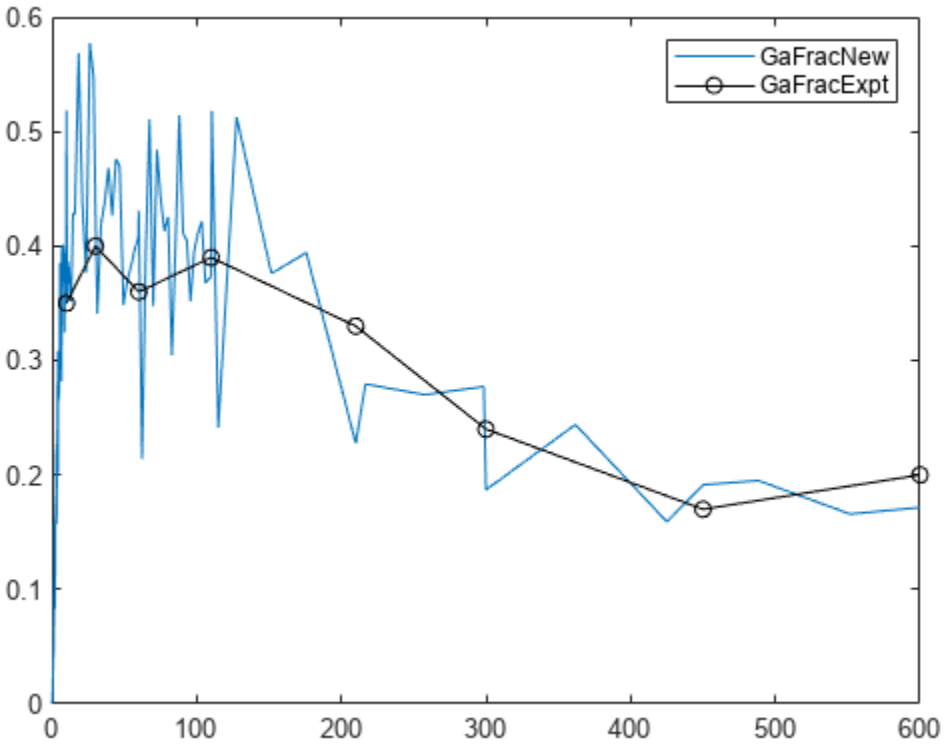
Plot the simulation results.

```
plot(GaFracNew.Time,GaFracNew.Data)
hold on
```



Plot the experimental data to compare it with the simulated data.

```
plot(time,GaFracExpt,'Color','k','Marker','o')
legend('GaFracNew','GaFracExpt')
```



Input Arguments

`resultsObj` — Estimation results

`OptimResults` object | `NLINResults` object

Estimation results, specified as an `OptimResults object` or `NLINResults object`, which contains estimation results returned by `sbiofit`. It must be a scalar object.

`data` — Grouped data or output times

`groupedData` object | vector | cell array of vectors

Grouped data or output times, specified as a `groupedData object`, vector, or cell array of vectors of output times.

If it is a vector of time points, `random` simulates the model with new time points using the parameter estimates from the results object `resultsObj`.

If it is a cell array of vectors of time points, `random` simulates the model *n* times using the output times from each time vector, where *n* is the length of `data`.

If it is a `groupedData` object, it must have an independent variable such as Time. It must also have a group variable if the training data used for fitting has such variable. You can use a `groupedData` object to query different combinations of categories if the `resultsObj` contains parameter estimates for each category. `random` simulates the model for each group with the specified categories. For

instance, suppose you have a set of parameter estimates for sex category (males versus females), and age category (young versus old) in your training data. You can use `random` to simulate the responses of an old male (or any other combination) although such patient may not exist in the training data.

If the `resultsObj` is from estimating category-specific parameters, `data` must be a `groupedData` object.

Note If `UnitConversion` is turned on for the underlying SimBiology model that was used for fitting and `data` is a `groupedData` object, `data` must specify valid variable units via `data.Properties.VariableUnits` property. If it is a numeric vector or cell array of vectors of time points, `random` uses the model's `TimeUnits`.

`dosing` — Dosing information

`[]` | `{}` | 2-D matrix of dose objects | cell vector of dose objects

Dosing information, specified as empty `[]` or `{}`, 2-D matrix or cell vector of SimBiology dose objects (`ScheduleDose object` or `RepeatDose object`).

If `dosing` is empty, no doses are applied during simulation, even if the model has active doses.

For a matrix of dose objects, it must have a single row or one row per group in the input data. If it has a single row, the same doses are applied to all groups during simulation. If it has multiple rows, each row is applied to a separate group, in the same order as the groups appear in the input data. Multiple columns are allowed so that you can apply multiple dose objects to each group.

For a cell vector of doses, it must have one element or one element per group in the input data. Each element must be `[]` or a vector of doses. Each element of the cell is applied to a separate group, in the same order as the groups appear in the input data.

In addition to manually constructing dose objects using `sbiodose`, if the input `groupedData` object has dosing information, you can use the `createDoses` method to construct doses.

Dose objects of the `dosing` input must be consistent with the original dosing data used with `sbiofit`. The objects must have the same values for dose properties (such as `TargetName`) or must be parameterized in the same way as the original dosing data. For instance, suppose that the original dosing matrix has two columns of doses, where the doses in the first column target species *x* and those in the second column target species *y*. Then `dosing` must have doses in the first column targeting species *x* and those in the second column targeting species *y*. A parameterized dose example is as follows. Suppose that the `Amount` property of a dose used in the original `sbiofit` call is parameterized to a model-scoped parameter `'A'`. All doses for the corresponding group (column) in the `dosing` matrix input must have the `Amount` property parameterized to `'A'`.

The number of rows in the `dosing` matrix or number of elements in the `dosing` cell vector and the number of groups or output time vectors in `data` determine the total number of simulation results in the output `ynew`. For details, see the table in the `ynew` argument description.

Note If `UnitConversion` is turned on for the underlying SimBiology model that was used for fitting, `dosing` must specify valid amount and time units.

`v` — Variants to apply

`[]` | `{}` | 2-D matrix of variants | cell vector of variants

Variants to apply, specified as an empty array (`[]`, `{}`), 2-D matrix or cell vector of variant objects.

If you do not specify this argument, the function has the following behavior depending on whether the second input argument (`data`) is specified also or not.

- If `data` is not specified, the function applies the group-specific variants from the original call to `sbiofit`.
- If `data` is a vector or cell array of output times, the function does not apply the group-specific variants.
- If `data` is a `groupedData` object, the function applies variants only to groups whose group identifier matches a group identifier in the original training data that was used in the call to `sbiofit`.

Note

- The baseline variants that were specified by the “variants” on page 1-0 positional input argument in the original call to `sbiofit` are always applied to the model, and they are applied before any group-specific variants.
- If there are no baseline variants, that is, you did not specify the `variants` input when calling `sbiofit`, the `random` function still applies the model active variants if there are any.

If the argument value is `[]` or `{}`, the function applies no group-specific variants.

If it is a matrix of variants, it must have either one row or one row per group. Each row is applied to a separate group, in the same order as the groups appear in `data` or `dosing`. If it has a single row, the same variants are applied to all groups during simulation. If there are multiple columns, the variants are applied in order from the first column to the last.

If it is a cell vector of variant objects, the number of cells must be one or must match the number of groups in the input data. Each element must be `[]` or a vector of variants. If there is a single cell containing a vector of variants, they are applied to all simulations. If there are multiple cells, the variants in the *i*th cell are applied to the simulation of the *i*th group.

The function defines the number of groups by examining the `data`, and `dosing` input arguments.

- `data` can have `1` or *N* groups.
- If `data` and `dosing` arguments are not specified, then the default data and dosing are determined as follows:
  - For unpooled fits, they are the data and dosing for the single group associated with that fit results.
  - For all other fits, they are the entire set of data and dosing associated with the call to `sbiofit`.

Output Arguments

`ynew` — Simulation results with noise

vector of `SimData` objects

Simulation results, returned as a vector of `SimData` objects. The states reported in `ynew` are the states that were included in the `responseMap` input argument of `sbiofit` as well as any other

states listed in the `StatesToLog` property of the runtime options (`RuntimeOptions`) of the SimBiology model.

The total number of simulation results in `ynew` depends on the number of groups or output time vectors in `data` and the number of rows in the `dosing` matrix.

Number of groups or output time vectors in `data`	Number of rows in the `dosing` matrix	Simulation results
1	`0`, that is, `dosing` is empty `[]`	The total number of `SimData` objects in `ynew` is 1. No doses are applied during simulation.
1	1	The total number of `SimData` objects in `ynew` is 1. The given row of doses is applied during the simulation.
1	*N*	The total number of `SimData` objects in `ynew` is *N*. Each row of `dosing` is applied to each simulation.
N	`0`, that is, `dosing` is empty `[]`	The total number of `SimData` objects in `ynew` is *N*. No doses are applied during simulation.
N	1	The total number of `SimData` objects in `ynew` is *N*. The same row of doses is applied to each simulation.
N	*N*	The total number of `SimData` objects in `ynew` is *N*. Each row of `dosing` is applied to a separate group, in the same order that groups appear in `data`.
M	*N*	The function throws an error when $M \neq N$.

`parameterEstimates` — Estimated parameter values
table

Estimated parameter values, returned as a table. This is identical to `resultsObj.ParameterEstimates` property.

Version History

Introduced in R2014a

References

[1] Yi, T-M., Kitano, H., and Simon, M. (2003). A quantitative characterization of the yeast heterotrimeric G protein cycle. PNAS. 100, 10764–10769.

See Also

`NLINResults object` | `OptimResults object` | `sbiofit`

random

Simulate a SimBiology model, adding variations by sampling the error model

Syntax

```
[ynew,parameterEstimates,randomEffects] = random(resultsObj)
[ynew,parameterEstimates] = random(resultsObj,data,dosing)
[ynew,parameterEstimates,randomEffects] = random( ___ ,Name,Value)
```

Description

`[ynew,parameterEstimates,randomEffects] = random(resultsObj)` returns simulation results `ynew` with added noise using the error model information specified by the `resultsObj.ErrorModelInfo` property and estimated parameter values `parameterEstimates` which are returned by `sbiofitmixed`.

`[ynew,parameterEstimates] = random(resultsObj,data,dosing)` uses the specified `data` and `dosing` information.

`[ynew,parameterEstimates,randomEffects] = random( ___ ,Name,Value)` uses additional options specified by one or more name-value arguments.

Note The noise is only added to states that are responses which are the states included in the `responseMap` input argument when you called `sbiofitmixed` or the "ResponseMap" on page 2-0 property of `fitproblem`.

Input Arguments

`resultsObj` — Estimation results

`NLMEResults` object

Estimation results, specified as an `NLMEResults object`, which contains estimation results returned by `sbiofitmixed`. It must be a scalar object.

The function calculates new parameter values using `sbiosampleparameters` with the covariate model returned by `resultsObj.covariateModel`, the fixed effect estimates (`resultsObj.FixedEffects`), and random effect covariance matrix (`resultsObj.RandomEffectCovarianceMatrix`). The function adds randomly sampled errors to the simulation results by calling `sbiosampleerror` using the error model and error model parameters from `resultsObj.ErrorModelInfo`.

`data` — Grouped data or output times

`groupedData` object | vector | cell array of vectors

Grouped data or output times, specified as a `groupedData object`, vector, or cell array of vectors of output times.

If it is a vector of time points, `random` simulates the model with new time points.

If it is a cell array of vectors of time points, `random` simulates the model *n* times using the output times from each time vector, where *n* is the length of `data`.

If the mixed-effects model from the original fit (using `sbiofitmixed`) uses a covariate model with covariates, the `data` must be a `groupedData` object containing covariate data with the same labels for the covariates (`CovariateLabels` property) specified in the original covariate model.

`dosing` — Dosing information

`[]` | `{}` | 2-D matrix of dose objects | cell vector of dose objects

Dosing information, specified as empty `[]` or `{}`, 2-D matrix or cell vector of SimBiology dose objects (`ScheduleDose object` or `RepeatDose object`).

If `dosing` is empty, no doses are applied during simulation, even if the model has active doses.

For a matrix of dose objects, it must have a single row or one row per group in the input data. If it has a single row, the same doses are applied to all groups during simulation. If it has multiple rows, each row is applied to a separate group, in the same order as the groups appear in the input data. Multiple columns are allowed so that you can apply multiple dose objects to each group.

For a cell vector of doses, it must have one element or one element per group in the input data. Each element must be `[]` or a vector of doses. Each element of the cell is applied to a separate group, in the same order as the groups appear in the input data.

In addition to manually constructing dose objects using `sbiodose`, if the input `groupedData` object has dosing information, you can use the `createDoses` method to construct doses.

Dose objects of the `dosing` input must be consistent with the original dosing data used with `sbiofitmixed`. The objects must have the same values for dose properties (such as `TargetName`) or must be parameterized in the same way as the original dosing data. For instance, suppose that the original dosing matrix has two columns of doses, where the doses in the first column target species *x* and those in the second column target species *y*. Then `dosing` must have doses in the first column targeting species *x* and those in the second column targeting species *y*. A parameterized dose example is as follows. Suppose that the `Amount` property of a dose used in the original `sbiofitmixed` call is parameterized to a model-scoped parameter `'A'`. All doses for the corresponding group (column) in the `dosing` matrix input must have the `Amount` property parameterized to `'A'`.

The number of rows in the `dosing` matrix or number of elements in the `dosing` cell vector and the number of groups or output time vectors in `data` determine the total number of simulation results in the output `ynew`. For details, see the table in the `ynew` argument description.

Note If `UnitConversion` is turned on for the underlying SimBiology model that was used for fitting, `dosing` must specify valid amount and time units.

Name-Value Pair Arguments

Specify optional pairs of arguments as `Name1=Value1,...,NameN=ValueN`, where `Name` is the argument name and `Value` is the corresponding value. Name-value arguments must appear after other arguments, but the order of the pairs does not matter.

Before R2021a, use commas to separate each name and value, and enclose `Name` *in quotes.*

Example: `'ParameterType','population'` specifies to use population parameter estimates.

`ParameterType` — Parameter type
`'individual'` (default) | `'population'`

Parameter type, specified as `'population'` or `'individual'` (default).

If `value` is `'individual'`, estimated parameter values and random effect values are resampled by calling `sbiosampleparameters` with the covariate model (specified by the `data` argument or returned by the `covariateModel` method of `resultsObj`), the fixed effect estimates (`resultsObj.FixedEffects`), and random effect covariance matrix (`resultsObj.RandomEffectCovarianceMatrix`). Parameter estimates and random effects are resampled for all groups. The function adds randomly sampled errors to the simulation results by calling `sbiosampleerror` using the error model and error model parameters from `resultsObj.ErrorModelInfo`.

If `value` is `'population'`, the method returns simulation results with noise using population parameter estimates. The estimated parameter values used in simulation are identical to `resultsObj.PopulationParameterEstimates` property unless you specify a new `groupedData` object `data` with new covariate data. In this case, the method will reevaluate the covariate model and this could change the parameter estimates.

Data Types: `char` | `string`

`Variants` — Variants to apply
`[]` | `{}` | 2-D matrix of variants | cell vector of variants

Variants to apply, specified as an empty array (`[]`, `{}`), 2-D matrix or cell vector of variant objects.

If you do not specify this argument, the function has the following behavior depending on whether the second input argument (`data`) is specified also or not.

- If `data` is not specified, the function applies the group-specific variants from the original call to `sbiofitmixed`.
- If `data` is a vector or cell array of output times, the function does not apply the group-specific variants.
- If `data` is a `groupedData` object, the function applies variants only to groups whose group identifier matches a group identifier in the original training data that was used in the call to `sbiofitmixed`.

Note

- The baseline variants that were specified by the “variants” on page 1-0 positional input argument in the original call to `sbiofitmixed` are always applied to the model, and they are applied before any group-specific variants.
- If there are no baseline variants, that is, you did not specify the `variants` input when calling `sbiofitmixed`, the function still applies the model active variants if there are any.

If the argument value is `[]` or `{}`, the function applies no group-specific variants.

If it is a matrix of variants, it must have either one row or one row per group. Each row is applied to a separate group, in the same order as the groups appear in `data` or `dosing`. If it has a single row, the

same variants are applied to all groups during simulation. If there are multiple columns, the variants are applied in order from the first column to the last.

If it is a cell vector of variant objects, the number of cells must be one or must match the number of groups in the input data. Each element must be `[]` or a vector of variants. If there is a single cell containing a vector of variants, they are applied to all simulations. If there are multiple cells, the variants in the *i*th cell are applied to the simulation of the *i*th group.

The function defines the number of groups by examining the `data`, and `dosing` input arguments.

- `data` can have `1` or *N* groups.
- If `data` and `dosing` arguments are not specified, then the default data and dosing are determined as follows:
  - For unpooled fits, they are the data and dosing for the single group associated with that fit results.
  - For all other fits, they are the entire set of data and dosing associated with the call to `sbiofitmixed`.

Output Arguments

`ynew` — Simulation results with noise

vector of `SimData` objects

Simulation results, returned as a vector of `SimData` objects. The states reported in `ynew` are the states included in the `responseMap` input argument of `sbiofitmixed` and any other states listed in the `StatesToLog` property of the runtime options (`RuntimeOptions`) of the SimBiology model.

The total number of simulation results in `ynew` depends on the number of groups or output time vectors in `data` and the number of rows in the `dosing` matrix.

Number of groups or output time vectors in `data`	Number of rows in the `dosing` matrix	Simulation results
`1`	`0`, that is, `dosing` is empty `[]`	The total number of `SimData` objects in `ynew` is 1. No doses are applied during simulation.
`1`	`1`	The total number of `SimData` objects in `ynew` is 1. The given row of doses is applied during the simulation.
`1`	*N*	The total number of `SimData` objects in `ynew` is *N*. Each row of `dosing` is applied to each simulation.

Number of groups or output time vectors in `data`	Number of rows in the `dosing` matrix	Simulation results
N	`0`, that is, `dosing` is empty `[]`	The total number of `SimData` objects in `ynew` is *N*. No doses are applied during simulation.
N	`1`	The total number of `SimData` objects in `ynew` is *N*. The same row of doses is applied to each simulation.
N	*N*	The total number of `SimData` objects in `ynew` is *N*. Each row of `dosing` is applied to a separate group, in the same order that groups appear in `data`.
M	*N*	The function throws an error when $M \neq N$.

`parameterEstimates` — Estimated parameter values
table

Estimated parameter values, returned as a table.

If you specify the `value` argument as `'individual'`, these estimated values will differ from those values from the original fit since parameter values are recalculated using `sbiosampleparameters`.

If `'ParameterType'` is `'population'`, the estimated parameter values are identical to `resultsObj.PopulationParameterEstimates` property unless you specify a new `groupedData` object `data` with new covariate data.

`randomEffects` — Random effect values
table

Random effect values, specified as a table.

Version History

Introduced in R2014a

See Also

`NLMEResults object` | `sbiofitmixed` | `sbiosampleparameters` | `sbiosampleerror`

ParameterConfidenceInterval

Object containing confidence interval results for estimated parameters

Description

The `ParameterConfidenceInterval` object contains confidence interval results for the estimated parameters.

Creation

Create a parameter confidence interval object using `sbioparameterci`.

Properties

`Type` — Confidence interval type
`'gaussian'` | `'profileLikelihood'` | `'bootstrap'`

This property is read-only.

Confidence interval type, specified as `'gaussian'`, `'profileLikelihood'`, or `'bootstrap'`.

Example: `'bootstrap'`

`Alpha` — Confidence level
positive scalar

This property is read-only.

Confidence level, `(1-`*`Alpha`*`) * 100%`, specified as a positive scalar between 0 and 1.

Example: `0.01`

`GroupNames` — Original group names from data used for fitting
cell array of character vectors

This property is read-only.

Original group names from the data used for fitting the model, specified as a cell array of character vectors. Each cell contains the name of a group.

Example: `{'1'}{'2'}{'3'}`

`Results` — Confidence interval results
table

This property is read-only.

Confidence interval results, specified as a table. The table contains the following columns.

Column Name	Description
Name	Name of the estimated parameter
Estimate	Estimated parameter value
Bounds	Lower and upper parameter bounds (if defined in the original fit)
Group	Group name (if available)
CategoryVariableName	Name of category (if defined in the original fit)
CategoryValue	Value of the category variable specified by *CategoryVariableName*
ConfidenceInterval	Confidence interval values
Status	Confidence interval estimation status, specified as one of the following categorical values: `success`, `constrained`, `estimable`, `not estimable` (for details, see “Parameter Confidence Interval Estimation Status” on page 2-666)

`ExitFlags` — Exit flags returned during calculation of `bootstrap` confidence intervals
vector

This property is read-only.

Exit flags returned during the calculation of `bootstrap` confidence intervals only, specified as a vector of integers. Each integer is an exit flag returned by the estimation function (except `nlinfit`) used to fit parameters during bootstrapping. The same estimation function used in the original fit is used for bootstrapping.

Each flag indicates the success or failure status of the fitting performed to create a bootstrap sample. Refer to the reference page of the corresponding estimation function for the meaning of the exit flag.

If the estimation function does not return an exit flag, `ExitFlags` is set to `[]`. For the `gaussian` and `profileLikelihood` confidence intervals, `ExitFlags` is not supported and is always set to `[]`.

Object Functions

ci2table Return summary table of confidence interval results
plot Plot parameter confidence interval results

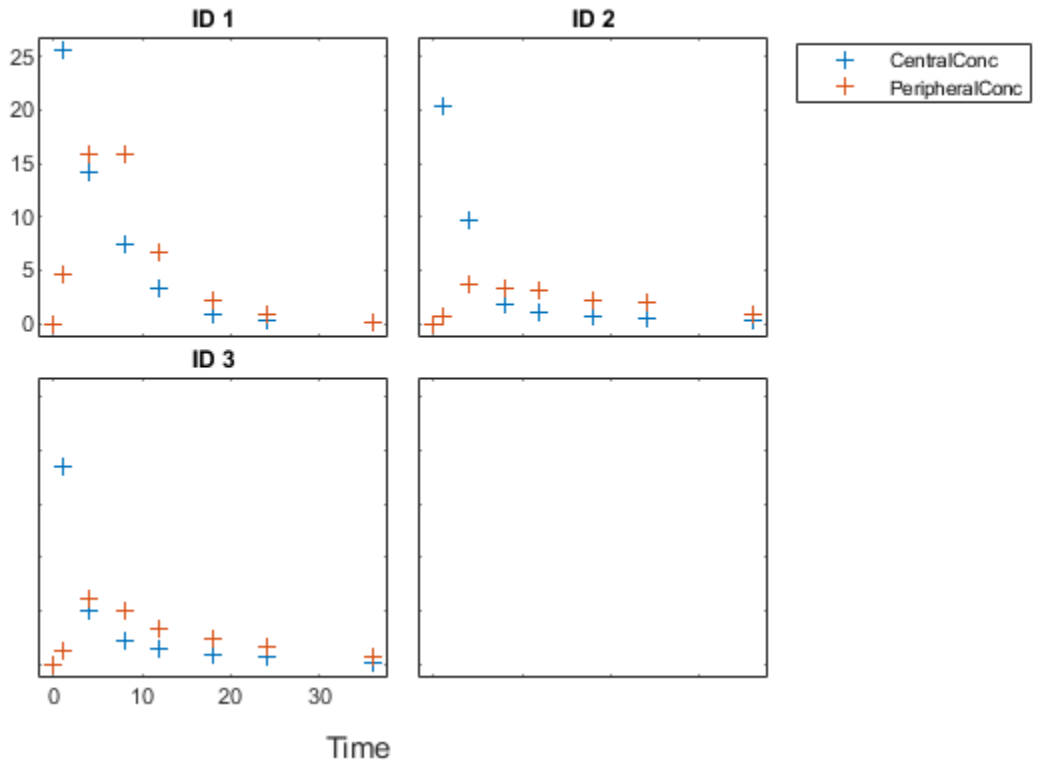
Examples

Compute Confidence Intervals for Estimated PK Parameters and Model Predictions

Load Data

Load the sample data to fit. The data is stored as a table with variables *ID* , *Time* , *CentralConc* , and *PeripheralConc*. This synthetic data represents the time course of plasma concentrations measured at eight different time points for both central and peripheral compartments after an infusion dose for three individuals.

```
load data10_32R.mat
gData = groupedData(data);
gData.Properties.VariableUnits = {'','hour','milligram/liter','milligram/liter'};
sbiotrellis(gData,'ID','Time',{'CentralConc','PeripheralConc'},'Marker','+',...
            'LineStyle','none');
```



Create Model

Create a two-compartment model.

```
pkmd                 = PKModelDesign;
pkc1                 = addCompartment(pkmd,'Central');
pkc1.DosingType      = 'Infusion';
pkc1.EliminationType = 'linear-clearance';
pkc1.HasResponseVariable = true;
pkc2                 = addCompartment(pkmd,'Peripheral');
model                = construct(pkmd);
configset            = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
```

Define Dosing

Define the infusion dose.

```
dose             = sbiodose('dose','TargetName','Drug_Central');
dose.StartTime   = 0;
dose.Amount      = 100;
dose.Rate        = 50;
```

```
dose.AmountUnits = 'milligram';
dose.TimeUnits   = 'hour';
dose.RateUnits   = 'milligram/hour';
```

Define Parameters

Define the parameters to estimate. Set the parameter bounds for each parameter. In addition to these explicit bounds, the parameter transformations (such as log, logit, or probit) impose implicit bounds.

```
responseMap = {'Drug_Central = CentralConc','Drug_Peripheral = PeripheralConc'};
paramsToEstimate   = {'log(Central)','log(Peripheral)','Q12','Cl_Central'};
estimatedParam     = estimatedInfo(paramsToEstimate,...
                                   'InitialValue',[1 1 1 1],...
                                   'Bounds',[0.1 3;0.1 10;0 10;0.1 2]);
```

Fit Model

Perform an unpooled fit, that is, one set of estimated parameters for each patient.

```
unpooledFit = sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',false);
```

Perform a pooled fit, that is, one set of estimated parameters for all patients.

```
pooledFit = sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',true);
```

Compute Confidence Intervals for Estimated Parameters

Compute 95% confidence intervals for each estimated parameter in the unpooled fit.

```
ciParamUnpooled = sbioparameterci(unpooledFit);
```

Display Results

Display the confidence intervals in a table format. For details about the meaning of each estimation status, see “Parameter Confidence Interval Estimation Status” on page 2-666.

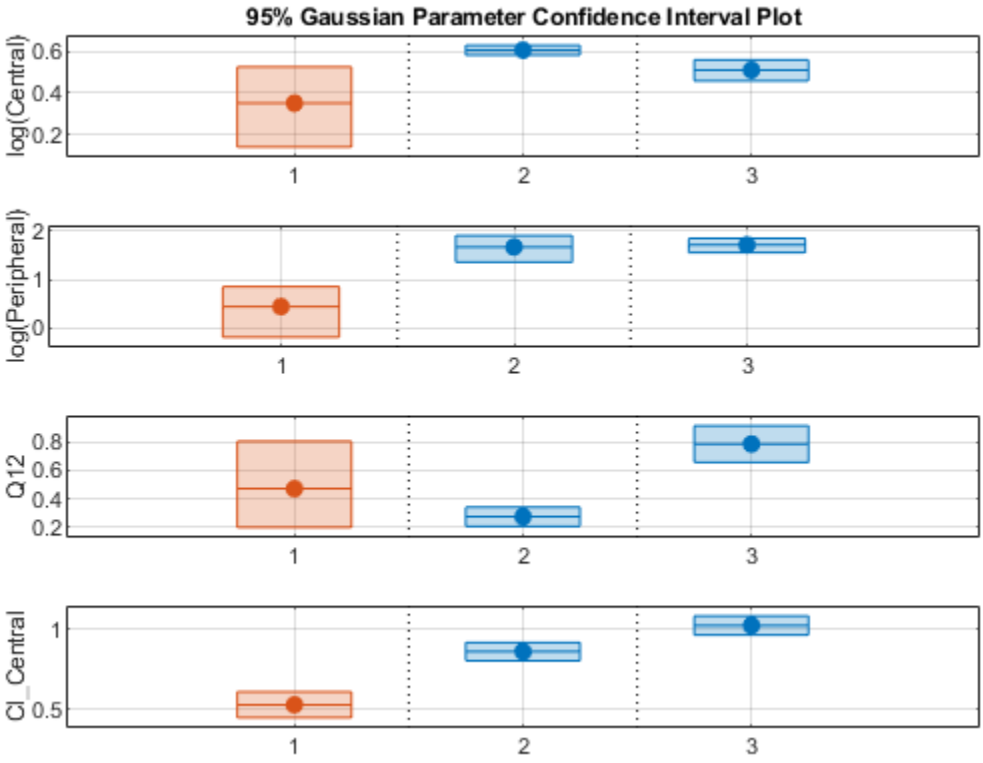
```
ci2table(ciParamUnpooled)
```

```
ans =

  12x7 table

    Group         Name         Estimate    ConfidenceInterval      Type      Alpha      Status
    _____    _____________     ________    __________________    ________    _____    __________

      1      {'Central'   }      1.422       1.1533     1.6906    Gaussian    0.05     estimable
      1      {'Peripheral'}     1.5629      0.83143     2.3551    Gaussian    0.05     constrained
      1      {'Q12'       }    0.47159      0.20093    0.80247    Gaussian    0.05     constrained
      1      {'Cl_Central'}    0.52898      0.44842    0.60955    Gaussian    0.05     estimable
      2      {'Central'   }     1.8322       1.7893     1.8751    Gaussian    0.05     success
      2      {'Peripheral'}     5.3368       3.9133     6.7602    Gaussian    0.05     success
      2      {'Q12'       }    0.27641       0.2093    0.34351    Gaussian    0.05     success
      2      {'Cl_Central'}    0.86034      0.80313    0.91755    Gaussian    0.05     success
      3      {'Central'   }     1.6657       1.5818     1.7497    Gaussian    0.05     success
      3      {'Peripheral'}     5.5632       4.7557     6.3708    Gaussian    0.05     success
      3      {'Q12'       }    0.78361      0.65581    0.91142    Gaussian    0.05     success
      3      {'Cl_Central'}     1.0233      0.96375     1.0828    Gaussian    0.05     success
```

Plot the confidence intervals. If the estimation status of a confidence interval is `success`, it is plotted in blue (the first default color). Otherwise, it is plotted in red (the second default color), which indicates that further investigation into the fitted parameters may be required. If the confidence interval is `not estimable`, then the function plots a red line with a centered cross. If there are any transformed parameters with estimated values 0 (for the log transform) and 1 or 0 (for the probit or logit transform), then no confidence intervals are plotted for those parameter estimates. To see the color order, type `get(groot,'defaultAxesColorOrder')`.

Groups are displayed from left to right in the same order that they appear in the `GroupNames` property of the object, which is used to label the x-axis. The y-labels are the transformed parameter names.

```
plot(ciParamUnpooled)
```



Compute the confidence intervals for the pooled fit.

```
ciParamPooled = sbioparameterci(pooledFit);
```

Display the confidence intervals.

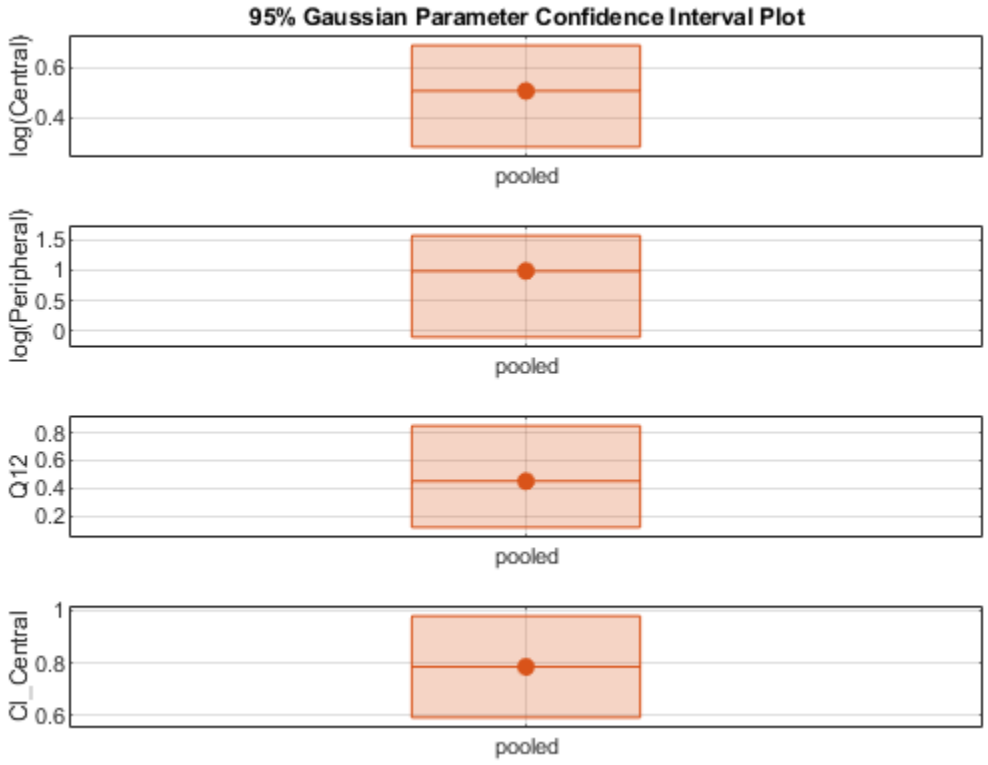
```
ci2table(ciParamPooled)
```

```
ans =

  4x7 table
```

Group	Name	Estimate	ConfidenceInterval		Type	Alpha	Status
pooled	{'Central' }	1.6626	1.3287	1.9965	Gaussian	0.05	estimable
pooled	{'Peripheral'}	2.687	0.89848	4.8323	Gaussian	0.05	constraine
pooled	{'Q12' }	0.44956	0.11445	0.85152	Gaussian	0.05	constraine
pooled	{'Cl_Central'}	0.78493	0.59222	0.97764	Gaussian	0.05	estimable

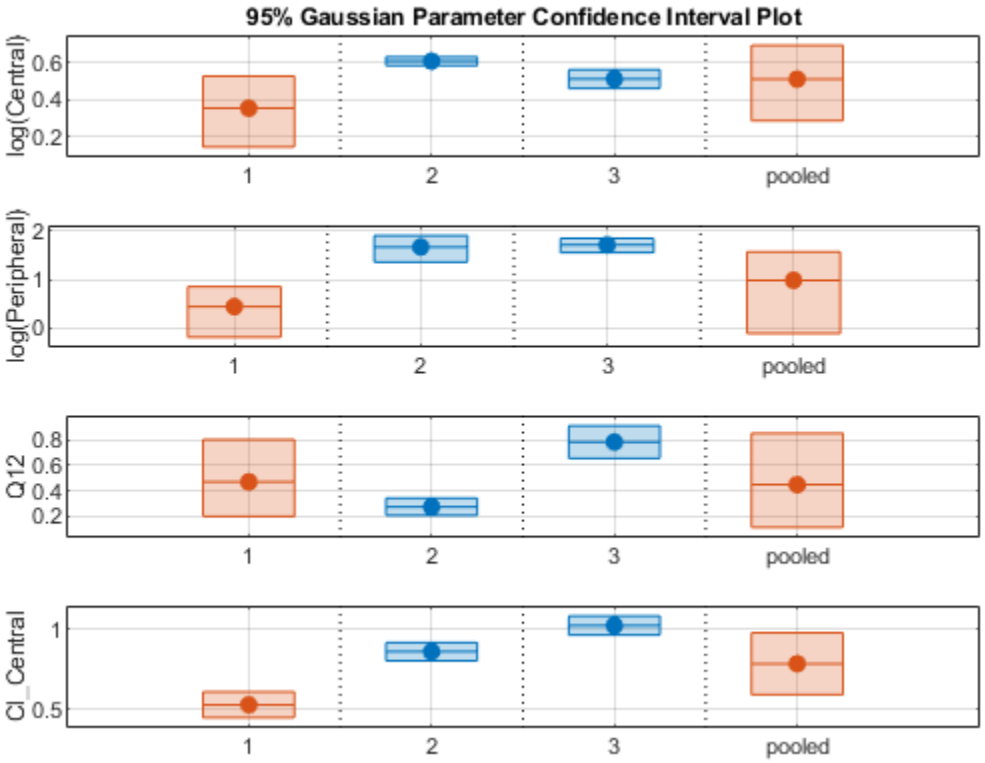
Plot the confidence intervals. The group name is labeled as "pooled" to indicate such fit.

```
plot(ciParamPooled)
```



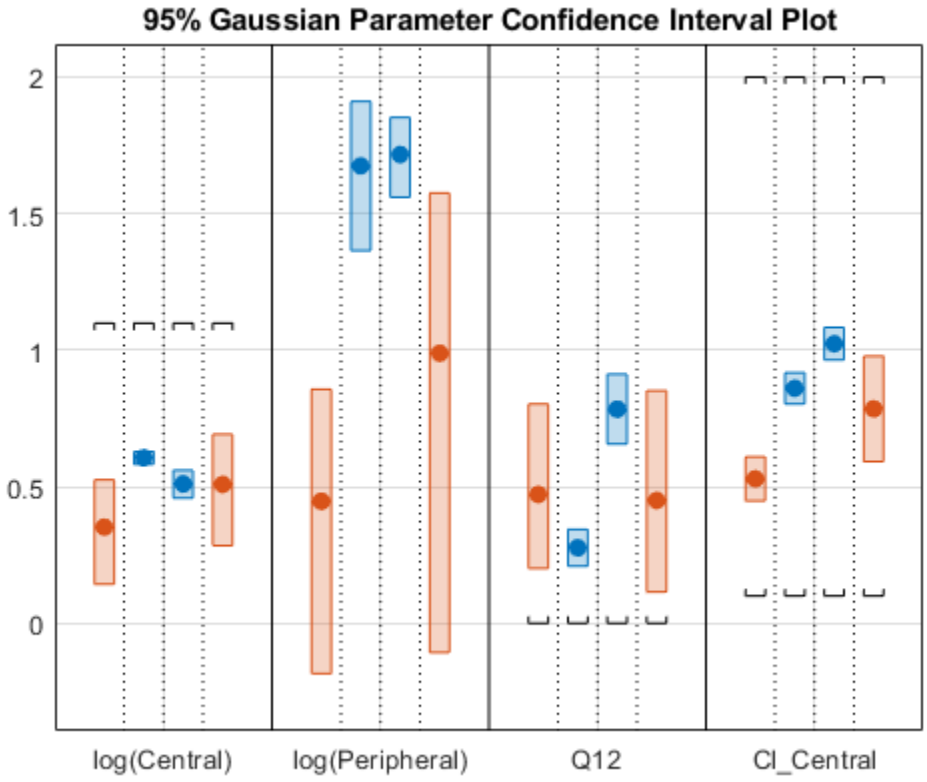
Plot all the confidence interval results together. By default, the confidence interval for each parameter estimate is plotted on a separate axes. Vertical lines group confidence intervals of parameter estimates that were computed in a common fit.

```
ciAll = [ciParamUnpooled;ciParamPooled];
plot(ciAll)
```



You can also plot all confidence intervals in one axes grouped by parameter estimates using the 'Grouped' layout.

```
plot(ciAll,'Layout','Grouped')
```



In this layout, you can point to the center marker of each confidence interval to see the group name. Each estimated parameter is separated by a vertical black line. Vertical dotted lines group confidence intervals of parameter estimates that were computed in a common fit. Parameter bounds defined in the original fit are marked by square brackets. Note the different scales on the y-axis due to parameter transformations. For instance, the y-axis of `Q12` is in the linear scale, but that of `Central` is in the log scale due to its log transform.

Compute Confidence Intervals for Model Predictions

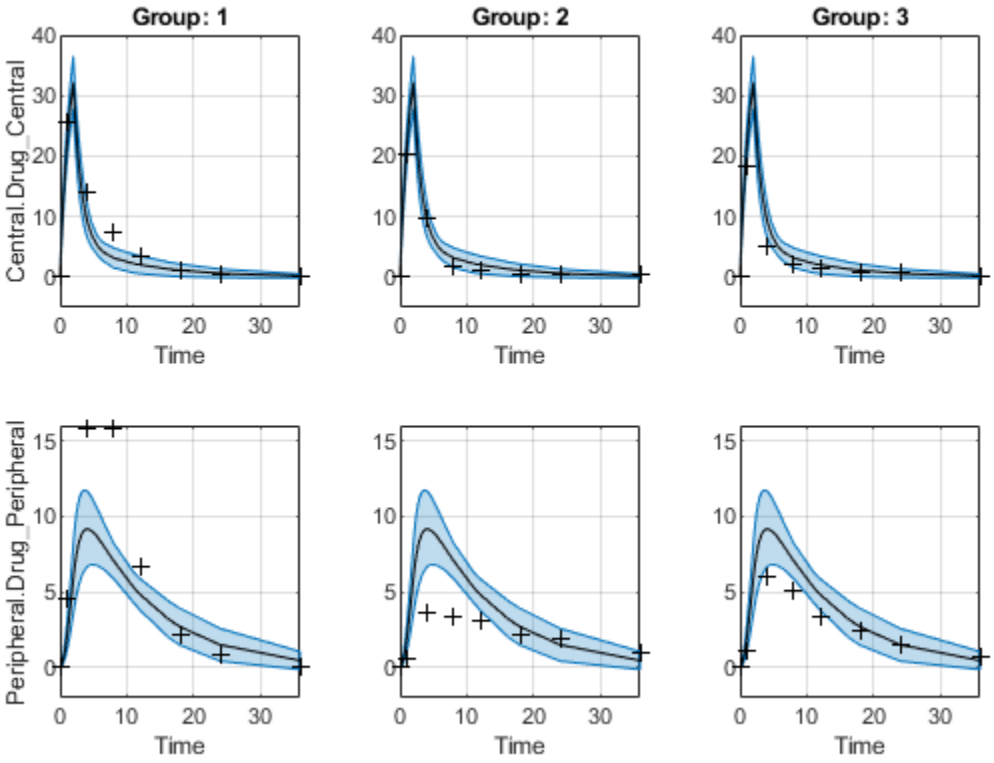
Calculate 95% confidence intervals for the model predictions, that is, simulation results using the estimated parameters.

```
% For the pooled fit
ciPredPooled = sbiopredictionci(pooledFit);
% For the unpooled fit
ciPredUnpooled = sbiopredictionci(unpooledFit);
```

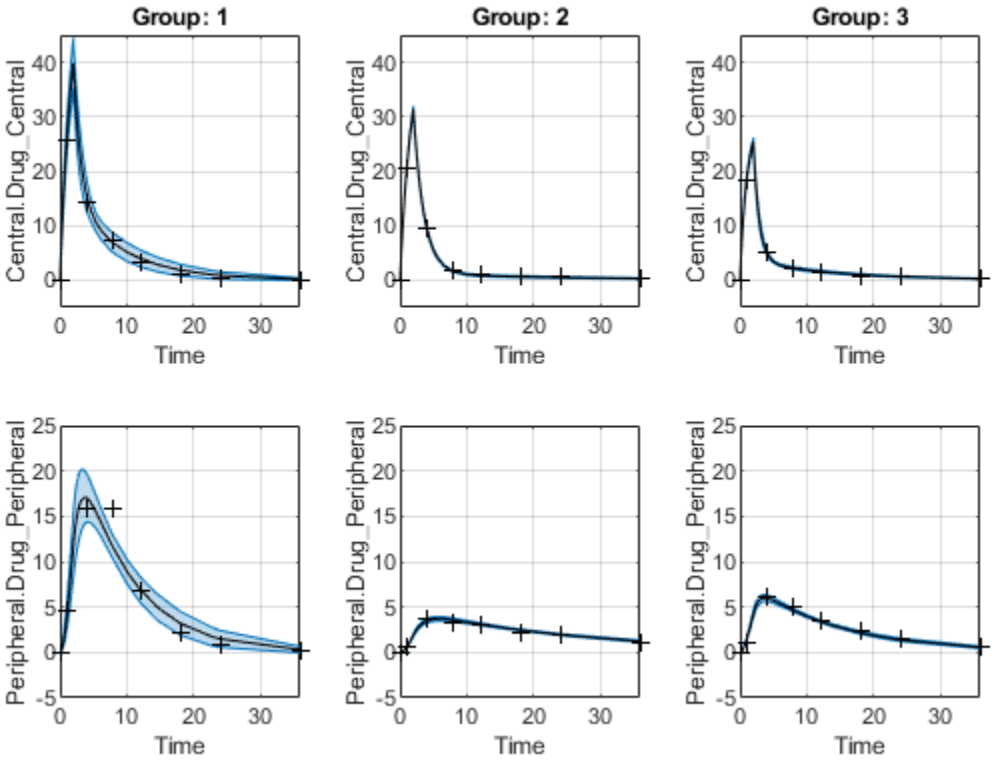
Plot Confidence Intervals for Model Predictions

The confidence interval for each group is plotted in a separate column, and each response is plotted in a separate row. Confidence intervals limited by the bounds are plotted in red. Confidence intervals not limited by the bounds are plotted in blue.

```
plot(ciPredPooled)
```




```
plot(ciPredUnpooled)
```



More About

Parameter Confidence Interval Estimation Status

The following are the definitions of confidence interval estimation statuses for different types of confidence intervals.

Gaussian Confidence Interval

- `not estimable` – The confidence interval is unbounded.
- `constrained` – The confidence interval is constrained by a parameter bound defined in the original fit. Parameter transformations (such as `log`, `probit`, or `logit`) impose implicit bounds on the estimated parameters, for example, positivity constraints. Such bounds can lead to the overestimation of the confidence, that is, the confidence interval can be smaller than expected.
- `success` – All confidence intervals for all parameters are computed successfully.
- `estimable` – The confidence interval is computed successfully, but other parameters have an estimation status of `not estimable` or `constrained`.

For more details about the algorithm, see “Gaussian Confidence Interval Calculation” on page 1-191.

Profile Likelihood Confidence Interval

- `not estimable` – The computation of the confidence interval is unsuccessful. This can happen when the profile likelihood curve is not strictly monotonically decreasing, or due to computation failures in the profile likelihood.

- `constrained` – The profile likelihood curve is bounded by the bounds on the estimated parameters defined in the original fit. Parameter transformations, such as `log`, `logit`, `probit`, impose implicit bounds on the estimated parameters, for example, positivity constraints.
- `success` – If there is no parameter estimate with the confidence interval estimation status `constrained` or `not estimable`, then the function sets all estimation statuses to `success`.
- `estimable` – The confidence interval is computed successfully, but other parameters have an estimation status of `not estimable` or `constrained`.

For more details about the algorithm, see “Profile Likelihood Confidence Interval Calculation” on page 1-191.

Bootstrap Confidence Interval

- `constrained` – The confidence interval is closer than `Tolerance` to the parameter bounds defined in the original fit.
- `success` – All confidence intervals were further away from the parameter bounds than `Tolerance`.
- `estimable` – The confidence interval is computed successfully, but other parameters have an estimation status of `constrained`.

For more details about the algorithm, see “Bootstrap Confidence Interval Calculation” on page 1-193.

Version History

Introduced in R2017b

See Also

`sbioparameterci` | `sbiopredictionci` | `PredictionConfidenceInterval`

PredictionConfidenceInterval

Object containing confidence interval results for model predictions

Description

The `PredictionConfidenceInterval` object contains confidence interval results for model predictions (that is, simulation results based on estimated parameters).

Creation

Create a prediction confidence interval object using `sbiopredictionci`.

Properties

`ResponseNames` — Names of model responses
cell array of character vectors

This property is read-only.

Names of model responses in the parameter fit, specified as a cell array of character vectors. Each cell contains the name of a response.

Example: `{'Central.Drug_Central' } {'Peripheral.Drug_Peripheral'}`

`Status` — Confidence interval estimation status
categorical

This property is read-only.

Confidence interval estimation status, specified as one of the following categorical values:

- `success` – The proper confidence intervals are found. That is, no model prediction is constrained by the parameter bounds defined in the original fit.
- `constrained` – The confidence intervals are found, but the confidence interval for the model response is constrained by a parameter bound defined in the original fit.
- `not estimable` – No confidence intervals are found.
- `estimable` – The proper confidence intervals are found, but other model predictions have an estimation status of either `constrained` or `not estimable`. For the bootstrap confidence interval, the status is always set to `estimable`.

For details, see “Gaussian Confidence Interval Calculation for Model Predictions” on page 1-214 and “Bootstrap Confidence Interval Calculation” on page 1-215.

Example: `success`

`Type` — Confidence interval type
`'gaussian'` | `'bootstrap'`

This property is read-only.

Confidence interval type, specified as `'gaussian'` or `'bootstrap'`.

Example: `'bootstrap'`

`Alpha` — Confidence level
positive scalar

This property is read-only.

Confidence level, `(1-`*`Alpha`*`) * 100%`, specified as a positive scalar between 0 and 1.

Example: `0.01`

`GroupNames` — Original group names from data used for fitting
cell array of character vectors

This property is read-only.

Original group names from the data used for fitting the model, specified as a cell array of character vectors. Each cell contains the name of a group.

Example: `{'1'}{'2'}{'3'}`

`Results` — Confidence interval results
table

This property is read-only.

Confidence interval results, specified as a table. The table contains the following columns.

Column Name	Description
Group	Group name
Response	Model response name
Time	Simulation time
Estimate	Estimated response value
ConfidenceInterval	Confidence interval values

`ExitFlags` — Exit flags returned during calculation of `bootstrap` confidence intervals
vector

This property is read-only.

Exit flags returned during the calculation of `bootstrap` confidence intervals only, specified as a vector of integers. Each integer is an exit flag returned by the estimation function (except `nlinfit`) used to fit parameters during bootstrapping. The same estimation function used in the original fit is used for bootstrapping.

Each flag indicates the success or failure status of the fitting performed to create a bootstrap sample. Refer to the reference page of the corresponding estimation function for the meaning of the exit flag.

If the estimation function does not return an exit flag, `ExitFlags` is set to `[]`. For the `gaussian` confidence intervals, `ExitFlags` is not supported and is always set to `[]`.

Object Functions

plot Plot confidence interval results for model predictions

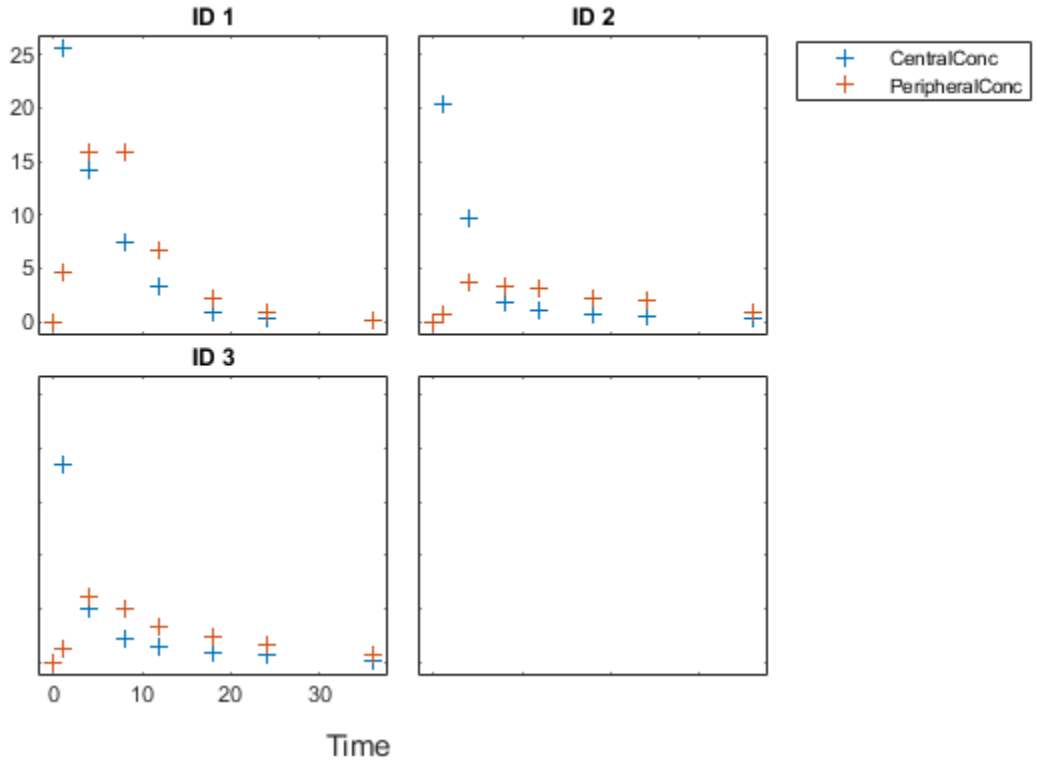
Examples

Compute Confidence Intervals for Estimated PK Parameters and Model Predictions

Load Data

Load the sample data to fit. The data is stored as a table with variables *ID* , *Time* , *CentralConc* , and *PeripheralConc*. This synthetic data represents the time course of plasma concentrations measured at eight different time points for both central and peripheral compartments after an infusion dose for three individuals.

```
load data10_32R.mat
gData = groupedData(data);
gData.Properties.VariableUnits = {'','hour','milligram/liter','milligram/liter'};
sbiotrellis(gData,'ID','Time',{'CentralConc','PeripheralConc'},'Marker','+',...
            'LineStyle','none');
```



Create Model

Create a two-compartment model.

```
pkmd                = PKModelDesign;
pkc1                = addCompartment(pkmd,'Central');
```

```
pkc1.DosingType      = 'Infusion';
pkc1.EliminationType = 'linear-clearance';
pkc1.HasResponseVariable = true;
pkc2                 = addCompartment(pkmd,'Peripheral');
model                = construct(pkmd);
configset            = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
```

Define Dosing

Define the infusion dose.

```
dose             = sbiodose('dose','TargetName','Drug_Central');
dose.StartTime   = 0;
dose.Amount      = 100;
dose.Rate        = 50;
dose.AmountUnits = 'milligram';
dose.TimeUnits   = 'hour';
dose.RateUnits   = 'milligram/hour';
```

Define Parameters

Define the parameters to estimate. Set the parameter bounds for each parameter. In addition to these explicit bounds, the parameter transformations (such as log, logit, or probit) impose implicit bounds.

```
responseMap = {'Drug_Central = CentralConc','Drug_Peripheral = PeripheralConc'};
paramsToEstimate   = {'log(Central)','log(Peripheral)','Q12','Cl_Central'};
estimatedParam     = estimatedInfo(paramsToEstimate,...
                                   'InitialValue',[1 1 1 1],...
                                   'Bounds',[0.1 3;0.1 10;0 10;0.1 2]);
```

Fit Model

Perform an unpooled fit, that is, one set of estimated parameters for each patient.

```
unpooledFit = sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',false);
```

Perform a pooled fit, that is, one set of estimated parameters for all patients.

```
pooledFit = sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',true);
```

Compute Confidence Intervals for Estimated Parameters

Compute 95% confidence intervals for each estimated parameter in the unpooled fit.

```
ciParamUnpooled = sbioparameterci(unpooledFit);
```

Display Results

Display the confidence intervals in a table format. For details about the meaning of each estimation status, see “Parameter Confidence Interval Estimation Status” on page 2-666.

```
ci2table(ciParamUnpooled)
```

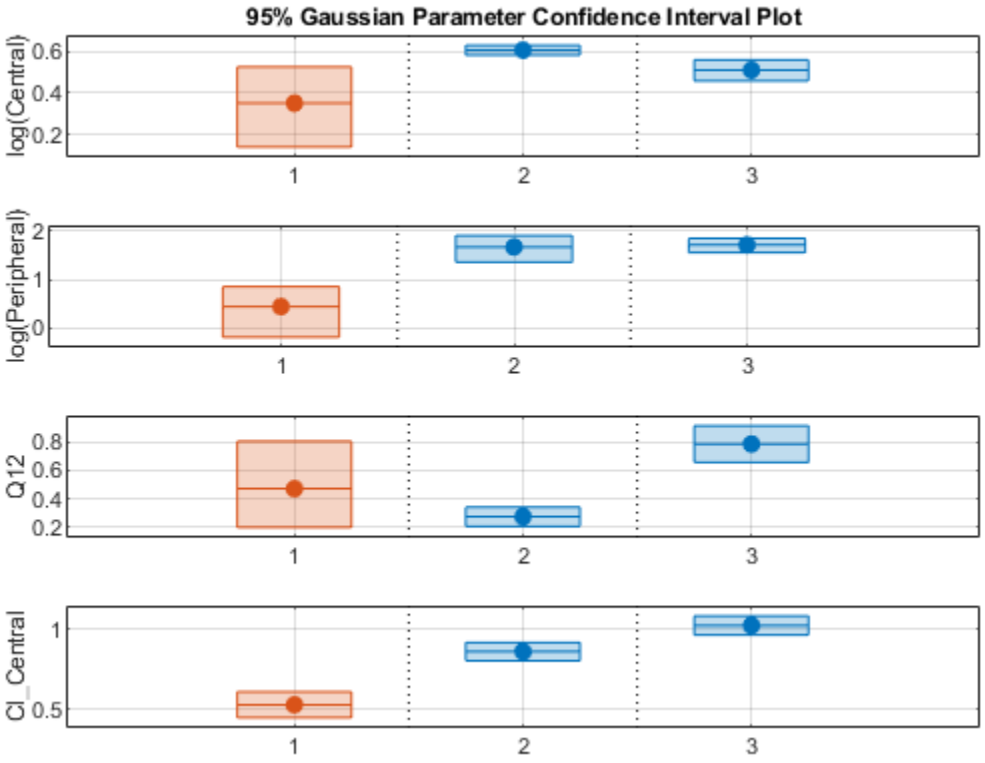
```
ans =

  12x7 table
```

Group	Name	Estimate	ConfidenceInterval		Type	Alpha	Status
1	{'Central' }	1.422	1.1533	1.6906	Gaussian	0.05	estimable
1	{'Peripheral'}	1.5629	0.83143	2.3551	Gaussian	0.05	constrained
1	{'Q12' }	0.47159	0.20093	0.80247	Gaussian	0.05	constrained
1	{'Cl_Central'}	0.52898	0.44842	0.60955	Gaussian	0.05	estimable
2	{'Central' }	1.8322	1.7893	1.8751	Gaussian	0.05	success
2	{'Peripheral'}	5.3368	3.9133	6.7602	Gaussian	0.05	success
2	{'Q12' }	0.27641	0.2093	0.34351	Gaussian	0.05	success
2	{'Cl_Central'}	0.86034	0.80313	0.91755	Gaussian	0.05	success
3	{'Central' }	1.6657	1.5818	1.7497	Gaussian	0.05	success
3	{'Peripheral'}	5.5632	4.7557	6.3708	Gaussian	0.05	success
3	{'Q12' }	0.78361	0.65581	0.91142	Gaussian	0.05	success
3	{'Cl_Central'}	1.0233	0.96375	1.0828	Gaussian	0.05	success

Plot the confidence intervals. If the estimation status of a confidence interval is `success`, it is plotted in blue (the first default color). Otherwise, it is plotted in red (the second default color), which indicates that further investigation into the fitted parameters may be required. If the confidence interval is `not estimable`, then the function plots a red line with a centered cross. If there are any transformed parameters with estimated values 0 (for the log transform) and 1 or 0 (for the probit or logit transform), then no confidence intervals are plotted for those parameter estimates. To see the color order, type `get(groot,'defaultAxesColorOrder')`.

Groups are displayed from left to right in the same order that they appear in the `GroupNames` property of the object, which is used to label the x-axis. The y-labels are the transformed parameter names.

```
plot(ciParamUnpooled)
```



Compute the confidence intervals for the pooled fit.

```
ciParamPooled = sbioparameterci(pooledFit);
```

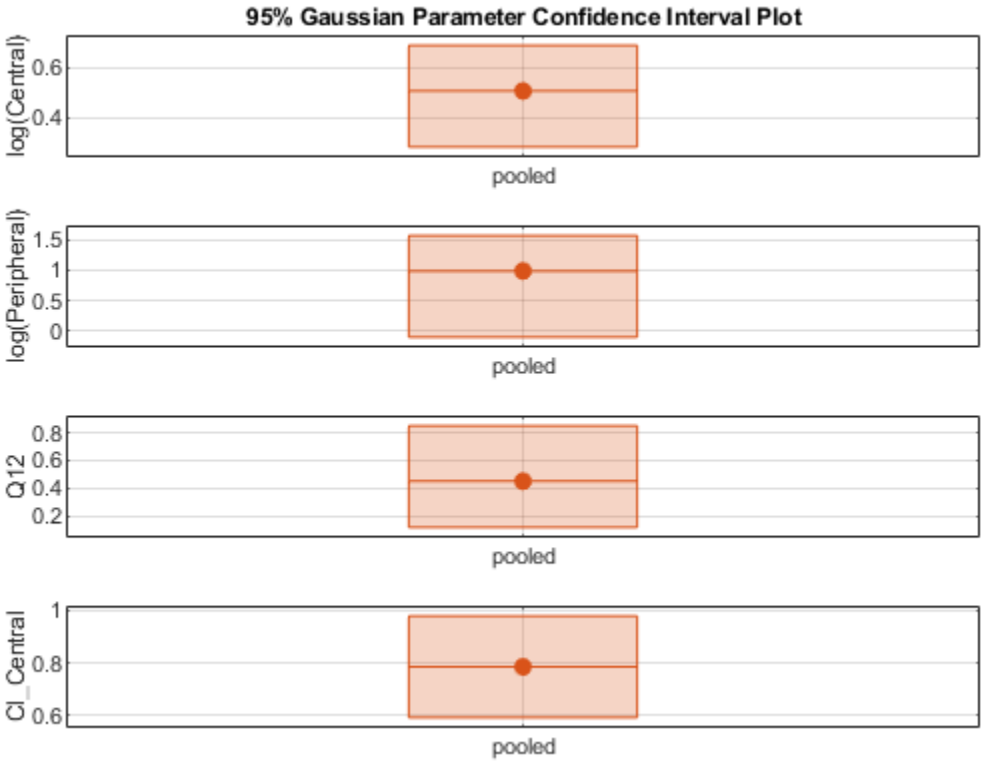
Display the confidence intervals.

```
ci2table(ciParamPooled)
```

```
ans =

  4x7 table

    Group         Name          Estimate    ConfidenceInterval      Type      Alpha      Status
    _______    _____________    ________    __________________    _________    _____    __________

    pooled     {'Central'   }      1.6626       1.3287     1.9965    Gaussian    0.05     estimable
    pooled     {'Peripheral'}       2.687      0.89848     4.8323    Gaussian    0.05     constraine
    pooled     {'Q12'       }     0.44956      0.11445    0.85152    Gaussian    0.05     constraine
    pooled     {'Cl_Central'}     0.78493      0.59222    0.97764    Gaussian    0.05     estimable
```

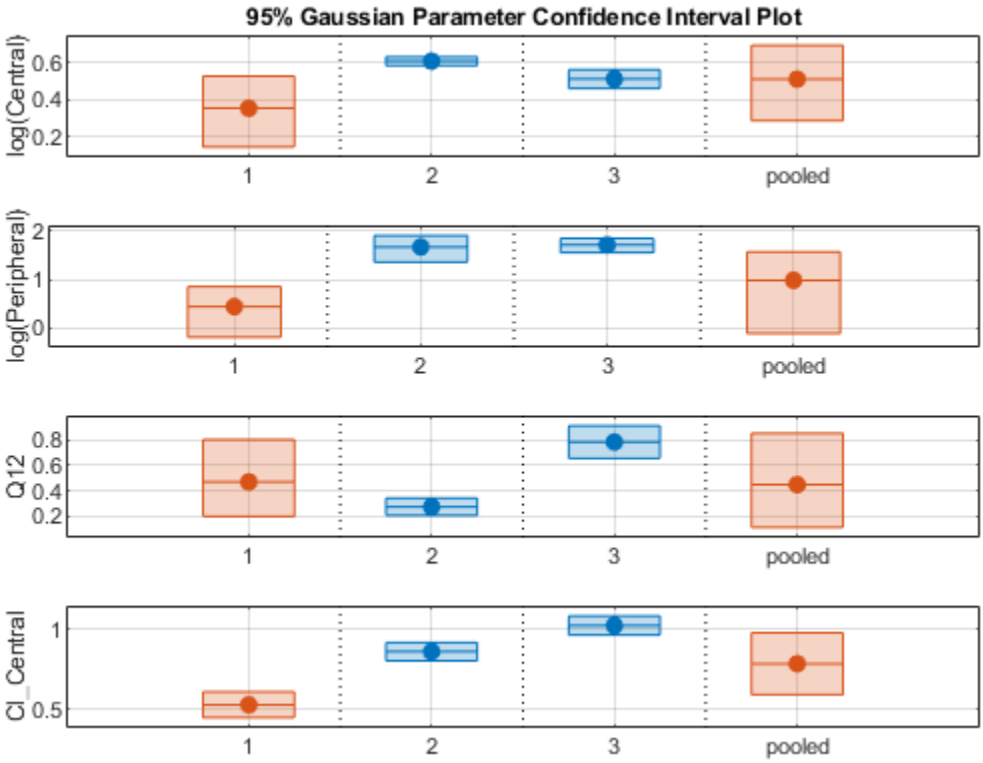
Plot the confidence intervals. The group name is labeled as "pooled" to indicate such fit.

```
plot(ciParamPooled)
```



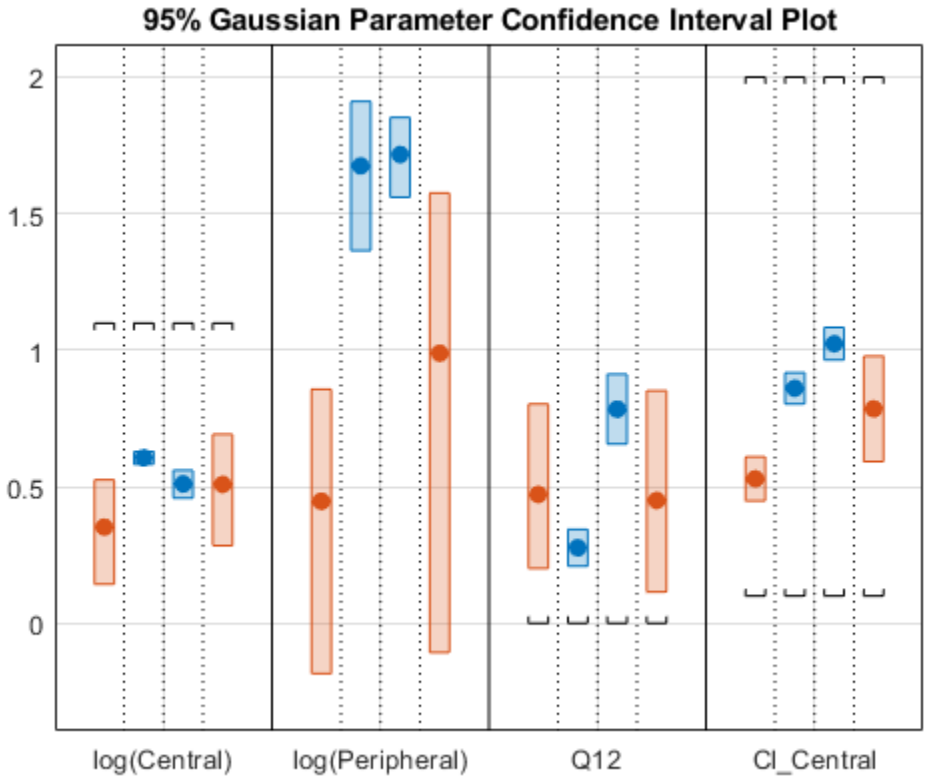
Plot all the confidence interval results together. By default, the confidence interval for each parameter estimate is plotted on a separate axes. Vertical lines group confidence intervals of parameter estimates that were computed in a common fit.

```
ciAll = [ciParamUnpooled;ciParamPooled];
plot(ciAll)
```



You can also plot all confidence intervals in one axes grouped by parameter estimates using the 'Grouped' layout.

```
plot(ciAll,'Layout','Grouped')
```



In this layout, you can point to the center marker of each confidence interval to see the group name. Each estimated parameter is separated by a vertical black line. Vertical dotted lines group confidence intervals of parameter estimates that were computed in a common fit. Parameter bounds defined in the original fit are marked by square brackets. Note the different scales on the y-axis due to parameter transformations. For instance, the y-axis of `Q12` is in the linear scale, but that of `Central` is in the log scale due to its log transform.

Compute Confidence Intervals for Model Predictions

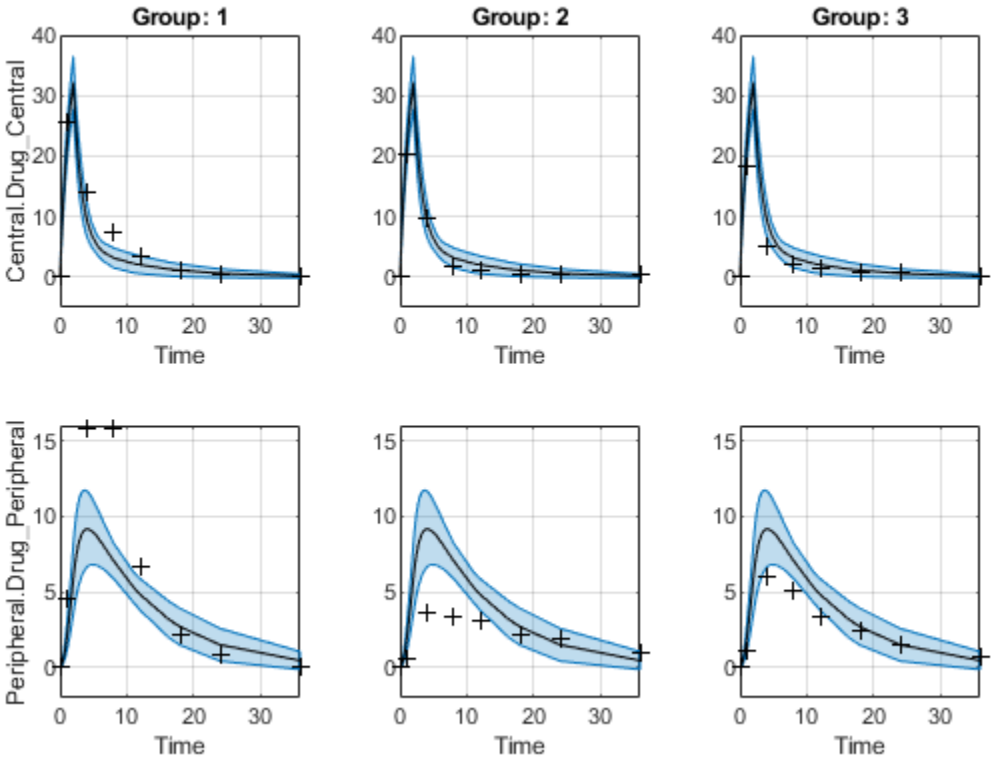
Calculate 95% confidence intervals for the model predictions, that is, simulation results using the estimated parameters.

```
% For the pooled fit
ciPredPooled = sbiopredictionci(pooledFit);
% For the unpooled fit
ciPredUnpooled = sbiopredictionci(unpooledFit);
```

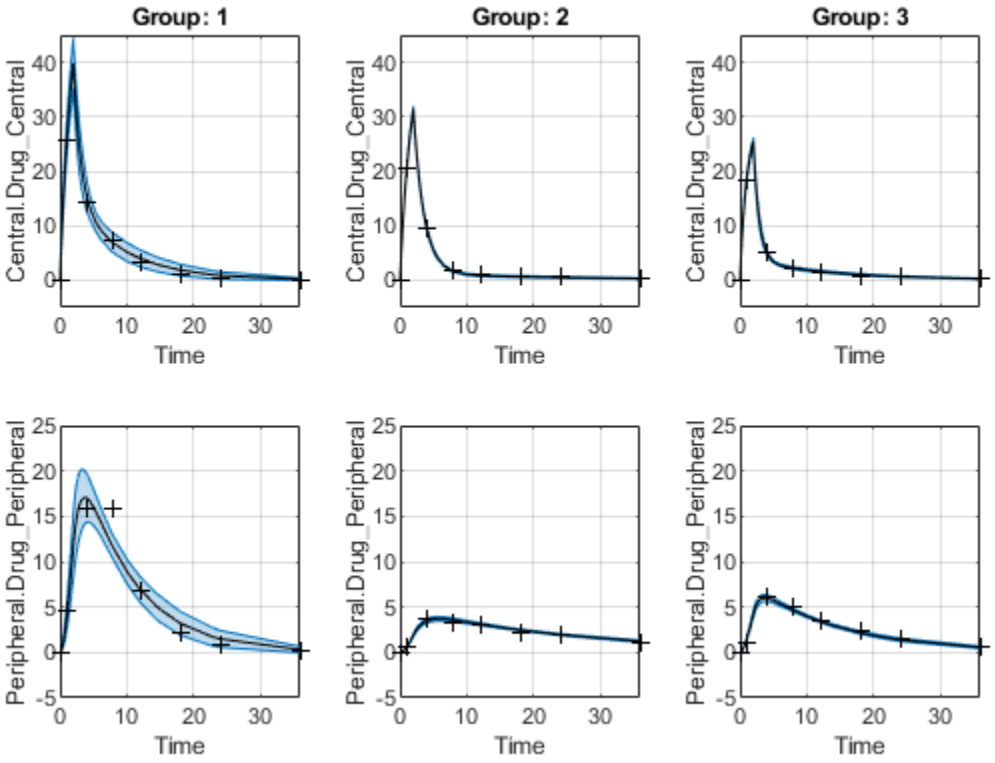
Plot Confidence Intervals for Model Predictions

The confidence interval for each group is plotted in a separate column, and each response is plotted in a separate row. Confidence intervals limited by the bounds are plotted in red. Confidence intervals not limited by the bounds are plotted in blue.

```
plot(ciPredPooled)
```




```
plot(ciPredUnpooled)
```



Version History

Introduced in R2017b

See Also

`sbioparameterci` | `sbiopredictionci` | `ParameterConfidenceInterval`

Reaction object

Object containing model reaction information

Description

The reaction object represents a *reaction*, which describes a transformation, transport, or binding process that changes one or more species. Typically, the change is the amount of a species. For example:

```
Creatine + ATP <-> ADP + phosphocreatine
```

```
glucose + 2 ADP + 2 Pi -> 2 lactic acid + 2 ATP + 2 H2O
```

Spaces are required before and after species names and stoichiometric values.

See “Property Summary” on page 2-680 for links to reaction object property reference pages.

Properties define the characteristics of an object. Use the `get` and `set` commands to list object properties and change their values at the command line. You can graphically change object properties in the graphical user interface.

Note If you create a new reaction at the command line and do not specify its name, the reaction gets an automatic name `Reaction_N`, where *N* is a positive integer. *N* increases monotonically as you add more reactions.

If you copy a reaction using `copyobj`, the name of the copied reaction is generated by appending `_N`, where *N* is the smallest integer not in use by that prefix. For example, `GivenName_1` gets copied to `GivenName_1_1`.

Constructor Summary

addreaction (model)	Create reaction object and add to model object

Method Summary

addkineticlaw (reaction)	Create kinetic law object and add to reaction object
addproduct (reaction)	Add product species object to reaction object
addreactant (reaction)	Add species object as reactant to reaction object
copyobj	Copy SimBiology object and its children
delete	Delete SimBiology object
display	Display summary of SimBiology object
get	Get SimBiology object properties
rename	Rename object and update expressions
rmproduct (reaction)	Remove species object from reaction object products
rmreactant (reaction)	Remove species object from reaction object reactants
set	Set SimBiology object properties

Property Summary

Active	Indicate object in use during simulation
KineticLaw	Show kinetic law used for `ReactionRate`
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Products	Array of reaction products
Reactants	Array of reaction reactants
Reaction	Reaction object reaction
ReactionRate	Reaction rate equation in reaction object
Reversible	Specify whether reaction is reversible or irreversible
Stoichiometry	Species coefficients in reaction
Tag	Specify label for SimBiology object
Type	Display SimBiology object type
UserData	Specify data to associate with object

See Also

"Definitions and Evaluations of Reactions in SimBiology Models", `AbstractKineticLaw object`, `Configset object`, `KineticLaw object`, `Model object`, `Parameter object`, `Root object`, `Rule object`, `Species object`

Version History

Introduced in R2006b

remove

Remove entries from `SimBiology.Scenarios` object

Syntax

```
sObj = remove(sObj,entryNameOrIndex)
sObj = remove(sObj,entryIndex,subIndex)
```

Description

`sObj = remove(sObj,entryNameOrIndex)` removes the entry (or subentry on page 2-799) `entryNameorIndex` from the `SimBiology.Scenarios` object `sObj`.

`sObj = remove(sObj,entryIndex,subIndex)` removes the subentry `subIndex` of the entry `entryIndex`.

Examples

Generate Different Simulation Scenarios for Glucose-Insulin Response

Load the model of glucose-insulin response. For details about the model, see the **Background** section in “Simulate the Glucose-Insulin Response”.

```
sbioloadproject('insulindemo','m1');
```

The model contains different parameter values and initial conditions that represents different insulin impairments (such as Type 2 diabetes, low insulin sensitivity, and so on) stored in five variants.

```
variants = getvariant(m1)
```

```
variants =
   SimBiology Variant Array

   Index:  Name:             Active:
   1       Type 2 diabetic   false
   2       Low insulin se... false
   3       High beta cell... false
   4       Low beta cell ... false
   5       High insulin s... false
```

Suppress an informational warning that is issued during simulations.

```
warnSettings = warning('off','SimBiology:DimAnalysisNotDone_MatlabFcn_Dimensionless');
```

Select a dose that represents a single meal of 78 grams of glucose.

```
singleMeal = sbioselect(m1,'Name','Single Meal');
```

Create a `Scenarios` object to represent different initial conditions combined with the dose. That is, create a `scenario` object where each variant is paired (or combined) with the dose, for a total of five simulation scenarios.

```
sObj = SimBiology.Scenarios;
add(sObj,'cartesian','variants',variants);
add(sObj,'cartesian','dose',singleMeal)
```

```
ans =
  Scenarios (5 scenarios)

                  Name            Content           Number
                ________    ____________________    ______

    Entry 1     variants    SimBiology variants       5
    x Entry 2   dose        SimBiology dose           1

  See also Expression property.
```

`sObj` contains two entries. Use the `generate` function to combine the entries and generate five scenarios. The function returns a scenarios table, where each row represents a scenario and each column represents an entry of the `Scenarios` object.

```
scenariosTbl = generate(sObj)
```

```
scenariosTbl=5×2 table
           variants                    dose
    ____________________    ____________________________

    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
```

Change the entry name of the first entry.

```
rename(sObj,1,'Insulin Impairements')
```

```
ans =
  Scenarios (5 scenarios)

                       Name                Content           Number
                ____________________    ____________________    ______

    Entry 1     Insulin Impairements    SimBiology variants       5
    x Entry 2   dose                    SimBiology dose           1

  See also Expression property.
```

Create a `SimFunction` object to simulate the generated scenarios. Use the `Scenarios` object as the input and specify the plasma glucose and insulin concentrations as reponses (outputs of the function to be plotted). Specify `[]` for the dose input argument since the `Scenarios` object already has the dosing information.

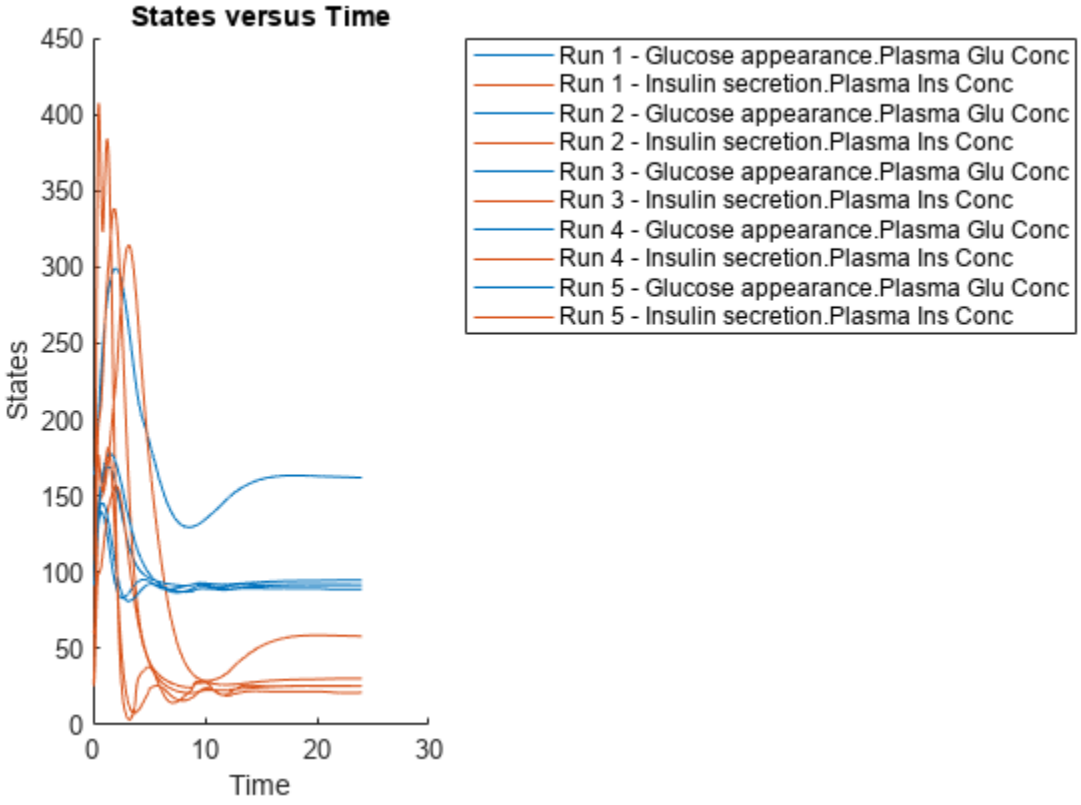
```
f = createSimFunction(m1,sObj,{'[Plasma Glu Conc]','[Plasma Ins Conc]'},[])
```

```
f =
SimFunction

Parameters:

            Name              Value        Type                      Units
    ____________________________    ______    ____________    ____________________________

    {'Plasma Volume (Glu)'  }      1.88    {'parameter'}    {'deciliter'
    {'k1'                   }     0.065    {'parameter'}    {'1/minute'
    {'k2'                   }     0.079    {'parameter'}    {'1/minute'
    {'Plasma Volume (Ins)'  }      0.05    {'parameter'}    {'liter'
    {'m1'                   }      0.19    {'parameter'}    {'1/minute'
    {'m2'                   }     0.484    {'parameter'}    {'1/minute'
    {'m4'                   }    0.1936    {'parameter'}    {'1/minute'
    {'m5'                   }    0.0304    {'parameter'}    {'minute/picomole'
    {'m6'                   }    0.6469    {'parameter'}    {'dimensionless'
    {'Hepatic Extraction'   }       0.6    {'parameter'}    {'dimensionless'
    {'kmax'                 }    0.0558    {'parameter'}    {'1/minute'
    {'kmin'                 }     0.008    {'parameter'}    {'1/minute'
    {'kabs'                 }    0.0568    {'parameter'}    {'1/minute'
    {'kgri'                 }         0    {'parameter'}    {'1/minute'
    {'f'                    }       0.9    {'parameter'}    {'dimensionless'
    {'a'                    }         0    {'parameter'}    {'1/milligram'
    {'b'                    }      0.82    {'parameter'}    {'dimensionless'
    {'c'                    }         0    {'parameter'}    {'1/milligram'
    {'d'                    }      0.01    {'parameter'}    {'dimensionless'
    {'kp1'                  }       2.7    {'parameter'}    {'milligram/minute'
    {'kp2'                  }    0.0021    {'parameter'}    {'1/minute'
    {'kp3'                  }     0.009    {'parameter'}    {'(milligram/minute)/(picomole/liter)
    {'kp4'                  }    0.0618    {'parameter'}    {'(milligram/minute)/picomole'
    {'ki'                   }    0.0079    {'parameter'}    {'1/minute'
    {'[Ins Ind Glu Util]'   }         1    {'parameter'}    {'milligram/minute'
    {'Vm0'                  }    2.5129    {'parameter'}    {'milligram/minute'
    {'Vmx'                  }     0.047    {'parameter'}    {'(milligram/minute)/(picomole/liter)
    {'Km'                   }    225.59    {'parameter'}    {'milligram'
    {'p2U'                  }    0.0331    {'parameter'}    {'1/minute'
    {'K'                    }      2.28    {'parameter'}    {'picomole/(milligram/deciliter)'
    {'alpha'                }      0.05    {'parameter'}    {'1/minute'
    {'beta'                 }      0.11    {'parameter'}    {'(picomole/minute)/(milligram/decili
    {'gamma'                }       0.5    {'parameter'}    {'1/minute'
    {'ke1'                  }    0.0005    {'parameter'}    {'1/minute'
    {'ke2'                  }       339    {'parameter'}    {'milligram'
    {'Basal Plasma Glu Conc'}     91.76    {'parameter'}    {'milligram/deciliter'
    {'Basal Plasma Ins Conc'}     25.49    {'parameter'}    {'picomole/liter'

Observables:

          Name              Type              Units
    ____________________    ___________    ____________________

    {'[Plasma Glu Conc]'}    {'species'}    {'milligram/deciliter'}
    {'[Plasma Ins Conc]'}    {'species'}    {'picomole/liter'     }

Dosed:

    TargetName       TargetDimension
    __________    ____________________
```

```
    {'Dose'}    {'Mass (e.g., gram)'}

TimeUnits: hour
```

Simulate the model for 24 hours and plot the simulation data. The data contains five runs, where each run represents a scenario in the Scenarios object.

```
sd = f(sObj,24);
sbioplot(sd)
```




```
ans =
  Axes (SbioPlot) with properties:

            XLim: [0 30]
            YLim: [0 450]
          XScale: 'linear'
          YScale: 'linear'
    GridLineStyle: '-'
         Position: [0.0920 0.1100 0.2956 0.8150]
            Units: 'normalized'

  Show all properties
```

If you have Statistics and Machine Learning Toolbox™, you can also draw sample values for model quantities from various probability distributions. For instance, suppose that the parameters `Vmx` and

kp3, which are known for the low and high insulin sensitivity, follow the lognormal distribution. You can generate sample values for these parameters from such a distribution, and perform a scan to explore model behavior.

Define the lognormal probability distribution object for Vmx.

```
pd_Vmx = makedist('lognormal')
```

```
pd_Vmx =
  LognormalDistribution

  Lognormal distribution
       mu = 0
    sigma = 1
```

By definition, the parameter mu is the mean of logarithmic values. To vary the parameter value around the base (model) value of the parameter, set mu to `log(`*`model_value`*`)`. Set the standard deviation (*sigma*) to 0.2. For a small *sigma* value, the mean of a lognormal distribtion is approximately equal to `log(`*`model_value`*`)`. For details, see “Lognormal Distribution” (Statistics and Machine Learning Toolbox).

```
Vmx = sbioselect(m1,'Name','Vmx');
pd_Vmx.mu = log(Vmx.Value);
pd_Vmx.sigma = 0.2
```

```
pd_Vmx =
  LognormalDistribution

  Lognormal distribution
       mu = -3.05761
    sigma =      0.2
```

Similarly define the probability distribution for kp3.

```
pd_kp3 = makedist('lognormal');
kp3 = sbioselect(m1,'Name','kp3');
pd_kp3.mu = log(kp3.Value);
pd_kp3.sigma = 0.2
```

```
pd_kp3 =
  LognormalDistribution

  Lognormal distribution
       mu = -4.71053
    sigma =      0.2
```

Now define a joint probability distribution to draw sample values for Vmx and kp3, with a rank correlation to specify some correlation between these two parameters. Note that this correlation assumption is for the illustration purposes of this example only and may not be biologically relevant.

First remove the variants entry (entry 1) from sObj.

```
remove(sObj,1)
```

```
ans =
  Scenarios (1 scenarios)
```

```
                Name         Content         Number
                ____    _________________    ______

    Entry 1     dose    SimBiology dose        1

  See also Expression property.
```

Add an entry that defines the joint probability distribution with a rank correlation matrix.

```
add(sObj,'cartesian',["Vmx","kp3"],[pd_Vmx, pd_kp3],'RankCorrelation',[1,0.5;0.5,1])
```

```
ans =
  Scenarios (2 scenarios)

                    Name           Content              Number
                    ____    ________________________    ___________

    Entry 1         dose    SimBiology dose             1
    x (Entry 2.1    Vmx     Lognormal distribution      2 (default)
    + Entry 2.2)    kp3     Lognormal distribution      2 (default)

  See also Expression property.
```

By default, the number of samples to draw from the joint distribution is set to 2. Increase the number of samples.

```
updateEntry(sObj,2,'Number',50)
```

```
ans =
  Scenarios (50 scenarios)

                    Name           Content              Number
                    ____    ________________________    ______

    Entry 1         dose    SimBiology dose               1
    x (Entry 2.1    Vmx     Lognormal distribution        50
    + Entry 2.2)    kp3     Lognormal distribution        50

  See also Expression property.
```

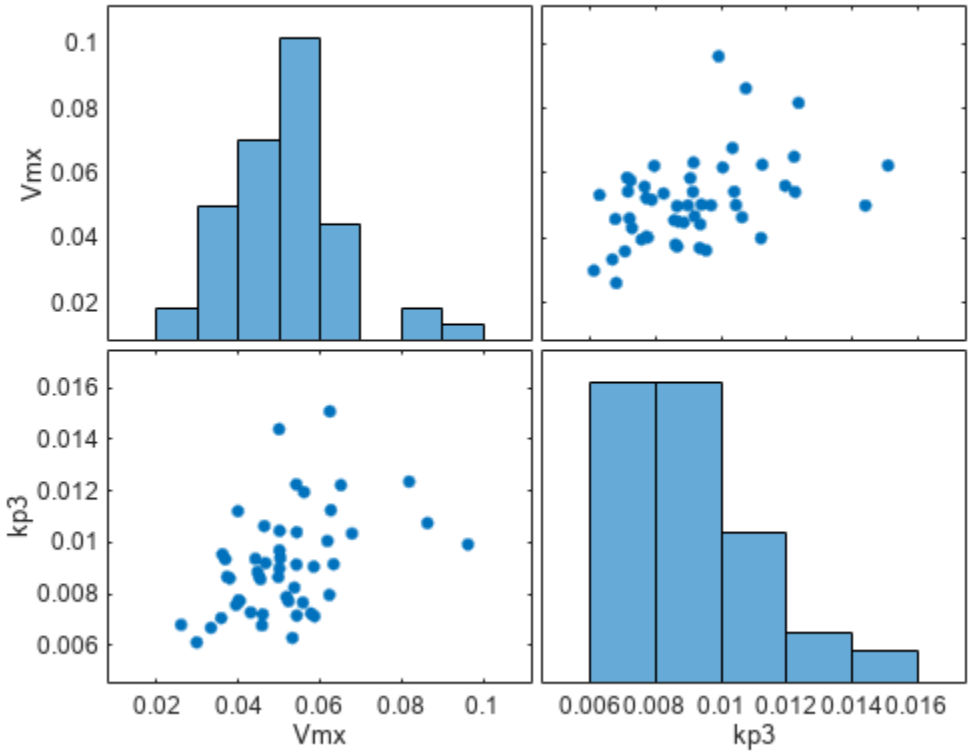
Verify that the `Scenarios` object can be simulated with the model. The `verify` function throws an error if any entry does not resolve uniquely to an object in the model or the entry contents have inconsistent lengths (sample sizes). The function throws a warning if multiple entries resolve to the same object in the model.

```
verify(sObj,m1)
```

Generate the simulation scenarios. Plot the sample values using `plotmatrix`. You can see the value of `Vmx` is varied around its model value 0.047 and that of `kp3` around 0.009.

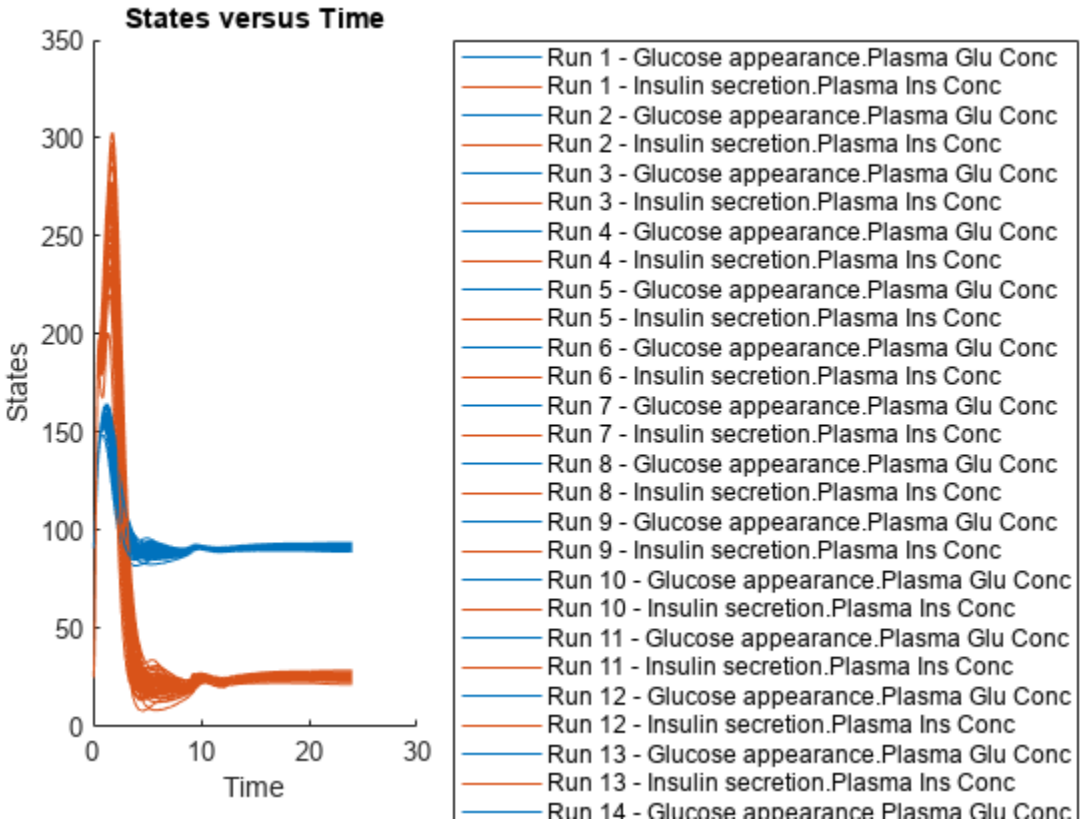
```
sTbl = generate(sObj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl.Vmx,sTbl.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
```

```
ax(2,1).XLabel.String = "Vmx";
ax(2,2).XLabel.String = "kp3";
```



Simulate the scenarios using the same SimFunction you created previously. You do not need to create a new SimFunction object even though the Scenarios object has been updated.

```
sd2 = f(sObj,24);
sbioplot(sd2);
```



By default, SimBiology uses the random sampling method. You can change it to the Latin hypercube sampling (or sobol or halton) for a more systematic space-filling approach.

```
entry2struct = getEntry(sObj,2)
```

```
entry2struct = struct with fields:
                Name: {'Vmx'  'kp3'}
             Content: [2x1 prob.LognormalDistribution]
              Number: 50
    RankCorrelation: [2x2 double]
          Covariance: []
      SamplingMethod: 'random'
    SamplingOptions: [0x0 struct]
```

```
entry2struct.SamplingMethod = 'lhs'
```

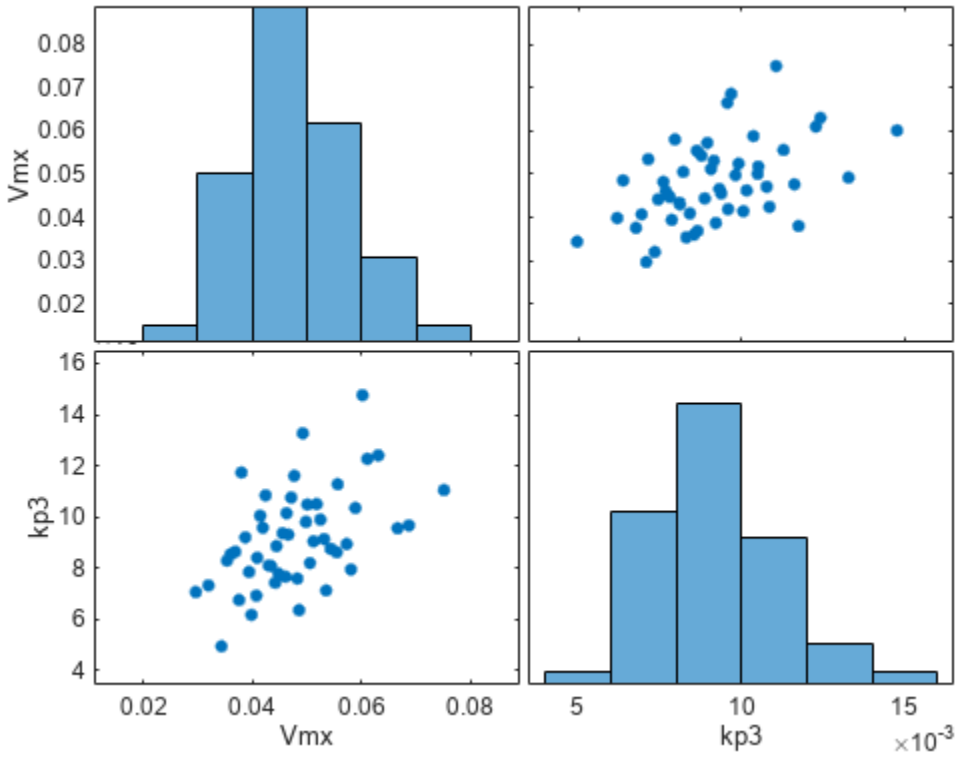
```
entry2struct = struct with fields:
                Name: {'Vmx'  'kp3'}
             Content: [2x1 prob.LognormalDistribution]
              Number: 50
    RankCorrelation: [2x2 double]
          Covariance: []
      SamplingMethod: 'lhs'
    SamplingOptions: [0x0 struct]
```

You can now use the updated structure to modify entry 2.

```
updateEntry(sObj,2,entry2struct)

ans =
  Scenarios (50 scenarios)

                    Name           Content              Number
                    ____    ____________________        ______

    Entry 1         dose    SimBiology dose               1
    x (Entry 2.1    Vmx     Lognormal distribution        50
    + Entry 2.2)    kp3     Lognormal distribution        50

  See also Expression property.
```

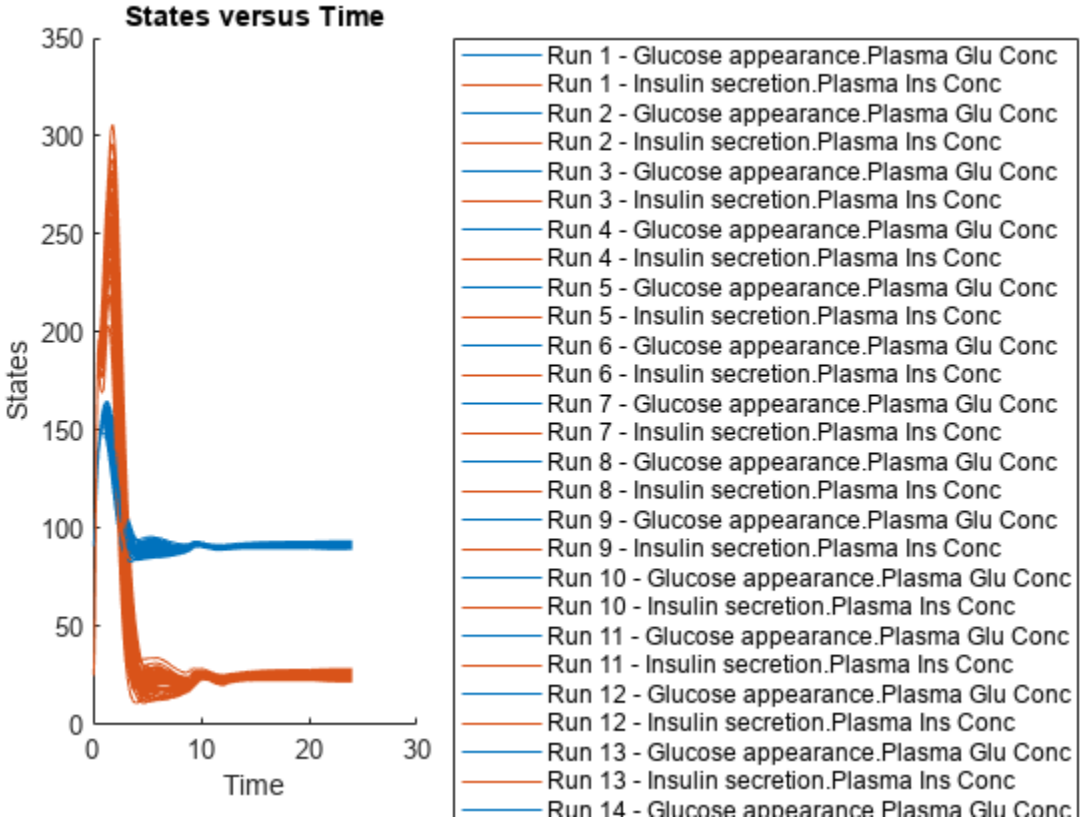
Visualize the sample values.

```
sTbl2 = generate(sObj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl2.Vmx,sTbl2.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
ax(2,1).XLabel.String = "Vmx";
ax(2,2).XLabel.String = "kp3";
```



Simulate the scenarios.

```
sd3 = f(sObj,24);
sbioplot(sd3);
```



Restore warning settings.

```
warning(warnSettings);
```

Input Arguments

`sObj` — Simulation scenarios

`SimBiology.Scenarios` object

Simulation scenarios, specified as a `SimBiology.Scenarios` object.

`entryNameOrIndex` — Entry name or index

character vector | string | scalar positive integer

Entry name or index, specified as a character vector, string, or scalar positive integer. You can also specify the name of a subentry.

If you are specifying an index, it must be smaller than or equal to the number of entries in the object.

Data Types: `double` | `char` | `string`

`entryIndex` — Entry index

scalar positive integer

Entry index, specified as a scalar positive integer. The entry index must be smaller than or equal to the number of entries in the object.

Data Types: `double`

`subIndex` — Entry subindex
scalar positive integer

Entry subindex, specified as a scalar positive integer. The subindex must be smaller than or equal to the number of subentries in the entry.

Data Types: `double`

Output Arguments

`sObj` — Simulation scenarios
`Scenarios` object

Simulation scenarios, returned as a `Scenarios` object.

Version History

Introduced in R2019b

See Also

`SimBiology.Scenarios` | `SimFunction object` | `createSimFunction (model)`

Topics

“SimBiology.Scenarios Terminology” on page 2-799
“Combine Simulation Scenarios in SimBiology”

remove

Remove simulation data from `SimData` object using expressions

Syntax

```
[t,x,names] = remove(simdata,query)
sdOut = remove(simdata,query)
___ = remove(simdata,query,'Format',formatValue)
```

Description

`[t,x,names] = remove(simdata,query)` returns the simulation time points `t`, the simulation data `x`, and corresponding `names` after removing the simulation data of model components that match `query`.

`sdOut = remove(simdata,query)` returns the simulation results after removing the simulation data of model components that match the `query` as a `SimData` object `sdOut`.

`___ = remove(simdata,query,'Format',formatValue)` returns the simulation data in the specified data format.

Examples

Remove Subset of Simulation Data from `SimData`

Load the model of glucose-insulin response. For details about the model, see the **Background** section in “Simulate the Glucose-Insulin Response”.

```
sbioloadproject('insulindemo.sbproj','m1');
```

Suppress an information warning that is issued during simulations.

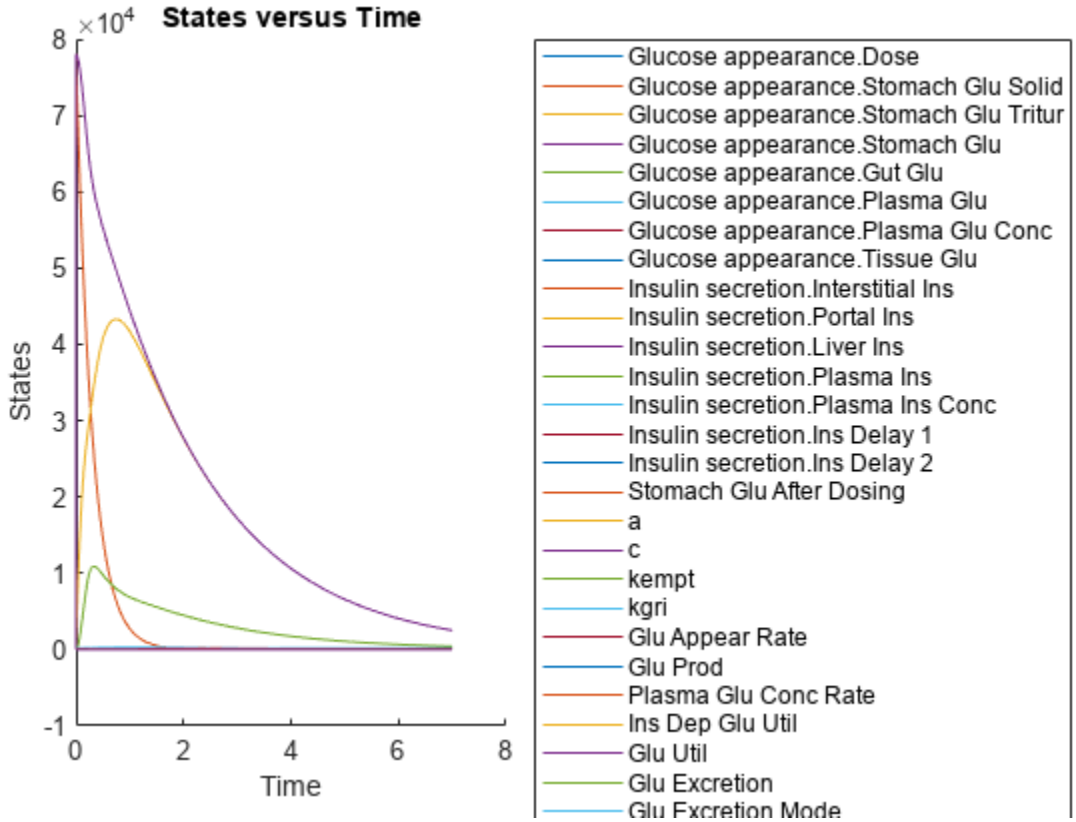
```
warnSettings = warning('off', 'SimBiology:DimAnalysisNotDone_MatlabFcn_Dimensionless');
```

Simulate a single meal for a normal subject for 7 hours.

```
singleMeal = sbioselect(m1,'Name','Single Meal');
cs = getconfigset(m1,'active');
cs.StopTime = 7;
sd1 = sbiosimulate(m1,singleMeal)
```

```
   SimBiology Simulation Data

   ModelName:        Cobelli's Glucose-Insulin System
   Logged Data:
     Species:        15
     Compartment:    0
     Parameter:      24
     Sensitivity:    0
```

```
     Observable:     0

sbioplot(sd1);
```

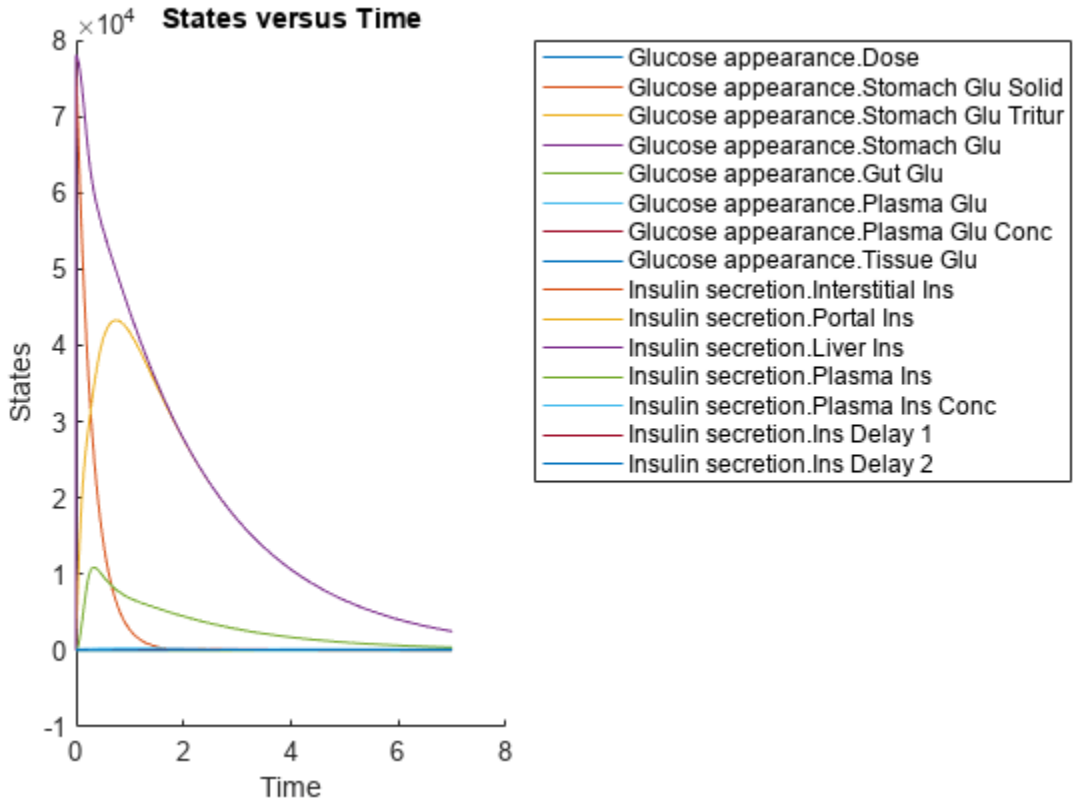


Remove all parameter data logged in the `SimData` object *sd*.

```
[t,x,names] = remove(sd1,{'Type','parameter'});
```

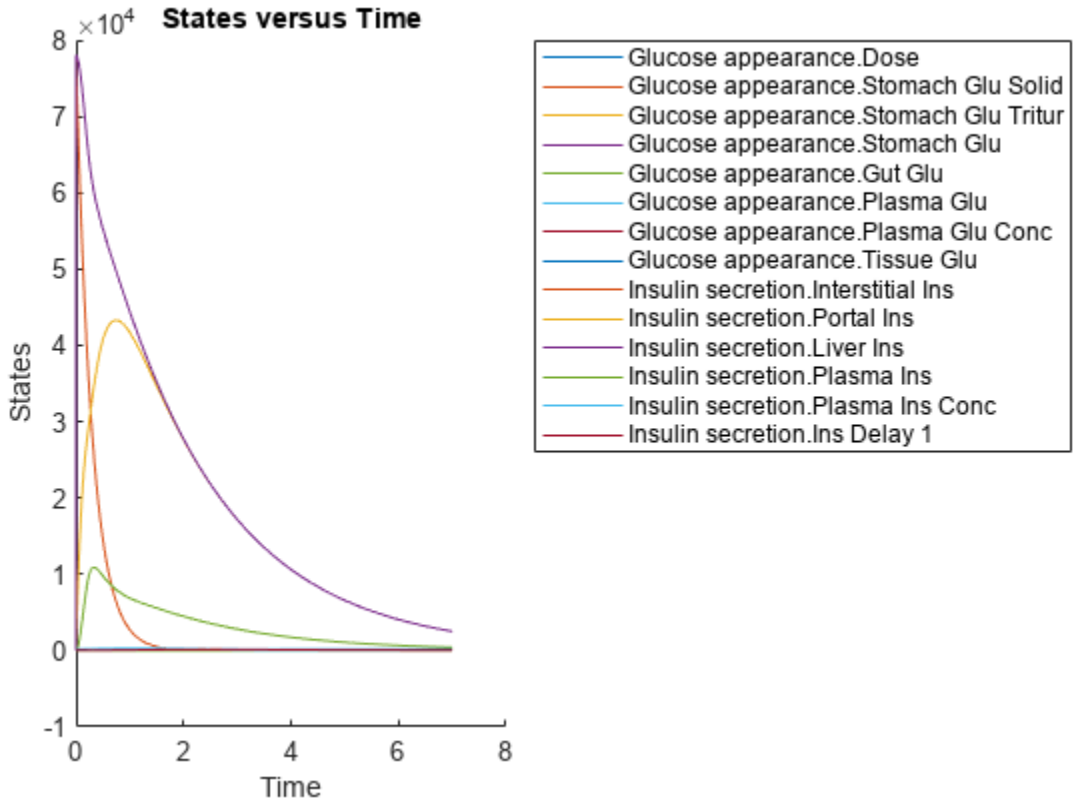
Remove all parameter data and return as a new `SimData` object.

```
sd2 = remove(sd1,{'Type','parameter'});
sbioplot(sd2);
```



Remove the simulation data of a species by specifying its name.

```
sd3 = removebyname(sd2,["[Insulin secretion].[Ins Delay 2]"]);
sbioplot(sd3);
```



Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

`simdata` — Simulation data

`SimData` object | array of `SimData` objects

Simulation data, specified as a `SimData` object or array of `SimData` objects.

`query` — Search query

cell array of character vectors | string vector

Search query, specified as a cell array of character vectors or a string vector. The query consists of some combination of name-value pair arguments or `'Where'` clauses. For a more complete description of the query syntax, including `'Where'` clauses and their supported condition types, see `sbioselect`.

You can use any of the metadata fields available in the `DataInfo` property of a `SimData` object in the query. The fields include `'Type'`, `'Name'`, `'Units'`, `'Compartment'` (for species only), and `'Reaction'` (for parameters only).

Example: `{'Type','species'}`

Data Types: `string` | `cell`

`formatValue` — Simulation data format
character vector | string

Simulation data format, specified as a character vector or string. Some formats require you to specify only one output argument. The valid formats follow.

- `'num'` — This format returns simulation time points and simulation data in numeric arrays and the names of quantities and sensitivities as a cell array. This format is the default when you run `getdata` with multiple output arguments.
- `'nummetadata'` — This format returns a cell array of metadata structures instead of the names of quantities and sensitivities as the third output argument.
- `'numqualnames'` — This format returns qualified names in the third output argument to resolve ambiguities.

You must specify only one output argument for the following formats.

- `'simdata'` — This format returns data in a new `SimData` object or an array of `SimData` objects. This format is the default when you specify a single output argument.
- `'struct'` — This format returns a structure or structure array that contains both data and metadata.
- `'ts'` — This format returns data as a cell array.
  - If `simdata` is scalar, the cell array is an *m*-by-1 array, where each element is a `timeseries` object. *m* is the number of quantities and sensitivities logged during the simulation.
  - If `simdata` is not scalar, the cell array is *k*-by-1, where each element of the cell array is an *m*-by-1 cell array of `timeseries` objects. *k* is the size of `simdata`, and *m* is the number of quantities or sensitivities in each `SimData` object in `simdata`. In other words, the function returns an individual time series for each state or column and for each `SimData` object in `simdata`.
- `'tslumped'` — This format returns the data as a cell array of `timeseries` objects, combining data from each `SimData` object into a single time series.

Output Arguments

`t` — Simulation time points
numeric vector | cell array

Simulation time points, returned as a numeric vector or cell array. If `simdata` is scalar, `t` is an *n*-by-1 vector, where *n* is the number of time points. If `simdata` is an array of objects, `t` is a *k*-by-1 cell array, where *k* is the size of `simdata`.

`x` — Simulation data
numeric matrix | cell array

Simulation data, returned as a numeric matrix or cell array. If `simdata` is scalar, `x` is an *n*-by-*m* matrix, where *n* is the number of time points and *m* is the number of quantities and sensitivities logged during the simulation. If `simdata` is an array of objects, `x` is a *k*-by-1 cell array, where *k* is the size of `simdata`.

`names` — Names of quantities and sensitivities
cell array

Names of quantities and sensitivities logged during the simulation, returned as a cell array. If `simdata` is scalar, `names` is an *m*-by-1 cell array. If `simdata` is an array of objects, `names` is a *k*-by-1 cell array, where *k* is the size of `simdata`.

`sdOut` — Simulation results
`SimData` object

Simulation results, returned as a `SimData` object.

Version History

Introduced in R2020a

See Also

`SimData` | `select` | `selectbyname`

removebyname

Remove simulation data by name from `SimData` object

Syntax

```
[t,x,names] = removebyname(simdata,selectNames)
sdOut = removebyname(simdata,selectNames)
___ = removebyname(simdata,selectNames,'Format',formatValue)
```

Description

`[t,x,names] = removebyname(simdata,selectNames)` returns the simulation time points `t`, the simulation data `x`, and corresponding `names` after removing the simulation data of model components specified by `selectNames`.

`sdOut = removebyname(simdata,selectNames)` returns the simulation results after removing the simulation data of model components specified by `selectNames` as a `SimData` object `sdOut`.

`___ = removebyname(simdata,selectNames,'Format',formatValue)` returns the simulation data in the specified data format.

Examples

Remove Subset of Simulation Data from SimData

Load the model of glucose-insulin response. For details about the model, see the **Background** section in “Simulate the Glucose-Insulin Response”.

```
sbioloadproject('insulindemo.sbproj','m1');
```

Suppress an information warning that is issued during simulations.

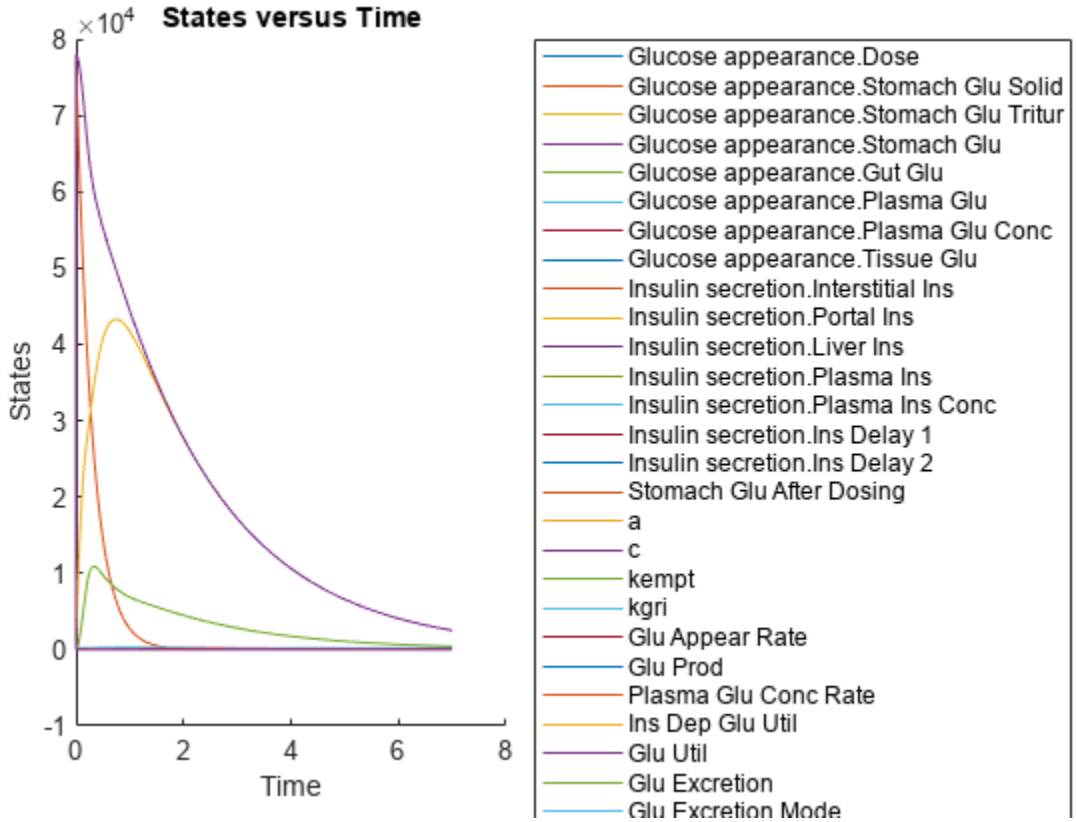
```
warnSettings = warning('off', 'SimBiology:DimAnalysisNotDone_MatlabFcn_Dimensionless');
```

Simulate a single meal for a normal subject for 7 hours.

```
singleMeal = sbioselect(m1,'Name','Single Meal');
cs = getconfigset(m1,'active');
cs.StopTime = 7;
sd1 = sbiosimulate(m1,singleMeal)
```

```
   SimBiology Simulation Data

   ModelName:        Cobelli's Glucose-Insulin System
   Logged Data:
     Species:        15
     Compartment:    0
     Parameter:      24
     Sensitivity:    0
```

```
     Observable:     0

sbioplot(sd1);
```

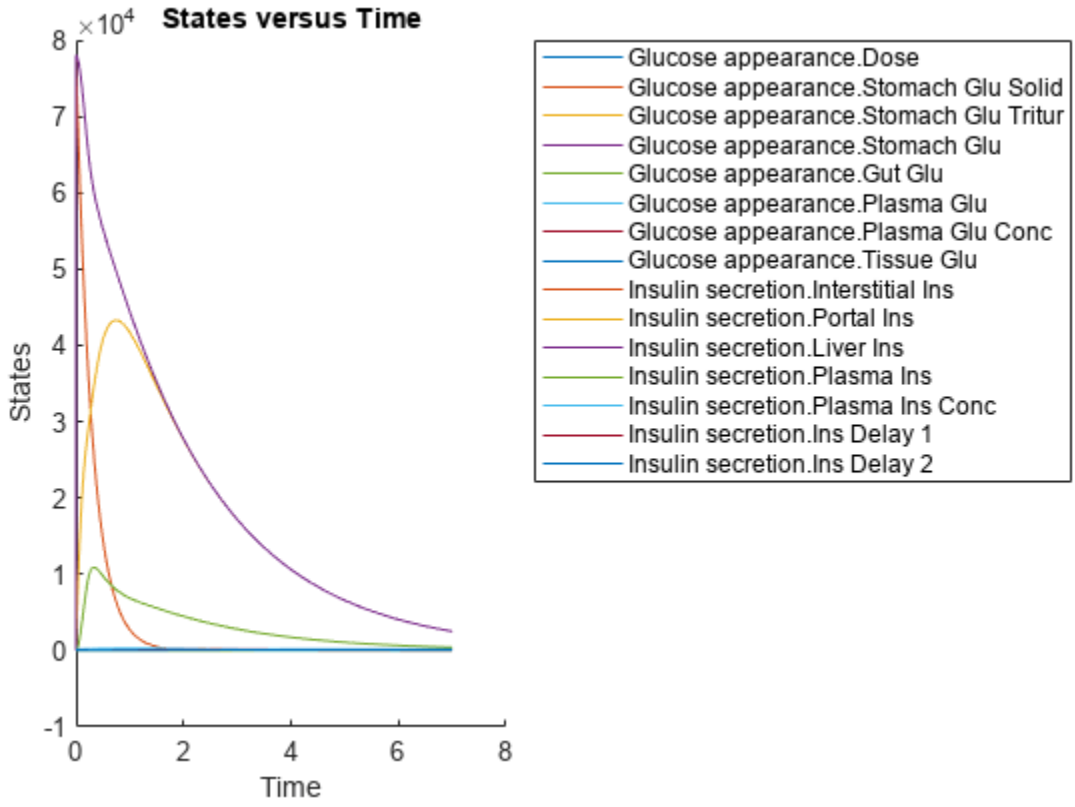


Remove all parameter data logged in the `SimData` object *sd*.

```
[t,x,names] = remove(sd1,{'Type','parameter'});
```

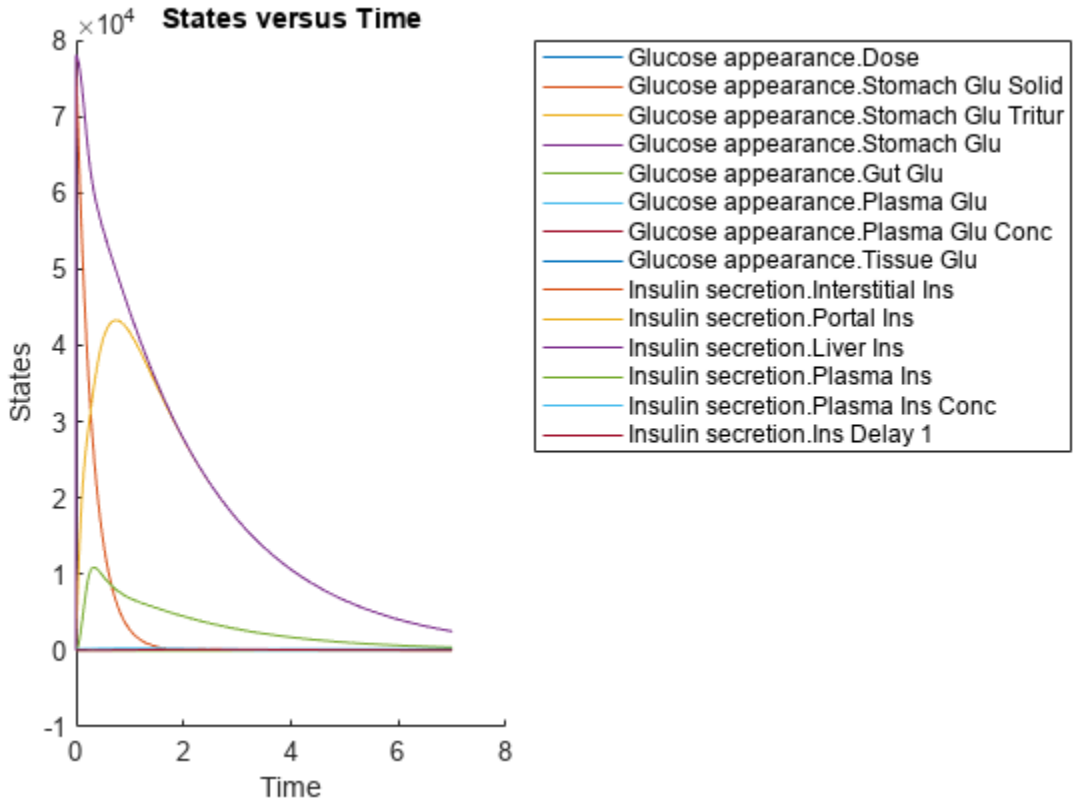
Remove all parameter data and return as a new `SimData` object.

```
sd2 = remove(sd1,{'Type','parameter'});
sbioplot(sd2);
```



Remove the simulation data of a species by specifying its name.

```
sd3 = removebyname(sd2,["[Insulin secretion].[Ins Delay 2]"]);
sbioplot(sd3);
```



Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

`simdata` — Simulation data

`SimData` object | array of `SimData` objects

Simulation data, specified as a `SimData` object or array of `SimData` objects.

`selectNames` — Names of states

character vector | string | string vector | cell array of character vectors

Names of states that you want to select data for, specified as a character vector, string, string vector, or cell array of character vectors.

Example: `{'x1','x2','x3'}`

Data Types: `char` | `string` | `cell`

`formatValue` — Simulation data format

character vector | string

Simulation data format, specified as a character vector or string. Some formats require you to specify only one output argument. The valid formats follow.

- `'num'` — This format returns simulation time points and simulation data in numeric arrays and the names of quantities and sensitivities as a cell array. This format is the default when you run `getdata` with multiple output arguments.
- `'nummetadata'` — This format returns a cell array of metadata structures instead of the names of quantities and sensitivities as the third output argument.
- `'numqualnames'` — This format returns qualified names in the third output argument to resolve ambiguities.

You must specify only one output argument for the following formats.

- `'simdata'` — This format returns data in a new `SimData` object or an array of `SimData` objects. This format is the default when you specify a single output argument.
- `'struct'` — This format returns a structure or structure array that contains both data and metadata.
- `'ts'` — This format returns data as a cell array.
  - If `simdata` is scalar, the cell array is an *m*-by-1 array, where each element is a `timeseries` object. *m* is the number of quantities and sensitivities logged during the simulation.
  - If `simdata` is not scalar, the cell array is *k*-by-1, where each element of the cell array is an *m*-by-1 cell array of `timeseries` objects. *k* is the size of `simdata`, and *m* is the number of quantities or sensitivities in each `SimData` object in `simdata`. In other words, the function returns an individual time series for each state or column and for each `SimData` object in `simdata`.
- `'tslumped'` — This format returns the data as a cell array of `timeseries` objects, combining data from each `SimData` object into a single time series.

Output Arguments

`t` — Simulation time points

numeric vector | cell array

Simulation time points, returned as a numeric vector or cell array. If `simdata` is scalar, `t` is an *n*-by-1 vector, where *n* is the number of time points. If `simdata` is an array of objects, `t` is a *k*-by-1 cell array, where *k* is the size of `simdata`.

`x` — Simulation data

numeric matrix | cell array

Simulation data, returned as a numeric matrix or cell array. If `simdata` is scalar, `x` is an *n*-by-*m* matrix, where *n* is the number of time points and *m* is the number of quantities and sensitivities logged during the simulation. If `simdata` is an array of objects, `x` is a *k*-by-1 cell array, where *k* is the size of `simdata`.

`names` — Names of quantities and sensitivities

cell array

Names of quantities and sensitivities logged during the simulation, returned as a cell array. If `simdata` is scalar, `names` is an *m*-by-1 cell array. If `simdata` is an array of objects, `names` is a *k*-by-1 cell array, where *k* is the size of `simdata`.

`sdOut` — Simulation results

`SimData` object

Simulation results, returned as a `SimData` object.

Version History

Introduced in R2020a

See Also

`SimData` | `select` | `selectbyname`

removeconfigset (model)

Remove configuration set from model

Syntax

```
removeconfigset(modelObj, 'NameValue')
removeconfigset(modelObj, configsetObj)
```

Arguments

modelObj	`Model object` from which to remove the configuration set.
NameValue	Name of the configuration set.
configsetObj	`Configset object` that is to be removed from the model object.

Description

`removeconfigset(`*`modelObj`*`, '`*`NameValue`*`')` removes and deletes the configset object with the name *`NameValue`* from the SimBiology model object *`modelObj`*. A configuration set object stores simulation-specific information. A SimBiology model can contain multiple configuration sets with one being active at any given time. The active configuration set contains the settings that are used during the simulation. *`modelObj`* always contains at least one configuration set object with name configured to `'default'`. You cannot remove the default configuration set from *`modelObj`*. If the active configuration set is removed from *`modelObj`*, then the default configuration set will be made active.

`removeconfigset(`*`modelObj`*`, `*`configsetObj`*`)` removes and deletes the configuration set object, *`configsetObj`*, from the SimBiology model, *`modelObj`*.

Examples

1 Create a model object by importing the file `oscillator.xml` and add a configset.

```
modelObj  = sbmlimport('oscillator');
configsetObj = addconfigset(modelObj, 'myset');
```

2 Remove the configset from `modelObj` by name or alternatively by indexing.

```
% Remove the configset with name 'myset'.
  removeconfigset(modelObj, 'myset');

 % Get all configset objects and remove the second.
  configsetObj = getconfigset(modelObj);
  removeconfigset(modelObj, configsetObj(2));
```

See Also

`Model object`, `Configset object`, `addconfigset`, `getconfigset`, `setactiveconfigset`

Version History

Introduced in R2006a

removedose (model)

Remove dose object from model

Syntax

```
doseObj2 = removedose(modelObj, 'DoseName')
doseObj2 = removedose(modelObj, doseObj)
```

Arguments

modelObj	`Model object` from which you remove a dose object.
DoseName	Name of the dose object to remove from a model object. *DoseName* is the value of the dose object property `Name`.
doseObj	Dose object to remove from a model object.

Outputs

doseObj2	ScheduleDose or RepeatDose object.

Description

`doseObj2 = removedose(`*modelObj*`, '`*DoseName*`')` removes a SimBiology ScheduleDose or RepeatDose object with the name *DoseName* from a model object (*modelObj*). returns the dose object (*doseObj*), and assigns [] to the dose object property `Parent`.

You can add a removed dose object back to a model object using the method `adddose`.

`doseObj2 = removedose(`*modelObj*`, `*doseObj*`)` removes a SimBiology ScheduleDose or RepeatDose object *doseObj*.

Examples

Remove a dose object from a model object.

1. Create model and dose objects, and then add dose to model.

   ```
   modelObj = sbiomodel('mymodel');
   dose1Obj = adddose(modelObj, 'dose1');
   ```

2. Remove dose object from model object.

   ```
   removedose(mymodel, 'dose1');
   ```

Get all dose objects from a model object, and then remove the second dose object.

```
AllDoseObjects = getdose(mymodel);
removedose(mymodel, AllDoseObjects(2));
```

See Also

`Model` methods:

- `adddose` — add a dose object to a model object
- `getdose` — get dose information from a model object
- `removedose` — remove a dose object from a model object

Dose object constructor `sbiodose`.

`ScheduleDose object` and `RepeatDose object` methods:

- `copyobj` — copy a dose object from one model object to another model object
- `get` — view properties for a dose object
- `set` — define or modify properties for a dose object

Version History

Introduced in R2010a

removeobservable

Remove Sobol indices or elementary effects of observables

Syntax

```
results = removeobservable(gsaObj,obsNames)
```

Description

`results = removeobservable(gsaObj,obsNames)` removes the Sobol indices or elementary effects computed for the specified observables `obsNames` from `gsaResults`.

Examples

Perform Global Sensitivity Analysis by Computing First- and Total-Order Sobol Indices

Load the “Tumor Growth Model”.

```
sbioloadproject tumor_growth_vpop_sa.sbproj
```

Get a variant with the estimated parameters and the dose to apply to the model.

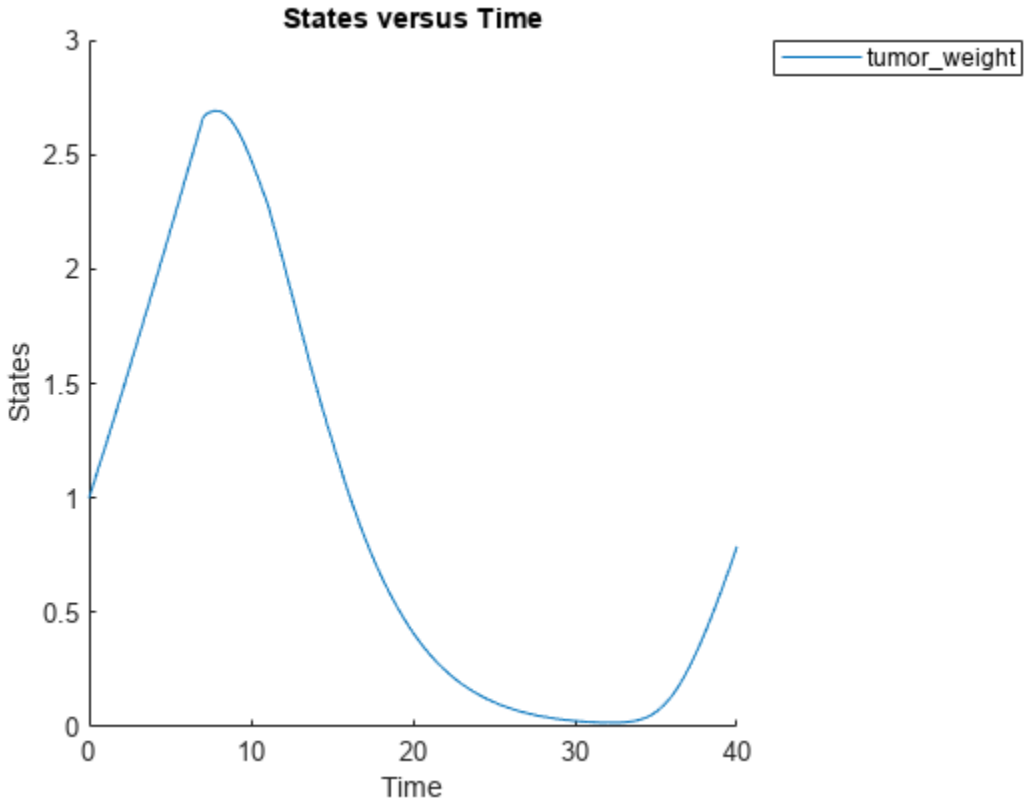
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

Get the active configset and set the tumor weight as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'tumor_weight';
```

Simulate the model and plot the tumor growth profile.

```
sbioplot(sbiosimulate(m1,cs,v,d));
```



Perform global sensitivity analysis (GSA) on the model to find the model parameters that the tumor growth is sensitive to.

First, retrieve model parameters of interest that are involved in the pharmacodynamics of the tumor growth. Define the model response as the tumor weight.

```
modelParamNames = {'L0','L1','w0','k1','k2'};
outputName = 'tumor_weight';
```

Then perform GSA by computing the first- and total-order Sobol indices using `sbiosobol`. Set `'ShowWaitBar'` to `true` to show the simulation progress. By default, the function uses 1000 parameter samples to compute the Sobol indices [1].

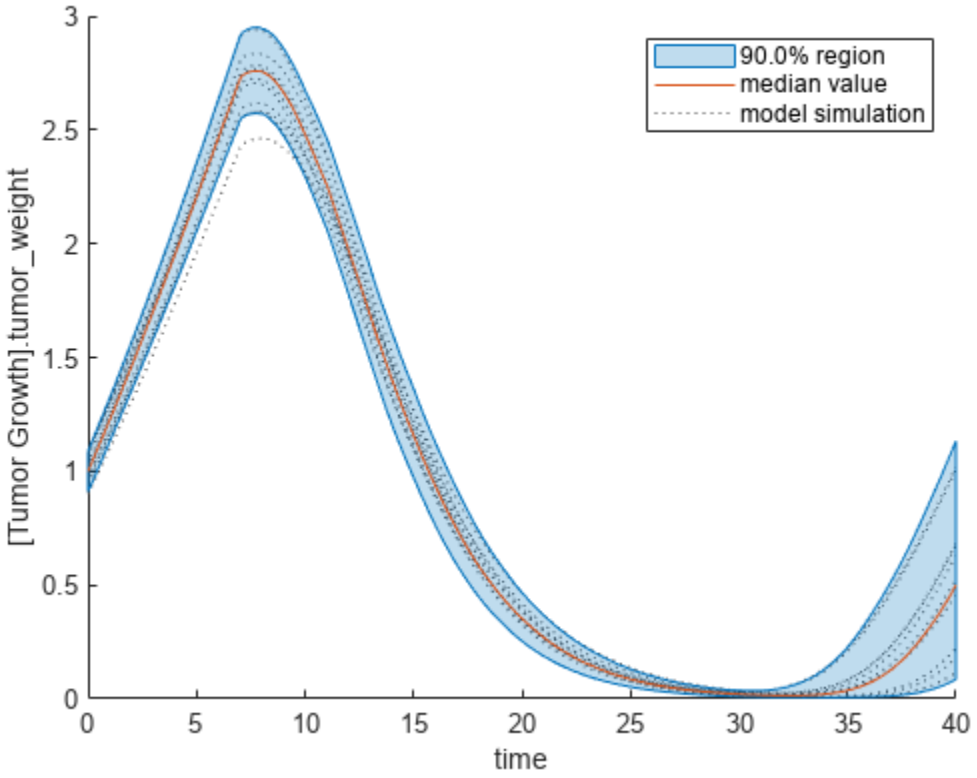
```
rng('default');
sobolResults = sbiosobol(m1,modelParamNames,outputName,Variants=v,Doses=d,ShowWaitBar=true)
```

```
sobolResults =
  Sobol with properties:

                Time: [444x1 double]
        SobolIndices: [5x1 struct]
            Variance: [444x1 table]
    ParameterSamples: [1000x5 table]
         Observables: {'[Tumor Growth].tumor_weight'}
      SimulationInfo: [1x1 struct]
```

You can change the number of samples by specifying the `'NumberSamples'` name-value pair argument. The function requires a total of `(number of input parameters + 2) * NumberSamples` model simulations.

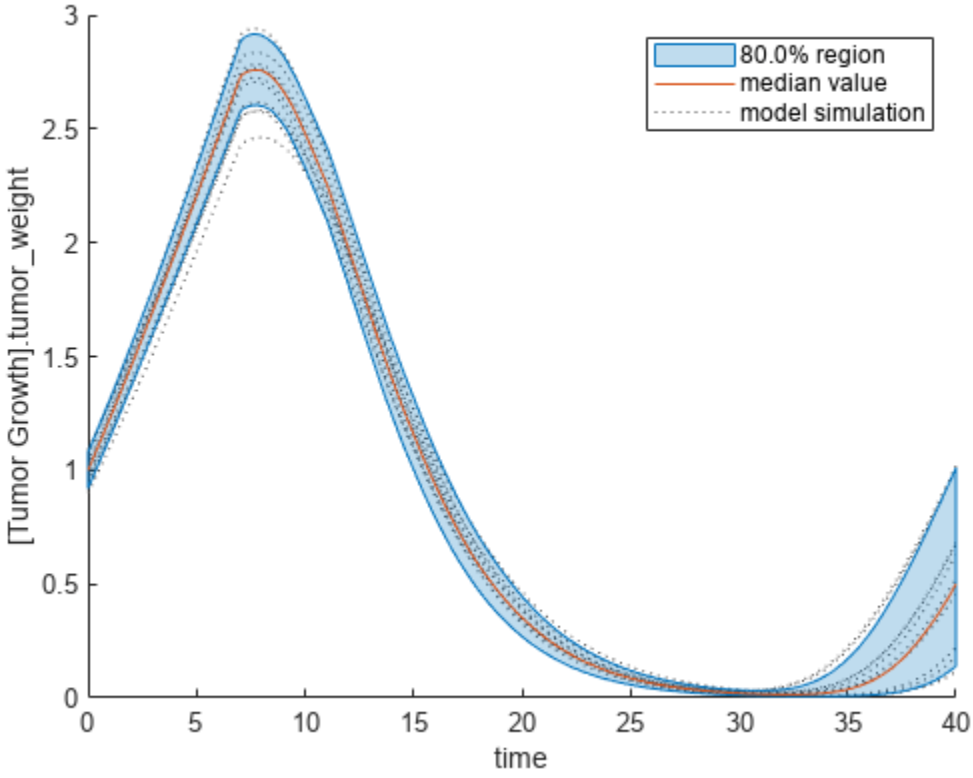
Show the mean model response, the simulation results, and a shaded region covering 90% of the simulation results.

```
plotData(sobolResults,ShowMedian=true,ShowMean=false);
```



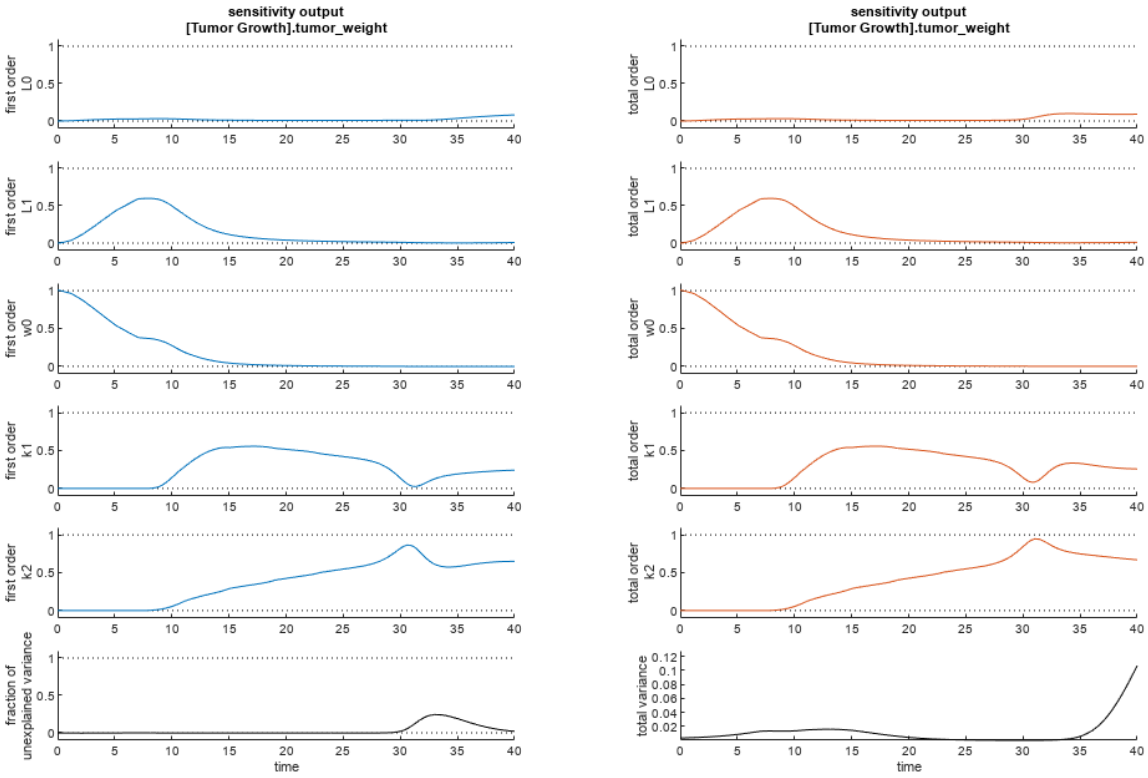
You can adjust the quantile region to a different percentage by specifying `'Alphas'` for the lower and upper quantiles of all model responses. For instance, an alpha value of 0.1 plots a shaded region between the `100 * alpha` and `100 * (1 - alpha)` quantiles of all simulated model responses.

```
plotData(sobolResults,Alphas=0.1,ShowMedian=true,ShowMean=false);
```



Plot the time course of the first- and total-order Sobol indices.

```
h = plot(sobolResults);
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```

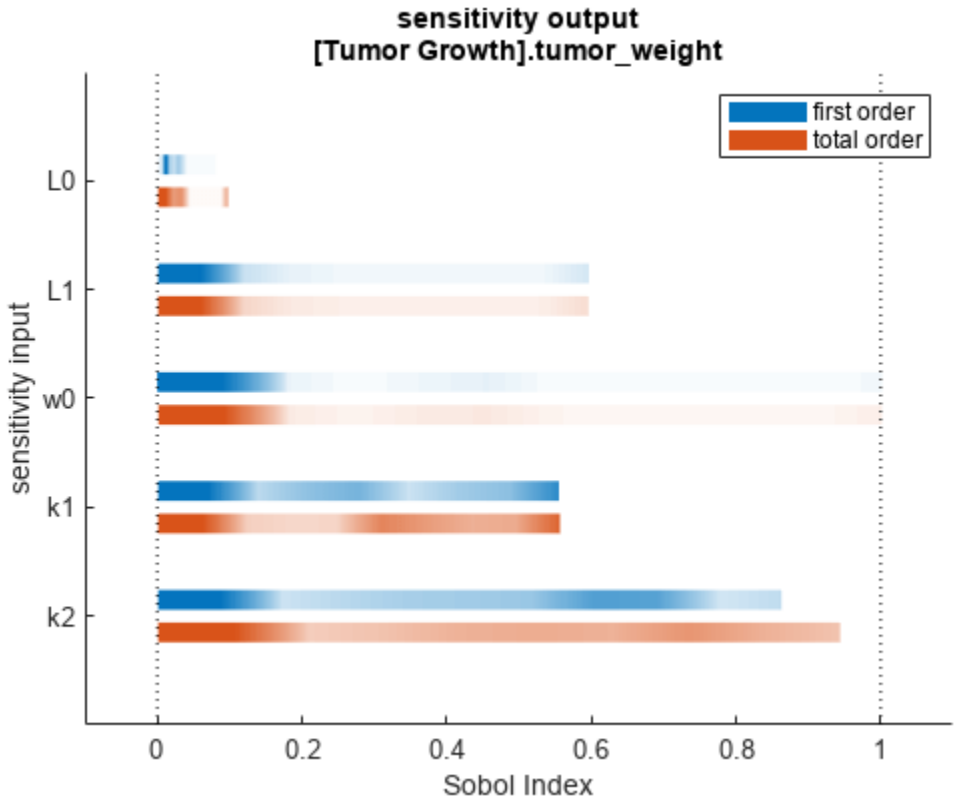


The first-order Sobol index of an input parameter gives the fraction of the overall response variance that can be attributed to variations in the input parameter alone. The total-order index gives the fraction of the overall response variance that can be attributed to any joint parameter variations that include variations of the input parameter.

From the Sobol indices plots, parameters `L1` and `w0` seem to be the most sensitive parameters to the tumor weight before the dose was applied at t = 7. But after the dose is applied, `k1` and `k2` become more sensitive parameters and contribute most to the after-dosing stage of the tumor weight. The total variance plot also shows a larger variance for the after-dose stage at t > 35 than for the before-dose stage of the tumor growth, indicating that `k1` and `k2` might be more important parameters to investigate further. The fraction of unexplained variance shows some variance at around t = 33, but the total variance plot shows little variance at t = 33, meaning the unexplained variance could be insignificant. The fraction of unexplained variance is calculated as 1 - (sum of all the first-order Sobol indices), and the total variance is calculated using `var(response)`, where `response` is the model response at every time point.

You can also display the magnitudes of the sensitivities in a bar plot. Darker colors mean that those values occur more often over the whole time course.

```
bar(sobolResults);
```



You can specify more samples to increase the accuracy of the Sobol indices, but the simulation can take longer to finish. Use `addsamples` to add more samples. For example, if you specify 1500 samples, the function performs `1500 * (2 + number of input parameters)` simulations.

```
gsaMoreSamples = addsamples(gsaResults,1500)
```

The “SimulationInfo” on page 2-0 property of the result object contains various information for computing the Sobol indices. For instance, the model simulation data (SimData) for each simulation using a set of parameter samples is stored in the `SimData` field of the property. This field is an array of `SimData` objects.

```
sobolResults.SimulationInfo.SimData
```

```
SimBiology SimData Array : 1000-by-7

Index:    Name:         ModelName:         DataCount:
1           -           Tumor Growth Model 1
2           -           Tumor Growth Model 1
3           -           Tumor Growth Model 1
...
7000        -           Tumor Growth Model 1
```

You can find out if any model simulation failed during the computation by checking the `ValidSample` field of `SimulationInfo`. In this example, the field shows no failed simulation runs.

```
all(sobolResults.SimulationInfo.ValidSample)
```

```
ans = 1x7 logical array

   1   1   1   1   1   1   1
```

`SimulationInfo.ValidSample` is a table of logical values. It has the same size as `SimulationInfo.SimData`. If `ValidSample` indicates that any simulations failed, you can get more information about those simulation runs and the samples used for those runs by extracting information from the corresponding column of `SimulationInfo.SimData`. Suppose that the fourth column contains one or more failed simulation runs. Get the simulation data and sample values used for that simulation using `getSimulationResults`.

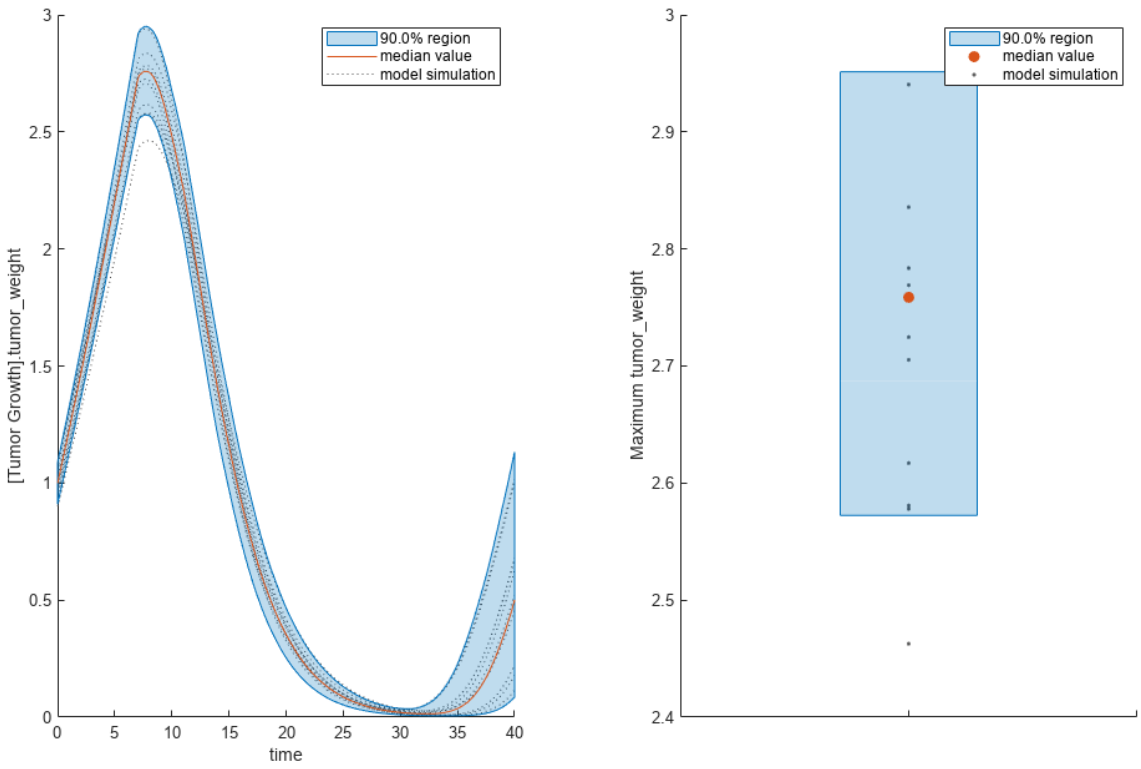
```
[samplesUsed,sd,validruns] = getSimulationResults(sobolResults,4);
```

You can add custom expressions as observables and compute Sobol indices for the added observables. For example, you can compute the Sobol indices for the maximum tumor weight by defining a custom expression as follows.

```
% Suppress an information warning that is issued during simulation.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
% Add the observable expression.
sobolObs = addobservable(sobolResults,'Maximum tumor_weight','max(tumor_weight)','Units','gram');
```

Plot the computed simulation results showing the 90% quantile region.

```
h2 = plotData(sobolObs,ShowMedian=true,ShowMean=false);
h2.Position(:) = [100 100 1280 800];
```



You can also remove the observable by specifying its name.

```
gsaNoObs = removeobservable(sobolObs,'Maximum tumor_weight');
```

Restore the warning settings.

```
warning(warnSettings);
```

Perform GSA by Computing Elementary Effects

Load the “Tumor Growth Model”.

```
sbioloadproject tumor_growth_vpop_sa.sbproj
```

Get a variant with estimated parameters and the dose to apply to the model.

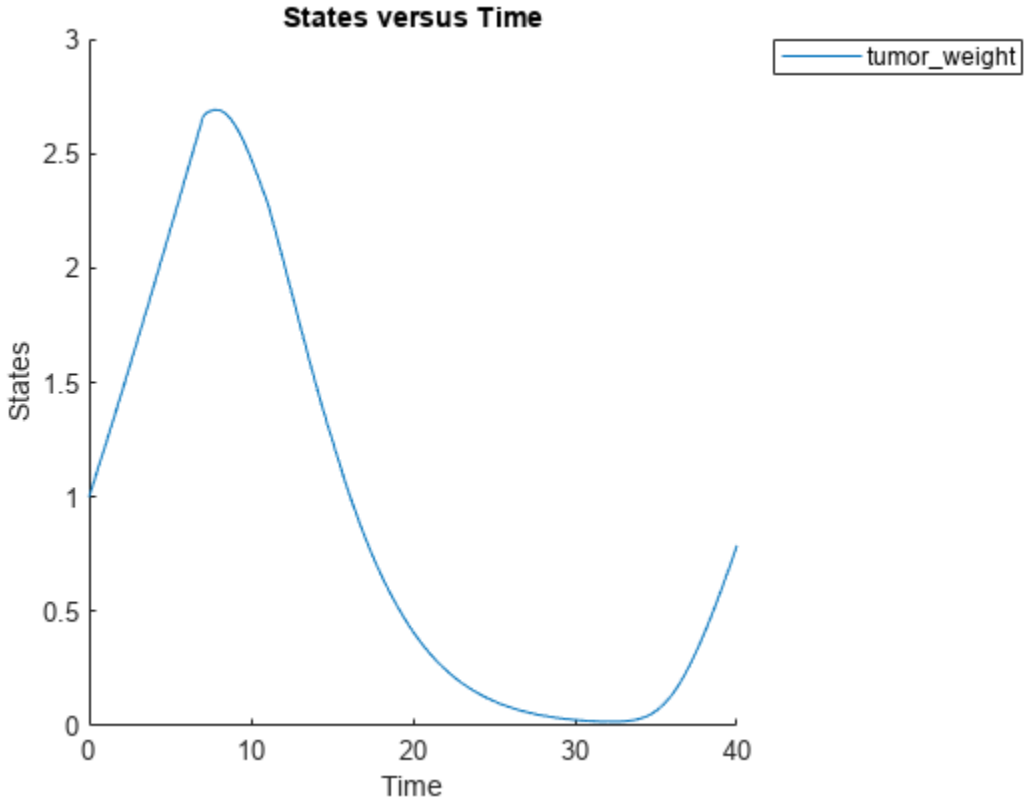
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

Get the active configset and set the tumor weight as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'tumor_weight';
```

Simulate the model and plot the tumor growth profile.

```
sbioplot(sbiosimulate(m1,cs,v,d));
```



Perform global sensitivity analysis (GSA) on the model to find the model parameters that the tumor growth is sensitive to.

First, define model parameters of interest, which are involved in the pharmacodynamics of the tumor growth. Define the model response as the tumor weight.

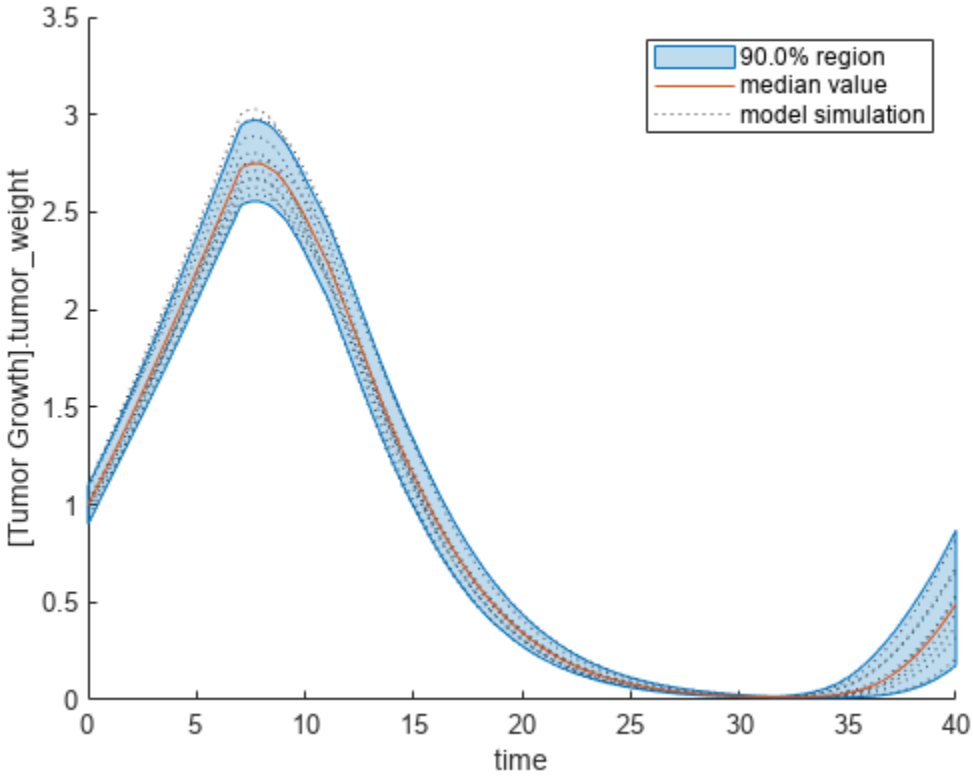
```
modelParamNames = {'L0','L1','w0','k1'};
outputName = 'tumor_weight';
```

Then perform GSA by computing the elementary effects using `sbioelementaryeffects`. Use `100` as the number of samples and set `ShowWaitBar` to `true` to show the simulation progress.

```
rng('default');
eeResults = sbioelementaryeffects(m1,modelParamNames,outputName,Variants=v,Doses=d,NumberSamples=
```

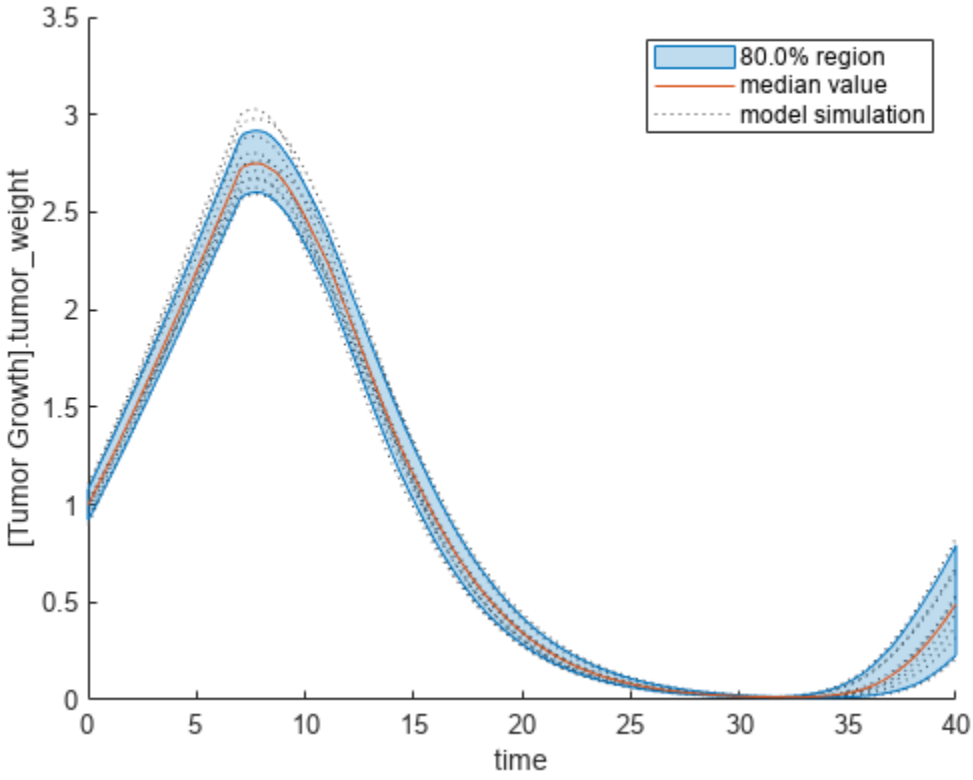
Show the median model response, the simulation results, and a shaded region covering 90% of the simulation results.

```
plotData(eeResults,ShowMedian=true,ShowMean=false);
```



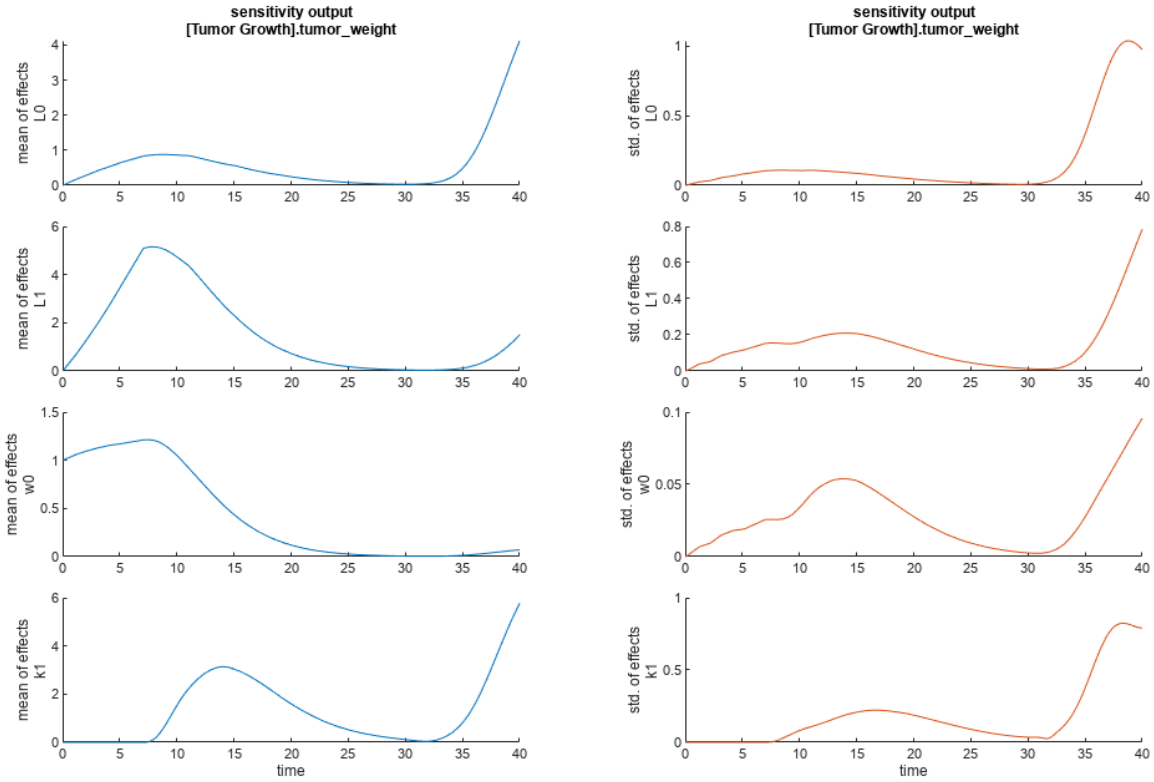
You can adjust the quantile region to a different percentage by specifying `Alphas` for the lower and upper quantiles of all model responses. For instance, an `alpha` value of 0.1 plots a shaded region between the `100*alpha` and `100*(1-alpha)` quantiles of all simulated model responses.

```
plotData(eeResults,Alphas=0.1,ShowMedian=true,ShowMean=false);
```



Plot the time course of the means and standard deviations of the elementary effects.

```
h = plot(eeResults);
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```

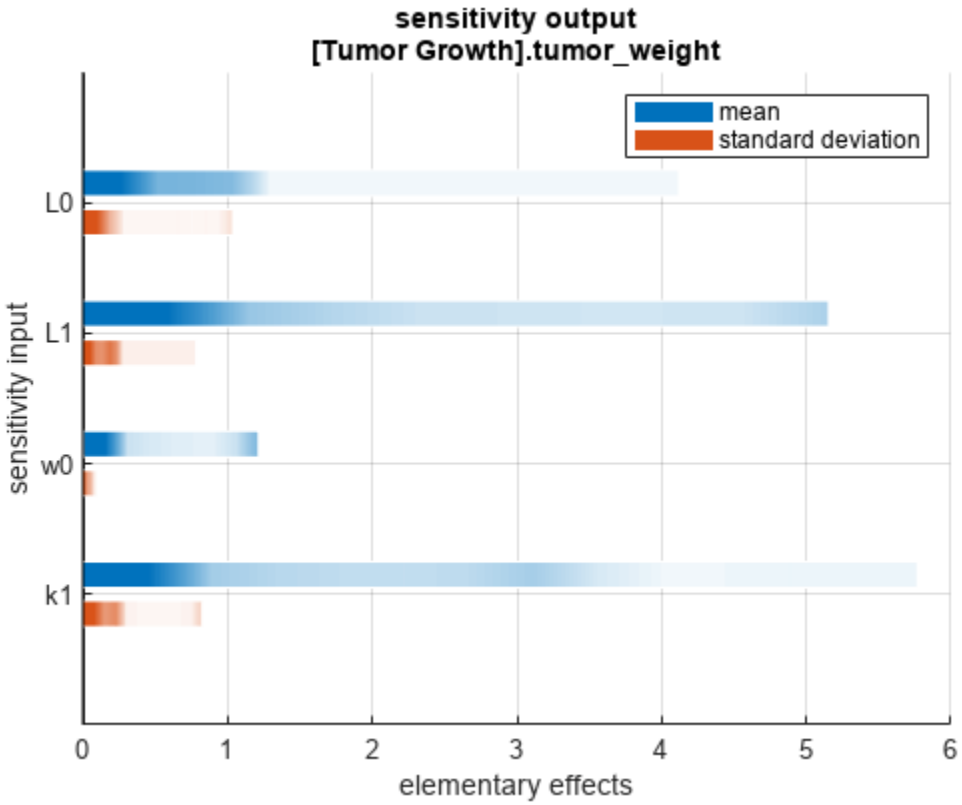


The mean of effects explains whether variations in input parameter values have any effect on the tumor weight response. The standard deviation of effects explains whether the sensitivity change is dependent on the location in the parameter domain.

From the mean of effects plots, parameters `L1` and `w0` seem to be the most sensitive parameters to the tumor weight before the dose is applied at t = 7. But, after the dose is applied, `k1` and `L0` become more sensitive parameters and contribute most to the after-dosing stage of the tumor weight. The plots of standard deviation of effects show more deviations for the larger parameter values in the later stage (t > 35) than for the before-dose stage of the tumor growth.

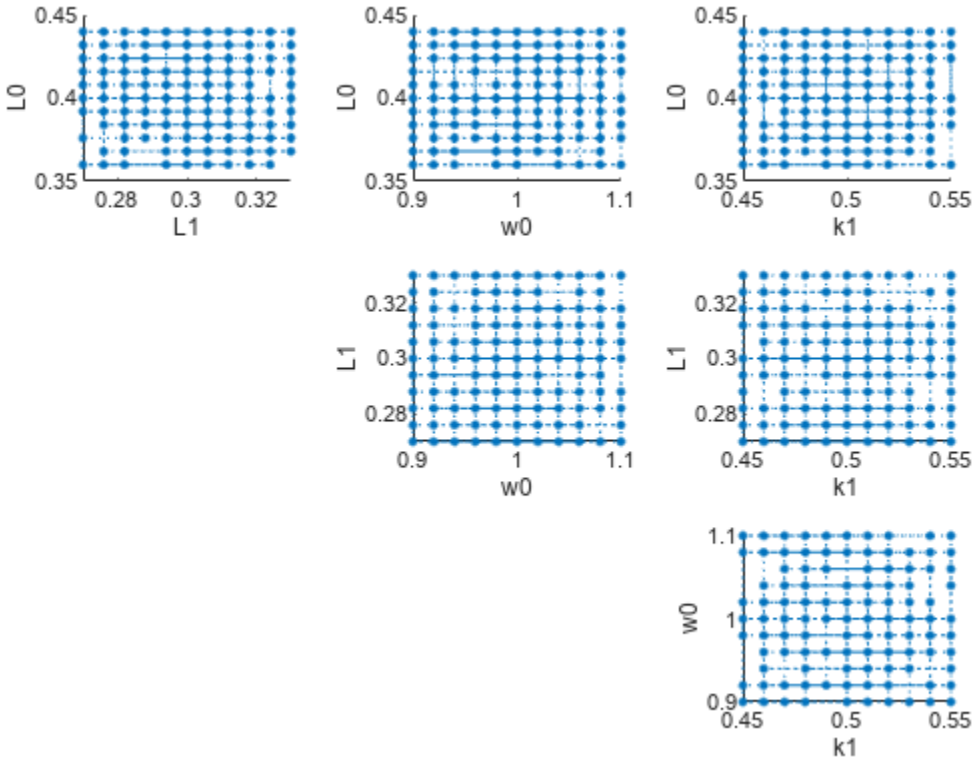
You can also display the magnitudes of the sensitivities in a bar plot. Each color shading represents a histogram representing values at different times. Darker colors mean that those values occur more often over the whole time course.

```
bar(eeResults);
```



You can also plot the parameter grids and samples used to compute the elementary effects.

```
plotGrid(eeResults)
```



You can specify more samples to increase the accuracy of the elementary effects, but the simulation can take longer to finish. Use `addsamples` to add more samples.

```
eeResults2 = addsamples(eeResults,200);
```

The `SimulationInfo` property of the result object contains various information for computing the elementary effects. For instance, the model simulation data (SimData) for each simulation using a set of parameter samples is stored in the `SimData` field of the property. This field is an array of `SimData` objects.

```
eeResults2.SimulationInfo.SimData
```

```
SimBiology SimData Array : 1500-by-1

Index:    Name:         ModelName:         DataCount:
1           -           Tumor Growth Model 1
2           -           Tumor Growth Model 1
3           -           Tumor Growth Model 1
...
1500        -           Tumor Growth Model 1
```

You can find out if any model simulation failed during the computation by checking the `ValidSample` field of `SimulationInfo`. In this example, the field shows no failed simulation runs.

```
all(eeResults2.SimulationInfo.ValidSample)
```

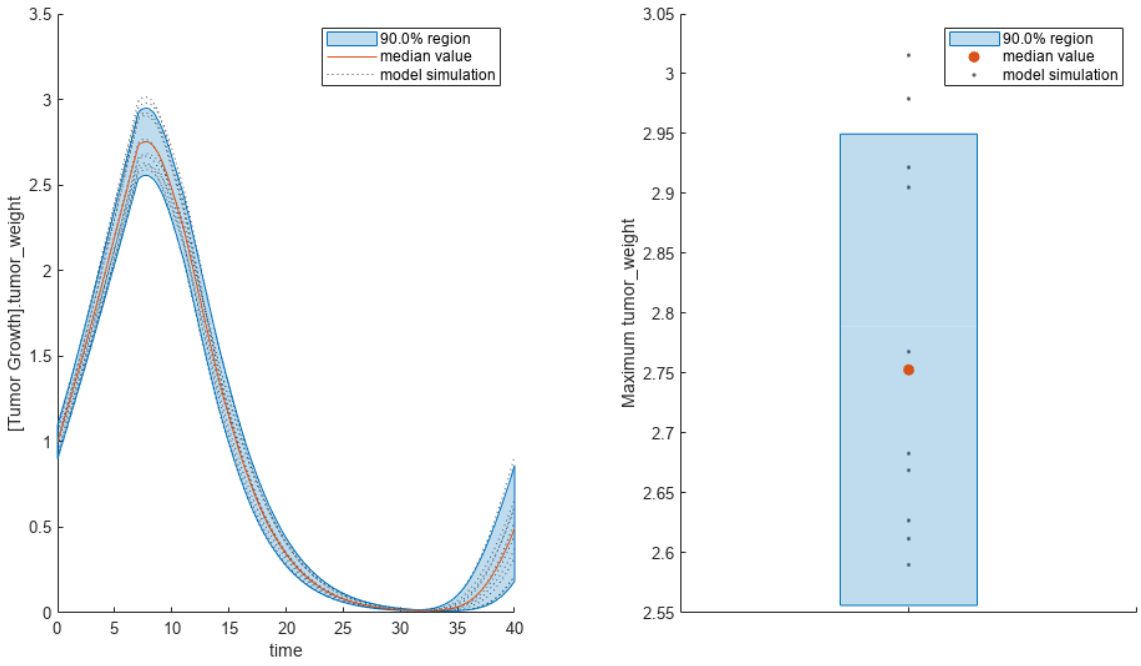
```
ans = logical
   1
```

You can add custom expressions as observables and compute the elementary effects of the added observables. For example, you can compute the effects for the maximum tumor weight by defining a custom expression as follows.

```
% Suppress an information warning that is issued.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
% Add the observable expression.
eeObs = addobservable(eeResults2,'Maximum tumor_weight','max(tumor_weight)','Units','gram');
```

Plot the computed simulation results showing the 90% quantile region.

```
h2 = plotData(eeObs,ShowMedian=true,ShowMean=false);
h2.Position(:) = [100 100 1500 800];
```



You can also remove the observable by specifying its name.

```
eeNoObs = removeobservable(eeObs,'Maximum tumor_weight');
```

Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

gsaObj — Results from global sensitivity analysis

`SimBiology.gsa.Sobol` object | `SimBiology.gsa.ElementaryEffects` object

Results from global sensitivity analysis, specified as a `SimBiology.gsa.Sobol` or `SimBiology.gsa.ElementaryEffects` object.

`obsNames` — Names of observable expressions
character vector | string | string vector | cell array of character vector

Names of observable expressions, specified as a character vector, string, string vector, or cell array of character vectors.

Data Types: `char` | `string` | `cell`

Output Arguments

`results` — Updated results
`SimBiology.gsa.Sobol` | `SimBiology.gsa.ElementaryEffects`

Updated results after removal of the Sobol indices or elementary effects for specified observables, returned as a `SimBiology.gsa.Sobol` or `SimBiology.gsa.ElementaryEffects` object.

Version History

Introduced in R2020a

References

[1] Saltelli, Andrea, Paola Annoni, Ivano Azzini, Francesca Campolongo, Marco Ratto, and Stefano Tarantola. “Variance Based Sensitivity Analysis of Model Output. Design and Estimator for the Total Sensitivity Index.” *Computer Physics Communications* 181, no. 2 (February 2010): 259–70. https://doi.org/10.1016/j.cpc.2009.09.018.

[2] Morris, Max D. “Factorial Sampling Plans for Preliminary Computational Experiments.” *Technometrics* 33, no. 2 (May 1991): 161–74.

[3] Sohier, Henri, Jean-Loup Farges, and Helene Piet-Lahanier. “Improvement of the Representativity of the Morris Method for Air-Launch-to-Orbit Separation.” *IFAC Proceedings Volumes* 47, no. 3 (2014): 7954–59.

See Also

`SimBiology.gsa.Sobol` | `SimBiology.gsa.ElementaryEffects` | `sbiosobol` | `sbioelementaryeffects`

Topics
“Sensitivity Analysis in SimBiology”

removevariant (model)

Remove variant from model

Syntax

```
variantObj = removevariant(modelObj, 'NameValue')

variantObj = removevariant(modelObj, variantObj)
```

Arguments

modelObj	Specify the `Model object` from which you want to remove the variant.
variantObj	Specify the `Variant object` to return from the model object.

Description

variantObj = removevariant(*modelObj*, '*NameValue*') removes a SimBiology variant object with the name *NameValue* from the model object *modelObj* and returns the variant object to *variantObj*. The variant object `Parent` property is assigned `[]` (empty).

A SimBiology variant object stores alternate values for properties on a SimBiology model. For more information on variants, see `Variant object`.

variantObj = removevariant(*modelObj*, *variantObj*) removes a SimBiology variant object (*variantObj*) and returns the variant object *variantObj*.

To view the variants stored on a model object, use the `getvariant` method. To copy a variant object to another model, use `copyobj`. To add a variant object to a SimBiology model, use the `addvariant` method.

Examples

1 Create a model containing several variants.

```
modelObj = sbiomodel('mymodel');
variantObj1 = addvariant(modelObj, 'v1');
variantObj2 = addvariant(modelObj, 'v2');
variantObj3 = addvariant(modelObj, 'v3');
```

2 Remove a variant object using its name.

```
removevariant(modelObj, 'v1');
```

3 Remove a variant object using its index number.

a Get the index number of the variant in the model.

```
vObjs = getvariant(modelObj)
```

```
SimBiology Variant Array

   Index:  Name:             Active:
   1       v2                false
   2       v3                false
```

b Remove the variant object.

```
removevariant(modelObj, vObjs(2));
```

See Also

`addvariant`, `getvariant`, `Model object`, `Variant object`

Version History

Introduced in R2007b

rename

Rename object and update expressions

Syntax

`rename(`*`Obj`*`, '`*`NewNameValue`*`')`

Arguments

`Obj`	Abstractkineticlaw, compartment, event, kinetic law, model, parameter, RepeatDose, reaction, rule, ScheduleDose, species, unit, unitprefix, variant, or observable object.
'*`NewNameValue`*'	Specify the new name.

Description

`rename(`*`Obj`*`, '`*`NewNameValue`*`')`, changes the `Name` property of the object, *`Obj`* to *`NewNameValue`* and updates any uses of it in the model such as rules, events, reactions, variants, and doses to use the new name.

If the new name is already being used by another model component, the new name will be qualified to ensure that it is unique. For example if you change a species named `A` to `K`, and a parameter with the name `K` exists, the species will be qualified as *`CompartmentName`*`.K` to indicate that the reference is to the species. If you are referring to an object by its qualified name, for example *`CompartmentName`*`.A` and you change the species name, the reference will contain the qualified name in its updated form, for example, *`CompartmentName`*`.K`

When you want to change the name of a compartment, parameter, species, or reaction object, use this method instead of `set`.

Note The `set` method only changes the `Name` property of the object, except for species and compartments. The method updates the species or compartment object's `Name` property and any reaction strings referring to the species or compartment to use the new name.

Examples

1. Create a model object that contains a species `A` in a rule.

```
m = sbiomodel('cell');
s = addspecies(m, 'A');
r = addrule(m, 'A = 4');
```

2. Rename the species to `Y`

```
rename(s, 'Y');
```

3. See that the rule expression is now updated.

```
r
```

```
SimBiology Rule Array

Index:    RuleType:            Rule:
1         initialAssignment    Y = 4
```

See Also

`set`

Version History

Introduced in R2008b

resetoptions

Reset optional SimBiology fit problem properties

Syntax

```
fitProblem2 = resetoptions(fitProblem1,propertyNames)
```

Description

`fitProblem2 = resetoptions(fitProblem1,propertyNames)` resets the specified properties `propertyNames` of a SimBiology `fitproblem` object `fitProblem1` back to their default values.

Examples

Reset Optional SimBiology Fit Problem Properties

Create a `fitproblem` object.

```
fp1 = fitproblem
```

```
fp1 =
  fitproblem with properties:

   Required:
                    Data: [0x0 groupedData]
               Estimated: [1x0 estimatedInfo]
             FitFunction: "sbiofit"
                   Model: [0x0 SimBiology.Model]
             ResponseMap: [1x0 string]

   Optional:
                   Doses: [0x0 SimBiology.Dose]
            FunctionName: "auto"
                 Options: []
            ProgressPlot: 0
             UseParallel: 0
                Variants: [0x0 SimBiology.Variant]

   sbiofit options:
              ErrorModel: "constant"
                  Pooled: "auto"
    SensitivityAnalysis: "auto"
                Weights: []
```

The object has required and optional properties. `resetoptions` lets you reset the optional properties back to default values.

Change two of the optional properties to some nondefault values.

```
fp1.ProgressPlot = true;
fp1.FunctionName = "lsqnonlin";
```

Reset the properties back to their default values.

```
fp2 = resetoptions(fp1,["ProgressPlot","FunctionName"]);
fp2.ProgressPlot
```

```
ans = logical
   0
```

```
fp2.FunctionName
```

```
ans =
"auto"
```

Input Arguments

`fitProblem1` — SimBiology fit problem

`fitproblem` object

SimBiology fit problem, specified as a `fitproblem` object.

`propertyNames` — Names of fit problem object properties

character vector | string scalar | string vector | cell array of character vectors

Names of fit problem object properties to reset to default values, specified as a character vector, string scalar, string vector, or cell array of character vectors.

Data Types: `char` | `string` | `cell`

Output Arguments

`fitProblem2` — New SimBiology fit problem object

`fitproblem` object

New SimBiology fit problem object after resetting the specified properties to default values, returned as a `fitproblem` object.

Version History

Introduced in R2021b

See Also

`fitproblem`

rename

Rename entry from `SimBiology.Scenarios` object

Syntax

```
sObj = rename(sObj,entryNameOrIndex,newName)
sObj = rename(sObj,entryIndex,subIndex,newName)
```

Description

`sObj = rename(sObj,entryNameOrIndex,newName)` renames the entry (or subentry on page 2-799) `entryNameorIndex` to `newName`.

`sObj = rename(sObj,entryIndex,subIndex,newName)` renames the subentry `subIndex` to `newName`.

Examples

Generate Different Simulation Scenarios for Glucose-Insulin Response

Load the model of glucose-insulin response. For details about the model, see the **Background** section in “Simulate the Glucose-Insulin Response”.

```
sbioloadproject('insulindemo','m1');
```

The model contains different parameter values and initial conditions that represents different insulin impairments (such as Type 2 diabetes, low insulin sensitivity, and so on) stored in five variants.

```
variants = getvariant(m1)
```

```
variants =
   SimBiology Variant Array

   Index:  Name:             Active:
   1       Type 2 diabetic   false
   2       Low insulin se... false
   3       High beta cell... false
   4       Low beta cell ... false
   5       High insulin s... false
```

Suppress an informational warning that is issued during simulations.

```
warnSettings = warning('off','SimBiology:DimAnalysisNotDone_MatlabFcn_Dimensionless');
```

Select a dose that represents a single meal of 78 grams of glucose.

```
singleMeal = sbioselect(m1,'Name','Single Meal');
```

Create a `Scenarios` object to represent different initial conditions combined with the dose. That is, create a `scenario` object where each variant is paired (or combined) with the dose, for a total of five simulation scenarios.

```
sObj = SimBiology.Scenarios;
add(sObj,'cartesian','variants',variants);
add(sObj,'cartesian','dose',singleMeal)
```

```
ans =
  Scenarios (5 scenarios)

                  Name            Content          Number
                ________    ____________________    ______

    Entry 1     variants    SimBiology variants      5
    x Entry 2   dose        SimBiology dose          1

  See also Expression property.
```

`sObj` contains two entries. Use the `generate` function to combine the entries and generate five scenarios. The function returns a scenarios table, where each row represents a scenario and each column represents an entry of the `Scenarios` object.

```
scenariosTbl = generate(sObj)
```

```
scenariosTbl=5×2 table
           variants                    dose
    ___________________________    ____________________________

    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
```

Change the entry name of the first entry.

```
rename(sObj,1,'Insulin Impairements')
```

```
ans =
  Scenarios (5 scenarios)

                       Name                Content          Number
                ____________________    ____________________    ______

    Entry 1     Insulin Impairements    SimBiology variants      5
    x Entry 2   dose                    SimBiology dose          1

  See also Expression property.
```

Create a `SimFunction` object to simulate the generated scenarios. Use the `Scenarios` object as the input and specify the plasma glucose and insulin concentrations as reponses (outputs of the function to be plotted). Specify `[]` for the dose input argument since the `Scenarios` object already has the dosing information.

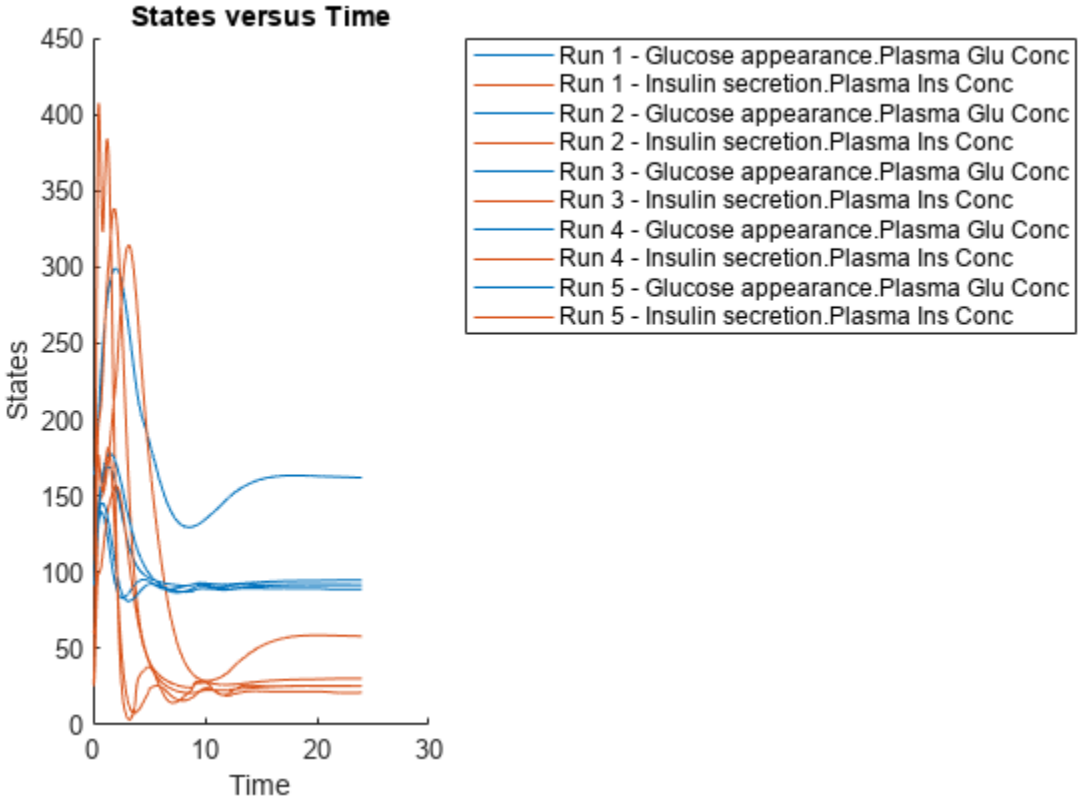
```
f = createSimFunction(m1,sObj,{'[Plasma Glu Conc]','[Plasma Ins Conc]'},[])
```

```
f = 
SimFunction

Parameters:

              Name                 Value         Type                            Units                   
    _________________________    ______    _____________    _______________________________________

    {'Plasma Volume (Glu)'  }      1.88    {'parameter'}    {'deciliter'                           
    {'k1'                   }     0.065    {'parameter'}    {'1/minute'                            
    {'k2'                   }     0.079    {'parameter'}    {'1/minute'                            
    {'Plasma Volume (Ins)'  }      0.05    {'parameter'}    {'liter'                               
    {'m1'                   }      0.19    {'parameter'}    {'1/minute'                            
    {'m2'                   }     0.484    {'parameter'}    {'1/minute'                            
    {'m4'                   }    0.1936    {'parameter'}    {'1/minute'                            
    {'m5'                   }    0.0304    {'parameter'}    {'minute/picomole'                     
    {'m6'                   }    0.6469    {'parameter'}    {'dimensionless'                       
    {'Hepatic Extraction'   }       0.6    {'parameter'}    {'dimensionless'                       
    {'kmax'                 }    0.0558    {'parameter'}    {'1/minute'                            
    {'kmin'                 }     0.008    {'parameter'}    {'1/minute'                            
    {'kabs'                 }    0.0568    {'parameter'}    {'1/minute'                            
    {'kgri'                 }         0    {'parameter'}    {'1/minute'                            
    {'f'                    }       0.9    {'parameter'}    {'dimensionless'                       
    {'a'                    }         0    {'parameter'}    {'1/milligram'                         
    {'b'                    }      0.82    {'parameter'}    {'dimensionless'                       
    {'c'                    }         0    {'parameter'}    {'1/milligram'                         
    {'d'                    }      0.01    {'parameter'}    {'dimensionless'                       
    {'kp1'                  }       2.7    {'parameter'}    {'milligram/minute'                    
    {'kp2'                  }    0.0021    {'parameter'}    {'1/minute'                            
    {'kp3'                  }     0.009    {'parameter'}    {'(milligram/minute)/(picomole/liter)
    {'kp4'                  }    0.0618    {'parameter'}    {'(milligram/minute)/picomole'         
    {'ki'                   }    0.0079    {'parameter'}    {'1/minute'                            
    {'[Ins Ind Glu Util]'   }         1    {'parameter'}    {'milligram/minute'                    
    {'Vm0'                  }    2.5129    {'parameter'}    {'milligram/minute'                    
    {'Vmx'                  }     0.047    {'parameter'}    {'(milligram/minute)/(picomole/liter)
    {'Km'                   }    225.59    {'parameter'}    {'milligram'                           
    {'p2U'                  }    0.0331    {'parameter'}    {'1/minute'                            
    {'K'                    }      2.28    {'parameter'}    {'picomole/(milligram/deciliter)'      
    {'alpha'                }      0.05    {'parameter'}    {'1/minute'                            
    {'beta'                 }      0.11    {'parameter'}    {'(picomole/minute)/(milligram/decil
    {'gamma'                }       0.5    {'parameter'}    {'1/minute'                            
    {'ke1'                  }    0.0005    {'parameter'}    {'1/minute'                            
    {'ke2'                  }       339    {'parameter'}    {'milligram'                           
    {'Basal Plasma Glu Conc'}     91.76    {'parameter'}    {'milligram/deciliter'                 
    {'Basal Plasma Ins Conc'}     25.49    {'parameter'}    {'picomole/liter'                      

Observables: 

            Name                Type                 Units          
    ____________________    ___________    ______________________

    {'[Plasma Glu Conc]'}    {'species'}    {'milligram/deciliter'}
    {'[Plasma Ins Conc]'}    {'species'}    {'picomole/liter'     }

Dosed: 

    TargetName       TargetDimension     
    __________    ____________________
```

```
    {'Dose'}    {'Mass (e.g., gram)'}

TimeUnits: hour
```

Simulate the model for 24 hours and plot the simulation data. The data contains five runs, where each run represents a scenario in the Scenarios object.

```
sd = f(sObj,24);
sbioplot(sd)
```




```
ans =
  Axes (SbioPlot) with properties:

            XLim: [0 30]
            YLim: [0 450]
          XScale: 'linear'
          YScale: 'linear'
    GridLineStyle: '-'
         Position: [0.0920 0.1100 0.2956 0.8150]
            Units: 'normalized'

  Show all properties
```

If you have Statistics and Machine Learning Toolbox™, you can also draw sample values for model quantities from various probability distributions. For instance, suppose that the parameters `Vmx` and

kp3, which are known for the low and high insulin sensitivity, follow the lognormal distribution. You can generate sample values for these parameters from such a distribution, and perform a scan to explore model behavior.

Define the lognormal probability distribution object for Vmx.

```
pd_Vmx = makedist('lognormal')
```

```
pd_Vmx =
  LognormalDistribution

  Lognormal distribution
       mu = 0
    sigma = 1
```

By definition, the parameter mu is the mean of logarithmic values. To vary the parameter value around the base (model) value of the parameter, set mu to log(*model_value*). Set the standard deviation (*sigma*) to 0.2. For a small *sigma* value, the mean of a lognormal distribtion is approximately equal to log(*model_value*). For details, see “Lognormal Distribution” (Statistics and Machine Learning Toolbox).

```
Vmx = sbioselect(m1,'Name','Vmx');
pd_Vmx.mu = log(Vmx.Value);
pd_Vmx.sigma = 0.2
```

```
pd_Vmx =
  LognormalDistribution

  Lognormal distribution
       mu = -3.05761
    sigma =      0.2
```

Similarly define the probability distribution for kp3.

```
pd_kp3 = makedist('lognormal');
kp3 = sbioselect(m1,'Name','kp3');
pd_kp3.mu = log(kp3.Value);
pd_kp3.sigma = 0.2
```

```
pd_kp3 =
  LognormalDistribution

  Lognormal distribution
       mu = -4.71053
    sigma =      0.2
```

Now define a joint probability distribution to draw sample values for Vmx and kp3, with a rank correlation to specify some correlation between these two parameters. Note that this correlation assumption is for the illustration purposes of this example only and may not be biologically relevant.

First remove the variants entry (entry 1) from sObj.

```
remove(sObj,1)
```

```
ans =
  Scenarios (1 scenarios)
```

```
                Name         Content         Number
                ____    _________________    ______

    Entry 1     dose    SimBiology dose        1

  See also Expression property.
```

Add an entry that defines the joint probability distribution with a rank correlation matrix.

```
add(sObj,'cartesian',["Vmx","kp3"],[pd_Vmx, pd_kp3],'RankCorrelation',[1,0.5;0.5,1])
```

```
ans =
  Scenarios (2 scenarios)

                    Name           Content              Number
                    ____    ____________________    ____________

    Entry 1         dose    SimBiology dose           1
    x (Entry 2.1    Vmx     Lognormal distribution    2 (default)
    + Entry 2.2)    kp3     Lognormal distribution    2 (default)

  See also Expression property.
```

By default, the number of samples to draw from the joint distribution is set to 2. Increase the number of samples.

```
updateEntry(sObj,2,'Number',50)
```

```
ans =
  Scenarios (50 scenarios)

                    Name           Content             Number
                    ____    ____________________    ______

    Entry 1         dose    SimBiology dose           1
    x (Entry 2.1    Vmx     Lognormal distribution    50
    + Entry 2.2)    kp3     Lognormal distribution    50

  See also Expression property.
```

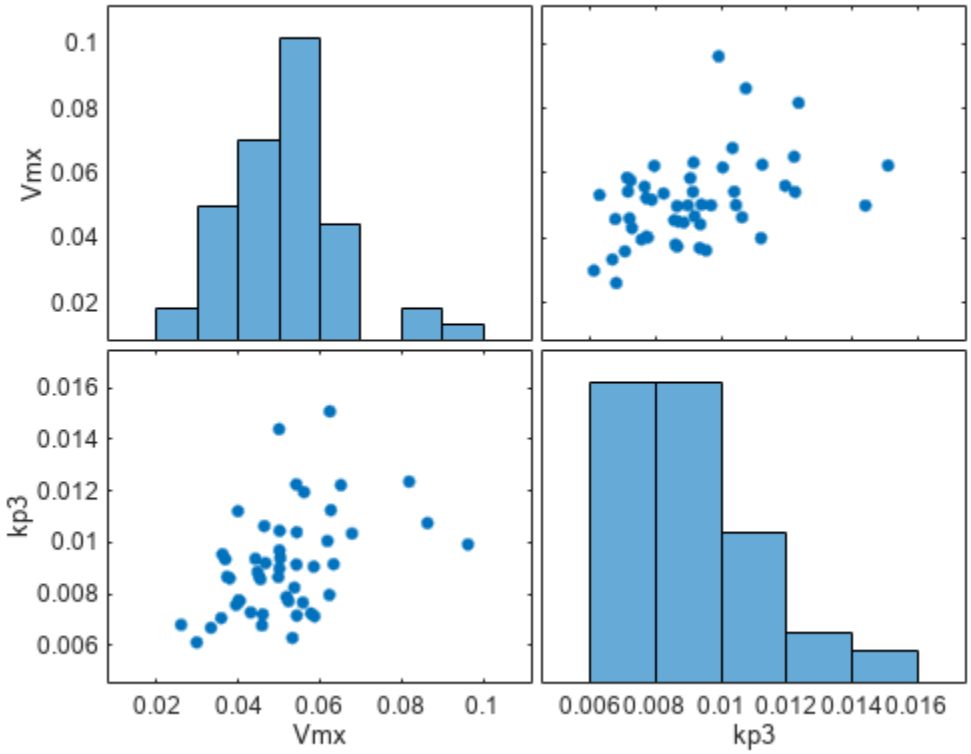
Verify that the `Scenarios` object can be simulated with the model. The `verify` function throws an error if any entry does not resolve uniquely to an object in the model or the entry contents have inconsistent lengths (sample sizes). The function throws a warning if multiple entries resolve to the same object in the model.

```
verify(sObj,m1)
```

Generate the simulation scenarios. Plot the sample values using `plotmatrix`. You can see the value of `Vmx` is varied around its model value 0.047 and that of `kp3` around 0.009.

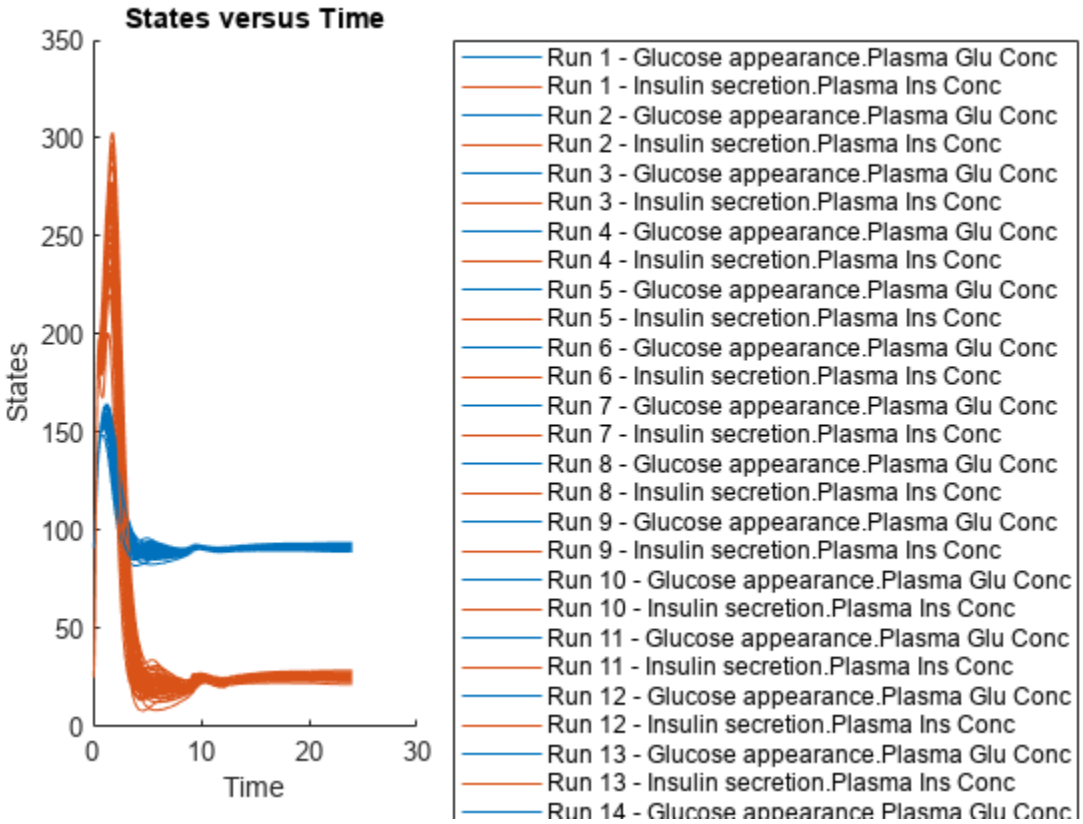
```
sTbl = generate(sObj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl.Vmx,sTbl.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
```

```
ax(2,1).XLabel.String = "Vmx";
ax(2,2).XLabel.String = "kp3";
```



Simulate the scenarios using the same SimFunction you created previously. You do not need to create a new SimFunction object even though the Scenarios object has been updated.

```
sd2 = f(sObj,24);
sbioplot(sd2);
```



By default, SimBiology uses the random sampling method. You can change it to the Latin hypercube sampling (or sobol or halton) for a more systematic space-filling approach.

```
entry2struct = getEntry(sObj,2)
```

```
entry2struct = struct with fields:
                Name: {'Vmx'  'kp3'}
             Content: [2x1 prob.LognormalDistribution]
              Number: 50
    RankCorrelation: [2x2 double]
          Covariance: []
      SamplingMethod: 'random'
    SamplingOptions: [0x0 struct]
```

```
entry2struct.SamplingMethod = 'lhs'
```

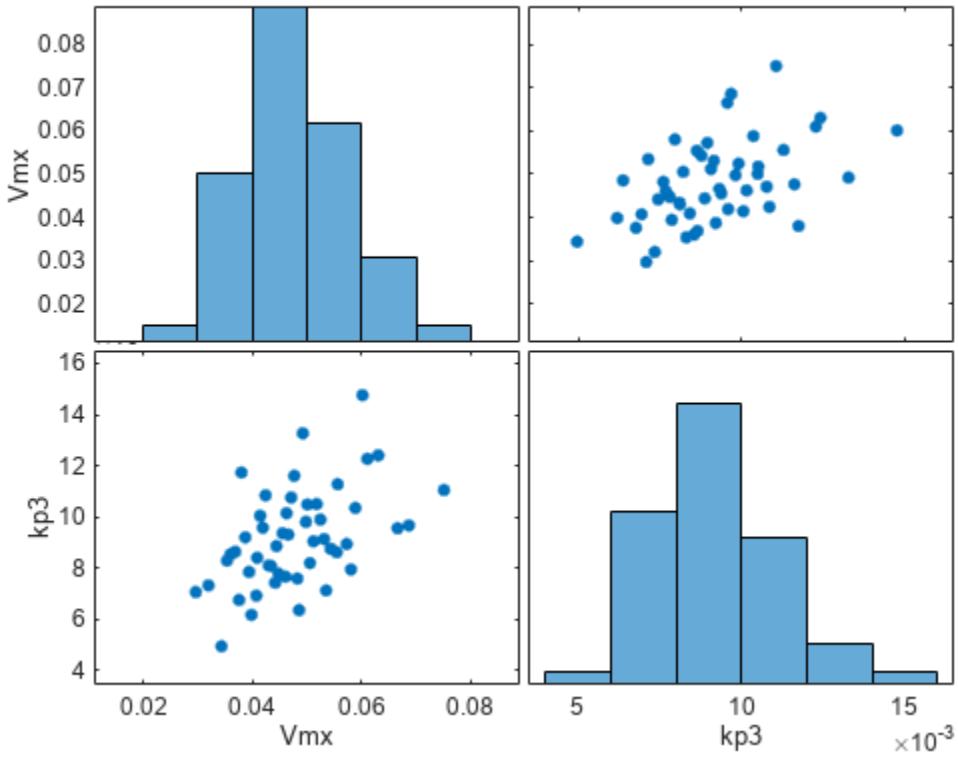
```
entry2struct = struct with fields:
                Name: {'Vmx'  'kp3'}
             Content: [2x1 prob.LognormalDistribution]
              Number: 50
    RankCorrelation: [2x2 double]
          Covariance: []
      SamplingMethod: 'lhs'
    SamplingOptions: [0x0 struct]
```

You can now use the updated structure to modify entry 2.

```
updateEntry(sObj,2,entry2struct)

ans =
  Scenarios (50 scenarios)

                    Name           Content             Number
                    ____    ____________________      ______

    Entry 1         dose    SimBiology dose             1
    x (Entry 2.1    Vmx     Lognormal distribution      50
    + Entry 2.2)    kp3     Lognormal distribution      50

  See also Expression property.
```

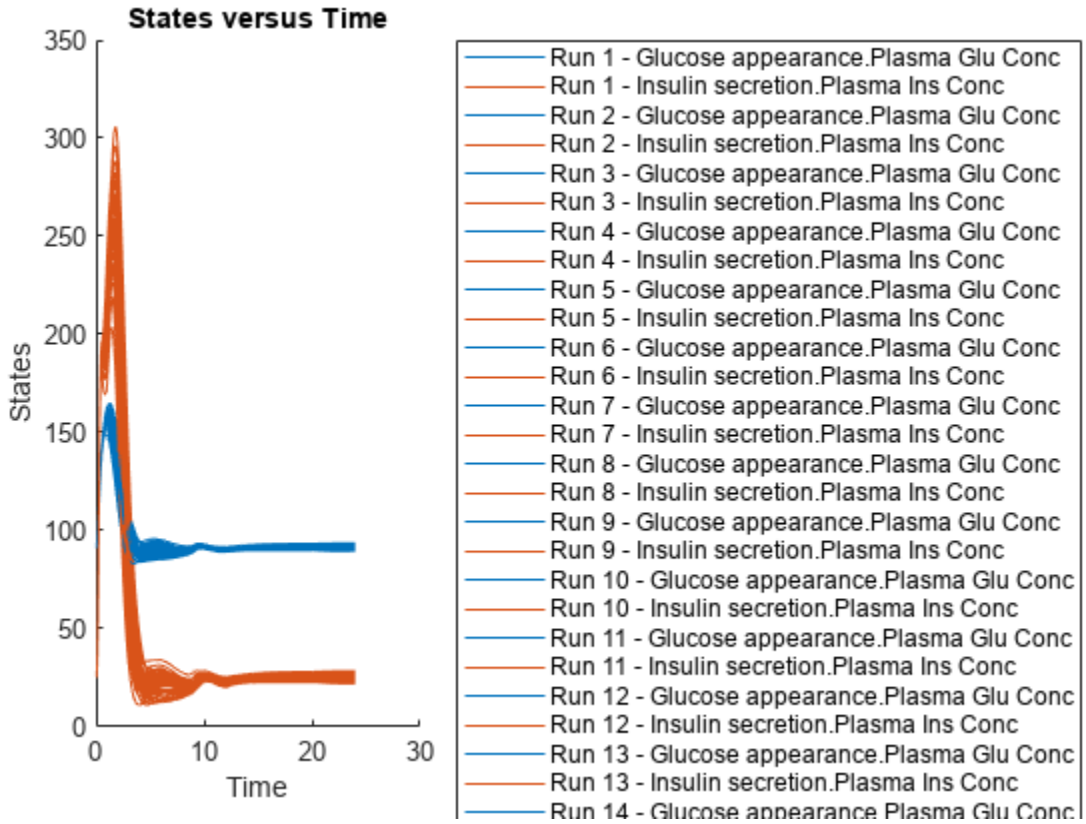
Visualize the sample values.

```
sTbl2 = generate(sObj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl2.Vmx,sTbl2.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
ax(2,1).XLabel.String = "Vmx";
ax(2,2).XLabel.String = "kp3";
```



Simulate the scenarios.

```
sd3 = f(sObj,24);
sbioplot(sd3);
```



Restore warning settings.

```
warning(warnSettings);
```

Input Arguments

`sObj` — Simulation scenarios

`SimBiology.Scenarios` object

Simulation scenarios, specified as a `SimBiology.Scenarios` object.

`entryNameOrIndex` — Entry name or index

character vector | string | scalar positive integer

Entry name or index, specified as a character vector, string, or scalar positive integer. You can also specify the name of a subentry.

If you are specifying an index, it must be smaller than or equal to the number of entries in the object.

Data Types: `double` | `char` | `string`

`newName` — New name

character vector | string

New name for the entry, specified as a character vector or string.

Example: `'k2'`

Data Types: `char` | `string`

`entryIndex` — Entry index
scalar positive integer

Entry index, specified as a scalar positive integer. The entry index must be smaller than or equal to the number of entries in the object.

Data Types: `double`

`subIndex` — Entry subindex
scalar positive integer

Entry subindex, specified as a scalar positive integer. The subindex must be smaller than or equal to the number of subentries in the entry.

Data Types: `double`

Output Arguments

`sObj` — Simulation scenarios
`Scenarios` object

Simulation scenarios, returned as a `Scenarios` object.

Version History

Introduced in R2019b

See Also

`SimBiology.Scenarios` | `SimFunction object` | `createSimFunction (model)`

Topics

“SimBiology.Scenarios Terminology” on page 2-799
“Combine Simulation Scenarios in SimBiology”

renameobservable

Rename observables in SimData

Syntax

```
sdout = renameobservable(sdin,oldNames,newNames)
```

Description

`sdout = renameobservable(sdin,oldNames,newNames)` returns a new `SimData` object (or array of objects) `sdout` after renaming observables in `sdin` and recalculating all observable expressions.

Examples

Calculate Statistics After Model Simulation Using Observables

Load the “Target-Mediated Drug Disposition (TMDD) Model”.

```
sbioloadproject tmdd_with_TO.sbproj
```

Set the target occupancy (`TO`) as a response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'TO';
```

Get the dosing information.

```
d = getdose(m1,'Daily Dose');
```

Scan over different dose amounts using a `SimBiology.Scenarios` object. To do so, first parameterize the `Amount` property of the dose. Then vary the corresponding parameter value using the `Scenarios` object.

```
amountParam = addparameter(m1,'AmountParam','Units',d.AmountUnits);
d.Amount = 'AmountParam';
d.Active = 1;
doseSamples = SimBiology.Scenarios('AmountParam',linspace(0,300,31));
```

Create a `SimFunction` to simulate the model. Set `TO` as the simulation output.

```
% Suppress informational warnings that are issued during simulation.
warning('off','SimBiology:SimFunction:DOSES_NOT_EMPTY');
f = createSimFunction(m1,doseSamples,'TO',d)
```

```
f =
SimFunction

Parameters:

         Name          Value        Type            Units
```

```
    ________________    _____    _____________    _____________

    {'AmountParam'}       1      {'parameter'}    {'nanomole'}

Observables:

     Name          Type                Units
    ______    _____________    ________________

    {'TO'}    {'parameter'}    {'dimensionless'}

Dosed:

      TargetName                TargetDimension                      Amount          AmountValue    A
    ________________    ____________________________________    ________________    ___________    -

    {'Plasma.Drug'}    {'Amount (e.g., mole or molecule)'}    {'AmountParam'}          1          -

TimeUnits: day
```

```
warning('on','SimBiology:SimFunction:DOSES_NOT_EMPTY');
```

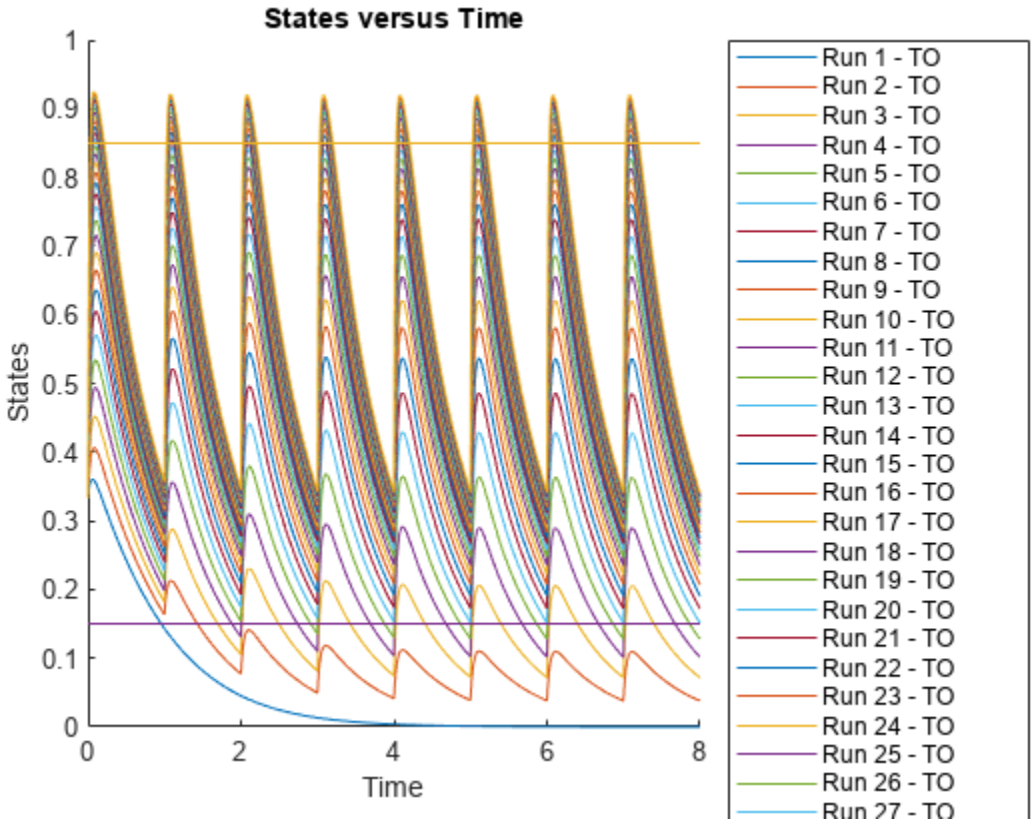
Simulate the model using the dose amounts generated by the `Scenarios` object. In this case, the object generates 31 different doses; hence the model is simulated 31 times and generates a `SimData` array.

```
doseTable = getTable(d);
sd = f(doseSamples,cs.StopTime,doseTable)
```

```
   SimBiology Simulation Data Array: 31-by-1

   ModelName:        TMDD
   Logged Data:
     Species:        0
     Compartment:    0
     Parameter:      1
     Sensitivity:    0
     Observable:     0
```

Plot the simulation results. Also add two reference lines that represent the safety and efficacy thresholds for `T0`. In this example, suppose that any `T0` value above 0.85 is unsafe, and any `T0` value below 0.15 has no efficacy.

```
h = sbioplot(sd);
time = sd(1).Time;
h.NextPlot = 'add';
safetyThreshold = plot(h,[min(time), max(time)],[0.85, 0.85],'DisplayName','Safety Threshold');
efficacyThreshold = plot(h,[min(time), max(time)],[0.15, 0.15],'DisplayName','Efficacy Threshold
```



Postprocess the simulation results. Find out which dose amounts are effective, corresponding to the `TO` responses within the safety and efficacy thresholds. To do so, add an observable expression to the simulation data.

```
% Suppress informational warnings that are issued during simulation.
warning('off','SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
newSD = addobservable(sd,'stat1','max(TO) < 0.85 & min(TO) > 0.15','Units','dimensionless')
```

```
SimBiology Simulation Data Array: 31-by-1

ModelName:        TMDD
Logged Data:
  Species:        0
  Compartment:    0
  Parameter:      1
  Sensitivity:    0
  Observable:     1
```

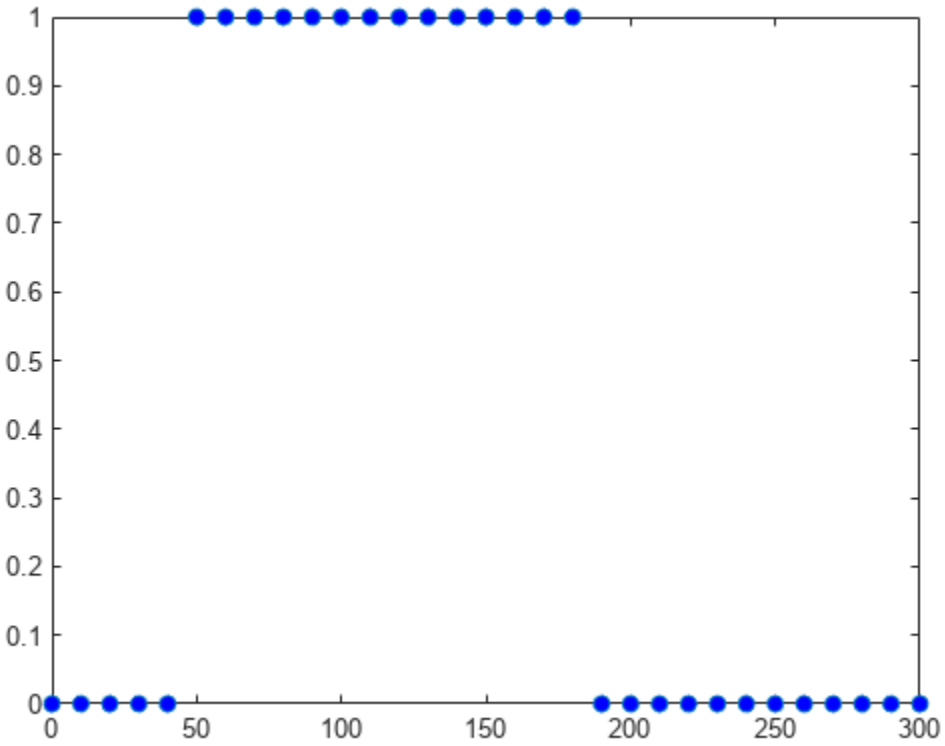
The addobservable function evaluates the new observable expression for each `SimData` in `sd` and returns the evaluated results as a new `SimData` array, `newSD`, which now has the added observable (`stat1`).

SimBiology stores the observable results in two different properties of a `SimData` object. If the results are scalar-valued, they are stored in `SimData.ScalarObservables`. Otherwise, they are

stored in `SimData.VectorObservables`. In this example, the `stat1` observable expression is scalar-valued.

Extract the scalar observable values and plot them against the dose amounts.

```
scalarObs = vertcat(newSD.ScalarObservables);
doseAmounts = generate(doseSamples);
figure
plot(doseAmounts.AmountParam,scalarObs.stat1,'o','MarkerFaceColor','b')
```



The plot shows that dose amounts ranging from 50 to 180 nanomoles provide `T0` responses that lie within the target efficacy and safety thresholds.

You can update the observable expression with different threshold amounts. The function recalculates the expression and returns the results in a new `SimData` object array.

```
newSD2 = updateobservable(newSD,'stat1','max(T0) < 0.75 & min(T0) > 0.30');
```

Rename the observable expression. The function renames the observable, updates any expressions that reference the renamed observable (if applicable), and returns the results in a new `SimData` object array.

```
newSD3 = renameobservable(newSD2,'stat1','EffectiveDose');
```

Restore the warning settings.

```
warning('on','SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
```

Input Arguments

`sdin` — Input simulation data
`SimData` object | array of `SimData` objects

Input simulation data, specified as a `SimData` object or array of objects.

`oldNames` — Existing names of observables
character vector | string | string vector | cell array of character vectors

Existing names of the observables, specified as a character vector, string, string vector, or cell array of character vectors.

Example: `{'max_drug','mean_drug'}`

Data Types: `char` | `string` | `cell`

`newNames` — New names for observables
character vector | string | string vector | cell array of character vectors

New names for the observables, specified as a character vector, string, string vector, or cell array of character vectors. The number of new names must match the number of old names.

Each new name must be unique in the `SimData` object, meaning it cannot match the name of any other observable, species, compartment, parameter, or reaction referenced in the `SimData` object.

Example: `{'MAX','MEAN'}`

Data Types: `char` | `string` | `cell`

Output Arguments

`sdout` — Simulation data with observable results
`SimData` object | array of `SimData` objects

Simulation data with observable results, returned as a `SimData` object or array of objects.

Version History

Introduced in R2020a

See Also

`SimData` | `updateobservable` | `addobservable`

reorder (model, compartment, kinetic law)

Reorder component lists

Syntax

```
modelObj = reorder(Obj,NewOrder)
```

Input Arguments

`Obj`	Model, compartment, or kinetic law object.
`NewOrder`	Object vector in the new order. If `Obj` is a `model object`, `NewOrder` can be an array of compartment, event, parameter, reaction, rule, variant, or dose objects. If `Obj` is a compartment object, `NewOrder` must be an array of species objects. If `Obj` is a kinetic law object, `NewOrder` must be an array of parameter objects. **Warning** As of 2017b, reordering rules has no effect on simulation results because the rules are evaluated as a unified system of constraints. For details, see “Evaluation Order of Rules”.

Description

`modelObj = reorder(Obj,NewOrder)` reorders the component vector `modelObj` to be in the order specified.

Use this method to reorder any of the component vectors, such as compartments, events, parameters, rules, species, doses, and variants. When reordered, the vector of components must contain the same objects as the original list of objects, though they can be in a different order.

Examples

Reorder Reactions in SimBiology Model

Import a model.

```
modelObj = sbmlimport('lotka');
```

Display reactions in the model.

```
modelObj.Reactions
```

```
ans =
   SimBiology Reaction Array

   Index:    Reaction:
   1         x + y1 -> 2 y1 + x
   2         y1 + y2 -> 2 y2
```

```
   3         y2 -> z
```

Reverse the order of reactions in the model.

```
reorder(modelObj,modelObj.Reactions([3 2 1]));
```

Display the new order of reactions.

```
modelObj.Reactions
```

```
ans =
   SimBiology Reaction Array

   Index:    Reaction:
   1         y2 -> z
   2         y1 + y2 -> 2 y2
   3         x + y1 -> 2 y1 + x
```

Version History

Introduced in R2007b

See Also

`Model object` | `Compartment object` | `KineticLaw object`

RepeatDose object

Define drug dosing protocol

Description

A `RepeatDose` object defines a series of doses to the amount of a species during a simulation. The `TargetName` property of a dose object defines the species that receives the dose.

Each dose is the same amount, as defined by the `Amount` property, and given at equally spaced times, as defined by the `Interval` property. The `RepeatCount` property defines the number of injections in the series, excluding the initial injection. The `Rate` property defines how fast each dose is given.

To use a dose object in a simulation you must add the dose object to a model object and set the `Active` property of the dose object to true. Set the `Active` property to true if you always want the dose to be applied before simulating the model.

Warning The `Active` property of the `RepeatDose object` will be removed in a future release. Explicitly specify a dose or an array of doses as an input argument when you simulate a model using `sbiosimulate`.

When there are multiple active RepeatDose objects on a model and if there are duplicate specifications for a property value, the last occurrence for the property value in the array of dose, is used during simulation. You can find out which dose is applied last by looking at the indices of the dose objects stored on the model.

You can set these dose properties to model parameters: `Amount`, `Interval`, `Rate`, `RepeatCount`, `StartTime`, `LagParameterName` and `DurationParameterName`. You can set these properties, except `LagParameterName` and `DurationParameterName`, to either a numeric value or the name of a model-scoped parameter (as a character vector or string). Parameterizing dose properties provides more flexibility for different dosing applications, such as scaling the dose amount by body weight. For details, see “Parameterized and Adaptive Doses”.

Constructor Summary

sbiodose	Construct dose object

Method Summary

Methods for `RepeatDose` objects

copyobj	Copy SimBiology object and its children
delete	Delete SimBiology object
display	Display summary of SimBiology object
get	Get SimBiology object properties
getTable(ScheduleDose,RepeatDose)	Return data from SimBiology dose object as table
rename	Rename object and update expressions
set	Set SimBiology object properties
setTable(ScheduleDose,RepeatDose)	Set dosing information from table to dose object

Property Summary

Properties for `RepeatDose` objects

Active	Indicate object in use during simulation
Amount	Amount of dose
AmountUnits	Dose amount units
DurationParameterName	Parameter specifying length of time to administer a dose
EventMode	Determine how events that change dose parameters affect in-progress dosing
Interval	Time between doses
LagParameterName	Parameter specifying time lag for dose
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Rate	Rate of dose
RateUnits	Units for dose rate
RepeatCount	Dose repetitions
StartTime	Start time for initial dose time
Tag	Specify label for SimBiology object
TargetName	Species receiving dose
TimeUnits	Show time units for dosing and simulation
Type	Display SimBiology object type
UserData	Specify data to associate with object

Examples

Scale Dose Amount by Body Weight

Parameterize the `Amount` property of a dose to scale it by the body weight of a patient.

Create a simple model with linear elimination and an amount parameter.

```
model                       = sbiomodel('simple model');
compartment                 = addcompartment(model,'Central',1);
compartment.CapacityUnits   = 'liter';
species                     = addspecies(model,'drug');
species.InitialAmountUnits  = 'milligram';

% Elimination rate
elimParam                   = addparameter(model,'kel',0.1);
elimParam.ValueUnits        = '1/hour';

% Elimination reaction
reaction                    = addreaction(model,'drug -> null');
reaction.ReactionRate       = 'kel*drug';
amountParam                 = addparameter(model,'A',50);
amountParam.ConstantValue   = false;
amountParam.ValueUnits      = 'milligram'
```

```
amountParam =
   SimBiology Parameter Array

   Index:    Name:    Value:    Units:
   1         A        50        milligram
```

Create a dose with its `Amount` property set to the amount parameter `'A'`.

```
dose                        = adddose(model,'adaptive dose','repeat');
dose.Amount                 = 'A';
```

Set other dose properties.

```
dose.TargetName             = 'drug';
dose.StartTime              = 0;
dose.TimeUnits              = 'hour';
dose.Interval               = 24;
dose.RepeatCount            = 7;
```

Add a parameter to represent the body weight.

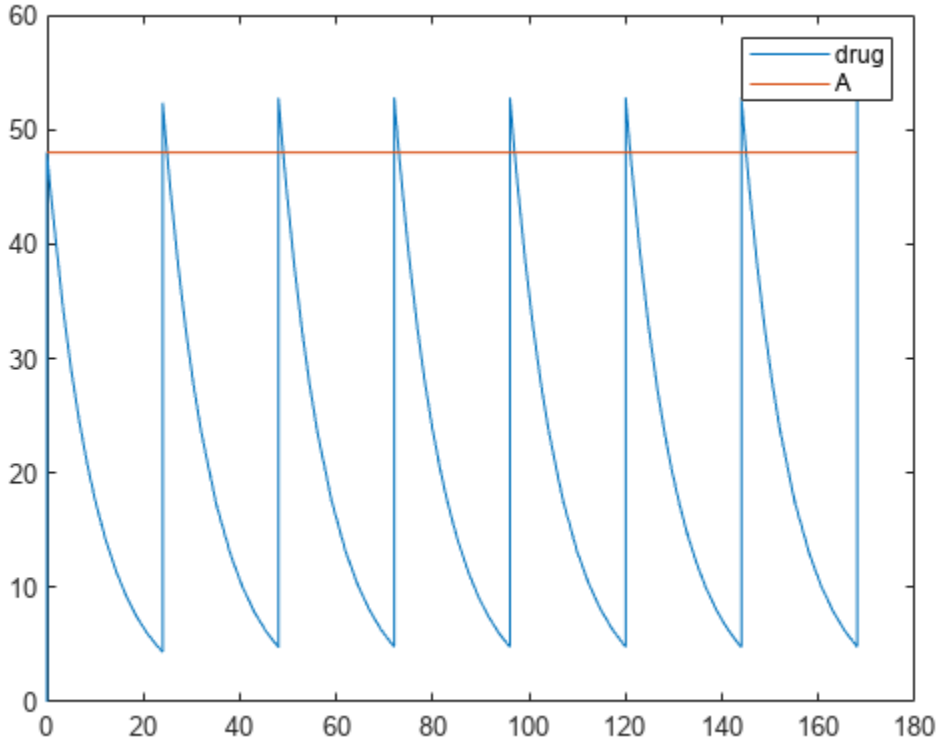
```
weightParam            = addparameter(model,'weight', 80);
weightParam.ValueUnits = 'kilogram';
```

Scale the dose amount by the body weight using an initial assignment rule.

```
scaleParam             = addparameter(model,'doseAmountPerWeight',0.6);
scaleParam.ValueUnits  = 'milligram/kilogram';
rule                   = addrule(model,'A = weight*doseAmountPerWeight','initialAssignment');
```

Simulate the model for 7 days and plot the results.

```
configset               = getconfigset(model);
configset.StopTime      = 7*24;
configset.TimeUnits     = 'hour';
[time, drugAndAmount]   = sbiosimulate(model,dose);
plot(time, drugAndAmount);
legend('drug','A');
```



Change Dose Behavior In Response to Changes in Model Parameters

Create a simple model with linear elimination, an amount parameter, and a rate parameter.

```
model                       = sbiomodel('simple model');
compartment                 = addcompartment(model,'Central',1);
compartment.CapacityUnits   = 'liter';
species                     = addspecies(model,'drug');
species.InitialAmountUnits  = 'milligram';

% Elimination rate
elimParam                   = addparameter(model,'kel',0.1);
elimParam.ValueUnits        = '1/hour';

% Elimination reaction
reaction                    = addreaction(model,'drug -> null');
reaction.ReactionRate       = 'kel*drug';

% Add amount and rate parameters
amountParam                 = addparameter(model,'A',50);
amountParam.ConstantValue   = false;
amountParam.ValueUnits      = 'milligram'

amountParam =
   SimBiology Parameter Array
```

```
   Index:    Name:    Value:    Units:
   1         A        50        milligram
```

```
rateParam                  = addparameter(model,'R',10);
rateParam.ValueUnits       = 'milligram/hour'
```

```
rateParam =
   SimBiology Parameter Array

   Index:    Name:    Value:    Units:
   1         R        10        milligram/hour
```

Create a dose with its `Amount` and `Rate` properties set to the amount and rate parameters 'A' and 'R', respectively.

```
dose                       = adddose(model,'adaptive dose','repeat');
dose.Amount                = 'A';
dose.Rate                  = 'R';
```

Set other dose properties.

```
dose.TargetName            = 'drug';
dose.StartTime             = 0;
dose.TimeUnits             = 'hour';
dose.Interval              = 24;
dose.RepeatCount           = 7;
```

Prepare the configuration set to simulate the model for 7 days.

```
configset           = getconfigset(model);
configset.StopTime  = 7*24;
configset.TimeUnits = 'hour';
```

Add an event to reset the dose amount to 10 at time >= 26.

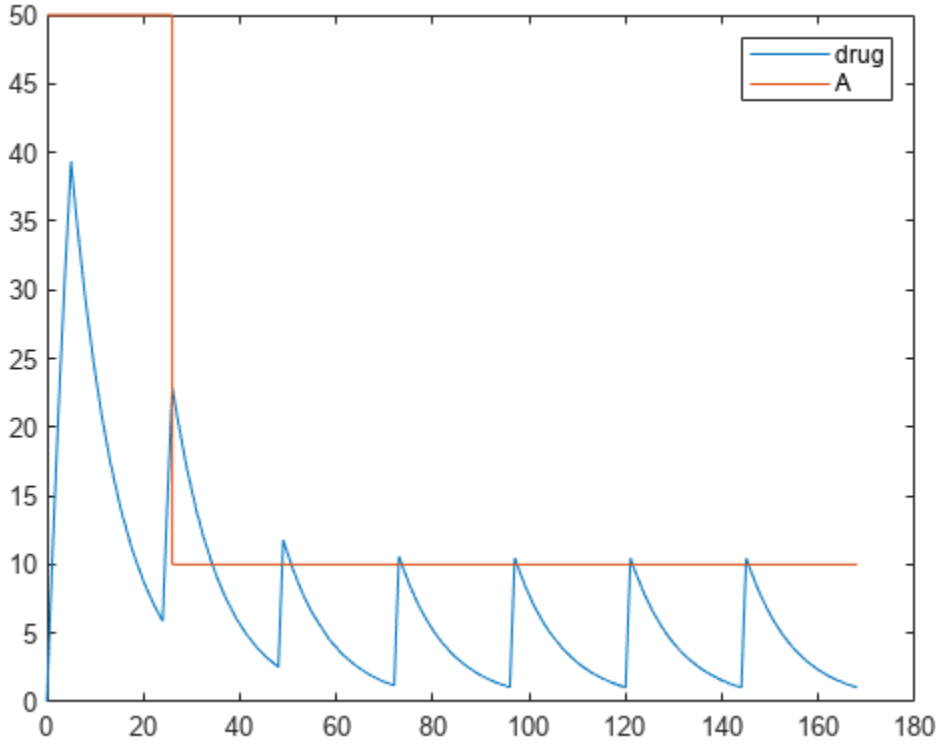
```
event = addevent(model,'time >= 26','A = 10');
```

Set the `EventMode` property to 'stop'. This setting causes any ongoing dose event to stop at 26 hours.

```
dose.EventMode = 'stop';
```

Simulate the model. The second dose event stops at 26 hours, and the subsequent dose events continue with the new dose amount of 10.

```
[time, drugAndAmount] = sbiosimulate(model,dose);
figure
plot(time, drugAndAmount);
legend('drug','A');
```

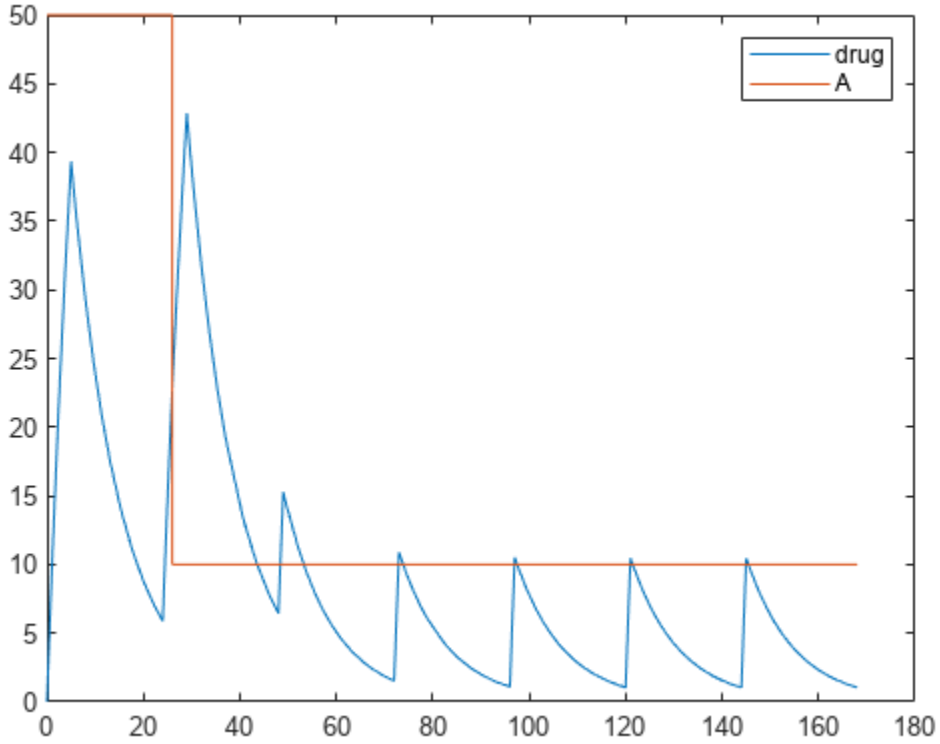


Alternatively, you can allow the ongoing dose event to finish before applying the new dose amount by setting `EventMode` to 'continue'.

```
dose.EventMode = 'continue';
```

Simulate the model. In this case, the second dose event continues to 26 hours.

```
[time, drugAndAmount] = sbiosimulate(model,dose);
figure
plot(time, drugAndAmount);
legend('drug','A');
```



Version History

Introduced in R2010a

See Also

`Model object` | `ScheduleDose object` | `sbiodose` | `sbiosimulate`

Topics

“Parameterized and Adaptive Doses”

resample

Resample simulation data onto new time vector

Syntax

```
newSimData = resample(simdata)
newSimData = resample(simdata,timeVector)
newSimData = resample(simdata,timeVector,method)
```

Description

`newSimData = resample(simdata)` resamples the simulation data in `simdata` to a common time vector and returns `newSimData`.

`newSimData = resample(simdata,timeVector)` resamples the simulation data to the specified time vector `timeVector`.

`newSimData = resample(simdata,timeVector,method)` resamples the simulation data using the specified interpolation `method`.

Examples

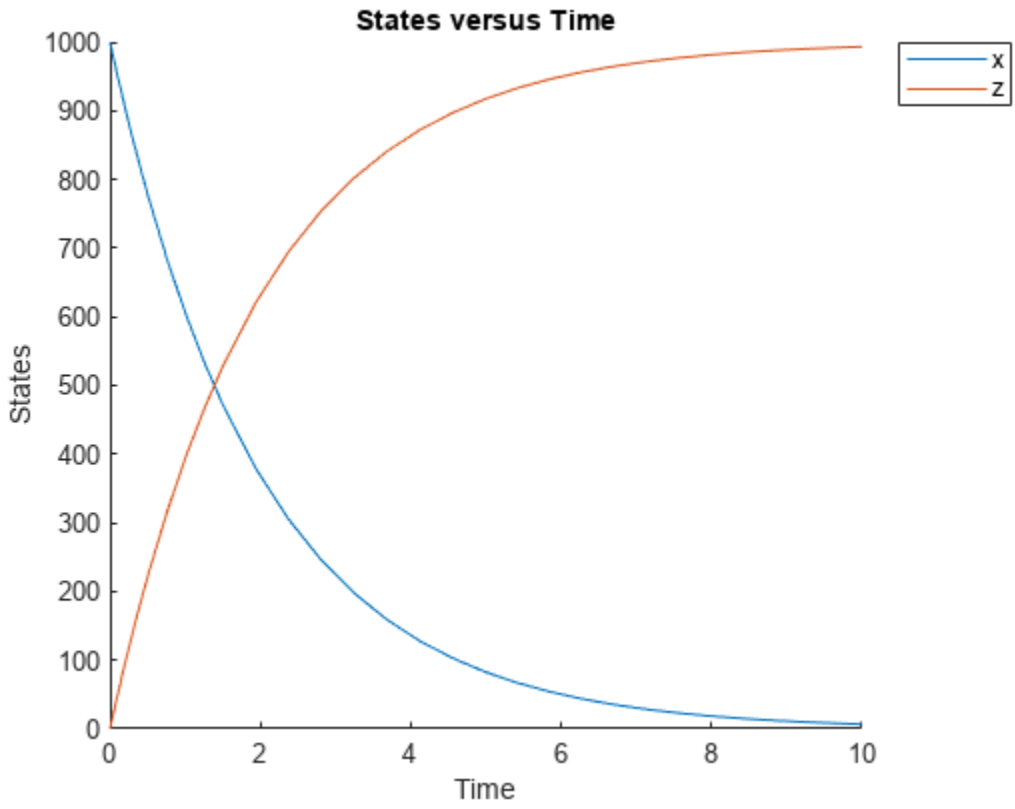
Resample Simulation Data

Load the radioactive decay model.

```
sbioloadproject('radiodecay');
```

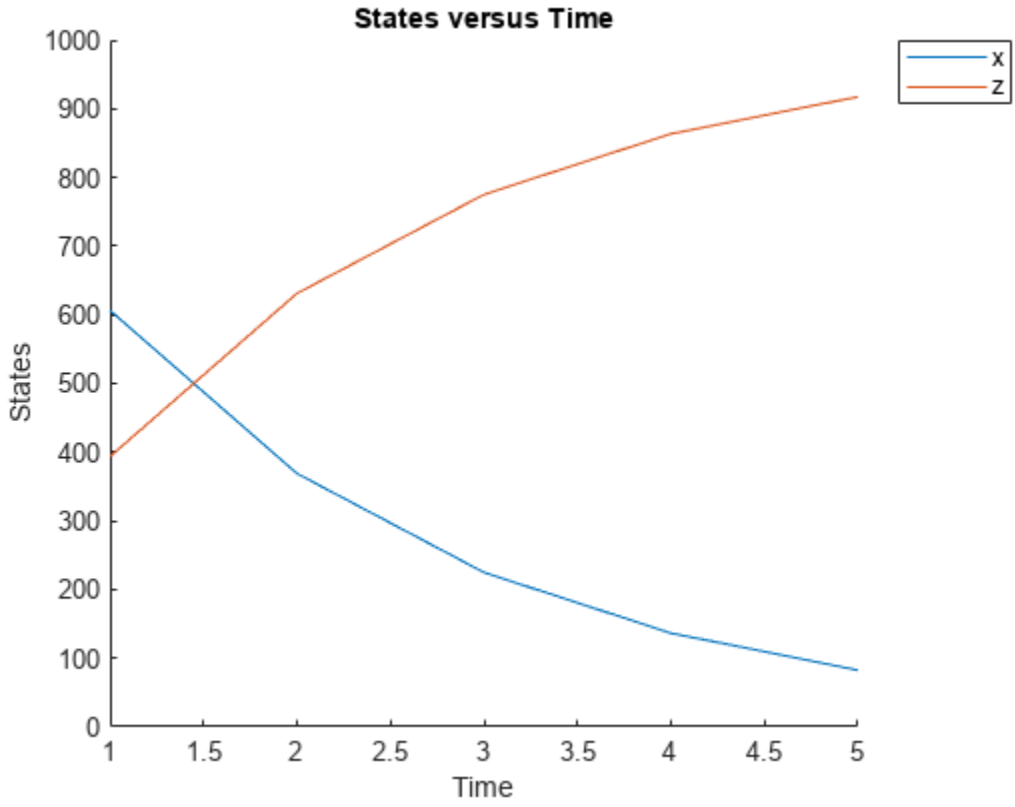
Simulate the model.

```
sd = sbiosimulate(m1);
sbioplot(sd);
```



Resample the simulation data between time points from 1 to 5 with the `linear` interpolation method.

```
newsd = resample(sd,[1:5],'linear');
sbioplot(newsd);
```



Change the solver to perform an ensemble run.

```
cs = getconfigset(m1);
cs.SolverType = 'ssa';
```

Perform an ensemble run.

```
sdEnsemble = sbioensemblerun(m1,10);
```

Resample the ensemble data between time points 1 and 10.

```
newsdEnsemble = resample(sdEnsemble,[1:10],'linear');
```

Compare the time steps.

```
newsdEnsemble(1).Time
```

```
ans = 10×1

     1
     2
     3
     4
     5
     6
     7
     8
     9
```

```
    10
```

```
sdEnsemble(1).Time
```

```
ans = 999×1

         0
    0.0004
    0.0006
    0.0047
    0.0049
    0.0058
    0.0105
    0.0131
    0.0143
    0.0144
      ⋮
```

Input Arguments

`simdata` — Simulation data

`SimData` object | array of `SimData` objects

Simulation data, specified as a `SimData` object or array of `SimData` objects. If you specify an array of `SimData` objects with different time courses, the function selects the time vector from a `SimData` object with the earliest stop time as the common time vector.

`timeVector` — Time vector

`[]` (default) | numeric vector

Time vector, specified as a numeric vector. The default value `[]` means that the function selects the time vector from `simdata` with the earliest stop time as the common time vector.

If `timeVector` includes time points outside the time interval of the `SimData` objects in `simdata`, `resample` performs extrapolation if the underlying interpolation "method" on page 2-0 supports it. Otherwise, the function returns `NaNs` for those time points. See the help for the MATLAB function corresponding to the interpolation method in use for information on how the function performs the extrapolation.

`method` — Interpolation method

`'interp1q'` (default) | character vector | string

Interpolation method for resampling, specified as a character vector or string. The valid choices follow.

- `'interp1q'` — Use the `interp1q` function.
- To use the `interp1` function, specify one of the following methods:
  - `'nearest'`
  - `'linear'`
  - `'spline'`

  - `'pchip'`
  - `'cubic'`
  - `'v5cubic'` (same as `'cubic'`)
- `'zoh'` — Specify the zero-order hold.

Note The `'cubic'` method changed in R2020b to perform cubic convolution. In previous releases, `'cubic'` was the same as `'pchip'`. For details, see `interp1`.

Output Arguments

`newSimData` — Resampled simulation data
`SimData` object | array of `SimData` objects

Resampled simulation data, returned as a `SimData` object or array of `SimData` objects.

Version History

Introduced in R2007b

See Also

`SimData` | `sbiosimulate`

resample

Resample Sobol indices or elementary effects to new time vector

Syntax

```
results = resample(gsaObj,timeVector)
results = resample(gsaObj,timeVector,method)
```

Description

`results = resample(gsaObj,timeVector)` resamples model evaluations to a vector of new time points. By default, the function uses the `interp1q` interpolation method.

`results = resample(gsaObj,timeVector,method)` specifies the interpolation `method`.

Examples

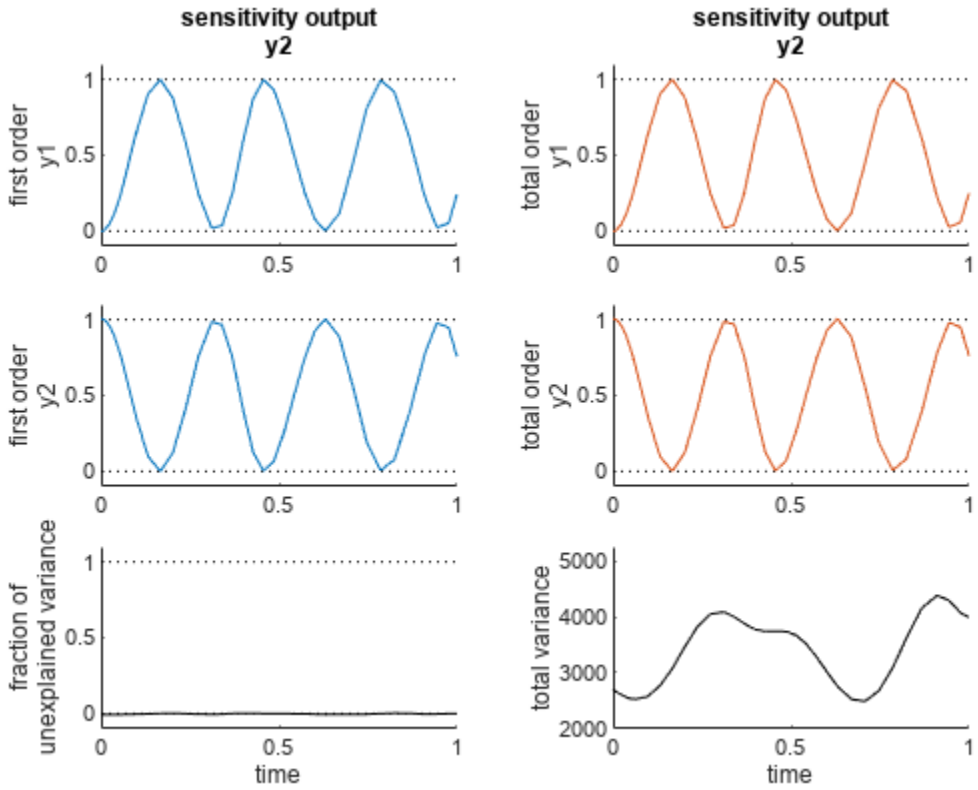
Resample Sobol Indices to New Time Points

Load the lotka model.

```
m = sbmlimport("lotka");
```

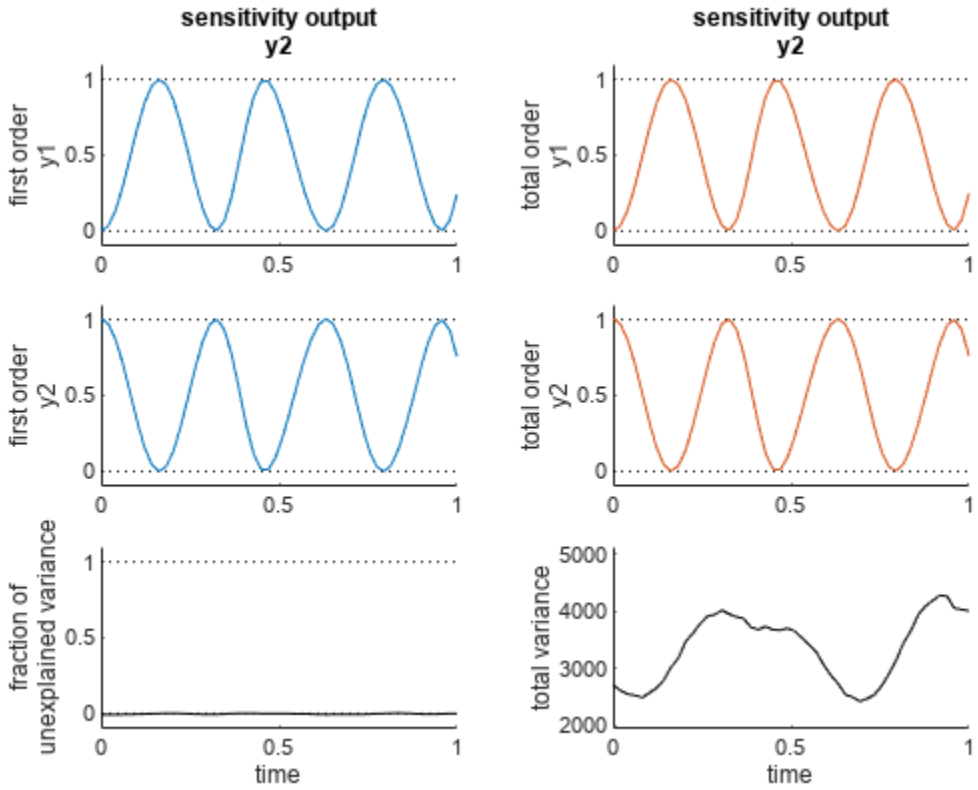
Decompose the variance of predators y2 into attributions of the initial values of the prey y1 and predators.

```
sobolResults = sbiosobol(m,["y1","y2"],"y2","StopTime",1);
plot(sobolResults);
```



Resample the Sobol indices to a new time vector.

```
newSobolResults = resample(sobolResults,linspace(0,1,50));
plot(newSobolResults);
```



Input Arguments

`gsaObj` — Results from global sensitivity analysis

`SimBiology.gsa.Sobol` object | `SimBiology.gsa.ElementaryEffects` object

Results from global sensitivity analysis, specified as a `SimBiology.gsa.Sobol` or `SimBiology.gsa.ElementaryEffects` object.

`timeVector` — New time points

numeric vector

New time points, specified as a nonempty real numeric vector containing finite and increasing values.

If `timeVector` includes time points outside the time interval encompassed by the simulation data in `sobolObj`, `resample` performs extrapolation. The function issues a warning and throws an error if resampling fails due to extrapolation.

See the help for the MATLAB function corresponding to the interpolation method in use for information on how the function performs the extrapolation.

Data Types: `double`

`method` — Interpolation method

`'interp1q'` (default) | string | character vector

Interpolation method, specified as a string or character vector. The valid options follows.

- `'interp1q'` — Use the `interp1q` function.
- Use the `interp1` function by specifying one of the following methods:
  - `'nearest'`
  - `'linear'`
  - `'spline'`
  - `'pchip'`
  - `'v5cubic'`
- `'zoh'` — Specify the zero-order hold.

Data Types: `char` | `string`

Output Arguments

`results` — Resampled results
`SimBiology.gsa.Sobol` object | `SimBiology.gsa.ElementaryEffects`

Resampled simulation results computed at new time points, returned as a `SimBiology.gsa.Sobol` or `SimBiology.gsa.ElementaryEffects` object. If the input is a `SimBiology.gsa.Sobol` object, the returned results contain resampled simulation results and Sobol indices computed at new time points. If the input is an `SimBiology.gsa.ElementaryEffects` object, the results contain resampled simulation results and elementary effects computed at new time points.

Version History

Introduced in R2020a

See Also

`SimBiology.gsa.Sobol` | `SimBiology.gsa.ElementaryEffects` | `sbiosobol` | `sbioelementaryeffects`

Topics
“Sensitivity Analysis in SimBiology”

reset (root)

Delete all model objects from root object

Syntax

```
reset(sbioroot)
```

Description

`reset(sbioroot)` deletes all SimBiology model objects contained by the root object. This call is equivalent to `sbioreset on page 1-224`.

The root object contains a list of model objects, available units, unit prefixes, and kinetic laws.

To add a kinetic law to the user-defined library, use the `sbioaddtolibrary` function. To add a unit to the user-defined library, use `sbiounit` followed by `sbioaddtolibrary`. To add a unit prefix to the user-defined library, use `sbiounitprefix` followed by `sbioaddtolibrary`.

Examples

1 Query `sbioroot`, which has two model objects.

```
sbioroot

   SimBiology Root Contains:

    Models:                          2
    Builtin Abstract Kinetic Laws:   3
    User Abstract Kinetic Laws:      1
    Builtin Units:                   54
    User Units:                      0
    Builtin Unit Prefixes:           13
    User Unit Prefixes:              0
```

2 Call `reset`.

```
sbioroot

   SimBiology Root Contains:

    Models:                          0
    Builtin Abstract Kinetic Laws:   3
    User Abstract Kinetic Laws:      1
    Builtin Units:                   54
    User Units:                      0
    Builtin Unit Prefixes:           13
    User Unit Prefixes:              0
```

See Also

`sbioaddtolibrary`, `sbioreset`, `sbioroot`, `sbiounit`, `sbiounitprefix`

Version History

Introduced in R2006a

rmcontent (variant)

Remove contents from variant object

Syntax

`rmcontent(variantObj, contents)`

`rmcontent(variantObj, idx)`

Arguments

<table>
<tr><td>variantObj</td><td colspan="3">Specify the variant object from which you want to remove data. The <code>Content</code> property is modified to remove the new data.</td></tr>
<tr><td>contents</td><td colspan="3">Specify the data you want to remove from a variant object. Contents can either be a cell array or an array of cell arrays. A valid cell array should have the form <code>{'Type', 'Name', 'PropertyName', PropertyValue}</code>, where <code>PropertyValue</code> is the new value to be applied for the <code>PropertyName</code>. Valid <code>Type</code>, <code>Name</code>, and <code>PropertyName</code> values are as follows.
<table>
<tr><th>'Type'</th><th>'Name'</th><th>'PropertyName'</th></tr>
<tr><td><code>'species'</code></td><td>Name of the species. If there are multiple species in the model with the same name, specify the species as [<code>compartmentName.speciesName</code>], where <code>compartmentName</code> is the name of the compartment containing the species.</td><td><code>'InitialAmount'</code></td></tr>
<tr><td><code>'parameter'</code></td><td>If the parameter scope is a model, specify the parameter name. If the parameter scope is a kinetic law, specify [<code>reactionName.parameterName</code>].</td><td><code>'Value'</code></td></tr>
<tr><td><code>'compartment'</code></td><td>Name of the compartment.</td><td><code>'Capacity'</code></td></tr>
</table></td></tr>
<tr><td>idx</td><td colspan="3">Specify the <code>ContentIndex</code> or indices of the data to be removed. To display the <code>ContentIndex</code>, enter the object name and press Enter.</td></tr>
</table>

Description

`rmcontent(variantObj, contents)` removes the data stored in the variable *`contents`* from the variant object (*`variantObj`*).

`rmcontent(variantObj, idx)` removes the data specified by the indices *`idx`* (also called `ContentIndex`) from the `Content` property of the variant object.

Examples

1 Create a model containing three species in one compartment.

```
modelObj = sbiomodel('mymodel');
compObj = addcompartment(modelObj, 'comp1');
A = addspecies(compObj, 'A');
B = addspecies(compObj, 'B');
C = addspecies(compObj, 'C');
```

2 Add a variant object that varies the species' `InitialAmount` property.

```
variantObj = addvariant(modelObj, 'v1');
addcontent(variantObj, {{'species','A', 'InitialAmount', 5}, ...
{'species', 'B', 'InitialAmount', 10}, ...
{ 'species', 'C', 'InitialAmount', 15}});% Display the variant
variantObj
```

```
SimBiology Variant - v1 (inactive)

   ContentIndex:     Type:        Name:             Property:           Value:
   1                 species      A                 InitialAmount       5
   2                 species      B                 InitialAmount       10
   3                 species      C                 InitialAmount       15
```

3 Use the `ContentIndex` number to remove a species from the `Content` property of the variant object.

```
rmcontent(variantObj, 2);
variantObj
```

```
SimBiology Variant - v1 (inactive)

   ContentIndex:     Type:        Name:             Property:           Value:
   1                 species      A                 InitialAmount       5
   2                 species      C                 InitialAmount       15
```

4 (Alternatively) Remove a species from the contents of the variant object using detailed reference to the species.

```
rmcontent(variantObj, {'species','A', 'InitialAmount', 5});
% Display variant object
variantObj
SimBiology Variant - v1 (inactive)

   ContentIndex:     Type:        Name:             Property:           Value:
   1                 species      C                 InitialAmount       15
```

See Also

`addvariant`, `rmcontent`, `sbiovariant`

Version History

Introduced in R2007b

rmproduct (reaction)

Remove species object from reaction object products

Syntax

```
rmproduct(reactionObj, SpeciesName)
rmproduct(reactionObj, speciesObj)
```

Arguments

reactionObj	Reaction object.
SpeciesName	Name for a model object. Enter a species name or a cell array of species names.
speciesObj	Species object. Enter a species object or an array of species objects.

Description

`rmproduct(reactionObj, SpeciesName)`, in a reaction object (`reactionObj`), removes a species object with a specified name (`SpeciesName`) from the property `Products`, removes the species name from the property `Reaction`, and updates the property `Stoichiometry` to exclude the species coefficient.

`rmproduct(reactionObj, speciesObj)` removes a species object as described above using a MATLAB variable for a species object.

The species object is not removed from the parent model property `Species`. If the species object is no longer used by any reaction, you can use the function `delete` to remove it from the parent object.

If one of the species specified does not exist as a product, a warning is returned.

Examples

Example 1

This example shows how to remove a product that was previously added to a reaction. You can remove the species object using the species name.

```
modelObj = sbiomodel('cell');
reactionObj = addreaction(modelObj, 'Phosphocreatine + ADP -> creatine + ATP + Pi');
rmproduct(reactionObj, 'Pi')

SimBiology Reaction Array

 Index:  Reaction:
  1      Phosphocreatine + ADP -> creatine + ATP
```

Example 2

Remove a species object using a model index to a species object.

```
modelObj = sbiomodel('cell');
reactionObj = addreaction(modelObj, 'A -> B + C');
```

```
reactionObj.Reaction
 ans =
    A -> B + C

rmproduct(reactionObj, modelObj.Species(2));
reactionObj.Reaction
  ans =
    A -> C
```

See Also

rmreactant

Version History

Introduced in R2006a

rmreactant (reaction)

Remove species object from reaction object reactants

Syntax

```
rmreactant(reactionObj, SpeciesName)
rmreactant(reactionObj, speciesObj)
```

Arguments

reactionObj	Reaction object.
SpeciesName	Name for a species object. Enter a species name or a cell array of species names.
speciesObj	Species object. Enter a species object or an array of species objects.

Description

`rmreactant(reactionObj, SpeciesName)`, in a reaction object (`reactionObj`), removes a species object with a specified name (`SpeciesName`) from the property `Reactants`, removes the species name from the property `Reaction`, and updates the property `Stoichiometry` to exclude the species coefficient.

`rmreactant(reactionObj, speciesObj)` removes a species object as described above using a MATLAB variable for a species object, or a model index for a species object.

The species object is not removed from the parent model property `Species`. If the species object is no longer used by any reaction, you can use the method `delete` to remove it from the parent object.

If one of the species specified does not exist as a reactant, a warning is returned.

Examples

Example 1

This example shows how to remove a reactant that was added to a reaction by mistake. You can remove the species object using the species name.

```
modelObj = sbiomodel('cell');
reactionObj = addreaction(modelObj, 'Phosphocreatine + ADP + Pi -> creatine + ATP');
rmreactant(reactionObj, 'Pi')

SimBiology Reaction Array

 Index:    Reaction:
  1        Phosphocreatine + ADP -> creatine + ATP
```

Example 2

Remove a species object using a model index to a species object.

```
modelObj = sbiomodel('cell');
reactionObj = addreaction(modelObj, 'A -> B + C');
```

```
reactionObj.Reaction
ans =
    A + B -> C

rmreactant(reactionObj, modelObj.Species(1));
reactionObj.Reaction

ans =
    A -> C
```

See Also

delete, rmproduct

Version History

Introduced in R2006a

Root object

Hold models, unit libraries, and abstract kinetic law libraries

Description

The SimBiology root object contains a list of the SimBiology model objects and SimBiology libraries. The components that the libraries contain are: all available units, unit prefixes, and available abstract kinetic law objects. There are two types of libraries: one contains components that are built in (`BuiltInLibrary`), and the other contains components that are user defined (`UserDefinedLibrary`).

You can retrieve SimBiology model objects from the SimBiology root object. A SimBiology model object has its `Parent` property set to the SimBiology root object.

See “Property Summary” on page 2-771 for links to root object property reference pages.

Properties define the characteristics of an object. Use the `get` and `set` commands to list object properties and change their values at the command line. You can interactively change object properties in the SimBiology desktop.

Constructor Summary

sbioroot	Return SimBiology root object

Method Summary

copyobj	Copy SimBiology object and its children
delete	Delete SimBiology object
display	Display summary of SimBiology object
get	Get SimBiology object properties
reset (root)	Delete all model objects from root object
set	Set SimBiology object properties

Property Summary

BuiltInLibrary	Library of built-in components
Models	Contain all model objects
Type	Display SimBiology object type
UserDefinedLibrary	Library of user-defined components

See Also

`AbstractKineticLaw object`, `Configset object`, `KineticLaw object`, `Model object`, `Parameter object`, `Reaction object`, `Rule object`, `Species object`

Version History

Introduced in R2006b

Rule object

Hold rule for species and parameters

Description

The SimBiology rule object represents a *rule*, which is a mathematical expression that modifies a species amount or a parameter value. For a description of the types of SimBiology rules, see `RuleType`.

See “Property Summary” on page 2-773 for links to rule property reference pages.

Properties define the characteristics of an object. Use the `get` and `set` commands to list object properties and change their values at the command line. You can graphically change object properties in the graphical user interface.

Constructor Summary

addrule (model)	Create rule object and add to model object

Method Summary

copyobj	Copy SimBiology object and its children
delete	Delete SimBiology object
display	Display summary of SimBiology object
get	Get SimBiology object properties
rename	Rename object and update expressions
set	Set SimBiology object properties

Property Summary

Active	Indicate object in use during simulation
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Rule	Specify species and parameter interactions
RuleType	Specify type of rule for rule object
Tag	Specify label for SimBiology object
Type	Display SimBiology object type
UserData	Specify data to associate with object

See Also

“Definitions and Evaluations of Rules in SimBiology Models”, `AbstractKineticLaw object`, `Configset object`, `KineticLaw object`, `Model object`, `Parameter object`, `Reaction object`, `Root object`, `Species object`

Version History

Introduced in R2006b

summary

Return structure array that contains estimated values and fit quality statistics

Syntax

```
stats = summary(resultsObj)
```

Description

`stats = summary(resultsObj)` returns a structure array `stats` that contains estimated values and estimation statistics.

Examples

Estimate Two-Compartment PK Parameters

Load the sample data set.

```
load data10_32R.mat
gData = groupedData(data);
gData.Properties.VariableUnits = ["","hour","milligram/liter","milligram/liter"];
```

Create a two-compartment PK model.

```
pkmd                 = PKModelDesign;
pkc1                 = addCompartment(pkmd,"Central");
pkc1.DosingType      = "Infusion";
pkc1.EliminationType = "linear-clearance";
pkc1.HasResponseVariable = true;
pkc2                 = addCompartment(pkmd,"Peripheral");
model                = construct(pkmd);
configset            = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
responseMap = ["Drug_Central = CentralConc","Drug_Peripheral = PeripheralConc"];
```

Provide model parameters to estimate.

```
paramsToEstimate   = ["log(Central)","log(Peripheral)","Q12","Cl_Central"];
estimatedParam     = estimatedInfo(paramsToEstimate,'InitialValue',[1 1 1 1]);
```

Assume every individual receives an infusion dose at time = 0, with a total infusion amount of 100 mg at a rate of 50 mg/hour.

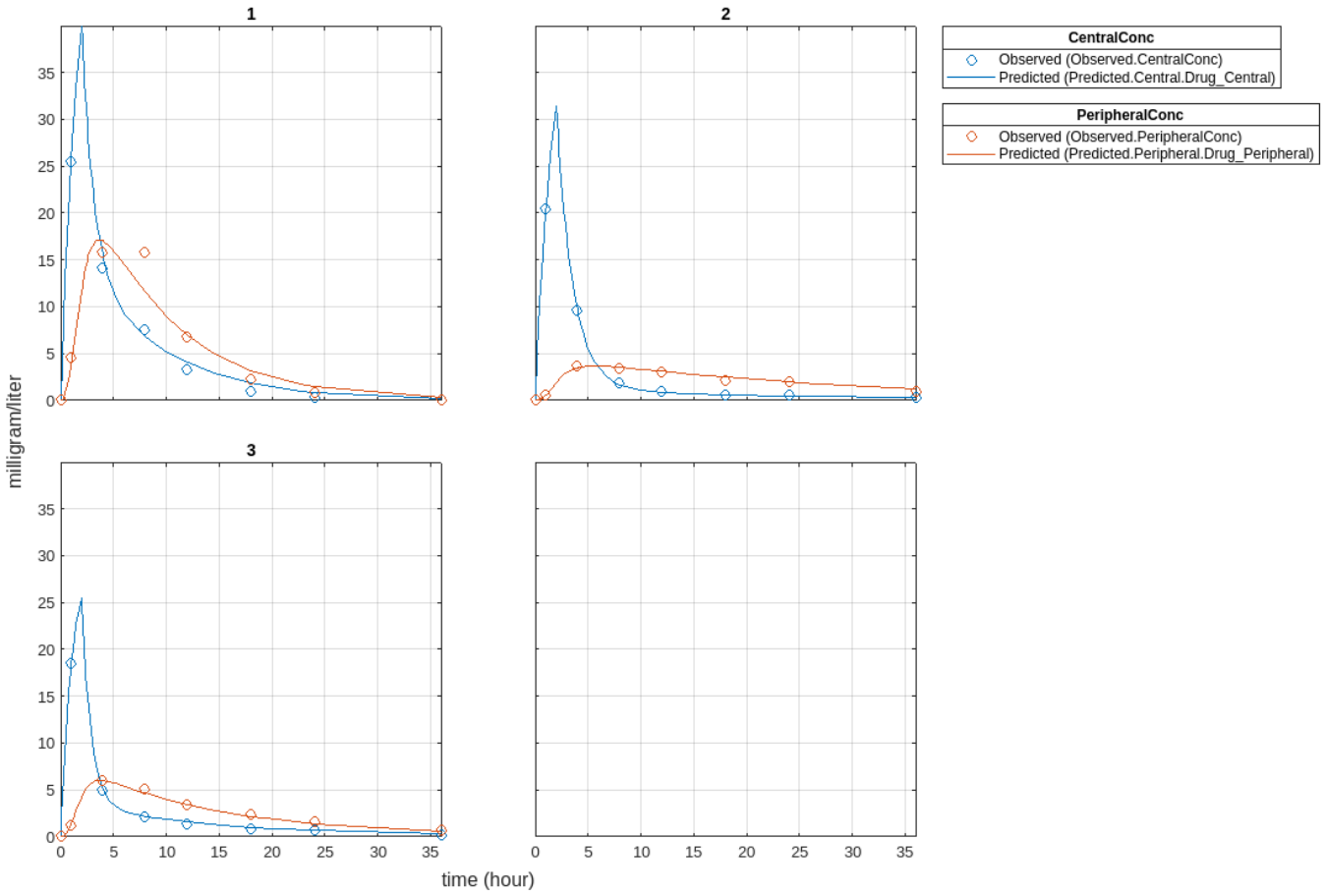
```
dose             = sbiodose("dose","TargetName","Drug_Central");
dose.StartTime   = 0;
dose.Amount      = 100;
dose.Rate        = 50;
dose.AmountUnits = "milligram";
dose.TimeUnits   = "hour";
dose.RateUnits   = "milligram/hour";
```

Estimate model parameters. By default, the function estimates a set of parameter for each individual (unpooled fit).

```
fitResults =  sbiofit(model,gData,responseMap,estimatedParam,dose);
```

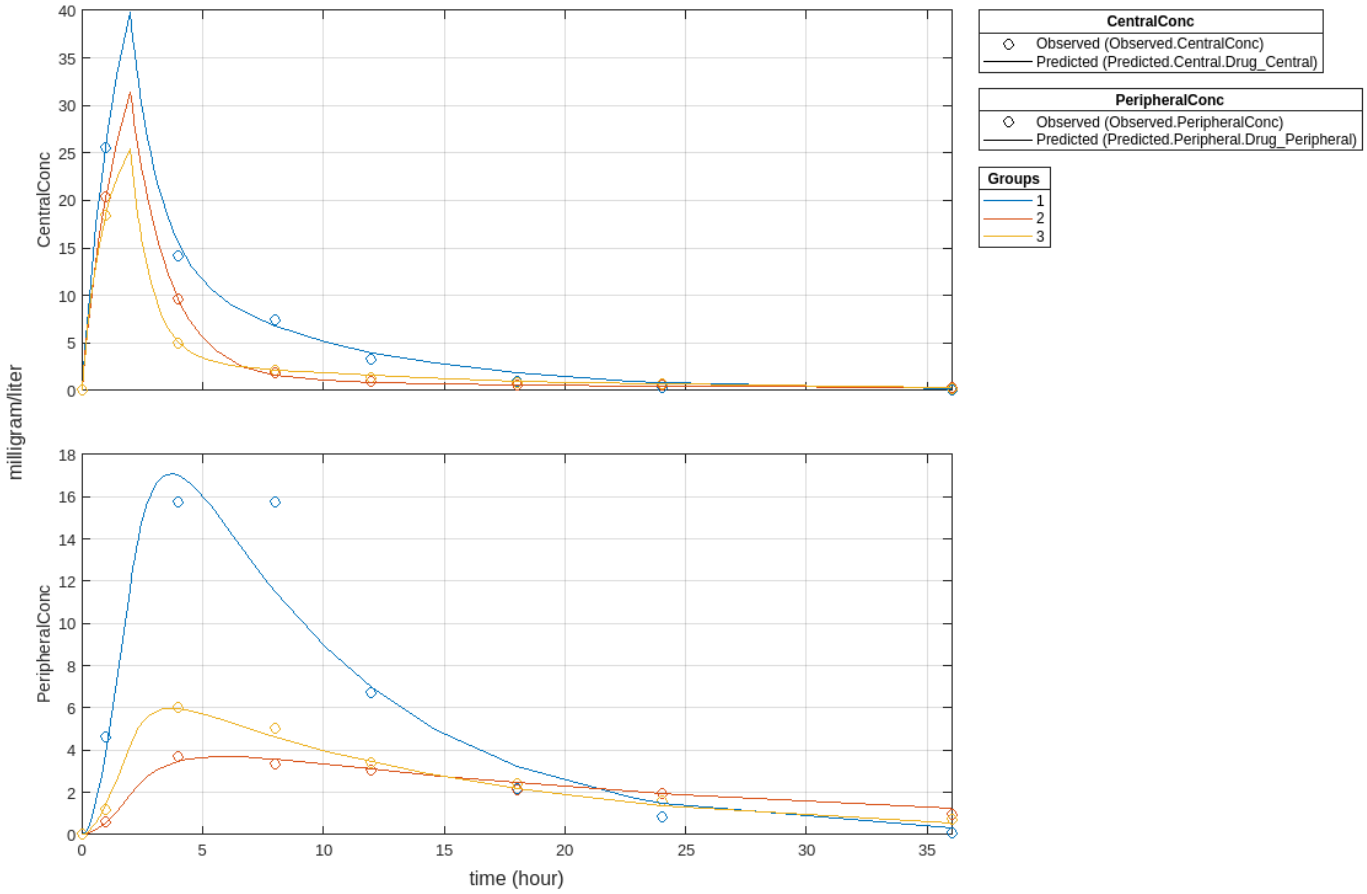
Plot the results.

```
plot(fitResults);
```



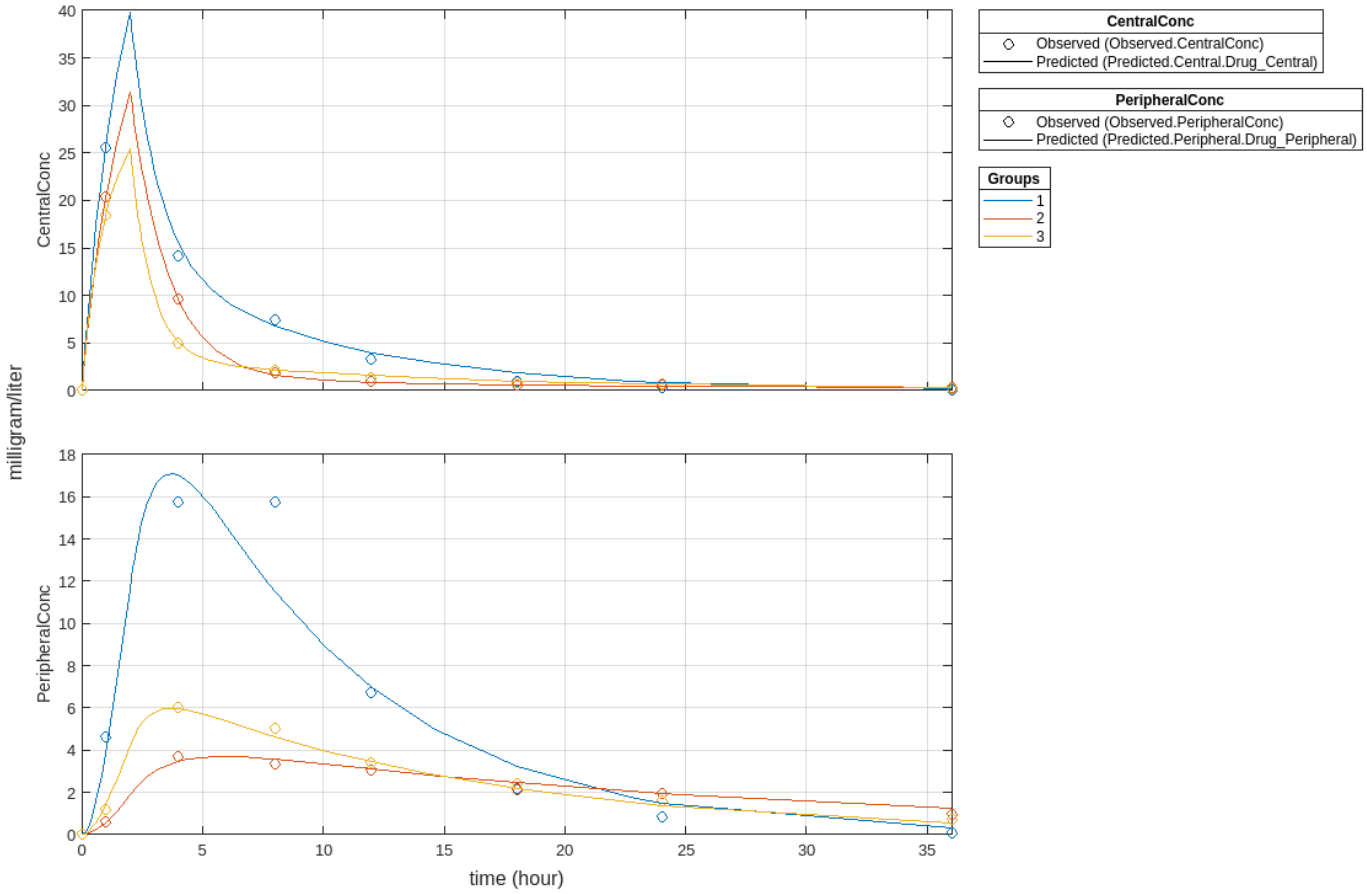
Plot all groups in one plot.

```
plot(fitResults,"PlotStyle","one axes");
```



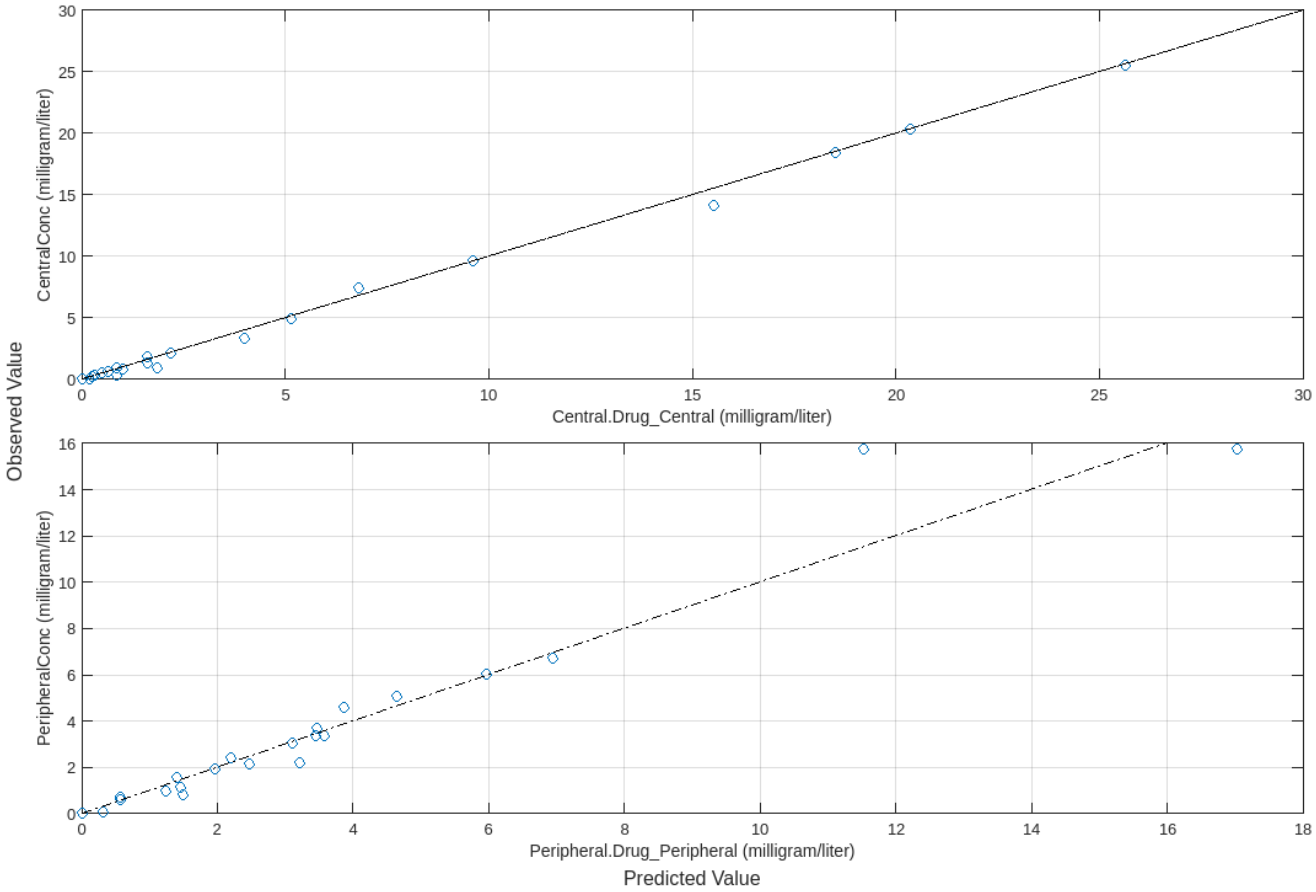
Change some axes properties.

```
s = struct;
s.Properties.XGrid = "on";
s.Properties.YGrid = "on";
plot(fitResults,"PlotStyle","one axes","AxesStyle",s);
```



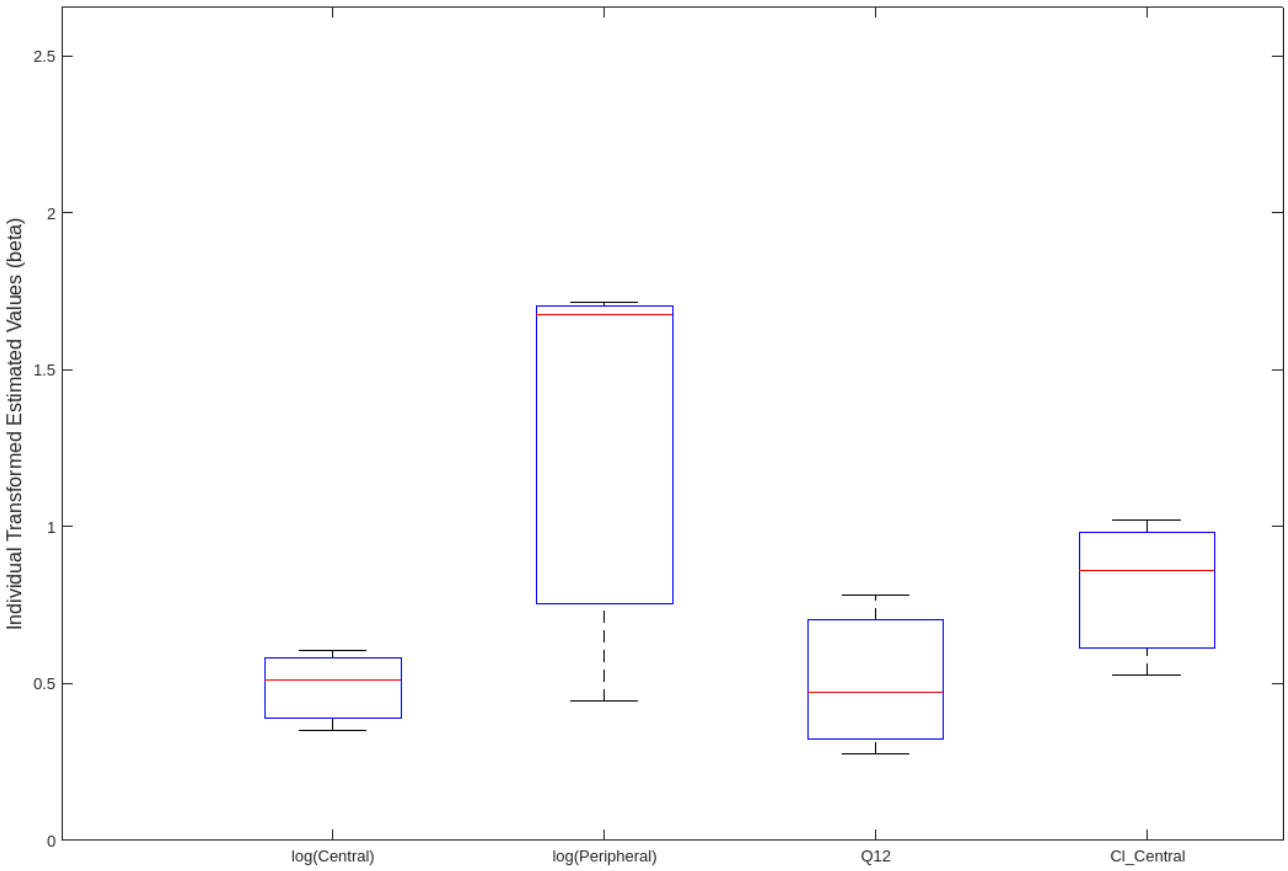
Compare the model predictions to the actual data.

```
plotActualVersusPredicted(fitResults)
```



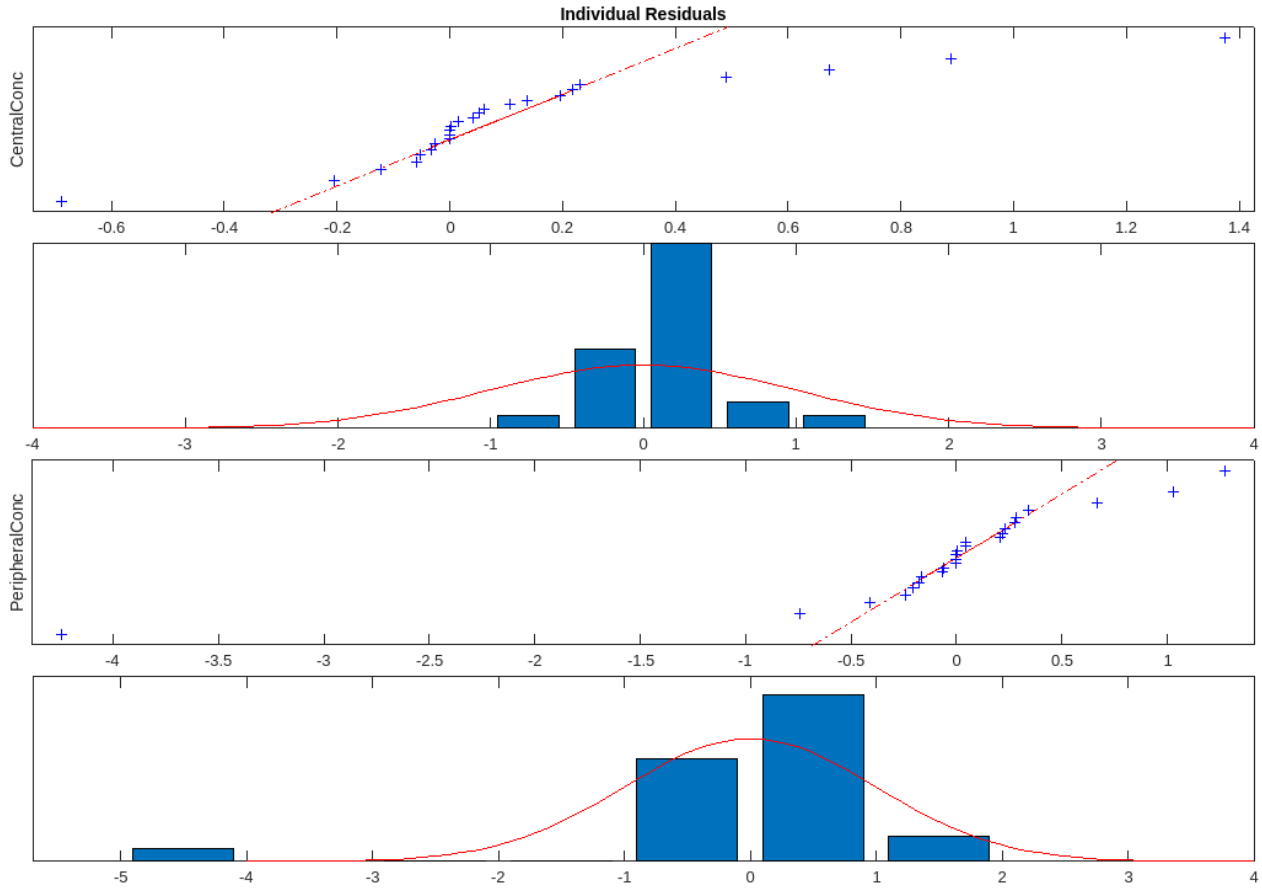
Use `boxplot` to show the variation of estimated model parameters.

```
boxplot(fitResults)
```



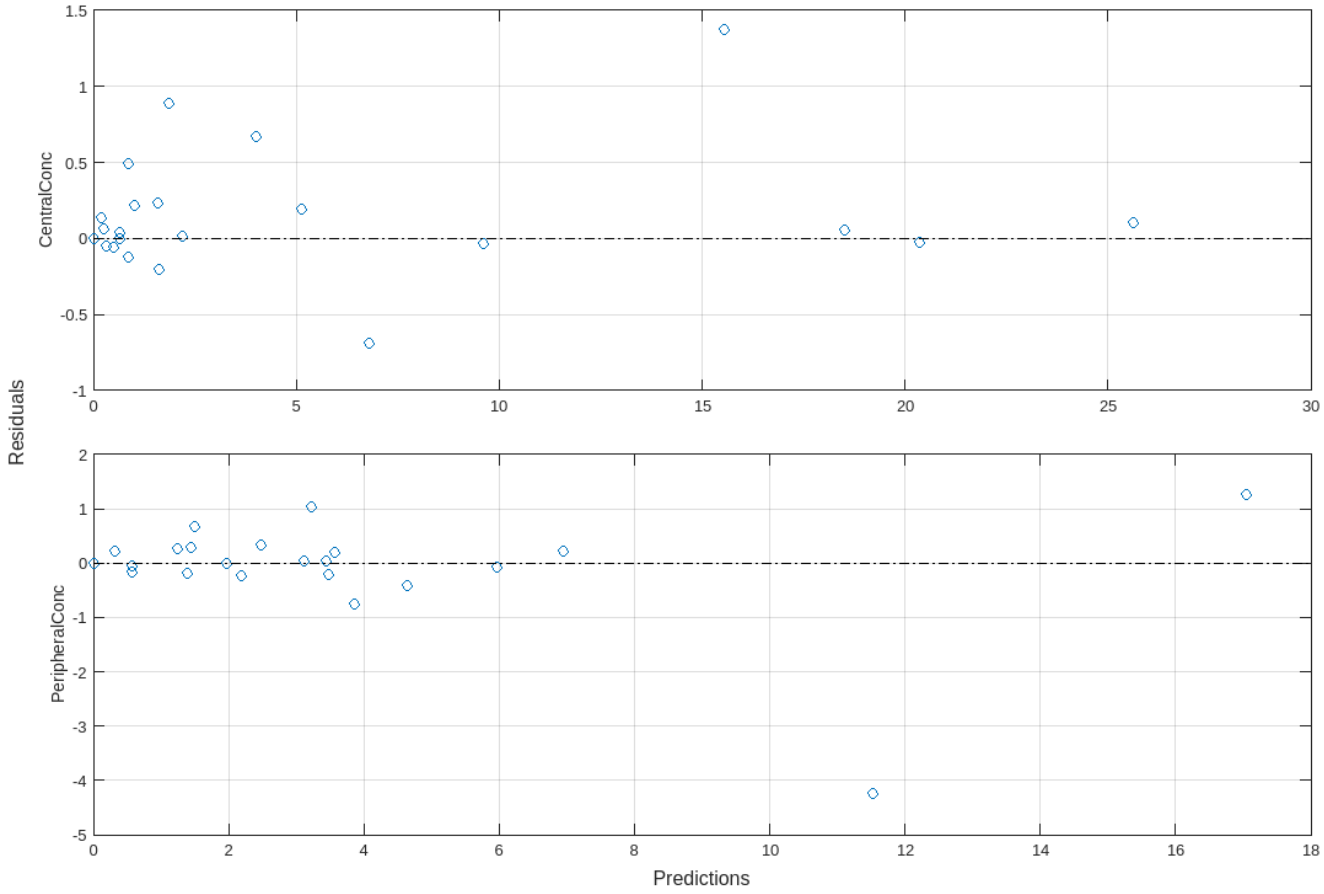
Plot the distribution of residuals. This normal probability plot shows the deviation from normality and the skewness on the right tail of the distribution of residuals. The default (constant) error model might not be the correct assumption for the data being fitted.

```
plotResidualDistribution(fitResults)
```



Plot residuals for each response using the model predictions on *x*-axis.

```
plotResiduals(fitResults,"Predictions")
```



Get the summary of the fit results. `stats.Name` contains the name for each table from `stats.Table`, which contains a list of tables with estimated parameter values and fit quality statistics.

```
stats = summary(fitResults);
stats.Name
```

```
ans =
'Unpooled Parameter Estimates'

ans =
'Statistics'

ans =
'Unpooled Beta'

ans =
'Residuals'

ans =
'Covariance Matrix'

ans =
'Error Model'
```

```
stats.Table
```

```
ans=3×9 table
    Group    Central Estimate    Central StandardError    Peripheral Estimate    Peripheral Stand
    _____    ________________    _____________________    ___________________    ________________

    {'1'}          1.422               0.12334                1.5619                0.36355
    {'2'}         1.8322              0.019672                5.3364                0.65327
    {'3'}         1.6657              0.038529                5.5632                0.37063

ans=3×7 table
    Group      AIC        BIC      LogLikelihood    DFE      MSE         SSE
    _____    _______    _______    _____________    ___    ________    _______

    {'1'}     60.961     64.051       -26.48        12        2.138     25.656
    {'2'}    -7.8379    -4.7475       7.9189        12     0.029012    0.34814
    {'3'}    -1.4336     1.6567       4.7168        12     0.043292     0.5195

ans=3×9 table
    Group    Central Estimate    Central StandardError    Peripheral Estimate    Peripheral Stand
    _____    ________________    _____________________    ___________________    ________________

    {'1'}        0.35208              0.086736               0.44589                0.23277
    {'2'}        0.60551              0.010737                1.6746                0.12242
    {'3'}        0.51027               0.02313                1.7162                0.06662

ans=24×4 table
    ID    Time    CentralConc    PeripheralConc
    __    ____    ___________    ______________

    1       0              0              0
    1       1        0.10646        -0.74394
    1       4         1.3745          1.2726
    1       8       -0.68825         -4.2435
    1      12        0.67383         0.21806
    1      18        0.88823          1.0269
    1      24        0.48941         0.66755
    1      36        0.13632         0.22948
    2       0              0              0
    2       1      -0.026731      -0.058311
    2       4      -0.033299       -0.20544
    2       8       -0.20466        0.20696
    2      12       -0.12223       0.045409
    2      18       0.041224        0.33883
    2      24      -0.059498      0.0036257
    2      36      -0.051645        0.27616
      ⋮

ans=12×6 table
    Group        Parameters         log(Central)    log(Peripheral)        Q12        Cl_Central
    _____    __________________    ____________    _______________    ___________    __________

    {'1'}    {'log(Central)'   }       0.015213        -0.022539       -0.0086672       0.00115
    {'1'}    {'log(Peripheral)'}      -0.022539          0.13217         0.045746     -0.007313
    {'1'}    {'Q12'            }     -0.0086672         0.045746         0.023092     -0.002148
    {'1'}    {'Cl_Central'     }       0.001159       -0.0073135       -0.0021484      0.001367
    {'2'}    {'log(Central)'   }     0.00038701        -0.002161      -0.00010177     9.7448e-05
```

```
    {'2'}    {'log(Peripheral)'}      -0.002161          0.42676          0.019101      -0.01575
    {'2'}    {'Q12'            }    -0.00010177         0.019101         0.00094857    -0.0007332
    {'2'}    {'Cl_Central'     }     9.7448e-05         -0.015755        -0.00073328     0.0006894
    {'3'}    {'log(Central)'   }      0.0014845        -0.0054648         -0.0013216     0.0001663
    {'3'}    {'log(Peripheral)'}     -0.0054648          0.13737           0.016903     -0.007272
    {'3'}    {'Q12'            }     -0.0013216         0.016903          0.0034406    -0.0008253
    {'3'}    {'Cl_Central'     }      0.00016639       -0.0072722        -0.00082538     0.0007458
```

```
ans=3×5 table
    Group     Response      ErrorModel        a        b
    _____    __________    _____________    _______    ___

    {'1'}    {0×0 char}    {'constant'}     1.2663    NaN
    {'2'}    {0×0 char}    {'constant'}    0.14751    NaN
    {'3'}    {0×0 char}    {'constant'}    0.18019    NaN
```

Input Arguments

`resultsObj` — Estimation results

`OptimResults` object | `NLINResults` object | vector of results objects

Estimation results, specified as an `OptimResults object` or `NLINResults object`, or vector of results objects which contains estimation results from running `sbiofit`.

Output Arguments

`stats` — Summary statistics

structure array

Summary statistics, returned as a structure array.

Each structure contains the fields:

- `Name` — Name of a fit statistics
- `Table` — Table containing values of the corresponding fit statistics

Version History

Introduced in R2014a

R2020a: `summary` returns structure array instead of figure

Behavior changed in R2020a

The summary function now returns a structure array instead of a figure.

See Also

`NLINResults object` | `OptimResults object` | `sbiofit`

SimBiology.Scenarios

Simulation scenarios

Description

`SimBiology.Scenarios` is an object that lets you generate different simulation scenarios based on different sample values of model quantities. You can combine these quantities with different doses or variants and simulate various scenarios to explore model behaviors under different experimental conditions and dosing regimens.

Creation

Syntax

```
sObj = SimBiology.Scenarios
sObj = SimBiology.Scenarios(name,content)
sObj = SimBiology.Scenarios(quantityNames,probDist,Name,Value)
```

Description

`sObj = SimBiology.Scenarios` returns a `Scenarios` object `sObj` that contains no entries on page 2-799.

`sObj = SimBiology.Scenarios(name,content)` returns a `Scenarios` object `sObj` with one entry. `name` is the name of a model quantity or the name of a group of variants or doses for scenario generation. `content` contains the corresponding numeric values for the model quantity or a vector of variant objects or vector of dose objects.

`sObj = SimBiology.Scenarios(quantityNames,probDist,Name,Value)` specifies to generate the sample values for one or more model quantities `quantityNames` from the joint probability distribution `probDist`. Specify additional options for the probability distributions and sampling method using one or more name-value pair arguments. To specify the probability distributions, you must have Statistics and Machine Learning Toolbox.

Input Arguments

`name` — Entry name

character vector | string

Entry name, specified as a character vector or string.

You can set the entry name to the name of a model quantity (species, parameter, or compartment). Alternatively, you can define a name for a group of doses or variants to be included in the sample (scenarios) generation.

Example: `"k1"`

Data Types: `char` | `string`

`content` — Model quantity values or vector of doses or variants

numeric vector | vector of `RepeatDose` or `ScheduleDose` objects | vector of variant objects

Model quantity values, or a vector of doses or variants, specified as a numeric vector, vector of `RepeatDose` or `ScheduleDose` objects, or vector of `variant` objects.

If you specify a quantity name for the `name` input argument, set `content` to a numeric vector.

If you specify a name for a group of doses or variants, set `content` to a vector of dose objects or vector of variant objects.

Example: `[0.5,1,1.5]`

`quantityNames` — Names of model quantities

character vector | string | string vector | cell array of character vectors

Names of model quantities for the sample (scenario) generation, specified as a character vector, string, string vector, or cell array of character vectors.

Example: `["k12","k21"]`

Data Types: `char` | `string` | `cell`

`probDist` — Probability distributions

vector of probability distribution objects | character vector | string | string vector | cell array of character vectors

Probability distributions to generate sample values for model quantities, specified as a vector of probability distribution objects, character vector, string, string vector, or cell array of character vectors containing the names of supported probability distributions. To specify the probability distributions, you must have Statistics and Machine Learning Toolbox.

Use the `makedist` function to create distribution objects. For a list of supported distributions, see “distname” (Statistics and Machine Learning Toolbox).

Example: `[pd1,pd2]`

Name-Value Pair Arguments

Specify optional comma-separated pairs of `Name,Value` arguments. `Name` is the argument name and `Value` is the corresponding value. `Name` must appear inside quotes. You can specify several name and value pair arguments in any order as `Name1,Value1,...,NameN,ValueN`.

Example: `'Number',10` specifies to generate 10 samples.

`Number` — Number of samples

`[]` (default) | positive scalar

Number of samples to draw from probability distributions, specified as the comma-separated pair consisting of `'Number'` and a positive scalar. The default value `[]` means that the function infers the number of samples from other entries. If the number cannot be inferred, the number is set to `2`.

Example: `'Number',5`

`RankCorrelation` — Rank correlation matrix

`[]` (default) | numeric matrix

Rank correlation matrix for the joint probability distribution, specified as the comma-separated pair consisting of `'RankCorrelation'` and a numeric matrix. The default behavior is that when both

`'RankCorrelation'` and `'Covariance'` are set to `[]`, `SimBiology.Scenarios` draws uncorrelated samples from the joint probability distribution.

You cannot specify `'RankCorrelation'` if `'Covariance'` is set. The number of columns in the matrix must match the number of specified distributions. The matrix must be symmetric with diagonal values of 1. All of its eigenvalues must also be positive.

Example: `'RankCorrelation',[1 0.3;0.3 1]`

`Mean` — Mean values
numeric vector

Mean values of quantities, specified as the comma-separated pair consisting of `'Mean'` and a numeric vector.

You can specify mean values for normal distributions only. The number of mean values must equal the number of specified probability distributions.

Example: `'Mean',[0.5,1.5]`

`Covariance` — Covariance matrix
`[]` (default) | numeric matrix

Covariance matrix for the joint probability distribution, specified as the comma-separated pair consisting of `'Covariance'` and a numeric matrix. The default behavior is that if both `'RankCorrelation'` and `'Covariance'` are set to `[]`, `SimBiology.Scenarios` draws uncorrelated samples from the joint probability distribution. You cannot specify `'Covariance'` if you specify `'RankCorrelation'`.

You can specify the covariance matrix for normal distributions only. The number of columns in the matrix must match the number of specified distributions. All of its eigenvalues must also be nonnegative.

Example: `'Covariance',[0.25 0.15;0.15 0.25]`

`SamplingMethod` — Sampling method
`'random'` (default) | `'lhs'` | `'copula'` | `'sobol'` | `'halton'`

Sampling method, specified as the comma-separated pair consisting of `'SamplingMethod'` and a character vector or string. Depending on whether probability distributions with `'RankCorrelation'` or normal distributions with `'Covariance'` are specified, the sampling techniques differ.

If an entry contains a (joint) normal distribution with `Covariance` specified, the sampling methods are:

- `'random'` – Draw random samples from the specified normal distribution using `mvnrnd`.
- `'lhs'` – Draw Latin hypercube samples from the specified normal distributions using `lhsnorm`. For details, see “Generating Quasi-Random Numbers” (Statistics and Machine Learning Toolbox).

If an entry contains a (joint) distribution with no `Covariance` specified, the sampling methods are:

- `'random'` – Draw random samples from the specified probability distributions using `random`.
- `'lhs'` – Draw Latin hypercube samples from the specified probability distributions using an algorithm similar to `lhsdesign`. This approach is a more systematic space-filling approach than

random sampling. For details, see “Generating Quasi-Random Numbers” (Statistics and Machine Learning Toolbox).

- `'copula'` – Draw random samples using a copula (Statistics and Machine Learning Toolbox). Use this option to impose correlations between samples using copulas.
- `'sobol'` – Use the sobol sequence (`sobolset`) which is transformed using the inverse cumulative distribution function (`icdf`) of the specified probability distributions. Use this method for highly systematic space-filling. For details, see “Generating Quasi-Random Numbers” (Statistics and Machine Learning Toolbox).
- `'halton'` – Use the halton sequence (`haltonset`) which is transformed using the inverse cumulative distribution function (`icdf`) of the specified probability distributions. For details, see “Generating Quasi-Random Numbers” (Statistics and Machine Learning Toolbox).

If no `Covariance` is specified, `SimBiology.Scenarios` essentially performs two steps. The first step is to generate samples using one of the above sampling methods. For `lhs`, `sobol`, and `halton` methods, the generated uniform samples are transformed to samples from the specified distribution using the inverse cumulative distribution function `icdf`. Then, as the second step, the samples are correlated using the Iman-Conover algorithm if `RankCorrelation` is specified. For `random`, the samples are drawn directly from the specified distributions and the samples are then correlated using the Iman-Conover algorithm.

Example: `'SamplingMethod','lhs'`

`SamplingOptions` — Options for sampling method
struct

Options for the sampling method, specified as a scalar struct. The options differ depending on the sampling method: `sobol`, `halton`, or `lhs`.

For `sobol` and `halton`, specify each field name and value of the structure according to each name-value argument of the `sobolset` or `haltonset` function. SimBiology uses the default value of `1` for the `Skip` argument for both methods. For all other name-value arguments, the software uses the same default values of `sobolset` or `haltonset`. For instance, set up a structure for the `Leap` and `Skip` options with nondefault values as follows.

```
s1.Leap = 50;
s1.Skip = 0;
```

For `lhs`, there are three samplers that support different sampling options.

- If you specify a covariance matrix, SimBiology uses `lhsnorm` for sampling. `SamplingOptions` argument is not allowed.
- Otherwise, use the field name `UseLhsdesign` to select a sampler.
  - If the value is `true`, SimBiology uses `lhsdesign`. You can use the name-value arguments of `lhsdesign` to specify the field names and values.
  - If the value is `false` (default), SimBiology uses a nonconfigurable Latin hypercube sampler that is different from `lhsdesign`. This sampler does not require Statistics and Machine Learning Toolbox. `SamplingOptions` cannot contain any other options, except `UseLhsdesign`.

For instance, set up a structure to use `lhsdesign` with the `Criterion` and `Iterations` options.

```
s2.UseLhsdesign  = true;
s2.Criterion     = "correlation";
s2.Iterations    = 10;
```

You cannot specify sampling options for the `random` and `copula` methods.

Data Types: `struct`

Properties

`Expression` — Combination expression

character vector

This property is read-only.

Combination expression summarizing the combination of entries in the object, specified as a character vector. The plus `+` sign indicates the *elementwise* combination, and the cross `x` sign indicates the *cartesian* combination. For details, see “Combine Simulation Scenarios in SimBiology”.

Example: `'(k1 + k2 + k3) x doses'`

Data Types: `char`

`NumberOfEntries` — Number of entries

positive integer

Number of entries in the scenarios object, specified as a positive integer.

Example: `4`

Data Types: `double`

`RandomSeed` — Seed or state for random number generation

`[]` (default) | nonnegative integer smaller than 2^{32} | structure returned by `rng`

Seed for random number generation to obtain reproducible scenarios, specified as a nonnegative integer smaller than 2^{32} or structure returned by `rng` that defines the random state. The default value `[]` means that the generated scenarios will be different every time the `generate` function is called unless you set the random seed before calling the function or use reproducible sequences such as Sobol or Halton.

Example: `10`

Data Types: `double` | `struct`

Object Functions

add	Add quantity values, doses, or variants to SimBiology.Scenarios object
getEntry	Get entry contents from SimBiology.Scenarios object
updateEntry	Update entry contents from SimBiology.Scenarios object
rename	Rename entry from SimBiology.Scenarios object
remove	Remove entries from SimBiology.Scenarios object
verify	Verify SimBiology.Scenarios object
generate	Generate scenarios from SimBiology.Scenarios object and return table
getNumberScenarios	Return number of scenarios from SimBiology.Scenarios object

Examples

Generate Different Simulation Scenarios for Glucose-Insulin Response

Load the model of glucose-insulin response. For details about the model, see the **Background** section in “Simulate the Glucose-Insulin Response”.

```
sbioloadproject('insulindemo','m1');
```

The model contains different parameter values and initial conditions that represents different insulin impairments (such as Type 2 diabetes, low insulin sensitivity, and so on) stored in five variants.

```
variants = getvariant(m1)
```

```
variants =
   SimBiology Variant Array

   Index:  Name:             Active:
   1       Type 2 diabetic   false
   2       Low insulin se... false
   3       High beta cell... false
   4       Low beta cell ... false
   5       High insulin s... false
```

Suppress an informational warning that is issued during simulations.

```
warnSettings = warning('off','SimBiology:DimAnalysisNotDone_MatlabFcn_Dimensionless');
```

Select a dose that represents a single meal of 78 grams of glucose.

```
singleMeal = sbioselect(m1,'Name','Single Meal');
```

Create a `Scenarios` object to represent different initial conditions combined with the dose. That is, create a `scenario` object where each variant is paired (or combined) with the dose, for a total of five simulation scenarios.

```
sObj = SimBiology.Scenarios;
add(sObj,'cartesian','variants',variants);
add(sObj,'cartesian','dose',singleMeal)
```

```
ans =
  Scenarios (5 scenarios)

                  Name           Content          Number
                ________    ____________________    ______

    Entry 1     variants    SimBiology variants      5
    x Entry 2   dose        SimBiology dose          1

  See also Expression property.
```

`sObj` contains two entries. Use the `generate` function to combine the entries and generate five scenarios. The function returns a scenarios table, where each row represents a scenario and each column represents an entry of the `Scenarios` object.

```
scenariosTbl = generate(sObj)

scenariosTbl=5×2 table
           variants                    dose
    ________________________    ____________________________

    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
```

Change the entry name of the first entry.

```
rename(sObj,1,'Insulin Impairements')

ans =
  Scenarios (5 scenarios)

                        Name                 Content          Number
                    _____________________    _____________________    _______

    Entry 1       Insulin Impairements     SimBiology variants       5
    x Entry 2     dose                     SimBiology dose           1

  See also Expression property.
```

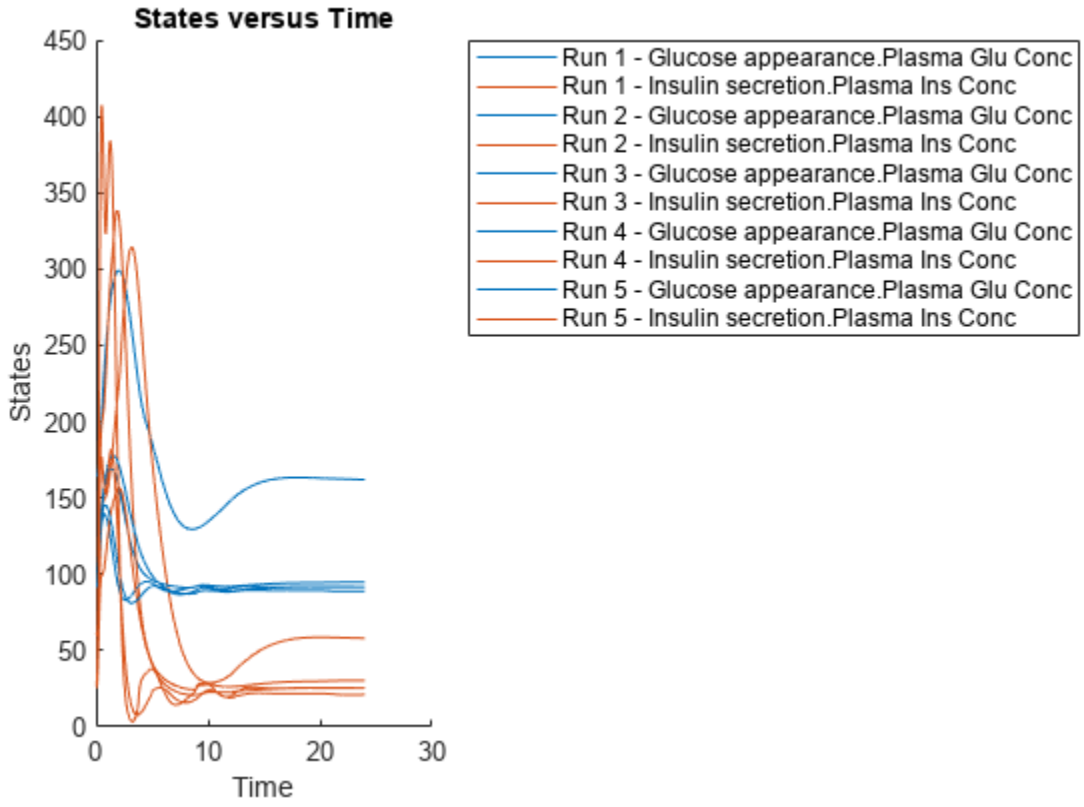
Create a `SimFunction` object to simulate the generated scenarios. Use the `Scenarios` object as the input and specify the plasma glucose and insulin concentrations as reponses (outputs of the function to be plotted). Specify `[]` for the dose input argument since the `Scenarios` object already has the dosing information.

```
f = createSimFunction(m1,sObj,{'[Plasma Glu Conc]','[Plasma Ins Conc]'},[])

f =
SimFunction

Parameters:

              Name                Value         Type                          Units
    ____________________________    ______    _____________    ____________________________________

    {'Plasma Volume (Glu)'  }      1.88    {'parameter'}    {'deciliter'
    {'k1'                   }     0.065    {'parameter'}    {'1/minute'
    {'k2'                   }     0.079    {'parameter'}    {'1/minute'
    {'Plasma Volume (Ins)'  }      0.05    {'parameter'}    {'liter'
    {'m1'                   }      0.19    {'parameter'}    {'1/minute'
    {'m2'                   }     0.484    {'parameter'}    {'1/minute'
    {'m4'                   }    0.1936    {'parameter'}    {'1/minute'
    {'m5'                   }    0.0304    {'parameter'}    {'minute/picomole'
    {'m6'                   }    0.6469    {'parameter'}    {'dimensionless'
    {'Hepatic Extraction'   }       0.6    {'parameter'}    {'dimensionless'
    {'kmax'                 }    0.0558    {'parameter'}    {'1/minute'
    {'kmin'                 }     0.008    {'parameter'}    {'1/minute'
    {'kabs'                 }    0.0568    {'parameter'}    {'1/minute'
    {'kgri'                 }         0    {'parameter'}    {'1/minute'
```

```
    {'f'                    }       0.9    {'parameter'}    {'dimensionless'
    {'a'                    }         0    {'parameter'}    {'1/milligram'
    {'b'                    }      0.82    {'parameter'}    {'dimensionless'
    {'c'                    }         0    {'parameter'}    {'1/milligram'
    {'d'                    }      0.01    {'parameter'}    {'dimensionless'
    {'kp1'                  }       2.7    {'parameter'}    {'milligram/minute'
    {'kp2'                  }    0.0021    {'parameter'}    {'1/minute'
    {'kp3'                  }     0.009    {'parameter'}    {'(milligram/minute)/(picomole/liter)
    {'kp4'                  }    0.0618    {'parameter'}    {'(milligram/minute)/picomole'
    {'ki'                   }    0.0079    {'parameter'}    {'1/minute'
    {'[Ins Ind Glu Util]'   }         1    {'parameter'}    {'milligram/minute'
    {'Vm0'                  }    2.5129    {'parameter'}    {'milligram/minute'
    {'Vmx'                  }     0.047    {'parameter'}    {'(milligram/minute)/(picomole/liter)
    {'Km'                   }    225.59    {'parameter'}    {'milligram'
    {'p2U'                  }    0.0331    {'parameter'}    {'1/minute'
    {'K'                    }      2.28    {'parameter'}    {'picomole/(milligram/deciliter)'
    {'alpha'                }      0.05    {'parameter'}    {'1/minute'
    {'beta'                 }      0.11    {'parameter'}    {'(picomole/minute)/(milligram/decili
    {'gamma'                }       0.5    {'parameter'}    {'1/minute'
    {'ke1'                  }    0.0005    {'parameter'}    {'1/minute'
    {'ke2'                  }       339    {'parameter'}    {'milligram'
    {'Basal Plasma Glu Conc'}     91.76    {'parameter'}    {'milligram/deciliter'
    {'Basal Plasma Ins Conc'}     25.49    {'parameter'}    {'picomole/liter'

Observables:

           Name                Type                Units
    ___________________    ___________    ____________________

    {'[Plasma Glu Conc]'}    {'species'}    {'milligram/deciliter'}
    {'[Plasma Ins Conc]'}    {'species'}    {'picomole/liter'     }

Dosed:

    TargetName       TargetDimension
    __________    ____________________

     {'Dose'}     {'Mass (e.g., gram)'}


TimeUnits: hour
```

Simulate the model for 24 hours and plot the simulation data. The data contains five runs, where each run represents a scenario in the Scenarios object.

```
sd = f(sObj,24);
sbioplot(sd)
```




```
ans =
  Axes (SbioPlot) with properties:

            XLim: [0 30]
            YLim: [0 450]
          XScale: 'linear'
          YScale: 'linear'
    GridLineStyle: '-'
         Position: [0.0920 0.1100 0.2956 0.8150]
            Units: 'normalized'

  Show all properties
```

If you have Statistics and Machine Learning Toolbox™, you can also draw sample values for model quantities from various probability distributions. For instance, suppose that the parameters `Vmx` and `kp3`, which are known for the low and high insulin sensitivity, follow the lognormal distribution. You can generate sample values for these parameters from such a distribution, and perform a scan to explore model behavior.

Define the lognormal probability distribution object for `Vmx`.

```
pd_Vmx = makedist('lognormal')
```

```
pd_Vmx =
  LognormalDistribution
```

```
  Lognormal distribution
       mu = 0
    sigma = 1
```

By definition, the parameter `mu` is the mean of logarithmic values. To vary the parameter value around the base (model) value of the parameter, set `mu` to `log(`*`model_value`*`)`. Set the standard deviation (*sigma*) to 0.2. For a small *sigma* value, the mean of a lognormal distribtion is approximately equal to `log(`*`model_value`*`)`. For details, see “Lognormal Distribution” (Statistics and Machine Learning Toolbox).

```
Vmx = sbioselect(m1,'Name','Vmx');
pd_Vmx.mu = log(Vmx.Value);
pd_Vmx.sigma = 0.2
```

```
pd_Vmx =
  LognormalDistribution

  Lognormal distribution
       mu = -3.05761
    sigma =      0.2
```

Similarly define the probability distribution for kp3.

```
pd_kp3 = makedist('lognormal');
kp3 = sbioselect(m1,'Name','kp3');
pd_kp3.mu = log(kp3.Value);
pd_kp3.sigma = 0.2
```

```
pd_kp3 =
  LognormalDistribution

  Lognormal distribution
       mu = -4.71053
    sigma =      0.2
```

Now define a joint probability distribution to draw sample values for Vmx and kp3, with a rank correlation to specify some correlation between these two parameters. Note that this correlation assumption is for the illustration purposes of this example only and may not be biologically relevant.

First remove the variants entry (entry 1) from `sObj`.

```
remove(sObj,1)
```

```
ans =
  Scenarios (1 scenarios)

               Name        Content        Number
               ____    ________________    ______

    Entry 1    dose    SimBiology dose       1

  See also Expression property.
```

Add an entry that defines the joint probability distribution with a rank correlation matrix.

```
add(sObj,'cartesian',["Vmx","kp3"],[pd_Vmx, pd_kp3],'RankCorrelation',[1,0.5;0.5,1])

ans =
  Scenarios (2 scenarios)

                    Name           Content              Number
                    ____    ______________________    ___________

    Entry 1         dose    SimBiology dose           1
    x (Entry 2.1    Vmx     Lognormal distribution    2 (default)
    + Entry 2.2)    kp3     Lognormal distribution    2 (default)

  See also Expression property.
```

By default, the number of samples to draw from the joint distribution is set to 2. Increase the number of samples.

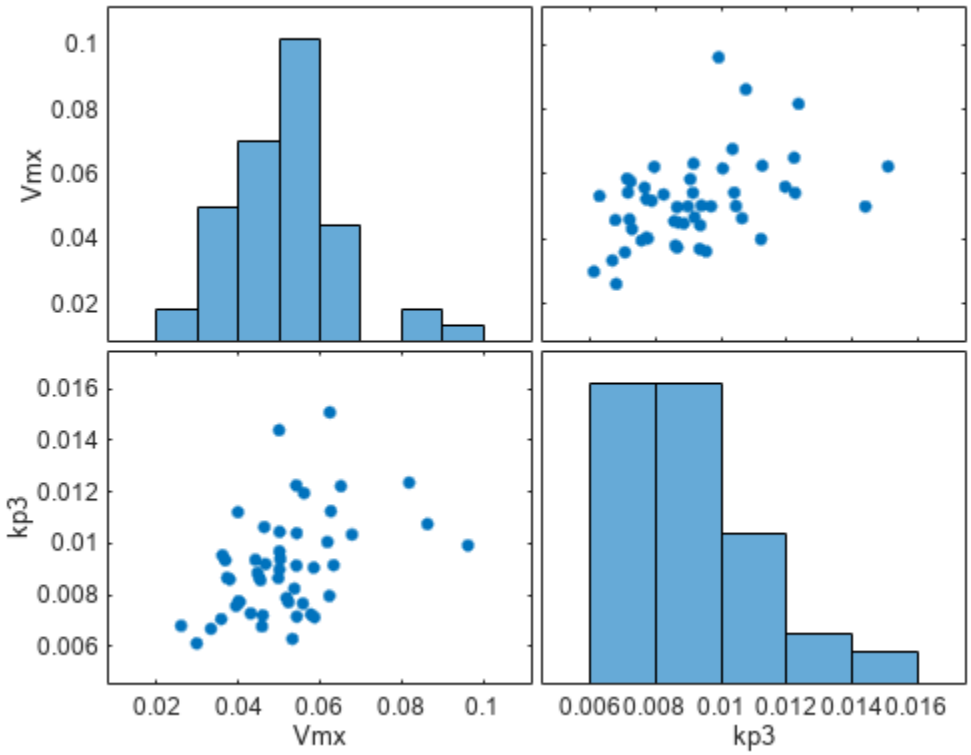
```
updateEntry(sObj,2,'Number',50)

ans =
  Scenarios (50 scenarios)

                    Name           Content             Number
                    ____    ______________________    ______

    Entry 1         dose    SimBiology dose             1
    x (Entry 2.1    Vmx     Lognormal distribution      50
    + Entry 2.2)    kp3     Lognormal distribution      50

  See also Expression property.
```

Verify that the `Scenarios` object can be simulated with the model. The `verify` function throws an error if any entry does not resolve uniquely to an object in the model or the entry contents have inconsistent lengths (sample sizes). The function throws a warning if multiple entries resolve to the same object in the model.

```
verify(sObj,m1)
```

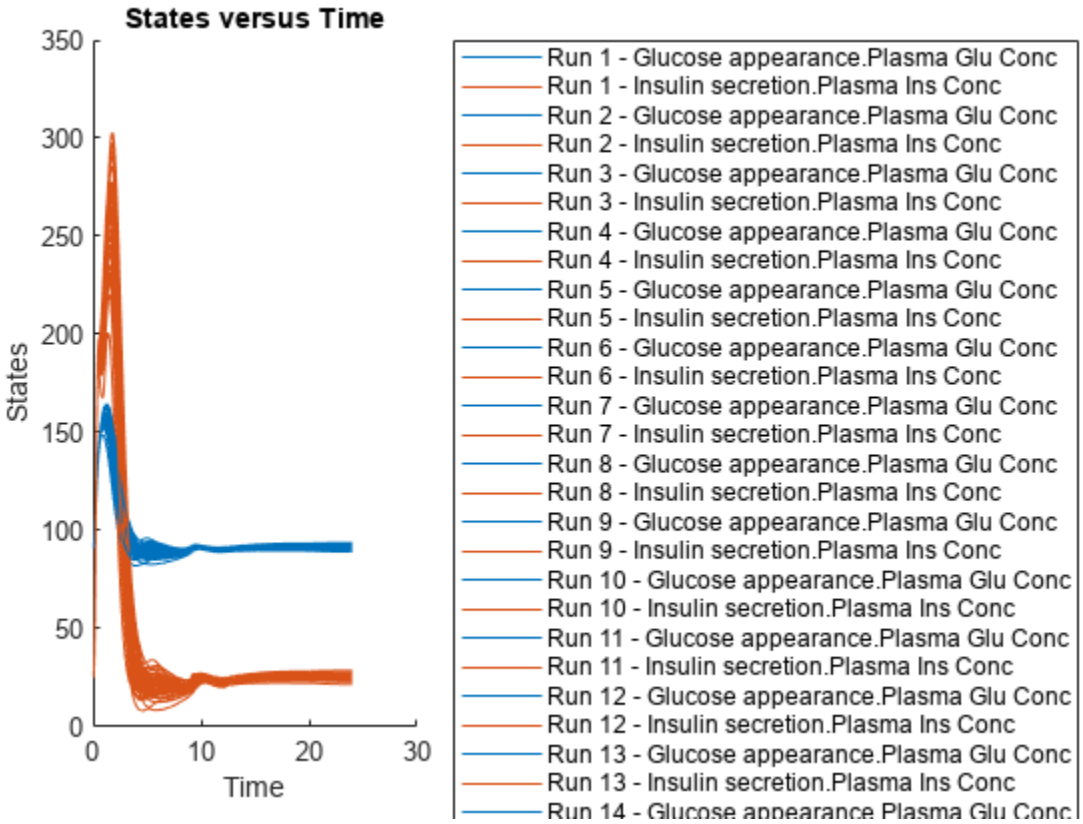
Generate the simulation scenarios. Plot the sample values using `plotmatrix`. You can see the value of `Vmx` is varied around its model value 0.047 and that of `kp3` around 0.009.

```
sTbl = generate(sObj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl.Vmx,sTbl.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
ax(2,1).XLabel.String = "Vmx";
ax(2,2).XLabel.String = "kp3";
```



Simulate the scenarios using the same SimFunction you created previously. You do not need to create a new SimFunction object even though the Scenarios object has been updated.

```
sd2 = f(sObj,24);
sbioplot(sd2);
```



By default, SimBiology uses the random sampling method. You can change it to the Latin hypercube sampling (or sobol or halton) for a more systematic space-filling approach.

```
entry2struct = getEntry(sObj,2)
```

```
entry2struct = struct with fields:
                Name: {'Vmx'  'kp3'}
             Content: [2x1 prob.LognormalDistribution]
              Number: 50
    RankCorrelation: [2x2 double]
          Covariance: []
      SamplingMethod: 'random'
     SamplingOptions: [0x0 struct]
```

```
entry2struct.SamplingMethod = 'lhs'
```

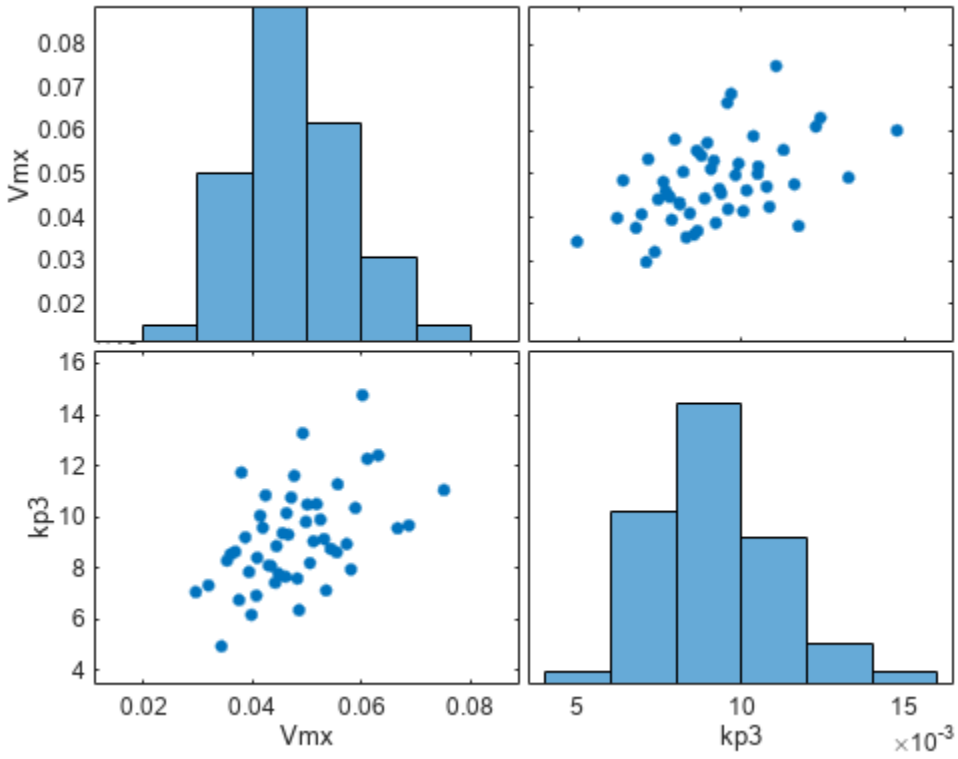
```
entry2struct = struct with fields:
                Name: {'Vmx'  'kp3'}
             Content: [2x1 prob.LognormalDistribution]
              Number: 50
    RankCorrelation: [2x2 double]
          Covariance: []
      SamplingMethod: 'lhs'
     SamplingOptions: [0x0 struct]
```

You can now use the updated structure to modify entry 2.

```
updateEntry(sObj,2,entry2struct)

ans =
  Scenarios (50 scenarios)

                    Name           Content             Number
                    ____    ____________________      ______

    Entry 1         dose    SimBiology dose             1
    x (Entry 2.1    Vmx     Lognormal distribution      50
    + Entry 2.2)    kp3     Lognormal distribution      50

  See also Expression property.
```

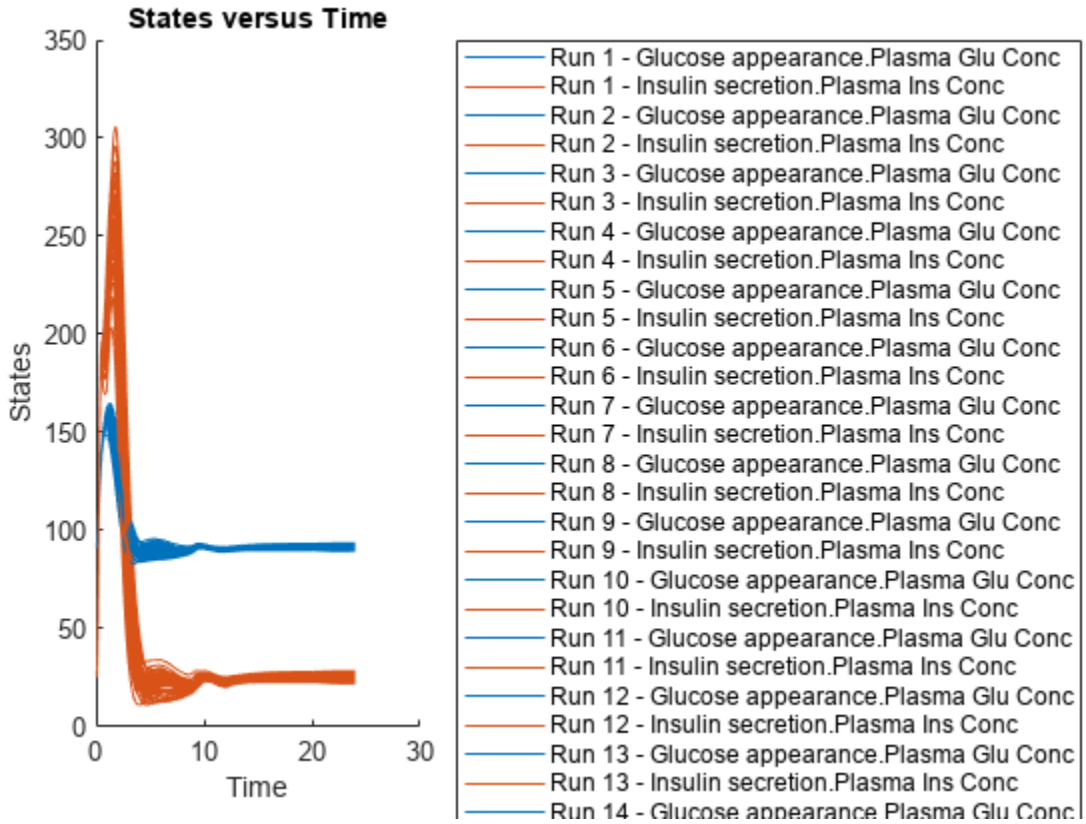
Visualize the sample values.

```
sTbl2 = generate(sObj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl2.Vmx,sTbl2.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
ax(2,1).XLabel.String = "Vmx";
ax(2,2).XLabel.String = "kp3";
```



Simulate the scenarios.

```
sd3 = f(sObj,24);
sbioplot(sd3);
```



Restore warning settings.

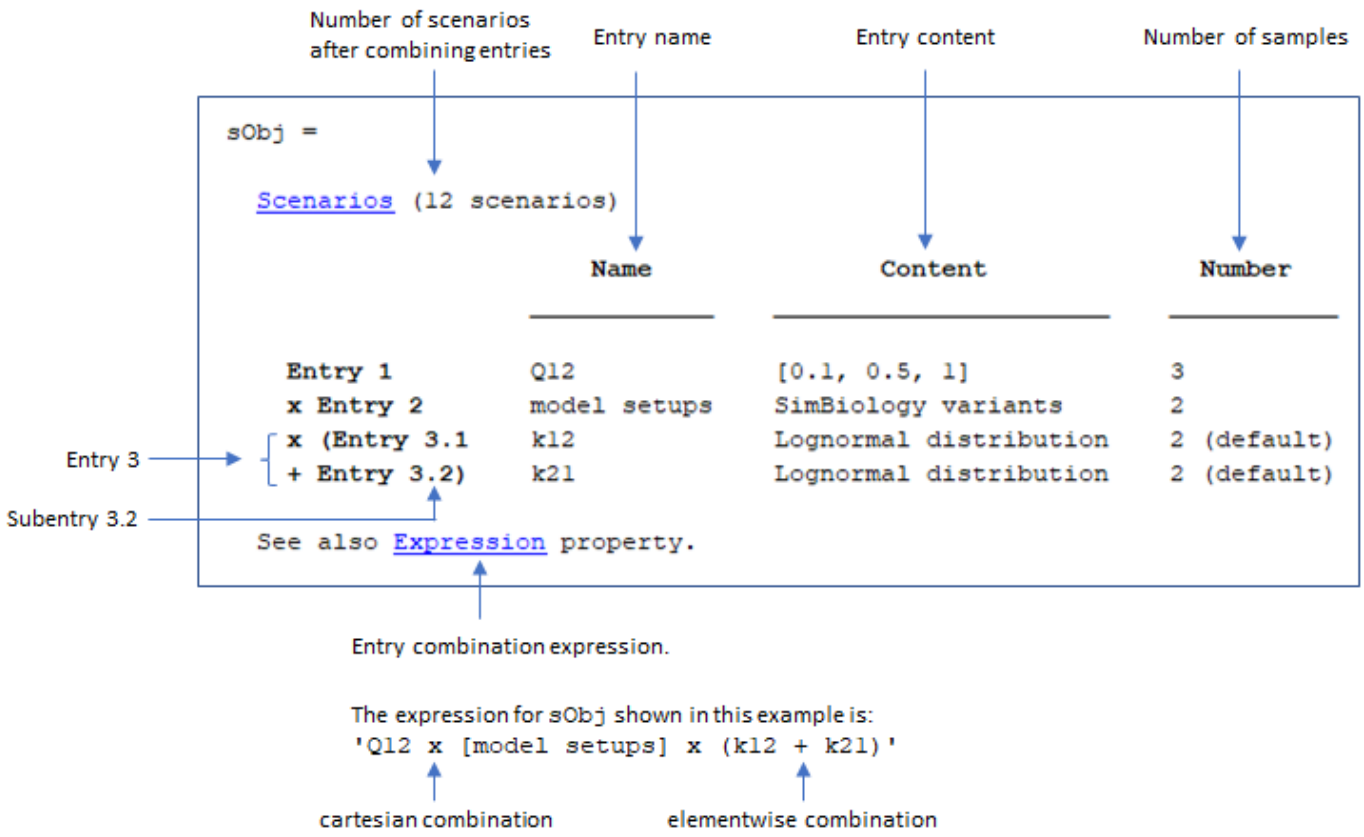
```
warning(warnSettings);
```

More About

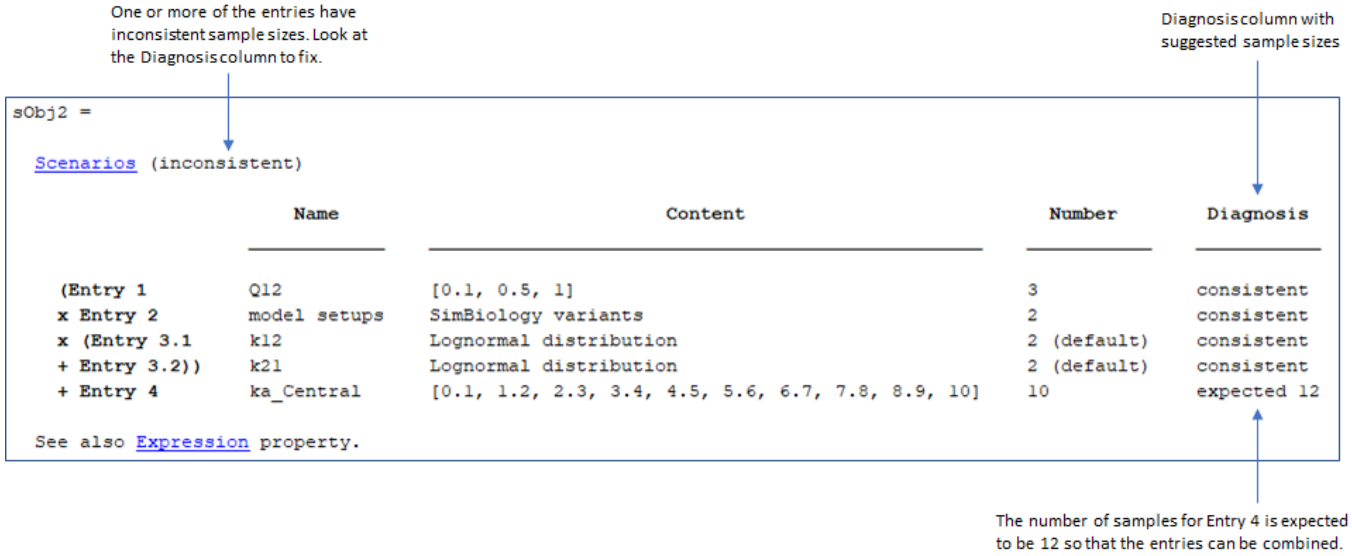
`SimBiology.Scenarios` Terminology

This section annotates the command line display of the `SimBiology.Scenarios` object and explains the terms shown in the output. Specifically, it explains these terminologies: `Scenarios`, `Entry`, `Subentry`, `Name`, `Content`, `Number`, `Expression`, `inconsistent` and `Diagnosis`.

A *consistent* `Scenarios` object has entries that have the correct number of samples so that entries can be combined without error. An example of a consistent `Scenarios` object is shown next.



An *inconsistent* Scenarios object has one or more entries with incorrect number of samples. You need to correct these entries before you can use the object for simulation. An example of an inconsistent object is shown next.



The `Diagnosis` column suggests which entries to fix to have the correct number of samples. Use `updateEntry`, `rename`, and `remove` to edit the entries.

Version History

Introduced in R2019b

References

[1] Iman, R., and W.J. Conover. 1982. A distribution-free approach to inducing rank correlation among input variables. *Communications in Statistics - Simulation and Computation*. 11(3):311–334.

See Also

`SimFunction object` | `createSimFunction (model)`

Topics

“Combine Simulation Scenarios in SimBiology”

ScheduleDose object

Define drug dosing protocol

Description

A `ScheduleDose` object defines a series of doses to the amount of a species during a simulation. The `TargetName` property defines the species that receives the dose.

Each dose can have a different amount, as defined by an amount array in the `Amount` property. Each dose can be given at specified times, as defined by a time array in the `Time` property. A rate array in the `Rate` property defines how fast each dose is given. At each time point in the time array, a dose is given with the corresponding amount and rate.

To use a dose object in a simulation you must add the dose object to a model object and set the `Active` property of the dose object to true. Set the `Active` property to true if you always want the dose to be applied before simulating the model.

Warning The `Active` property of the `ScheduleDose object` will be removed in a future release. Explicitly specify a dose or an array of doses as an input argument when you simulate a model using `sbiosimulate`.

When there are multiple active `ScheduleDdose` objects on a model, and there are duplicate specifications for a property value, the simulation uses the last occurrence for the property value in the array of doses. You can find out which dose you applied last by looking at the indices of the dose objects stored on the model.

Tip You can create a combination of bolus and infusion doses by setting the `rate` property of a `ScheduleDose` object to a vector containing zeros and non-zeros.

Constructor Summary

sbiodose	Construct dose object

Method Summary

Methods for `ScheduleDose` objects

copyobj	Copy SimBiology object and its children
delete	Delete SimBiology object
display	Display summary of SimBiology object
get	Get SimBiology object properties
getTable(ScheduleDose,RepeatDose)	Return data from SimBiology dose object as table
rename	Rename object and update expressions
set	Set SimBiology object properties
setTable(ScheduleDose,RepeatDose)	Set dosing information from table to dose object

Property Summary

Properties for `ScheduleDose` objects

Active	Indicate object in use during simulation
Amount	Amount of dose
AmountUnits	Dose amount units
DurationParameterName	Parameter specifying length of time to administer a dose
EventMode	Determine how events that change dose parameters affect in-progress dosing
LagParameterName	Parameter specifying time lag for dose
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Rate	Rate of dose
RateUnits	Units for dose rate
Tag	Specify label for SimBiology object
TargetName	Species receiving dose
Time	Simulation time steps or schedule dose times
TimeUnits	Show time units for dosing and simulation
Type	Display SimBiology object type
UserData	Specify data to associate with object

See Also

`Model object`, `RepeatDose object`, `sbiodose`, `sbiosimulate`

Version History

Introduced in R2010a

select

Select simulation data from `SimData` object using expressions

Syntax

```
[t,x,names] = select(simdata,query)
sdOut = select(simdata,query)
___ = select(simdata,query,'Format',formatValue)
```

Description

`[t,x,names] = select(simdata,query)` returns the simulation time points `t`, the simulation data `x`, and corresponding `names` for the data columns that match `query`.

`sdOut = select(simdata,query)` returns the simulation results that match the `query` as a `SimData` object `sdOut`.

`___ = select(simdata,query,'Format',formatValue)` returns the queried simulation data in the specified data format.

Examples

Select Simulation Data Using Names and Regular Expressions

Load the model of glucose-insulin response. For details about the model, see the **Background** section in “Simulate the Glucose-Insulin Response”.

```
sbioloadproject('insulindemo.sbproj','m1');
```

Suppress an information warning that is issued during simulations.

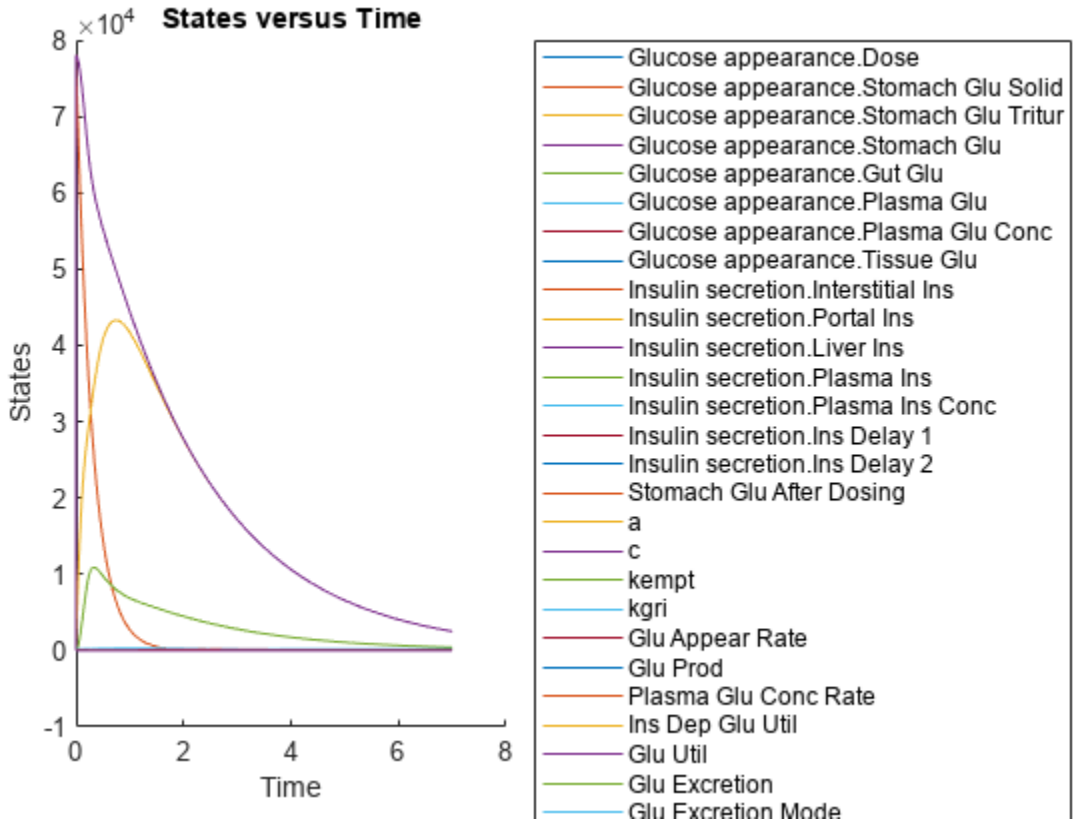
```
warnSettings = warning('off', 'SimBiology:DimAnalysisNotDone_MatlabFcn_Dimensionless');
```

Simulate a single meal for a normal subject for 7 hours.

```
singleMeal = sbioselect(m1,'Name','Single Meal');
cs = getconfigset(m1,'active');
cs.StopTime = 7;
sd = sbiosimulate(m1,singleMeal)
```

```
   SimBiology Simulation Data

   ModelName:        Cobelli's Glucose-Insulin System
   Logged Data:
     Species:        15
     Compartment:    0
     Parameter:      24
     Sensitivity:    0
     Observable:     0
```

```
sbioplot(sd);
```



Select all species data logged in the `SimData` object *sd*.

```
[t,x,names] = select(sd,{'Type','species'});
names
```

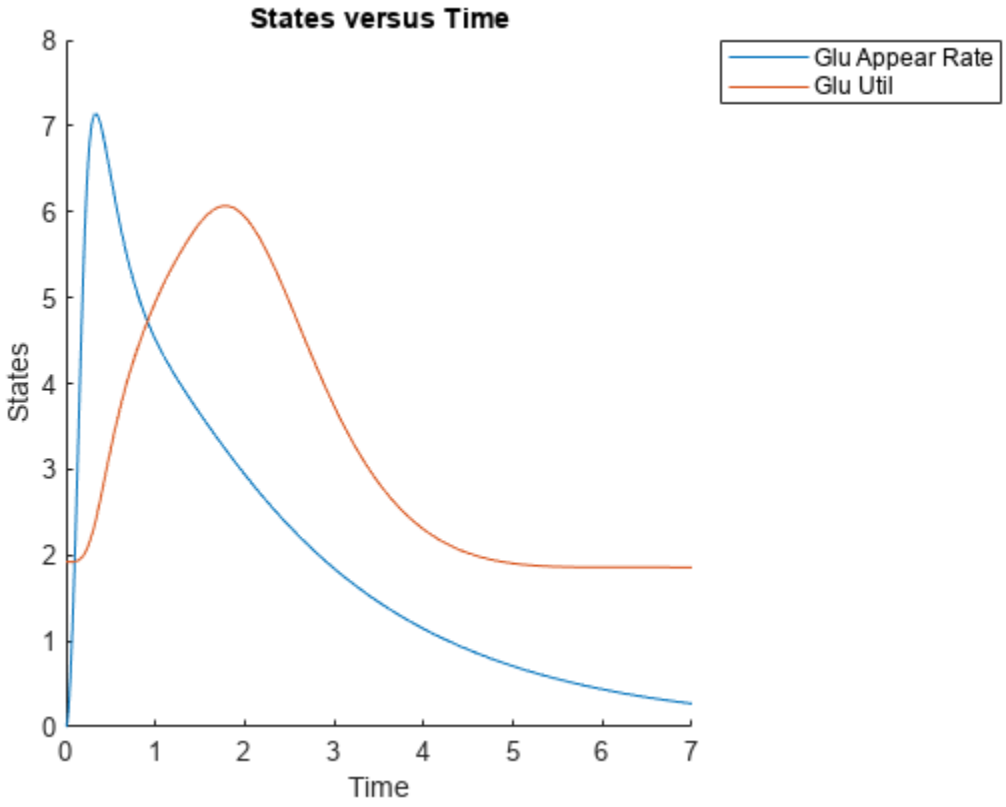
```
names = 15x1 cell
    {'Glucose appearance.Dose'              }
    {'Glucose appearance.Stomach Glu Solid' }
    {'Glucose appearance.Stomach Glu Tritur'}
    {'Glucose appearance.Stomach Glu'       }
    {'Glucose appearance.Gut Glu'           }
    {'Glucose appearance.Plasma Glu'        }
    {'Glucose appearance.Plasma Glu Conc'   }
    {'Glucose appearance.Tissue Glu'        }
    {'Insulin secretion.Interstitial Ins'   }
    {'Insulin secretion.Portal Ins'         }
    {'Insulin secretion.Liver Ins'          }
    {'Insulin secretion.Plasma Ins'         }
    {'Insulin secretion.Plasma Ins Conc'    }
    {'Insulin secretion.Ins Delay 1'        }
    {'Insulin secretion.Ins Delay 2'        }
```

Plot data for the glucose rate of appearance and glucose utilization, namely *Glu Appear Rate* and *Glu Util*.

```
newsd = select(sd,{'Type','parameter','name',{'Glu Appear Rate'; 'Glu Util'}})
```

```
   SimBiology Simulation Data

   ModelName:        Cobelli's Glucose-Insulin System
   Logged Data:
     Species:        0
     Compartment:    0
     Parameter:      2
     Sensitivity:    0
     Observable:     0
```

```
sbioplot(newsd);
```



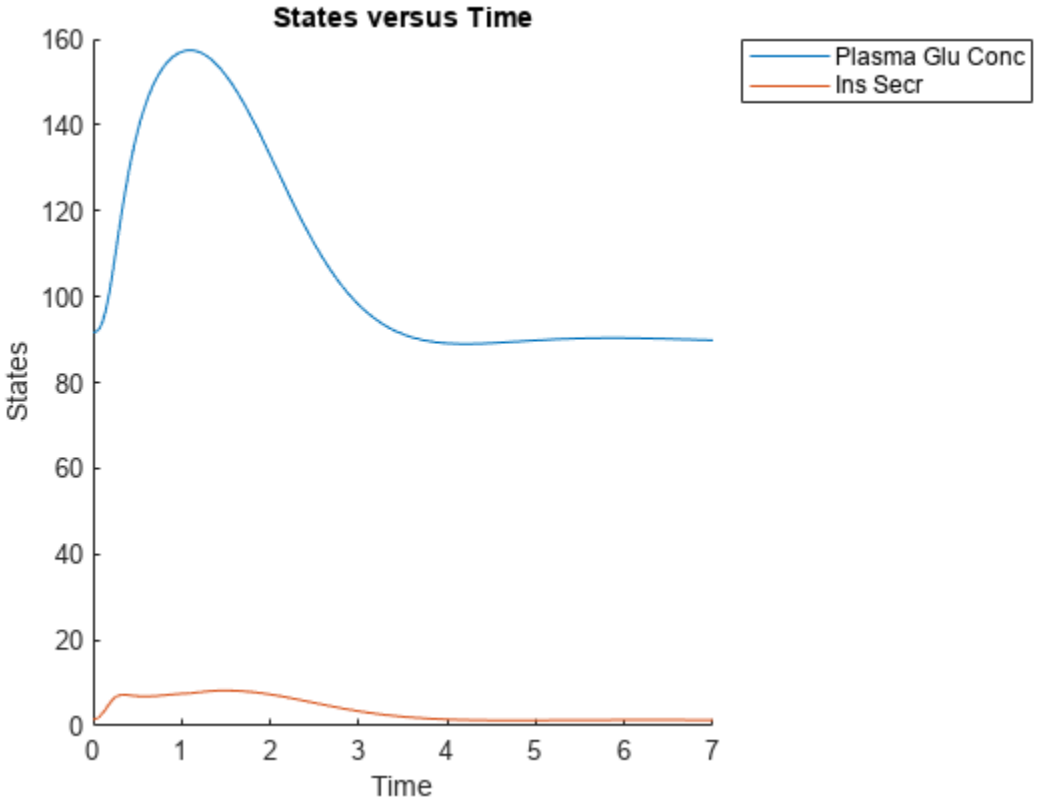
Compare data for the plasma glucose concentration (the species named `Plasma Glu Conc`) and insulin secretion rate (the parameter named *Ins Secr*). Use `selectbyname` to extract data by specifying the corresponding names.

```
newsd2 = selectbyname(sd,{'Plasma Glu Conc','Ins Secr'})
```

```
   SimBiology Simulation Data

   ModelName:        Cobelli's Glucose-Insulin System
   Logged Data:
     Species:        1
```

```
    Compartment:    0
    Parameter:      1
    Sensitivity:    0
    Observable:     0
```

```
sbioplot(newsd2);
```



Select data for all species and parameters that have *Glu* in their names.

```
newsd3 = select(sd,{'Where','Name','regexp','Glu'})
```

```
   SimBiology Simulation Data

   ModelName:        Cobelli's Glucose-Insulin System
   Logged Data:
     Species:        7
     Compartment:    0
     Parameter:      11
     Sensitivity:    0
     Observable:     0
```

```
newsd3.DataNames
```

```
ans = 18x1 cell
    {'Stomach Glu Solid'       }
```

```
    {'Stomach Glu Tritur'      }
    {'Stomach Glu'             }
    {'Gut Glu'                 }
    {'Plasma Glu'              }
    {'Plasma Glu Conc'         }
    {'Tissue Glu'              }
    {'Stomach Glu After Dosing'}
    {'Glu Appear Rate'         }
    {'Glu Prod'                }
    {'Plasma Glu Conc Rate'    }
    {'Ins Dep Glu Util'        }
    {'Glu Util'                }
    {'Glu Excretion'           }
    {'Glu Excretion Mode'      }
    {'Delayed Glu Signal'      }
    {'Delayed Glu Signal Mode' }
    {'Basal Glu Prod'          }
```

You can also return the selected data as a structure.

```
sdStruct = select(sd,{'Where','Name','regexp','Glu'},'Format','struct');
```

Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

`simdata` — Simulation data

`SimData` object | array of `SimData` objects

Simulation data, specified as a `SimData` object or array of `SimData` objects.

`query` — Search query

cell array of character vectors | string vector

Search query, specified as a cell array of character vectors or a string vector. The query consists of some combination of name-value pair arguments or `'Where'` clauses. For a more complete description of the query syntax, including `'Where'` clauses and their supported condition types, see `sbioselect`. However, the only boolean operator that the function supports is `and`.

You can use any of the metadata fields available in the `DataInfo` property of a `SimData` object in the query. The fields include `'Type'`, `'Name'`, `'Units'`, `'Compartment'` (for species only), and `'Reaction'` (for parameters only).

Example: `{'Type','species'}`

Data Types: `string` | `cell`

`formatValue` — Simulation data format

character vector | string

Simulation data format, specified as a character vector or string. Some formats require you to specify only one output argument. The valid formats follow.

- `'num'` — This format returns simulation time points and simulation data in numeric arrays and the names of quantities and sensitivities as a cell array. This format is the default when you run `getdata` with multiple output arguments.
- `'nummetadata'` — This format returns a cell array of metadata structures instead of the names of quantities and sensitivities as the third output argument.
- `'numqualnames'` — This format returns qualified names in the third output argument to resolve ambiguities.

You must specify only one output argument for the following formats.

- `'simdata'` — This format returns data in a new `SimData` object or an array of `SimData` objects. This format is the default when you specify a single output argument.
- `'struct'` — This format returns a structure or structure array that contains both data and metadata.
- `'ts'` — This format returns data as a cell array.
  - If `simdata` is scalar, the cell array is an *m*-by-1 array, where each element is a `timeseries` object. *m* is the number of quantities and sensitivities logged during the simulation.
  - If `simdata` is not scalar, the cell array is *k*-by-1, where each element of the cell array is an *m*-by-1 cell array of `timeseries` objects. *k* is the size of `simdata`, and *m* is the number of quantities or sensitivities in each `SimData` object in `simdata`. In other words, the function returns an individual time series for each state or column and for each `SimData` object in `simdata`.
- `'tslumped'` — This format returns the data as a cell array of `timeseries` objects, combining data from each `SimData` object into a single time series.

Output Arguments

`t` — Simulation time points

numeric vector | cell array

Simulation time points, returned as a numeric vector or cell array. If `simdata` is scalar, `t` is an *n*-by-1 vector, where *n* is the number of time points. If `simdata` is an array of objects, `t` is a *k*-by-1 cell array, where *k* is the size of `simdata`.

`x` — Simulation data

numeric matrix | cell array

Simulation data, returned as a numeric matrix or cell array. If `simdata` is scalar, `x` is an *n*-by-*m* matrix, where *n* is the number of time points and *m* is the number of quantities and sensitivities logged during the simulation. If `simdata` is an array of objects, `x` is a *k*-by-1 cell array, where *k* is the size of `simdata`.

`names` — Names of quantities and sensitivities

cell array

Names of quantities and sensitivities logged during the simulation, returned as a cell array. If `simdata` is scalar, `names` is an *m*-by-1 cell array. If `simdata` is an array of objects, `names` is a *k*-by-1 cell array, where *k* is the size of `simdata`.

`sdOut` — Simulation results

`SimData` object

Simulation results, returned as a `SimData` object.

Version History

Introduced in R2007b

See Also

`get` | `set` | `SimData`

selectbyname

Select simulation data by name from `SimData` object

Syntax

```
[t,x,names] = selectbyname(simdata,selectNames)
sdOut = selectbyname(simdata,selectNames)
___ = selectbyname(simdata,selectNames,'Format',formatValue)
```

Description

`[t,x,names] = selectbyname(simdata,selectNames)` returns the simulation time points `t`, the simulation data `x`, and corresponding `names` for the states specified by `selectNames`.

`sdOut = selectbyname(simdata,selectNames)` returns the simulation results of the states specified by `selectNames` as a `SimData` object `sdOut`.

`___ = selectbyname(simdata,selectNames,'Format',formatValue)` returns the simulation data in the specified data format.

Examples

Select Simulation Data Using Names and Regular Expressions

Load the model of glucose-insulin response. For details about the model, see the **Background** section in “Simulate the Glucose-Insulin Response”.

```
sbioloadproject('insulindemo.sbproj','m1');
```

Suppress an information warning that is issued during simulations.

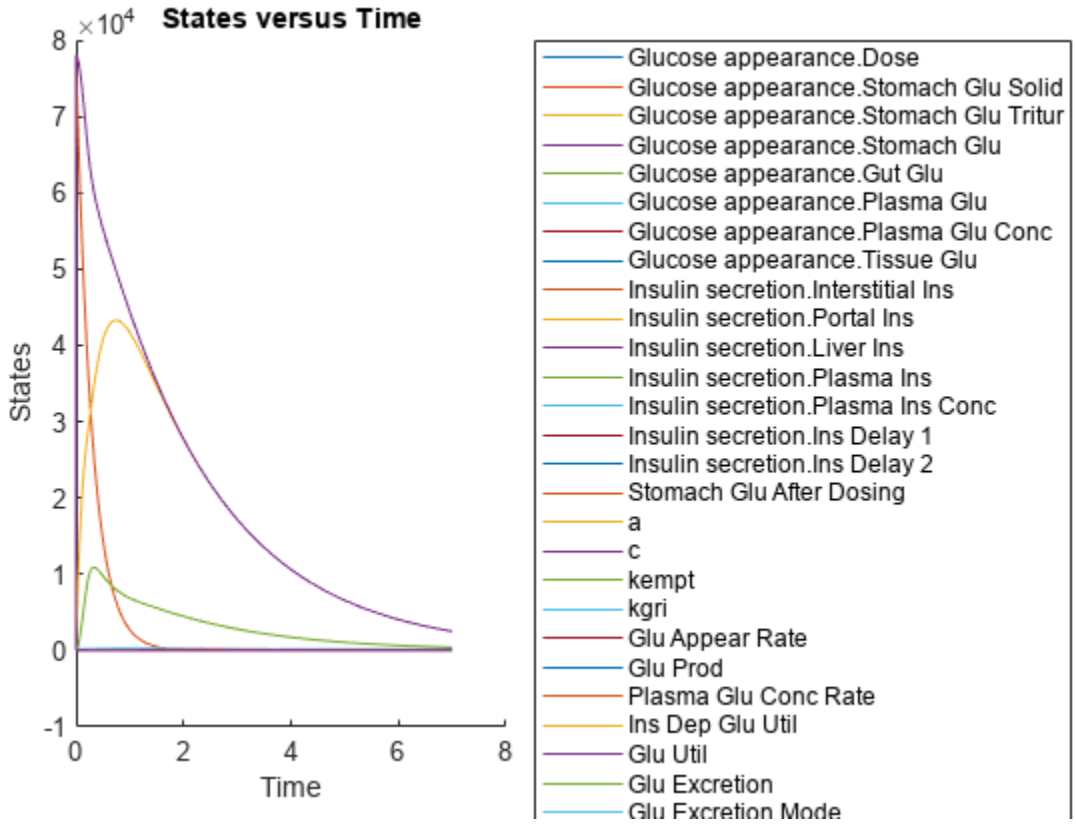
```
warnSettings = warning('off', 'SimBiology:DimAnalysisNotDone_MatlabFcn_Dimensionless');
```

Simulate a single meal for a normal subject for 7 hours.

```
singleMeal = sbioselect(m1,'Name','Single Meal');
cs = getconfigset(m1,'active');
cs.StopTime = 7;
sd = sbiosimulate(m1,singleMeal)
```

```
   SimBiology Simulation Data

   ModelName:        Cobelli's Glucose-Insulin System
   Logged Data:
     Species:        15
     Compartment:    0
     Parameter:      24
     Sensitivity:    0
     Observable:     0
```

```
sbioplot(sd);
```



Select all species data logged in the `SimData` object *sd*.

```
[t,x,names] = select(sd,{'Type','species'});
names
```

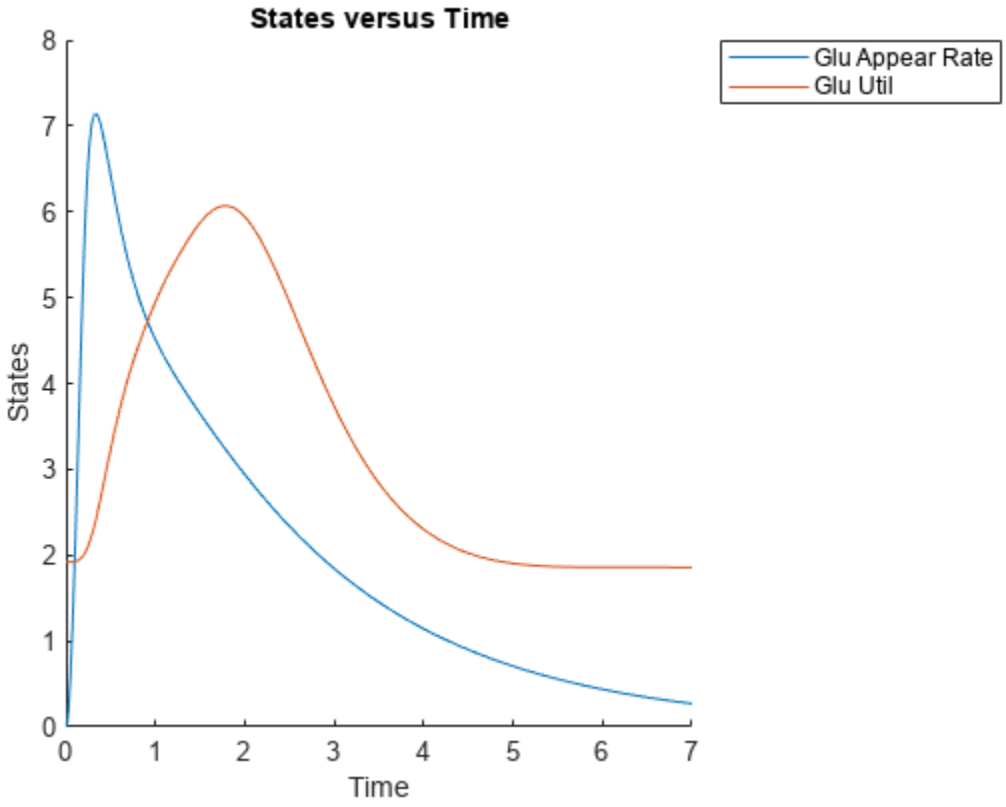
```
names = 15x1 cell
    {'Glucose appearance.Dose'              }
    {'Glucose appearance.Stomach Glu Solid' }
    {'Glucose appearance.Stomach Glu Tritur'}
    {'Glucose appearance.Stomach Glu'       }
    {'Glucose appearance.Gut Glu'           }
    {'Glucose appearance.Plasma Glu'        }
    {'Glucose appearance.Plasma Glu Conc'   }
    {'Glucose appearance.Tissue Glu'        }
    {'Insulin secretion.Interstitial Ins'   }
    {'Insulin secretion.Portal Ins'         }
    {'Insulin secretion.Liver Ins'          }
    {'Insulin secretion.Plasma Ins'         }
    {'Insulin secretion.Plasma Ins Conc'    }
    {'Insulin secretion.Ins Delay 1'        }
    {'Insulin secretion.Ins Delay 2'        }
```

Plot data for the glucose rate of appearance and glucose utilization, namely *Glu Appear Rate* and *Glu Util*.

```
newsd = select(sd,{'Type','parameter','name',{'Glu Appear Rate'; 'Glu Util'}})
```

```
   SimBiology Simulation Data

   ModelName:        Cobelli's Glucose-Insulin System
   Logged Data:
     Species:        0
     Compartment:    0
     Parameter:      2
     Sensitivity:    0
     Observable:     0
```

```
sbioplot(newsd);
```



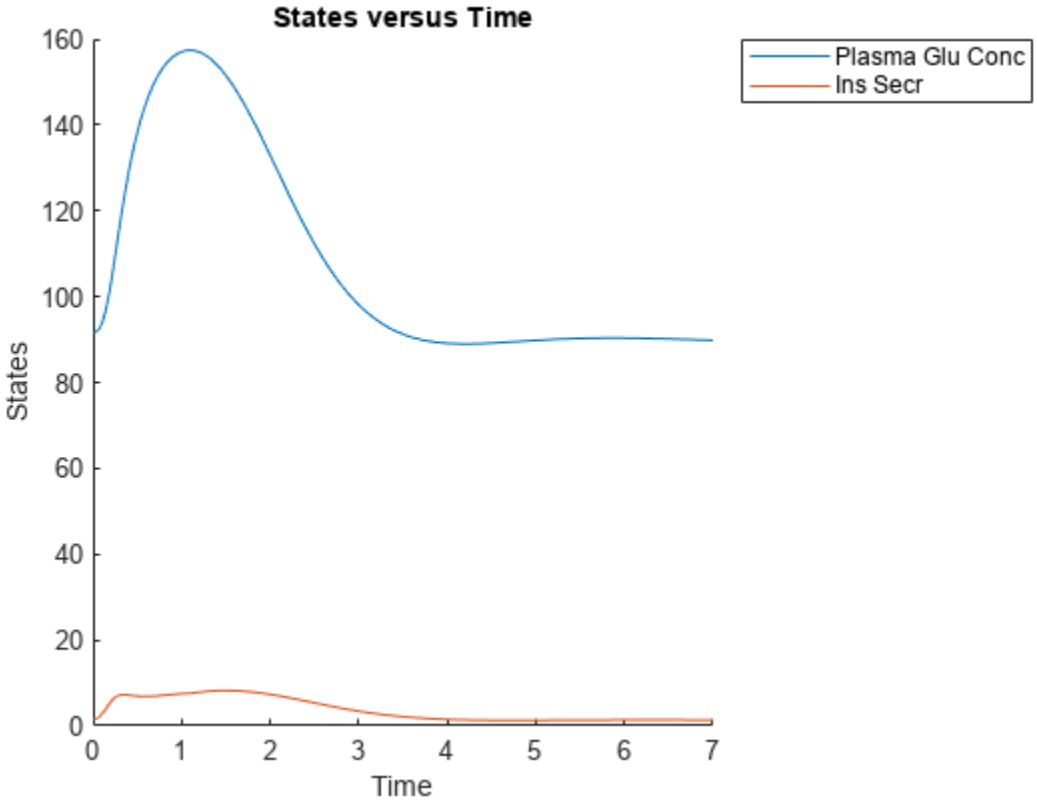
Compare data for the plasma glucose concentration (the species named `Plasma Glu Conc`) and insulin secretion rate (the parameter named *Ins Secr*). Use `selectbyname` to extract data by specifying the corresponding names.

```
newsd2 = selectbyname(sd,{'Plasma Glu Conc','Ins Secr'})
```

```
   SimBiology Simulation Data

   ModelName:        Cobelli's Glucose-Insulin System
   Logged Data:
     Species:        1
```

```
    Compartment:    0
    Parameter:      1
    Sensitivity:    0
    Observable:     0
```

```
sbioplot(newsd2);
```



Select data for all species and parameters that have *Glu* in their names.

```
newsd3 = select(sd,{'Where','Name','regexp','Glu'})
```

```
   SimBiology Simulation Data

   ModelName:        Cobelli's Glucose-Insulin System
   Logged Data:
     Species:        7
     Compartment:    0
     Parameter:      11
     Sensitivity:    0
     Observable:     0
```

```
newsd3.DataNames
```

```
ans = 18x1 cell
    {'Stomach Glu Solid'       }
```

```
    {'Stomach Glu Tritur'      }
    {'Stomach Glu'             }
    {'Gut Glu'                 }
    {'Plasma Glu'              }
    {'Plasma Glu Conc'         }
    {'Tissue Glu'              }
    {'Stomach Glu After Dosing'}
    {'Glu Appear Rate'         }
    {'Glu Prod'                }
    {'Plasma Glu Conc Rate'    }
    {'Ins Dep Glu Util'        }
    {'Glu Util'                }
    {'Glu Excretion'           }
    {'Glu Excretion Mode'      }
    {'Delayed Glu Signal'      }
    {'Delayed Glu Signal Mode' }
    {'Basal Glu Prod'          }
```

You can also return the selected data as a structure.

```
sdStruct = select(sd,{'Where','Name','regexp','Glu'},'Format','struct');
```

Restore the warning settings.

```
warning(warnSettings);
```

Input Arguments

`simdata` — Simulation data

`SimData` object | array of `SimData` objects

Simulation data, specified as a `SimData` object or array of `SimData` objects.

`selectNames` — Names of states

character vector | string | string vector | cell array of character vectors

Names of states that you want to select data for, specified as a character vector, string, string vector, or cell array of character vectors.

Example: `{'x1','x2','x3'}`

Data Types: `char` | `string` | `cell`

`formatValue` — Simulation data format

character vector | string

Simulation data format, specified as a character vector or string. Some formats require you to specify only one output argument. The valid formats follow.

- `'num'` — This format returns simulation time points and simulation data in numeric arrays and the names of quantities and sensitivities as a cell array. This format is the default when you run `getdata` with multiple output arguments.
- `'nummetadata'` — This format returns a cell array of metadata structures instead of the names of quantities and sensitivities as the third output argument.

- `'numqualnames'` — This format returns qualified names in the third output argument to resolve ambiguities.

You must specify only one output argument for the following formats.

- `'simdata'` — This format returns data in a new `SimData` object or an array of `SimData` objects. This format is the default when you specify a single output argument.
- `'struct'` — This format returns a structure or structure array that contains both data and metadata.
- `'ts'` — This format returns data as a cell array.
  - If `simdata` is scalar, the cell array is an *m*-by-1 array, where each element is a `timeseries` object. *m* is the number of quantities and sensitivities logged during the simulation.
  - If `simdata` is not scalar, the cell array is *k*-by-1, where each element of the cell array is an *m*-by-1 cell array of `timeseries` objects. *k* is the size of `simdata`, and *m* is the number of quantities or sensitivities in each `SimData` object in `simdata`. In other words, the function returns an individual time series for each state or column and for each `SimData` object in `simdata`.
- `'tslumped'` — This format returns the data as a cell array of `timeseries` objects, combining data from each `SimData` object into a single time series.

Output Arguments

`t` — Simulation time points

numeric vector | cell array

Simulation time points, returned as a numeric vector or cell array. If `simdata` is scalar, `t` is an *n*-by-1 vector, where *n* is the number of time points. If `simdata` is an array of objects, `t` is a *k*-by-1 cell array, where *k* is the size of `simdata`.

`x` — Simulation data

numeric matrix | cell array

Simulation data, returned as a numeric matrix or cell array. If `simdata` is scalar, `x` is an *n*-by-*m* matrix, where *n* is the number of time points and *m* is the number of quantities and sensitivities logged during the simulation. If `simdata` is an array of objects, `x` is a *k*-by-1 cell array, where *k* is the size of `simdata`.

`names` — Names of quantities and sensitivities

cell array

Names of quantities and sensitivities logged during the simulation, returned as a cell array. If `simdata` is scalar, `names` is an *m*-by-1 cell array. If `simdata` is an array of objects, `names` is a *k*-by-1 cell array, where *k* is the size of `simdata`.

`sdOut` — Simulation results

`SimData` object

Simulation results, returned as a `SimData` object.

Version History

Introduced in R2007b

See Also

`get` | `set` | `SimData`

set

Set SimBiology object properties

Syntax

```
set(sobj,Name,Value)
```

Description

`set(sobj,Name,Value)` sets the properties of `sobj`, a SimBiology object, using one or more name-value pair arguments. `Name` is the property name and `Value` is the corresponding value. The property cannot be a read-only property. `Name` must appear inside quotes. You can specify several name and value pair arguments in any order as `Name1,Value1,...,NameN,ValueN`.

Examples

Set SimBiology Object Properties

Load the G-protein model.

```
sbioloadproject('gprotein.sbproj');
```

Select the kGd parameter.

```
kgd = sbioselect(m1,'Name','kGd');
```

Display the properties of the parameter.

```
get(kgd)
```

```
ans = struct with fields:
           ValueUnits: ''
        ConstantValue: 1
             Constant: 1
                Value: 0.1100
                Units: ''
    BoundaryCondition: 0
                 Name: 'kGd'
               Parent: [1x1 SimBiology.Model]
                Notes: ''
                  Tag: ''
                 Type: 'parameter'
             UserData: []
```

Change the values of multiple properties of the object.

```
set(kgd,'Constant',false,'Value',0.06)
```

Check the updated property values.

```
get(kgd)
```

```
ans = struct with fields:
           ValueUnits: ''
        ConstantValue: 0
             Constant: 0
                Value: 0.0600
                Units: ''
    BoundaryCondition: 0
                 Name: 'kGd'
               Parent: [1x1 SimBiology.Model]
                Notes: ''
                  Tag: ''
                 Type: 'parameter'
             UserData: []
```

Update a common property of multiple objects.

```
set(m1.Parameters,'Constant',false)
```

Check the property values.

```
[m1.Parameters.Constant]
```

```
ans = 1x9 logical array

   0   0   0   0   0   0   0   0   0
```

Input Arguments

`sobj` — Object

SimBiology object | array of Simbiology objects

Object, specified as any SimBiology object or array of objects. You can use an array of objects to set the value of a common property.

Version History

Introduced in R2008b

See Also

`get` | `SimData`

setactiveconfigset (model)

Set active configuration set for model object

Syntax

```
configsetObj = setactiveconfigset(modelObj, 'NameValue')
configsetObj2 = setactiveconfigset(modelObj, configsetObj1)
```

Description

`configsetObj = setactiveconfigset(modelObj, 'NameValue')` sets the configuration set *NameValue* to be the active configuration set for the `model object` *modelObj* and returns to *configsetObj*.

`configsetObj2 = setactiveconfigset(modelObj, configsetObj1)` sets the `configset` *configsetObj1* to be the active `configset` for *modelObj* and returns to *configsetObj2*. Any change in one of these two configset objects *configsetObj1* and *configsetObj2* is reflected in the other. To copy over a `configset` object from one `model object` to another, use the `copyobj` method.

The active configuration set contains the settings that are be used during a simulation. A default configuration set is attached to any new model.

Examples

1. Create a model object by importing the `oscillator.xml` file, and add a `Configset` object to the model.

   ```
   modelObj  = sbmlimport('oscillator');
   configsetObj = addconfigset(modelObj, 'myset');
   ```

2. Configure the simulation stop criteria by setting the `StopTime`, `MaximumNumberOfLogs`, and `MaximumWallClock` properties of the `Configset` object. Set the stop criteria to a simulation time of `3000` seconds, `50` logs, or a wall clock time of `10` seconds, whichever comes first.

   ```
   set(configsetObj, 'StopTime', 3000, 'MaximumNumberOfLogs', 50,...
       'MaximumWallClock', 10)
   get(configsetObj)
   ```

   ```
                          Active: 0
                  CompileOptions: [1x1 SimBiology.CompileOptions]
                            Name: 'myset'
                           Notes: ''
                  RuntimeOptions: [1x1 SimBiology.RuntimeOptions]
      SensitivityAnalysisOptions: [1x1 SimBiology.SensitivityAnalysisOptions]
                   SolverOptions: [1x1 SimBiology.ODESolverOptions]
                      SolverType: 'ode15s'
                        StopTime: 3000
             MaximumNumberOfLogs: 50
                MaximumWallClock: 10
                       TimeUnits: 'second'
                            Type: 'configset'
   ```

3 Set the new `Configset` object to be active, simulate the model using the new `Configset` object, and plot the result.

```
 setactiveconfigset(modelObj, configsetObj);
[t,x] = sbiosimulate(modelObj);
plot (t,x)
```

See Also

`Model object`, `addconfigset`, `getconfigset`, `removeconfigset`

Version History

Introduced in R2006a

setparameter (kineticlaw)

Specify specific parameters in kinetic law object

Syntax

```
setparameter(kineticlawObj, 'ParameterVariablesValue',
'ParameterVariableNamesValue')
```

Arguments

ParameterVariableValue	Specify the value of the parameter variable in the kinetic law object.
ParameterVariableNamesValue	Specify the parameter name with which to configure the parameter variable in the kinetic law object. Determines parameters in the `ReactionRate` equation.

Description

Configure `ParameterVariableNames` in the kinetic law object.

`setparameter(kineticlawObj, 'ParameterVariablesValue', 'ParameterVariableNamesValue')` configures the `ParameterVariableNames` property of the kinetic law object (`kineticlawObj`). `ParameterVariableValue` corresponds to one of the character vectors in `kineticlawObj` `ParameterVariables` property. The corresponding element in the `kineticlawObjParameterVariableNames` property is configured to `ParameterVariableNamesValue`. For example, if `ParameterVariables` is `{'Vm', 'Km'}` and `ParameterVariablesValue` is specified as `Vm`, then the first element of the `ParameterVariableNames` cell array is configured to `ParameterVariableNamesValue`.

Examples

Create a model, add a reaction, and then assign the `ParameterVariableNames` for the reaction rate equation.

1. Create the model object, and then add a reaction object.

   ```
   modelObj = sbiomodel('my_model');
   reactionObj = addreaction(modelObj, 'a -> c + d');
   ```

2. Create a kinetic law object for the reaction object of the type `'Henri-Michaelis-Menten'`.

   ```
   kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
   ```

   `reactionObj` `KineticLaw` property is configured to `kineticlawObj`.

3. The `'Henri-Michaelis-Menten'` kinetic law has two parameter variables (`Vm` and `Km`) that should be set. To set these variables:

   ```
   setparameter(kineticlawObj,'Vm', 'Va');
   setparameter(kineticlawObj,'Km', 'Ka');
   ```

4 Verify that the parameter variables are correct.

```
get (kineticlawObj, 'ParameterVariableNames')
```

MATLAB returns:

```
ans =

    'Va'    'Ka'
```

See Also

`addparameter`, `getspecies`, `setspecies`

Version History

Introduced in R2006a

setspecies (kineticlaw)

Specify species in kinetic law object

Syntax

```
setspecies(kineticlawObj, 'SpeciesVariablesValue',
'SpeciesVariableNamesValue')
```

Arguments

SpeciesVariablesValue	Specify the species variable in the kinetic law object.
SpeciesVariableNamesValue	Specify the species name with which to configure the species variable in the kinetic law object. Determines the species in the `ReactionRate` equation.

Description

`setspecies` configures the kinetic law object `SpeciesVariableNames` property.

`setspecies(kineticlawObj, 'SpeciesVariablesValue', 'SpeciesVariableNamesValue')` configures the `SpeciesVariableNames` property of the kinetic law object, `kineticlawObj`. `SpeciesVariablesValue` corresponds to one of the character vectors in the `SpeciesVariables` property of `kineticlawObj`. The corresponding element in `kineticlawObj` `SpeciesVariableNames` property is configured to `SpeciesVariableNamesValue`.

For example, if `SpeciesVariables` are `{'S', 'S1'}` and `SpeciesVariablesValue` is specified as `S1`, the first element of the `SpeciesVariableNames` cell array is configured to `SpeciesVariableNamesValue`.

Examples

Create a model, add a reaction, and assign the `SpeciesVariableNames` for the reaction rate equation.

1. Create the model object, and then add a reaction object.

   ```
   modelObj = sbiomodel('my_model');
   reactionObj = addreaction(modelObj, 'a -> c + d');
   ```

2. Create a kinetic law object for the reaction object of the type `'Henri-Michaelis-Menten'`.

   ```
   kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
   ```

   `reactionObj` `KineticLaw` property is configured to `kineticlawObj`.

3. The `'Henri-Michaelis-Menten'` kinetic law has one species variable (`S`) that should be set. To set this variable:

```
setspecies(kineticlawObj,'S', 'a');
```

4 Verify that the species variable is correct.

```
get (kineticlawObj, 'SpeciesVariableNames')
```

MATLAB returns:

```
ans =

'a'
```

See Also

`addparameter`, `getspecies`, `setparameter`

Version History

Introduced in R2006a

setTable(ScheduleDose,RepeatDose)

Set dosing information from table to dose object

Syntax

```
setTable(doseObj,tbl)
```

Description

`setTable(doseObj,tbl)` sets the dosing data from a table `tbl` to a dose object `doseObj`.

Input Arguments

`doseObj` — Dose object
`ScheduleDose` object | `RepeatDose` object | array of dose objects

Dose object, specified as a `ScheduleDose object` or `RepeatDose object` or array of these objects.

`tbl` — Dosing data
table | cell array of tables

Dosing data, specified as a table or cell array of tables. If `doseObj` is an array of dose objects, then `tbl` must be a cell array of tables of the same size as `doseObj`.

If `doseObj` is a `ScheduleDose` object, `tbl` must have 2 or 3 variables (columns) representing dose time, amount, and rate (optional). The variable names (`tbl.Properties.VariableNames`) must be `'Time'`, `'Amount'`, and `'Rate'` (optional), respectively.

If `doseObj` is a `RepeatDose` object, `tbl` must have only one row with 4 or 5 variables (columns) representing dose start time, amount, interval, repeat count, and rate (optional). The variable names (`tbl.Properties.VariableNames`) must be `'StartTime'`, `'Amount'`, `'Interval'`, `'RepeatCount'`, and `'Rate'` (optional), respectively. The value of each variable can be a numeric scalar or the name of a parameter (if the property is parameterized).

The units of `tbl` variables (`tbl.Properties.VariableUnits`), if any, are copied over to the corresponding property units of `doseObj`.

Examples

Set a Table of Dosing Data to a RepeatDose Object

Create a table containing dose start time, amount, interval, repeat count, and rate.

```
StartTime = 5;
Amount = 500;
Interval = 1;
RepeatCount = 3;
```

```
Rate = 1;
tbl = table(StartTime,Amount,Interval,RepeatCount,Rate);
```

Create a `RepeatDose` object, and set the dosing information from the table.

```
rdose = sbiodose('rdose','repeat');
setTable(rdose,tbl);
```

Set a Table of Dosing Data to a ScheduleDose Object

Create a table containing dose time and amount.

```
Time = [1 2 3 4 5]';
Amount = [10 15 20 25 30]';
tbl = table(Time,Amount);
```

Create a `ScheduleDose` object, and set the dosing information from the table.

```
sdose = sbiodose('sdose','schedule');
setTable(sdose,tbl);
```

Set an Array of Dosing Tables to an Array of Dose Objects

Create a table containing dose time and amount.

```
Time = [1 2 3 4 5]';
Amount = [10 15 20 25 30]';
tbl1 = table(Time,Amount);
```

Create a table containing dose start time, amount, interval, repeat count, and rate.

```
StartTime = 5;
Amount = 500;
Interval = 1;
RepeatCount = 3;
Rate = 1;
tbl2 = table(StartTime,Amount,Interval,RepeatCount,Rate);
```

Create a cell array of dose tables.

```
tblArray = {tbl1,tbl2};
```

Create `ScheduleDose` and `RepeatDose` objects

```
sdose = sbiodose('sdose','schedule');
rdose = sbiodose('rdose','repeat');
doseArray = [sdose,rdose];
```

Set the cell array of dose tables to dose objects.

```
setTable(doseArray,tblArray);
```

Version History

Introduced in R2014a

See Also

`getTable` | `ScheduleDose object` | `RepeatDose object`

SimData

Simulation data

Description

The `SimData` object contains simulation data, which includes time and state data, as well as metadata, such as the types and names for the logged states or the configuration set used during simulation.

You can access time data, state data, and metadata stored in the object through the object properties. Use dot notation to query the object properties or change properties that are not read-only. You can also use the `get` and `set` commands.

You can store data from multiple simulation runs as an array of `SimData` objects. You can use any `SimData` function on an array of `SimData` objects.

Creation

Create a `SimData` object in one of the following ways.

- Return a `SimData` object after simulating a model using `sbiosimulate`.
- Return a `SimData` object after simulating a model using a `SimFunction object`.
- Return an array of `SimData` objects after multiple stochastic ensemble runs using `sbioensemblerun`.
- Export the simulation results to the command line after simulating a model using the **SimBiology Model Analyzer** app.

Properties

`Data` — Simulation data

m×`0` empty double matrix (default) | matrix

This property is read-only.

Simulation data, specified as an *m*-by-*n* matrix. *m* is the number of time steps in the simulation and *n* is the number of quantities and sensitivities logged during the simulation. View the corresponding time steps by accessing the `Time` property, and view the corresponding logged quantity information by accessing the `DataInfo` property.

Data Types: `double`

`DataCount` — Number of species, compartments, parameters, and sensitivities

structure

This property is read-only.

Number of species, compartments, parameters, and sensitivities, specified as a structure. The structure contains the fields `Species`, `Compartment`, `Parameter`, and `Sensitivity`. The default value for each field is `0`.

Data Types: `struct`

`DataInfo` — Metadata labels for simulation data

`0-by-1` empty cell array (default) | cell array of structures

This property is read-only.

Metadata labels for simulation data, specified as an *n*-by-1 cell array of structures. *n* is the number of quantities and sensitivities logged during simulation. The *i*th cell contains metadata labeling the *i*th column of the matrix in the `Data` property.

The possible types of structures follow.

Type	Fields
Species	• Type — `'species'` • Name — Species name • Compartment — Compartment that the species is in • Units — Species unit
Parameter	• Type — `'parameter'` • Name — Parameter name • Reaction — Name of the reaction that the parameter is scoped to, or `''` if the parameter is scoped to the model • Units — Parameter unit
Compartment	• Type — `'compartment'` • Owner — Compartment owner • Name — Compartment name • Units — Compartment unit

Type	Fields
Sensitivity	• Type — `'sensitivity'` • Name — Sensitivity name, for example, `'d[tumor_weight]/d[k2]'` • OutputType — Sensitivity output type (`'species'` or `'parameter'`). • OutputName — Sensitivity output name • OutputQualifier — Sensitivity output qualifier. If the output is a species, its output qualifier is the name of the compartment that the species is in. If the output is a model-scoped parameter, its output qualifier is `''`. If the output is a reaction-scoped parameter, its output qualifier is the name of the reaction that the parameter is scoped to. • InputType — Sensitivity input type (`'species'`, `'parameter'`, or `'compartment'`) • InputName — Sensitivity input name • InputQualifier — Sensitivity input qualifier. If the input is a species, its input qualifier is the name of the compartment that the species is in. If the input is a model-scoped parameter, its input qualifier is `''`. If the input is a reaction-scoped parameter, its input qualifier is the name of the reaction that the parameter is scoped to. If the input is a compartment, its input qualifier is either `''` or name of the parent compartment. • Units — Sensitivity unit
Observable	• Scalar — Flag to indicate if the observable is scalar-valued or vector-valued. • Expression — Observable expression • Type — `'observable'` • Name — Observable name • Units — Observable unit

Data Types: `cell`

`DataNames` — Labels for simulation data
`0-by-1` empty cell array (default) | *n*-by-1 cell array of character vectors

This property is read-only.

Labels for simulation data, specified as an *n*-by-1 cell array of character vectors. *n* is the number of logged quantities and sensitivities. In other words, the `DataNames` property contains the names that label the columns of the data matrix in the `Data` property.

Data Types: `cell`

`ScalarObservables` — Results from scalar-valued observable expressions
table

This property is read-only.

Results from scalar-valued observable expressions, specified as a table. Each table variable corresponds to each observable. The name of a variable is the same as that of a scalar-valued observable. However, if the observable name is too long, it is truncated and used as the table variable name. A suffix `'_N'` is also added, where N is a positive integer. The `VariableDescriptions` property of the table contains the untruncated names.

If you specified any units for the observable, the units are copied to the `VariableUnits` property of the table.

Data Types: `table`

`VectorObservables` — Results from vector-valued observable expressions
table

This property is read-only.

Results from vector-valued observable expressions, specified as a table. Each table variable corresponds to each observable. The name of a variable is the same as that of a vector-valued observable. However, if the observable name is too long, it is truncated and used as the table variable name. A suffix `'_N'` is also added, where N is a positive integer. The `VariableDescriptions` property of the table contains the untruncated names.

If you specified any units for the observable, the units are copied to the `VariableUnits` property of the table.

Data Types: `table`

`ModelName` — Name of model
`''` (default) | character vector

This property is read-only.

Name of the simulated model, specified as a character vector.

Data Types: `char`

`Name` — `SimData` object name
`0-by-0` empty character array (default) | character vector | string

`SimData` object name, specified as a character vector or string.

Data Types: `char` | `string`

`Notes` — Additional information
`0-by-0` empty character array (default) | character vector | string

Additional information that you can add for the `SimData` object, specified as a character vector or string.

Data Types: `char` | `string`

`RunInfo` — Information about simulation run
structure

This property is read-only.

Information about the simulation run that generated the simulation data, specified as a structure. The structure contains the following fields.

- `Configset` — A `struct` form of the configuration set used during simulation. The configuration set corresponds to the model active configset. The default is `[]`.
- `SimulationDate` — The date and time of simulation. The default is `''`.
- `SimulationType` — Either `'single run'` or `'ensemble run'`, depending on whether you create the object using `sbiosimulate` or `sbioensemblerun`. The default is `''`.

- `Variant` — A `struct` form of the variant(s) used during simulation. The default is `[]`.

Data Types: `struct`

`Time` — Simulation time steps
column vector

This property is read-only.

Simulation time steps, specified as a column vector.

Data Types: `double`

`TimeUnits` — Simulation time units
`'second'` (default) | character vector

This property is read-only.

Simulation time units, specified as a character vector.

If you simulate a model created using `sbiomodel`, the default `TimeUnits` value of the corresponding `SimData` object is `'second'`.

If you simulate model created using `PKModelDesign`, the default `TimeUnits` value is `'hour'`.

Data Types: `char`

`UserData` — Data to associate with object
`[]` (default) | any supported data type

Data to associate with the object, specified as any supported data type.

Object Functions

addobservable	Add observable expressions to SimData
display	Display summary of SimBiology object
getdata	Get simulation data from SimData object
getsensmatrix	Get 3-D sensitivity matrix from SimData object
remove	Remove simulation data from SimData object using expressions
removebyname	Remove simulation data by name from SimData object
renameobservable	Rename observables in SimData
resample	Resample simulation data onto new time vector
select	Select simulation data from SimData object using expressions
selectbyname	Select simulation data by name from SimData object
updateobservable	Update observable expressions or units in SimData

Examples

Initialize Simulation Using Previous Simulation Results

Load the G protein model.

```
sbioloadproject gprotein.sbproj;
```

Check the initial amounts of species.

```
m1.Species

ans =
   SimBiology Species Array

   Index:    Compartment:    Name:    Value:       Units:
   1         unnamed         G        7000
   2         unnamed         Gd       3000
   3         unnamed         Ga       0
   4         unnamed         RL       0
   5         unnamed         L        6.022e+17
   6         unnamed         R        10000
   7         unnamed         Gbg      3000
```

Select only the species as the states to log for simulation.

```
cs = getconfigset(m1);
allspecies = sbioselect(m1,'Type','species');
cs.RuntimeOptions.StatesToLog = allspecies;
```

Simulate the model.

```
sd = sbiosimulate(m1);
```

Use the Data property of the `SimData` object `sd` to get the states at the final time point. The Data property is an *m*-by-*n* matrix, where *m* is the number of time steps and *n* is the number of quantities logged.

```
finalData = sd.Data(end,:);
```

Use the `DataInfo` property to get the names of logged states.

```
info = sd.DataInfo;
```

Loop through the species and set their initial values.

```
numSpecies = length(info);
vObj = addvariant(m1,'initCond');
for i = 1:numSpecies
    addcontent(vObj,{'species',info{i}.Name,'Value',finalData(i)});
end
commit(vObj,m1);
```

Verify the species initial amounts.

```
m1.Species

ans =
   SimBiology Species Array

   Index:    Compartment:    Name:    Value:       Units:
   1         unnamed         G        8562.5
   2         unnamed         Gd       0.109565
   3         unnamed         Ga       1437.39
   4         unnamed         RL       1820.54
   5         unnamed         L        6.022e+17
   6         unnamed         R        11.1125
```

```
   7         unnamed         Gbg      1437.5
```

Calculate Statistics After Model Simulation Using Observables

Load the “Target-Mediated Drug Disposition (TMDD) Model”.

```
sbioloadproject tmdd_with_TO.sbproj
```

Set the target occupancy (`TO`) as a response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'TO';
```

Get the dosing information.

```
d = getdose(m1,'Daily Dose');
```

Scan over different dose amounts using a `SimBiology.Scenarios` object. To do so, first parameterize the `Amount` property of the dose. Then vary the corresponding parameter value using the `Scenarios` object.

```
amountParam = addparameter(m1,'AmountParam','Units',d.AmountUnits);
d.Amount = 'AmountParam';
d.Active = 1;
doseSamples = SimBiology.Scenarios('AmountParam',linspace(0,300,31));
```

Create a `SimFunction` to simulate the model. Set `TO` as the simulation output.

```
% Suppress informational warnings that are issued during simulation.
warning('off','SimBiology:SimFunction:DOSES_NOT_EMPTY');
f = createSimFunction(m1,doseSamples,'TO',d)
```

```
f =
SimFunction

Parameters:

        Name          Value        Type           Units
    ______________    _____    _____________    ___________

    {'AmountParam'}     1      {'parameter'}    {'nanomole'}

Observables:

     Name         Type              Units
    ______    _____________    _________________

    {'TO'}    {'parameter'}    {'dimensionless'}

Dosed:

      TargetName                TargetDimension                      Amount         AmountValue    A
    ______________    ____________________________________    _______________    ___________    _

    {'Plasma.Drug'}    {'Amount (e.g., mole or molecule)'}    {'AmountParam'}         1         -
```

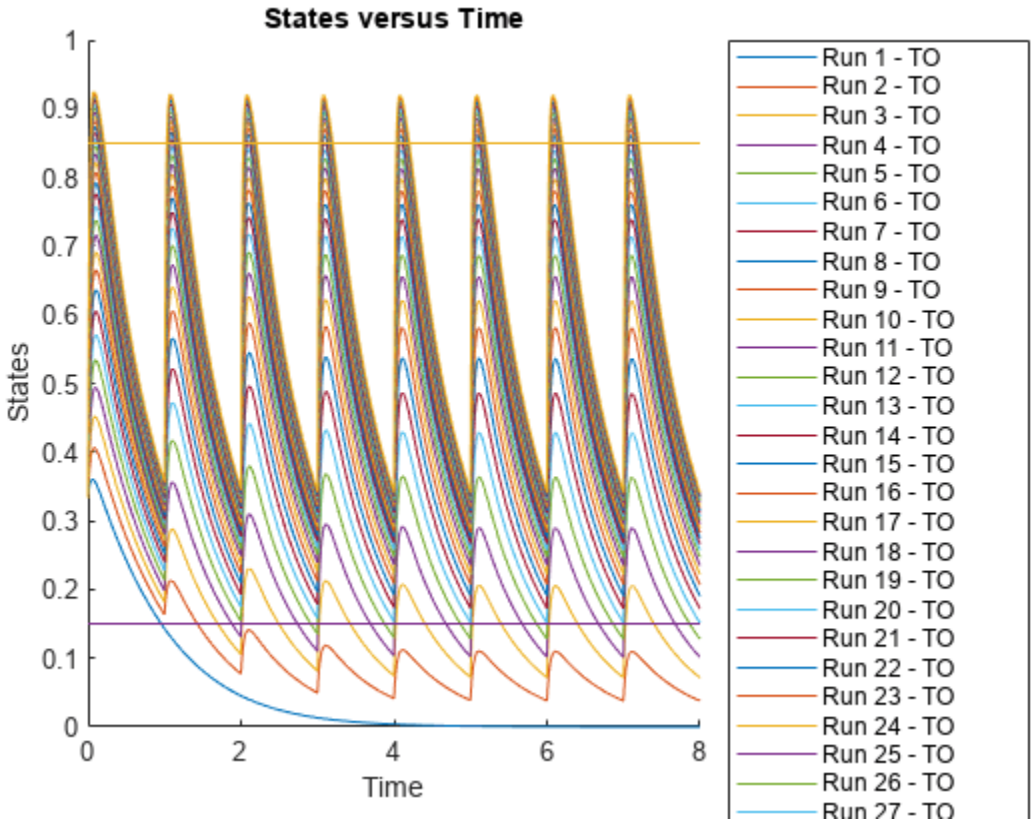
```
TimeUnits: day

warning('on','SimBiology:SimFunction:DOSES_NOT_EMPTY');
```

Simulate the model using the dose amounts generated by the `Scenarios` object. In this case, the object generates 31 different doses; hence the model is simulated 31 times and generates a `SimData` array.

```
doseTable = getTable(d);
sd = f(doseSamples,cs.StopTime,doseTable)


   SimBiology Simulation Data Array: 31-by-1

   ModelName:        TMDD
   Logged Data:
     Species:        0
     Compartment:    0
     Parameter:      1
     Sensitivity:    0
     Observable:     0
```

Plot the simulation results. Also add two reference lines that represent the safety and efficacy thresholds for `TO`. In this example, suppose that any `TO` value above 0.85 is unsafe, and any `TO` value below 0.15 has no efficacy.

```
h = sbioplot(sd);
time = sd(1).Time;
h.NextPlot = 'add';
safetyThreshold = plot(h,[min(time), max(time)],[0.85, 0.85],'DisplayName','Safety Threshold');
efficacyThreshold = plot(h,[min(time), max(time)],[0.15, 0.15],'DisplayName','Efficacy Threshold
```



Postprocess the simulation results. Find out which dose amounts are effective, corresponding to the `TO` responses within the safety and efficacy thresholds. To do so, add an observable expression to the simulation data.

```
% Suppress informational warnings that are issued during simulation.
warning('off','SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
newSD = addobservable(sd,'stat1','max(TO) < 0.85 & min(TO) > 0.15','Units','dimensionless')
```

```
  SimBiology Simulation Data Array: 31-by-1

  ModelName:        TMDD
  Logged Data:
    Species:        0
    Compartment:    0
    Parameter:      1
    Sensitivity:    0
    Observable:     1
```

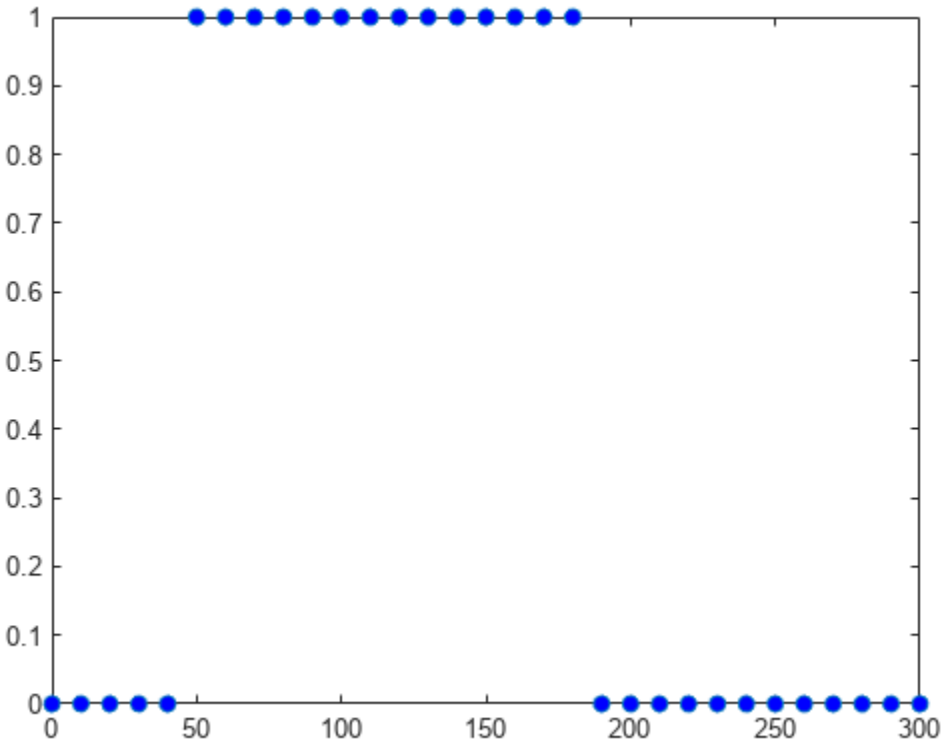
The addobservable function evaluates the new observable expression for each `SimData` in `sd` and returns the evaluated results as a new `SimData` array, `newSD`, which now has the added observable (`stat1`).

SimBiology stores the observable results in two different properties of a `SimData` object. If the results are scalar-valued, they are stored in `SimData.ScalarObservables`. Otherwise, they are

stored in `SimData.VectorObservables`. In this example, the `stat1` observable expression is scalar-valued.

Extract the scalar observable values and plot them against the dose amounts.

```
scalarObs = vertcat(newSD.ScalarObservables);
doseAmounts = generate(doseSamples);
figure
plot(doseAmounts.AmountParam,scalarObs.stat1,'o','MarkerFaceColor','b')
```



The plot shows that dose amounts ranging from 50 to 180 nanomoles provide `T0` responses that lie within the target efficacy and safety thresholds.

You can update the observable expression with different threshold amounts. The function recalculates the expression and returns the results in a new `SimData` object array.

```
newSD2 = updateobservable(newSD,'stat1','max(T0) < 0.75 & min(T0) > 0.30');
```

Rename the observable expression. The function renames the observable, updates any expressions that reference the renamed observable (if applicable), and returns the results in a new `SimData` object array.

```
newSD3 = renameobservable(newSD2,'stat1','EffectiveDose');
```

Restore the warning settings.

```
warning('on','SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
```

Version History

Introduced in R2007b

R2022a: `delete` function of `SimData` has been removed
Behavior changed in R2022a

The `delete` function of the `SimData` object has been removed.

See Also

`Model` | `Parameter` | `Species` | `Compartment` | `Reaction`

SimFunction object

Function-like interface to execute SimBiology models

Description

The `SimFunction` object provides an interface that allows you to execute a SimBiology model like a function and a workflow to perform parameter scans (in parallel if Parallel Computing Toolbox is available), Monte Carlo simulations, and scans with multiple or vectorized doses. Since a `SimFunction` object can be executed like a function handle, you can customize it to integrate SimBiology models with other MATLAB products and other custom analyses (such as visual predictive checks).

Use the `createSimFunction` method to construct the SimFunction object. SimFunction objects are immutable once created and automatically accelerated at the first function execution.

Syntax

If you specified any dosing information when you called `createSimFunction` to construct the `SimFunction` object `F`, then `F` has the following syntaxes.

`simdata = F(phi,t_stop,u,t_output)` returns a `SimData object` `simdata` after simulating a SimBiology model using the initial conditions or simulation scenarios specified in `phi`, simulation stop time, `t_stop`, dosing information, `u`, and output time, `t_output`.

`simdata = F(phi,t_stop,u)` runs simulations using the input arguments `phi`, `t_stop`, and `u`.

If you did *not* specify any dosing information when you called `createSimFunction`, then `F` has the following syntaxes:

`simdata = F(phi,t_stop)` returns a `SimData object` `simdata` after simulating the model using initial conditions or simulation scenarios specified in `phi`, and simulation stop time, `t_stop`.

`simdata = F(phi,t_stop,[],t_output)` uses the input arguments `phi`, `t_stop`, empty dosed argument `[]`, and `t_output`. You must specify `u`, the dosing information, as an empty array`[]` for this signature. When `t_output` is empty and `t_stop` is specified, the simulations report the solver time points until `t_stop`. When `t_output` is specified and `t_stop` is empty, only the time points in `t_output` are reported. When both are specified, the reported time points are the union of solver time points and the time points in `t_output`. If the last `t_output` is greater than the corresponding `t_stop`, then simulation proceeds until the last time point in `t_output`.

`simdata = F(phi,tbl)` uses the input arguments `phi` and `tbl`. Using this signature only lets you specify output times as one of the variables of `tbl`. Any data row in `tbl` where all dependent variable columns having `NaN` values is ignored.

`[T,Y] = F(_)` returns `T`, a cell array of numeric vector, and `Y`, a cell array of 2-D numeric matrices, using any of the input arguments in the preceding syntaxes.

Input Arguments

`phi`

One of the following:

- Empty array `[]` or empty cell array `{}`, meaning to perform simulations using the baseline initial values, that is, the values listed in the `Parameter` property of the `SimFunction` object, without altering them.
- Matrix of size *S*-by-*P*, where *S* is the number of simulations to perform and *P* is the number of parameters specified in the `params` argument when you called `createSimFunction` to construct `F`. Each simulation is performed with the parameters specified in the corresponding row of `phi`.
- *S*-by-*V* matrix of variant objects or a cell column vector of length *S*, where each element consists of a row vector of variant objects. *S* is the number of simulations to perform, and *V* is the number of variant objects. These variants are only allowed to modify the `SimFunction` input parameters, that is, model elements that were specified as the `params` input argument when you called `createSimFunction`. In other words, you must specify the variant parameters as the input parameters when you create the `SimFunction` object. Any `SimFunction` input parameters that are not specified in the variants use their baseline initial values.

  If, within a row of variants, multiple entries refer to the same model element, the last occurrence is used for simulation.
- Scalar `SimBiology.Scenarios` object containing *S* number of scenarios.

When `phi` is specified as a `1`-by-*P* or `1`-by-*V* matrix (or a `Scenarios` object with only one scenario), then all simulations use the same parameters, and the number of simulations is determined from the `t_stop`, `u`, or `t_output` argument in that order. For example, if `phi` and `t_stop` have a single row and `u` is a matrix of size *N*-by-*DoseTargets*, the number of simulations is determined as *N*.

When `phi` is specified as a `SimBiology.Scenarios` object, all scenarios are simulated. Variants are applied before values from the scenarios are set.

`t_stop`

- Scalar specifying the same stop time for all simulations
- Vector of size N specifying a stop time for each simulation for all N simulations

`u`

- Empty array `[]` to apply no doses during simulation unless you specify `phi` as a `Scenarios` object that has doses defined in its entries.
- `table` of dosing information with two or three variables containing `ScheduleDose` data (`ScheduleDose` table), namely, dose time, dose amount, and dose rate (optional). Name the table variables as follows.

  ```
  u.Properties.VariableNames = {'Time','Amount','Rate'};
  ```

  If `UnitConversion` is on, specify units for each variable. For instance, you can specify units as follows.

  ```
  u.Properties.VariableUnits = {'second','molecule','molecule/second'};
  ```

This table can have multiple rows, where each row represents a dose applied to the dose target at a specified dose time with a specified amount and rate if available.

- `table` with one row and five variables containing `RepeatDose` data (`RepeatDose` table). Dose rate variable is optional. Name the variables as follows.

  ```
  u.Properties.VariableNames = {'StartTime','Amount','Rate','Interval','RepeatCount'};
  ```

  If `UnitConversion` is on, specify units for each variable. Units for `'RepeatCount'` variable can be empty `''` or `'dimensionless'`. The unit of the `'Amount'` variable must be dimensionally consistent with that of the target species. For example, if the unit of target species is in an *amount* unit (such as mole or molecule), then the `'Amount'` variable unit must have the same dimension, i.e., its unit must be an *amount* unit and cannot be a *mass* unit (such as gram or kilogram). The unit for the `'Rate'` variable must be dimensionally consistent as well.

  ```
  u.Properties.VariableUnits = {'second','molecule','molecule/second','second','dimensionless'};
  ```

  Tip If you already have a dose object (`ScheduleDose` or `RepeatDose`), you can get this dose table by using the `getTable` method of the object.

- Cell array of tables of size 1-by-N, where N is the number of dose targets. Each cell can represent either table as described previously.
- Cell array of tables of size S-by-N, where S is the number of simulations and N is the number of dose targets. Each cell represents a table. S is equal to the number of rows in `phi`.

If `u` is a cell array of tables, then:

- If `phi` is also a `Scenarios` object, the combined number of doses in the `Scenarios` object and the number of columns in `u` must equal to the number of elements in the `Dosed` property of the `SimFunction` object. In other words, the dosing information that you specified during the creation of the `SimFunction` object must be consistent with the dosing information you specify in the execution of the object. The total number of elements for the `Dosed` property is equal to the combination of any doses from the input `Scenarios` object and doses in the dosed input argument on page 2-0 of `createSimFunction`.
- If `phi` is not a `Scenarios` object, the number of columns (*N*) in the cell array `u` must be equal to the number of elements in the `Dosed` property of the `SimFunction` object. The order of dose tables must also match the order of dosed species in `createSimFunction`. That is, SimBiology assumes one-to-one correspondence between the columns of `u` and dose targets specified in the `Dosed` property of the `SimFunction` object, meaning the doses (dose tables) in the first column of `u` are applied to the first dose target in the `Dosed` property and so on.
- The *i*th dose for the *j*th dose target is ignored if `u{i,j} = []`.
- If the *i*th dose is not parameterized, `u{i,j}` can be `[]` or either type of table (the `ScheduleDose` or `RepeatDose` table).
- If the *i*th dose is parameterized, `u{i,j}` must be `[]` or a `RepeatDose` table with one row and a column for each property (`StartTime`, `Amount`, `Rate`, `Interval`, `RepeatCount`) that is not parameterized. It is not required to create a column for a dose property that is parameterized. If all of the properties are parameterized, you can pass in a table with one row and no columns to specify the parameterized dose is applied during simulations. To create such table, use `table.empty(1,0)`.

`t_output`

- Vector of monotonically increasing output times that is applied to all simulations

- Cell array containing a single time vector that is applied to all simulations
- Cell array of vectors representing output times. The ith cell element provides the output times for the ith simulation. The number of elements in the cell array must match the number of rows (simulations) in `phi`.

`tbl`

`table` or `dataset` that has time and dosing information such as group labels, independent variable, dependent variable(s), amount(s), and rate(s). You must name the variables of the table or data set as `'GROUP','TIME','DEPENDENTVAR1','DEPENDENTVAR2',...,'AMOUNT1','RATE1','AMOUNT2','RATE2',...`. The rate variable is optional for each dose.

If the `Dosed` property of the SimFunction object `F` is empty, then amount- and rate-related variables are not required. The number of groups in `tbl` must be equal to the number of rows, or the number of scenarios, in `phi`. The combined dosing information in `phi`, if `phi` is a `SimBiology.Scenarios` object, and the number of amount and rate columns in `tbl` must be equal to the number of doses in the `Dosed` property of the object `F`. If `tbl` has additional columns, they are ignored.

If `UnitConversion` is on, specify a unit for each variable. The unit of `'Amount'` variable must be dimensionally consistent with that of the target species. See the description of the input argument `u` for details.

Output Arguments

`simdata`

Array of SimData objects that contains results from executing the SimFunction `F`. The number of elements in the `simdata` array is the same as the number of rows in `phi`. The number of columns in each element of the `simdata` array, that is, `simdata(i).Data`, is equal to the number of elements in the `observed` cell array which was specified when creating `F`.

`T`

Cell array containing a numeric vector of size `S x 1`. `S` is the number of simulations. The ith element of T contains the time point from the ith simulation.

`Y`

Cell array of 2-D numeric matrices. The i^{th} element of `Y` contains data from the i^{th} simulation. The number of rows in `T{i}` is equal to the number of rows in `Y{i}`.

Constructor Summary

createSimFunction (model)	Create SimFunction object

Method Summary

accelerate(SimFunction)	Prepare SimFunction object for accelerated simulations
isAccelerated(SimFunction)	Determine if SimFunction object is accelerated

Property Summary

`Parameters`	`table` with variables named: • `'Name'` • `'Value'` • `'Type'` • `'Units'` (only if `UnitConversion` is turned on) The table contains information about model quantities (species, compartments, or parameters) that define the inputs of a `SimFunction object`. For instance, this table can contain parameters or species whose values are being scanned by the `SimFunction object`. This property is read only.
`Observables`	`table` with variables named: • `'Name'` • `'Type'` • `'Units'` (only if `UnitConversion` is turned on) This table contains information about model quantities (species, compartments, or parameters) that define the output of a `SimFunction object`. This property is read only.
`Dosed`	`table` containing dosing information with variables named: • `'TargetName'` • `'TargetDimension'` (only if `UnitConversion` is turned on) In addition, the table also contains variables for each property that is parameterized. For each parameterized property, two variables are added to this table. The first variable has the same name as the property name and the value is the name of the specified parameter. The second variable has the property name suffixed by *Value* (*PropertyNameValue*), and the value is the default value of the parameter. If the `UnitConversion` is on, the unit column is also added with the name *PropertyNameUnits*. Suppose the `Amount` property of a repeat dose targeting the *Drug* species is parameterized by setting it to a model parameter called `AmountParam` with the value of `10` milligram, and `UnitConversion` is on. The `Dosed` table contains the following variables:

TargetName	TargetDimension	Amount	AmountValue	AmountUnits
`'Drug'`	`'Mass (e.g., gram)'`	`'AmountParam'`	10	`'milligram'`

`UseParallel`	Logical. If `true` and Parallel Computing Toolbox is available, SimFunction is executed in parallel. This property is read-only.

`UnitConversion`	Logical. If true: • During the execution of the `SimFunction` object, `phi` is assumed to be in the same units as units for corresponding model quantities specified in the `params` argument when the object was created using the `createSimFunction` method. • Time (`t_output` or `t_stop`) is assumed to be in the same unit as the `TimeUnits` property of the active `configset object` of the SimBiology model from which `F` was created. • Variables of dose tables (`u`) must have units specified by setting `u.Properties.VariableUnits` to a cell array of appropriate units. The dimension of the dose target such as an amount (molecule, mole, etc.) or mass (gram, kilogram, etc.), is stored on the `Dosed` property of `F`. • The simulation result is in the same units as those specified on the corresponding quantities in the SimBiology model from which `F` was created. This property is read only.
`AutoAccelerate`	Logical. When true, the model is accelerated on the first evaluation of the `SimFunction` object. This property is read only.
`DependentFiles`	Cell array of character vectors containing the names of files that the model depends on. This property is used for deployment. This property is read only.
`TimeUnits`	Character vector that represents the time units.

Examples

Simulate Model of Glucose-Insulin Response with Different Initial Conditions

This example shows how to simulate the glucose-insulin responses for the normal and diabetic subjects.

Load the model of glucose-insulin response. For details about the model, see the **Background** section in “Simulate the Glucose-Insulin Response”.

```
sbioloadproject('insulindemo', 'm1')
```

The model contains different initial conditions stored in various variants.

```
variants = getvariant(m1);
```

Get the initial conditions for the type 2 diabetic patient.

```
type2 = variants(1)
```

```
type2 =
   SimBiology Variant - Type 2 diabetic (inactive)

   ContentIndex:     Type:        Name:             Property:          Value:
   1                 parameter    Plasma Volume ... Value              1.49
   2                 parameter    k1                Value              .042
```

```
   3                parameter    k2                Value              .071
   4                parameter    Plasma Volume ... Value              .04
   5                parameter    m1                Value              .379
   6                parameter    m2                Value              .673
   7                parameter    m4                Value              .269
   8                parameter    m5                Value              .0526
   9                parameter    m6                Value              .8118
   10               parameter    Hepatic Extrac... Value              .6
   11               parameter    kmax              Value              .0465
   12               parameter    kmin              Value              .0076
   13               parameter    kabs              Value              .023
   14               parameter    kgri              Value              .0465
   15               parameter    f                 Value              .9
   16               parameter    a                 Value              6e-05
   17               parameter    b                 Value              .68
   18               parameter    c                 Value              .00023
   19               parameter    d                 Value              .09
   20               parameter    kp1               Value              3.09
   21               parameter    kp2               Value              .0007
   22               parameter    kp3               Value              .005
   23               parameter    kp4               Value              .0786
   24               parameter    ki                Value              .0066
   25               parameter    [Ins Ind Glu U... Value              1.0
   26               parameter    Vm0               Value              4.65
   27               parameter    Vmx               Value              .034
   28               parameter    Km                Value              466.21
   29               parameter    p2U               Value              .084
   30               parameter    K                 Value              .99
   31               parameter    alpha             Value              .013
   32               parameter    beta              Value              .05
   33               parameter    gamma             Value              .5
   34               parameter    ke1               Value              .0007
   35               parameter    ke2               Value              269.0
   36               parameter    Basal Plasma G... Value              164.18
   37               parameter    Basal Plasma I... Value              54.81
```

Suppress an informational warning that is issued during simulations.

```
warnSettings = warning('off','SimBiology:DimAnalysisNotDone_MatlabFcn_Dimensionless');
```

Create SimFunction objects to simulate the glucose-insulin response for the normal and diabetic subjects.

- Specify an empty array `{}` for the second input argument to denote that the model will be simulated using the base parameter values (that is, no parameter scanning will be performed).
- Specify the plasma glucose and insulin concentrations as responses (outputs of the function to be plotted).
- Specify the species `Dose` as the dosed species. This species represents the initial concentration of glucose at the start of the simulation.

```
normSim = createSimFunction(m1,{},...
            {'[Plasma Glu Conc]','[Plasma Ins Conc]'},'Dose')
```

```
normSim =
SimFunction
```

```
Parameters:

Observables:

           Name                Type                Units
    ___________________    ___________    ____________________

    {'[Plasma Glu Conc]'}    {'species'}    {'milligram/deciliter'}
    {'[Plasma Ins Conc]'}    {'species'}    {'picomole/liter'     }

Dosed:

    TargetName       TargetDimension
    __________    ____________________

     {'Dose'}     {'Mass (e.g., gram)'}


TimeUnits: hour
```

For the diabetic patient, specify the initial conditions using the variant `type2`.

```
diabSim = createSimFunction(m1,{},...
             {'[Plasma Glu Conc]','[Plasma Ins Conc]'},'Dose',type2)
```

```
diabSim =
SimFunction

Parameters:

Observables:

           Name                Type                Units
    ___________________    ___________    ____________________

    {'[Plasma Glu Conc]'}    {'species'}    {'milligram/deciliter'}
    {'[Plasma Ins Conc]'}    {'species'}    {'picomole/liter'     }

Dosed:

    TargetName       TargetDimension
    __________    ____________________

     {'Dose'}     {'Mass (e.g., gram)'}


TimeUnits: hour
```

Select a dose that represents a single meal of 78 grams of glucose at the start of the simulation.

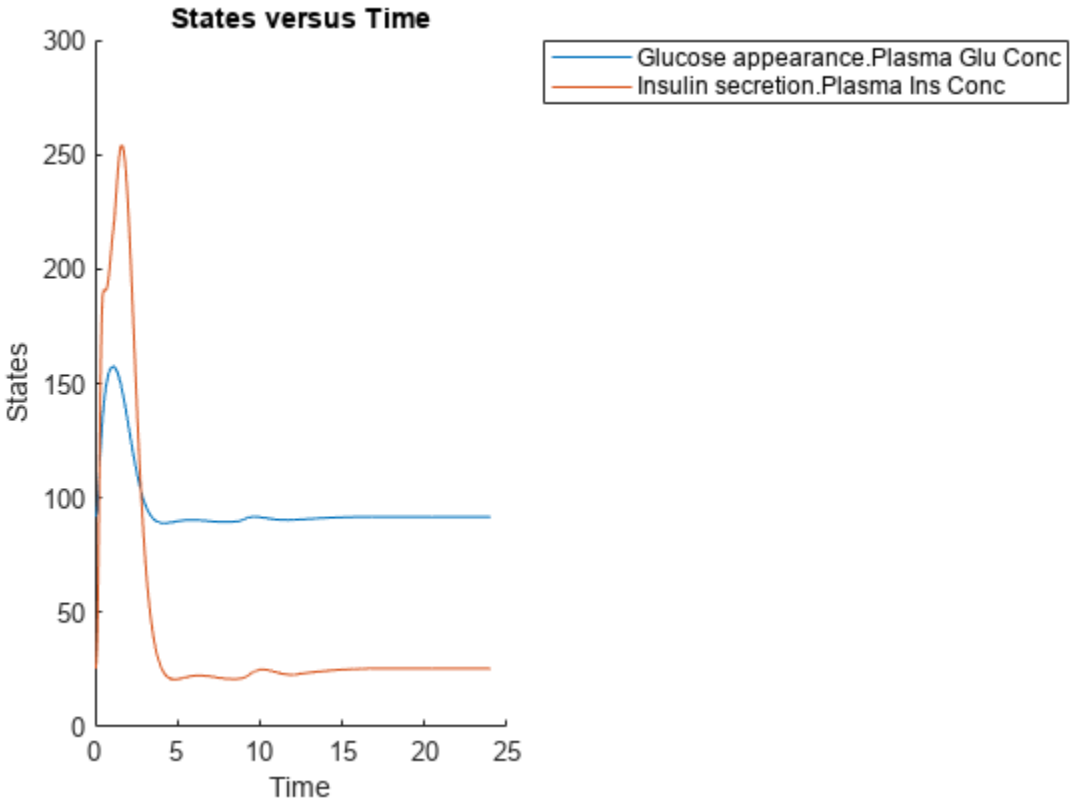
```
singleMeal = sbioselect(m1,'Name','Single Meal');
```

Convert the dosing information to the table format.

```
mealTable  = getTable(singleMeal);
```

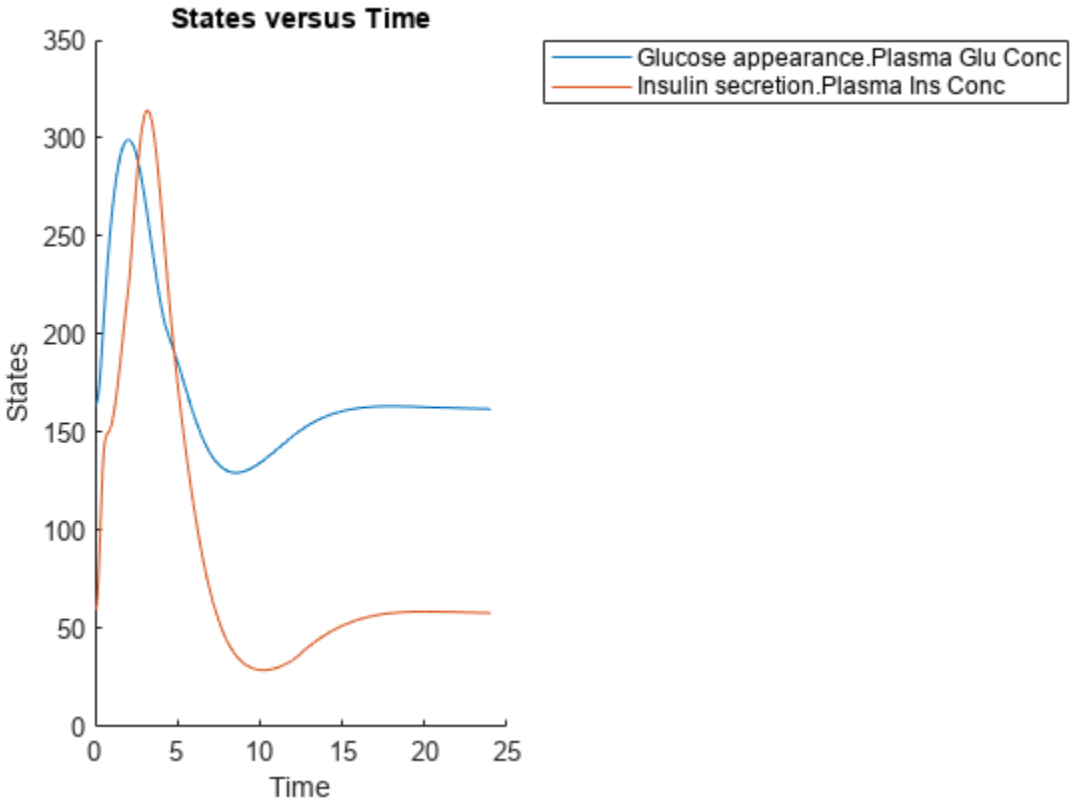
Simulate the glucose-insulin response for a normal subject for 24 hours.

```
sbioplot(normSim([],24,mealTable));
```



Simulate the glucose-insulin response for a diabetic subject for 24 hours.

```
sbioplot(diabSim([],24,mealTable));
```



Perform a Scan Using Variants

Suppose you want to perform a parameter scan using an array of variants that contain different initial conditions for different insulin impairments. For example, the model `m1` has variants that correspond to the low insulin sensitivity and high insulin sensitivity. You can simulate the model for both conditions via a single call to the SimFunction object.

Select the variants to scan.

```
varToScan = sbioselect(m1,'Name',...
                   {'Low insulin sensitivity','High insulin sensitivity'});
```

Check which model parameters are being stored in each variant.

```
varToScan(1)
```

```
ans =
   SimBiology Variant - Low insulin sensitivity (inactive)

   ContentIndex:     Type:        Name:            Property:          Value:
   1                 parameter    Vmx              Value              .0235
   2                 parameter    kp3              Value              .0045
```

```
varToScan(2)
```

```
ans =
   SimBiology Variant - High insulin sensitivity (inactive)
```

```
ContentIndex:     Type:        Name:            Property:          Value:
1                 parameter    Vmx              Value              .094
2                 parameter    kp3              Value              .018
```

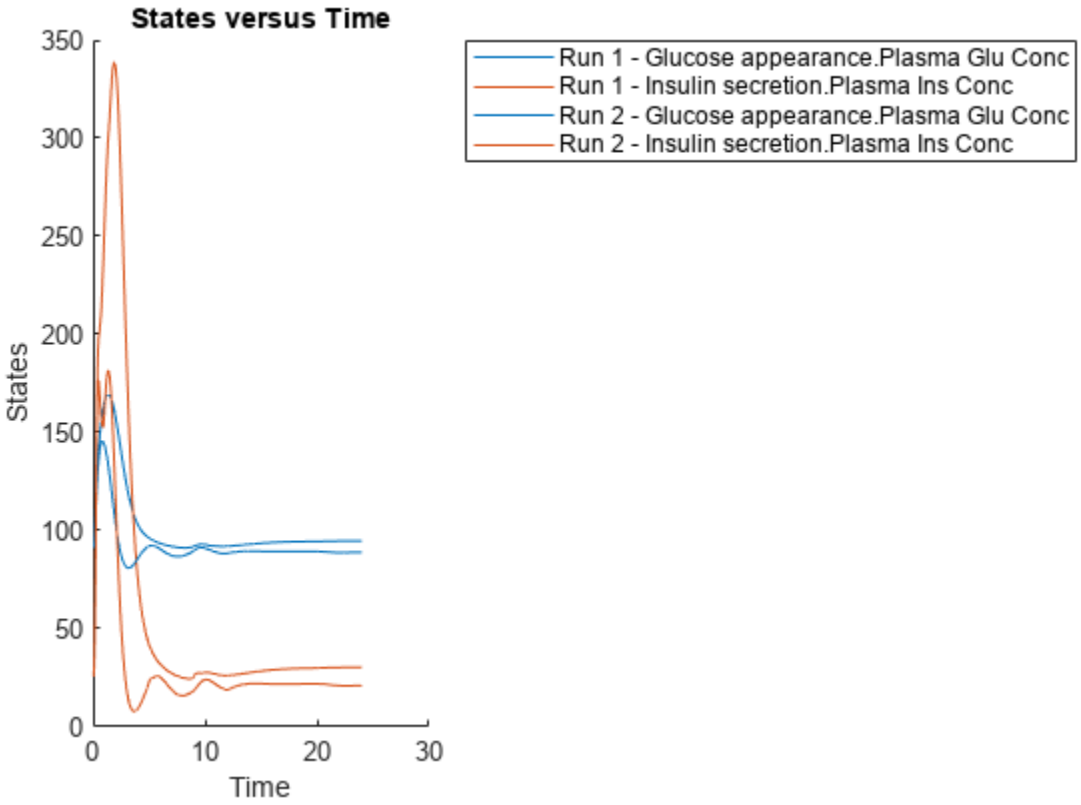
Both variants store alternate values for `Vmx` and `kp3` parameters. You need to specify them as input parameters when you create a SimFunction object.

Create a SimFunction object to scan the variants.

```
variantScan = createSimFunction(m1,{'Vmx','kp3'},...
          {'[Plasma Glu Conc]','[Plasma Ins Conc]'},'Dose');
```

Simulate the model and plot the results. `Run 1` include simulation results for the low insulin sensitivity and `Run 2` for the high insulin sensitivity.

```
sbioplot(variantScan(varToScan,24,mealTable));
```



Low insulin sensitivity lead to increased and prolonged plasma glucose concentration.

Restore warning settings.

```
warning(warnSettings);
```

Scan Initial Amounts of a Species from a Radioactive Decay Model

This example shows how to scan initial amounts of a species from a radioactive decay model with the first-order reaction $\frac{dz}{dt} = c \cdot x$, where `x` and `z` are species and `c` is the forward rate constant.

Load the sample project containing the radiodecay model `m1`.

```
sbioloadproject radiodecay;
```

Create a `SimFunction` object `f` to scan initial amounts of species `x`.

```
f = createSimFunction(m1,{'x'},{'x','z'},[])
```

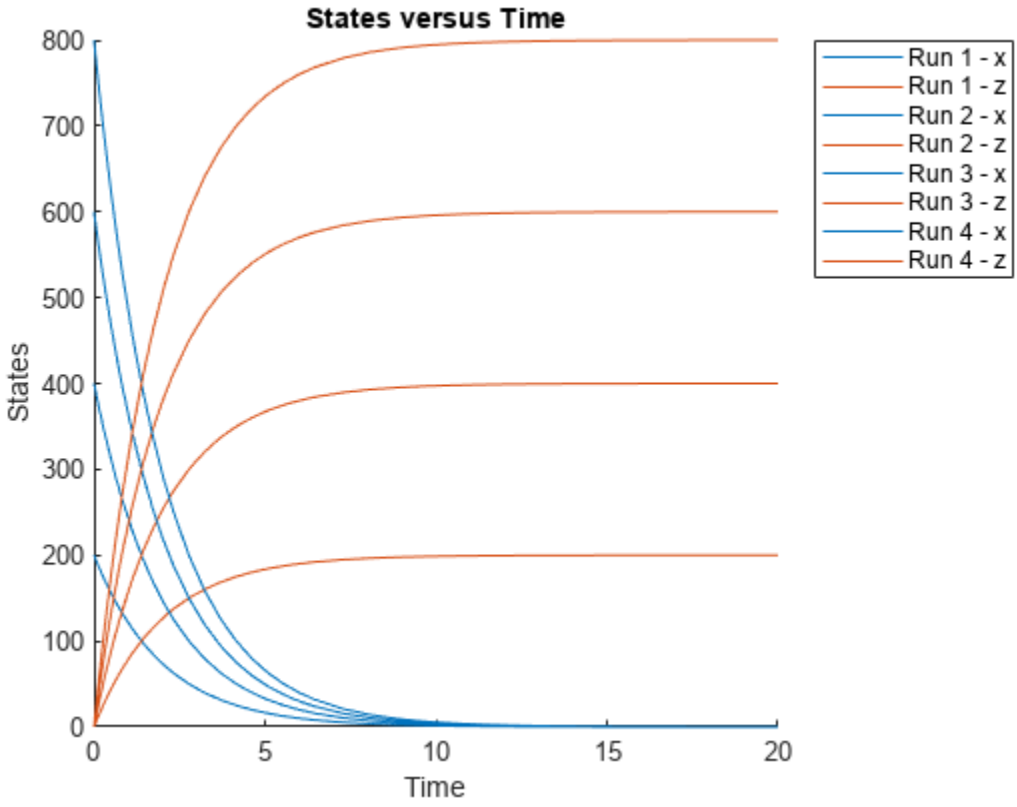
```
f =
SimFunction

Parameters:

    Name     Value       Type           Units
    _____    _____    ___________    ____________

    {'x'}    1000     {'species'}    {'molecule'}

Observables:

    Name        Type           Units
    _____    ___________    ____________

    {'x'}    {'species'}    {'molecule'}
    {'z'}    {'species'}    {'molecule'}

Dosed: None

TimeUnits: second
```

Define four different initial amounts of species x for scanning. The number of rows indicates the total number of simulations, and each simulation uses the parameter value specified in each row of the vector.

```
phi = [200; 400; 600; 800];
```

Run simulations until the stop time is 20 and plot the simulation results.

```
sbioplot(f(phi, 20));
```



Simulate a Model and Scan Parameters with Doses

This example shows how to simulate and scan a parameter of a radiodecay model while a species is being dosed.

Load the sample project containing the radiodecay model `m1`.

```
sbioloadproject radiodecay;
```

Create a `SimFunction` object `f` specifying parameter `Reaction1.c` to be scanned and species `x` as a dosed target.

```
f = createSimFunction(m1,{'Reaction1.c'},{'x','z'},{'x'});
```

Define a scalar dose of amount 200 molecules given at three time points (5, 10, and 15 seconds).

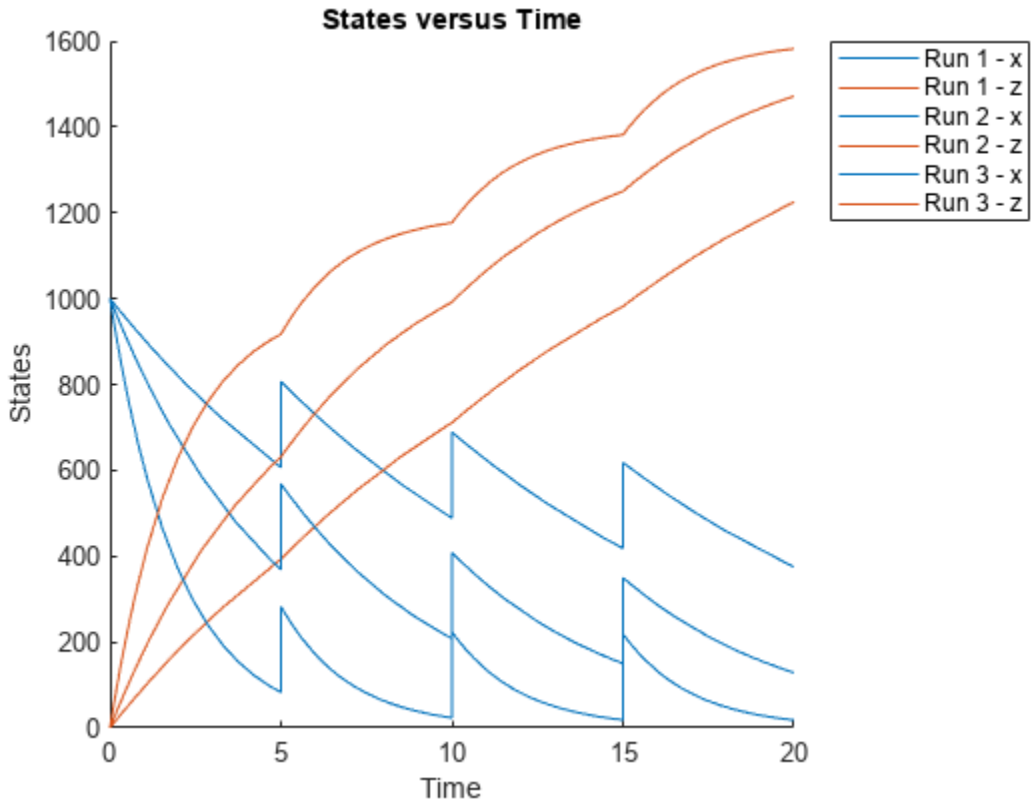
```
dosetime = [5 10 15];
dose = [200 200 200];
u = table(dosetime', dose');
u.Properties.VariableNames = {'Time','Amount'};
u.Properties.VariableUnits = {'second','molecule'};
```

Define the parameter values for `Reaction1.c` to scan.

```
phi = [0.1 0.2 0.5]';
```

Simulate the model for 20 seconds and plot the results.

```
sbioplot(f(phi,20,u));
```

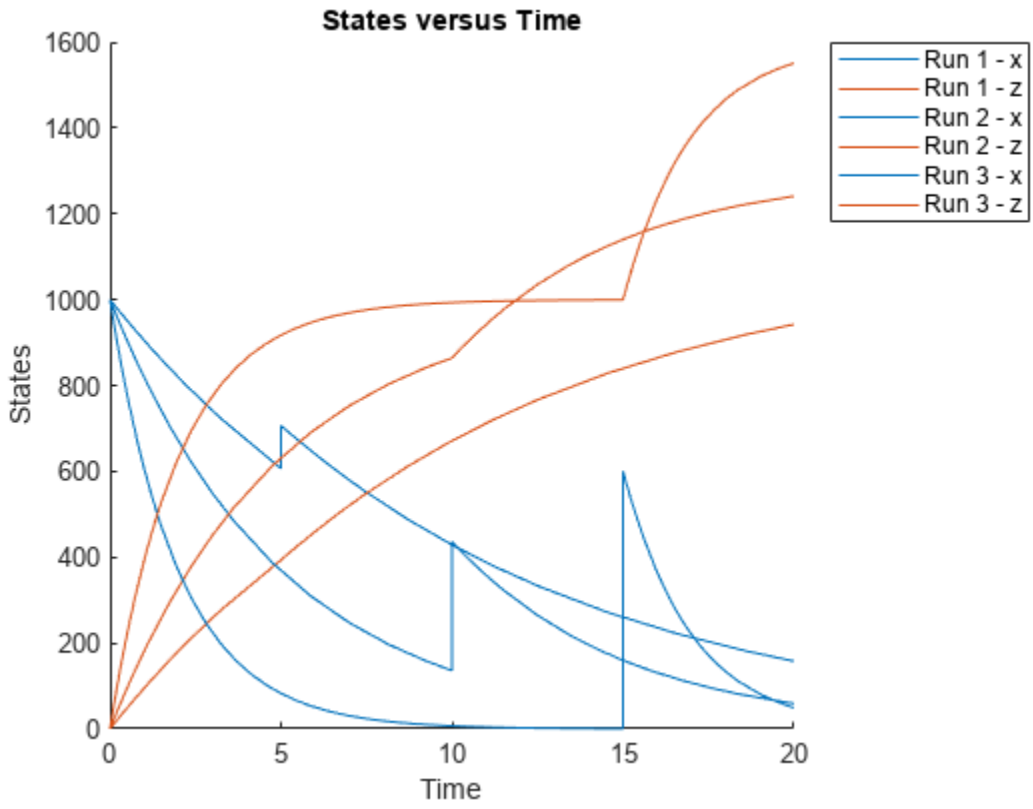


You can also specify different dose amounts at different times.

```
d1 = table(5,100);
d1.Properties.VariableNames = {'Time','Amount'};
d1.Properties.VariableUnits = {'second','molecule'};
d2 = table(10,300);
d2.Properties.VariableNames = {'Time','Amount'};
d2.Properties.VariableUnits = {'second','molecule'};
d3 = table(15,600);
d3.Properties.VariableNames = {'Time','Amount'};
d3.Properties.VariableUnits = {'second','molecule'};
```

Simulate the model using these doses and plot the results.

```
sbioplot(f(phi,20,{d1;d2;d3}));
```

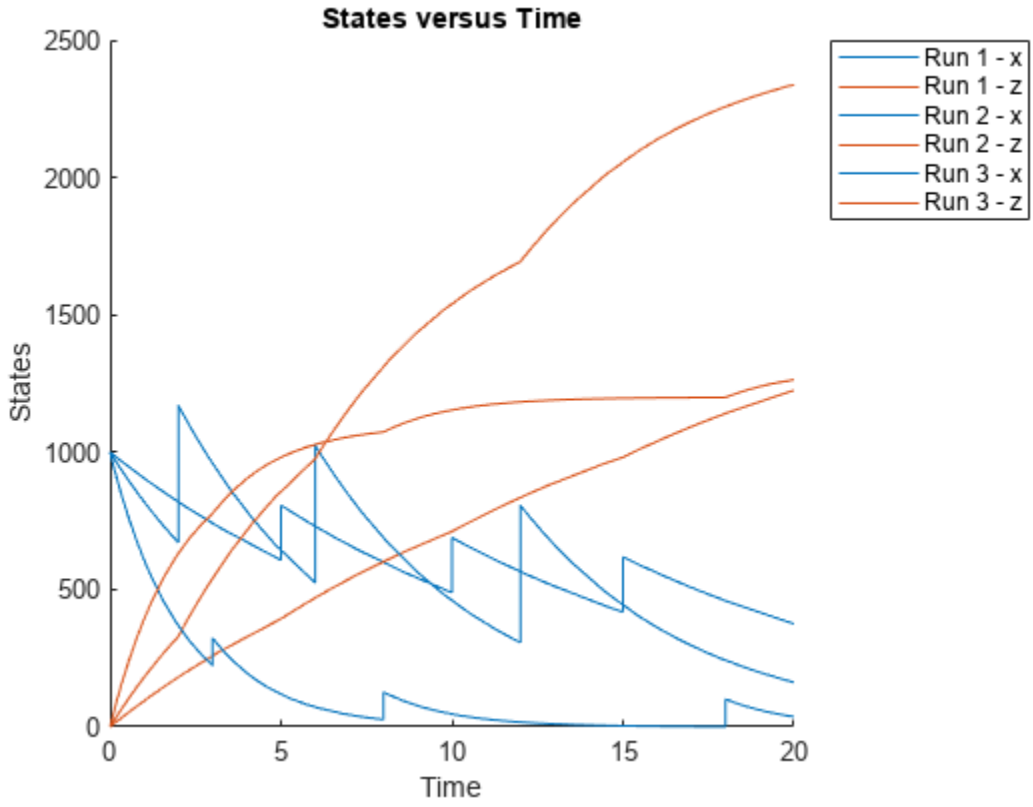


You can also define a cell array of dose tables.

```
u = cell(3,1);
dosetime = [5 10 15];
dose = [200 200 200];
u{1} = table(dosetime',dose');
u{1}.Properties.VariableNames = {'Time','Amount'};
u{1}.Properties.VariableUnits = {'second','molecule'};
dosetime2 = [2 6 12];
dose2 = [500 500 500];
u{2} = table(dosetime2', dose2');
u{2}.Properties.VariableNames = {'Time','Amount'};
u{2}.Properties.VariableUnits = {'second','molecule'};
dosetime3 = [3 8 18];
dose3 = [100 100 100];
u{3} = table(dosetime3', dose3');
u{3}.Properties.VariableNames = {'Time','Amount'};
u{3}.Properties.VariableUnits = {'second','molecule'};
```

Simulate the model using the dose tables and plot results.

```
sbioplot(f(phi,20,u));
```



Version History

Introduced in R2014a

References

[1] Gillespie, D.T. (1977). Exact Stochastic Simulation of Coupled Chemical Reactions. The Journal of Physical Chemistry. 81(25), 2340–2361.

See Also

`SimBiology.Scenarios` | `SimFunctionSensitivity object` | `createSimFunction` | `sbiosampleerror` | `sbiosampleparameters` | `ScheduleDose object` | `RepeatDose object`

Topics

“Perform PK/PD Modeling and Simulation to Guide Dosing Strategy for Antibiotics”
“Model Simulation”

SimFunctionSensitivity object

SimFunctionSensitivity object, subclass of `SimFunction` object

Description

The `SimFunctionSensitivity` object is a subclass of `SimFunction object`. It allows you to compute sensitivity.

Syntax

The `SimFunctionSensitivity` object shares all syntaxes of the `SimFunction` object. It has the following additional syntax.

`[T,Y,SensMatrix] = F( ___ )` returns `T`, a cell array of numeric vector, `Y`, a cell array of 2-D numeric matrices, and `SensMatrix`, a cell array of 3-D numeric matrix containing calculated sensitivities of model quantities. `SensMatrix` contains a matrix of size *TimePoints* x *Outputs* x *Inputs*. *TimePoints* is the total number of time points, *Outputs* is the total number of output factors, and *Inputs* is the total number of input factors.

If you specify a single output argument, the object returns an `SimData` object or array of `SimData` objects with sensitivity information.

Property Summary

The `SimFunctionSensitivity` object shares all properties of the `SimFunction object`. It has the following additional properties.

`SensitivityOutputs`

`table` with variables named:

- `'Name'`
- `'Type'`
- `'Units'` (only if UnitConversion is turned on)

This table contains information about model quantities (species or parameters) for which you want to compute the sensitivities. Sensitivity output factors are the numerators of time-dependent derivatives described in “Sensitivity Analysis in SimBiology”. This property is read only.

`SensitivityInputs`

`table` with variables named:

- `'Name'`
- `'Type'`
- `'Units'` (only if `UnitConversion` is turned on)

This table contains information about model quantities (species, compartments, or parameters) with respect to which you want to compute the sensitivities. Sensitivity input factors are the denominators of time-dependent derivatives described in “Sensitivity Analysis in SimBiology”. This property is read only.

`SensitivityNormalization` — Character vector specifying the normalization method for calculated sensitivities. The following examples show how sensitivities of a species x with respect to a parameter k are calculated for each normalization type.

- `'None'` — No normalization.

  $$\frac{\partial x(t)}{\partial k}$$

- `'Half'` — Normalization relative to the numerator only.

  $$\left(\frac{1}{x(t)}\right)\left(\frac{\partial x(t)}{\partial k}\right)$$

- `'Full'` — Full dedimensionalization

  $$\left(\frac{k}{x(t)}\right)\left(\frac{\partial x(t)}{\partial k}\right)$$

Examples

Calculate Local Sensitivities Using `SimFunctionSensitivity` Object

This example shows how to calculate the local sensitivities of some species in the Lotka-Volterra model using the `SimFunctionSensitivity` object.

Load the sample project.

```
sbioloadproject lotka;
```

Define the input parameters.

```
params = {'Reaction1.c1', 'Reaction2.c2'};
```

Define the observed species, which are the outputs of simulation.

```
observables  = {'y1', 'y2'};
```

Create a `SimFunctionSensitivity` object. Set the sensitivity output factors to all species (`y1` and `y2`) specified in the `observables` argument and input factors to those in the `params` argument (`c1` and `c2`) by setting the name-value pair argument to `'all'`.

```
f = createSimFunction(m1,params,observables,[],'SensitivityOutputs','all','SensitivityInputs','a
```

```
f =
SimFunction

Parameters:

          Name           Value        Type
    _________________    _____    _____________

    {'Reaction1.c1'}      10     {'parameter'}
    {'Reaction2.c2'}    0.01     {'parameter'}

Observables:
```

```
     Name        Type
    ______    ___________

    {'y1'}    {'species'}
    {'y2'}    {'species'}

Dosed: None

Sensitivity Input Factors:

          Name              Type
    ________________    _____________

    {'Reaction1.c1'}    {'parameter'}
    {'Reaction2.c2'}    {'parameter'}

Sensitivity Output Factors:

     Name        Type
    ______    ___________

    {'y1'}    {'species'}
    {'y2'}    {'species'}

Sensitivity Normalization:

Full
```

Calculate sensitivities by executing the object with `c1` and `c2` set to 10 and 0.1, respectively. Set the output times from 1 to 10. `t` contains time points, `y` contains simulation data, and `sensMatrix` is the sensitivity matrix containing sensitivities of `y1` and `y2` with respect to `c1` and `c2`.

```
[t,y,sensMatrix] = f([10,0.1],[],[],1:10);
```

Retrieve the sensitivity information at time point 5.

```
temp = sensMatrix{:};
sensMatrix2 = temp(t{:}==5,:,:);
sensMatrix2 = squeeze(sensMatrix2)
```

```
sensMatrix2 = 2×2

   37.6987   -6.8447
  -40.2791    5.8225
```

The rows of `sensMatrix2` represent the output factors (`y1` and `y2`). The columns represent the input factors (`c1` and `c2`).

$$sensMatrix2 = \begin{bmatrix} \frac{\partial y1}{\partial c1} & \frac{\partial y1}{\partial c2} \\ \frac{\partial y2}{\partial c1} & \frac{\partial y2}{\partial c2} \end{bmatrix}$$

Set the stop time to 15, without specifying the output times. In this case, the output times are the solver time points by default.

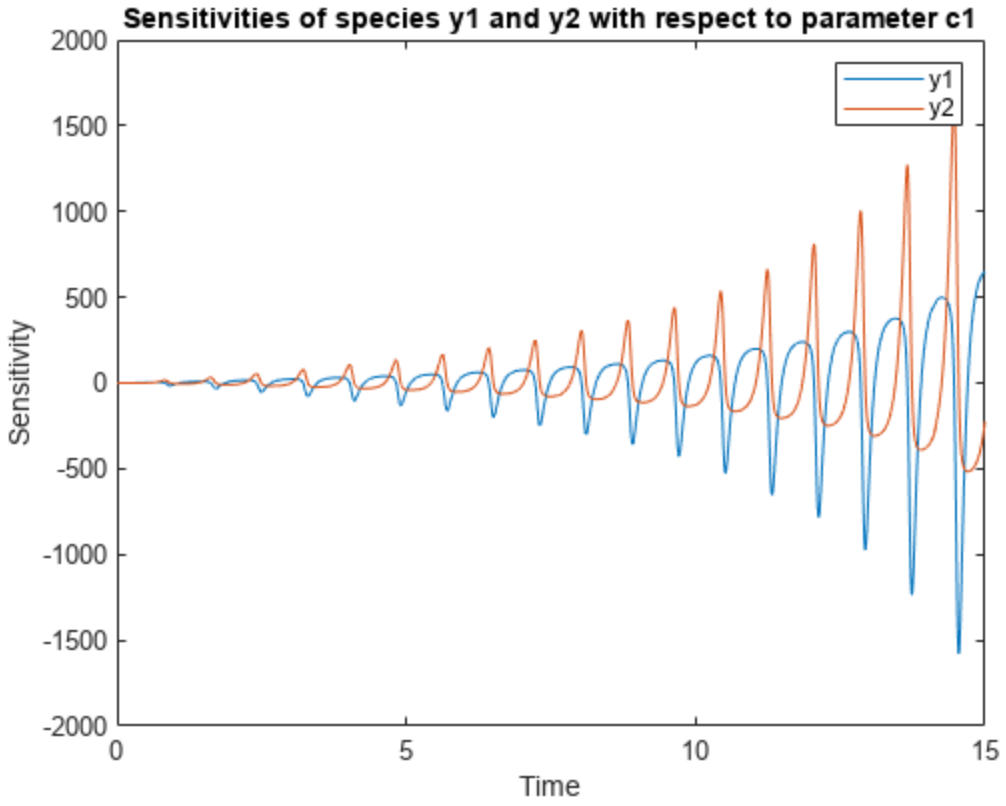
```
sd = f([10,0.1],15);
```

Retrieve the calculated sensitivities from the `SimData` object `sd`.

```
[t,y,outputs,inputs] = getsensmatrix(sd);
```

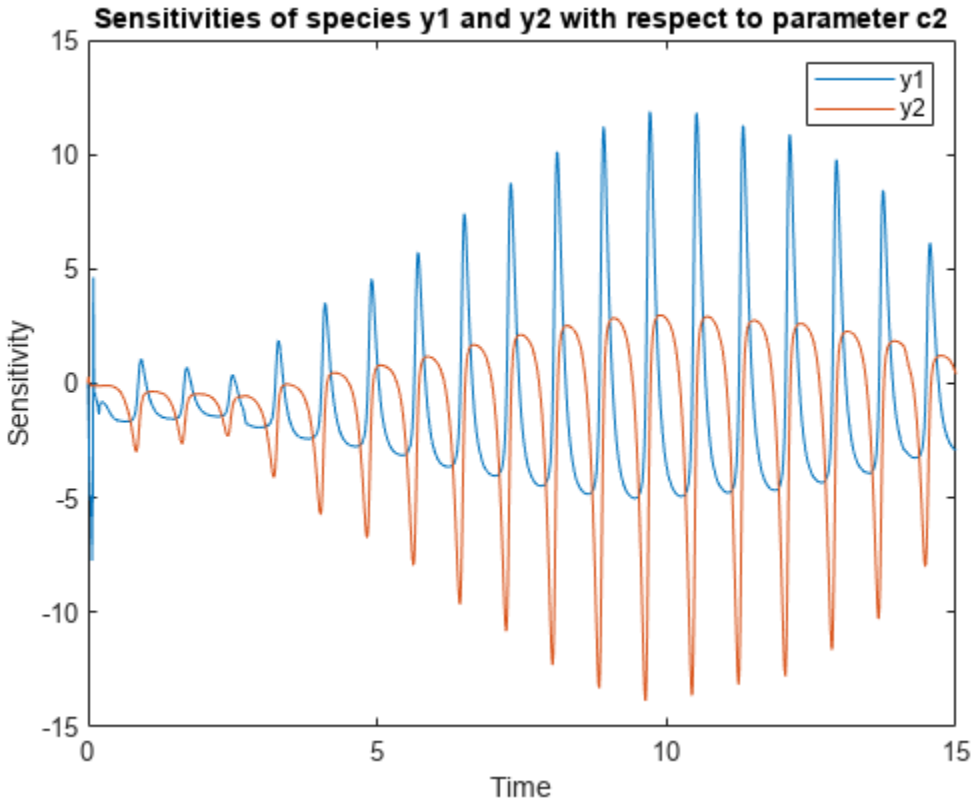
Plot the sensitivities of species `y1` and `y2` with respect to `c1`.

```
figure;
plot(t,y(:,:,1));
legend(outputs);
title('Sensitivities of species y1 and y2 with respect to parameter c1');
xlabel('Time');
ylabel('Sensitivity');
```



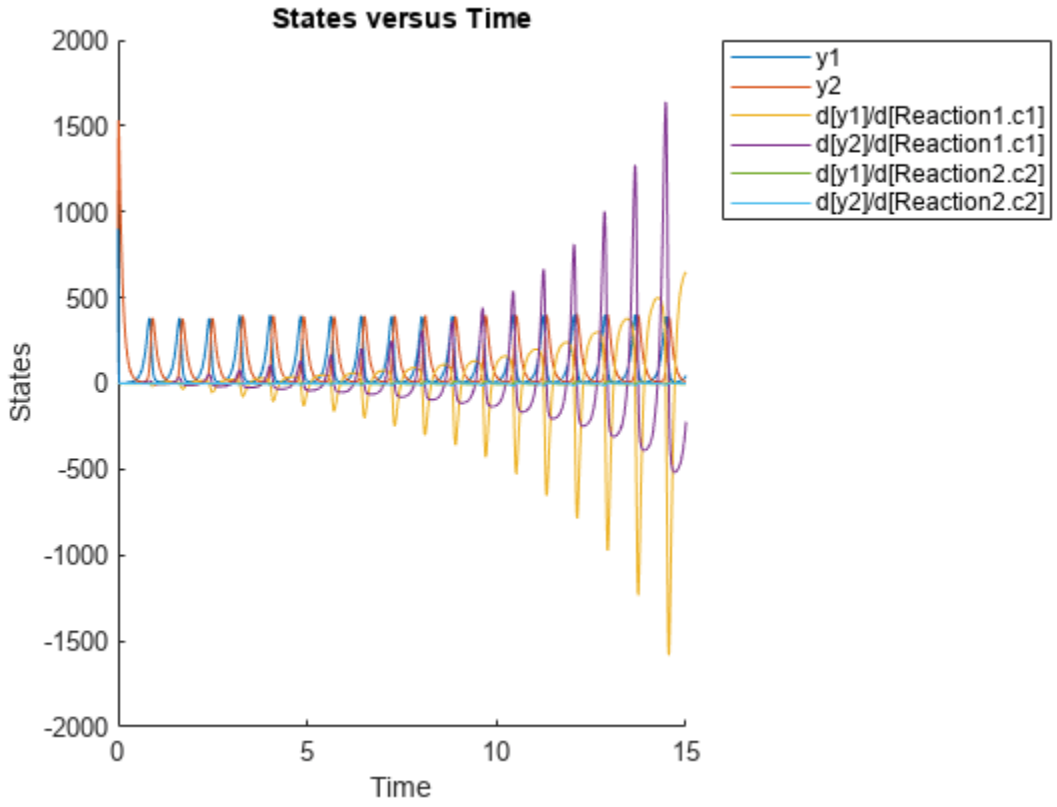
Plot the sensitivities of species `y1` and `y2` with respect to `c2`.

```
figure;
plot(t,y(:,:,2));
legend(outputs);
title('Sensitivities of species y1 and y2 with respect to parameter c2');
xlabel('Time');
ylabel('Sensitivity');
```



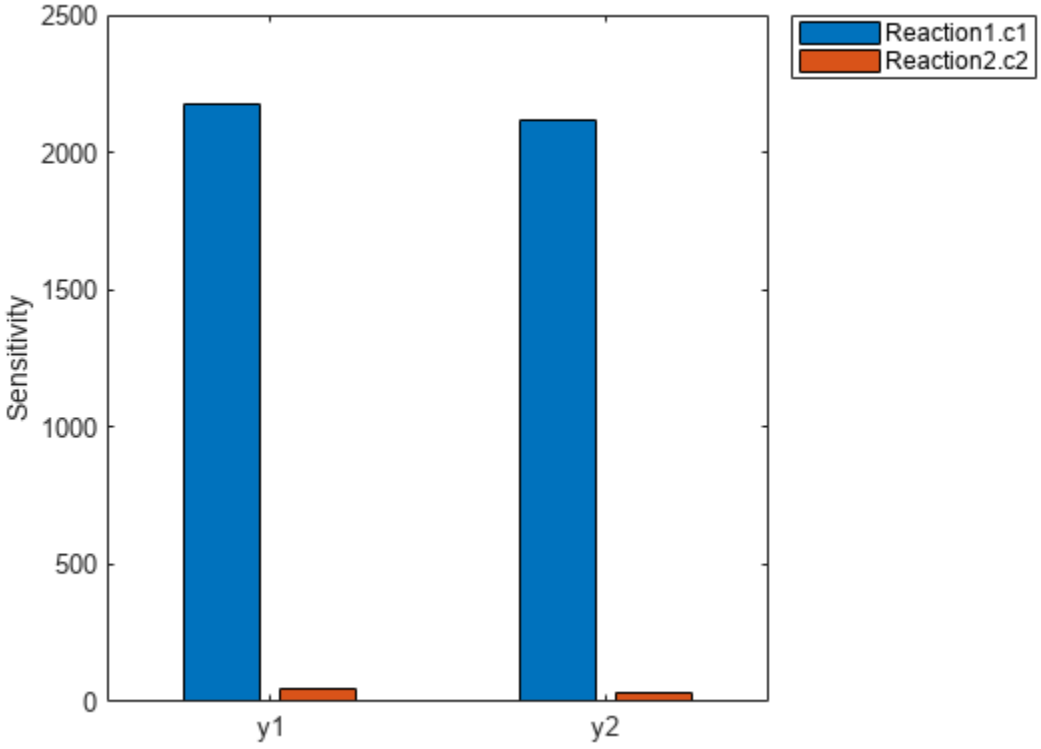
Alternatively, you can use `sbioplot`.

```
sbioplot(sd);
```



You can also plot the sensitivity matrix using the time integral for the calculated sensitivities of `y1` and `y2`. The plot indicates `y1` and `y2` are more sensitive to `c1` than `c2`.

```
[~, in, out] = size(y);
result = zeros(in, out);
for i = 1:in
    for j = 1:out
        result(i,j) = trapz(t(:),abs(y(:,i,j)));
    end
end
figure;
hbar = bar(result);
haxes = hbar(1).Parent;
haxes.XTick = 1:length(outputs);
haxes.XTickLabel = outputs;
legend(inputs,'Location','NorthEastOutside');
ylabel('Sensitivity');
```



Version History

Introduced in R2015a

See Also

`SimFunction object` | `createSimFunction` | `sbiosampleerror` | `sbiosampleparameters`

Topics

“Sensitivity Analysis in SimBiology”

simulate

Simulate exported SimBiology model

Syntax

```
[t,x,names] = simulate(model)
[t,x,names] = simulate(model,initialValues)
[t,x,names] = simulate(model,initialValues,doses)
simDataObj = simulate( ___ )
```

Description

`[t,x,names] = simulate(model)` simulates a model, using the default initial values specified by `model.InitialValues` (which are always equal to the `InitialValue` property on the corresponding `ValueInfo` object). `simulate` returns:

- `t`, time samples.
- `x`, simulation data that contain variation in the quantity of states over time.
- `names`, column labels of simulation data `x`.

You can set additional simulation options using the property `SimBiology.export.Model.SimulationOptions`.

`[t,x,names] = simulate(model,initialValues)` simulates a model, using the values specified in `initialValues` as the initial values of the simulation.

`[t,x,names] = simulate(model,initialValues,doses)` simulates the model, using the specified initial values and doses.

`simDataObj = simulate( ___ )` returns simulation data in a `SimData object` `simDataObj` using any of the input arguments in the previous syntaxes. The `simDataObj` contains time and state data, as well as metadata, such as the types and names for the reported states. You can access the time, data, and names stores in `simDataObj` using the properties `simDataObj.Time`, `simDataObj.Data`, and `simDataObj.DataNames`, respectively.

Examples

Simulate an Exported SimBiology Model

Load a sample SimBiology model object, and select the species `y1` and `y2` for simulation.

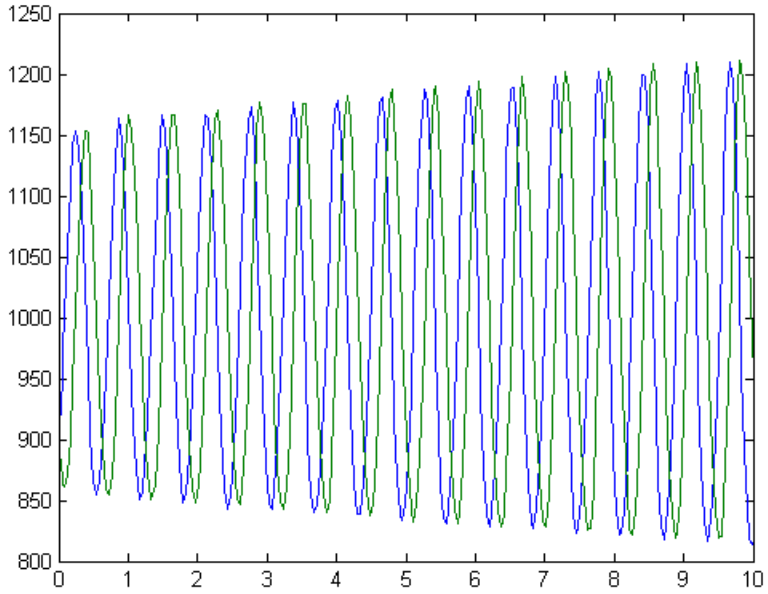
```
modelObj = sbmlimport('lotka');
modelObj.getconfigset.RuntimeOptions.StatesToLog = ...
       sbioselect(modelObj,'Name',{'y1','y2'});
```

Export the model object.

```
em = export(modelObj);
```

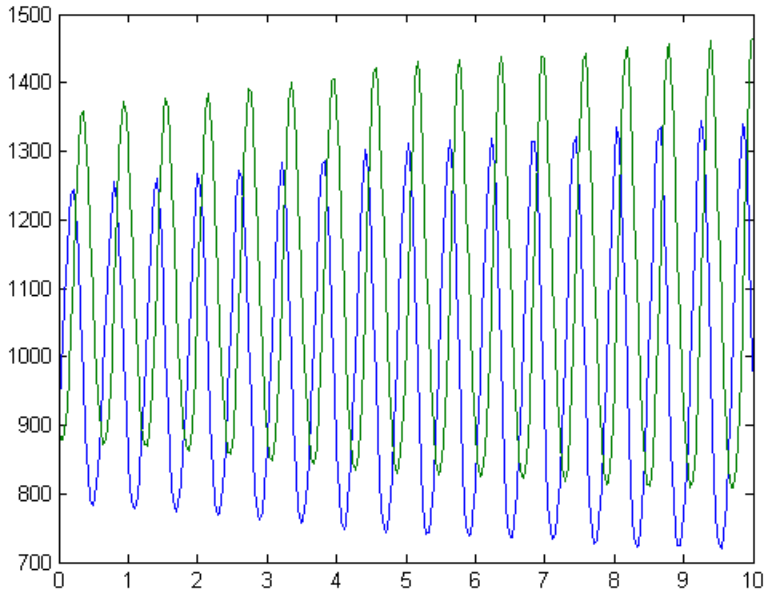
Simulate the exported model.

```
[t,y] = simulate(em);

figure()
plot(t,y)
```



Modify the initial conditions, and simulate again.

```
xIndex = em.getIndex('x');
em.InitialValues(xIndex) = em.InitialValues(xIndex)*1.1;
[t,y] = simulate(em);

figure()
plot(t,y)
```



Input Arguments

`model` — Input model
`SimBiology.export.Model` object

Input model, specified as a `SimBiology.export.Model` object.

`initialValues` — Initial values of the simulation
vector of values

Initial values of the simulation, specified as a vector of values for `simulate` to use. `initialValues` must have the same number of elements as `model.InitialValues`. If you do not specify `initialValues`, then `simulate` uses values specified in `model.InitialValues`.

`doses` — Doses used for simulation
vector of dose objects

Doses used for simulation, specified as a vector of dose objects. The input dose objects must be a subset of the doses in the exported model, as returned by `getdose`. If you do not specify `doses`, then `simulate` uses all dose objects in the exported model.

Output Arguments

`t` — Time samples
vector

Time samples, returned as an *n*-by-1 vector of time samples from the simulation, where *n* is the number of time samples.

`x` — Simulation data
matrix

Simulation data, returned as an *n*-by-*m* matrix, where *n* is the number of time samples and *m* is the number of states logged during the simulation. Each column of `x` describes the variation in the quantity of a state over time.

`names` — Names labelling the simulation data
cell array of character vectors

Names labelling the simulation data, returned as an *m*-by-1 cell array of character vectors with names labeling the rows and columns of `x`, respectively.

`simDataObj` — Simulation data
`SimData` object

Simulation data, returned as a `SimData` object containing simulation time and state data, as well as metadata, such as the types and names for the reported states.

Version History

Introduced in R2012b

See Also

`SimBiology.export.Model` | `getdose` | `SimBiology.export.ValueInfo` | `SimBiology.export.SimulationOptions` | `SimData object` | `export`

Topics

“Perform PK/PD Modeling and Simulation to Guide Dosing Strategy for Antibiotics”
“Deploy a SimBiology Exported Model”

SimBiology.gsa.Sobol

Object containing first- and total-order Sobol indices

Description

The `SimBiology.gsa.Sobol` object contains global sensitivity analysis results returned by `sbiosobol`. The object contains the computed first- and total-order Sobol indices related to the decomposition of the variance of model output with respect to sensitivity inputs [1].

Creation

Create a `SimBiology.gsa.Sobol` object using `sbiosobol`.

Properties

`ParameterSamples` — Sampled parameter values
table

This property is read-only.

Sampled parameter values, specified as a table. The parameter sample values are used for approximating the Sobol indices. For details, see “Saltelli Method to Compute Sobol Indices” on page 2-876.

Data Types: `table`

`Observables` — Names of model responses or observables
cell array of character vectors

This property is read-only.

Names of model responses or observables, specified as a cell array of character vectors.

Data Types: `char`

`Time` — Time points
column numeric vector

This property is read-only.

Time points at which Sobol indices are computed, specified as a column numeric vector. The property is `[]` if all observables are scalars.

Data Types: `double`

`SobolIndices` — Computed sobol indices
structure array

This property is read-only.

Computed sobol indices, specified as a structure array. The size of the array is `[params,observables]`, where *params* is the number of input parameters and *observables* is the number of observables.

Each structure contains the following fields.

- `Parameter` — Name of an input parameter, specified as a character vector
- `Observable` — Name of an observable, specified as a character vector
- `FirstOrder` — First-order Sobol index, specified as a numeric vector
- `TotalOrder` — Total-order Sobol index, specified as a numeric vector.

If all observables are scalar, then the `FirstOrder` and `TotalOrder` fields are specified as scalars. If some observables are scalars and some are vectors, `FirstOrder` and `TotalOrder` are numeric vectors of length `Time`. Scalar observables are scalar-expanded, where each time point has the same value.

Data Types: `struct`

`Variance` — Variance values for time courses of observables
table

This property is read-only.

Variance values for time courses of observables, specified as a table. Each column of the table contains the variance values for the time courses of each observable.

If all observables are scalars, then the `Variance` table has one row. If some observables are scalars and some are vectors, then the variances for scalar observables are scalar-expanded, where each row has the same value.

The `VariableNames` property of the table (`Variance.Properties.VariableNames`) is a cell array of character vectors containing the names of observables provided as inputs to `sbiosobol`. Names are truncated if needed. The `VariableDescriptions` property contains the untruncated observable names.

Data Types: `table`

`SimulationInfo` — Simulation information used for computing Sobol indices
structure

This property is read-only.

Simulation information, such as simulation data and parameter samples, used for computing Sobol indices, specified as a structure. The structure contains the following fields.

- `SimFunction` — `SimFunction` object used for simulating model responses or observables.
- `SimData` — `SimData` array of size `[NumberSamples,2 + params]`, where *NumberSamples* on page 1-0 is the number of samples and *params on page 1-0* is the number of input parameters.
  - The first column contains the model simulation results from `ParameterSamples`.
  - The second column contains simulation results from `SupportSamples`.
  - The rest of the columns contain simulation results from combinations of parameter values from `ParameterSamples` and `SupportSamples`. For information on retrieving the model

simulation results and samples for a specified column (index) from this `SimData` array, see `getSimulationResults`. For details on how Sobol indices are computed, see the "Saltelli Method to Compute Sobol Indices" on page 2-876.

- `OutputTimes` — Numeric column vector containing the common time vector of all `SimData` objects.
- `Bounds` — Numeric matrix of size `[params,2]`. *params* is the number of input parameters. The first column contains the lower bounds and the second column contains the upper bounds for sensitivity inputs.
- `DoseTables` — Cell array of dose tables used for the `SimFunction` evaluation. `DoseTables` is the output of `getTable(doseInput)`, where *doseInput* is the value specified for the `'Doses'` name-value pair argument in the call to `sbiosobol`, `sbiompgsa`, or `sbioelementaryeffects`. If no doses are applied, this field is set to `[]`.
- `ValidSample` — Logical matrix of size `[NumberSamples,2 + params]` indicating whether a simulation result for a particular sample failed. Resampling of the simulation data (SimData) can result in `NaN` values if the data is extrapolated. Such SimData are indicated as invalid.
- `InterpolationMethod` — Name of the interpolation method for `SimData`.
- `SamplingMethod` — Name of the sampling method used to draw `ParameterSamples`.
- `RandomState` — Structure containing the state of `rng` before drawing `ParameterSamples`.
- `SupportSamples` — Table of parameter sample values used for approximating the Sobol indices. For details, see "Saltelli Method to Compute Sobol Indices" on page 2-876.

Data Types: `struct`

Object Functions

resample	Resample Sobol indices or elementary effects to new time vector
addobservable	Compute Sobol indices or elementary effects for new observable expression
removeobservable	Remove Sobol indices or elementary effects of observables
getSimulationResults	Retrieve model simulation results and sample values used for computing Sobol indices
addsamples	Add additional samples to increase accuracy of Sobol indices or elementary effects analysis
plotData	Plot quantile summary of model simulations from global sensitivity analysis (requires Statistics and Machine Learning Toolbox)
plot	Plot first- and total-order Sobol indices and variances
bar	Create bar plot of first- and total-order Sobol indices

Examples

Perform Global Sensitivity Analysis by Computing First- and Total-Order Sobol Indices

Load the "Tumor Growth Model".

```
sbioloadproject tumor_growth_vpop_sa.sbproj
```

Get a variant with the estimated parameters and the dose to apply to the model.

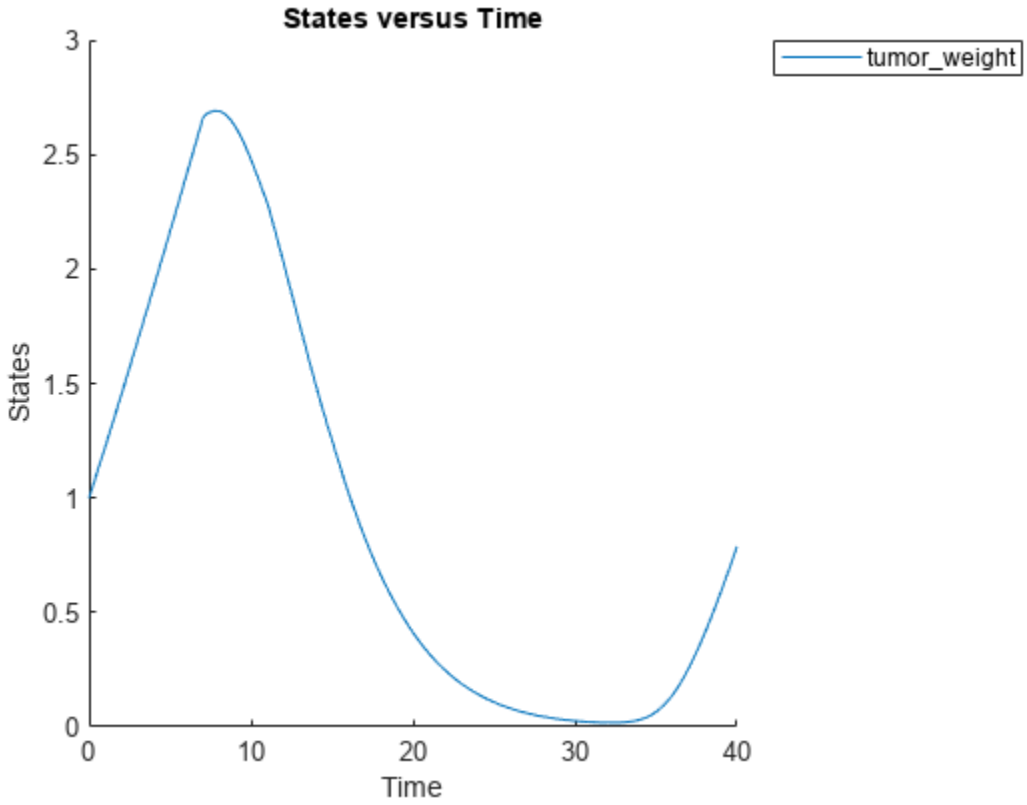
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

Get the active configset and set the tumor weight as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'tumor_weight';
```

Simulate the model and plot the tumor growth profile.

```
sbioplot(sbiosimulate(m1,cs,v,d));
```



Perform global sensitivity analysis (GSA) on the model to find the model parameters that the tumor growth is sensitive to.

First, retrieve model parameters of interest that are involved in the pharmacodynamics of the tumor growth. Define the model response as the tumor weight.

```
modelParamNames = {'L0','L1','w0','k1','k2'};
outputName = 'tumor_weight';
```

Then perform GSA by computing the first- and total-order Sobol indices using `sbiosobol`. Set `'ShowWaitBar'` to `true` to show the simulation progress. By default, the function uses 1000 parameter samples to compute the Sobol indices [1].

```
rng('default');
sobolResults = sbiosobol(m1,modelParamNames,outputName,Variants=v,Doses=d,ShowWaitBar=true)
```

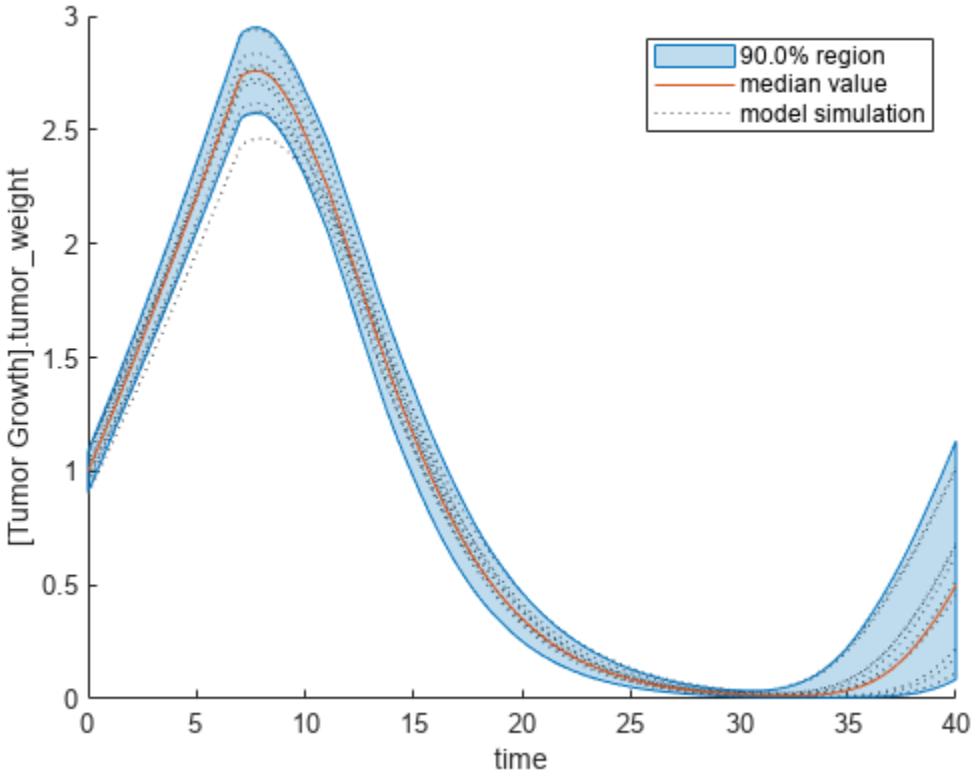
```
sobolResults =
  Sobol with properties:

                Time: [444x1 double]
        SobolIndices: [5x1 struct]
```

```
        Variance: [444x1 table]
ParameterSamples: [1000x5 table]
     Observables: {'[Tumor Growth].tumor_weight'}
  SimulationInfo: [1x1 struct]
```

You can change the number of samples by specifying the `'NumberSamples'` name-value pair argument. The function requires a total of `(number of input parameters + 2) * NumberSamples` model simulations.

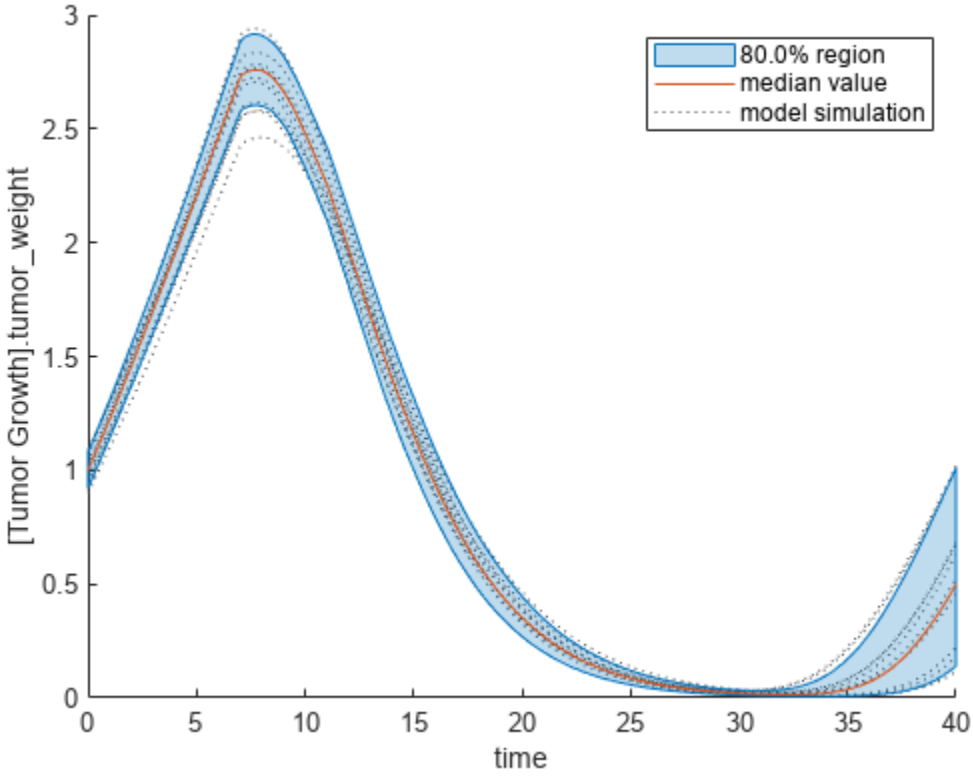
Show the mean model response, the simulation results, and a shaded region covering 90% of the simulation results.

```
plotData(sobolResults,ShowMedian=true,ShowMean=false);
```



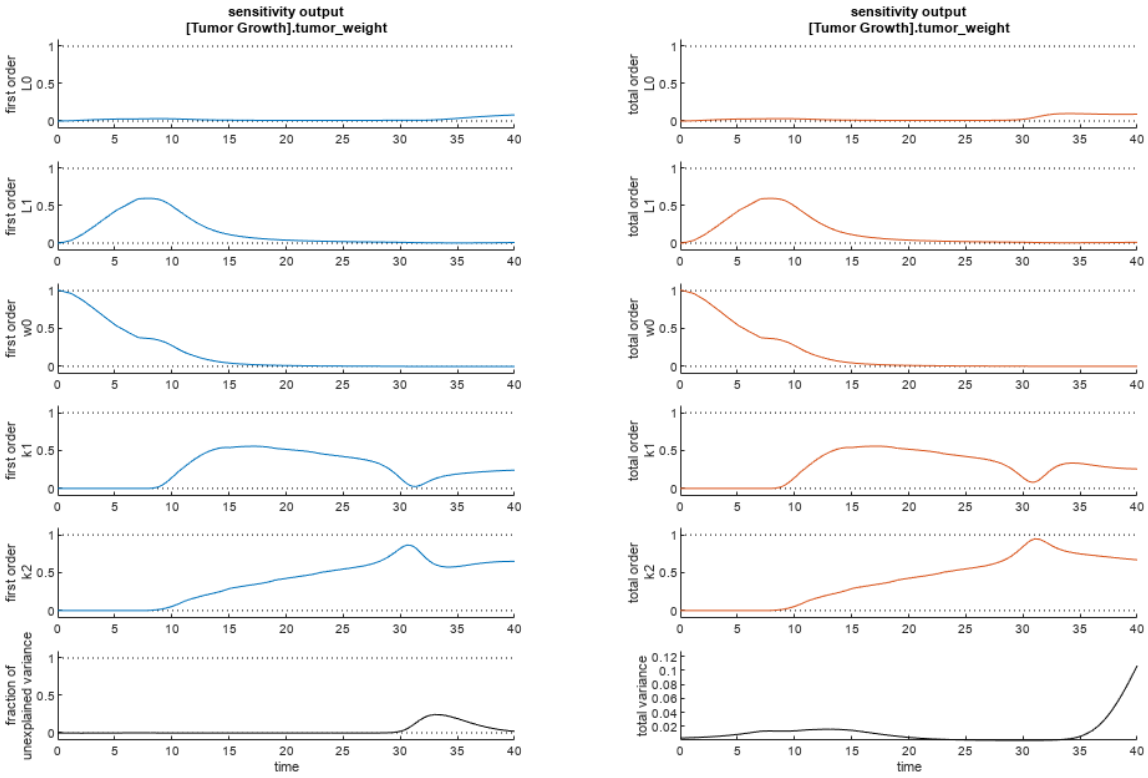
You can adjust the quantile region to a different percentage by specifying `'Alphas'` for the lower and upper quantiles of all model responses. For instance, an alpha value of 0.1 plots a shaded region between the `100 * alpha` and `100 * (1 - alpha)` quantiles of all simulated model responses.

```
plotData(sobolResults,Alphas=0.1,ShowMedian=true,ShowMean=false);
```



Plot the time course of the first- and total-order Sobol indices.

```
h = plot(sobolResults);
% Resize the figure.
h.Position(:) = [100 100 1280 800];
```

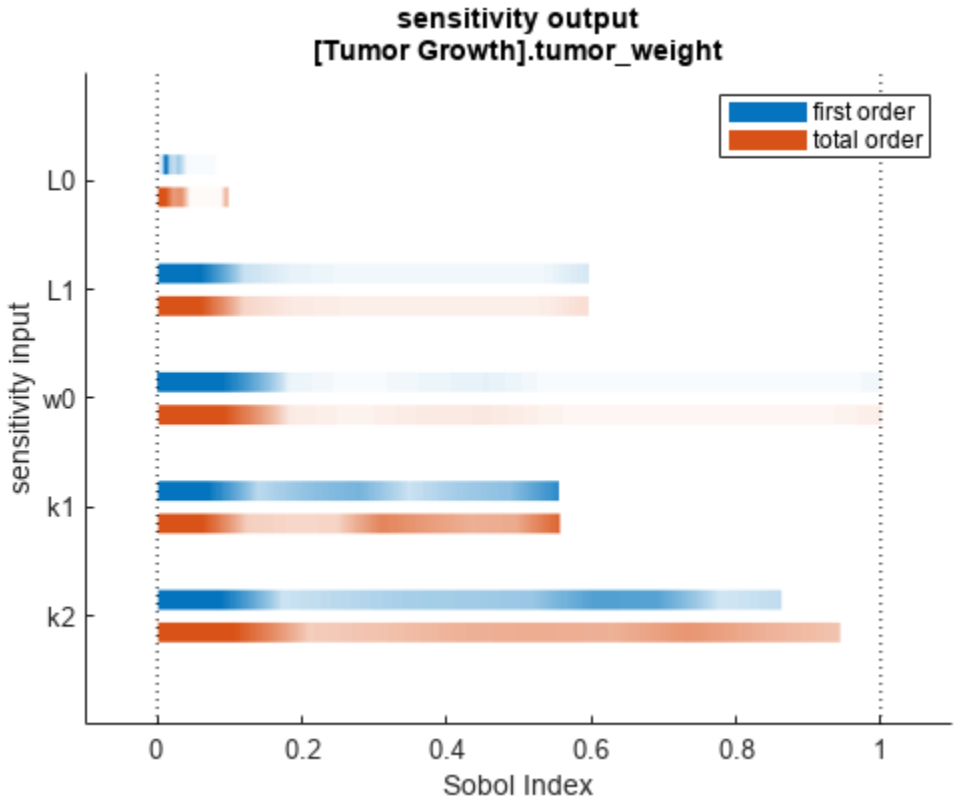


The first-order Sobol index of an input parameter gives the fraction of the overall response variance that can be attributed to variations in the input parameter alone. The total-order index gives the fraction of the overall response variance that can be attributed to any joint parameter variations that include variations of the input parameter.

From the Sobol indices plots, parameters `L1` and `w0` seem to be the most sensitive parameters to the tumor weight before the dose was applied at t = 7. But after the dose is applied, `k1` and `k2` become more sensitive parameters and contribute most to the after-dosing stage of the tumor weight. The total variance plot also shows a larger variance for the after-dose stage at t > 35 than for the before-dose stage of the tumor growth, indicating that `k1` and `k2` might be more important parameters to investigate further. The fraction of unexplained variance shows some variance at around t = 33, but the total variance plot shows little variance at t = 33, meaning the unexplained variance could be insignificant. The fraction of unexplained variance is calculated as 1 - (sum of all the first-order Sobol indices), and the total variance is calculated using `var(response)`, where `response` is the model response at every time point.

You can also display the magnitudes of the sensitivities in a bar plot. Darker colors mean that those values occur more often over the whole time course.

```
bar(sobolResults);
```



You can specify more samples to increase the accuracy of the Sobol indices, but the simulation can take longer to finish. Use `addsamples` to add more samples. For example, if you specify 1500 samples, the function performs `1500 * (2 + number of input parameters)` simulations.

```
gsaMoreSamples = addsamples(gsaResults,1500)
```

The “SimulationInfo” on page 2-0 property of the result object contains various information for computing the Sobol indices. For instance, the model simulation data (SimData) for each simulation using a set of parameter samples is stored in the `SimData` field of the property. This field is an array of `SimData` objects.

```
sobolResults.SimulationInfo.SimData
```

```
SimBiology SimData Array : 1000-by-7

Index:    Name:         ModelName:         DataCount:
1           -           Tumor Growth Model 1
2           -           Tumor Growth Model 1
3           -           Tumor Growth Model 1
...
7000        -           Tumor Growth Model 1
```

You can find out if any model simulation failed during the computation by checking the `ValidSample` field of `SimulationInfo`. In this example, the field shows no failed simulation runs.

```
all(sobolResults.SimulationInfo.ValidSample)
```

```
ans = 1x7 logical array

   1   1   1   1   1   1   1
```

`SimulationInfo.ValidSample` is a table of logical values. It has the same size as `SimulationInfo.SimData`. If `ValidSample` indicates that any simulations failed, you can get more information about those simulation runs and the samples used for those runs by extracting information from the corresponding column of `SimulationInfo.SimData`. Suppose that the fourth column contains one or more failed simulation runs. Get the simulation data and sample values used for that simulation using `getSimulationResults`.

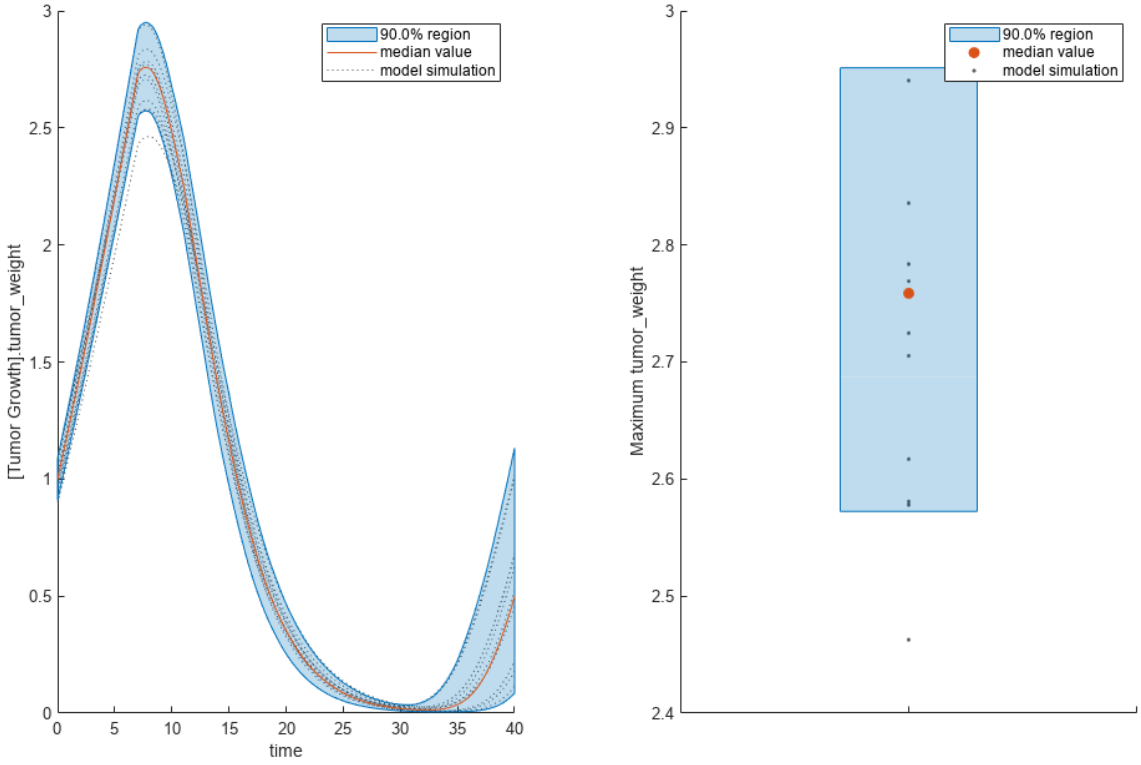
```
[samplesUsed,sd,validruns] = getSimulationResults(sobolResults,4);
```

You can add custom expressions as observables and compute Sobol indices for the added observables. For example, you can compute the Sobol indices for the maximum tumor weight by defining a custom expression as follows.

```
% Suppress an information warning that is issued during simulation.
warnSettings = warning('off', 'SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
% Add the observable expression.
sobolObs = addobservable(sobolResults,'Maximum tumor_weight','max(tumor_weight)','Units','gram');
```

Plot the computed simulation results showing the 90% quantile region.

```
h2 = plotData(sobolObs,ShowMedian=true,ShowMean=false);
h2.Position(:) = [100 100 1280 800];
```



You can also remove the observable by specifying its name.

```
gsaNoObs = removeobservable(sobolObs,'Maximum tumor_weight');
```

Restore the warning settings.

```
warning(warnSettings);
```

More About

Saltelli Method to Compute Sobol Indices

`sbiosobol` implements the Saltelli method [1] to compute Sobol indices.

Consider a SimBiology model response Y expressed as a mathematical model $Y = f(X_1, X_2, X_3, ..., X_k)$, where X_i is a model parameter and `i = 1,…,k`.

The first-order Sobol index (S_i) gives the fraction of the overall response variance `V(Y)` that can be attributed to variations in X_i alone. S_i is defined as follows.

$$S_i = \frac{V_{X_i}\left(E_{X\sim i}(Y|X_i)\right)}{V(Y)}$$

The total-order Sobol index (S_{Ti}) gives the fraction of the overall response variance `V(Y)` that can be attributed to any joint parameter variations that include variations of X_i. S_{Ti} is defined as follows.

$$S_{Ti} = 1 - \frac{V_{X\sim i}\left(E_{X_i}(Y|X\sim i)\right)}{V(Y)} = \frac{E_{X\sim i}\left(V_{X_i}(Y|X\sim i)\right)}{V(Y)}$$

To compute individual values for Y corresponding to samples of parameters X_1, X_1, ..., X_k, consider two independent sampling matrices A and B.

$$A = \begin{pmatrix} X_{11} & X_{12} & \dots & X_{1k} \\ X_{21} & X_{22} & \dots & X_{2k} \\ \dots & \dots & \dots & \dots \\ X_{n1} & X_{n2} & \dots & X_{nk} \end{pmatrix}$$

$$B = \begin{pmatrix} X'_{11} & X'_{12} & \dots & X'_{1k} \\ X'_{21} & X'_{22} & \dots & X'_{2k} \\ \dots & \dots & \dots & \dots \\ X'_{n1} & X'_{n2} & \dots & X'_{nk} \end{pmatrix}$$

n is the sample size. Each row of the matrices A and B corresponds to one parameter sample set, which is a single realization of model parameter values.

Estimates for S_i and S_{Ti} are obtained from model simulation results using sample values from the matrices A, B, and A_B^i, which is a matrix where all columns are from A except the ith column, which is from B for `i = 1, 2, …, params`.

$$A_B^i = \begin{pmatrix} X_{11} & X_{12} & \dots & X'_{1i} & \dots & X_{1k} \\ X_{21} & X_{22} & \dots & X'_{2i} & \dots & X_{2k} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ X_{n1} & X_{n2} & \dots & X'_{ni} & \dots & X_{nk} \end{pmatrix}$$

The formulas to approximate the first- and total-order Sobol indices are as follows.

$$\widehat{S}_i = \frac{\frac{1}{n}\sum_{j=1}^{n} f(B)_j \left(f\left(A_B^i\right)_j - f(A)_j \right)}{V(Y)}$$

$$\widehat{S}_{Ti} = \frac{\frac{1}{2n}\sum_{j=1}^{n} \left(f(A)_j - f\left(A_B^i\right)_j \right)^2}{V(Y)}$$

`f(A)`, `f(B)`, and $f\left(A_B^i\right)_j$ are the model simulation results using the parameter sample values from matrices A, B, and A_B^i.

The matrix A corresponds to the `ParameterSamples` property of the Sobol results object (`resultsObj.ParameterSamples`). The matrix B corresponds to the `SupportSamples` property (`resultsObj.SimulationInfo.SupportSamples`).

The A_B^i matrices are stored in the `SimData` structure of the `SimulationInfo` on page 2-0 property (`resultsObj.SimulationInfo.SimData`). The size of `SimulationInfo.SimData` is *`NumberSamples`*`-by-`*`params`*` + 2`, where *NumberSamples* on page 1-0 is the number of samples and *param on page 1-0* is the number of input parameters. The number of columns is `2 +` *`params`* because the first column of `SimulationInfo.SimData` contains the model simulation results using the sample matrix A. The second column contains simulation results using `SupportSamples`, which is another sample matrix B. The rest of the columns contain simulation results using A_B^1, A_B^2, ..., A_B^i, ..., A_B^{params}. See `getSimulationResults` to retrieve the model simulation results and samples for a specified ith index (A_B^i) from the `SimulationInfo.SimData` array.

Tips

The results object can contain a significant amount of simulation data (SimData). The size of the object exceeds `(1 + number of observables) * number of output time points * (2 + number of parameters) * number of samples * 8` bytes. For example, if you have one observable, 500 output time points, 8 parameters, and 100,000 samples, the object size is `(1 + 1) * 500 * (2 + 8) * 100000 * 8` bytes = 8 GB. If you need to save such large objects, use this syntax:

```
save(fileName,variableName,'-v7.3');
```

For details, see MAT-file version.

Version History

Introduced in R2020a

References

[1] Saltelli, Andrea, Paola Annoni, Ivano Azzini, Francesca Campolongo, Marco Ratto, and Stefano Tarantola. “Variance Based Sensitivity Analysis of Model Output. Design and Estimator for the Total Sensitivity Index.” *Computer Physics Communications* 181, no. 2 (February 2010): 259–70. https://doi.org/10.1016/j.cpc.2009.09.018.

See Also

`sbiosobol` | `sbiompgsa` | `Observable`

Topics

“Sensitivity Analysis in SimBiology”

SolverOptions

SimBiology model solver options

Description

The `SolverOptions` object holds the model solver options, and it is a property of the `configset` object.

Changing the `SolverType` property of `configset` changes the options specified in the `SolverOptions` object (or property).

You can add a number of `configset` objects with different `SolverOptions` to the model object with the `addconfigset` method. Only one `configset` object in the model object can be `Active on page 3-2` at any given time. To change or update any of properties of the `SolverOptions` property object, use dot notation syntax: *`csObj`*`.SolverOptions.`*`PropertyName`* `= value`, where *csObj* is the configset object of a SimBiology model and *PropertyName* is the name of the property of `SolverOptions`.

Creation

Use dot notation syntax on a `configset` object to return the property object. That is, *`csObj`*`.SolverOptions` returns the `SolverOptions` property object of the `configset` object *csObj*.

Properties

`AbsoluteTolerance` — Absolute error tolerance applied to state value during simulation
`1e-6` (default) | positive scalar

Absolute error tolerance applied to a state value during simulation, specified as a positive scalar. This property is available for the ODE solvers (`ode15s`, `ode23t`, `ode45`, and `sundials`).

SimBiology uses `AbsoluteTolerance` to determine the largest allowable absolute error at any step in a simulation. How the software uses `AbsoluteTolerance` to determine this error depends on whether the `AbsoluteToleranceScaling` property is enabled. For details, see “Selecting Absolute Tolerance and Relative Tolerance for Simulation”.

Data Types: `double`

`AbsoluteToleranceScaling` — Control scaling of absolute error tolerance during simulation
`true` or 1 (default) | `false` or 0

Control scaling of absolute error tolerance during simulation, specified as a numeric or logical 1 (`true`) or 0 (`false`).

When `AbsoluteToleranceScaling` is enabled (by default), each state has its own absolute tolerance that can increase over the course of simulation. Sometimes the automatic scaling is

inadequate for models that have kinetics at largely different scales. For example, the reaction rate of one reaction can be on the order of 10^{22}, while another is 0.1. By turning off `AbsoluteToleranceScaling`, you might be able to simulate the model. For more tips, see "Troubleshooting Simulation Problems".

Data Types: `double` | `logical`

`AbsoluteToleranceStepSize` — Initial guess for time step size for scaling of absolute error tolerance
`[]` (default) | positive scalar

Initial guess for time step size for scaling of absolute error tolerance, specified as a positive scalar. The property uses the time units specified by the `TimeUnits` property of the corresponding `configset` object.

Data Types: `double`

`ErrorTolerance` — Error tolerance of explicit or implicit tau stochastic solver
`3e-2` (default) | positive scalar between 0 and 1

Error tolerance of an explicit or implicit tau stochastic solver, specified as a positive scalar between 0 and 1.

The explicit and implicit tau solvers automatically chooses a time interval (tau) such that the relative change in the propensity function for each reaction is less than the user-specified error tolerance. A propensity function describes the probability that the reaction will occur in the next smallest time interval, given the conditions and constraints. If the error tolerance is too large, there may not be a solution to the problem and that could lead to an error. If the error tolerance is small, the solver will take more steps than when the error tolerance is large leading to longer simulation times. The error tolerance should be adjusted depending upon the problem, but a good value for the error tolerance is between 1% and 5%.

Data Types: `double`

`LogDecimation` — Specify frequency to log stochastic simulation output
1 (default) | positive integer

Specify the frequency to log stochastic simulation output, specified as a positive integer. This property is available only for stochastic solvers (`ssa`, `expltau`, and `impltau`).

Use `LogDecimation` to specify how frequently you want to record the output of the simulation. For example, if you set `LogDecimation` to 1, for the command `[t,x] = sbiosimulate(modelObj)`, at each simulation step the time will be logged in *t* and the quantity of each logged species will be logged as a row in *x*. If `LogDecimation` is 10, then every 10th simulation step will be logged in *t* and *x*.

Data Types: `double`

`MaxIterations` — Maximum number of iterations for nonlinear solver in implicit tau
15 (default) | positive integer

Maximum number of iterations for the nonlinear solver in implicit tau (`impltau`), specified as a positive integer.

The implicit tau solver in SimBiology internally uses a nonlinear solver to solve a set of algebraic nonlinear equations at every simulation step. Starting with an initial guess at the solution, the

nonlinear solver iteratively tries to find the solution to the algebraic equations. The closer the initial guess is to the solution, the fewer the iterations the nonlinear solver will take before it finds a solution. `MaxIterations` specifies the maximum number of iterations the nonlinear solver should take before it issues a *failed to converge* error. If you get this error during simulation, try increasing `MaxIterations`.

Data Types: `double`

`MaxStep` — Maximum step size
`[]` (default) | positive scalar

Maximum step size taken by an ODE solver, specified as a positive scalar. This property sets an upper bound on the size of any step taken by the solver. This property is available only for the ODE solvers (`ode15s`, `ode23t`, `ode45`, and `sundials`).

By default, `MaxStep` is set to `[]`, which is equivalent to setting the value to infinity.

If the differential equation has periodic coefficients or solutions, it might be a good idea to set `MaxStep` to some fraction (such as 1/4) of the period. This guarantees that the solver does not enlarge the time step too much and step over a period of interest. For more information, see `odeset`.

Data Types: `double`

`OutputTimes` — Times to log deterministic simulation output
`[]` (default) | vector of nonnegative values

Times to log deterministic (ODE) simulation output, specified as a vector of nonnegative monotonically increasing values. This property specifies the times during an ODE simulation that data is recorded. This property is available only for the ODE solvers (`ode15s`, `ode23t`, `ode45`, and `sundials`).

By default, the property is set to `[]`, which instructs SimBiology to log data every time the solver takes a step. The unit for this property is specified by the `TimeUnits` property of the corresponding `configset` object.

If the criteria set in the `MaximumWallClock` property causes a simulation to stop before all time values in `OutputTimes` are reached, then no data is recorded for the latter time values.

The `OutputTimes` property can also control when a simulation stops:

- The last value in `OutputTimes` overrides the `StopTime` property as criteria for stopping a simulation.
- The length of `OutputTimes` overrides the `MaximumNumberOfLogs` property as criteria for stopping a simulation.

Data Types: `double`

`RandomState` — State of random number generator
`[]` (default) | integer

State of the random number generator for stochastic solvers, specified as an integer. This property is available only for these solvers: `ssa`, `expltau`, and `impltau`.

SimBiology uses a pseudorandom number generator. The sequence of numbers generated is determined by the state of the generator, which can be specified by the `RandomState` property. If

`RandomState` is set to an integer *J*, the random number generator is initialized to its *J*th state. The random number generator can generate all the floating-point numbers in the closed interval [2^{-53}, $1-2^{-53}$]. Theoretically, it can generate over 2^{1492} values before repeating itself. But for a given state, the sequence of numbers generated will be the same. To change the sequence, change `RandomState`. SimBiology resets the state at startup. The default value of `RandomState` is `[]`.

Data Types: `double`

`RelativeTolerance` — Allowable error tolerance relative to state value during a simulation
`1e-3` (default) | positive scalar less than 1

Allowable error tolerance relative to a state value during a simulation, specified as a positive scalar less than 1. This property is available only for the ODE solvers (`ode15s`, `ode23t`, `ode45`, and `sundials`).

The `RelativeTolerance` property specifies the allowable error tolerance relative to the state vector at each simulation step. The state vector contains values for all the state variables, for example, amounts for all the species.

For example, if you set the `RelativeTolerance` to `1e-2`, you are specifying that an error of 1% relative to each state value is acceptable at each simulation step. For details, see "Selecting Absolute Tolerance and Relative Tolerance for Simulation".

Data Types: `double`

`SensitivityAnalysis` — Flag to enable or disable sensitivity analysis
`false` or 0 (default) | `true` or 1

Flag to enable or disable sensitivity analysis, specified as a numeric or logical 1 (`true`) or 0 (`false`).

This property lets you compute the time-dependent sensitivities of all the species states defined by the `StatesToLog` property with respect to the `Inputs` that you specify in the SensitivityAnalysisOptions property of the configuration set object.

SimBiology always uses the SUNDIALS solver to perform sensitivity analysis on a model, regardless of what you have selected as the SolverType in the configuration set.

For more information on setting up sensitivity analysis, see SensitivityAnalysisOptions. For a description of sensitivity analysis calculations, see "Sensitivity Analysis in SimBiology".

Note Models containing the following active components do not support sensitivity analysis:

- Nonconstant compartments
- Algebraic rules
- Events

Data Types: `double` | `logical`

`Type` — SimBiology object type
`'solveroptions'` (default)

This property is read-only.

SimBiology object type, specified as `'solveroptions'`.

Data Types: `char`

Examples

Change Solver Options and Simulation Options

The solver and simulation options are stored in the configuration set (`configset` object) of a SimBiology model. Solver options contain settings such as relative and absolute tolerances. Simulation options are settings such as `MaximumNumberOfLogs` and `MaximumWallClock`.

Depending on the solver type, the available solver options differ. Inspect the default ODE solver.

```
m1 = sbiomodel("m1");
cs = getconfigset(m1);
cs.SolverType
```

```
ans =
'ode15s'
```

Change the ODE solver to `ode45`, which is one of the supported ODE solvers. For details, see “Choosing a Simulation Solver”.

```
cs.SolverType = "ode45";
cs.SolverOptions
```

```
ans =
   SimBiology Solver Settings: (ode)

     AbsoluteTolerance:            1e-06
     AbsoluteToleranceScaling:     true
     RelativeTolerance:            0.001
     SensitivityAnalysis:          false
```

If you change a common option for the ODE solvers, that change is persistant across all the ODE solver types. For example, change the `AbsoluteTolerance` of the current solver.

```
cs.SolverOptions.AbsoluteTolerance = 1e-3
```

```
cs =
   Configuration Settings - default (active)
     SolverType:                   ode45
     StopTime:                     10

   SolverOptions:
     AbsoluteTolerance:            0.001
     AbsoluteToleranceScaling:     true
     RelativeTolerance:            0.001
     SensitivityAnalysis:          false

   RuntimeOptions:
     StatesToLog:                  all

   CompileOptions:
     UnitConversion:               false
```

```
     DimensionalAnalysis:          true

   SensitivityAnalysisOptions:
     Inputs:                       0
     Outputs:                      0
```

Change the solver to `ode23t` and check the value of `AbsoluteTolerance`, which is still the value you set previously.

```
cs.SolverType = "ode23t";
cs.SolverOptions.AbsoluteTolerance

ans = 1.0000e-03
```

If you specify a stochastic solver as the solver type, the associated solver options are updated automatically, and these options are different from the ODE solver options. For details on the supported stochastic solvers, see “Stochastic Solvers”.

Change to the explicit tau-leaping algorithm.

```
cs.SolverType = "expltau"

cs =
   Configuration Settings - default (active)
     SolverType:                   expltau
     StopTime:                     10

   SolverOptions:
     ErrorTolerance:               0.03
     LogDecimation:                1

   RuntimeOptions:
     StatesToLog:                  all

   CompileOptions:
     UnitConversion:               false
     DimensionalAnalysis:          true

   SensitivityAnalysisOptions:
     Inputs:                       0
     Outputs:                      0
```

You can also change the simulation settings, which are the properties of the `configset` object. For example, change the maximum number of logs criterion to decide when to stop the simulation. Setting it to 1 returns simulated values of the model quantities immediately after applying initial and repeated assignment rules of the model. If you change the value to 2, and the subsequent simulation fails with the integration error, then it probably indicates an error with the assignment rules. For more tips on how to use these simulation settings to troubleshoot some of the common simulation problems, see “Troubleshooting Simulation Problems”.

```
cs.MaximumNumberOfLogs = 1;
```

Specify Times to Log Deterministic Simulation Output

Specify the times during a deterministic (ODE) simulation that data is recorded.

Create a `model` object named `cell` and save it in a variable named `modelObj`.

```
modelObj  = sbiomodel('cell');
```

Retrieve the configuration set from `modelObj` and save it in a variable named `configsetObj`.

```
configsetObj = getconfigset(modelObj);
```

Specify to log output every second for the first `10` seconds of the simulation. Do this by setting the `OutputTimes` property of the `SolverOptions` property of `ConfigsetObj`.

```
sopt = configsetObj.SolverOptions;
sopt.OutputTimes = [1:10];
sopt.OutputTimes
```

```
ans = 10×1

     1
     2
     3
     4
     5
     6
     7
     8
     9
    10
```

When you simulate `modelObj`, output is logged every second for the first `10` seconds of the simulation. Also, the simulation stops after the 10th log.

Version History

Introduced in R2006b

See Also

Topics

“Selecting Absolute Tolerance and Relative Tolerance for Simulation”
“Troubleshooting Simulation Problems”

Species object

Object containing species information

Description

The SimBiology species object represents a *species*, which is a chemical or entity that participates in reactions, for example, `DNA`, `ATP`, `Pi`, `creatine`, `G-Protein`, or `Mitogen-Activated Protein Kinase (MAPK)`. Species amounts can vary or remain constant during a simulation. The name of each species must be unique within the same compartment and the species object cannot have the same name as any `observable` object in the model.

To add species that participate in reactions, add the reaction to the model. The process of adding the reaction to the model creates a compartment object (*`unnamed`*) and the necessary species objects.

Alternatively, create and add a species object to a compartment object, using the `addspecies` method at the command line.

See “Property Summary” on page 2-886 for links to species property reference pages. Properties define the characteristics of an object. Use the `get` and `set` commands to list object properties and change their values at the command line. You can graphically change object properties in the graphical user interface.

Constructor Summary

addspecies (model, compartment)	Create species object and add to compartment object within model object

Method Summary

Methods for species objects

copyobj	Copy SimBiology object and its children
delete	Delete SimBiology object
display	Display summary of SimBiology object
findUsages	Find out how a species, parameter, or compartment is used in a model
get	Get SimBiology object properties
move	Move SimBiology species or parameter object to new parent
rename	Rename object and update expressions
set	Set SimBiology object properties

Property Summary

Properties for species objects

BoundaryCondition	Indicate species boundary condition
Constant	Specify variable or constant species amount, parameter value, or compartment capacity
ConstantAmount	Specify variable or constant species amount
InitialAmount	Species initial amount
InitialAmountUnits	Species initial amount units
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Tag	Specify label for SimBiology object
Type	Display SimBiology object type
Units	Units for species amount, parameter value, compartment capacity, observable expression
UserData	Specify data to associate with object
Value	Value of species, compartment, or parameter object

See Also

`Compartment object`, `Configset object`, `KineticLaw object`, `Model object`, `Parameter object`, `Reaction object`, `Root object`, `Rule object`

Version History

Introduced in R2006b

Unit object

Hold information about user-defined unit

Description

The SimBiology unit object holds information about user-defined units. To create a unit, create the unit object and add the unit to the library using the `sbioaddtolibrary` function.

Use the unit object property `Composition` to specify the composition of your units. See “Property Summary” on page 2-888 for links to unit object property reference pages.

Properties define the characteristics of an object. Use the `get` and `set` commands to list object properties and change their values at the command line. You can graphically change unit object properties in the SimBiology desktop. For more information, see “SimBiology Model Component Libraries”.

Constructor Summary

sbiounit	Create user-defined unit

Method Summary

delete	Delete SimBiology object
display	Display summary of SimBiology object
findUsages	Find out how a unit or unit prefix is used
get	Get SimBiology object properties
rename	Rename object and update expressions
set	Set SimBiology object properties

Property Summary

Composition	Unit composition
Multiplier	Relationship between defined unit and base unit
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Tag	Specify label for SimBiology object
Type	Display SimBiology object type
UserData	Specify data to associate with object

See Also

`AbstractKineticLaw object`, `KineticLaw object`, `Model object`, `Parameter object`, `Reaction object`, `Root object`, `Rule object`, `Species object`, `UnitPrefix object`

Version History

Introduced in R2008a

UnitPrefix object

Hold information about user-defined unit prefix

Description

The SimBiology unit prefix object holds information about user-defined unit prefixes. To create a unit prefix, create the unit prefix object and add the unit prefix to the library using the `sbioaddtolibrary` function.

Use the unit prefix object property `Exponent`, to specify the exponent of your unit prefix. See “Property Summary” on page 2-890 for links to unit prefix object property reference pages.

Properties define the characteristics of an object. Use the `get` and `set` commands to list object properties and change their values at the command line. You can graphically change unit prefix object properties in the SimBiology desktop. For more information, see “SimBiology Model Component Libraries”.

Constructor Summary

sbiounitprefix	Create user-defined unit prefix

Method Summary

delete	Delete SimBiology object
display	Display summary of SimBiology object
findUsages	Find out how a unit or unit prefix is used
get	Get SimBiology object properties
rename	Rename object and update expressions
set	Set SimBiology object properties

Property Summary

Exponent	Exponent value of unit prefix
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Tag	Specify label for SimBiology object
Type	Display SimBiology object type
UserData	Specify data to associate with object

See Also

`AbstractKineticLaw object`, `KineticLaw object`, `Model object`, `Parameter object`, `Reaction object`, `Root object`, `Rule object`, `Species object`, `Unit object`

Version History

Introduced in R2008a

updateEntry

Update entry contents from `SimBiology.Scenarios` object

Syntax

```
sObj = updateEntry(sObj,entryNameOrIndex,Name,Value)
sObj = updateEntry(sObj,entryIndex,subIndex,Name,Value)
```

Description

`sObj = updateEntry(sObj,entryNameOrIndex,Name,Value)` updates the contents of the entry (or subentry on page 2-799) `entryNameOrIndex` as specified by one or more name-value pair arguments. You must specify at least one name-value pair argument.

`sObj = updateEntry(sObj,entryIndex,subIndex,Name,Value)` updates the contents of the subentry `subIndex` as specified by one or more name-value arguments. You must specify at least one name-value pair argument.

Examples

Generate Different Simulation Scenarios for Glucose-Insulin Response

Load the model of glucose-insulin response. For details about the model, see the **Background** section in “Simulate the Glucose-Insulin Response”.

```
sbioloadproject('insulindemo','m1');
```

The model contains different parameter values and initial conditions that represents different insulin impairments (such as Type 2 diabetes, low insulin sensitivity, and so on) stored in five variants.

```
variants = getvariant(m1)
```

```
variants =
   SimBiology Variant Array

   Index:  Name:             Active:
   1       Type 2 diabetic   false
   2       Low insulin se... false
   3       High beta cell... false
   4       Low beta cell ... false
   5       High insulin s... false
```

Suppress an informational warning that is issued during simulations.

```
warnSettings = warning('off','SimBiology:DimAnalysisNotDone_MatlabFcn_Dimensionless');
```

Select a dose that represents a single meal of 78 grams of glucose.

```
singleMeal = sbioselect(m1,'Name','Single Meal');
```

Create a `Scenarios` object to represent different initial conditions combined with the dose. That is, create a `scenario` object where each variant is paired (or combined) with the dose, for a total of five simulation scenarios.

```
sObj = SimBiology.Scenarios;
add(sObj,'cartesian','variants',variants);
add(sObj,'cartesian','dose',singleMeal)
```

```
ans =
  Scenarios (5 scenarios)

                  Name            Content          Number
                ________    ____________________    ______

    Entry 1     variants    SimBiology variants      5
    x Entry 2   dose        SimBiology dose          1

  See also Expression property.
```

`sObj` contains two entries. Use the `generate` function to combine the entries and generate five scenarios. The function returns a scenarios table, where each row represents a scenario and each column represents an entry of the `Scenarios` object.

```
scenariosTbl = generate(sObj)
```

```
scenariosTbl=5×2 table
           variants                    dose
    ____________________    ____________________________

    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
```

Change the entry name of the first entry.

```
rename(sObj,1,'Insulin Impairements')
```

```
ans =
  Scenarios (5 scenarios)

                       Name                Content          Number
                ____________________    ____________________    ______

    Entry 1     Insulin Impairements    SimBiology variants      5
    x Entry 2   dose                    SimBiology dose          1

  See also Expression property.
```

Create a `SimFunction` object to simulate the generated scenarios. Use the `Scenarios` object as the input and specify the plasma glucose and insulin concentrations as reponses (outputs of the function to be plotted). Specify `[]` for the dose input argument since the `Scenarios` object already has the dosing information.

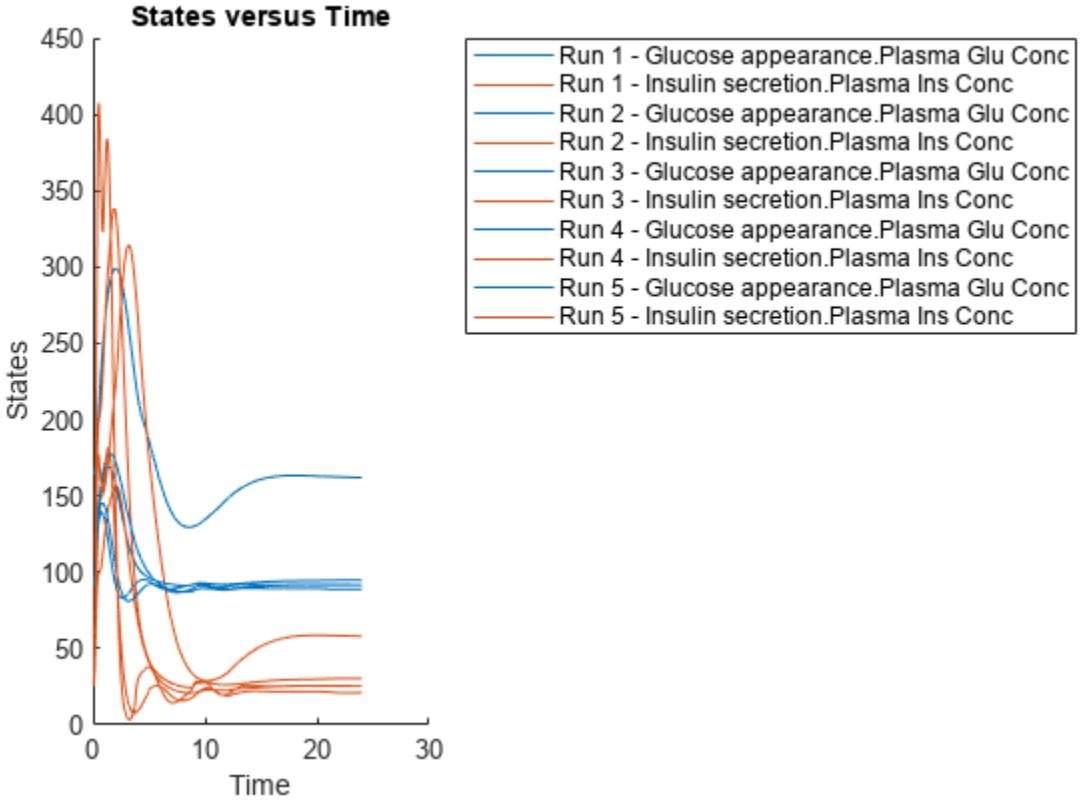
```
f = createSimFunction(m1,sObj,{'[Plasma Glu Conc]','[Plasma Ins Conc]'},[])
```

```
f =
SimFunction

Parameters:

            Name              Value        Type                        Units
    ______________________    ______    ____________    ____________________________________

    {'Plasma Volume (Glu)'  }      1.88    {'parameter'}    {'deciliter'
    {'k1'                   }     0.065    {'parameter'}    {'1/minute'
    {'k2'                   }     0.079    {'parameter'}    {'1/minute'
    {'Plasma Volume (Ins)'  }      0.05    {'parameter'}    {'liter'
    {'m1'                   }      0.19    {'parameter'}    {'1/minute'
    {'m2'                   }     0.484    {'parameter'}    {'1/minute'
    {'m4'                   }    0.1936    {'parameter'}    {'1/minute'
    {'m5'                   }    0.0304    {'parameter'}    {'minute/picomole'
    {'m6'                   }    0.6469    {'parameter'}    {'dimensionless'
    {'Hepatic Extraction'   }       0.6    {'parameter'}    {'dimensionless'
    {'kmax'                 }    0.0558    {'parameter'}    {'1/minute'
    {'kmin'                 }     0.008    {'parameter'}    {'1/minute'
    {'kabs'                 }    0.0568    {'parameter'}    {'1/minute'
    {'kgri'                 }         0    {'parameter'}    {'1/minute'
    {'f'                    }       0.9    {'parameter'}    {'dimensionless'
    {'a'                    }         0    {'parameter'}    {'1/milligram'
    {'b'                    }      0.82    {'parameter'}    {'dimensionless'
    {'c'                    }         0    {'parameter'}    {'1/milligram'
    {'d'                    }      0.01    {'parameter'}    {'dimensionless'
    {'kp1'                  }       2.7    {'parameter'}    {'milligram/minute'
    {'kp2'                  }    0.0021    {'parameter'}    {'1/minute'
    {'kp3'                  }     0.009    {'parameter'}    {'(milligram/minute)/(picomole/liter)
    {'kp4'                  }    0.0618    {'parameter'}    {'(milligram/minute)/picomole'
    {'ki'                   }    0.0079    {'parameter'}    {'1/minute'
    {'[Ins Ind Glu Util]'   }         1    {'parameter'}    {'milligram/minute'
    {'Vm0'                  }    2.5129    {'parameter'}    {'milligram/minute'
    {'Vmx'                  }     0.047    {'parameter'}    {'(milligram/minute)/(picomole/liter)
    {'Km'                   }    225.59    {'parameter'}    {'milligram'
    {'p2U'                  }    0.0331    {'parameter'}    {'1/minute'
    {'K'                    }      2.28    {'parameter'}    {'picomole/(milligram/deciliter)'
    {'alpha'                }      0.05    {'parameter'}    {'1/minute'
    {'beta'                 }      0.11    {'parameter'}    {'(picomole/minute)/(milligram/decili
    {'gamma'                }       0.5    {'parameter'}    {'1/minute'
    {'ke1'                  }    0.0005    {'parameter'}    {'1/minute'
    {'ke2'                  }       339    {'parameter'}    {'milligram'
    {'Basal Plasma Glu Conc'}     91.76    {'parameter'}    {'milligram/deciliter'
    {'Basal Plasma Ins Conc'}     25.49    {'parameter'}    {'picomole/liter'

Observables:

          Name              Type              Units
    ____________________    __________    ____________________

    {'[Plasma Glu Conc]'}    {'species'}    {'milligram/deciliter'}
    {'[Plasma Ins Conc]'}    {'species'}    {'picomole/liter'     }

Dosed:

    TargetName       TargetDimension
    __________    ____________________
```

```
    {'Dose'}    {'Mass (e.g., gram)'}

TimeUnits: hour
```

Simulate the model for 24 hours and plot the simulation data. The data contains five runs, where each run represents a scenario in the Scenarios object.

```
sd = f(sObj,24);
sbioplot(sd)
```




```
ans =
  Axes (SbioPlot) with properties:

            XLim: [0 30]
            YLim: [0 450]
          XScale: 'linear'
          YScale: 'linear'
    GridLineStyle: '-'
         Position: [0.0920 0.1100 0.2956 0.8150]
            Units: 'normalized'

  Show all properties
```

If you have Statistics and Machine Learning Toolbox™, you can also draw sample values for model quantities from various probability distributions. For instance, suppose that the parameters `Vmx` and

kp3, which are known for the low and high insulin sensitivity, follow the lognormal distribution. You can generate sample values for these parameters from such a distribution, and perform a scan to explore model behavior.

Define the lognormal probability distribution object for Vmx.

```
pd_Vmx = makedist('lognormal')
```

```
pd_Vmx =
  LognormalDistribution

  Lognormal distribution
       mu = 0
    sigma = 1
```

By definition, the parameter mu is the mean of logarithmic values. To vary the parameter value around the base (model) value of the parameter, set mu to `log(model_value)`. Set the standard deviation (*sigma*) to 0.2. For a small *sigma* value, the mean of a lognormal distribtion is approximately equal to `log(model_value)`. For details, see "Lognormal Distribution" (Statistics and Machine Learning Toolbox).

```
Vmx = sbioselect(m1,'Name','Vmx');
pd_Vmx.mu = log(Vmx.Value);
pd_Vmx.sigma = 0.2
```

```
pd_Vmx =
  LognormalDistribution

  Lognormal distribution
       mu = -3.05761
    sigma =      0.2
```

Similarly define the probability distribution for kp3.

```
pd_kp3 = makedist('lognormal');
kp3 = sbioselect(m1,'Name','kp3');
pd_kp3.mu = log(kp3.Value);
pd_kp3.sigma = 0.2
```

```
pd_kp3 =
  LognormalDistribution

  Lognormal distribution
       mu = -4.71053
    sigma =      0.2
```

Now define a joint probability distribution to draw sample values for Vmx and kp3, with a rank correlation to specify some correlation between these two parameters. Note that this correlation assumption is for the illustration purposes of this example only and may not be biologically relevant.

First remove the variants entry (entry 1) from sObj.

```
remove(sObj,1)
```

```
ans =
  Scenarios (1 scenarios)
```

```
                Name         Content         Number
                ____    _________________    ______

    Entry 1     dose    SimBiology dose       1

  See also Expression property.
```

Add an entry that defines the joint probability distribution with a rank correlation matrix.

```
add(sObj,'cartesian',["Vmx","kp3"],[pd_Vmx, pd_kp3],'RankCorrelation',[1,0.5;0.5,1])
```

```
ans =
  Scenarios (2 scenarios)

                    Name           Content              Number
                    ____    ________________________    ___________

    Entry 1         dose    SimBiology dose             1
    x (Entry 2.1    Vmx     Lognormal distribution      2 (default)
    + Entry 2.2)    kp3     Lognormal distribution      2 (default)

  See also Expression property.
```

By default, the number of samples to draw from the joint distribution is set to 2. Increase the number of samples.

```
updateEntry(sObj,2,'Number',50)
```

```
ans =
  Scenarios (50 scenarios)

                    Name           Content              Number
                    ____    ________________________    ______

    Entry 1         dose    SimBiology dose               1
    x (Entry 2.1    Vmx     Lognormal distribution        50
    + Entry 2.2)    kp3     Lognormal distribution        50

  See also Expression property.
```

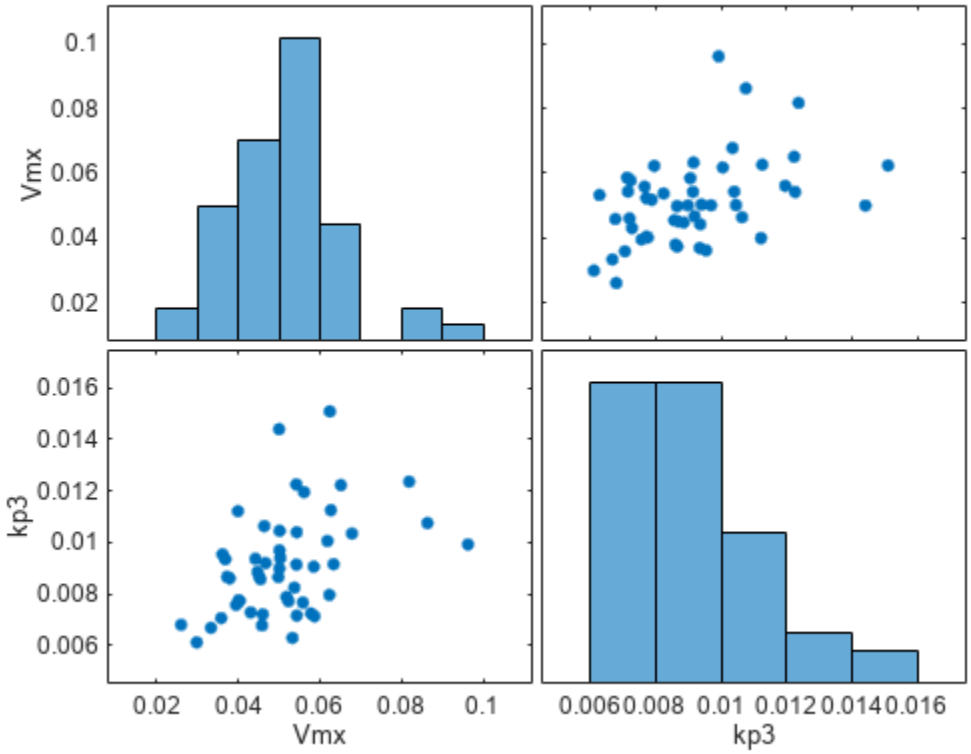
Verify that the `Scenarios` object can be simulated with the model. The `verify` function throws an error if any entry does not resolve uniquely to an object in the model or the entry contents have inconsistent lengths (sample sizes). The function throws a warning if multiple entries resolve to the same object in the model.

```
verify(sObj,m1)
```

Generate the simulation scenarios. Plot the sample values using `plotmatrix`. You can see the value of `Vmx` is varied around its model value 0.047 and that of `kp3` around 0.009.

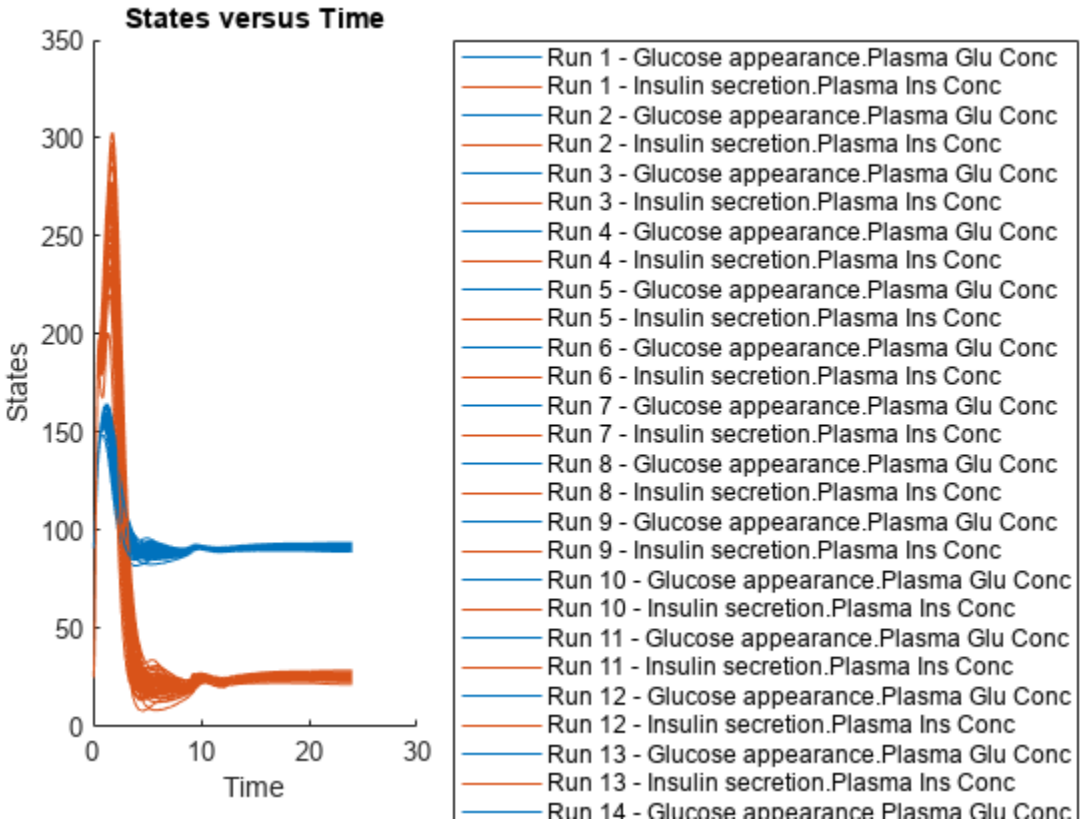
```
sTbl = generate(sObj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl.Vmx,sTbl.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
```

```
ax(2,1).XLabel.String = "Vmx";
ax(2,2).XLabel.String = "kp3";
```



Simulate the scenarios using the same SimFunction you created previously. You do not need to create a new SimFunction object even though the Scenarios object has been updated.

```
sd2 = f(sObj,24);
sbioplot(sd2);
```



By default, SimBiology uses the random sampling method. You can change it to the Latin hypercube sampling (or sobol or halton) for a more systematic space-filling approach.

```
entry2struct = getEntry(sObj,2)
```

```
entry2struct = struct with fields:
                Name: {'Vmx'  'kp3'}
             Content: [2x1 prob.LognormalDistribution]
              Number: 50
    RankCorrelation: [2x2 double]
          Covariance: []
      SamplingMethod: 'random'
    SamplingOptions: [0x0 struct]
```

```
entry2struct.SamplingMethod = 'lhs'
```

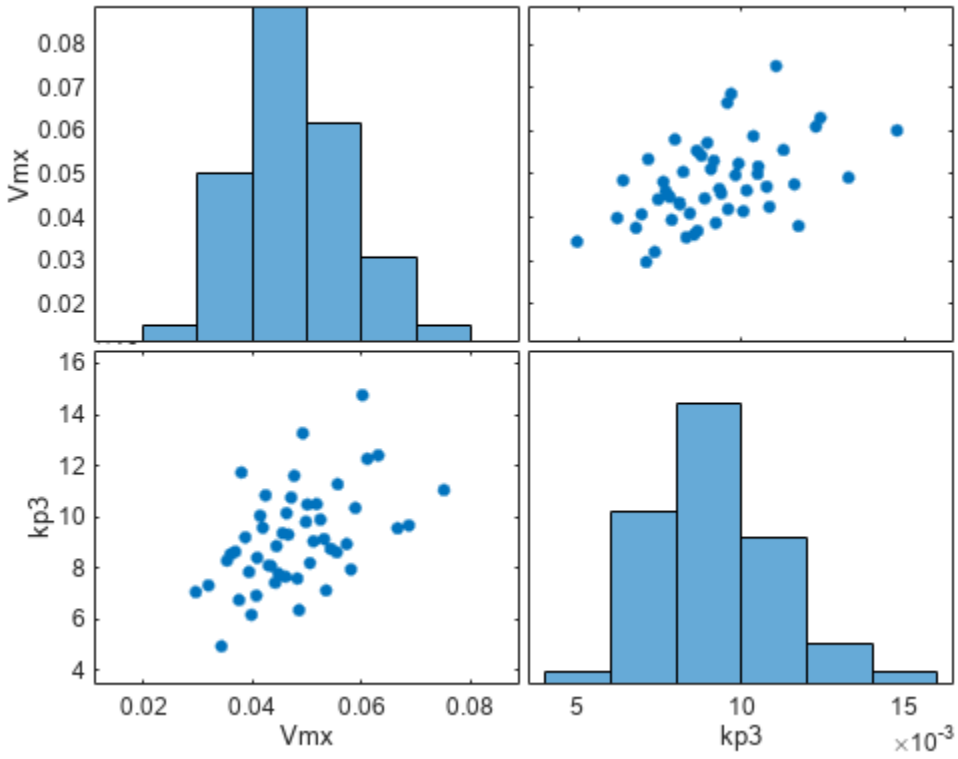
```
entry2struct = struct with fields:
                Name: {'Vmx'  'kp3'}
             Content: [2x1 prob.LognormalDistribution]
              Number: 50
    RankCorrelation: [2x2 double]
          Covariance: []
      SamplingMethod: 'lhs'
    SamplingOptions: [0x0 struct]
```

You can now use the updated structure to modify entry 2.

```
updateEntry(sObj,2,entry2struct)

ans =
  Scenarios (50 scenarios)

                    Name           Content             Number
                    ____    ____________________      ______

    Entry 1         dose    SimBiology dose             1
    x (Entry 2.1    Vmx     Lognormal distribution      50
    + Entry 2.2)    kp3     Lognormal distribution      50

  See also Expression property.
```

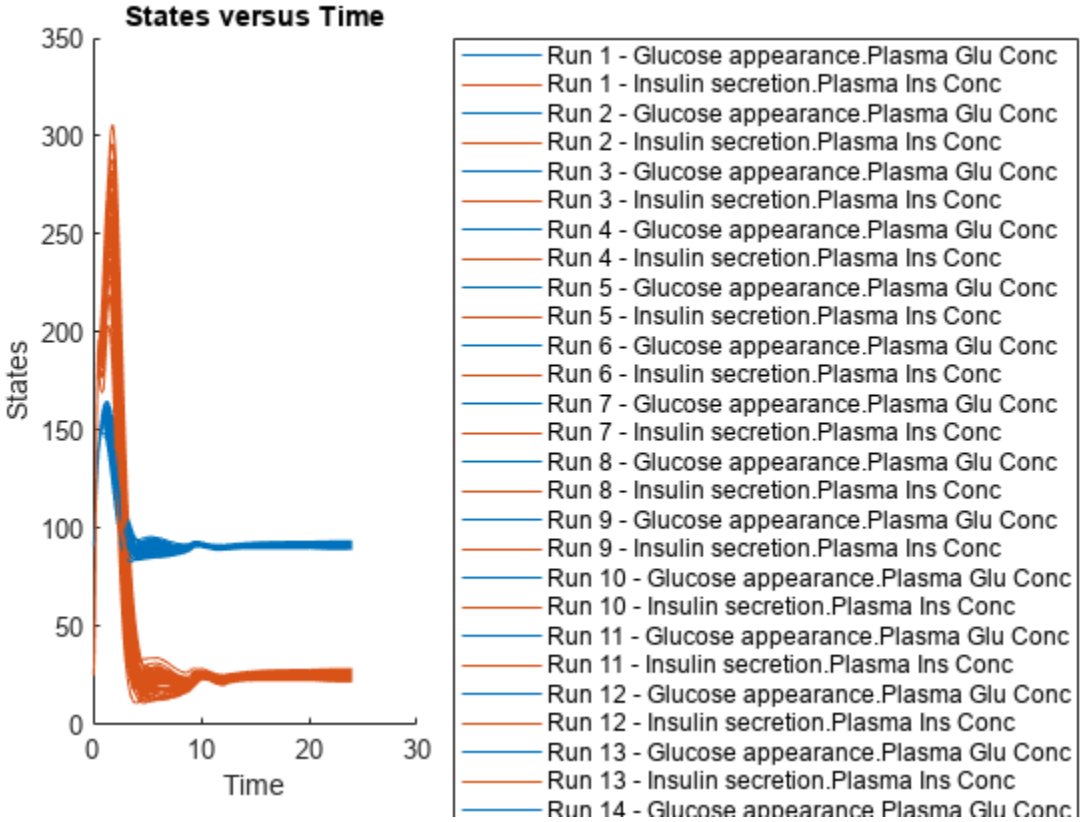
Visualize the sample values.

```
sTbl2 = generate(sObj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl2.Vmx,sTbl2.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
ax(2,1).XLabel.String = "Vmx";
ax(2,2).XLabel.String = "kp3";
```



Simulate the scenarios.

```
sd3 = f(sObj,24);
sbioplot(sd3);
```



Restore warning settings.

```
warning(warnSettings);
```

Input Arguments

`sObj` — Simulation scenarios

`SimBiology.Scenarios` object

Simulation scenarios, specified as a `SimBiology.Scenarios` object.

`entryNameOrIndex` — Entry name or index

character vector | string | scalar positive integer

Entry name or index, specified as a character vector, string, or scalar positive integer. You can also specify the name of a subentry.

If you are specifying an index, it must be smaller than or equal to the number of entries in the object.

Data Types: `double` | `char` | `string`

`entryIndex` — Entry index

scalar positive integer

Entry index, specified as a scalar positive integer. The entry index must be smaller than or equal to the number of entries in the object.

Data Types: `double`

`subIndex` — Entry subindex
scalar positive integer

Entry subindex, specified as a scalar positive integer. The subindex must be smaller than or equal to the number of subentries in the entry.

Data Types: `double`

Name-Value Pair Arguments

Specify one or more comma-separated pairs of `Name,Value` arguments. `Name` is the argument name and `Value` is the corresponding value. `Name` must appear inside quotes. You can specify several name and value pair arguments in any order as `Name1,Value1,...,NameN,ValueN`.

Note You must specify at least one name-value argument.

Instead of using name-value arguments, you can also use a structure containing the corresponding filed names and values. For instance, you can get such a structure by using the `getEntry` function.

Example: `object = updateEntry(object,1,'Name','k1','Content',[0.4,0.5,0.6])` updates the name of entry 1 to `'k1'` and its values to `[0.4,0.5,0.6]`.

For Entries Defining Numeric Vectors, Doses, or Variants

`Name` — New entry name
character vector | string

New entry name, specified as the comma-separated pair consisting of `'Name'` and a character vector or string.

Example: `'Name','k_forward'`

Data Types: `char` | `string`

`Content` — New content
numeric vector | vector of doses | vector of variants

New content, specified as the comma-separated pair consisting of `'Content'` and a numeric vector, vector of `RepeatDose` or `ScheduleDose` objects, or vector of `variant` objects.

Example: `'Content',[0.1 0.5 0.9]`

Data Types: `double`

For Entries Defining Multivariate Distributions

`Name` — New entry names
character vector | string | string vector | cell array of character vectors

New entry names, specified as the comma-separated pair consisting of `'Name'` and a character vector, string, string vector, or cell array of character vectors.

Example: `["kel","Cl"]`

Data Types: `char` | `string` | `cell`

`Content` — Probability distributions
vector of probability distribution objects

Probability distributions, specified as the comma-separated pair consisting of `'Content'` and a vector of probability distribution objects. If the entry has only one distribution, specify a scalar probability distribution object. Use `makedist` to create the object.

Example: `'Content',[pd1,pd2]`

`Mean` — Expected values
numeric vector

Expected values of normal distributions, specified as the comma-separated pair consisting of `'Mean'` and a numeric vector. If the entry has only one distribution, specify a numeric scalar. This name-value pair is valid for normal distributions only.

The number of mean values must be equal to the number of distributions specified in `'Content'`.

Example: `'Mean',[0.5,0.8]`

Data Types: `double`

`Number` — Number of samples
`[]` (default) | positive scalar

Number of samples to draw from probability distributions, specified as the comma-separated pair consisting of `'Number'` and a positive scalar. The default value `[]` means that the function infers the number of samples from other entries. If the number cannot be inferred, the number is set to `2`.

Example: `'Number',5`

`RankCorrelation` — Rank correlation matrix
`[]` (default) | numeric matrix

Rank correlation matrix for the joint probability distribution, specified as the comma-separated pair consisting of `'RankCorrelation'` and a numeric matrix. The default behavior is that when both `'RankCorrelation'` and `'Covariance'` are set to `[]`, `SimBiology.Scenarios` draws uncorrelated samples from the joint probability distribution.

You cannot specify `'RankCorrelation'` if `'Covariance'` is set. The number of columns in the matrix must match the number of specified distributions. The matrix must be symmetric with diagonal values of 1. All of its eigenvalues must also be positive.

Example: `'RankCorrelation',[1 0.3;0.3 1]`

`Covariance` — Covariance matrix
`[]` (default) | numeric matrix

Covariance matrix for the joint probability distribution, specified as the comma-separated pair consisting of `'Covariance'` and a numeric matrix. The default behavior is that if both `'RankCorrelation'` and `'Covariance'` are set to `[]`, `SimBiology.Scenarios` draws uncorrelated samples from the joint probability distribution. You cannot specify `'Covariance'` if you specify `'RankCorrelation'`.

You can specify the covariance matrix for normal distributions only. The number of columns in the matrix must match the number of specified distributions. All of its eigenvalues must also be nonnegative.

Example: `'Covariance',[0.25 0.15;0.15 0.25]`

`SamplingMethod` — Sampling method
`'random'` (default) | `'lhs'` | `'copula'` | `'sobol'` | `'halton'`

Sampling method, specified as the comma-separated pair consisting of `'SamplingMethod'` and a character vector or string. Depending on whether probability distributions with `'RankCorrelation'` or normal distributions with `'Covariance'` are specified, the sampling techniques differ.

If an entry contains a (joint) normal distribution with `Covariance` specified, the sampling methods are:

- `'random'` – Draw random samples from the specified normal distribution using `mvnrnd`.
- `'lhs'` – Draw Latin hypercube samples from the specified normal distributions using `lhsnorm`. For details, see “Generating Quasi-Random Numbers” (Statistics and Machine Learning Toolbox).

If an entry contains a (joint) distribution with no `Covariance` specified, the sampling methods are:

- `'random'` – Draw random samples from the specified probability distributions using `random`.
- `'lhs'` – Draw Latin hypercube samples from the specified probability distributions using an algorithm similar to `lhsdesign`. This approach is a more systematic space-filling approach than random sampling. For details, see “Generating Quasi-Random Numbers” (Statistics and Machine Learning Toolbox).
- `'copula'` – Draw random samples using a copula (Statistics and Machine Learning Toolbox). Use this option to impose correlations between samples using copulas.
- `'sobol'` – Use the sobol sequence (`sobolset`) which is transformed using the inverse cumulative distribution function (`icdf`) of the specified probability distributions. Use this method for highly systematic space-filling. For details, see “Generating Quasi-Random Numbers” (Statistics and Machine Learning Toolbox).
- `'halton'` – Use the halton sequence (`haltonset`) which is transformed using the inverse cumulative distribution function (`icdf`) of the specified probability distributions. For details, see “Generating Quasi-Random Numbers” (Statistics and Machine Learning Toolbox).

If no `Covariance` is specified, `SimBiology.Scenarios` essentially performs two steps. The first step is to generate samples using one of the above sampling methods. For `lhs`, `sobol`, and `halton` methods, the generated uniform samples are transformed to samples from the specified distribution using the inverse cumulative distribution function `icdf`. Then, as the second step, the samples are correlated using the Iman-Conover algorithm if `RankCorrelation` is specified. For `random`, the samples are drawn directly from the specified distributions and the samples are then correlated using the Iman-Conover algorithm.

Example: `'SamplingMethod','lhs'`

`SamplingOptions` — Options for sampling method
struct

Options for the sampling method, specified as a scalar struct. The options differ depending on the sampling method: `sobol`, `halton`, or `lhs`.

For `sobol` and `halton`, specify each field name and value of the structure according to each name-value argument of the `sobolset` or `haltonset` function. SimBiology uses the default value of `1` for the `Skip` argument for both methods. For all other name-value arguments, the software uses the

same default values of `sobolset` or `haltonset`. For instance, set up a structure for the `Leap` and `Skip` options with nondefault values as follows.

```
s1.Leap = 50;
s1.Skip = 0;
```

For `lhs`, there are three samplers that support different sampling options.

- If you specify a covariance matrix, SimBiology uses `lhsnorm` for sampling. `SamplingOptions` argument is not allowed.
- Otherwise, use the field name `UseLhsdesign` to select a sampler.
  - If the value is `true`, SimBiology uses `lhsdesign`. You can use the name-value arguments of `lhsdesign` to specify the field names and values.
  - If the value is `false` (default), SimBiology uses a nonconfigurable Latin hypercube sampler that is different from `lhsdesign`. This sampler does not require Statistics and Machine Learning Toolbox. `SamplingOptions` cannot contain any other options, except `UseLhsdesign`.

For instance, set up a structure to use `lhsdesign` with the `Criterion` and `Iterations` options.

```
s2.UseLhsdesign  = true;
s2.Criterion     = "correlation";
s2.Iterations    = 10;
```

Example: `'SamplingOptions',struct("Skip",5)`

Data Types: `struct`

For Subentries of Multivariate Distributions

`Name` — New subentry name

character vector | string

New subentry name, specified as the comma-separated pair consisting of `'Name'` and a character vector or string.

Example: `'Name','pd2'`

Data Types: `char` | `string`

`Content` — Probability distribution

probability distribution object

Probability distribution, specified as the comma-separated pair consisting of `'Content'` and a probability distribution object. Use `makedist` to create such an object.

Example: `'Content',pd2`

`Mean` — Expected value

numeric scalar

Expected value of a normal distribution, specified as the comma-separated pair consisting of `'Mean'` and a numeric scalar. This name-value pair is valid for normal distributions only.

Example: `'Mean',0.5`

Data Types: `double`

Output Arguments

`sObj` — Simulation scenarios
`Scenarios` object

Simulation scenarios, returned as a `Scenarios` object.

Version History

Introduced in R2019b

See Also

`SimBiology.Scenarios` | `SimFunction object` | `createSimFunction (model)`

Topics
“SimBiology.Scenarios Terminology” on page 2-799
“Combine Simulation Scenarios in SimBiology”

updateobservable

Update observable expressions or units in SimData

Syntax

```
sdout = updateobservable(sdin,obsNames,obsExpressions)
sdout = updateobservable(sdin,obsNames,obsExpressions,'Units',units)
sdout = updateobservable(sdin,obsNames,'Units',units)
```

Description

`sdout = updateobservable(sdin,obsNames,obsExpressions)` returns a new `SimData` object (or array of objects) `sdout` after copying the input `SimData` `sdin` and recalculating the observables using updated expressions. `obsNames` and `obsExpressions` are the existing observable names and their corresponding expressions to update, respectively. The number of expressions must match the number of observable names.

`sdout = updateobservable(sdin,obsNames,obsExpressions,'Units',units)` recalculates the observables `obsNames` using the updated expressions `obsExpressions` and the specified `units`. The number of units must match the number of observable names.

`sdout = updateobservable(sdin,obsNames,'Units',units)` recalculates the observables `obsNames` using the specified `units`. The number of units must match the number of observable names.

Examples

Calculate Statistics After Model Simulation Using Observables

Load the “Target-Mediated Drug Disposition (TMDD) Model”.

```
sbioloadproject tmdd_with_TO.sbproj
```

Set the target occupancy (`TO`) as a response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'TO';
```

Get the dosing information.

```
d = getdose(m1,'Daily Dose');
```

Scan over different dose amounts using a `SimBiology.Scenarios` object. To do so, first parameterize the `Amount` property of the dose. Then vary the corresponding parameter value using the `Scenarios` object.

```
amountParam = addparameter(m1,'AmountParam','Units',d.AmountUnits);
d.Amount = 'AmountParam';
d.Active = 1;
doseSamples = SimBiology.Scenarios('AmountParam',linspace(0,300,31));
```

Create a `SimFunction` to simulate the model. Set `T0` as the simulation output.

```
% Suppress informational warnings that are issued during simulation.
warning('off','SimBiology:SimFunction:DOSES_NOT_EMPTY');
f = createSimFunction(m1,doseSamples,'T0',d)
```

```
f =
SimFunction

Parameters:

         Name          Value        Type           Units
    _______________    _____    _____________    ___________

    {'AmountParam'}      1      {'parameter'}    {'nanomole'}

Observables:

     Name         Type              Units
    ______    _____________    _________________

    {'T0'}    {'parameter'}    {'dimensionless'}

Dosed:

      TargetName                TargetDimension                      Amount          AmountValue    A
    _______________    ____________________________________    _______________    ___________    _

    {'Plasma.Drug'}    {'Amount (e.g., mole or molecule)'}    {'AmountParam'}          1          -

TimeUnits: day
```

```
warning('on','SimBiology:SimFunction:DOSES_NOT_EMPTY');
```

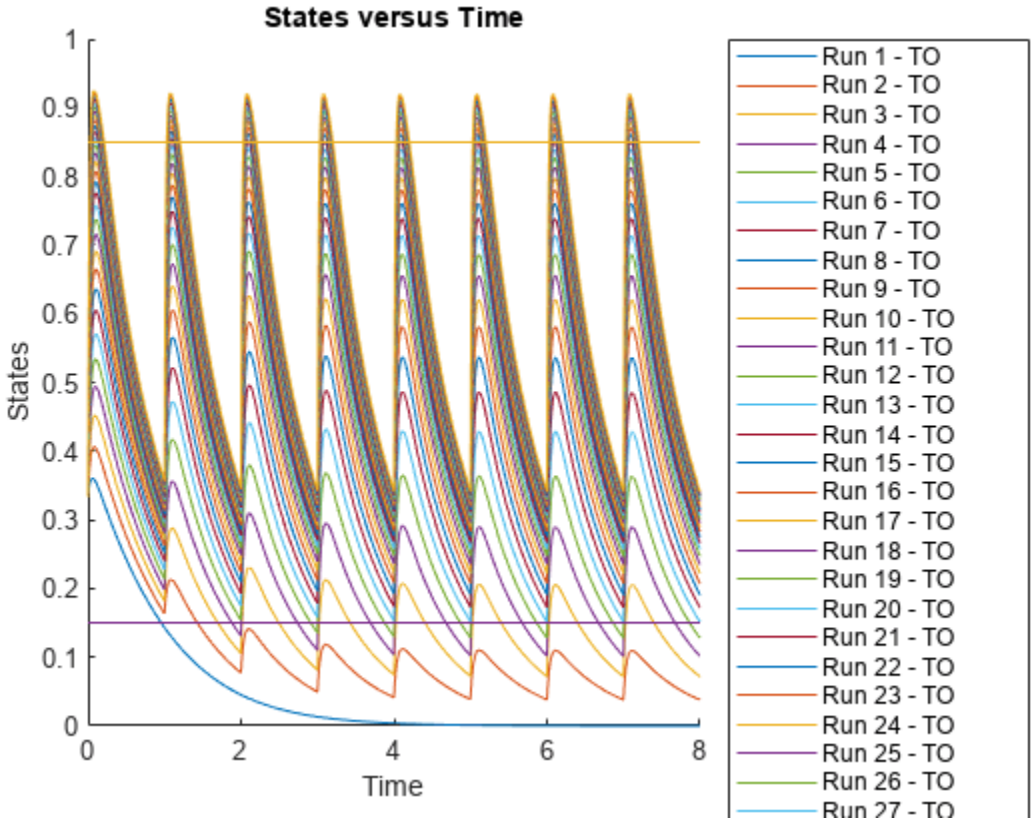
Simulate the model using the dose amounts generated by the `Scenarios` object. In this case, the object generates 31 different doses; hence the model is simulated 31 times and generates a `SimData` array.

```
doseTable = getTable(d);
sd = f(doseSamples,cs.StopTime,doseTable)
```

```
   SimBiology Simulation Data Array: 31-by-1

   ModelName:        TMDD
   Logged Data:
     Species:        0
     Compartment:    0
     Parameter:      1
     Sensitivity:    0
     Observable:     0
```

Plot the simulation results. Also add two reference lines that represent the safety and efficacy thresholds for `T0`. In this example, suppose that any `T0` value above 0.85 is unsafe, and any `T0` value below 0.15 has no efficacy.

```
h = sbioplot(sd);
time = sd(1).Time;
h.NextPlot = 'add';
safetyThreshold = plot(h,[min(time), max(time)],[0.85, 0.85],'DisplayName','Safety Threshold');
efficacyThreshold = plot(h,[min(time), max(time)],[0.15, 0.15],'DisplayName','Efficacy Threshold
```



Postprocess the simulation results. Find out which dose amounts are effective, corresponding to the `TO` responses within the safety and efficacy thresholds. To do so, add an observable expression to the simulation data.

```
% Suppress informational warnings that are issued during simulation.
warning('off','SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
newSD = addobservable(sd,'stat1','max(TO) < 0.85 & min(TO) > 0.15','Units','dimensionless')
```

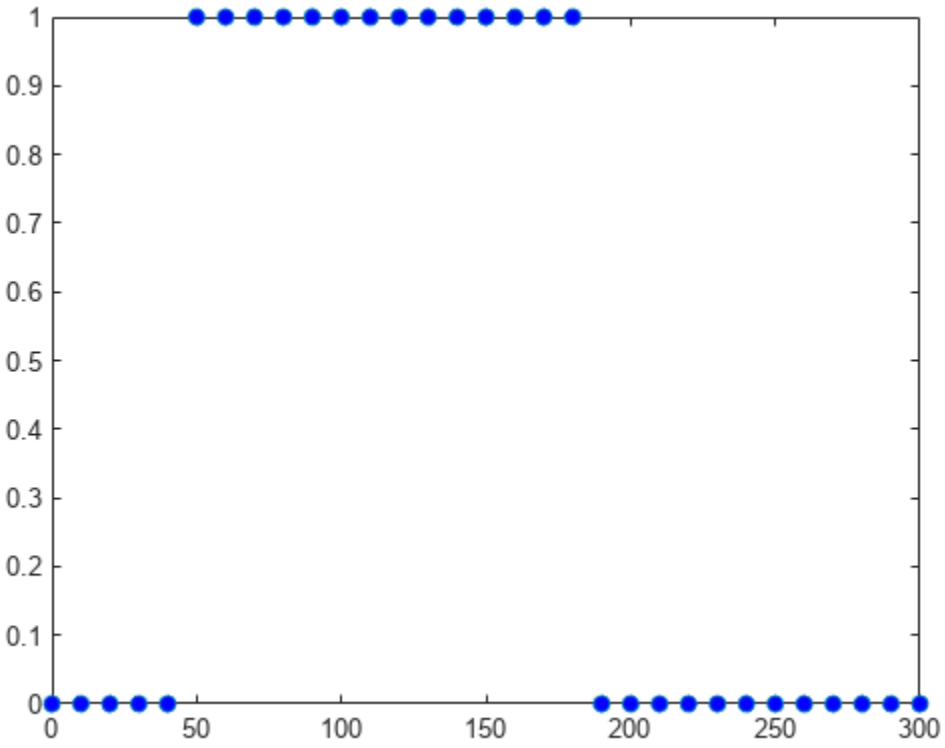
```
SimBiology Simulation Data Array: 31-by-1

ModelName:        TMDD
Logged Data:
  Species:        0
  Compartment:    0
  Parameter:      1
  Sensitivity:    0
  Observable:     1
```

The addobservable function evaluates the new observable expression for each `SimData` in `sd` and returns the evaluated results as a new `SimData` array, `newSD`, which now has the added observable (`stat1`).

SimBiology stores the observable results in two different properties of a `SimData` object. If the results are scalar-valued, they are stored in `SimData.ScalarObservables`. Otherwise, they are stored in `SimData.VectorObservables`. In this example, the `stat1` observable expression is scalar-valued.

Extract the scalar observable values and plot them against the dose amounts.

```
scalarObs = vertcat(newSD.ScalarObservables);
doseAmounts = generate(doseSamples);
figure
plot(doseAmounts.AmountParam,scalarObs.stat1,'o','MarkerFaceColor','b')
```



The plot shows that dose amounts ranging from 50 to 180 nanomoles provide `T0` responses that lie within the target efficacy and safety thresholds.

You can update the observable expression with different threshold amounts. The function recalculates the expression and returns the results in a new `SimData` object array.

```
newSD2 = updateobservable(newSD,'stat1','max(T0) < 0.75 & min(T0) > 0.30');
```

Rename the observable expression. The function renames the observable, updates any expressions that reference the renamed observable (if applicable), and returns the results in a new `SimData` object array.

```
newSD3 = renameobservable(newSD2,'stat1','EffectiveDose');
```

Restore the warning settings.

```
warning('on','SimBiology:sbservices:SB_DIMANALYSISNOTDONE_MATLABFCN_UCON');
```

Input Arguments

`sdin` — Input simulation data

`SimData` object | array of `SimData` objects

Input simulation data, specified as a `SimData` object or array of objects.

`obsNames` — Names of existing observable expressions

character vector | string | string vector | cell array of character vector

Names of existing observable expressions, specified as a character vector, string, string vector, or cell array of character vector.

Example: `{'max_drug','mean_drug'}`

Data Types: `char` | `string` | `cell`

`obsExpressions` — Observable expressions

character vector | string | string vector | cell array of character vectors

Observable expressions, specified as a character vector, string, string vector, or cell array of character vectors. The number of expressions must match the number of observable names.

Example: `{'max(drug)','mean(drug)'}`

Data Types: `char` | `string` | `cell`

`units` — Units for observable expressions

character vector | string | string vector | cell array of character vectors

Units for the observable expressions, specified as a character vector, string, string vector, or cell array of character vectors. The number of units must match the number of observable names.

Example: `{'nanomole/liter','nanomole/liter'}`

Data Types: `char` | `string` | `cell`

Output Arguments

`sdout` — Simulation data with observable results

`SimData` object | array of `SimData` objects

Simulation data with observable results, returned as a `SimData` object or array of objects.

Version History

Introduced in R2020a

See Also

SimData | renameobservable | addobservable

Variant object

Store alternate component values

Description

The SimBiology variant object stores the names and values of model components and allows you to use the values stored in a variant object as the alternate value to be applied during a simulation. You can store values for species `InitialAmount`, parameter `Value`, and compartment `Capacity` in a variant object. Simulating using a variant does not alter the model component values. The values specified in the variant temporarily apply during simulation.

Using one or more variant objects associated with a model allows you to evaluate model behavior during simulation, with different values for the various model components without having to search and replace these values, or having to create additional models with these values. If you determine that the values in a variant object accurately define your model, you can permanently replace the values in your model with the values stored in the variant object, using the `commit` method.

To use a variant in a simulation you must add the variant object to the model object and set the `Active` property of the variant to true. Set the `Active` property to true if you always want the variant to be applied before simulating the model. You can also enter the variant object as an argument to `sbiosimulate`; this applies the variant only for the current simulation and supersedes any active variant objects on the model.

Warning The `Active` property of the `Variant object` will be removed in a future release. Explicitly specify a variant or an array of variants as an input argument when you simulate a model using `sbiosimulate`.

When there are multiple active variant objects on a model, if there are duplicate specifications for a property's value, the last occurrence for the property value in the array of variants, is used during simulation. You can find out which variant is applied last by looking at the indices of the variant objects stored on the model. Similarly, in the `Content` property, if there are duplicate specifications for a property's value, the last occurrence for the property in the `Content` property, is used during simulation.

Use the `addcontent` method to append contents to a variant object.

See “Property Summary” on page 2-914 for links to species property reference pages. Properties define the characteristics of an object. Use the `get` and `set` commands to list object properties and change their values at the command line. You can graphically change object properties in the graphical user interface.

Constructor Summary

sbiovariant	Construct variant object

Method Summary

Methods for variant objects

addcontent (variant)	Append content to variant object
commit (variant)	Commit variant contents to model
copyobj	Copy SimBiology object and its children
delete	Delete SimBiology object
display	Display summary of SimBiology object
get	Get SimBiology object properties
rename	Rename object and update expressions
rmcontent (variant)	Remove contents from variant object
set	Set SimBiology object properties
verify (model, variant)	Validate and verify SimBiology model

Property Summary

Properties for variant objects

Active	Indicate object in use during simulation
Content	Contents of variant object
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Tag	Specify label for SimBiology object
Type	Display SimBiology object type
UserData	Specify data to associate with object

See Also

`Compartment object`, `Configset object`, `Model object`, `Parameter object`, `Species object`

`sbiosimulate`

Version History

Introduced in R2008a

verify (model, variant)

Validate and verify SimBiology model

Syntax

```
verify(modelObj)
verify(modelObj,csObj)
verify(modelObj,dvObj)

verify(modelObj,csObj,dvObj)

verify(modelObj,csObj,variantObj,doseObj)
```

Description

`verify(modelObj)` performs checks on a `Model` `modelObj` to verify that you can simulate the model. This function generates stacked errors and warnings if it finds any problems. To see the entire list of errors and warnings, use `sbiolasterror` and `sbiolastwarning`. The function uses the active configuration set, any active doses and active variants for verification.

`verify(modelObj,csObj)` verifies a model `modelObj` using the specified configset object `csObj` and any active variants and active doses. Any other configsets are ignored. If you set `csObj` to empty `[]`, the function uses the active configset.

`verify(modelObj,dvObj)` verifies a model `modelObj` using doses or variants specified by `dvObj` and the active configset. `dvObj` can be one of the following:

- `Variant object`
- `ScheduleDose object`
- `RepeatDose object`
- Array of doses or variants

If you set `dvObj` to empty `[]`, the function uses the active configset, active variants, and active doses.

If you specify `dvObj` as variants, the function uses the specified variants and active doses. Any other variants are ignored.

If you specify `dvObj` as doses, the function uses the specified doses and active variants. Any other doses are ignored.

`verify(modelObj,csObj,dvObj)` verifies a model `modelObj` using a configset object `csObj` and doses or variants specified by `dvObj`.

If you set `csObj` to `[]`, then the function uses the active configset object.

If you set `dvObj` to `[]`, then the function uses no variants, but uses active doses.

If you specify `dvObj` as variants, the function uses the specified variants and active doses. Any other variants are ignored.

If you specify `dvObj` as doses, the function uses the specified doses and active variants. Any other doses are ignored.

`verify(modelObj,csObj,variantObj,doseObj)` verifies a model `modelObj` using a configset object `csObj`, variants (`variantObj`) and doses (`doseObj`). Any other configset, doses, and variants are ignored.

If you set `csObj` to `[]`, then the function uses the active configset object.

If you set `variantObj` to `[]`, then the function uses no variants.

If you set `doseObj` to `[]`, then the function uses no doses.

Input Arguments

`modelObj` — SimBiology model
SimBiology model object

SimBiology model, specified as a SimBiology model object.

`csObj` — Configuration set object
configset object

Configuration set object, specified as a `Configset object` that stores simulation-specific information.

`dvObj` — Dose or variant object
dose object or array of dose objects | variant object or array of variant objects

Dose or variant object, specified as a `ScheduleDose object` , `RepeatDose object` , an array of dose objects, `Variant object` , or an array of variant objects.

- When `dvObj` is a dose object, `verify` uses the specified dose object as well as any active variant objects if available.
- When `dvObj` is a variant object, `verify` uses the specified variant object as well as any active dose objects if available.

`variantObj` — Variant object
variant object or array of variant objects

Variant object, specified as a `Variant object` or an array of variant objects.

`doseObj` — Dose object
dose object or array of dose objects

Dose object, specified as a `ScheduleDose object` , `RepeatDose object` , or an array of dose objects. A dose object defines additions that are made to species amounts or parameter values.

Examples

Verify a SimBiology Model While Using a User-Defined Configset Object

Load a sample SimBiology model.

```
sbioloadproject radiodecay.sbproj
```

Add a new configuration set using a different stop time of 15 seconds.

```
csObj = addconfigset(m1,'newStopTimeConfigSet');
csObj.StopTime = 15;
```

Verify the model while using the configset object.

```
verify(m1,csObj);
```

After verification, check the latest errors and warnings if there is any.

```
sbiolasterror
```

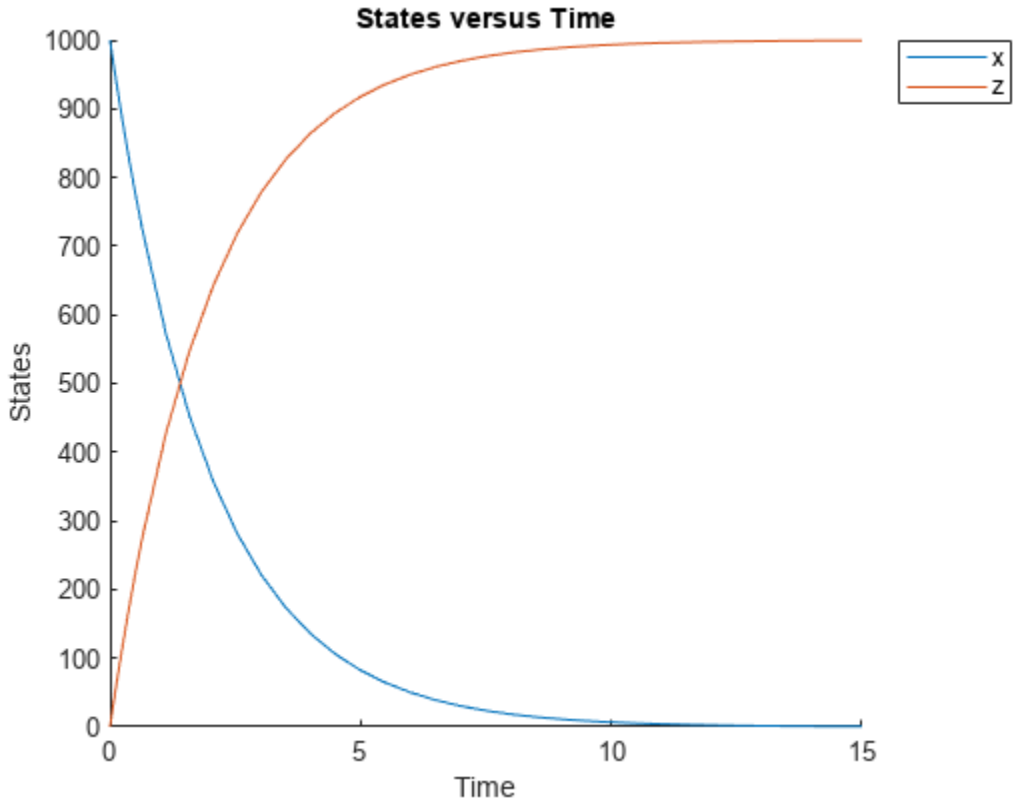
```
ans =

  0x1 empty struct array with fields:

    Type
    MessageID
    Message
```

```
sbiolastwarning
```

```
ans=3×1 struct array with fields:
    Type
    MessageID
    Message
```

Simulate the model.

```
sim = sbiosimulate(m1,csObj);
sbioplot(sim);
```



Verify a SimBiology Model While Using Configset and Dose Objects

Load a sample SimBiology model.

```
sbioloadproject radiodecay.sbproj
```

Get the default configuration set from the model.

```
defaultConfigSet = getconfigset(m1,'default');
```

Add a scheduled dose of 100 molecules at 2 seconds for species `x`.

```
dObj = adddose(m1,'d1','schedule');
dObj.Amount = 100;
dObj.AmountUnits = 'molecule';
dObj.TimeUnits = 'second';
dObj.Time = 2;
dObj.TargetName = 'unnamed.x';
```

Verify the model while using the default configset object and added dose object.

```
verify(m1,defaultConfigSet,dObj);
```

After verification, check the latest errors and warnings if there is any.

```
sbiolasterror
```

```
ans =

  0x1 empty struct array with fields:

    Type
    MessageID
    Message
```

```
sbiolastwarning
```

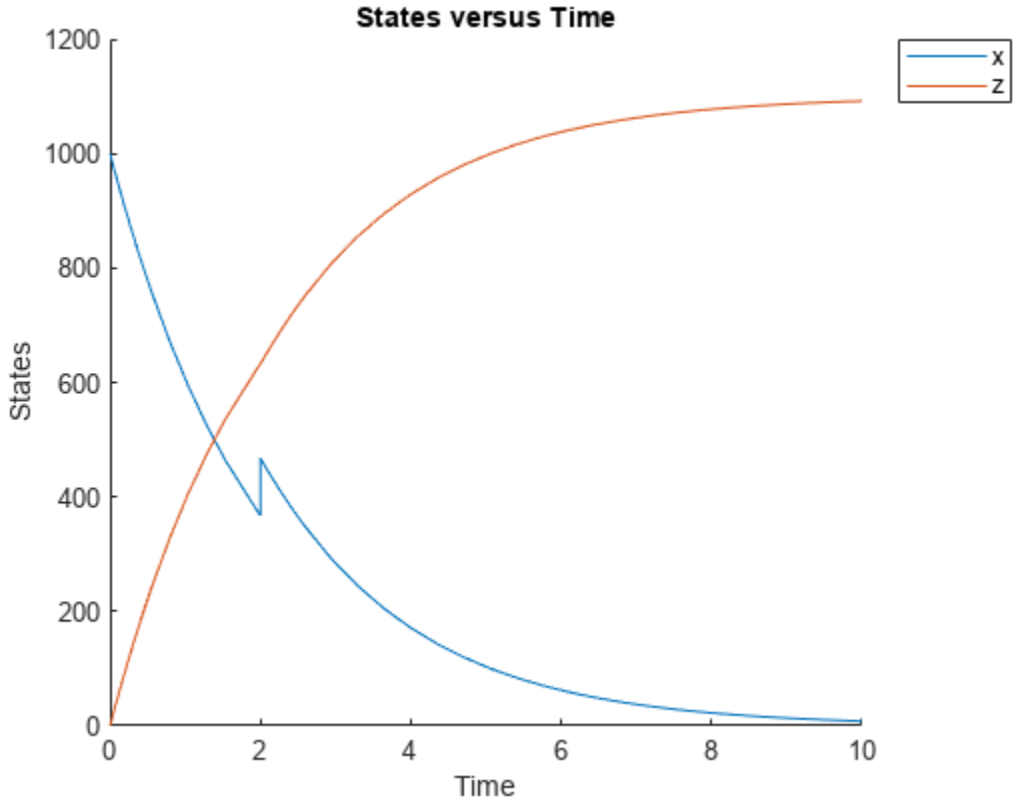
```
ans=3×1 struct array with fields:
    Type
    MessageID
    Message
```

Simulate the model using the same configset and dose objects.

```
sim = sbiosimulate(m1,defaultConfigSet,dObj);
```

Plot the result.

```
sbioplot(sim);
```



Verify SimBiology Model While Using Configset, Dose, and Variant Objects

Load a sample SimBiology model.

```
sbioloadproject radiodecay.sbproj
```

Add a new configuration set using a different stop time of 15 seconds.

```
csObj = m1.addconfigset('newStopTimeConfigSet');
csObj.StopTime = 15;
```

Add a scheduled dose of 100 molecules at 2 seconds for species x.

```
dObj = adddose(m1,'d1','schedule');
dObj.Amount = 100;
dObj.AmountUnits = 'molecule';
dObj.TimeUnits = 'second';
dObj.Time = 2;
dObj.TargetName = 'unnamed.x';
```

Add a variant of species x using a different initial amount of 500 molecules.

```
vObj = addvariant(m1,'v1');
addcontent(vObj,{'species','x','InitialAmount',500});
```

Verify the model while using the configset, dose, and variant objects. Note that the order of arguments should be as described.

```
verify(m1,csObj,vObj,dObj);
```

After verification, check the latest errors and warnings if there is any.

```
sbiolasterror
```

```
ans =

  0x1 empty struct array with fields:

    Type
    MessageID
    Message
```

```
sbiolastwarning
```

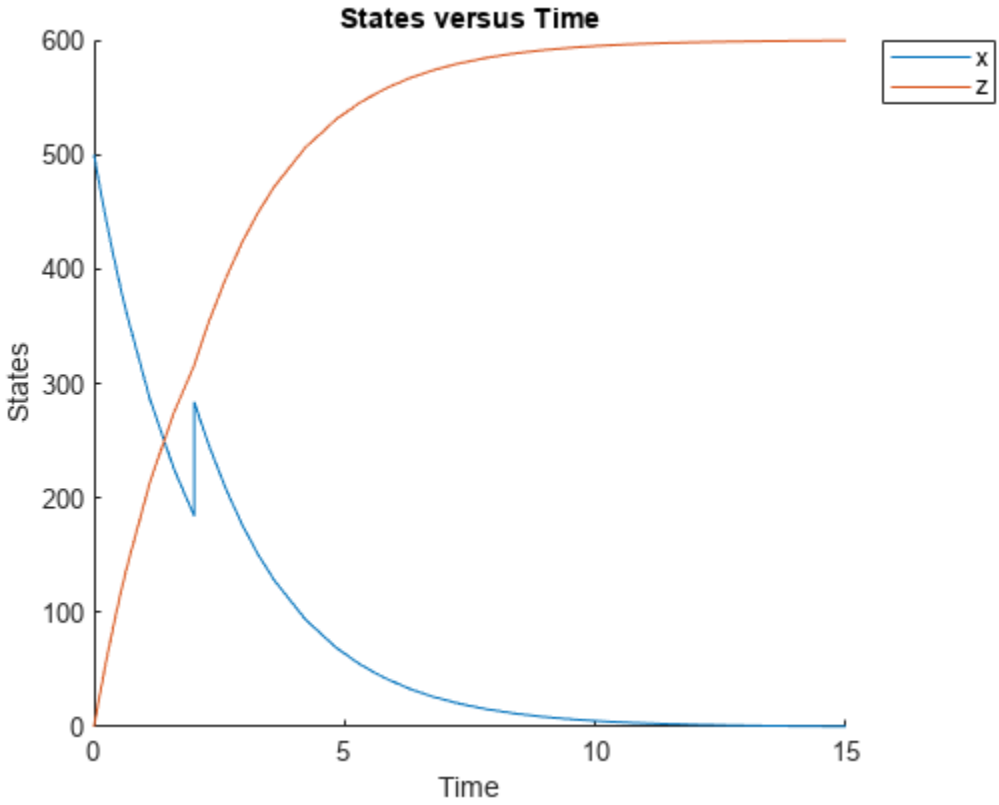
```
ans=3×1 struct array with fields:
    Type
    MessageID
    Message
```

Simulate the model using the same configset, variant, and dose objects.

```
sim = sbiosimulate(m1,csObj,vObj,dObj);
```

Plot the result.

```
sbioplot(sim);
```



See Also

`sbiolasterror`, `sbiolastwarning`

Version History

Introduced in R2006a

verify

Verify `SimBiology.Scenarios` object

Syntax

```
verify(sObj,model)
```

Description

`verify(sObj,model)` verifies the `SimBiology.Scenarios` object `sObj` and checks whether you can simulate its scenarios with a given SimBiology `model`.

The function throws an error if any entry does not resolve uniquely to an object in the `model` or the entry contents have inconsistent lengths. The function throws a warning if multiple entries resolve to the same object in the `model`.

Examples

Generate Different Simulation Scenarios for Glucose-Insulin Response

Load the model of glucose-insulin response. For details about the model, see the **Background** section in “Simulate the Glucose-Insulin Response”.

```
sbioloadproject('insulindemo','m1');
```

The model contains different parameter values and initial conditions that represents different insulin impairments (such as Type 2 diabetes, low insulin sensitivity, and so on) stored in five variants.

```
variants = getvariant(m1)
```

```
variants =
   SimBiology Variant Array

   Index:  Name:             Active:
   1       Type 2 diabetic   false
   2       Low insulin se... false
   3       High beta cell... false
   4       Low beta cell ... false
   5       High insulin s... false
```

Suppress an informational warning that is issued during simulations.

```
warnSettings = warning('off','SimBiology:DimAnalysisNotDone_MatlabFcn_Dimensionless');
```

Select a dose that represents a single meal of 78 grams of glucose.

```
singleMeal = sbioselect(m1,'Name','Single Meal');
```

Create a `Scenarios` object to represent different initial conditions combined with the dose. That is, create a `scenario` object where each variant is paired (or combined) with the dose, for a total of five simulation scenarios.

```
sObj = SimBiology.Scenarios;
add(sObj,'cartesian','variants',variants);
add(sObj,'cartesian','dose',singleMeal)
```

```
ans =
  Scenarios (5 scenarios)

                  Name            Content           Number
                ________    ____________________    ______

    Entry 1     variants    SimBiology variants       5
    x Entry 2   dose        SimBiology dose           1

  See also Expression property.
```

`sObj` contains two entries. Use the `generate` function to combine the entries and generate five scenarios. The function returns a scenarios table, where each row represents a scenario and each column represents an entry of the `Scenarios` object.

```
scenariosTbl = generate(sObj)
```

```
scenariosTbl=5×2 table
           variants                    dose
    ________________________    ____________________________

    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
    1x1 SimBiology.Variant    1x1 SimBiology.RepeatDose
```

Change the entry name of the first entry.

```
rename(sObj,1,'Insulin Impairements')
```

```
ans =
  Scenarios (5 scenarios)

                       Name                Content           Number
                ____________________    ____________________    ______

    Entry 1     Insulin Impairements    SimBiology variants       5
    x Entry 2   dose                    SimBiology dose           1

  See also Expression property.
```

Create a `SimFunction` object to simulate the generated scenarios. Use the `Scenarios` object as the input and specify the plasma glucose and insulin concentrations as reponses (outputs of the function to be plotted). Specify `[]` for the dose input argument since the `Scenarios` object already has the dosing information.

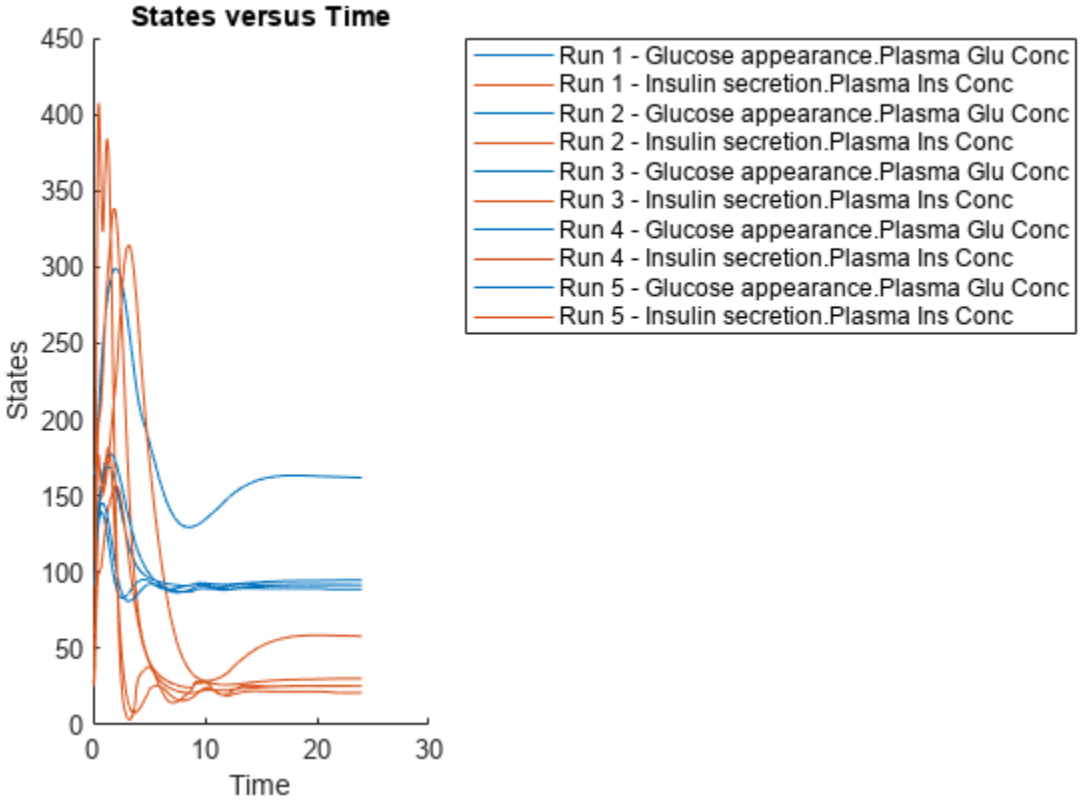
```
f = createSimFunction(m1,sObj,{'[Plasma Glu Conc]','[Plasma Ins Conc]'},[])
```

```
f =
SimFunction

Parameters:

            Name              Value        Type                        Units
    ______________________    ______    ____________    ____________________________________

    {'Plasma Volume (Glu)'  }      1.88    {'parameter'}    {'deciliter'
    {'k1'                   }     0.065    {'parameter'}    {'1/minute'
    {'k2'                   }     0.079    {'parameter'}    {'1/minute'
    {'Plasma Volume (Ins)'  }      0.05    {'parameter'}    {'liter'
    {'m1'                   }      0.19    {'parameter'}    {'1/minute'
    {'m2'                   }     0.484    {'parameter'}    {'1/minute'
    {'m4'                   }    0.1936    {'parameter'}    {'1/minute'
    {'m5'                   }    0.0304    {'parameter'}    {'minute/picomole'
    {'m6'                   }    0.6469    {'parameter'}    {'dimensionless'
    {'Hepatic Extraction'   }       0.6    {'parameter'}    {'dimensionless'
    {'kmax'                 }    0.0558    {'parameter'}    {'1/minute'
    {'kmin'                 }     0.008    {'parameter'}    {'1/minute'
    {'kabs'                 }    0.0568    {'parameter'}    {'1/minute'
    {'kgri'                 }         0    {'parameter'}    {'1/minute'
    {'f'                    }       0.9    {'parameter'}    {'dimensionless'
    {'a'                    }         0    {'parameter'}    {'1/milligram'
    {'b'                    }      0.82    {'parameter'}    {'dimensionless'
    {'c'                    }         0    {'parameter'}    {'1/milligram'
    {'d'                    }      0.01    {'parameter'}    {'dimensionless'
    {'kp1'                  }       2.7    {'parameter'}    {'milligram/minute'
    {'kp2'                  }    0.0021    {'parameter'}    {'1/minute'
    {'kp3'                  }     0.009    {'parameter'}    {'(milligram/minute)/(picomole/liter)
    {'kp4'                  }    0.0618    {'parameter'}    {'(milligram/minute)/picomole'
    {'ki'                   }    0.0079    {'parameter'}    {'1/minute'
    {'[Ins Ind Glu Util]'   }         1    {'parameter'}    {'milligram/minute'
    {'Vm0'                  }    2.5129    {'parameter'}    {'milligram/minute'
    {'Vmx'                  }     0.047    {'parameter'}    {'(milligram/minute)/(picomole/liter)
    {'Km'                   }    225.59    {'parameter'}    {'milligram'
    {'p2U'                  }    0.0331    {'parameter'}    {'1/minute'
    {'K'                    }      2.28    {'parameter'}    {'picomole/(milligram/deciliter)'
    {'alpha'                }      0.05    {'parameter'}    {'1/minute'
    {'beta'                 }      0.11    {'parameter'}    {'(picomole/minute)/(milligram/decili
    {'gamma'                }       0.5    {'parameter'}    {'1/minute'
    {'ke1'                  }    0.0005    {'parameter'}    {'1/minute'
    {'ke2'                  }       339    {'parameter'}    {'milligram'
    {'Basal Plasma Glu Conc'}     91.76    {'parameter'}    {'milligram/deciliter'
    {'Basal Plasma Ins Conc'}     25.49    {'parameter'}    {'picomole/liter'

Observables:

          Name              Type              Units
    ____________________    __________    ____________________

    {'[Plasma Glu Conc]'}    {'species'}    {'milligram/deciliter'}
    {'[Plasma Ins Conc]'}    {'species'}    {'picomole/liter'     }

Dosed:

    TargetName       TargetDimension
    __________    ____________________
```

```
     {'Dose'}     {'Mass (e.g., gram)'}

TimeUnits: hour
```

Simulate the model for 24 hours and plot the simulation data. The data contains five runs, where each run represents a scenario in the Scenarios object.

```
sd = f(sObj,24);
sbioplot(sd)
```




```
ans =
  Axes (SbioPlot) with properties:

            XLim: [0 30]
            YLim: [0 450]
          XScale: 'linear'
          YScale: 'linear'
    GridLineStyle: '-'
         Position: [0.0920 0.1100 0.2956 0.8150]
            Units: 'normalized'

  Show all properties
```

If you have Statistics and Machine Learning Toolbox™, you can also draw sample values for model quantities from various probability distributions. For instance, suppose that the parameters `Vmx` and

kp3, which are known for the low and high insulin sensitivity, follow the lognormal distribution. You can generate sample values for these parameters from such a distribution, and perform a scan to explore model behavior.

Define the lognormal probability distribution object for Vmx.

```
pd_Vmx = makedist('lognormal')
```

```
pd_Vmx =
  LognormalDistribution

  Lognormal distribution
       mu = 0
    sigma = 1
```

By definition, the parameter mu is the mean of logarithmic values. To vary the parameter value around the base (model) value of the parameter, set mu to `log(`*`model_value`*`)`. Set the standard deviation (*sigma*) to 0.2. For a small *sigma* value, the mean of a lognormal distribtion is approximately equal to `log(`*`model_value`*`)`. For details, see “Lognormal Distribution” (Statistics and Machine Learning Toolbox).

```
Vmx = sbioselect(m1,'Name','Vmx');
pd_Vmx.mu = log(Vmx.Value);
pd_Vmx.sigma = 0.2
```

```
pd_Vmx =
  LognormalDistribution

  Lognormal distribution
       mu = -3.05761
    sigma =      0.2
```

Similarly define the probability distribution for kp3.

```
pd_kp3 = makedist('lognormal');
kp3 = sbioselect(m1,'Name','kp3');
pd_kp3.mu = log(kp3.Value);
pd_kp3.sigma = 0.2
```

```
pd_kp3 =
  LognormalDistribution

  Lognormal distribution
       mu = -4.71053
    sigma =      0.2
```

Now define a joint probability distribution to draw sample values for Vmx and kp3, with a rank correlation to specify some correlation between these two parameters. Note that this correlation assumption is for the illustration purposes of this example only and may not be biologically relevant.

First remove the variants entry (entry 1) from sObj.

```
remove(sObj,1)
```

```
ans =
  Scenarios (1 scenarios)
```

```
                Name        Content         Number
                ____    ________________    ______

    Entry 1     dose    SimBiology dose       1

  See also Expression property.
```

Add an entry that defines the joint probability distribution with a rank correlation matrix.

```
add(sObj,'cartesian',["Vmx","kp3"],[pd_Vmx, pd_kp3],'RankCorrelation',[1,0.5;0.5,1])
```

```
ans =
  Scenarios (2 scenarios)

                    Name           Content              Number
                    ____    ________________________    ___________

    Entry 1         dose    SimBiology dose             1
    x (Entry 2.1    Vmx     Lognormal distribution      2 (default)
    + Entry 2.2)    kp3     Lognormal distribution      2 (default)

  See also Expression property.
```

By default, the number of samples to draw from the joint distribution is set to 2. Increase the number of samples.

```
updateEntry(sObj,2,'Number',50)
```

```
ans =
  Scenarios (50 scenarios)

                    Name           Content              Number
                    ____    ________________________    ______

    Entry 1         dose    SimBiology dose               1
    x (Entry 2.1    Vmx     Lognormal distribution        50
    + Entry 2.2)    kp3     Lognormal distribution        50

  See also Expression property.
```

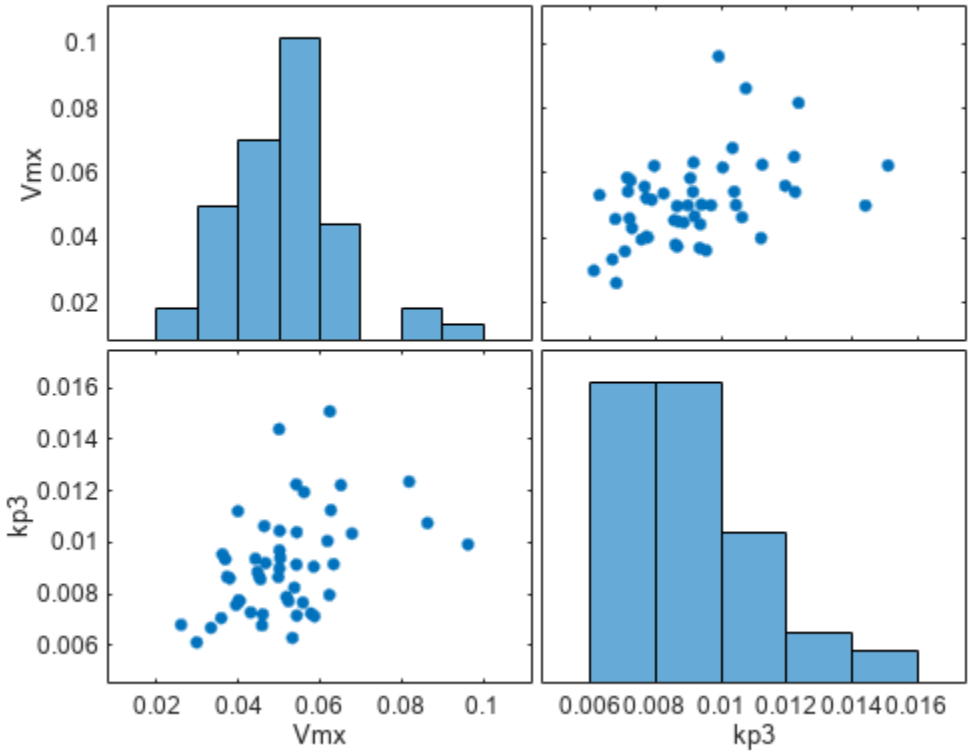
Verify that the `Scenarios` object can be simulated with the model. The `verify` function throws an error if any entry does not resolve uniquely to an object in the model or the entry contents have inconsistent lengths (sample sizes). The function throws a warning if multiple entries resolve to the same object in the model.

```
verify(sObj,m1)
```

Generate the simulation scenarios. Plot the sample values using `plotmatrix`. You can see the value of `Vmx` is varied around its model value 0.047 and that of `kp3` around 0.009.

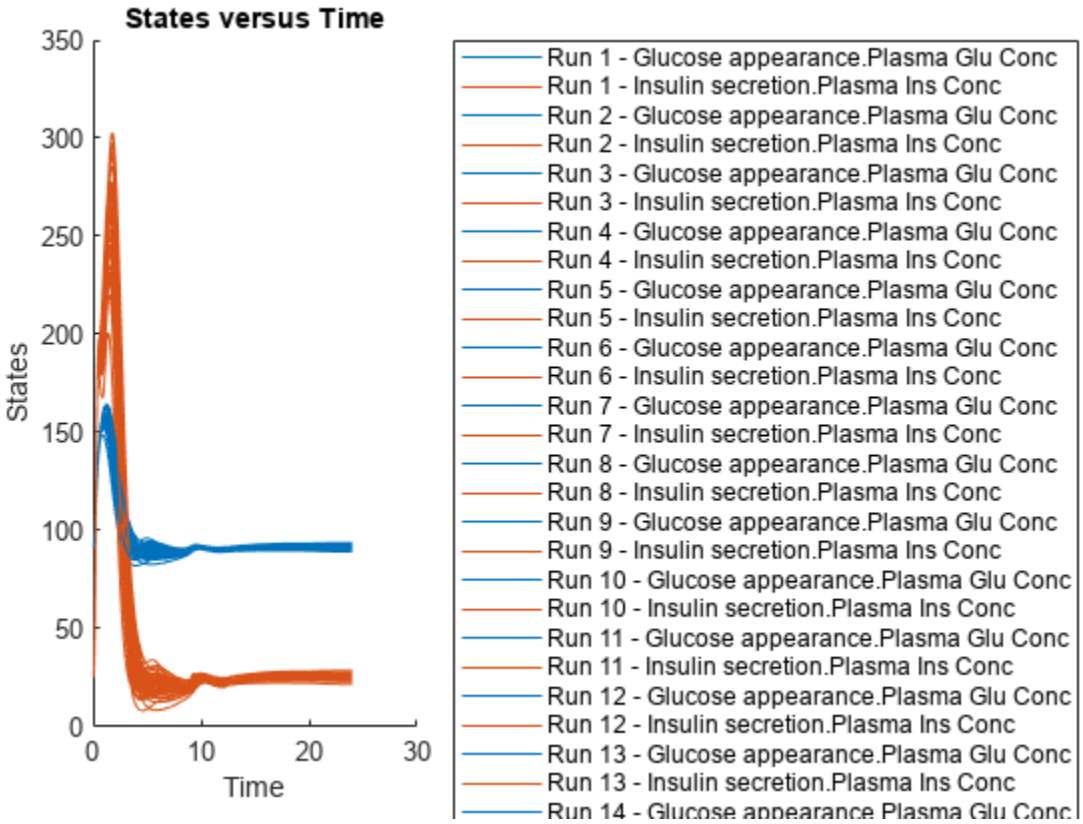
```
sTbl = generate(sObj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl.Vmx,sTbl.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
```

```
ax(2,1).XLabel.String = "Vmx";
ax(2,2).XLabel.String = "kp3";
```



Simulate the scenarios using the same SimFunction you created previously. You do not need to create a new SimFunction object even though the Scenarios object has been updated.

```
sd2 = f(sObj,24);
sbioplot(sd2);
```



By default, SimBiology uses the random sampling method. You can change it to the Latin hypercube sampling (or sobol or halton) for a more systematic space-filling approach.

```
entry2struct = getEntry(sObj,2)
```

```
entry2struct = struct with fields:
               Name: {'Vmx'  'kp3'}
            Content: [2x1 prob.LognormalDistribution]
             Number: 50
    RankCorrelation: [2x2 double]
         Covariance: []
     SamplingMethod: 'random'
    SamplingOptions: [0x0 struct]
```

```
entry2struct.SamplingMethod = 'lhs'
```

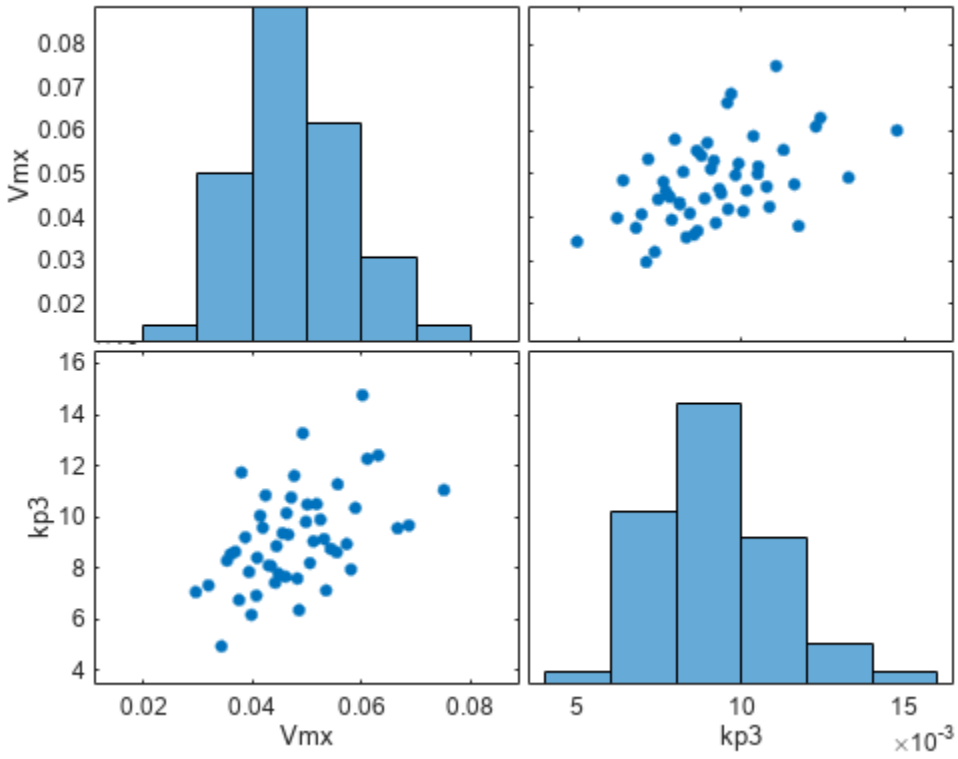
```
entry2struct = struct with fields:
               Name: {'Vmx'  'kp3'}
            Content: [2x1 prob.LognormalDistribution]
             Number: 50
    RankCorrelation: [2x2 double]
         Covariance: []
     SamplingMethod: 'lhs'
    SamplingOptions: [0x0 struct]
```

You can now use the updated structure to modify entry 2.

```
updateEntry(sObj,2,entry2struct)

ans =
  Scenarios (50 scenarios)

                    Name           Content             Number
                    ____    ____________________      ______

    Entry 1         dose    SimBiology dose             1
    x (Entry 2.1    Vmx     Lognormal distribution      50
    + Entry 2.2)    kp3     Lognormal distribution      50

  See also Expression property.
```

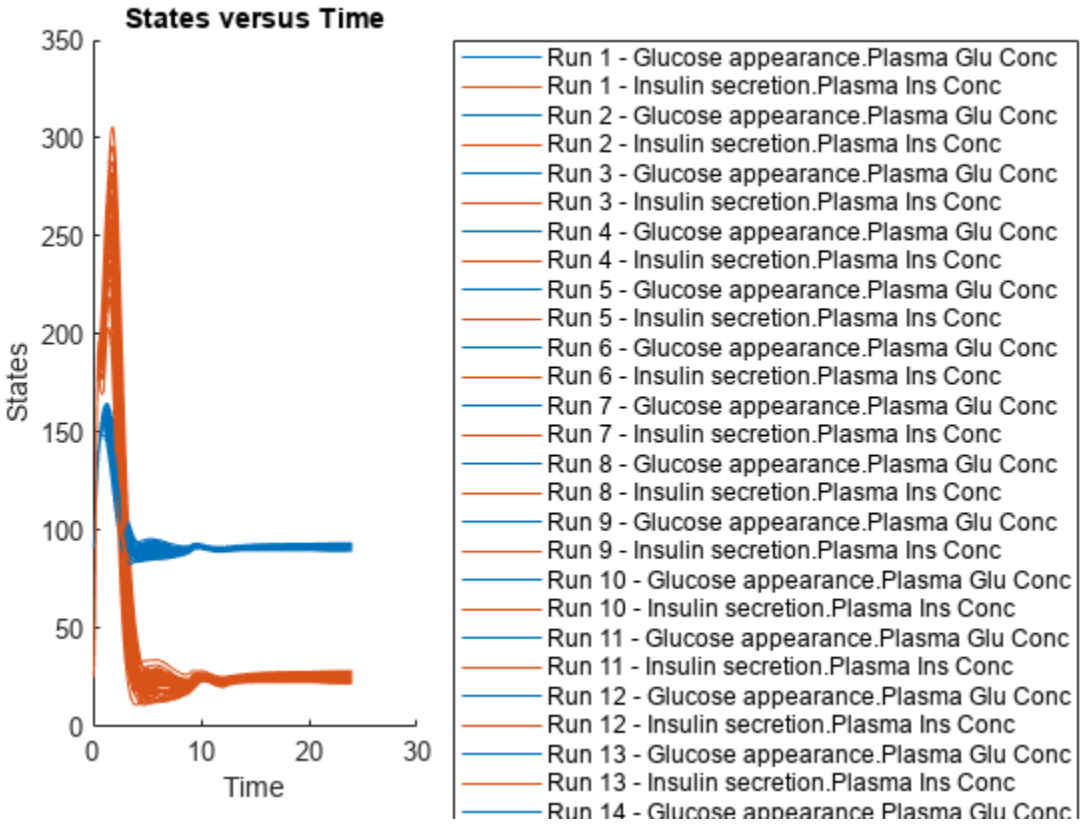
Visualize the sample values.

```
sTbl2 = generate(sObj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl2.Vmx,sTbl2.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
ax(2,1).XLabel.String = "Vmx";
ax(2,2).XLabel.String = "kp3";
```



Simulate the scenarios.

```
sd3 = f(sObj,24);
sbioplot(sd3);
```



Restore warning settings.

```
warning(warnSettings);
```

Input Arguments

`sObj` — Simulation scenarios

`SimBiology.Scenarios` object

Simulation scenarios, specified as a `SimBiology.Scenarios` object.

`model` — SimBiology model

`Model` object

SimBiology model, specified as a `Model` object.

Output Arguments

`sObj` — Simulation scenarios

`Scenarios` object

Simulation scenarios, returned as a `Scenarios` object.

Version History

Introduced in R2019b

See Also

`SimBiology.Scenarios` | `SimFunction object` | `createSimFunction (model)`

Topics

“SimBiology.Scenarios Terminology” on page 2-799
“Combine Simulation Scenarios in SimBiology”

verify

Check covariate model for errors

Syntax

```
verify(CovModel)
```

Description

`verify(CovModel)` verifies that the following are true about the `Expression` property of the `CovariateModel` object, `CovModel`:

- The expressions are valid MATLAB code.
- Each expression is linear with a transformation.
- There is exactly one expression for each parameter.
- In each expression, a covariate is used in at most one term.
- In each expression, there is at most one random effect (`eta`)
- Fixed effect (`theta`) and random effect (`eta`) names are unique within and across expressions. That is, each covariate has its own fixed effect.

Examples

Specify a Covariate Model

Create an empty `CovariateModel` object.

```
covModel = CovariateModel;
```

Set its Expression property to define the relationships between parameters (*Cl*, *V*, and *k*) and covariate (*w*). You must use `theta` as a prefix for all fixed effects and `eta` for random effects.

```
covModel.Expression = ["Cl = theta1 + theta2*w + eta1","V = theta3 + eta2","k = theta4 + eta3"];
```

Display the names of fixed effects.

```
covModel.FixedEffectNames
```

```
ans = 4x1 cell
    {'theta1'}
    {'theta3'}
    {'theta4'}
    {'theta2'}
```

The `FixedEffectDescription` property displays which fixed effects correspond to which parameter. For instance, *theta1* is the fixed effect for the *Cl* parameter, and *theta2* is the fixed effect for the weight covariate that has a correlation with *Cl* parameter, denoted as *Cl*/*w*.

```
covModel.FixedEffectDescription
```

```
ans = 4x1 cell
    {'Cl'  }
    {'V'   }
    {'k'   }
    {'Cl/w'}
```

Specify initial estimates for the fixed effects. Create a default structure containing initial estimates using the `constructDefaultFixedEffectValues` function.

```
initialEstimates = constructDefaultFixedEffectValues(covModel)
```

```
initialEstimates = struct with fields:
    theta1: 0
    theta3: 0
    theta4: 0
    theta2: 0
```

Update the initial estimate value of each fixed effects.

```
initialEstimates.theta1 = 1.20;
initialEstimates.theta2 = 0.30;
initialEstimates.theta3 = 0.90;
initialEstimates.theta4 = 0.10;
```

Update the `FixedEffectValues` property to use the updated initial estimates.

```
covModel.FixedEffectValues = initialEstimates;
```

Check the covariate model for errors.

```
verify(covModel)
```

Input Arguments

`CovModel` — Covariate model

`CovariateModel` object

Covariate model, specified as a `CovariateModel` object.

Version History

Introduced in R2011b

See Also

`CovariateModel`

Topics

“Specify a Covariate Model”
“Model the Population Pharmacokinetics of Phenobarbital in Neonates”

visdiff

Visualize SimBiology model comparison results

Syntax

```
visdiff(diffResults)
```

Description

`visdiff(diffResults)` opens the Comparison tool and shows the comparison results `diffResults` of SimBiology models.

Tip Alternatively, you can also use two SBPROJ files as inputs. For details, see “Compare Models in Comparison Tool”.

Examples

Compare SimBiology Models

Load a source model.

```
model1      = sbmlimport("lotka");
y1          = sbioselect(model1, "Type", "species", "Name", "y1");
y1.Value    = 880;
```

Load a target model to compare against the source model.

```
model2      = sbmlimport("lotka");
y1          = sbioselect(model2, "Type", "species", "Name", "y1");
y1.Value    = 920;
```

Compare the models using `sbiodiff` and display the comparison table.

```
diffResults = sbiodiff(model1,model2);
diffTable   = diffResults.Comparisons
```

```
diffTable=1×6 table
           Class      Source    Target    Property    SourceValue    TargetValue
          _________    ______    ______    ________    ___________    ___________

    1    "Species"     "y1"      "y1"     "Value"       {[880]}        {[920]}
```

You can also view the comparison results graphically in the Comparison tool.

```
visdiff(diffResults);
```

Get a table of model components associated with the changes reported in the comparison table.

```
tbl = getComponents(diffResults)
```

```
tbl=1×2 table
                Source                          Target
        ____________________________    ____________________________

    1   {1x1 SimBiology.Species}        {1x1 SimBiology.Species}
```

Input Arguments

`diffResults` — Model comparison results

`SimBiology.DiffResults` object

Model comparison results, specified as a `SimBiology.DiffResults` object. Use `sbiodiff` to generate this object.

Version History

Introduced in R2022a

See Also

`sbiodiff` | `SimBiology.DiffResults` | `getComponents` | `visdiff`

Topics

“Compare SimBiology Models”
“SimBiology Model Matching Policy”

Properties

Active

Indicate object in use during simulation

Description

The `Active` property indicates whether a simulation is using a SimBiology object. A SimBiology model is organized into a hierarchical group of objects. Use the `Active` property to include or exclude objects during a simulation.

- **Event, Reaction, or Rule** — When an event, a reaction, or rule object `Active` property is set to `false`, the simulation does not include the event, reaction, or rule. This is a convenient way to test a model with and without a reaction or rule.
- **Configuration set** — For the `configset` object, use the method `setactiveconfigset` to set the object `Active` property to `true`.

  Warning This property of the `Configset object` will be removed in a future release. Explicitly specify a configset as an input argument when you simulate a model using `sbiosimulate`.
- **Variant** — Set the `Active` property to `true` if you always want the variant to be applied before simulating the model. You can also pass the variant object as an argument to `sbiosimulate`; this applies the variant only for the current simulation. For more information on using the `Active` property for variants, see `Variant object`.

  Warning This property of the `Variant object` will be removed in a future release. Explicitly specify a variant or an array of variants as an input argument when you simulate a model using `sbiosimulate`.

  .
- **Schedule dose** and **Repeat dose** — To use a dose object in a simulation, you must add the dose object to a model object and set the Active property of the dose object to true.

  Warning This property of the `ScheduleDose object` and `RepeatDose object` will be removed in a future release. Explicitly specify a dose or an array of doses as an input argument when you simulate a model using `sbiosimulate`.

Characteristics

Applies to	Objects: configset, event, observable, reaction, RepeatDose, rule, ScheduleDose, variant
Data type	`boolean`
Data values	`true` or `false`. The default value for events, reactions, rules, and observables is `true`. For the `configset` object, default is `true`. For added configset object, the default is `false`. For variants, the default is `false`.

Access	Read/write

Examples

1 Create a model object.

```
modelObj = sbiomodel ('my_model');
```

2 Add a reaction object and verify that the `Active` property setting is `'true'` or `1`.

```
reactionObj = addreaction (modelObj, 'a + b -> c + d');
get (reactionObj, 'Active')
```

MATLAB returns:

```
ans =

1
```

3 Set the `Active` property to `'false'` and verify.

```
set (reactionObj, 'Active', false);
get (reactionObj, 'Active')
```

MATLAB returns:

```
ans =

0
```

See Also

`addconfigset`, `addreaction`, `addrule`, `Event object`, `Reaction object`,`RepeatDose object`, `Rule object` , `ScheduleDose object`, `Variant object`,

Amount

Amount of dose

Note The property of a `ScheduleDose` object is a column vector instead of a row vector. For details, see “Compatibility Considerations”.

Description

`Amount` is a property of a RepeatDose or ScheduleDose object. It defines an increase in the amount of a SimBiology species that receives a dose.

A `RepeatDose` object defines a series of doses. Each dose is the same amount, as defined by the `Amount` property, and given at equally spaced times, as defined by the `Interval` property.

The number of injections in the series, excluding the initial injection, is defined by the `RepeatCount` property, and the `Rate` property defines how fast each dose is given.

For `RepeatDose` objects, you can parameterize the property by setting it to the name of a model-scoped parameter that is not being modified by a repeated assignment rule, an algebraic rule, or a rate rule. However, the parameter can be modified by an event.

A `ScheduleDose` object defines a series of doses. Each dose can have a different amount, as defined by an amount array in the `Amount` property, and given at specified times, as defined by a time array in the `Time` property. A rate array in the `Rate` property defines how fast each dose is given. At each time point in the time array, a dose is given with the corresponding amount and rate.

Characteristics

Applies to	Object: `RepeatDose`, `ScheduleDose`.
Data type	double or character vector (`RepeatDose`) or double coulmn (`ScheduleDose`).
Data values	Nonnegative value or name of a model-scoped parameter object. The default value is `0` (`RepeatDose`) or `0x1` empty double column vector (`ScheduleDose`).
Access	Read/write.

Version History

R2019b: `Amount` property of `ScheduleDose` is a column vector
Behavior changed in R2019b

The Amount property of a `ScheduleDose` object is a column vector instead of a row vector. The default value is `0x1` empty double column vector, instead of `[]`.

See Also

`RepeatDose object` | `ScheduleDose object`

Topics
“Parameterized and Adaptive Doses”

AmountUnits

Dose amount units

Description

`AmountUnits` is a property of a `RepeatDose` or `ScheduleDose` object. This property defines units for the `Amount` property.

If the `TargetName` property defines a species, then `AmountUnits` for a dose must be a chemical amount (for example, milligram, mole, or molecule), not a concentration. To get a list of the defined units in the library, use the `sbioshowunits` function. To add a user-defined unit to the list, see `sbioaddtolibrary`.

Characteristics

Applies to	Objects: `RepeatDose`, `ScheduleDose`
Data type	Character vector
Data values	Units from library with dimensions of amount. Default = '' (empty)
Access	Read/write

Note SimBiology uses units including empty units in association with DimensionalAnalysis and UnitConversion features.

- When `DimensionalAnalysis` and `UnitConversion` are both `false`, units are not used. However, SimBiology still performs a minimum level of dimensional analysis to decide whether a reaction rate is in dimensions of amount/time or concentration/time.
- When `DimensionalAnalysis` is `true` and `UnitConversion` is `false`, units (if not empty) must have consistent dimensions so that SimBiology can perform dimensional analysis. However, the units are not converted.
- When `UnitConversion` is set to `true` (which requires `DimensionalAnalysis` to be `true`), SimBiology performs a dimensional analysis and converts everything to consistent units. Hence, you must specify consistent units, and no units can be empty. If you have a dimensionless parameter, you must still set its unit to `dimensionless`.

See Also

`ScheduleDose object` and `RepeatDose object`

AmountUnits

Amount unit used internally during simulation when UnitConversion is on

Description

This property defines the amount unit that SimBiology uses internally during model simulation when UnitConversion is on. You can set this to any character vector representing an amount unit such as molecule, mole, or mole with any valid prefix. It can also be a custom unit if it is consistent with amount as its dimension. The default is `<automatic>`, which means SimBiology automatically selects an amount unit for simulation. SimBiology examines the units on all of the states and selects an amount unit such that AbsoluteTolerance of the states in amount, or amount per volume is at least as stringent as the simulation absolute tolerance multiplied by the smallest amount unit. This stringency is relaxed appropriately for states that become large when AbsoluteToleranceScaling is on.

Note It is recommended that you use the default unit (`<automatic>`) or choose units for states such that the simulated values are neither too large (greater than 10^6) or too small (less than 10^{-6}).

However, for some edge cases, you may need to change `AmountUnits`. Suppose you have a model with a state that takes on values around 10^{-12} moles for the entire simulation, and you need to use `mole` as its unit. Then it may be appropriate to set `AmountUnits` to `picomole`. In this case, the internal simulation values would be around 1, instead of around 10^{-12} as in the default case. AbsoluteTolerance of the simulation is determined using this internal value. Thus by choosing `picomole` as the amount unit, you effectively reduce the size of `AbsoluteTolerance`. Changing the `AmountUnits` property is closely related to changing `AbsoluteTolerance` when considering the effects on simulation results.

Even when using the default unit, it may be still necessary to change AbsoluteTolerance. For details, see “Selecting Absolute Tolerance and Relative Tolerance for Simulation”.

If you need to recover the simulation behavior from releases prior to R2015b:

- Set the `AmountUnit` to `mole`. However, if the model has quantity units in `molecule`, set the unit to `molecule` instead.
- Set the MassUnits to `kilogram`.

Tip If you have a custom function and UnitConversion is on (whether or not you are using the default unit `<automatic>`), follow the recommendation below.

- Non-dimensionalize the parameters that are passed to the function if they are not already dimensionless.

  Suppose you have a custom function defined as `y = f(t)` where `t` is the time in hour and `y` is the concentration of a species in mole/liter. When you use this function in your model to define a repeated assignment rule for instance, define it as: `s1 = f(time/t0)*s0`, where `time` is the simulation time, `t0` is a parameter defined as 1.0 hour, `s0` is a parameter defined as 1.0 mole/liter, and `s1` is the concentration of a species in mole/liter. Note that `time` and `s1` do not have to be in the same units as `t0` and `s0`, but they must be dimensionally consistent. For example, the `time` and `s1` units can be set to minute and picomole/liter, respectively.

Characteristics

Applies to	Object: `Configset`
Data type	Character vector
Data values	Character vector specifying any amount unit. The default is `<automatic>`.
Access	Read/write for properties of `Configset`

See Also

`Configset object`, MassUnits

BoundaryCondition

Indicate species boundary condition

Description

The `BoundaryCondition` property indicates whether reactions affect a species quantity.

When the `BoundaryCondition` of a species is `false` (default), the reactions can modify the species quantity. If a species is modified by reactions, then rules (repeated assignment rule, rate rule, or algebraic rule) cannot modify its value. SimBiology considers a reaction to modify a species when the net stoichiometry for the species is non-zero. For example, the reaction `X -> 2*X` modifies *X*, but the reaction `X + E -> Y + E` does not modify *E*.

When the `BoundaryCondition` of a species is `true`, then the value of the species is not changed by reactions during model simulation, even if the net stoichiometry is non-zero. Set the `BoundaryCondition` of a species to `true` if you want the species to participate in the reaction but you want to determine the value of that species using a rule instead. For example, set the `BoundaryCondition` of species *X* to `true` to specify its value using a repeated assignment rule but also to use species *X* in a reaction with `MassAction` kinetics, for example, `X + Y -> Z`.

For details on how these two properties affect a species quantity during simulation, see “How Species Amounts Change During Simulations”.

More Information

Consider the following two use cases of boundary conditions:

- Modeling receptor-ligand interactions that affect the rate of change of the receptor but not the ligand. For example, in response to hormone, steroid receptors such as the glucocorticoid receptor (GR) translocate from the cytoplasm (`cyt`) to the nucleus (`nuc`). The hsp90/ hsp70 chaperone complex directs this nuclear translocation [Pratt 2004 on page 3-12]. The natural ligand for GR is cortisol; the synthetic hormone dexamethasone (`dex`) is used in place of cortisol in experimental systems. In this system dexamethasone participates in the reaction but the quantity of dexamethasone in the cell is regulated using a rule. To simply model translocation of GR you could use the following reactions:

  Formation of the chaperone-receptor complex,

  ```
  Hsp90_complex + GR_cyt -> Hsp90_complex:GR_cyt
  ```

  In response to the synthetic hormone dexamethasone (`dex`), GR moves from the cytoplasm to the nucleus.

  ```
  Hsp90_complex:GR_cyt + dex -> Hsp90_complex + GR_nuc + dex
  ```

  For `dex`,

  ```
  BoundaryCondition = true; ConstantAmount = false
  ```

  In this example `dex` is modeled as a boundary condition with a rule to regulate the rate of change of `dex` in the system. Here, the quantity of `dex` is not determined by the rate of the second reaction but by a rate rule such as

```
ddex/dt = 0.001
```

which is specified in the SimBiology software as

```
dex = 0.001
```

- Modeling the role of nucleotides (for example, GTP, ATP, cAMP) and cofactors (for example, Ca^{++}, NAD^{+}, coenzyme A). Consider the role of GTP in the activation of Ras by receptor tyrosine kinases.

  ```
  Ras-GDP + GTP  -> Ras-GTP + GDP
  ```

  ```
  For GTP, BoundaryCondition = true; ConstantAmount = true
  ```

  Model GTP and GDP with boundary conditions, thus making them *boundary species*. In addition, you can set the `ConstantAmount on page 3-24` property of these species to `true` to indicate that their quantity does not vary during a simulation.

Characteristics

Applies to	Object: species
Data type	`boolean`
Data values	`true` or `false`. The default value is `false`.
Access	Read/write

Examples

Simulate a Model with a Boundary Condition for a Species

This example illustrates how to use the `BoundaryCondition` property of a species so that the species amount is not modified by the reaction it participates in, but by a user-defined dose object.

Load a sample project.

```
sbioloadproject radiodecay.sbproj
```

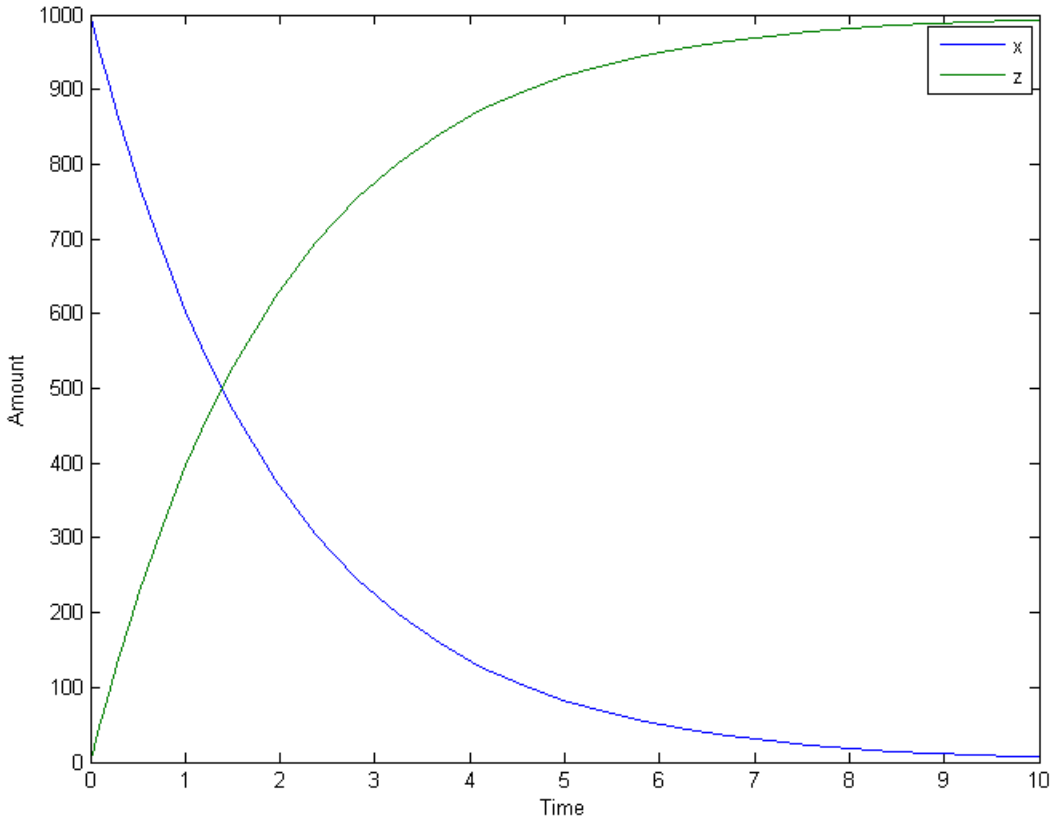
A SimBiology model named `m1` is loaded to the MATLAB Workspace. The model is a simple radioactive decay model in which two species (`x` and `z`) are modified by the following reaction.

```
m1.Reactions
```

```
   SimBiology Reaction Array

   Index:    Reaction:
   1         x -> z
```

Simulate the model and view results before adding any boundary conditions.

```
[t,x,names] = sbiosimulate(m1);
plot(t,x);
legend(names)
xlabel('Time');
ylabel('Amount');
```



Add a `RepeatDose` object to the model and specify the species to be dosed, dose amount, dose schedule, and units.

```
d1 = adddose(m1,'d1','repeat');
set(d1,'TargetName','z','Amount',100.0,'Interval',1.0,'RepeatCount',8);
set(d1,'TimeUnits','second','AmountUnits','molecule');
```

Set the `BoundaryCondition` of species `z` to be true so that the species will be modified by the dose object `d1`, but not by the reaction.

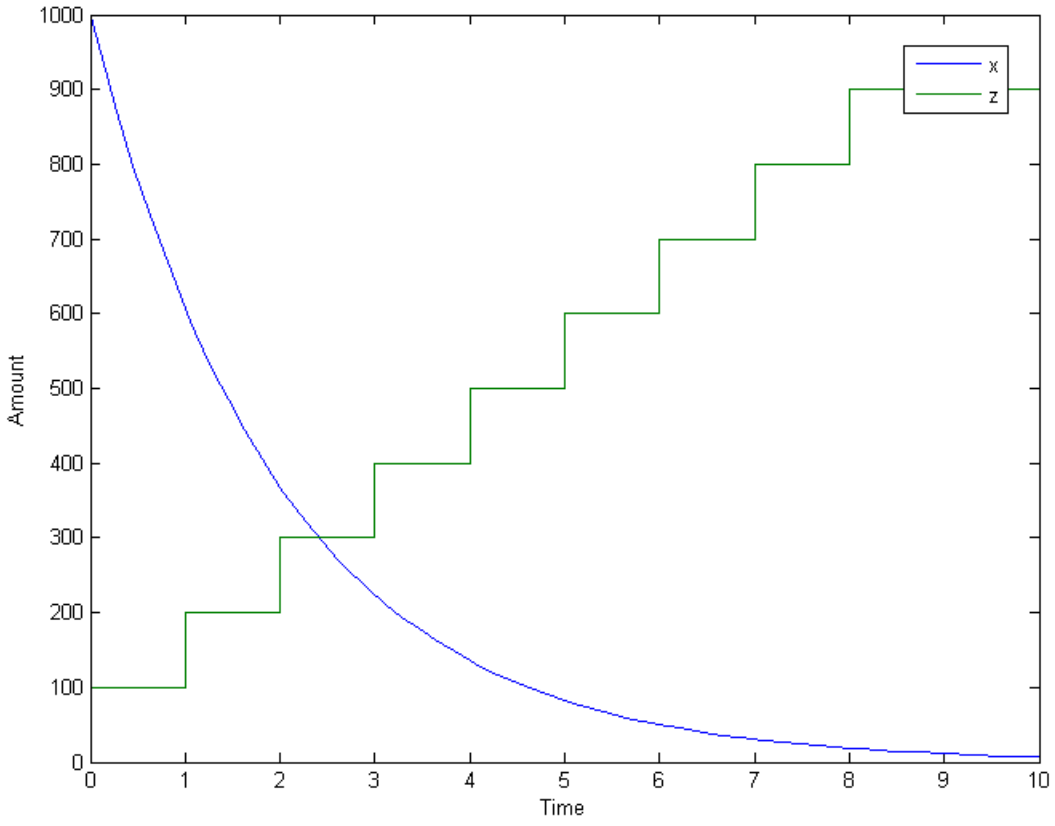
```
set(m1.species(2),'BoundaryCondition',true);
```

Simulate the model by applying the dose object.

```
[t2,x2,names] = sbiosimulate(m1,d1);
```

Plot the results. Notice that the amount of species `z` is now modified by the repeated dose object, but not by the reaction.

```
[t2,x2,names] = sbiosimulate(m1,d1);
plot(t2,x2);
legend(names);
xlabel('Time');
ylabel('Amount');
```



References

Pratt, W.B., Galigniana, M.D., Morishima, Y., Murphy, P.J. (2004), Role of molecular chaperones in steroid receptor action, *Essays Biochem*, 40:41-58.

See Also

`addrule`, `addspecies`, ConstantAmount, InitialAmount

BuiltInLibrary

Library of built-in components

Description

`BuiltInLibrary` is a SimBiology root object property containing all built-in components namely, unit, unit-prefixes, and kinetic laws that are shipped with the SimBiology product. You cannot add, modify, or delete components in the built-in library. The `BuiltInLibrary` property is an object that contains the following properties:

- `Units` — contains all units that are shipped with the SimBiology product. You can specify units for compartment capacity, species amounts and parameter values, to do dimensional analysis and unit conversion during simulation. You can display the built-in units either by using the command `sbiowhos -builtin -unit`, or by accessing the root object.
- `UnitPrefixes` — contains all unit-prefixes that are shipped with the SimBiology product. You can specify unit—prefixes in combination with a valid unit for compartment capacity, species amounts and parameter values, to do dimensional analysis and unit conversion during simulation. You can display the built-in unit-prefixes either by using the command `sbiowhos -builtin -unitprefix`, or by accessing the root object.
- `KineticLaws` — contains all kinetic laws that are shipped with the SimBiology product. Use the command `sbiowhos -builtin -kineticlaw` to see the list of built-in kinetic laws. You can use built-in kinetic laws when you use the command `addkineticlaw` to create a kinetic law object for a reaction object. Refer to the kinetic law by name when you create the kinetic law object, for example, `kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');`

  See “Kinetic Law Definition” on page 3-58 for a definition and more information.

Characteristics

`BuiltInLibrary`

Applies to	Object: root
Data type	object
Data values	Unit, unit-prefix, and abstract kinetic law objects
Access	Read-only

Characteristics for `BuiltInLibrary` properties:

- `Units`

Applies to	`BuiltInLibrary` property
Data type	unit objects
Data values	units
Access	Read-only

- `UnitPrefixes`

Applies to	`BuiltInLibrary` property
Data type	unit prefix objects
Data values	unit prefixes
Access	Read-only

- `KineticLaws`

Applies to	`BuiltInLibrary` property
Data type	Abstract kinetic law object
Data values	kinetic laws
Access	Read-only

Examples

Example 1

This example uses the command `sbiowhos` to show the current list of built-in components.

```
sbiowhos -builtin -kineticlaw
sbiowhos -builtin -unit
sbiowhos -builtin -unitprefix
```

Example 2

This example shows the current list of built-in components by accessing the root object.

```
rootObj = sbioroot;
get(rootObj.BuiltinLibrary, 'KineticLaws')
get(rootObj.BuiltinLibrary, 'Units')
get(rootObj.BuiltinLibrary, 'UnitPrefixes')
```

See Also

Functions — `sbioaddtolibrary`, `sbioremovefromlibrary`, `sbioroot`, `sbiounit`, `sbiounitprefix`

Properties — `UserDefinedLibrary`

Capacity

Compartment capacity

Description

The `Capacity` property indicates the size of the SimBiology compartment object. If the size of the compartment does not vary during simulation, set the property ConstantCapacity to `true`.

You can vary compartment capacity using rules or events.

Note Remember to set the `ConstantCapacity` property to false for varying capacity.

Events cannot result in the capacity having a negative value. Rules could result in the capacity having a negative value.

The `Capacity` property and Value property are identical.

Characteristics

Applies to	Object: compartment
Data type	`double`
Data values	Positive real number. The default value is `1`.
Access	Read/write

Examples

Add a compartment to a model and set the compartment capacity.

1. Create a model object named `my_model`.

```
modelObj = sbiomodel ('comp_model');
```

2. Add the compartment object named `nucleus` with a capacity of `0.5`.

```
compartmentObj = addcompartment(modelObj, 'nucleus', 0.5);
```

See Also

`addcompartment` | `addspecies` | CapacityUnits | ConstantCapacity | Value

Topics
“Model Simulation”
“Conservation of Amounts During Simulation”

CapacityUnits

Compartment capacity units

Description

The `CapacityUnits` property indicates the unit definition for the `Capacity` property of a compartment object. `CapacityUnits` can be any unit from the units library. To get a list of the defined units in the library, use the `sbioshowunits` function. If `CapacityUnits` changes from one unit definition to another, the `Capacity` does not automatically convert to the new units. The `sbioconvertunits` function does this conversion. To add a user-defined unit to the list, see `sbioaddtolibrary`.

The `CapacityUnits` property is identical to the `Units` property.

Characteristics

Applies to	Object: compartment
Data type	Character vector
Data values	Units from library with dimensions of length, area, or volume. Default = `''` (empty).
Access	Read/write

Note SimBiology uses units including empty units in association with DimensionalAnalysis and UnitConversion features.

- When `DimensionalAnalysis` and `UnitConversion` are both `false`, units are not used. However, SimBiology still performs a minimum level of dimensional analysis to decide whether a reaction rate is in dimensions of amount/time or concentration/time.
- When `DimensionalAnalysis` is `true` and `UnitConversion` is `false`, units (if not empty) must have consistent dimensions so that SimBiology can perform dimensional analysis. However, the units are not converted.
- When `UnitConversion` is set to `true` (which requires `DimensionalAnalysis` to be `true`), SimBiology performs a dimensional analysis and converts everything to consistent units. Hence, you must specify consistent units, and no units can be empty. If you have a dimensionless parameter, you must still set its unit to `dimensionless`.

Examples

1. Create a model object named `my_model`.

```
modelObj = sbiomodel ('my_model');
```

2. Add a compartment object named `cytoplasm` with a capacity of `0.5`.

```
compObj = addcompartment (modelObj, 'cytoplasm', 0.5);
```

3 Set the `CapacityUnits` to `femtoliter`, and verify.

```
set (compObj,'CapacityUnits', 'femtoliter');
get (compObj,'CapacityUnits')
```

MATLAB returns:

```
ans =

femtoliter
```

See Also

InitialAmount, `sbioaddtolibrary`, `sbioconvertunits`, `sbioshowunits`, ValueUnits

Compartments

Array of compartments in model or compartment

Description

`Compartments` shows you a read-only array of SimBiology compartment objects in the model object and the compartment object. In the model object, the `Compartments` property indicates all the compartments in a `Model` object as a flat list. In the compartment object, the `Compartments` property indicates other compartments that are referenced within the compartment. The two instances of `Compartments` are illustrated in “Examples” on page 3-18.

You can add a compartment object using the method `addcompartment`.

Characteristics

Applies to	Objects: compartment, model
Data type	Array of compartment objects
Data values	Compartment object. Default is `[]` (empty).
Access	Read-only

Examples

1 Create a model object named `modelObj`.

```
modelObj = sbiomodel('cell');
```

2 Add two compartments to the model object.

```
compartmentObj1 = addcompartment(modelObj, 'nucleus');
compartmentObj2 = addcompartment(modelObj, 'mitochondrion');
```

3 Add a compartment to one of the compartment objects.

```
compartmentObj3 = addcompartment(compartmentObj2, 'matrix');
```

4 Display the `Compartments` property in the model object.

```
get(modelObj, 'Compartments')
```

```
SimBiology Compartment Array

   Index:    Name:            Capacity:    CapacityUnits:
   1         nucleus          1
   2         mitochondrion    1
   3         matrix           1
```

5 Display the `Compartments` property in the compartment object.

```
get(compartmentObj2, 'Compartments')
```

```
SimBiology Compartment - matrix

   Compartment Components:
```

```
Capacity:          1
CapacityUnits:
Compartments:      0
ConstantCapacity:  true
Owner:             mitochondrion
Species:           0
```

See Also

addcompartment, addreaction, addspecies, Compartment object

CompileOptions

Dimensional analysis and unit conversion options

Description

The SimBiology `CompileOptions` property is an object that defines the compile options available for simulation; you can specify whether dimensional analysis and unit conversion is necessary for simulation. Compile options are checked during compile time. The compile options object can be accessed through the `CompileOptions` property of the `configset` object. Retrieve `CompileOptions` object properties with the `get` function and configure the properties with the `set` function.

Property Summary

DefaultSpeciesDimension	Dimension of species name in expression
DimensionalAnalysis	(To be removed) Perform dimensional analysis on model
Type	Display SimBiology object type
UnitConversion	Perform unit conversion

Characteristics

Applies to	Object: `configset`
Data type	Object
Data values	Compile-time options
Access	Read-only

Examples

1. Retrieve the `configset` object of `modelObj`.

```
modelObj = sbiomodel('cell');
configsetObj = getconfigset(modelObj);
```

2. Retrieve the `CompileOptions` object (`optionsObj`) from the `configsetObj`.

```
optionsObj = get(configsetObj, 'CompileOptions');

Compile Settings:

     UnitConversion:       false
     DimensionalAnalysis:  true
```

See Also

`get`, `set`

Composition

Unit composition

Description

The `Composition` property holds the composition of a unit object. The `Composition` property shows the combination of base and derived units that defines the unit. For example, molarity is the name of the unit and the composition is mole/liter. Base units are the set of units used to define all unit quantity equations. Derived units are defined using base units or mixtures of base and derived units.

Valid physical quantities for reaction rates are amount/time, mass/time, or concentration/time.

Characteristics

Applies to	Object: `Unit`
Data type	Character vector
Data values	Valid combination of units and prefixes from the library. Default is `''` (empty).
Access	Read/write

Examples

This example shows you how to create a user-defined unit, add it to the user-defined library, and query the `Composition` property.

1. Create a unit for the rate constants of a second-order reaction.

```
unitObj = sbiounit('secondconstant', '1/molarity*second', 1);
```

2. Query the `Composition` property.

```
get(unitObj, 'Composition')

ans =

1/molarity*second
```

3. Change the `Composition` property.

```
set(unitObj, 'Composition', 'liter/mole*second'))

ans =

liter/mole*second
```

4. Add the unit to the user-defined library.

```
sbioaddtolibrary(unitObj);
```

See Also

`get`, `Multiplier`, `sbiounit`, `set`

Constant

Specify variable or constant species amount, parameter value, or compartment capacity

Description

The `Constant` property is an alias for the following existing properties.

- ConstantAmount
- ConstantCapacity
- ConstantValue

Characteristics

Applies to	Object: species, parameter, compartment
Data type	`boolean`
Data values	`true` or `false`.
Access	Read/write

Version History

Introduced in R2019b

See Also

`addspecies` | BoundaryCondition | ConstantAmount | ConstantCapacity | ConstantValue | StatesToLog

Topics

“Model Simulation”
“Conservation of Amounts During Simulation”
“How Species Amounts Change During Simulations”

ConstantAmount

Specify variable or constant species amount

Description

The `ConstantAmount` property indicates whether the quantity of the species object can vary during the simulation. `ConstantAmount` can be either `true` or `false`. If `ConstantAmount` is `true`, the quantity of the species cannot vary during the simulation. By default, `ConstantAmount` is `false` and the quantity of the species can vary during the simulation. If `ConstantAmount` is `false`, the quantity of the species can be determined by reactions and rules.

The property `ConstantAmount` is for species objects; the property `ConstantValue on page 3-27` is for parameter objects.

Note When you want the species to participate in a reaction, but do not want any reactions to modify its quantity, set its BoundaryCondition to `true`, and `ConstantAmount` to `false`.

More Information

The following is an example of modeling species as constant amounts:

Modeling the role of nucleotides (GTP, ATP, cAMP) and cofactors (Ca^{++}, NAD^{+}, coenzyme A). Consider the role of GTP in the activation of Ras by receptor tyrosine kinases.

```
Ras-GDP + GTP  -> Ras-GTP + GDP
```

Model GTP and GDP with constant amount set to `true`. In addition, you can set the `BoundaryCondition` of these species to `true`, thus making them *boundary species*.

Characteristics

Applies to	Object: species
Data type	`boolean`
Data values	`true` or `false`. The default value is `false`.
Access	Read/write

Examples

1. Create a model object named `my_model`.

   ```
   modelObj = sbiomodel ('my_model');
   ```

2. Add a species object and verify that the `ConstantAmount` property setting is `'false'` or `0`.

   ```
   speciesObj = addspecies (modelObj, 'glucose');
   get (speciesObj, 'ConstantAmount')
   ```

   MATLAB returns:

```
ans =

     0
```

3 Set the constant amount to `'true'` and verify.

```
set (speciesObj, 'ConstantAmount', true);
get (speciesObj, 'ConstantAmount')
```

MATLAB returns:

```
ans =

     1
```

See Also

`addspecies`, BoundaryCondition

ConstantCapacity

Specify variable or constant compartment capacity

Description

The `ConstantCapacity` property indicates whether the capacity of the compartment object can vary during the simulation. `ConstantCapacity` can be either `true` (`1`) or `false` (`0`). If `ConstantCapacity` is `true`, the quantity of the compartment cannot vary during the simulation. By default, `ConstantCapacity` is `true` and the quantity of the compartment cannot vary during the simulation. If `ConstantCapacity` is `false`, the quantity of the compartment can be determined by rules and events.

Characteristics

Applies to	Object: compartment
Data type	`boolean`
Data values	`true` or `false`. The default value is `true`.
Access	Read/write

Examples

Add a compartment to a model and check the `ConstantCapacity` property of the compartment.

1. Create a model object named `comp_model`.

```
modelObj = sbiomodel ('comp_model');
```

2. Add the compartment object named `nucleus` with a capacity of `0.5`.

```
compartmentObj = addcompartment(modelObj, 'nucleus', 0.5);
```

3. Display the `ConstantCapacity` property.

```
get(compartmentObj, 'ConstantCapacity')
```

```
ans =
```

```
     1
```

See Also

`addcompartment` | ConstantAmount | ConstantValue

Topics

“Model Simulation”
“Conservation of Amounts During Simulation”

ConstantValue

Specify variable or constant parameter value

Description

The `ConstantValue` property indicates whether the value of a parameter can change during a simulation. Enter either `true` (value is constant) or `false` (value can change).

You can allow the value of the parameter to change during a simulation by specifying a rule that changes the `Value` property of the parameter object.

The property `ConstantValue` is for parameter objects; the property `ConstantAmount` is for species objects.

More Information

As an example, consider feedback inhibition of an enzyme such as aspartate kinase by threonine. Aspartate kinase has three isozymes that are independently inhibited by the products of downstream reactions (threonine, homoserine, and lysine). Although threonine is made through a series of reactions in the synthesis pathway, for illustration, the reactions are simplified as follows:

$$Aspartic\ \text{acid} \xrightarrow{\text{aspartate kinase}} \beta - Aspartylphosphate$$
$$\beta - Aspartylphosphate \rightarrow Threonine$$

To model inhibition of aspartate kinase by threonine, you could use a rule like the `algebraic` rule below to vary the rate of the above reaction and simulate inhibition. In the rule, the rate constant for the above reaction is denoted by `k_aspartate_kinase` and the quantity of threonine is `threonine`.

```
k_aspartate_kinase -(1/threonine)
```

Characteristics

Applies to	Object: parameter
Data type	`boolean`
Data values	`true` or `false`. The default value is `'true'`.
Access	Read/write

Examples

1. Create a model object.

   ```
   modelObj = sbiomodel ('my_model');
   ```

2. Add a parameter object.

   ```
   parameterObj = addparameter (modelObj, 'kf');
   ```

3. Change the `ConstantValue` property of the parameter object from default (`true`) to `false` and verify.

MATLAB returns `1` for `true` and `0` for `false`.

```
set (parameterObj, 'ConstantValue', false);
get(parameterObj, 'ConstantValue')
```

MATLAB returns:

```
ans =

     0
```

See Also

`addparameter`

Content

Contents of variant object

Description

The `Content` property contains the data for the variant object. `Content` is a cell array with the structure `{'Type', 'Name', 'PropertyName', 'PropertyValue'}`. You can store values for species `InitialAmount`, parameter `Value`, and compartment `Capacity`, in a variant object.

For more information about variants, see `Variant object`.

Characteristics

Applies to	Object: variant
Data type	`cell array`
Data values	Default value is `[]` (empty).
Access	Read/write

Examples

1 Create a model containing three species in one compartment.

```
modelObj = sbiomodel('mymodel');
compObj = addcompartment(modelObj, 'comp1');
A = addspecies(compObj, 'A');
B = addspecies(compObj, 'B');
C = addspecies(compObj, 'C');
```

2 Add a variant object that varies the species' `InitialAmount` property.

```
variantObj = addvariant(modelObj, 'v1');
addcontent(variantObj, {{'species','A', 'InitialAmount', 5}, ...
{'species', 'B', 'InitialAmount', 10}});
% Display the variant
variantObj

SimBiology Variant - v1 (inactive)

   ContentIndex:     Type:        Name:             Property:           Value:
   1                 species      A                 InitialAmount       5
   2                 species      B                 InitialAmount       10
```

3 Append data to the `Content` property.

```
addcontent(variantObj, {'species', 'C', 'InitialAmount', 15});

SimBiology Variant - v1 (inactive)

   ContentIndex:     Type:        Name:             Property:           Value:
   1                 species      A                 InitialAmount        5
   2                 species      B                 InitialAmount       10
   3                 species      C                 InitialAmount       15
```

4 Remove a species from the `Content` property.

```
rmcontent(variantObj, 3);
```

5 Replace the data in the `Content` property.

```
set(variantObj, 'Content', {'species', 'C', 'InitialAmount', 15});
```

See Also

`addcontent`, `rmcontent`, `sbiovariant`

CovariateLabels

Identify covariate columns in data set

Description

`CovariateLabels` is a property of the `PKData` object. It specifies the column in DataSet on page 3-32 that contains the covariate data.

Characteristics

Applies to	Object: `PKData`
Data type	Character vector or cell array of character vectors
Data values	Column headers from imported data set
Access	Read/write

See Also

`PKData object`

DataSet

`Dataset` object containing imported data

Description

`DataSet` is a property of the `PKData` object. It contains the imported data set. The `PKData` object constructor (`PKData`) assigns the specified data set to its `DataSet` property during construction.

Characteristics

Applies to	Object: `PKData`
Data type	`dataset` object
Data values	Variable containing `dataset` object
Access	Read-only

See Also

`PKData object`

DefaultSpeciesDimension

Dimension of species name in expression

Description

The `DefaultSpeciesDimension` property specifies how SimBiology interprets species names in expressions (namely reaction rate, rule, or event expressions). The valid property values are `substance` or `concentration`. If you specify `InitialAmountUnits`, SimBiology interprets species names appearing in expressions as concentration or substance amount according to the units specified, regardless of the value in `DefaultSpeciesDimension`. Thus, if `DefaultSpeciesDimension` is `concentration` and you specify species units as `molecule`, SimBiology interprets species names in expressions as `substance`. This interpretation applies even when `DimensionalAnalysis` is off.

You can find `DefaultSpeciesDimension` in the `CompileOptions` property.

When you set `DefaultSpeciesDimension` to `substance`, if you do not specify units, SimBiology interprets species names appearing in expressions as substance amounts, and does not scale by compartment capacity. To include a species concentration in an expression, divide by the appropriate compartment capacity in the expression. To specify compartment capacity in an expression enter the compartment name.

When you set `DefaultSpeciesDimension` to `concentration`, SimBiology interprets species names appearing in expressions as concentrations, and scales by compartment capacity in the expressions. To include a species amount in an expression, multiply by the species name by the appropriate compartment name in the expression.

For information on dimensional analysis for reaction rates, see “How Reaction Rates Are Evaluated”.

Characteristics

Applies to	Object: `CompileOptions` (in `configset` object)
Data type	Character vector
Data values	`concentration` or `substance`. Default value is `concentration`.
Access	Read/write

See Also

`CompileOptions`, `DimensionalAnalysis`, `get`, `getconfigset`, `sbiosimulate`, `set`

DependentVarLabel

Identify dependent variable column in data set

Description

`DependentVarLabel` is a property of a `PKData` object. It specifies the column(s) in DataSet on page 3-32 that contain the dependent variable(s), for example, measured response(s). The column must contain numeric values, and cannot contain `Inf` or `–Inf`.

Characteristics

Applies to	Object: `PKData`
Data type	Character vector or cell array of character vectors
Data values	Column header from an imported data set
Access	Read/write

See Also

`PKData object`

DependentVarUnits

Response units in PKData object

Description

`DependentVarUnits` is a property of a `PKData` object. It specifies the units for the column(s) containing the dependent variable(s) (responses) in the imported data set. If unit conversion is on, plot results in the SimBiology desktop show the units specified in `DependentVarUnits`.

To get a list of units, use the `sbioshowunits` on page 1-254 function.

Characteristics

Applies to	Object: `PKData`
Data type	Character vector or cell array of character vectors
Data values	Units from the units library. Default is an empty cell array. **Tip** If there are no units associated with the dependent variable(s) in your data set, you can set this property to a cell array of empty character vectors, or simply an empty cell array.
Access	Read/write

See Also

DependentVarLabel, `PKData object`

DimensionalAnalysis

(To be removed) Perform dimensional analysis on model

Note will be removed in a future release. Use UnitConversion instead.

Description

The `DimensionalAnalysis` property specifies whether to perform dimensional analysis on the model before simulation. It is a property of the `CompileOptions` object. `CompileOptions` holds the model's compile time options and is the object property of the `configset` object. When `DimensionalAnalysis` is set to `true`, the SimBiology software checks whether the physical quantities of the units involved in reactions and rules, match and are applicable.

For example, consider a reaction `a + b –> c`. Using mass action kinetics, the reaction rate is defined as `a*b*k`, where `k` is the rate constant of the reaction. If you specify that initial amounts of `a` and `b` are 0.01M and 0.005M respectively, then units of `k` are `1/(M*second)`. If you specify `k` with another equivalent unit definition, for example, `1/[(moles/liter)*second]`, `DimensionalAnalysis` checks whether the physical quantities match. If the physical quantities do not match, you see an error and the model is not simulated.

Unit conversion requires dimensional analysis. If `DimensionalAnalysis` is off, and you turn `UnitConversion` on, then `DimensionalAnalysis` is turned on automatically. If `UnitConversion` is on and you turn off `DimensionalAnalysis`, then `UnitConversion` is turned off automatically.

If you have MATLAB function calls in your model, dimensional analysis ignores any expressions containing function calls and generates a warning.

Valid physical quantities for reaction rates are amount/time, mass/time, or concentration/time.

Characteristics

Applies to	Object: `CompileOptions` (in `configset` object)
Data type	`boolean`
Data values	`true` or `false`. Default value is `true`.
Access	Read/write

Note SimBiology allows exponentiation of any dimensionless quantity to any dimensionless power. For example, you can write the following expression if both `x` and `a` are dimensionless: `(x + 3)^(a + 0.5)`

Note SimBiology uses units including empty units in association with DimensionalAnalysis and UnitConversion features.

- When `DimensionalAnalysis` and `UnitConversion` are both `false`, units are not used. However, SimBiology still performs a minimum level of dimensional analysis to decide whether a reaction rate is in dimensions of amount/time or concentration/time.

- When `DimensionalAnalysis` is `true` and `UnitConversion` is `false`, units (if not empty) must have consistent dimensions so that SimBiology can perform dimensional analysis. However, the units are not converted.
- When `UnitConversion` is set to `true` (which requires `DimensionalAnalysis` to be `true`), SimBiology performs a dimensional analysis and converts everything to consistent units. Hence, you must specify consistent units, and no units can be empty. If you have a dimensionless parameter, you must still set its unit to `dimensionless`.

Tip If you have a custom function and UnitConversion is on, follow the recommendation below.

- Non-dimensionalize the parameters that are passed to the function if they are not already dimensionless.

  Suppose you have a custom function defined as `y = f(t)` where `t` is the time in hour and `y` is the concentration of a species in mole/liter. When you use this function in your model to define a repeated assignment rule for instance, define it as: `s1 = f(time/t0)*s0`, where `time` is the simulation time, `t0` is a parameter defined as 1.0 hour, `s0` is a parameter defined as 1.0 mole/liter, and `s1` is the concentration of a species in mole/liter. Note that `time` and `s1` do not have to be in the same units as `t0` and `s0`, but they must be dimensionally consistent. For example, the `time` and `s1` units can be set to minute and picomole/liter, respectively.

Examples

This example shows how to retrieve and set `DimensionalAnalysis` from the default `true` to `false` in the default configuration set in a model object.

1 Import a model.

```
modelObj = sbmlimport('oscillator')

SimBiology Model - Oscillator

   Model Components:
     Models:            0
     Parameters:        0
     Reactions:         42
     Rules:             0
     Species:           23
```

2 Retrieve the `configset` object of the model object.

```
configsetObj = getconfigset(modelObj)

 Configuration Settings - default (active)
     SolverType:           ode15s
     StopTime:             10.000000

   SolverOptions:
     AbsoluteTolerance:    1.000000e-006
     RelativeTolerance:    1.000000e-003

   RuntimeOptions:
     StatesToLog:          all
```

```
   CompileOptions:
     UnitConversion:       true
     DimensionalAnalysis:  true
```

3 Retrieve the `CompileOptions` object.

```
optionsObj = get(configsetObj,'CompileOptions')

Compile Settings:

     UnitConversion:       true
     DimensionalAnalysis:  true
```

4 Assign a value of `false` to `DimensionalAnalysis`.

```
 set(optionsObj,'DimensionalAnalysis', false)
```

See Also

UnitConversion, `get`, `getconfigset`, `sbiosimulate`, `set`

Version History

R2023a: To be removed
Not recommended starting in R2023a

`DimensionalAnalysis` will be removed in a future release. Use UnitConversion instead.

Dosed

Dosed object name

Description

`Dosed` is a property of the `PKModelMap` object. It specifies the name(s) of species object(s) that receive an input, such as a drug in a compartment or a ligand.

When dosing multiple compartments, a one-to-one relationship must exist between the number and order of elements in the `Dosed` property and the `DosingType` property.

Characteristics

Applies to	Object: `PKModelMap`
Data type	Character vector or cell array of character vectors
Data values	Name of a species object or empty. Default is an empty cell array.
Access	Read/write

See Also

DosingType, Estimated, Observed, `PKModelMap object`

DoseLabel

Dose column in data set

Description

`DoseLabel` is a property of the `PKData` object. `DoseLabel` specifies the column that contains that contains the dosing information, in DataSet on page 3-32. The column must contain positive values, and cannot contain `Inf` or `–Inf`.

Characteristics

Applies to	Object: `PKData`
Data type	Character vector or array of character vectors
Data values	Column headers from imported data set
Access	Read/write

See Also

`PKData object`, `sbionmimport`, `sbionmfiledef`

DoseUnits

Dose units in PKData object

Description

The `DoseUnits` property indicates the units for dose values in the PKData object. Dose units must have dimensions of amount or mass. The length of `DoseUnits` must be the same as `DoseLabel`. For example, if the `DoseLabel` property defines two columns containing dosing information, `DoseUnits` must also define units for both columns. If unit conversion is on, dose and rate units must be consistent with each other (that is in terms of amount or mass) and must be consistent with the species object that is being dosed.

To get a list of units, use the `sbioshowunits` on page 1-254 function.

Characteristics

Applies to	Object: PKData
Data type	Character vector or cell array of character vectors
Data values	Units from units library. Default is `''` (empty).
Access	Read/write

See Also

DoseLabel, `PKData object`

DosingType

Drug dosing type in compartment

Description

`DosingType` is a property of the `PKCompartment` and `PKModelMap` objects. It specifies the type of dosing of a drug in a compartment. You can only dose one compartment in the model at any given time. For a description of the types of dosing supported, the model components created for each type of dosing, and the parameters to estimate, see “Dosing Types”.

Characteristics

Applies to	Objects: `PKCompartment`, `PKModelMap`
Data type	Character vector or cell array of character vectors
Data values	`''`, `'Bolus'`, `'Infusion'`, `'ZeroOrder'`, `'FirstOrder'`
Access	Read/write

See Also

EliminationType, `PKCompartment object`, `PKModelMap object`

DurationParameterName

Parameter specifying length of time to administer a dose

Description

`DurationParameterName` is a property of a `RepeatDose` or `ScheduleDose` object.

Specify the name of a parameter object that is scoped to a model. This parameter defines the length of time it takes to administer a dose.

you can parameterize the property by setting it to the name of a model-scoped parameter that is not being modified by a repeated assignment rule, an algebraic rule, or a rate rule. However, the parameter can be modified by an event.

Note If you set the `DurationParameterName` property of a dose, you must also specify the `Amount` property of the dose, and set the `Rate` property to `0`. This is because the rate is calculated from the amount and duration.

Characteristics

Applies to	Objects: `RepeatDose`, `ScheduleDose`.
Data type	Character vector.
Data values	Name of a model-scoped parameter object. The default value is an empty character vector `''`.
Access	Read/write.

Examples

Estimate Time Lag and Duration of a Dose

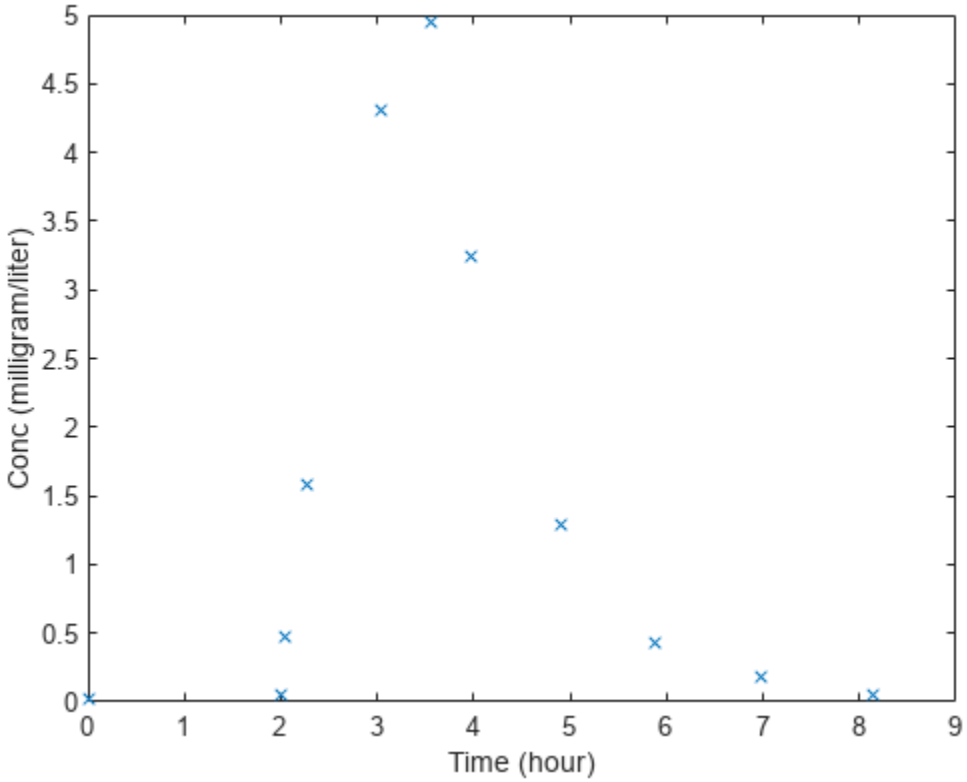
This example shows how to estimate the time lag before a bolus dose was administered and the duration of the dose using a one-compartment model.

Load a sample data set.

```
load lagDurationData.mat
```

Plot the data.

```
plot(data.Time,data.Conc,'x')
xlabel('Time (hour)')
ylabel('Conc (milligram/liter)')
```



Convert to groupedData.

```
gData = groupedData(data);
gData.Properties.VariableUnits = {'hour','milligram/liter'};
```

Create a one-compartment model.

```
pkmd                    = PKModelDesign;
pkc1                    = addCompartment(pkmd,'Central');
pkc1.DosingType         = 'Bolus';
pkc1.EliminationType    = 'linear-clearance';
pkc1.HasResponseVariable = true;
model                   = construct(pkmd);
configset               = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
```

Add two parameters that represent the time lag and duration of a dose. The lag parameter specifies the time lag before the dose is administered. The duration parameter specifies the length of time it takes to administer a dose.

```
lagP = addparameter(model,'lagP');
lagP.ValueUnits = 'hour';
durP = addparameter(model,'durP');
durP.ValueUnits = 'hour';
```

Create a dose object. Set the `LagParameterName` and `DurationParameterName` properties of the dose to the names of the lag and duration parameters, respectively. Set the dose amount to 10 milligram which was the amount used to generate the data.

```
dose                = sbiodose('dose');
dose.TargetName     = 'Drug_Central';
dose.StartTime      = 0;
dose.Amount         = 10;
dose.AmountUnits    = 'milligram';
dose.TimeUnits      = 'hour';
dose.LagParameterName = 'lagP';
dose.DurationParameterName = 'durP';
```

Map the model species to the corresponding data.

```
responseMap = {'Drug_Central = Conc'};
```

Specify the lag and duration parameters as parameters to estimate. Log-transform the parameters. Initialize them to 2 and set the upper bound and lower bound.

```
paramsToEstimate    = {'log(lagP)','log(durP)'};
estimatedParams     = estimatedInfo(paramsToEstimate,'InitialValue',2,'Bounds',[1 5]);
```

Perform parameter estimation.

```
fitResults = sbiofit(model,gData,responseMap,estimatedParams,dose,'fminsearch')
```

```
fitResults =
  OptimResults with properties:

                  ExitFlag: 1
                    Output: [1x1 struct]
                 GroupName: One group
                      Beta: [2x4 table]
        ParameterEstimates: [2x4 table]
                         J: [11x2 double]
                      COVB: [2x2 double]
          CovarianceMatrix: [2x2 double]
                         R: [11x1 double]
                       MSE: 0.0024
                       SSE: 0.0213
                   Weights: []
              LogLikelihood: 18.7511
                       AIC: -33.5023
                       BIC: -32.7065
                       DFE: 9
            DependentFiles: {1x2 cell}
                      Data: [11x2 groupedData]
   EstimatedParameterNames: {'lagP'  'durP'}
             ErrorModelInfo: [1x3 table]
         EstimationFunction: 'fminsearch'
```

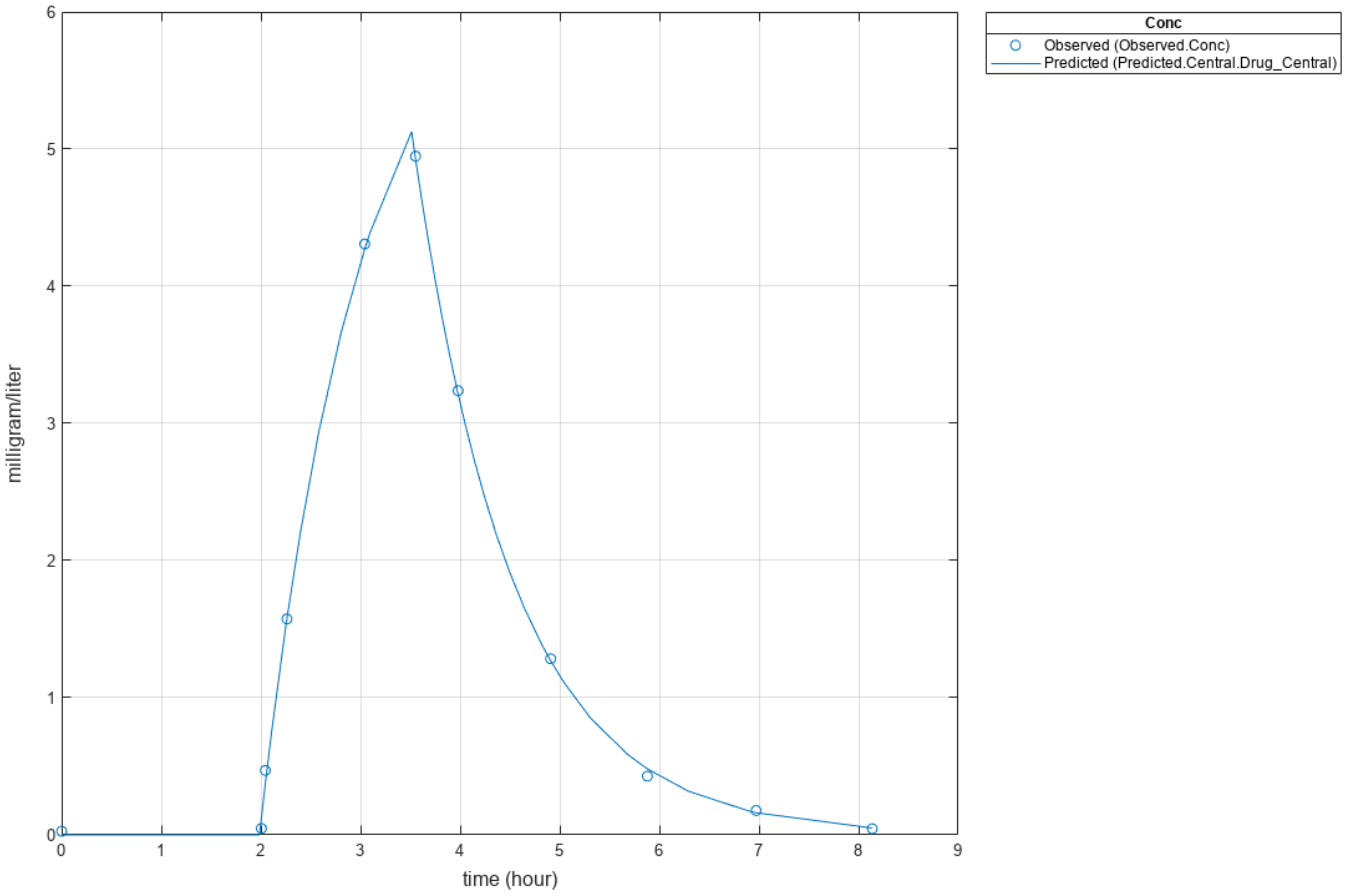
Display the result.

```
fitResults.ParameterEstimates
```

```
ans=2×4 table
      Name      Estimate    StandardError    Bounds
    ________    ________    _____________    ______

    {'lagP'}     1.986        0.0051568      1    5
```

```
    {'durP'}     1.527         0.012956      1    5
```

```
plot(fitResults)
```



See Also

`RepeatDose object` | `ScheduleDose object`

Topics

“Parameterized and Adaptive Doses”

EliminationType

Drug elimination type from compartment

Description

`EliminationType` is a property of the `PKCompartment` object. It specifies the type of elimination of a drug from a compartment. For a description of the types of elimination supported, the model components created for each type of elimination, and the parameters to estimate, see “Elimination Types”.

Characteristics

Applies to	Object: `PKCompartment`
Data type	Character vector
Data values	`'Linear'`, `'Linear-Clearance'`, `'Enzymatic'`, and `''`
Access	Read/write

See Also

`addCompartment`, DosingType, `PKCompartment object`

Estimated

Names of parameters to estimate

Description

`Estimated` is a property of the `PKModelMap` object. It specifies the name(s) of the object(s) to estimate. Specify the name(s) of species, compartment, or parameter object(s) that are scoped to a model.

Note If you specify a species object, you are estimating the InitialAmount property of the species object.

Characteristics

Applies to	Object: `PKModelMap`
Data type	Character vector or cell array of character vectors
Data values	Name of a species, compartment, or parameter object or empty. Default is an empty cell array.
Access	Read/write

See Also

Dosed, InitialAmount, Observed, `PKModelMap object`

EventFcns

Event expression

Description

Property of the event object that defines what occurs when the event is triggered. Specify a cell array of character vectors.

`EventFcns` can be any MATLAB assignment or expression that defines what is executed when the event is triggered. All `EventFcn` expressions are assignments of the form '*`objectname = expression`*', where *`objectname`* is the name of a valid SimBiology object.

For more information about how SimBiology handles events, see “How Events Are Evaluated”. For examples of event functions, see “Specifying Event Functions”.

Characteristics

Applies to	Object: event
Data type	Cell array of character vectors
Data values	Expressions for `EventFcn` (default is an empty character vector `''`)
Access	Read/write

Tip If UnitConversion is on and your model has any event, follow the recommendation below.

Non-dimensionalize any parameters used in the event `Trigger` if they are not already dimensionless. For example, suppose you have a trigger `x > 1`, where *x* is the species concentration in mole/liter. Non-dimensionalize *x* by scaling (dividing) it with a constant such as `x/x0 > 1`, where *x0* is a parameter defined as 1.0 mole/liter. Note that *x* does not have to have the same unit as the constant *x0*, but must be dimensionally consistent with it. For example, the unit of *x* can be picomole/liter instead of mole/liter.

Examples

1. Create a model object, and then add an event object.

```
modelObj = sbmlimport('oscillator');
eventObj = addevent(modelObj, 'time>= 5', 'OpC = 200');
```

2. Set the `EventFcns` property of the event object.

```
set(eventObj, 'EventFcns', {'pA = OpA','mA = pol'});
```

3. Get the `EventFcns` property.

```
get(eventObj, 'EventFcns')
```

See Also

`Event`, Trigger

EventMode

Determine how events that change dose parameters affect in-progress dosing

Description

`EventMode` is a property of `RepeatDose` and `ScheduleDose` objects. This property determines whether to continue the ongoing dose, that is, a dose with a nondefault infusion rate or dose duration, to completion when an event changes a parameter that is referenced by a dose property. Dose properties that you can parameterize are: Amount, Rate, Interval, StartTime, RepeatCount, LagParameterName, and DurationParameterName.

If `EventMode` is set to `'continue'`, the ongoing dose continues to completion when the event changes dose parameters, and updated parameters affect only subsequent doses. If `EventMode` is set to `'stop'`, the ongoing dose stops immediately when dose parameters change, and subsequent doses use the updated parameters.

To decide whether a parameter has been changed, SimBiology compares the old value of a parameter to the new value. For instance, the following event does not change the `doseStartTime` parameter value: `addevent(model,'time >= 5','doseStartTime = doseStartTime * 1')`.

Any change in dose parameters affects the schedule of doses generated. If the simulation reaches a time point for a scheduled dose, the dose is applied. If an event changes dose parameters, SimBiology updates the dose schedule, ignores any doses scheduled before the current simulation time, and applies only the subsequent doses. Suppose that you have parameterized the `StartTime` property of a dose. Updating the parameter with an event causes to regenerate the dose schedule. If there are any previously-scheduled doses before the current simulation time, they are ignored.

By default, SimBiology uses the following MATLAB expression to generate a list of dose times (dose schedule) whenever an event changes any dose parameter, using the updated parameter values:

scheduledDoseTimes = *StartTime* + (0:*RepeatCount*) * *Interval* + *Lag*,

where *StartTime*, *RepeatCount*, and *Interval* are properties of the dose object. *Lag* is the time lag parameter for a dose, referenced by the `LagParameterName` property.

Characteristics

Applies to	Objects: `RepeatDose`, `ScheduleDose`
Data type	Character vector
Data values	`'stop'` (default) or `'continue'`
Access	Read/write

Examples

Change Dose Behavior In Response to Changes in Model Parameters

Create a simple model with linear elimination, an amount parameter, and a rate parameter.

```
model                       = sbiomodel('simple model');
compartment                 = addcompartment(model,'Central',1);
compartment.CapacityUnits   = 'liter';
species                     = addspecies(model,'drug');
species.InitialAmountUnits  = 'milligram';

% Elimination rate
elimParam                   = addparameter(model,'kel',0.1);
elimParam.ValueUnits        = '1/hour';

% Elimination reaction
reaction                    = addreaction(model,'drug -> null');
reaction.ReactionRate       = 'kel*drug';

% Add amount and rate parameters
amountParam                 = addparameter(model,'A',50);
amountParam.ConstantValue   = false;
amountParam.ValueUnits      = 'milligram'

amountParam =
   SimBiology Parameter Array

   Index:    Name:    Value:    Units:
   1         A        50        milligram


rateParam                   = addparameter(model,'R',10);
rateParam.ValueUnits        = 'milligram/hour'

rateParam =
   SimBiology Parameter Array

   Index:    Name:    Value:    Units:
   1         R        10        milligram/hour
```

Create a dose with its `Amount` and `Rate` properties set to the amount and rate parameters 'A' and 'R', respectively.

```
dose                        = adddose(model,'adaptive dose','repeat');
dose.Amount                 = 'A';
dose.Rate                   = 'R';
```

Set other dose properties.

```
dose.TargetName             = 'drug';
dose.StartTime              = 0;
dose.TimeUnits              = 'hour';
dose.Interval               = 24;
dose.RepeatCount            = 7;
```

Prepare the configuration set to simulate the model for 7 days.

```
configset           = getconfigset(model);
configset.StopTime  = 7*24;
configset.TimeUnits = 'hour';
```

Add an event to reset the dose amount to 10 at time >= 26.

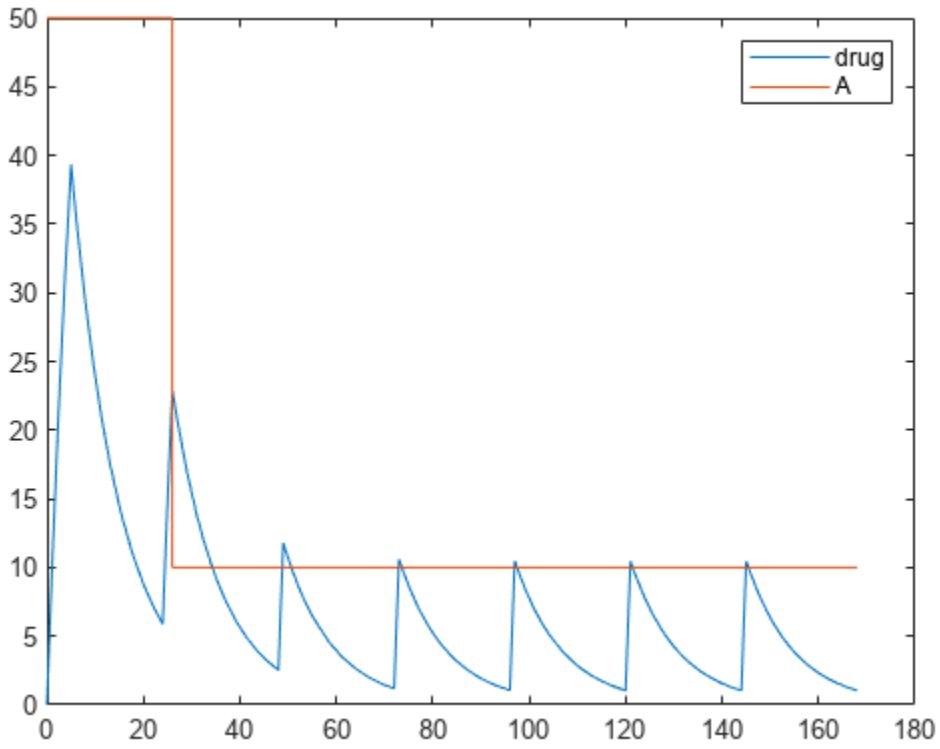
```
event = addevent(model,'time >= 26','A = 10');
```

Set the `EventMode` property to 'stop'. This setting causes any ongoing dose event to stop at 26 hours.

```
dose.EventMode = 'stop';
```

Simulate the model. The second dose event stops at 26 hours, and the subsequent dose events continue with the new dose amount of 10.

```
[time, drugAndAmount] = sbiosimulate(model,dose);
figure
plot(time, drugAndAmount);
legend('drug','A');
```

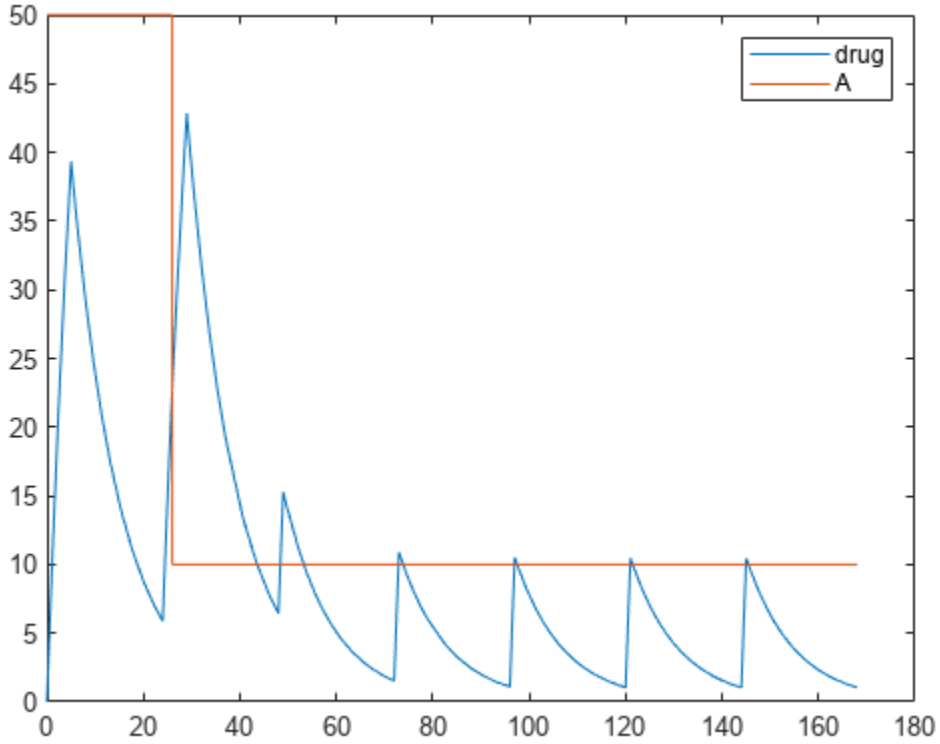


Alternatively, you can allow the ongoing dose event to finish before applying the new dose amount by setting `EventMode` to 'continue'.

```
dose.EventMode = 'continue';
```

Simulate the model. In this case, the second dose event continues to 26 hours.

```
[time, drugAndAmount] = sbiosimulate(model,dose);
figure
plot(time, drugAndAmount);
legend('drug','A');
```



See Also

`RepeatDose object` | `ScheduleDose object`

Topics

“Parameterized and Adaptive Doses”

Events

Contain all event objects

Description

Property to indicate events in a model object. Read-only array of `Event` objects.

An event defines an action when a defined condition is met. For example, the quantity of a species may double when the quantity of species `B` is `100`. An event is triggered when the conditions specified in the event are met by the model. For more information, see “Events” and “Events in SimBiology Models”.

Add an event to a `Model` object with the method `addevent (model)` method and remove an event with the `delete` method. See `Event` for more information.

You can view event object properties with the `get` command and modify the properties with the `set` command.

Characteristics

Applies to	Object: model
Data type	Array of event objects
Data values	Event object. The default is `[]` (empty).
Access	Read-only

Examples

1 Create a model object, and then add an event object.

```
modelObj = sbmlimport('oscillator')
eventObj = addevent(modelObj, 'time>= 5', 'OpC = 200');
```

2 Get a list of properties for an event object.

```
get(modelObj.Events(1));
```

Or

```
get(eventObj)
```

MATLAB displays a list of event properties.

```
            Active: 1
        Annotation: ''
         EventFcns: {'OpC = 200'}
              Name: ''
             Notes: ''
            Parent: [1x1 SimBiology.Model]
               Tag: ''
           Trigger: 'time >= 5'
      TriggerDelay: 0
```

```
    TriggerDelayUnits: 'second'
                 Type: 'event'
             UserData: []
```

See Also

EventFcns, Event, Model, Trigger

Exponent

Exponent value of unit prefix

Description

`Exponent` shows the value of `10^Exponent` that defines the numerical value of the unit prefix *`Name`*. You can use the unit prefix in conjunction with any built-in or user-defined units. For example, for the unit `mole`, specify as `picomole` to use the `Exponent`, `-12`.

Characteristics

Applies to	Object: Unit prefix
Data type	`double`
Data values	Real number. Default is `0`.
Access	Read/write

Examples

This example shows you how to create a user-defined unit prefix, add it to the user-defined library, and query the `Exponent` property.

1. Create a unit prefix.

```
unitprefixObj1 = sbiounitprefix('peta', 15);
```

2. Add the unit prefix to the user-defined library.

```
sbioaddtolibrary(unitprefixObj1);
```

3. Query the `Exponent` property.

```
get(unitprefixObj1, 'Exponent')

ans =

    15
```

See Also

`get`, `sbioaddtolibrary`, `sbiounitprefix`, `set`, `UnitPrefix object`

Expression

Expression to determine reaction rate equation or expression of observable object

Description

The `Expression` property can be a property of `KineticLaw` (or `AbstractKineticLaw`) object or an `observable` object.

For an `observable` object, the `Expression` property is a mathematical expression that lets you perform post-simulation calculations. For details, see `Observable`.

For a `KineticLaw` object, the `Expression` property indicates the mathematical expression that is used to determine the `ReactionRate on page 3-116` property of the reaction object. `Expression` is a reaction rate expression assigned by the kinetic law definition used by the reaction. The kinetic law being used is indicated by the property `KineticLawName on page 3-76`. You can configure `Expression` for user-defined kinetic laws, but not for built-in kinetic laws. `Expression` is read only for kinetic law objects.

Note If you set the `Expression` property to a reaction rate expression that is not continuous and differentiable, see “Using Events to Address Discontinuities in Rule and Reaction Rate Expressions” before simulating your model.

Kinetic Law Definition

The *kinetic law definition* provides a mechanism for applying a specific rate law to multiple reactions. It acts as a mapping template for the reaction rate. The kinetic law is defined by a mathematical expression, (defined in the property `Expression`), and includes the species and parameter variables used in the expression. The species variables are defined in the `SpeciesVariables on page 3-138` property, and the parameter variables are defined in the `ParameterVariables on page 3-105` property of the kinetic law object.

If a reaction is using a kinetic law definition, the `ReactionRate` property of the reaction object shows the result of a mapping from the kinetic law definition. To determine `ReactionRate`, the species variables and parameter variables that participate in the reaction rate should be mapped in the kinetic law for the reaction. In this case, SimBiology software determines the `ReactionRate` by using the `Expression` property of the abstract kinetic law object, and by mapping `SpeciesVariableNames on page 3-136` to `SpeciesVariables` and `ParameterVariableNames on page 3-103` to `ParameterVariables`.

For example, the kinetic law definition `Henri-Michaelis-Menten` has the `Expression` Vm*S/(Km +S), where `Vm` and `Km` are defined as parameters in the `ParameterVariables` property of the abstract kinetic law object, and `S` is defined as a species in the `SpeciesVariable` property of the abstract kinetic law object.

By applying the `Henri-Michaelis-Menten` kinetic law to a reaction `A -> B` with `Va` mapping to `Vm`, `A` mapping to `S`, and `Ka` mapping to `Km`, the rate equation for the reaction becomes Va*A/(Ka+A).

The exact expression of a reaction using `MassAction` kinetic law varies depending upon the number of reactants. Thus, for mass action kinetics the `Expression` property is set to `MassAction` because in general for mass action kinetics the reaction rate is defined as

$$r = k \prod_{i=1}^{nr} [Si]^{m_i}$$

where `[Si]` is the concentration of the `ith` reactant, m_i is the stoichiometric coefficient of `[Si]`, n_r is the number of reactants, and `k` is the mass action reaction rate constant.

SimBiology software contains some built-in kinetic laws. You can also define your own kinetic laws. To find the list of available kinetic laws, use the `sbiowhos -kineticlaw` command (`sbiowhos on page 1-311`). You can create a kinetic law definition with the function `sbioabstractkineticlaw` and add it to the library using `sbioaddtolibrary on page 1-16`.

Characteristics

Applies to	Objects: abstract kinetic law, kinetic law, observable
Data type	Character vector
Data values	Defined by kinetic law definition
Access	Read-only in kinetic law object. Read/write in user-defined kinetic law.

Examples

Example 1

Example with `Henri-Michaelis-Menten` kinetics

1. Create a model object, and add a reaction object to the model.

```
modelObj = sbiomodel ('my_model');
reactionObj = addreaction (modelObj, 'a + b -> c + d');
```

2. Define a kinetic law for the reaction object.

```
kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
```

3. Verify that the `Expression` property for the kinetic law object is `Henri-Michaelis-Menten`.

```
get (kineticlawObj, 'Expression')
```

MATLAB returns:

```
ans =

Vm*S/(Km + S)
```

4. The `'Henri-Michaelis-Menten'` kinetic law has two parameter variables (`Vm` and `Km`) and one species variable (`S`) that you should set. To set these variables, first create the parameter variables as parameter objects (`parameterObj1, parameterObj2`) with names `Vm_d, Km_d`, and assign the objects' `Parent` property value to the `kineticlawObj`. The species object with `Name a` is created when `reactionObj`is created and need not be redefined.

```
parameterObj1 = addparameter(kineticlawObj, 'Vm_d');
parameterObj2 = addparameter(kineticlawObj, 'Km_d');
```

5 Set the variable names for the kinetic law object.

```
set(kineticlawObj,'ParameterVariableNames', {'Vm_d' 'Km_d'});
set(kineticlawObj,'SpeciesVariableNames', {'a'});
```

6 Verify that the reaction rate is expressed correctly in the reaction object `ReactionRate` property.

```
get (reactionObj, 'ReactionRate')
```

MATLAB returns:

```
ans =

Vm_d*a/(Km_d+a)
```

Example 2

Example with `Mass Action` kinetics.

1 Create a model object, and then add a reaction object.

```
modelObj = sbiomodel ('my_model');
reactionObj = addreaction (modelObj, 'a + b -> c + d');
```

2 Define a kinetic law for the reaction object.

```
kineticlawObj = addkineticlaw(reactionObj, 'MassAction');
get(kineticlawObj, 'Expression')
```

MATLAB returns:

```
ans =

MassAction
```

3 Assign the rate constant for the reaction.

```
set (kineticlawObj, 'ParameterVariablenames', 'k');

get (reactionObj, 'ReactionRate')
```

MATLAB returns:

```
ans =

k*a*b
```

See Also

KineticLawName, Parameters, ParameterVariableNames, ParameterVariables, ReactionRate, `sbioaddtolibrary`, `sbiowhos`, SpeciesVariables, SpeciesVariableNames

GroupID

Integer identifying each group in data set

Description

`GroupID` is a property of the `PKData` object. It is an array of the same length as the DataSet on page 3-32 property containing an integer to identify each group. `PKData` sets this property during construction of the `PKData` object.

Characteristics

Applies to	Object: `PKData`
Data type	`double`
Data values	Index value for each group
Access	Read-only

See Also

`PKData object`

GroupLabel

Identify group column in data set

Description

`GroupLabel` is a property of the `PKData` object. It specifies the column in DataSet on page 3-32 that contains the group identification labels.

Characteristics

Applies to	Object: `PKData`
Data type	Character vector
Data values	Column header from imported data set
Access	Read/write

See Also

`PKData object`, GroupNames

GroupNames

Unique values from `GroupLabel` in data set

Description

`GroupNames` is a property of the `PKData` object. It contains unique values from the data column specified by the `GroupLabel` property. `PKData` sets this property during construction of the `PKData` object.

Characteristics

Applies to	Object: `PKData`
Data type	Character vector or cell array of character vectors
Data values	Unique values in `GroupLabel`
Access	Read-only

See Also

`PKData object`, GroupLabel

HasLag

Lag associated with dose targeting compartment

Description

`HasLag` is a property of the `PKCompartment` object. It is a logical indicating if the dose targeting the compartment has a time lag or not.

Characteristics

Applies to	Object: `PKCompartment`
Data type	logical
Data values	`1` (true) or `0` (false). Default is `0` (false).
Access	Read/write

See Also

`addCompartment`, DosingType, EliminationType, `PKCompartment object`

HasResponseVariable

Compartment drug concentration reported

Description

`HasResponseVariable` is a property of the `PKCompartment` object. It is a logical indicating if the drug concentration in this compartment is reported.

Note The `HasResponseVariable` property can be `true` for more than one `PKCompartment` object in the model. If you perform a parameter fit on a model, at least one `PKCompartment` object in the model must have a `HasResponseVariable` property set to `true`.

Characteristics

Applies to	Object: `PKCompartment`
Data type	Logical
Data values	`1` (true) or `0` (false). Default is `0` (false).
Access	Read/write

See Also

`addCompartment`, DosingType, EliminationType, `PKCompartment object`

IndependentVarLabel

Identify independent variable column in data set

Description

`IndependentVarLabel` is a property of the `PKData` object. It specifies the column in DataSet on page 3-32 that contains the independent variable (for example, time).

The column must contain positive values, and cannot contain, `NaN`, `Inf` or `–Inf`.

Characteristics

Applies to	Object: `PKData`
Data type	Character vector
Data values	Column header from imported data set
Access	Read/write

See Also

`PKData object`

IndependentVarUnits

Time units in PKData object

Description

The `IndependentVarUnits` property indicates the units for the column containing the independent variable (time) in the `PKData` object. If unit conversion is on, plot results in the SimBiology desktop show the units specified in `IndependentVarUnits`.

To get a list of units, use the `sbioshowunits` on page 1-254 function.

Characteristics

Applies to	Object: PKData
Data type	Character vector
Data values	Time units. Default is `''` (empty).
Access	Read/write

See Also

`DependentVarLabel`, `PKData object`

InitialAmount

Species initial amount

Description

The `InitialAmount` property indicates the initial quantity of the SimBiology species object. `InitialAmount` is the quantity of the species before the simulation starts.

The `InitialAmount` property and Value property are identical.

Characteristics

Applies to	Object: species
Data type	`double`
Data values	Positive real number. Default value is `0`.
Access	Read/write

Examples

Add a species to a model and set the initial amount of the species.

1. Create a model object named `my_model`.

```
modelObj = sbiomodel ('my_model');
```

2. Add the species object named `glucose`.

```
speciesObj = addspecies (modelObj, 'glucose');
```

3. Set the initial amount to `100` and verify.

```
set (speciesObj, 'InitialAmount',100);
get (speciesObj, 'InitialAmount')
```

MATLAB returns:

```
ans =

   100
```

See Also

Value`addspecies`, InitialAmountUnits

InitialAmountUnits

Species initial amount units

Description

The `InitialAmountUnits` property indicates the unit definition for the `InitialAmount` property of a species object. `InitialAmountUnits` can be one of the built-in units. To get a list of the defined units, use the `sbioshowunits` on page 1-254 function. If `InitialAmountUnits` changes from one unit definition to another, `InitialAmount` does not automatically convert to the new units. The `sbioconvertunits` function does this conversion. To add a user-defined unit to the list, use `sbiounit` followed by `sbioaddtolibrary`.

See DefaultSpeciesDimension for more information on specifying dimensions for species quantities. `InitialAmountUnits` must have corresponding dimensions to `CapacityUnits`. For example, if the `CapacityUnits` are $\texttt{meter}^2$, then species must be $\texttt{amount/meter}^2$ or `amount`.

The `InitialAmountUnits` property is identical to the `Units` property.

Characteristics

Applies to	Object: species
Data type	Character vector
Data values	Units from library with dimensions of amount, amount/length, amount/area, or amount/volume. Default is `''` (empty).
Access	Read/write

Note SimBiology uses units including empty units in association with DimensionalAnalysis and UnitConversion features.

- When `DimensionalAnalysis` and `UnitConversion` are both `false`, units are not used. However, SimBiology still performs a minimum level of dimensional analysis to decide whether a reaction rate is in dimensions of amount/time or concentration/time.
- When `DimensionalAnalysis` is `true` and `UnitConversion` is `false`, units (if not empty) must have consistent dimensions so that SimBiology can perform dimensional analysis. However, the units are not converted.
- When `UnitConversion` is set to `true` (which requires `DimensionalAnalysis` to be `true`), SimBiology performs a dimensional analysis and converts everything to consistent units. Hence, you must specify consistent units, and no units can be empty. If you have a dimensionless parameter, you must still set its unit to `dimensionless`.

Examples

1 Create a model object named `my_model`.

```
modelObj = sbiomodel ('my_model');
compObj = addcompartment(modelObj, 'cell');
```

2 Add a species object named `glucose`.

```
speciesObj = addspecies (compObj, 'glucose');
```

3 Set the initial amount to `100`, `InitialAmountUnits` to `molecule`, and verify.

```
set (speciesObj,'InitialAmountUnits','molecule');
get (speciesObj,'InitialAmountUnits')
```

MATLAB returns:

```
ans =

molecule
```

See Also

DefaultSpeciesDimension, InitialAmount, `sbioaddtolibrary`, `sbioconvertunits`, `sbioshowunits`, `sbiounit`, ValueUnits

Inputs

Specify species and parameter input factors for sensitivity analysis

Description

`Inputs` is a property of the `SensitivityAnalysisOptions` object.
`SensitivityAnalysisOptions` is a property of the configuration set object.

Use `Inputs` to specify the species, parameters, or compartments with respect to which you want to compute the sensitivities of the species or parameter states in your model.

The SimBiology software calculates sensitivities with respect to the values of the parameters, capacities of compartments, and the initial amounts of the species specified in the `Inputs` property. When you simulate a model with `SensitivityAnalysis` enabled in the active configuration set object, sensitivity analysis returns the computed sensitivities of the species and parameters specified in the Outputs property. For a description of the output, see the SensitivityAnalysisOptions property description.

Characteristics

Applies to	Object: `SensitivityAnalysisOptions`
Data type	Species, parameter, or compartment object or an array of objects **Note** • If this object is determined by a repeated assignment rule, then you cannot use it as an `Inputs` property. • To be an input factor, a compartment object must have a constant capacity, that is, its `ConstantCapacity` property must be set to `true`. • If a parameter is referenced by the `LagParameterName` and `DurationParameterName` property of a `RepeatDose object`, the parameter must be constant to be an input for sensitivity analysis. • If a parameter is referenced by any other `RepeatDose object` properties, namely, `Amount`, `Rate`, `Interval`, `StartTime`, and `RepeatCount`, you cannot use the parameter as an input for sensitivity analysis.
Data values	Species, compartment, or parameter object, or an array of objects. Default is `[]` (empty array).
Access	Read/write

Examples

This example shows how to set `Inputs` for sensitivity analysis.

1. Import the radio decay model from the SimBiology demos.

```
modelObj  = sbmlimport('radiodecay');
```

2. Retrieve the configuration set object from `modelObj`.

```
configsetObj = getconfigset(modelObj);
```

3. Add a parameter to the `Inputs` property and display it. Use the `sbioselect` function to retrieve the parameter object from the model.

```
SimBiology Parameter Array

Index:    Name:    Value:    ValueUnits:
 1         c        0.5       1/second
```

See Also

Outputs, `sbioselect`, SensitivityAnalysis, SensitivityAnalysisOptions

Interval

Time between doses

Description

`Interval` is a property of a `RepeatDose` object. This property defines the equally spaced times between repeated doses.

For `RepeatDose` objects, you can parameterize the property by setting it to the name of a model-scoped parameter that is not being modified by a repeated assignment rule, an algebraic rule, or a rate rule. However, the parameter can be modified by an event.

Note When the `Interval` property is `0`, `RepeatDose` ignores the `RepeatCount` property, that is, it treats it as though it is set to `0`.

Characteristics

Applies to	Object: `RepeatDose`.
Data type	double or character vector.
Data values	Nonnegative real number or name of a model-scoped parameter object. The default value is `0`.
Access	Read/Write.

See Also

`RepeatDose object` | `ScheduleDose object`

Topics

“Parameterized and Adaptive Doses”

KineticLaw

Show kinetic law used for `ReactionRate`

Description

The `KineticLaw` property shows the kinetic law that determines the reaction rate specified in the `ReactionRate` property of the reaction object. This property shows the kinetic law used to define `ReactionRate`.

`KineticLaw` can be configured with the `addkineticlaw on page 2-43` method. The `addkineticlaw` function configures the `ReactionRate` based on the `KineticLaw` and the species and parameters specified in the kinetic law object properties `SpeciesVariableNames on page 3-136` and `ParameterVariableNames on page 3-103`. `SpeciesVariableNames` are determined automatically for mass action kinetics.

If you update the reaction, the `ReactionRate` property automatically updates only for mass action kinetics. For all other kinetics, you must set the `SpeciesVariableNames` property of the kinetic law object.

For information on dimensional analysis for reaction rates, see “How Reaction Rates Are Evaluated”.

Characteristics

Applies to	Object: reaction
Data type	Kinetic law object
Data values	Kinetic law object. Default is `[]` (empty).
Access	Read-only

Examples

Example with `Henri-Michaelis-Menten` kinetics

1. Create a model object, and then add a reaction object.

```
modelObj = sbiomodel ('my_model');
reactionObj = addreaction (modelObj, 'a + b -> c + d');
```

2. Define a kinetic law for the reaction object.

```
kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
```

3. Verify that the `KineticLaw` property for the reaction object is `Henri-Michaelis-Menten`.

```
get (reactionObj, 'KineticLaw')
```

MATLAB returns:

```
SimBiology Kinetic Law Array

 Index:    KineticLawName:
   1       Henri-Michaelis-Menten
```

See Also

KineticLawName, Parameters, ParameterVariableNames, ReactionRate, SpeciesVariableNames, Expression (AbstractKineticLaw, KineticLaw)

KineticLawName

Name of kinetic law applied to reaction

Description

The `KineticLawName` property of the kinetic law object indicates the name of the kinetic law definition applied to the reaction. `KineticLawName` can be any valid name from the built-in or user-defined kinetic law library. See “Kinetic Law Definition” on page 3-58 for more information.

You can find the `KineticLawName` list in the kinetic law library by using the command `sbiowhos -kineticlaw` (`sbiowhos on page 1-311`). You can create a kinetic law definition with the function `sbioabstractkineticlaw` and add it to the library using `sbioaddtolibrary on page 1-16`.

Characteristics

Applies to	Object: kineticlaw
Data type	Character vector
Data values	Character vector specified by kinetic law definition
Access	Read-only

Examples

1 Create a model object, add a reaction object, and define a kinetic law for the reaction object.

```
modelObj = sbiomodel ('my_model');
reactionObj = addreaction (modelObj, 'a + b -> c + d');
kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
```

2 Verify the `KineticLawName` of `kineticlawObj`.

```
get (kineticlawObj, 'KineticLawName')
```

MATLAB returns:

```
ans =

Henri-Michaelis-Menten
```

See Also

Expression(AbstractKineticLaw, KineticLaw), Parameters, ParameterVariableNames, ParameterVariables, ReactionRate, `sbioaddtolibrary`, `sbiowhos`, SpeciesVariables, SpeciesVariableNames

LagParameter

Parameter specifying time lag for doses

Description

`LagParameter` is a property of the `PKModelMap` object. It specifies the name(s) of parameter object(s) that represent the time lag(s) of doses associated with the `PKModelMap` object.

Specify the name(s) of parameter object(s) that are:

- Scoped to a model
- Constant, that is, their `ConstantValue` property is `true`

When dosing multiple compartments, a one-to-one relationship must exist between the number and order of elements in the `LagParameter` property and the `DosingType` property. For a dose that has no lag, use `''` (an empty character vector).

Characteristics

Applies to	Object: `PKModelMap`
Data type	Character vector or cell array of character vectors **Tip** If you are not using any doses with time lags, you can set this property to a cell array of empty character vectors, or simply an empty cell array.
Data values	Name(s) of parameter object(s) or empty. Default is an empty cell array. The parameter objects must be: • Scoped to a model • Constant, that is, have a `ConstantValue` property set to `true`.
Access	Read/write

See Also

DosingType, `PKModelMap object`

LagParameterName

Parameter specifying time lag for dose

Description

`LagParameterName` is a property of a `RepeatDose` or `ScheduleDose` object.

Specify the name of a parameter object that is scoped to a model. The parameter defines the length of time it takes for the dose to reach its target after being introduced.

You can parameterize the property by setting it to the name of a model-scoped parameter that is not being modified by a repeated assignment rule, an algebraic rule, or a rate rule. However, the parameter can be modified by an event.

Characteristics

Applies to	Objects: `RepeatDose`, `ScheduleDose`.
Data type	Character vector.
Data values	Name of a model-scoped parameter object. The default value is an empty character vector `''`.
Access	Read/write.

Examples

Estimate Time Lag and Duration of a Dose

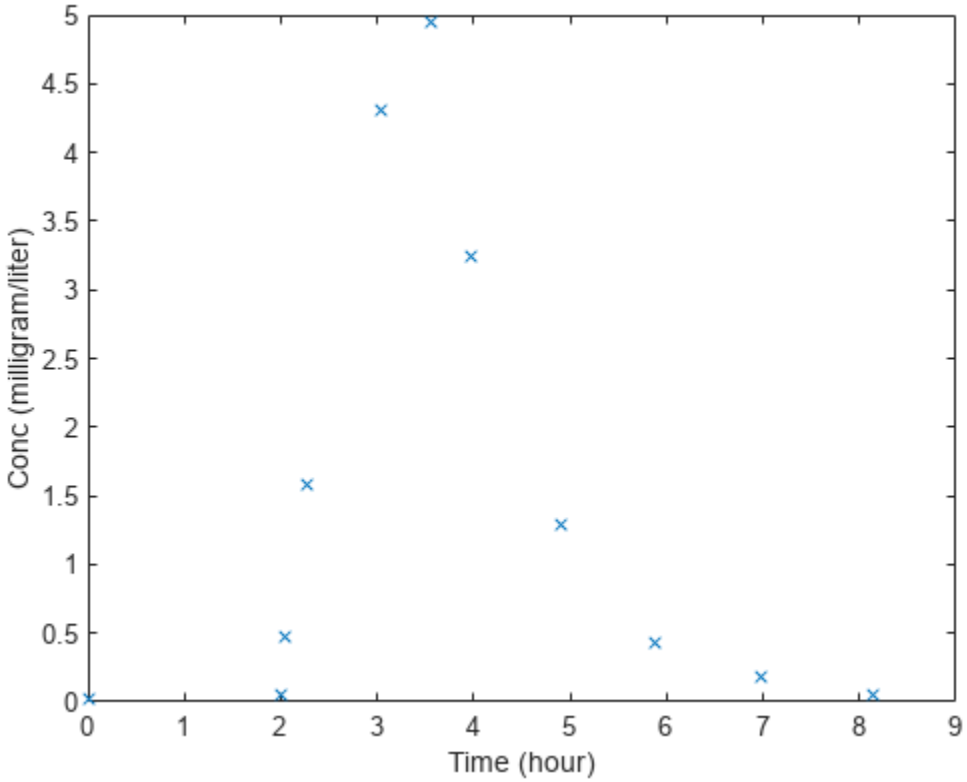
This example shows how to estimate the time lag before a bolus dose was administered and the duration of the dose using a one-compartment model.

Load a sample data set.

```
load lagDurationData.mat
```

Plot the data.

```
plot(data.Time,data.Conc,'x')
xlabel('Time (hour)')
ylabel('Conc (milligram/liter)')
```



Convert to groupedData.

```
gData = groupedData(data);
gData.Properties.VariableUnits = {'hour','milligram/liter'};
```

Create a one-compartment model.

```
pkmd                    = PKModelDesign;
pkc1                    = addCompartment(pkmd,'Central');
pkc1.DosingType         = 'Bolus';
pkc1.EliminationType    = 'linear-clearance';
pkc1.HasResponseVariable = true;
model                   = construct(pkmd);
configset               = getconfigset(model);
configset.CompileOptions.UnitConversion = true;
```

Add two parameters that represent the time lag and duration of a dose. The lag parameter specifies the time lag before the dose is administered. The duration parameter specifies the length of time it takes to administer a dose.

```
lagP = addparameter(model,'lagP');
lagP.ValueUnits = 'hour';
durP = addparameter(model,'durP');
durP.ValueUnits = 'hour';
```

Create a dose object. Set the `LagParameterName` and `DurationParameterName` properties of the dose to the names of the lag and duration parameters, respectively. Set the dose amount to 10 milligram which was the amount used to generate the data.

```
dose                = sbiodose('dose');
dose.TargetName     = 'Drug_Central';
dose.StartTime      = 0;
dose.Amount         = 10;
dose.AmountUnits    = 'milligram';
dose.TimeUnits      = 'hour';
dose.LagParameterName = 'lagP';
dose.DurationParameterName = 'durP';
```

Map the model species to the corresponding data.

```
responseMap = {'Drug_Central = Conc'};
```

Specify the lag and duration parameters as parameters to estimate. Log-transform the parameters. Initialize them to 2 and set the upper bound and lower bound.

```
paramsToEstimate    = {'log(lagP)','log(durP)'};
estimatedParams     = estimatedInfo(paramsToEstimate,'InitialValue',2,'Bounds',[1 5]);
```

Perform parameter estimation.

```
fitResults = sbiofit(model,gData,responseMap,estimatedParams,dose,'fminsearch')
```

```
fitResults =
  OptimResults with properties:

                  ExitFlag: 1
                    Output: [1x1 struct]
                 GroupName: One group
                      Beta: [2x4 table]
        ParameterEstimates: [2x4 table]
                         J: [11x2 double]
                      COVB: [2x2 double]
          CovarianceMatrix: [2x2 double]
                         R: [11x1 double]
                       MSE: 0.0024
                       SSE: 0.0213
                   Weights: []
              LogLikelihood: 18.7511
                       AIC: -33.5023
                       BIC: -32.7065
                       DFE: 9
            DependentFiles: {1x2 cell}
                      Data: [11x2 groupedData]
    EstimatedParameterNames: {'lagP'  'durP'}
             ErrorModelInfo: [1x3 table]
         EstimationFunction: 'fminsearch'
```

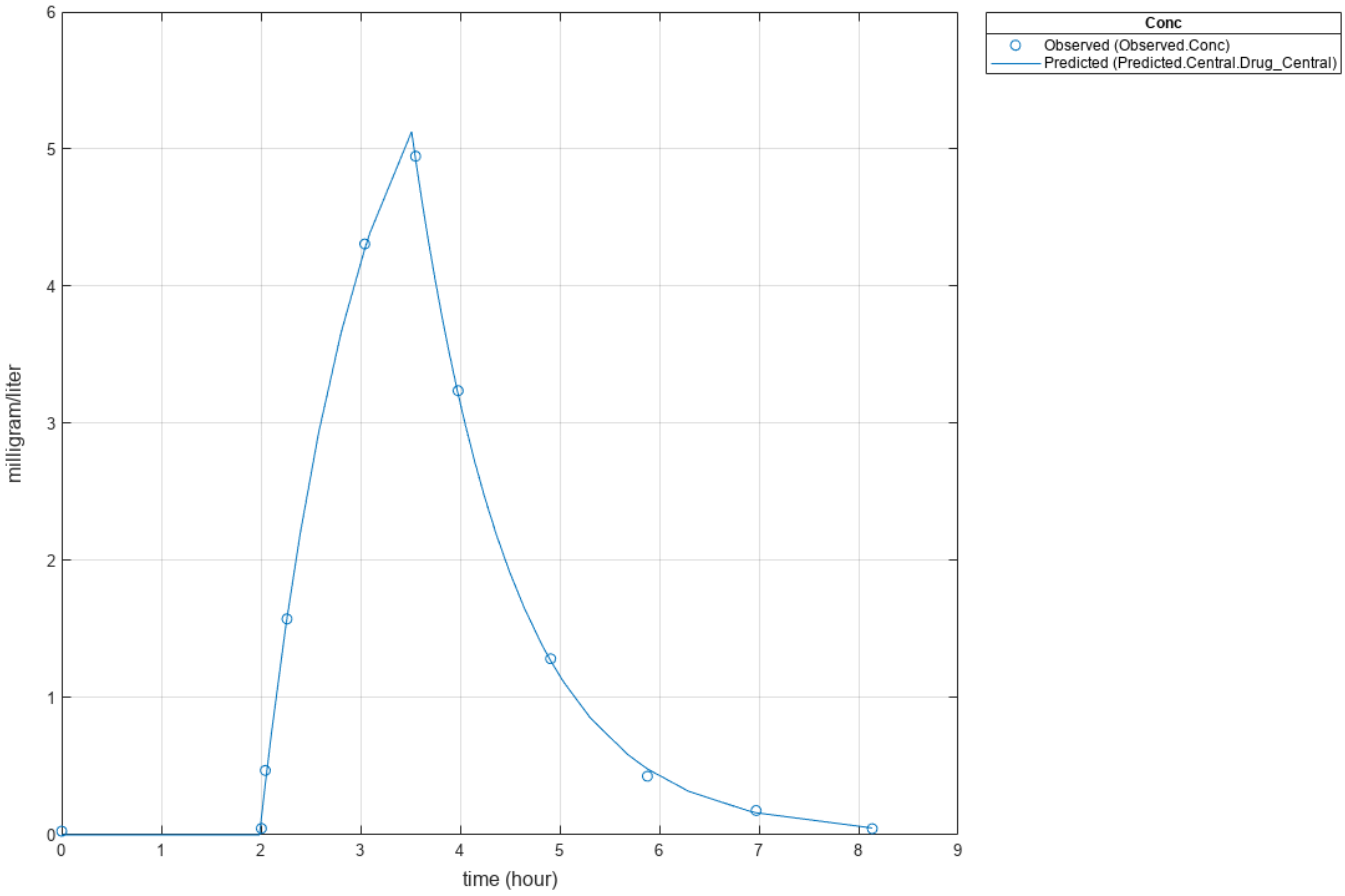
Display the result.

```
fitResults.ParameterEstimates
```

```
ans=2×4 table
      Name      Estimate    StandardError    Bounds
    ________    ________    _____________    ______

    {'lagP'}     1.986        0.0051568      1    5
```

```
    {'durP'}     1.527         0.012956      1    5
```

```
plot(fitResults)
```



See Also

`RepeatDose object` | `ScheduleDose object`

Topics

“Parameterized and Adaptive Doses”

MassUnits

Mass unit used internally during simulation when UnitConversion is on

Description

This property defines the mass unit that SimBiology uses internally during model simulation when UnitConversion is on. You can set this to any string representing a mass unit such as gram, or gram with any valid prefix. It can also be a custom unit if it is consistent with mass as its dimension. The default is `<automatic>`, which means SimBiology automatically selects a mass unit for simulation. SimBiology examines the units on all of the states and selects a mass unit such that AbsoluteTolerance of the states in mass or mass per volume is at least as stringent as the simulation absolute tolerance multiplied by the smallest mass unit. This stringency is relaxed appropriately for states that become large when AbsoluteToleranceScaling is on.

Note It is recommended that you use the default unit (`<automatic>`) or choose units for states such that the simulated values are neither too large (greater than 10^6) or too small (less than 10^{-6}).

However, for some edge cases, you may need to change `MassUnits`. Suppose you have a model with a state that takes on values around 10^{-12} `gram` for the entire simulation, and you need to use `gram` as its unit. Then it may be appropriate to set `MassUnits` to `picogram`. In this case, the internal simulation values would be around 1, instead of around 10^{-12} as in the default case. AbsoluteTolerance of the simulation is determined using this internal value. Thus by choosing `picogram` as the mass unit, you effectively reduce the size of `AbsoluteTolerance`. Changing the `MassUnits` property is closely related to changing `AbsoluteTolerance` when considering the effects on simulation results.

Even when using the default unit, it may be still necessary to change AbsoluteTolerance. For details, see “Selecting Absolute Tolerance and Relative Tolerance for Simulation”.

If you need to recover the simulation behavior from releases prior to R2015b:

- Set the `MassUnits` to `kilogram`.
- Set the AmountUnits to `mole`. However, if the model has quantity units in `molecule`, set the unit to `molecule` instead.

Tip If you have a custom function and UnitConversion is on (whether or not you are using the default unit `<automatic>`), follow the recommendation below.

- Non-dimensionalize the parameters that are passed to the function if they are not already dimensionless.

  Suppose you have a custom function defined as `y = f(t)` where `t` is the time in hour and `y` is the concentration of a species in mole/liter. When you use this function in your model to define a repeated assignment rule for instance, define it as: `s1 = f(time/t0)*s0`, where `time` is the simulation time, `t0` is a parameter defined as 1.0 hour, `s0` is a parameter defined as 1.0 mole/liter, and `s1` is the concentration of a species in mole/liter. Note that `time` and `s1` do not have to be in the same units as `t0` and `s0`, but they must be dimensionally consistent. For example, the `time` and `s1` units can be set to minute and picomole/liter, respectively.

Characteristics

Applies to	Object: `Configset`
Data type	Character vector
Data values	Character vector specifying any mass unit. The default is `<automatic>`.
Access	Read/write for properties of `Configset`

See Also

`Configset object`, AmountUnits

MaximumNumberOfLogs

Maximum number of logs criteria to stop simulation

Description

`MaximumNumberOfLogs` is a property of a `Configset` object. This property sets the maximum number of logs criteria to stop a simulation.

A simulation stops when it meets any of the criteria specified by `StopTime`, `MaximumNumberOfLogs`, or `MaximumWallClock`. However, if you specify the `OutputTimes` property of the `SolverOptions` property of the `Configset` object, then `StopTime` and `MaximumNumberOfLogs` are ignored. Instead, the last value in `OutputTimes` is used as the `StopTime` criteria, and the length of `OutputTimes` is used as the `MaximumNumberOfLogs` criteria.

Characteristics

Applies to	Object: `Configset`
Data type	`double`
Data values	Positive value. Default is `Inf`.
Access	Read/write

Examples

Set Maximum Number of Logs Criteria to Stop Simulation

Set the maximum number of logs that triggers a simulation to stop.

Create a `model` object named `cell` and save it in a variable named `modelObj`.

```
modelObj  = sbiomodel('cell');
```

Retrieve the configuration set from `modelObj` and save it in a variable named `configsetObj`.

```
configsetObj = getconfigset(modelObj);
```

Configure the simulation stop criteria by setting the `MaximumNumberOfLogs` property to `50`. Leave the `StopTime` and `MaximumWallClock` properties at their default values of `10` seconds and `Inf`, respectively.

```
set(configsetObj, 'MaximumNumberOfLogs', 50)
```

View the properties of `configsetObj`.

```
get(configsetObj)
```

```
                 Active: 1
         CompileOptions: [1x1 SimBiology.CompileOptions]
                   Name: 'default'
                  Notes: ''
```

```
            RuntimeOptions: [1x1 SimBiology.RuntimeOptions]
SensitivityAnalysisOptions: [1x1 SimBiology.SensitivityAnalysisOptions]
             SolverOptions: [1x1 SimBiology.ODESolverOptions]
                SolverType: 'ode15s'
                  StopTime: 10
       MaximumNumberOfLogs: 50
          MaximumWallClock: Inf
                  TimeUnits: 'second'
                AmountUnits: '<automatic>'
                  MassUnits: '<automatic>'
                       Type: 'configset'
```

When you simulate `modelObj`, the simulation stops when `50` logs are created or when the simulation time reaches `10` seconds, whichever comes first.

See Also

`Configset object`, MaximumWallClock, OutputTimes, StopTime

MaximumWallClock

Maximum elapsed wall clock time to stop simulation

Description

`MaximumWallClock` is a property of a `Configset` object. This property sets the maximum elapsed wall clock time (seconds) criteria to stop a simulation.

A simulation stops when it meets any of the criteria specified by `StopTime`, `MaximumNumberOfLogs`, or `MaximumWallClock`. However, if you specify the `OutputTimes` property of the `SolverOptions` property of the `Configset` object, then `StopTime` and `MaximumNumberOfLogs` are ignored. Instead, the last value in `OutputTimes` is used as the `StopTime` criteria, and the length of `OutputTimes` is used as the `MaximumNumberOfLogs` criteria.

Characteristics

Applies to	Object: `Configset`
Data type	`double`
Data values	Positive scalar. Default is `Inf`.
Access	Read/write

Examples

Set Maximum Wall Clock Criteria to Stop Simulation

Set the maximum wall clock time (in seconds) that triggers a simulation to stop.

Create a `model` object named `cell` and save it in a variable named `modelObj`.

```
modelObj  = sbiomodel('cell');
```

Retrieve the configuration set from `modelObj` and save it in a variable named `configsetObj`.

```
configsetObj = getconfigset(modelObj);
```

Configure the simulation stop criteria by setting the `MaximumWallClock` property to `20` seconds. Leave the `StopTime` and `MaximumNumberOfLogs` properties at their default values of `10` seconds and `Inf`, respectively.

```
set(configsetObj, 'MaximumWallClock', 20)
```

View the properties of `configsetObj`.

```
get(configsetObj)
```

```
                Active: 1
        CompileOptions: [1x1 SimBiology.CompileOptions]
                  Name: 'default'
                 Notes: ''
```

```
            RuntimeOptions: [1x1 SimBiology.RuntimeOptions]
SensitivityAnalysisOptions: [1x1 SimBiology.SensitivityAnalysisOptions]
             SolverOptions: [1x1 SimBiology.ODESolverOptions]
                SolverType: 'ode15s'
                  StopTime: 10
       MaximumNumberOfLogs: Inf
          MaximumWallClock: 20
                 TimeUnits: 'second'
               AmountUnits: '<automatic>'
                 MassUnits: '<automatic>'
                      Type: 'configset'
```

When you simulate `modelObj`, the simulation stops when the simulation time reaches `10` seconds or the wall clock time reaches `20` seconds, whichever comes first.

See Also

`Configset object`, MaximumNumberOfLogs, OutputTimes, StopTime

Models

Contain all model objects

Description

The `Models` property shows the models in the SimBiology root. It is a read-only array of model objects.

SimBiology has a hierarchical organization. A model object has the SimBiology root as its `Parent`. Parameter objects can have a model object or kinetic law object as `Parent`. You can display all the component objects with *`modelObj`*`.Models` or `get (`*`modelObj`*`, 'Models')`.

Characteristics

Applies to	Objects: root
Data type	Array of model objects
Data values	Model object. Default is `[]` (empty).
Access	Read-only

See Also

`sbiomodel`

Multiplier

Relationship between defined unit and base unit

Description

The `Multiplier` is the numerical value that defines the relationship between the unit `Name` and the base unit as a product of the `Multiplier` and the base unit. For example, in `1 mole = 6.0221e23*molecule`, the `Multiplier` is `6.0221e23`.

Characteristics

Applies to	Object: Unit
Data type	`double`
Data values	Nonzero real number. Default value is 1.
Access	Read/write

Examples

This example shows how to create a user-defined unit, add it to the user-defined library, and query the library.

1. Create a user-defined unit called `usermole`, whose composition is `molecule` and `Multiplier` property is `6.0221e23`.

   ```
   unitObj = sbiounit('usermole', 'molecule', 6.0221e23);
   ```

2. Add the unit to the user-defined library.

   ```
   sbioaddtolibrary(unitObj);
   ```

3. Query the `Multiplier` property.

   ```
   get(unitObj, 'Multiplier')

   ans =

   1/molarity*second
   ```

See Also

`Composition`, `get`, `sbiounit`, `set`

Name

Specify name of object

Description

The `Name` property identifies a SimBiology object. Compartments, species, parameters, observables, and model objects can be referenced by other objects using the `Name` property, therefore `Name` must be unique for these objects. However, species names need only be unique within each compartment. Parameter names must be unique within a model (if at the model level), or within each kinetic law (if at the kinetic law level). This means that you can have nonunique species names if the species are in different compartments, and nonunique parameter names if the parameters are in different kinetic laws or at different levels. Note that having nonunique parameter names can cause the model to have shadowed parameters and that may not be best modeling practice.

Use the function `sbioselect` to find an object with the same `Name` property value.

In addition, note the following constraints and reserved characters for the `Name` property in objects:

- Model and parameter names cannot be empty, the word `time`, all whitespace, or contain the characters `[` or `]`.
- Compartment and species names cannot be empty, the word `null`, the word `time` or contain the characters `->`, `<->`, `[` or `]`.
  - However, compartment and species names can contain the words `null` and `time` within the name, such as `nulldrug` or `nullreceptor`.
- Reaction, event, and rule names cannot be the word `time` or contain the characters `[` or `]`.
- If you have a parameter, a species, or compartment name that is not a valid MATLAB variable name, when you write an event function, an event trigger, a reaction, reaction rate equation, or a rule you must enclose that name in brackets. For example, enclose `[DNA polymerase+]` in brackets. In addition, if you have the same species in multiple compartments you must qualify the species with the compartment name, for example, `nucleus.[DNA polymerase+]`, `[nuclear complex].[DNA polymerase+]`.

For more information on valid MATLAB variable names, see `matlab.lang.makeValidName`, `matlab.lang.makeUniqueStrings`, and `isvarname`.

Characteristics

Applies to	Objects: abstract kinetic law, configuration set, compartment, event, kinetic law, model, observable, parameter, reaction, RepeatDose, rule, ScheduleDose, species, unit, or variant
Data type	Character vector
Data values	Any character vector except reserved words and characters
Access	Read/write

Examples

1. Create a model object named `my_model`.

   ```
   modelObj = sbiomodel ('my_model');
   ```

2. Add a reaction object to the model object. Note the use of brackets because the names are not valid MATLAB variable names.

   ```
   reactionObj = addreaction(modelObj, '[Aspartic acid] -> [beta-Aspartyl-PO4]')
   ```

   MATLAB returns:

   ```
   SimBiology Reaction Array

   Index:    Reaction:
     1       [Aspartic acid] -> [beta-Aspartyl-PO4]
   ```

3. Set the reaction `Name` and verify.

   ```
   set (reactionObj, 'Name', 'Aspartate kinase reaction');
   get (reactionObj, 'Name')
   ```

   MATLAB returns:

   ```
   ans =

     Aspartate kinase reaction
   ```

Version History

R2022b: Having duplicate model component names issues a warning
Warns starting in R2022b

- SimBiology issues a warning if multiple model components (model, compartment, species, parameter, reaction, rule, event, observable, dose, and variant) have the same name. In a future release, within a single model, these components will be required to have unique names even when they are of different types with the following two exceptions:

  - Species in different compartments can have the same name.
  - Parameters can have the same name if they are scoped to different parents. Specifically, you can use the same name for a model-scoped parameter and reaction-scoped parameters, where each reaction-scoped parameter belongs to a different reaction.

  The purpose of this naming restriction is to ensure that every model component can be unambiguously referenced by its unique name within a model. For details on how to reference model component names in expressions, see “Guidelines for Referencing Names in Expressions”.
- To disambiguate duplicate names from your model, use the `updateDuplicateNames` function at the command line. The function takes in a SimBiology model as an input and updates the component names as necessary. You can also specify optional outputs, such as a logical flag to check whether any update occurred, a list of model changes, and a copy of the original model before any updates were made.
- The `updateDuplicateNames` function disambiguates the duplicate names by adding a suffix "`_N`", where *N* is the first positive integer that results in a unique name. If there is an existing suffix, *N* will be incremented from that suffix. For example, if there are two model components

named *x_3*, the function updates one of the names to *x_4*. If the existing suffix has leading zeros, the function omits the zeros in the new name. For instance, if *x_003* is a duplicate name, it gets renamed to *x_4*. However, the function assumes that names with leading zeros and without leading zeros are different. For instance, *x_005* and *x_5* are considered to be different names.

R2022a: Having duplicate model component names will not be allowed in a future release
Behavior change in future release

SimBiology will not allow you to have duplicate names for model components within a model.

See Also

`addcompartment` | `addkineticlaw` | `addparameter` | `addreaction` | `addrule` | `addspecies` | `RepeatDose object` | `sbiomodel` | `sbiounit` | `sbiounitprefix` | `ScheduleDose object`

Normalization

Specify normalization type for sensitivity analysis

Description

`Normalization` is a property of the `SensitivityAnalysisOptions` object. `SensitivityAnalysisOptions` is a property of the configuration set object. Use `Normalization` to specify the normalization for the computed sensitivities.

The following values let you specify the type of normalization. The examples show you how sensitivities of a species `x` with respect to a parameter `k` are calculated for each normalization type:

- `'None'` specifies no normalization.

  $$\frac{\partial x(t)}{\partial k}$$

- `'Half'` specifies normalization relative to the numerator (species quantity) only.

  $$\left(\frac{1}{x(t)}\right)\left(\frac{\partial x(t)}{\partial k}\right)$$

- `'Full'` specifies that the data should be made dimensionless.

  $$\left(\frac{k}{x(t)}\right)\left(\frac{\partial x(t)}{\partial k}\right)$$

Characteristics

Applies to	Object: `SensitivityAnalysisOptions`
Data type	`enum`
Data values	`'None'`, `'Half'`, `'Full'`. Default is `'None'`.
Access	Read/write

See Also

Inputs, Outputs, SensitivityAnalysis, SensitivityAnalysisOptions

Notes

HTML text describing SimBiology object

Description

Use the `Notes` property of an object to store comments about the object.

Characteristics

Applies to	Objects: compartment, kinetic law, model, observable, parameter, reaction, RepeatDose, rule, ScheduleDose, species, unit, or unit prefix
Data type	Character vector
Data values	Any character vector
Access	Read/write

Examples

1. Create a model object.

   ```
   modelObj = sbiomodel ('my_model');
   ```

2. Write notes for the model object.

   ```
   set (modelObj, 'notes', '09/01/05 experimental data')
   ```

3. Verify the assignment.

   ```
   get (modelObj, 'notes')
   ```

   MATLAB returns:

   ```
   ans =

   09/01/05 experimental data
   ```

See Also

`addkineticlaw`, `addparameter`, `addreaction`, `addrule`, `addspecies`, `RepeatDose object`, `sbiomodel`, `sbiounit`, `sbiounitprefix`, `ScheduleDose object`

Observables

Array of observable objects

Description

The `Observables` property indicates the observable objects in a model object. The property is a read-only array of `observable` objects.

You can add an observable object to a model object using `addobservable`.

You can view and configure observable object properties by using dot notation or the `get` and `set` functions.

Characteristics

Applies to	Model object
Data type	Array of observable objects
Data values	Observable objects; default value is `[]` (empty)
Access	Read-only

See Also

`Observable`, `addobservable`, `delete`, `get`, `set`, `findUsages`

Version History

Introduced in R2020a

Observed

Measured response object name

Description

`Observed` is a property of the `PKModelMap` object. It specifies the name(s) of one or more objects that represent the measured response (the response variable). Specify the name(s) of species or parameter object(s) that are scoped to a model.

Characteristics

Applies to	Object: `PKModelMap`
Data type	Character vector or cell array of character vectors
Data values	Name of a species or parameter object or empty. Default is an empty cell array.
Access	Read/write

See Also

Dosed, Estimated, `PKModelMap object`

Outputs

Specify species and parameter outputs for sensitivity analysis

Description

`Outputs` is a property of the `SensitivityAnalysisOptions` object.
`SensitivityAnalysisOptions` is a property of the configuration set object.

Use `Outputs` to specify the species and parameters for which you want to compute sensitivities.

The SimBiology software calculates sensitivities with respect to the values of the parameters and the initial amounts of the species specified in the Inputs property. When you simulate a model with `SensitivityAnalysis` enabled in the active configuration set object, sensitivity analysis returns the computed sensitivities of the species and parameters specified in `Outputs`. For a description of the output, see the SensitivityAnalysisOptions property description.

Characteristics

Applies to	Object: `SensitivityAnalysisOptions`
Data type	Species or parameter object or array of objects **Note** If a species or parameter object is determined by a repeated assignment rule, then you cannot use it as an `Outputs` property.
Data values	Species or parameter object, or an array of objects. Default is `[]` (empty array).
Access	Read/write

Examples

This example shows how to set `Outputs` for sensitivity analysis.

1. Import the radio decay model from the SimBiology demos.

```
modelObj  = sbmlimport('radiodecay');
```

2. Retrieve the configuration set object from `modelObj`.

```
configsetObj = getconfigset(modelObj);
```

3. Add a species to the `Outputs` property and display it. Use the `sbioselect` function to retrieve the species object from the model.

```
SimBiology Species Array

Index:  Compartment:  Name:  InitialAmount: InitialAmountUnits:
  1       unnamed      z        0              molecule
```

See Also

Inputs, `sbioselect`, SensitivityAnalysis, SensitivityAnalysisOptions

Owner

Owning compartment

Description

`Owner` shows you the SimBiology compartment object that owns the compartment object. In the compartment object, the `Owner` property shows you whether the compartment resides within another compartment. The `Compartments` property indicates whether other compartments reside within the compartment. You can add a compartment object using the method `addcompartment`.

Characteristics

Applies to	Object: compartment
Data type	Character vector
Data values	Name of compartment object. Default is `[]`.
Access	Read-only

Examples

1. Create a model object named `modelObj`.

```
modelObj = sbiomodel('cell');
```

2. Add two compartments to the model object.

```
compartmentObj1 = addcompartment(modelObj, 'nucleus');
compartmentObj2 = addcompartment(modelObj, 'mitochondrion');
```

3. Add a compartment to one of the compartment objects.

```
compartmentObj3 = addcompartment(compartmentObj2, 'matrix');
```

4. Display the `Owner` property in the compartment objects.

```
get(compartmentObj3, 'Owner')
```

The result shows you the owning compartment and its components:

```
SimBiology Compartment - mitochondrion

   Compartment Components:
     Capacity:          1
     CapacityUnits:
     Compartments:      1
     ConstantCapacity:  true
     Owner:
     Species:           0
```

5. Change the owning compartment.

```
set(compartmentObj3, 'Owner', compartmentObj1)
```

See Also

`Compartments`, `Parent`

Parameters

Array of parameter objects

Description

The `Parameters` property indicates the parameters in a `Model` or `KineticLaw` object. Read-only array of `Parameter` objects.

The scope of a parameter object is hierarchical and is defined by the parameter's parent. If a parameter is defined with a kinetic law object as its parent, then only the kinetic law object can use the parameter. If a parameter object is defined with a model object as its parent, then components such as rules, events, and kinetic laws (reaction rate equations) can use the parameter.

You can add a parameter to a model object, or kinetic law object with the method `addparameter on page 2-75` and delete it with the method `delete on page 2-185`.

You can view parameter object properties with the `get` command and configure properties with the `set` command.

Characteristics

Applies to	Objects: `model`, `kineticlaw`
Data type	Array of parameter objects
Data values	Parameter objects. Default value is `[]` (empty).
Access	Read-only

Examples

1. Create a model object, and then add a reaction object.

```
modelObj = sbiomodel ('my_model');
reactionObj = addreaction (modelObj, 'a + b -> c + d');
```

2. Define a kinetic law for the reaction object.

```
kineticlawObj = addkineticlaw(reactionObj, 'MassAction');
```

3. Add a parameter and assign it to the kinetic law object `(kineticlawObj);`.

```
parameterObj1 = addparameter (kineticlawObj, 'K1');
get (kineticlawObj, 'Parameters')

SimBiology Parameter Array

Index:    Name:    Value:    ValueUnits:
 1         K1       1
```

4. Add a parameter and assign it to the model object (`modelObj`).

```
parameterObj1 = addparameter(modelObj, 'K2');
get(modelObj, 'Parameters')
SimBiology Parameter Array
```

```
    Index:    Name:    Value:    ValueUnits:
      1         K2       1
```

See Also

`addparameter`, `delete`, `get`, `set`

ParameterVariableNames

Cell array of reaction rate parameters

Description

The `ParameterVariableNames` property shows the parameters used by the kinetic law object to determine the `ReactionRate on page 3-116` equation in the reaction object. Use `setparameter on page 2-822` to assign `ParameterVariableNames`. When you assign species to `ParameterVariableNames`, SimBiology software maps these parameter names to `ParameterVariables on page 3-105` in the kinetic law object.

If the reaction is using a kinetic law, the `ReactionRate` property of a reaction object shows the result of a mapping from a "Kinetic Law Definition" on page 3-58. The `ReactionRate` is determined by the kinetic law object `Expression` property by mapping `ParameterVariableNames` to `ParameterVariables` and `SpeciesVariableNames` to `SpeciesVariables`.

Characteristics

Applies to	Object: `kineticlaw`
Data type	Cell array of character vectors
Data values	Cell array of parameters
Access	Read/write

Examples

Create a model, add a reaction, and assign the `SpeciesVariableNames` for the reaction rate equation.

1. Create a model object, and then add a reaction object.

   ```
   modelObj = sbiomodel('my_model');
   reactionObj = addreaction(modelObj, 'a -> c + d');
   ```

2. Create a kinetic law object for the reaction object of type `'Henri-Michaelis-Menten'`.

   ```
   kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
   ```

   `reactionObj` `KineticLaw` property is configured to `kineticlawObj`.

3. The `'Henri-Michaelis-Menten'` kinetic law has two parameter variables (`Vm` and `Km`) that should to be set. To set these variables:

   ```
   setparameter(kineticlawObj,'Vm', 'Va');
   setparameter(kineticlawObj,'Km', 'Ka');
   ```

4. Verify that the parameter variables are correct.

   ```
   get (kineticlawObj, 'ParameterVariableNames')
   ```

   MATLAB returns:

```
ans =

    'Va'    'Ka'
```

See Also

Expression(AbstractKineticLaw, KineticLaw), ParameterVariables, ReactionRate, `setparameter`, SpeciesVariables, SpeciesVariableNames

ParameterVariables

Parameters in kinetic law definition

Description

The `ParameterVariables` property shows the parameter variables that are used in the `Expression` on page 3-58 property of the abstract kinetic law object. Use this property to specify the parameters in the `ReactionRate on page 3-116` equation. Use the method `set` to assign `ParameterVariables` to a kinetic law definition. For more information, see “Kinetic Law Definition” on page 3-58.

Characteristics

Applies to	Objects: abstract kinetic law, kineticlaw
Data type	Cell array of character vectors
Data values	Specified by kinetic law definition
Access	Read/write in kinetic law definition. Read-only in kinetic law.

Examples

Create a model, add a reaction, and assign the `SpeciesVariableNames` for the reaction rate equation.

1. Create a model object, and then add a reaction object.

   ```
   modelObj = sbiomodel('my_model');
   reactionObj = addreaction(modelObj, 'a -> c + d');
   ```

2. Create a kinetic law object for the reaction object of the type `'Henri-Michaelis-Menten'` .

   ```
   kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
   ```

   `reactionObj` `KineticLaw` property is configured to `kineticlawObj`.

3. The `'Henri-Michaelis-Menten'` kinetic law has two parameter variables. To set these variables:

   ```
   get (kineticlawObj, 'ParameterVariables')
   ```

   MATLAB returns:

   ```
   ans =

       'Vm' 'Km'
   ```

See Also

Expression(AbstractKineticLaw, KineticLaw), ParameterVariableNames, ReactionRate, `set`, `setparameter`, SpeciesVariables, SpeciesVariableNames

Parent

Indicate parent object

Description

The `Parent` property indicates the parent object for a SimBiology object (read-only). The `Parent` property indicates accessibility of the object. The object is accessible to the `Parent` object and other objects within the `Parent` object. The value of `Parent` depends on the type of object and how it was created. All models always have the SimBiology root as the `Parent`.

More Information

The following table shows you the different objects and the possible `Parent` value.

Object	Parent
abstract kinetic law	• `[]` (empty) until added to library • root object upon addition to library
compartment	model object
event	model object or `[]` (empty)
kinetic law	reaction object
model	root object
observable	model object
parameter	model object, kinetic law object, or `[]` (empty)
reaction	model object or `[]` (empty)
RepeatDose	model object or `[]` (empty)
rule	model object or `[]` (empty)
ScheduleDose	model object or `[]` (empty)
species	compartment
variant	model object or `[]` (empty)
unit and unit prefixes	• `[]` (empty) until added to library • root object upon addition to library

Characteristics

Applies to	Objects: abstract kinetic law, compartment, event, kinetic law, model, observable, parameter, reaction, RepeatDose, rule, ScheduleDose, species, variant, unit, or unit prefix
Data type	Object
Data values	SimBiology component object or `[]` (empty)
Access	Read-only

See Also

addkineticlaw, addparameter, addreaction, RepeatDose object, sbiomodel, ScheduleDose object

PKCompartments

Hold compartments in PK model

Description

`PKCompartments` is a property of the `PKModelDesign` object. It is used to specify the compartments in the `PKModelDesign` object. Each compartment is a `PKCompartment` object added using the `addCompartment` method.

Characteristics

Applies to	Objects: `PKModelDesign`
Data type	object
Data values	`PKCompartment` object
Access	Read-only

See Also

“Create Pharmacokinetic Models” in the SimBiology User's Guide, `addCompartment`, `PKCompartment object`, `PKModelDesign object`

Products

Array of reaction products

Description

The `Products` property contains an array of `SimBiology.Species` objects.

`Products` is a `1-by-n` species object array that indicates the species that are changed by the reaction. If the `Reaction` property is modified to use a different species, the `Products` property is updated accordingly.

You can add product species to the reaction with `addproduct on page 2-80` function. You can remove product species from the reaction with `rmproduct on page 2-767`. You can also update reaction products by setting the `Reaction` property with the function `set`.

Characteristics

Applies to	Object: reaction
Data type	Array of objects
Data values	Species objects. Default is `[]` (empty).
Access	Read-only

Examples

1. Create a model object.

   ```
   modelObj = sbiomodel ('my_model');
   ```

2. Add reaction objects.

   ```
   reactionObj = addreaction (modelObj, 'a + b -> c + d');
   ```

3. Verify the assignment.

   ```
   productsObj = get(reactionObj, 'Products')
   ```

   MATLAB returns:

   ```
   SimBiology Species Array

   Index:  Compartment:  Name:  InitialAmount: InitialAmountUnits:
    1       unnamed        c        0
    2       unnamed        d        0
   ```

See Also

`addkineticlaw`, `addproduct`, `addspecies`, `rmproduct`

Rate

Rate of dose

Note The property of a `ScheduleDose` object is a column vector instead of a row vector. For details, see “Compatibility Considerations”.

Description

`Rate` is a property of a `RepeatDose` or `ScheduleDose` object.

This property defines how fast a dose is given. If the rate is set to `0` or an empty array `[]`, then it is interpreted as a bolus (instantaneous) dose.

For `RepeatDose` objects, you can parameterize the property by setting it to the name of a model-scoped parameter that is not being modified by a repeated assignment rule, an algebraic rule, or a rate rule. However, the parameter can be modified by an event.

Note If you set the `Rate` property of a dose, you must also specify the `Amount` property of the dose, and set the `DurationParameterName` property to `''`. This is because the duration is calculated from the amount and rate.

Tip You can create a combination of bolus and infusion doses by setting the `rate` property of a `ScheduleDose object` to a vector containing zeros and non-zeros.

Characteristics

Applies to	Objects: `RepeatDose`, `ScheduleDose`.
Data type	double or character vector (`RepeatDose`) or double column (`ScheduleDose`).
Data values	Nonnegative real number or name of a model-scoped parameter object. The default value is `0` (`RepeatDose`) or `0x1` empty double column vector (`ScheduleDose`), that is, the dose is interpreted as a bolus (instantaneous) dose.
Access	Read/write.

Version History

R2019b: `Rate` property of `ScheduleDose` is a column vector
Behavior changed in R2019b

The Rate property of a `ScheduleDose` object is a column vector instead of a row vector. The default value is `0x1` empty double column vector, instead of `[]`.

See Also

`RepeatDose object` | `ScheduleDose object`

Topics

“Parameterized and Adaptive Doses”

RateUnits

Units for dose rate

Description

`RateUnits` is a property of a `PKData`, `RepeatDose` or `ScheduleDose` object.

- In `RepeatDose` or `ScheduleDose` objects, this property defines units for the `Rate` property.
- In `PKData` object, this property defines units for the `RateLabel` property.

Characteristics

Applies to	Object: `RepeatDose`, `ScheduleDose`, `PKData`
Data type	Character vector
Data values	Units from library with dimensions of amount divided by time. You cannot use units of concentration divided by time. Default = '' (empty).
Access	Read/write

Note SimBiology uses units including empty units in association with DimensionalAnalysis and UnitConversion features.

- When `DimensionalAnalysis` and `UnitConversion` are both `false`, units are not used. However, SimBiology still performs a minimum level of dimensional analysis to decide whether a reaction rate is in dimensions of amount/time or concentration/time.
- When `DimensionalAnalysis` is `true` and `UnitConversion` is `false`, units (if not empty) must have consistent dimensions so that SimBiology can perform dimensional analysis. However, the units are not converted.
- When `UnitConversion` is set to `true` (which requires `DimensionalAnalysis` to be `true`), SimBiology performs a dimensional analysis and converts everything to consistent units. Hence, you must specify consistent units, and no units can be empty. If you have a dimensionless parameter, you must still set its units to `dimensionless`.

See Also

`PKData object`, `ScheduleDose object`, `RepeatDose object`, `Rate`, `RateLabel`

RateLabel

Rate of infusion column in data set

Description

`RateLabel` is a property of the `PKData` object. It specifies the column in DataSet on page 3-32 that contains the rate of infusion. This applies only when dosing type is infusion. The data set must contain the rate and not an infusion time. The values must be positive and the column cannot contain `Inf` or `–Inf`. `0` specifies an infinite rate (equivalent to a bolus dose), and `NaN` specifies no rate.

Characteristics

Applies to	Objects: `PKData`
Data type	Character vector
Data values	Column header
Access	Read/write

See Also

`PKData object`, DosingType

Reactants

Array of reaction reactants

Description

The `Reactants` property is a `1-by-n` species object array of reactants in the reaction. If the `Reaction` property is modified to use a different reactant, the `Reactants` property will be updated accordingly.

You can add reactant species to the reaction with the `addreactant on page 2-82` method.

You can remove reactant species from the reaction with the `rmreactant on page 2-769 method`. You can also update reactants by setting the `Reaction` property with the function `set`.

Characteristics

Applies to	Object: reaction
Data type	Species object or array of species objects
Data values	Species objects. Default is `[]` (empty).
Access	Read-only

Examples

1. Create a model object.

   ```
   modelObj = sbiomodel ('my_model');
   ```

2. Add reaction objects.

   ```
   reactionObj = addreaction (modelObj, 'a + b -> c + d');
   ```

3. View the reactants for `reactionObj`.

   ```
   get(reactionObj, 'Reactants')
   ```

   MATLAB returns:

   ```
   SimBiology Species Array

   Index:  Compartment:  Name:  InitialAmount: InitialAmountUnits:
    1       unnamed        a        0
    2       unnamed        b        0
   ```

See Also

`addreactant`, `addreaction`, `addspecies`, `rmreactant`

Reaction

Reaction object reaction

Description

Property to indicate the reaction represented in the reaction object. Indicates the chemical reaction that can change the amount of one or more species, for example, `'A + B –> C'`. This property is different from the model object property called `Reactions`.

See `addreaction` for more information on how the `Reaction` property is set.

Characteristics

Applies to	Object: reaction
Data type	Character vector
Data values	Character vector containing a valid reaction. Default is `''` (empty character vector).
Access	Read/write

Examples

1. Create a model object, and then add a reaction object.

```
modelObj = sbiomodel ('my_model');
reactionObj = addreaction (modelObj, 'a + b -> c + d');
```

2. Verify that the reaction property records the input.

```
get (reactionObj, 'Reaction')
```

MATLAB returns:

```
ans =

a + b -> c + d
```

See Also

`addreaction`

ReactionRate

Reaction rate equation in reaction object

Description

The `ReactionRate` property defines the reaction rate equation. You can define a `ReactionRate` with or without the `KineticLaw` property. `KineticLaw` defines the type of reaction rate. The `addkineticlaw` function configures the `ReactionRate` based on the `KineticLaw` and the species and parameters specified in the kinetic law object properties `SpeciesVariableNames` and `ParameterVariableNames`.

The reaction takes place in the reverse direction if the `Reversible` property is true. This is reflected in `ReactionRate`. The `ReactionRate` includes the forward and reverse rate if reversible.

You can specify `ReactionRate` without `KineticLaw`. Use the `set` function to specify the reaction rate equation. SimBiology software adds species variables while creating `reactionObj` using the `addreaction` method. You must add the parameter variables (to the `modelObj` in this case). See the example below.

After you specify the `ReactionRate` without `KineticLaw` and you later configure the `reactionObj` to use `KineticLaw`, the `ReactionRate` is unset until you specify `SpeciesVariableNames` and `ParameterVariableNames`.

For information on dimensional analysis for reaction rates, see “How Reaction Rates Are Evaluated” .

Note If you set the `ReactionRate` property to an expression that is not continuous and differentiable, see “Using Events to Address Discontinuities in Rule and Reaction Rate Expressions” before simulating your model.

Characteristics

Applies to	Object: reaction
Data type	Character vector
Data values	Character vector defining the reaction rate. Default is `''` (empty character vector).
Access	Read/write

Examples

Add a Reaction Defined by Michaelis-Menten Kinetic Law

Create a model, add a reaction, and assign the expression for the reaction rate equation.

1 Create a model object, and then add a reaction object.

```
modelObj = sbiomodel('my_model');
reactionObj = addreaction(modelObj, 'a -> c + d');
```

2. Create a kinetic law object for the reaction object of the type `'Henri-Michaelis-Menten'`.

```
kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
```

`reactionObj` KineticLaw property is configured to `kineticlawObj`.

3. The `'Henri-Michaelis-Menten'` kinetic law has two parameter variables (`Vm` and `Km`) and one species variable (`S`) that you should set. To set these variables, first create the parameter variables as parameter objects (`parameterObj1, parameterObj2`) with names `Vm_d` and `Km_d` and assign them to `kineticlawObj`.

```
parameterObj1 = addparameter(kineticlawObj, 'Vm_d');
parameterObj2 = addparameter(kineticlawObj, 'Km_d');
```

4. Set the variable names for the kinetic law object.

```
set(kineticlawObj,'ParameterVariableNames', {'Vm_d' 'Km_d'});
set(kineticlawObj,'SpeciesVariableNames', {'a'});
```

5. Verify that the reaction rate is expressed correctly in the reaction object `ReactionRate` property.

```
get (reactionObj, 'ReactionRate')
```

MATLAB returns:

```
ans =

Vm_d*a/(Km_d + a)
```

Add a Reaction without a Kinetic Law

Create a model, add a reaction, and specify `ReactionRate` without a kinetic law.

1. Create a model object, and then add a reaction object.

```
modelObj = sbiomodel('my_model');
reactionObj = addreaction(modelObj, 'a + b -> c + d');
```

2. Specify `ReactionRate` and verify the assignment.

```
set (reactionObj, 'ReactionRate', 'k*a');
get(reactionObj, 'ReactionRate')
```

MATLAB returns:

```
ans =

k*a
```

3. You cannot simulate the model until you add the parameter `k` to the `modelObj`.

```
parameterObj = addparameter(modelObj, 'k');
```

SimBiology adds the parameter to the `modelObj` with default `Value = 1.0` for the parameter.

Define a Custom Hill Kinetic Law that Works with Dimensional Analysis

This example shows how to define a custom reaction rate for the Hill kinetics that is compatible with DimensionalAnalysis feature of SimBiology.

This example is useful especially if you are using the built-in Hill kinetic law, but have the kinetic reaction with a non-integer exponent and cannot verify the model because dimensional analysis

failed. The built-in Hill kinetic law has the following expression: $\frac{V_m * S^n}{K_p + S^n}$. Suppose $K_p = K_h{}^n$, then you can rewrite the equation as follows: $\frac{V_m}{\left(\frac{K_h}{S}\right)^n + 1}$. The redefined Hill kinetic equation is compatible with Dimensional Analysis and allows you to have a non-integer exponent.

Create a SimBiology model.

```
m1 = sbiomodel('m1');
```

Add a compartment, two species, and a reaction.

```
c1 = addcompartment(m1, 'cell');
s1 = addspecies(m1,'a');
s2 = addspecies(m1,'b');
r1 = addreaction(m1, 'a -> b');
```

Add a predefined a Hill kinetic law for the reaction.

```
k1 = addkineticlaw(r1, 'Hill-Kinetics');
```

Display the rate expression of the built-in kinetic law.

```
k1.Expression
```

```
ans =

Vm*S^n/(Kp + S^n)
```

Define parameters, values, and units.

```
p1 = addparameter(k1, 'Vm', 1.0);
p2 = addparameter(k1, 'n', 1.5);
p3 = addparameter(k1, 'Kp', 2.828);

set(k1, 'ParameterVariableNames', {'Vm','n','Kp'});
set(k1, 'SpeciesVariableNames', {'a'});
set(s1, 'InitialAmount', 2.0);

set(s1, 'InitialAmountUnits', 'mole/liter');
set(s2, 'InitialAmountUnits', 'mole/liter');
set(c1, 'CapacityUnits', 'liter');
set(p1, 'ValueUnits', 'mole/liter/second');
set(p2, 'ValueUnits', 'dimensionless');
set(p3, 'ValueUnits', 'mole/liter');
```

Verify the model.

```
verify(m1)
```

```
Error using SimBiology.Model/verify
--> Error reported from Dimensional Analysis:
Dimensional analysis failed for reaction 'a -> b'.
When using the power function, both the base and exponent must be dimensionless or the exponent r
integer constant (for example 2 in 'x^2').
```

You are seeing the error message because SimBiology only allows exponentiation of any dimensionless quantity to any dimensionless power.

Redefine the reaction rate so that it is compatible with dimensional analysis and allows a non-integer exponent.

```
r1.ReactionRate = 'Vm / ( (Kh/a)^n + 1 )';
k1.KineticLaw = 'Unknown';
```

Define the value and units for Kh parameter.

```
p4 = addparameter(k1, 'Kh', 2.0);
set(p4, 'ValueUnits', 'mole/liter');
```

Verify the model.

```
verify(m1)
```

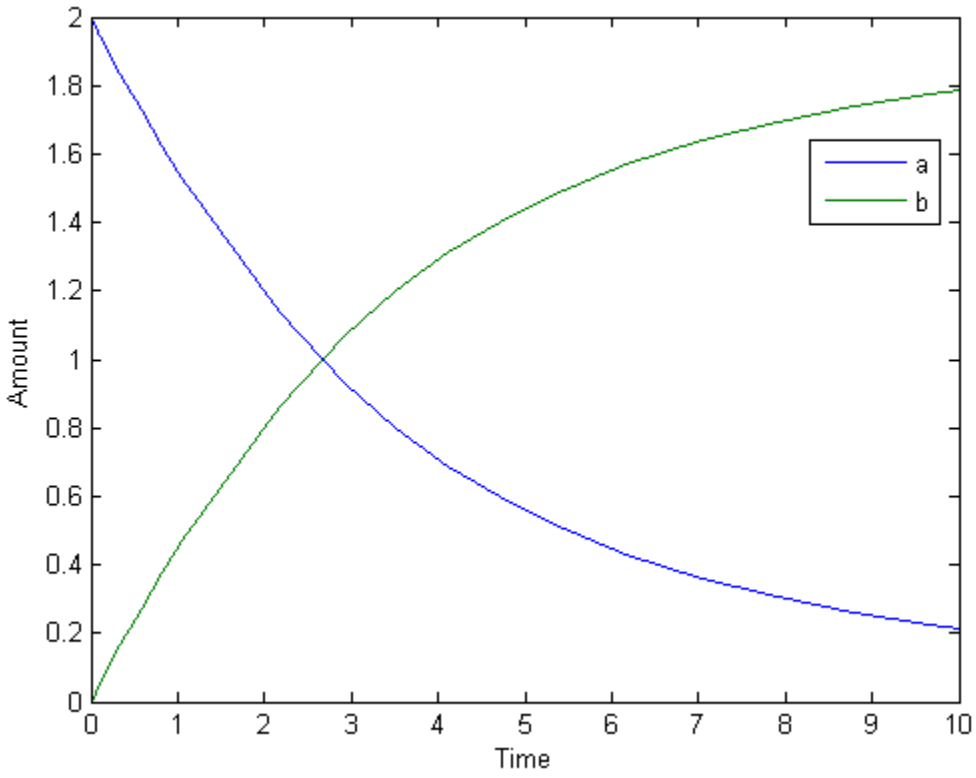
You no longer see the error message.

Simulate the model.

```
[t,x,names] = sbiosimulate(m1);
```

Plot the results.

```
plot(t,x);
xlabel('Time');
ylabel('Amount');
legend(names);
```



See Also

`addparameter`, `addreaction`, Reversible

Reactions

Array of reaction objects

Description

Property to indicate the reactions in a `Model` object. Read-only array of reaction objects.

A reaction object defines a chemical reaction that occurs between species. The species for the reaction are defined in the `Model` object property `Species`.

You can add a reaction to a model object with the method `addreaction on page 2-84`, and you can remove a reaction from the model object with the method `delete on page 2-185`.

Characteristics

Applies to	Object: model
Data type	Array of reaction objects
Data values	Reaction object
Access	Read-only

Examples

1. Create a model object, and then add a reaction object.

```
modelObj = sbiomodel ('my_model');
reactionObj = addreaction (modelObj, 'a + b -> c + d');
```

2. Verify that the reactions property records the input.

```
get (modelObj, 'Reactions')
```

MATLAB returns:

```
SimBiology Reaction Array

 Index:    Reaction:
   1       a + b -> c + d
```

See Also

`addreaction`, `delete`

RepeatCount

Dose repetitions

Description

`RepeatCount` is a property of a `RepeatDose` object. This property defines the number of doses after the initial dose in a repeat dose series.

For `RepeatDose` objects, you can parameterize the property by setting it to the name of a model-scoped parameter that is not being modified by a repeated assignment rule, an algebraic rule, or a rate rule. However, the parameter can be modified by an event.

Note When the `Interval` property is `0`, `RepeatDose` ignores the `RepeatCount` property, that is, it treats it as though it is set to `0`.

Characteristics

Applies to	Object: `RepeatDose`.
Data type	double or character vector.
Data values	Nonnegative integer or name of a model-scoped parameter object. The default value is `0`.
Access	Read/Write.

See Also

`RepeatDose object` | `ScheduleDose object`

Topics

“Parameterized and Adaptive Doses”

Reversible

Specify whether reaction is reversible or irreversible

Description

The `Reversible` property defines whether a reaction is reversible or irreversible. The rate of the reaction is defined by the `ReactionRate` property. For a reversible reaction, the reaction rate equation is the sum of the rate of the forward and reverse reactions. The type of reaction rate is defined by the `KineticLaw` property. If a reaction is changed from reversible to irreversible or vice versa after `KineticLaw` is assigned, the new `ReactionRate` is determined only if `Type` is `MassAction`. All other `Types` result in unchanged `ReactionRate`. For `MassAction`, the first parameter specified is assumed to be the rate of the forward reaction.

Characteristics

Applies to	Object: reaction
Data type	`boolean`
Data values	`true`, `false`. Default value is `false`.
Access	Read/write

Examples

Create a model, add a reaction, and assign the expression for the reaction rate equation.

1. Create model object, and then add a reaction object.

```
modelObj = sbiomodel('my_model');
reactionObj = addreaction(modelObj, 'a -> c + d');
```

2. Set the `Reversible` property for the `reactionObj` to `true` and verify this setting.

```
set (reactionObj, 'Reversible', true)
get (reactionObj, 'Reversible')
```

MATLAB returns:

```
ans =

     1
```

MATLAB returns `1` for `true` and `0` for `false`.

In the next steps the example illustrates how the reaction rate equation is assigned for reversible reactions.

3. Create a kinetic law object for the reaction object of the type `'MassAction'`.

```
kineticlawObj = addkineticlaw(reactionObj, 'MassAction');
```

`reactionObj` `KineticLaw` property is configured to `kineticlawObj`.

4 The 'MassAction' kinetic law for reversible reactions has two parameter variables ('Forward Rate Parameter' and 'Reverse Rate Parameter') that you should set. The species variables for MassAction are automatically determined. To set the parameter variables, first create the parameter variables as parameter objects (parameterObj1, parameterObj2) named Kf and Kr and assign the object to kineticlawObj.

```
parameterObj1 = addparameter(kineticlawObj, 'Kf');
parameterObj2 = addparameter(kineticlawObj, 'Kr');
```

5 Set the variable names for the kinetic law object.

```
set(kineticlawObj,'ParameterVariableNames', {'Kf' 'Kr'});
```

6 Verify that the reaction rate is expressed correctly in the reaction object ReactionRate property.

```
get (reactionObj, 'ReactionRate')
```

MATLAB returns:

```
ans =

Kf*a*b - Kr*c*d
```

See Also

addparameter, addreactant, addreaction, ParameterVariableNames, ReactionRate

Rule

Specify species and parameter interactions

Description

The `Rule` property contains a rule that defines how certain species and parameters should interact with one another. For example, a rule could state that the total number of species `A` and species `B` must be some value. `Rule` is a MATLAB expression that defines the change in the species object quantity or a parameter object `Value on page 3-162` when the rule is evaluated.

You can add a rule to a model object with the `addrule on page 2-89` method and remove the rule with the `delete on page 2-185` method. For more information on rules, see `addrule on page 2-89` and `RuleType on page 3-126`.

Note If you set the `Rule` property for an algebraic rule, rate rule, or repeated assignment rule, and the rule expression is not continuous and differentiable, see "Using Events to Address Discontinuities in Rule and Reaction Rate Expressions" before simulating your model.

Characteristics

Applies to	Object: rule
Data type	Character vector
Data values	Character vector defined as species or parameter objects. Default is an empty character vector `''`.
Access	Read/write

Examples

1. Create a model object, and then add a reaction object.

```
modelObj = sbiomodel ('my_model');
reactionObj = addreaction (modelObj, 'a + b -> c + d');
```

2. Add a rule.

```
ruleObj = addrule(modelObj, '10-a+b')
```

MATLAB returns:

```
SimBiology Rule Array

Index:    RuleType:    Rule:
1         algebraic    10-a+b
```

See Also

`addrule`, `delete`, "Definitions and Evaluations of Rules in SimBiology Models"

RuleType

Specify type of rule for rule object

Description

The `RuleType` property indicates the type of rule defined by the rule object. A `Rule` object defines how certain species, parameters, and compartments should interact with one another. For example, a rule could state that the total number of species A and species B must be some value. `Rule` is a MATLAB expression that defines the change in the species object quantity or a parameter object `Value on page 3-162` when the rule is evaluated.

You can add a rule to a model object with the `addrule on page 2-89` method and remove the rule with the `delete on page 2-185` method. For more information on rules, see `addrule on page 2-89`.

The types of rules in SimBiology are as follows:

- `initialAssignment` — Lets you specify the initial value of a parameter, species, or compartment capacity, as a function of other model component values in the model.
- `repeatedAssignment` — Lets you specify a value that holds at all times during simulation, and is a function of other model component values in the model.
- `algebraic` — Lets you specify mathematical constraints on one or more parameters, species, or compartments that must hold during a simulation.
- `rate` — Lets you specify the time derivative of a parameter value, species amount, or compartment capacity.

Constraints on Varying Species Using a Rate Rule

If the model has a species defined in concentration, being varied by a `rate` rule, and it is in a compartment with varying volume, you can only use `rate` or `initialAssignment` rules to vary the compartment volume.

Conversely, if you are varying a compartment's volume using a `repeatedAssignment` or `algebraic` rules, then you cannot vary a species (defined in concentration) within that compartment, with a `rate` rule.

The reason for these constraints is that, if a species is defined in concentration and it is in a compartment with varying volume, the time derivative of that species is a function of the compartment's rate of change. For compartments varied by rate rules, the solver has that information.

Note that if you specify the species in amounts there are no constraints.

Characteristics

Applies to	Object: rule
Data type	Character vector

Data values	`'initialAssignment'`, `'repeatedAssignment''algebraic'`, `'rate'`. Default value is `'initialAssignment'`.
Access	Read/write

Examples

1 Create a model object, and then add a reaction object.

```
modelObj = sbiomodel ('my_model');
reactionObj = addreaction (modelObj, 'a -> b');
```

2 Add a rule that specifies the quantity of a species `c`. In the rule expression, `k` is the rate constant for `a -> b`.

```
ruleObj = addrule(modelObj, 'c = k*(a+b)')
```

3 Change the `RuleType` from the default (`'initialAssignment'`) to `'rate'` and verify it using the `get` command.

```
set(ruleObj, 'RuleType', 'rate');
get(ruleObj)
```

MATLAB returns all the properties for the rule object.

```
    Active: 1
Annotation: ''
      Name: ''
     Notes: ''
    Parent: [1x1 SimBiology.Model]
      Rule: 'c = k*(a+b)'
  RuleType: 'rate'
       Tag: ''
      Type: 'rule'
  UserData: []
```

See Also

“Definitions and Evaluations of Rules in SimBiology Models”, `addrule`, `delete`

Rules

Array of rules in model object

Description

The `Rules` property shows the rules in a `Model` object. Read-only array of `SimBiology.Rule` objects.

A *rule* is a mathematical expression that modifies a species amount or a parameter value. A rule defines how certain species and parameters should interact with one another. For example, a rule could state that the total number of species `A` and species `B` must be some value.

You can add a rule to a model object with the `addrule on page 2-89` method and remove the rule with the `delete on page 2-185` method. For more information on rules, see `addrule` and `RuleType on page 3-126`.

Characteristics

Applies to	Object: model
Data type	Array of rule objects
Data values	Rule object
Access	Read-only

Examples

1. Create a model object, and then add a reaction object.

```
modelObj = sbiomodel ('my_model');
reactionObj = addreaction (modelObj, 'a + b -> c + d');
```

2. Add a rule.

```
ruleobj = addrule(modelObj, '10-a+b')
```

MATLAB returns:

```
SimBiology Rule Array

Index:    RuleType:    Rule:
 1        algebraic    10-a+b
```

See Also

`addrule`, `delete`, “Definitions and Evaluations of Rules in SimBiology Models”

RuntimeOptions

Options for logged species

Description

The `RuntimeOptions` property holds options for species that will be logged during the simulation run. The run-time options object can be accessed through this property.

The `LogDecimation` property of the configuration set object defines how often data is logged.

Property Summary

StatesToLog	Specify species, compartment, or parameter data recorded
Type	Display SimBiology object type

Characteristics

Applies to	Object: `configset`
Data type	Object
Data values	Run-time options
Access	Read-only

Examples

1. Create a model object, and retrieve its configuration set.

```
modelObj  = sbiomodel('cell');
configsetObj = getconfigset(modelObj);
```

2. Retrieve the `RuntimeOptions` object from the `configset` object.

```
runtimeObj = get(configsetObj, 'RunTimeOptions')
Runtime Settings:

     StatesToLog:          all
```

See Also

`get`, `set`

SensitivityAnalysisOptions

Specify sensitivity analysis options

Description

The `SensitivityAnalysisOptions` property is an object that holds the sensitivity analysis options in the configuration set object. Sensitivity analysis is supported only for deterministic (ODE) simulations.

Note The `SensitivityAnalysisOptions` property controls the settings related to sensitivity analysis. To enable or disable sensitivity analysis, use the SensitivityAnalysis property.

Properties of `SensitivityAnalysisOptions` are summarized in "Property Summary" on page 3-130.

When sensitivity analysis is enabled, the following command

```
[t,x,names] = sbiosimulate(modelObj)
```

returns `[t,x,names]`, where

- `t` is an `n-by-1` vector, where `n` is the number of steps taken by the ode solver and `t` defines the time steps of the solver.
- `x` is an `n-by-m` matrix, where `n` is the number of steps taken by the ode solver and `m` is:

  ```
  Number of species and parameters specified in StatesToLog +
  (Number of sensitivity outputs * Number of sensitivity input factors)
  ```

  A SimBiology state includes species and nonconstant parameters.
- `names` is the list of states logged and the list of sensitivities of the species specified in `StatesToLog` with respect to the input factors.

For an example of the output, see "Examples" on page 3-131.

You can add a number of configuration set objects with different `SensitivityAnalysisOptions` to the model object with the `addconfigset` method. Only one configuration set object in the model object can have the `Active on page 3-2` property set to `true` at any given time.

Property Summary

Inputs	Specify species and parameter input factors for sensitivity analysis
Normalization	Specify normalization type for sensitivity analysis
Outputs	Specify species and parameter outputs for sensitivity analysis

Characteristics

Applies to	Object: configuration set

Data type	Object
Data values	`SensitivityAnalysisOptions` properties as summarized in “Property Summary” on page 3-130.
Access	Read-only

Examples

This example shows how to set `SensitivityAnalysisOptions`.

1. Import the radio decay model from SimBiology demos.

```
modelObj  = sbmlimport('radiodecay');
```

2. Retrieve the configuration settings and the sensitivity analysis options from `modelObj`.

```
configsetObj = getconfigset(modelObj);
sensitivityObj = get(configsetObj, 'SensitivityAnalysisOptions');
```

3. Add a species and a parameter to the `Inputs` property. Use the `sbioselect` function to retrieve the species and parameter objects from the model.
4. Add a species to the `Outputs` property and display.

```
SimBiology Species Array

   Index:    Compartment:    Name:    InitialAmount:    InitialAmountUnits:
   1         unnamed         z        0                 molecule
```

5. Enable `SensitivityAnalysis`.

```
set(configsetObj.SolverOptions, 'SensitivityAnalysis', true);
get(configsetObj.SolverOptions, 'SensitivityAnalysis')

ans =

  1
```

6. Simulate and return the results to three output variables. See “Description” on page 3-130 for more information.

```
[t,x,names] = sbiosimulate(modelObj);
```

7. Display the `names`.

```
names

names =

    'x'
    'z'
    'd[z]/d[z]_0'
    'd[z]/d[Reaction1.c]'
```

Display state values `x`.

```
x
```

The display follows the column order shown in `names` for the values in `x`. The rows correspond to `t`.

See Also

`addconfigset`, `getconfigset`, SensitivityAnalysis

SolverType

Select solver type for simulation

Description

The `SolverType` property lets you specify the solver to use for a simulation. For a discussion about solver types, see “Choosing a Simulation Solver”.

Changing the solver type changes the options (properties) specified in the `SolverOptions` property of the `configset` object. If you change any `SolverOptions`, these changes are persistent when you switch `SolverType`. For example, if you set the `ErrorTolerance` for the `expltau` solver and then change to `impltau` when you switch back to `expltau`, the `ErrorTolerance` will have the value you assigned.

Characteristics

Applies to	Object: `Configset`
Data type	`enum`
Data values	`'ode15s'`, `'ode23t'`, `'ode45'`, `'sundials'`, `'ssa'`, `'expltau'`, `'impltau'`. Default is `'ode15s'`. **Note** • If your model contains events, you cannot specify `'expltau'` or `'impltau'` for the `SolverType` property. • If your model contains doses, you cannot specify `'ssa'`, `'expltau'`, or `'impltau'` for the `SolverType` property. • If your model contains algebraic rules, you cannot use `'ode45'`. • SimBiology always uses the SUNDIALS solver to perform sensitivity analysis on a model, regardless of what you have selected as the SolverType in the configuration set.
Access	Read/write

Examples

1 Retrieve the `configset` object from the `modelObj`.

```
modelObj  = sbiomodel('cell');
configsetObj = getconfigset(modelObj)


Configuration Settings - default (active)
     SolverType:                  ode15s
     StopTime:                    10.000000

   SolverOptions:
```

```
    AbsoluteTolerance:           1.000000e-006
    RelativeTolerance:           1.000000e-003
    SensitivityAnalysis:         false

  RuntimeOptions:
    StatesToLog:                 all

  CompileOptions:
    UnitConversion:              false
    DimensionalAnalysis:         true

  SensitivityAnalysisOptions:
    Inputs:                      0
    Outputs:                     0
```

2 Configure the `SolverType` to `ode45`.

```
set(configsetObj, 'SolverType', 'ode45')
configsetObj

  Configuration Settings - default (active)
    SolverType:                  ode45
    StopTime:                    10.000000

  SolverOptions:
    AbsoluteTolerance:           1.000000e-006
    RelativeTolerance:           1.000000e-003
    SensitivityAnalysis:         false

  RuntimeOptions:
    StatesToLog:                 all

  CompileOptions:
    UnitConversion:              false
    DimensionalAnalysis:         true

  SensitivityAnalysisOptions:
    Inputs:                      0
    Outputs:                     0
```

See Also

`getconfigset`, `set`

Species

Array of species in compartment object

Description

The `Species` property is a property of the compartment object and indicates all the species in a compartment object. `Species` is a read-only array of SimBiology species objects.

In the model object, `Species` contains a flat list of all the species that exist within all the compartments in the model. You should always access a species through its compartment rather than the model object. Use the format *`compartmentName.speciesName`*, for example, `nucleus.DNA`. Another example of the syntax is `modelObj.Compartments(2).Species(1)`. The `Species` property in the model object might not be available in a future version of the software.

Species are entities that take part in reactions. A species object is added to the `Species` property when a reaction is added to the model object with the method `addreaction on page 2-84`. A species object can also be added to the `Species` property with the method `addspecies on page 2-108`.

If you remove a reaction with the method `delete on page 2-239`, and a species is no longer being used by any of the remaining reactions, the species object is *not* removed from the `Species` property. You have to use the `delete` method to remove species.

There are reserved characters that cannot be used in species object names. See Name for more information.

Characteristics

Applies to	Object: compartment
Data type	Array of species objects
Data values	Species object. Default is `[]` (empty).
Access	Read-only

See Also

`addcompartment`, `addreaction`, `addspecies`, `delete`

SpeciesVariableNames

Cell array of species in reaction rate equation

Description

The SpeciesVariableNames property shows the species used by the kinetic law object to determine the ReactionRate on page 3-116 equation in the reaction object. Use setspecies to assign SpeciesVariableNames. When you assign species to SpeciesVariableNames, SimBiology software maps these species names to SpeciesVariables on page 3-138 in the kinetic law object.

The ReactionRate property of a reaction object shows the result of a mapping from kinetic law definition on page 3-58. The ReactionRate is determined by the kinetic law object Expression property by mapping ParameterVariableNames to ParameterVariables and SpeciesVariableNames to SpeciesVariables.

Characteristics

Applies to	Object: kinetic law
Data type	Cell array of character vectors
Data values	Cell array of species names
Access	Read/write

Examples

Create a model, add a reaction, and assign the SpeciesVariableNames for the reaction rate equation.

1. Create a model object, and then add a reaction object.

   ```
   modelObj = sbiomodel('my_model');
   reactionObj = addreaction(modelObj, 'a -> c + d');
   ```

2. Create a kinetic law object for the reaction object, of the type 'Henri-Michaelis-Menten'

   ```
   kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
   ```

   The reactionObj KineticLaw property is configured to kineticlawObj.

3. The 'Henri-Michaelis-Menten' kinetic law has one species variable (S) that you should set. To set this variable:

   ```
   setspecies(kineticlawObj,'S', 'a');
   ```

4. Verify that the species variable is correct.

   ```
   get (kineticlawObj, 'SpeciesVariableNames')
   ```

   MATLAB returns:

```
ans =

'a'
```

See Also

Expression(AbstractKineticLaw, KineticLaw), ParameterVariables, ParameterVariableNames, ReactionRate, `setparameter`, SpeciesVariables

SpeciesVariables

Species in abstract kinetic law

Description

This property shows species variables that are used in the `Expression on page 3-58` property of the kinetic law object to determine the `ReactionRate on page 3-116` equation in the reaction object. Use the function `set` to assign `SpeciesVariables` to an abstract kinetic law. For more information, see abstract kinetic law on page 3-58.

Characteristics

Applies to	Objects: abstract kinetic law, kineticlaw
Data type	Cell array of character vectors
Data values	Defined by abstract kinetic law
Access	Read/write in abstract kinetic law. Read-only in kinetic law.

Examples

Create a model, add a reaction, and assign the `SpeciesVariableNames` for the reaction rate equation.

1. Create a model object, and then add a reaction object.

   ```
   modelObj = sbiomodel('my_model');
   reactionObj = addreaction(modelObj, 'a -> c + d');
   ```

2. Create a kinetic law object for the reaction object, of the type `'Henri-Michaelis-Menten'`.

   ```
   kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
   ```

   `reactionObj` `KineticLaw` property is configured to `kineticlawObj`.

3. View the species variable for`'Henri-Michaelis-Menten'` kinetic law.

   ```
   get (kineticlawObj, 'SpeciesVariables')
   ```

   MATLAB returns:

   ```
   ans =

       'S'
   ```

See Also

Expression(AbstractKineticLaw, KineticLaw), ParameterVariables, ParameterVariableNames, ReactionRate, `set`, `setparameter`, SpeciesVariableNames

StartTime

Start time for initial dose time

Description

`StartTime` is a property of a `RepeatDose` object. For a series of repeated doses, the `StartTime` property defines the amount of time that elapses before the first (initial) dose is given.

For `RepeatDose` objects, you can parameterize the property by setting it to the name of a model-scoped parameter that is not being modified by a repeated assignment rule, an algebraic rule, or a rate rule. However, the parameter can be modified by an event.

Characteristics

Applies to	Objects: `RepeatDose`.
Data type	double or character vector.
Data values	Nonnegative real number or name of a model-scoped parameter object. The default value is `0`.
Access	Read-write.

See Also

`RepeatDose object` | `ScheduleDose object`

Topics

“Parameterized and Adaptive Doses”

StatesToLog

Specify species, compartment, or parameter data recorded

Description

The `StatesToLog` property specifies the species, compartment, or parameter data to log during a simulation. This is the data returned in `x` during execution of `[t,x] = sbiosimulate(modelObj)`. By default, all species, nonconstant compartments, and nonconstant parameters are logged.

If you specify a particular list of species, compartments, or parameters to be logged, the order of the states in the result `SimData` after simulation is the same as the order specified.

Characteristics

Applies to	Object: `RuntimeOptions`
Data type	Character vector, cell array of character vectors, object or vector of objects
Data values	Species objects, compartment objects, or parameter objects. Default is `'all'`, which means all species objects, all nonconstant compartment objects and all nonconstant parameter objects are logged. A nonconstant compartment or parameter means that its Constant property is set to false.
Access	Read/write

Examples

Specify a List of Species to be Logged During Simulation

Load the Lotka-Volterra model.

```
sbioloadproject lotka;
```

Get the configset object of the lotka model `m1`.

```
configset = getconfigset(m1);
```

Display the list of species whose data are logged by default during the simulation.

```
configset.RuntimeOptions.StatesToLog
```

```
ans =
   SimBiology Species Array

   Index:    Compartment:    Name:    Value:    Units:
   1         unnamed         x        1
   2         unnamed         y1       900
   3         unnamed         y2       900
   4         unnamed         z        0
```

Suppose you want to log just species `y1` and `y2` data. You can specify their names as a cell array of strings and set it to `StatesToLog` property.

```
configset.RuntimeOptions.StatesToLog = {'y1','y2'};
```

Confirm the setting.

```
configset.RuntimeOptions.StatesToLog
```

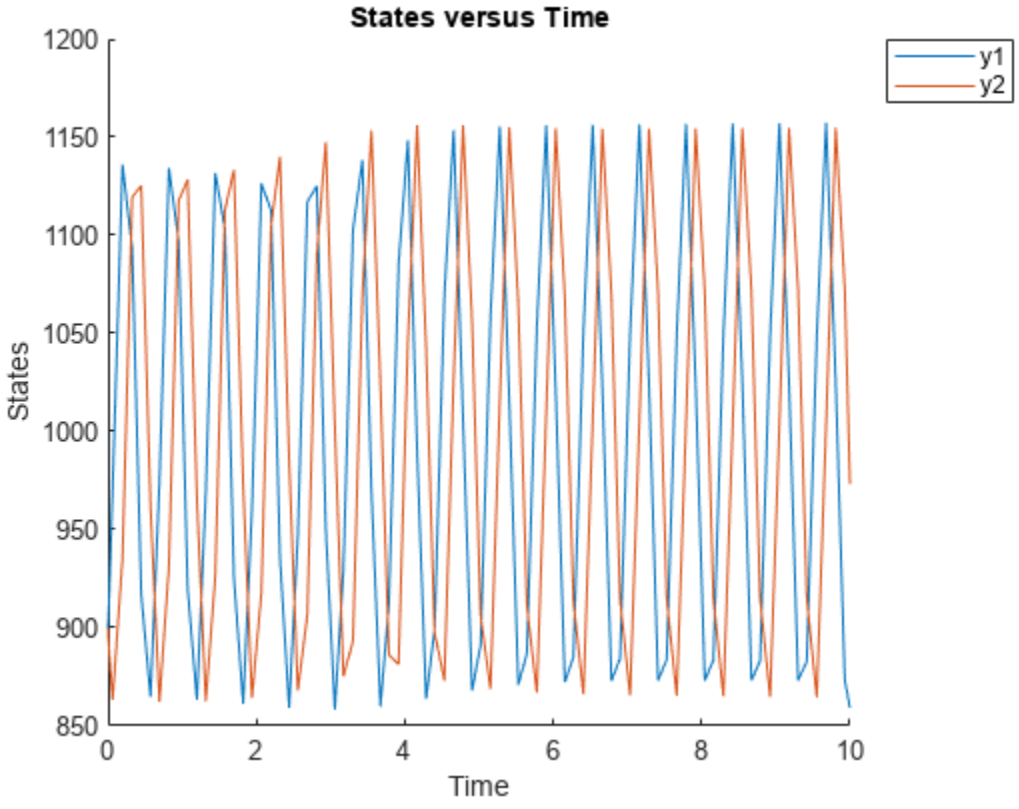
```
ans =
   SimBiology Species Array

   Index:    Compartment:    Name:    Value:    Units:
   1         unnamed         y1       900
   2         unnamed         y2       900
```

Alternatively, you can specify an array of species objects (instead of strings) to `StatesToLog` property.

```
y1 = m1.Species(2);
y2 = m1.Species(3);
configset.RuntimeOptions.StatesToLog = [y1, y2];
```

Simulate and plot the results. Notice that simulation results of only `y1` and `y2` are plotted.

```
sbioplot(sbiosimulate(m1));
```

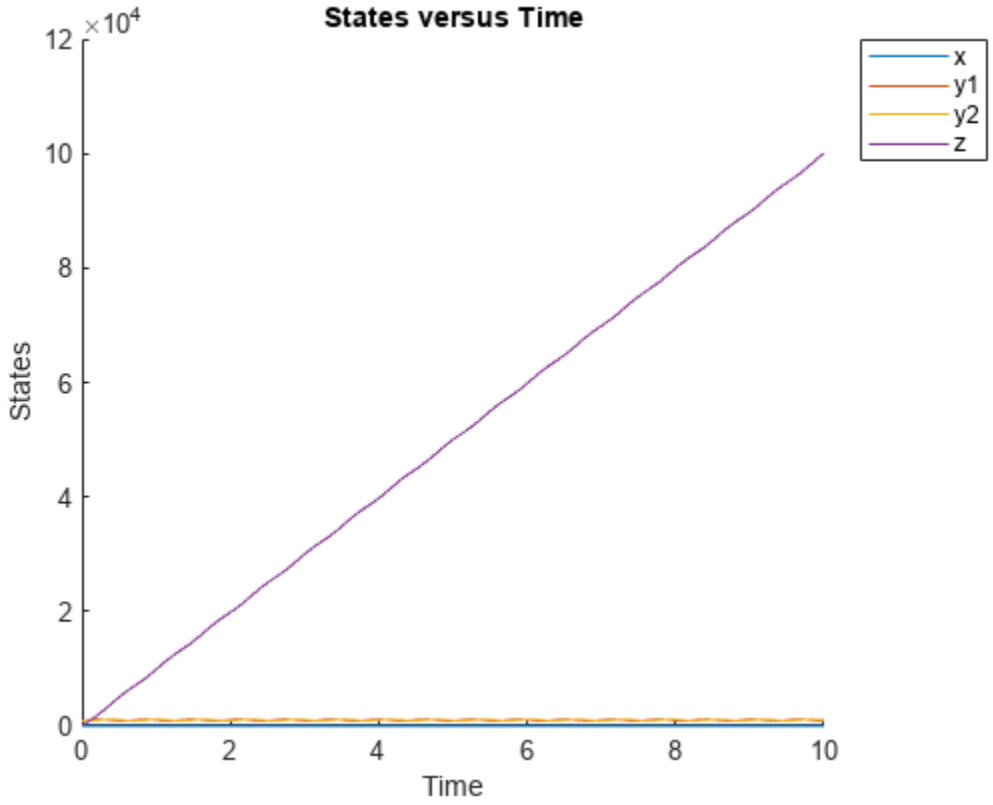


To reset to the default list, set `StatesToLog` to a string `'all'`, which means all species objects, all nonconstant compartment objects and all nonconstant parameter objects are logged by default. A nonconstant compartment or parameter means that its Constant property is set to false.

```
configset.RuntimeOptions.StatesToLog = 'all';
```

Simulate again. Notice all the species data are plotted.

```
sbioplot(sbiosimulate(m1));
```



Do not specify `'all'` as a cell string such as `{'all'}`. If so, SimBiology interprets it as a species named `all`.

See Also

Constant, Configset on page 2-170, RuntimeOptions on page 3-129

Stoichiometry

Species coefficients in reaction

Description

The `Stoichiometry` property specifies the species coefficients in a reaction. Enter an array of `doubles` indicating the stoichiometry of reactants (negative value) and products (positive value). Example: [-1 -1 2].

The `double` specified cannot be `0`. The reactants of the reaction are defined with a negative number. The products of the reaction are defined with a positive number. For example, the reaction 3 H + A-> 2 C + F has the `Stoichiometry` value of [-3 -1 2 1].

When this property is configured, the `Reaction` property updates accordingly. In the above example, if the `Stoichiometry` value was set to [-2 -1 2 3], the reaction is updated to 2H + A -> 2C + 3F.

The length of the `Stoichiometry` array is the sum of the `Reactants` array and the `Products` array. To remove a product or reactant from a reaction, use the `rmproduct on page 2-767` or `rmreactant on page 2-769` function. Add a product or reactant and set stoichiometry with methods `addproduct` on page 2-80 and `addreactant on page 2-82`.

ODE solvers support `double` stoichiometry values such as `0.5`. Stochastic solvers and dimensional analysis currently support only integers in `Stoichiometry`, therefore you must balance the reaction equation and specify integer values for these two cases.

`A -> null` has a stoichiometry value of `[-1]`. `null -> B` has a stoichiometry value of `[1]`.

Characteristics

Applies to	Object: reaction
Data type	Double array
Data values	1-by-n double, where n is length (products) + length (reactants). Default is [ ] (empty).
Access	Read/write

Examples

1 Create a reaction object.

```
modelObj = sbiomodel('cell');
reactionObj = addreaction(modelObj, '2 a + 3 b -> d + 2 c');
```

2 Verify the `Reaction` and `Stoichiometry` properties for `reactionObj`.

```
get(reactionObj,'Stoichiometry')
```

MATLAB returns:

```
ans =

-2    -3     1     2
```

3 Set stoichiometry to `[-1 -2 2 2]`.

```
set (reactionObj, 'Stoichiometry', [-1 -2 2 2]);
get (reactionObj, 'Stoichiometry')
```

MATLAB returns:

```
ans =

 -1    -2     2     2
```

4 Note with `get` that the `Reaction` property updates automatically.

```
get (reactionObj, 'Reaction')
```

MATLAB returns:

```
ans =

a + 2 b -> 2 d + 2 c
```

See Also

`addproduct`, `addreactant`, `addreaction`, Reaction, `rmproduct`, `rmreactant`

StopTime

Simulation time criteria to stop simulation

Description

`StopTime` is a property of a `Configset` object. This property sets the maximum simulation time criteria to stop a simulation. Time units are specified by the `TimeUnits` property of the `Configset` object.

A simulation stops when it meets any of the criteria specified by `StopTime`, `MaximumNumberOfLogs`, or `MaximumWallClock`. However, if you specify the `OutputTimes` property of the `SolverOptions` property of the `Configset` object, then `StopTime` and `MaximumNumberOfLogs` are ignored. Instead, the last value in `OutputTimes` is used as the `StopTime` criteria, and the length of `OutputTimes` is used as the `MaximumNumberOfLogs` criteria.

Characteristics

Applies to	Object: `Configset`
Data type	`double`
Data values	Nonnegative scalar. Default is `10`.
Access	Read/write

Examples

Set Simulation Time Criteria to Stop Simulation

1. Create a `model` object named `cell` and save it in a variable named `modelObj`. Retrieve the configuration set from `modelObj` and save it in a variable named `configsetObj`.

```
modelObj  = sbiomodel('cell');
configsetObj = getconfigset(modelObj);
```

2. Configure the simulation stop criteria by setting the `StopTime` property to `20` seconds. Leave the `MaximumNumberOfLogs`and `MaximumWallClock` properties at their default values of `Inf`.

```
set(configsetObj, 'StopTime', 20)
get(configsetObj)
```

```
                       Active: 1
               CompileOptions: [1x1 SimBiology.CompileOptions]
                         Name: 'default'
                        Notes: ''
               RuntimeOptions: [1x1 SimBiology.RuntimeOptions]
    SensitivityAnalysisOptions: [1x1 SimBiology.SensitivityAnalysisOptions]
                SolverOptions: [1x1 SimBiology.ODESolverOptions]
                   SolverType: 'ode15s'
                     StopTime: 20
          MaximumNumberOfLogs: Inf
             MaximumWallClock: Inf
                    TimeUnits: 'second'
                         Type: 'configset'
```

When you simulate `modelObj`, the simulation stops when the simulation time reaches `20` seconds.

See Also

`Configset object`, MaximumNumberOfLogs, MaximumWallClock, OutputTimes, TimeUnits, MassUnits, AmountUnits

Tag

Specify label for SimBiology object

Description

The `Tag` property specifies a label associated with a SimBiology object. Use this property to group objects and then use `sbioselect` to retrieve. For example, use the `Tag` property in reaction objects to group synthesis or degradation reactions. You can then retrieve all synthesis reactions using `sbioselect`. Similarly, for species objects you can enter and store classification information, for example, membrane protein, transcription factor, enzyme classifications, or whether a species is an independent variable. You can also enter the full form of the name of the species.

Characteristics

Applies to	Objects: abstract kinetic law, kinetic law, model, observable, parameter, reaction, RepeatDose, rule, ScheduleDose, species
Data type	Character vector
Data values	Any character vector
Access	Read/write

Examples

1. Create a model object.

```
modelObj = sbiomodel ('my_model');
```

2. Add a reaction object and set the `Tag` property to `'Synthesis Reaction'`.

```
reactionObj = addreaction (modelObj, 'a + b -> c + d');
set (reactionObj, 'Tag', 'Synthesis Reaction')
```

3. Verify the `Tag` assignment.

```
get (reactionObj, 'Tag');
```

MATLAB returns:

```
ans =

     'Synthesis Reaction'
```

See Also

`addkineticlaw`, `addparameter`, `addreaction`, `addrule`, `addspecies`, `RepeatDose object`, `sbioabstractkineticlaw`, `sbiomodel`, `sbioroot`, `ScheduleDose object`

TargetName

Species receiving dose

Description

`TargetName` is a property of a `RepeatDose` or `ScheduleDose` object. This property defines the SimBiology species receiving the dose. The dose amount increases the species amount at each time interval defined by a repeat dose or at each time point defined by a schedule dose.

The value of `TargetName` is the name of a species. If the model has more than one species with the same name, `TargetName` is defined as *compartmentName.speciesName*, where *compartmentName* is the name of the compartment containing the species.

Characteristics

Applies to	Objects: `RepeatDose`, `ScheduleDose`
Data type	Character vector
Data values	Species name. Default value is '' (empty).
Access	Read/Write

See Also

`ScheduleDose object` and `RepeatDose object`

Trigger

Event trigger

Description

`Trigger` is a property of an `Event` object

A `Trigger` is a condition that must become true for an event to execute. You can use a combination of relational and logical operators to build a trigger expression. `Trigger` can be a character vector, an expression, or a function handle that when evaluated returns a value of `true` or `false`. A `Trigger` can access species, parameters, and compartments.

A trigger can contain the keyword `time` and relational operators to trigger an event that occurs at a specific time during the simulation. For example, `time >= x`. In this example trigger, note that:

- The units associated with the keyword `time` are the units for the `TimeUnits` property for the `Configset` object associated with the simulation.
- If `x` is an expression containing compartments, species, or parameters, then any units associated with the expression must have the same dimensions as the keyword `time`.
- If `x` is a raw number, then its dimensions (and units, if unit conversion is on) are assumed to be the same as the keyword `time`.

For more information about how the SimBiology software handles events, see “How Events Are Evaluated”. For examples of event functions, see “Specifying Event Triggers”.

Tip If UnitConversion is on and your model has any event, follow the recommendation below.

Non-dimensionalize any parameters used in the event `Trigger` if they are not already dimensionless. For example, suppose you have a trigger `x > 1`, where *x* is the species concentration in mole/liter. Non-dimensionalize *x* by scaling (dividing) it with a constant such as `x/x0 > 1`, where *x0* is a parameter defined as 1.0 mole/liter. Note that *x* does not have to have the same unit as the constant *x0*, but must be dimensionally consistent with it. For example, the unit of *x* can be picomole/liter instead of mole/liter.

Characteristics

Applies to	Object: `event`
SimBiology type	Character vector, function handle
SimBiology values	Specify a MATLAB expression as a character vector. Default is `''` (empty character vector).
Access	Read/write

Examples

1 Create a model object, and then add an event object.

```
modelObj = sbmlimport('oscillator');
eventObj = addevent(modelObj, 'time>= 5', 'OpC = 200');
```

2 Set the `Trigger` property of the event object.

```
set(eventObj, 'Trigger', '(time >=5) && (speciesA<1000)');
```

3 Get the `Trigger` property.

```
get(eventObj, 'Trigger')
```

See Also

`Event`, `EventFcns`

Time

Simulation time steps or schedule dose times

Note The property of a `ScheduleDose` object is a column vector instead of a row vector. For details, see “Compatibility Considerations”.

Description

`Time` is a property of a `SimData` or `ScheduleDose` object.

SimData Object

For a simulation, the `Time` property records the time steps.

ScheduleDose Object

For a series of scheduled doses, the `Time` property defines the times to give a dose.

A ScheduleDose object defines a series of doses. Each dose can have a different amount, as defined by an amount array in the `Amount` property, and given at specified times, as defined by a time array in the `Time` property. A rate array in the `Rate` property defines how fast each dose is given. At each time point in the time array, a dose is given with the corresponding amount and rate.

Characteristics

Applies to	Objects: `SimData`, `ScheduleDose`.
Data type	double (`SimData`), double column (`ScheduleDose`) .
Data values	Vector of doubles (`SimData`) or column of nonnegative real numbers. Default property value for `ScheduleDose` is `0x1` empty double column vector.
Access	Read-only.

See Also

`ScheduleDose object`, `SimData object`, StopTime

Version History

R2019b: `Time` property of `ScheduleDose` is a column vector

Behavior changed in R2019b

The Time property of a `ScheduleDose` object is a column vector instead of a row vector. The default value is `0x1` empty double column vector, instead of `[]`.

TimeUnits

Show time units for dosing and simulation

Description

The `TimeUnits` property specifies time units for these properties:

- `StopTime` property of a `Configset` object
- `OutputTimes` and `AbsoluteToleranceStepSize` properties of the `SolverOptions` property of a `Configset` object
- `StartTime` and `Interval` properties of a `RepeatDose` object
- `Time` property of a `ScheduleDose` object
- `Time` property of a `SimData` object

Note If you change the value of the `TimeUnits` property, make sure:

- You update the values of the `Time`, `StartTime`, `Interval`, `StopTime`, and `OutputTimes` properties accordingly.
- You update raw numbers used in any event triggers that use the keyword `time` accordingly. For more information, see Trigger.
- The units, if any, associated with expressions used in any event triggers that use the keyword `time`, are consistent with the updated `TimeUnits` property. For more information, see Trigger.

Tip If UnitConversion is on and your model has any event, follow the recommendation below.

Non-dimensionalize any parameters used in the event `Trigger` if they are not already dimensionless. For example, suppose you have a trigger `x > 1`, where *x* is the species concentration in mole/liter. Non-dimensionalize *x* by scaling (dividing) it with a constant such as `x/x0 > 1`, where *x0* is a parameter defined as 1.0 mole/liter. Note that *x* does not have to have the same unit as the constant *x0*, but must be dimensionally consistent with it. For example, the unit of *x* can be picomole/liter instead of mole/liter.

Characteristics

Applies to	Objects: `Configset`, `RepeatDose`, `ScheduleDose`, `SimData`
Data type	Character vector

Data values	Empty character vector or a character vector specifying any unit defined in the Units Library. Default value is: • `second` — properties of a `Configset` object or `SimData` object for a `model` object created using `sbiomodel` • `hour` — properties of a `Configset` object or `SimData` object for a `model` object created from a `PKModelDesign` object • `''` (empty character vector) — properties of `RepeatDose` and `ScheduleDose` objects
Access	Read/write for properties of `Configset`, `RepeatDose`, and `ScheduleDose` objects Read only for properties of `SimData` objects

See Also

`Configset object`, `RepeatDose object`, `ScheduleDose object`, `SimData object`, Interval, OutputTimes, StartTime, StopTime, Time, MassUnits, AmountUnits

Type

Display SimBiology object type

Description

The `Type` property indicates a SimBiology object type. When you create a SimBiology object, the value of `Type` is automatically defined.

For example, when a `Species` object is created, the value of the `Type` property is automatically defined as `'species'`.

Characteristics

Applies to	Objects: abstract kinetic law, compartment, configuration set, `CompileOptions`, event, kinetic law, model, observable, parameter, reaction, RepeatDose, root, rule, ScheduleDose, species, `RuntimeOptions`, `SolverOptions`, unit, unitprefix, and variant
Data type	Character vector
Data values	`abstract_kinetic_law`, `compartment`, `configset`, `compileoptions`, `event`, `kineticlaw`, `observable` `parameter`, `reaction`, `repeatdose`, `root`, `rule`, `runtimeoptions`, `sbiomodel`, `scheduledose`, `species`, `solveroptions`, `unit`, `unitprefix`, and `variant`
Access	Read-only

See Also

`RepeatDose object`, `sbiomodel`, `sbioroot`, `ScheduleDose object`, `setactiveconfigset`

UnitConversion

Perform unit conversion

Description

The `UnitConversion` property specifies whether to perform unit conversion for the model before simulation. It is a property of the `CompileOptions` object. `CompileOptions` holds the model's compile time options and is the object property of the `configset` object.

When `UnitConversion` is set to `true`, the SimBiology software converts the matching physical quantities to one consistent unit system in order to resolve them. This conversion is in preparation for correct simulation, but species amounts are returned in the user-specified units.

For example, consider a reaction `a + b -> c`. Using mass action kinetics the reaction rate is defined as `a*b*k` where `k` is the rate constant of the reaction. If you specify that initial amounts of `a` and `b` are 0.01M and 0.005M respectively, then units of `k` are `1/(M*second)`. If you specify `k` with another equivalent unit definition, for example, `1/((molecules/liter)*second)`, `UnitConversion` occurs after `DimensionalAnalysis`.

Unit conversion requires dimensional analysis. If `DimensionalAnalysis` is off, and you turn `UnitConversion` on, then `DimensionalAnalysis` is turned on automatically. If `UnitConversion` is on and you turn off `DimensionalAnalysis`, then `UnitConversion` is turned off automatically.

If `UnitConversion` fails, then you see an error when you simulate (`sbiosimulate`).

If `UnitConversion` is set to `false`, the simulation uses the given object values.

Characteristics

Applies to	Object: `CompileOptions` (in `configset` object)
Data type	`boolean`
Data values	`true` or `false`. Default value is `false`.
Access	Read/write

Note SimBiology uses units including empty units in association with DimensionalAnalysis and UnitConversion features.

- When `DimensionalAnalysis` and `UnitConversion` are both `false`, units are not used. However, SimBiology still performs a minimum level of dimensional analysis to decide whether a reaction rate is in dimensions of amount/time or concentration/time.
- When `DimensionalAnalysis` is `true` and `UnitConversion` is `false`, units (if not empty) must have consistent dimensions so that SimBiology can perform dimensional analysis. However, the units are not converted.
- When `UnitConversion` is set to `true` (which requires `DimensionalAnalysis` to be `true`), SimBiology performs a dimensional analysis and converts everything to consistent units. Hence, you must specify consistent units, and no units can be empty. If you have a dimensionless parameter, you must still set its unit to `dimensionless`.

Tip If you have a custom function and UnitConversion is on, follow the recommendation below.

- Non-dimensionalize the parameters that are passed to the function if they are not already dimensionless.

  Suppose you have a custom function defined as `y = f(t)` where `t` is the time in hour and `y` is the concentration of a species in mole/liter. When you use this function in your model to define a repeated assignment rule for instance, define it as: `s1 = f(time/t0)*s0`, where `time` is the simulation time, `t0` is a parameter defined as 1.0 hour, `s0` is a parameter defined as 1.0 mole/liter, and `s1` is the concentration of a species in mole/liter. Note that `time` and `s1` do not have to be in the same units as `t0` and `s0`, but they must be dimensionally consistent. For example, the `time` and `s1` units can be set to minute and picomole/liter, respectively.

Examples

This example shows how to retrieve and set `unitconversion` from the default `true` to `false` in the default configuration set in a model object.

1 Import a model.

```
modelObj = sbmlimport('oscillator')

SimBiology Model - Oscillator

   Model Components:
     Models:            0
     Parameters:        0
     Reactions:         42
     Rules:             0
     Species:           23
```

2 Retrieve the `configset` object of the model object.

```
configsetObj = getconfigset(modelObj)

 Configuration Settings - default (active)
     SolverType:           ode15s
     StopTime:             10.000000

   SolverOptions:
     AbsoluteTolerance:    1.000000e-006
     RelativeTolerance:    1.000000e-003

   RuntimeOptions:
     StatesToLog:          all

   CompileOptions:
     UnitConversion:       false
     DimensionalAnalysis:  true
```

3 Retrieve the `CompileOptions` object.

```
optionsObj = get(configsetObj,'CompileOptions')

Compile Settings:
```

```
    UnitConversion:       false
    DimensionalAnalysis:  true
```

4 Assign a value of false to `UnitConversion`.

```
set(optionsObj,'UnitConversion', true)
```

See Also

`get`, `getconfigset`, `sbiosimulate`, `set`

Units

Units for species amount, parameter value, compartment capacity, observable expression

Description

The `Units` property is an alias for the following existing properties.

- InitialAmountUnits
- CapacityUnits
- ValueUnits

Characteristics

Applies to	Object: species, parameter, compartment, observable
Data type	`boolean`
Data values	`true` or `false`.
Access	Read/write

See Also

InitialAmountUnits, CapacityUnits, ValueUnits

Version History

Introduced in R2019b

UserData

Specify data to associate with object

Description

Property to specify data that you want to associate with a SimBiology object. The object does not use this data directly, but you can access it using the function `get` or dot notation.

Characteristics

Applies to	Objects: abstract kinetic law, configuration set, compartment, data, event, kinetic law, model, observable, parameter, reaction, RepeatDose, rule, ScheduleDose, species, or unit
Data type	Any
Data values	Any. Default is empty.
Access	Read/write

See Also

`RepeatDose object`, `sbioabstractkineticlaw`, `sbiomodel`, `sbioroot`, `sbiounit`, `sbiounitprefix`, `ScheduleDose object`

UserDefinedLibrary

Library of user-defined components

Description

`UserDefinedLibrary` is a SimBiology root object property containing all user-defined components of unit, unit prefixes, and kinetic laws that you define. You can add, modify, or delete components in the user-defined library. The `UserDefinedLibrary` property is an object that contains the following properties:

- `Units` — Contains any user-defined units. You can specify units for compartment capacity, species amounts and parameter values, to do dimensional analysis and unit conversion during simulation. You can display the user-defined units either by using the command `sbiowhos -userdefined -unit`, or by accessing the root object.
- `UnitPrefixes` — Contains any user-defined unit prefixes. You can specify unit prefixes in combination with a valid unit for compartment capacity, species amounts and parameter values, to do dimensional analysis and unit conversion during simulation. You can display the user-defined unit prefixes either by using the command `sbiowhos -userdefined -unitprefix`, or by accessing the root object.
- `KineticLaws` — Contains any user-defined kinetic laws. Use the command `sbiowhos -userdefined -kineticlaw` to see the list of user-defined kinetic laws. You can use user-defined kinetic laws when you use the command `addkineticlaw` to create a kinetic law object for a reaction object. Refer to the kinetic law by name when you create the kinetic law object, for example, `kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');`.

  See “Kinetic Law Definition” on page 3-58 for a definition and more information.

Characteristics

Applies to	Object: root
Data type	object
Data values	Unit, unit prefix, and abstract kinetic law objects
Access	Read-only

Characteristics for `UserDefinedLibrary` properties:

- `Units`

Applies to	`UserDefinedLibrary` property
Data type	Unit objects
Data values	Units
Access	Read/write

- `UnitPrefixes`

Applies to	`UserDefinedLibrary` property
Data type	Unit prefix objects
Data values	Unit prefixes
Access	Read/write

- `KineticLaws`

Applies to	`UserDefinedLibrary` property
Data type	Abstract kinetic law object
Data values	Kinetic laws
Access	Read/write

Examples

Example 1

This example uses the command `sbiowhos` to show the current list of user-defined components.

```
sbiowhos -userdefined -kineticlaw
sbiowhos -userdefined -unit
sbiowhos -userdefined -unitprefix
```

Example 2

This example shows the current list of user-defined components by accessing the root object.

```
rootObj = sbioroot;
get(rootObj.UserDefinedLibrary, 'KineticLaws')
get(rootObj.UserDefinedLibrary, 'Units')
get(rootObj.UserDefinedLibrary, 'UnitPrefixes')
```

See Also

`BuiltInLibrary`, `sbioaddtolibrary`, `sbioremovefromlibrary`, `sbioroot`, `sbiounit`, `sbiounitprefix`

Value

Value of species, compartment, or parameter object

Description

The `Value` property is the value of a parameter, species, or compartment object.

A parameter object defines an assignment that can be used by the model object and/or the kinetic law object. Create parameters and assign `Value` using the method `addparameter on page 2-75`.

For a species object, this property is identical to the InitialAmount property. For a compartment object, this property is identical to the Capacity property.

Characteristics

Applies to	Object: species, compartment, parameter
Data type	`double`
Data values	Any `double`. Default value is `1.0` for parameter and compartment objects, and `0.0` for the species object.
Access	Read/write

Examples

Assign a parameter with a value to the model object.

1. Create a model object, and then add a reaction object.

```
modelObj = sbiomodel ('my_model');
```

2. Add a parameter to the model object (`modelObj`) with `Value` `0.5`.

```
parameterObj1 = addparameter (modelObj, 'K1', 0.5)
```

MATLAB returns:

```
SimBiology Parameter Array

Index:    Name:    Value:    ValueUnits:
 1         K1       0.5
```

See Also

`addparameter`

ValueUnits

Parameter value units

Description

The `ValueUnits` property indicates the unit definition of the `Value` property of a parameter object.

`ValueUnits` can be one of the built-in units. To get a list of the built-in units, use the `sbioshowunits` on page 1-254 function. If `ValueUnits` changes from one unit definition to another, the `Value` does not automatically convert to the new units. The `sbioconvertunits` on page 1-21 function does this conversion.

The `ValueUnits` property is identical to the `Units` property.

Characteristics

Applies to	Object: species, compartment, parameter
Data type	Character vector
Data values	Unit from units library. Default is `''` (empty character vector). Note that the default value of an empty character vector means unspecified. Unspecified units are permitted during dimensional analysis, but not during unit conversion. (Use `'dimensionless'` to specify dimensionless units.)
Access	Read/write

Note SimBiology uses units including empty units in association with DimensionalAnalysis and UnitConversion features.

- When `DimensionalAnalysis` and `UnitConversion` are both `false`, units are not used. However, SimBiology still performs a minimum level of dimensional analysis to decide whether a reaction rate is in dimensions of amount/time or concentration/time.
- When `DimensionalAnalysis` is `true` and `UnitConversion` is `false`, units (if not empty) must have consistent dimensions so that SimBiology can perform dimensional analysis. However, the units are not converted.
- When `UnitConversion` is set to `true` (which requires `DimensionalAnalysis` to be `true`), SimBiology performs a dimensional analysis and converts everything to consistent units. Hence, you must specify consistent units, and no units can be empty. If you have a dimensionless parameter, you must still set its unit to `dimensionless`.

Examples

Assign a parameter with a value to the model object.

1 Create a model object, and then add a reaction object.

```
modelObj = sbiomodel('my_model');
```

2 Add a parameter with `Value` `0.5`, and assign it to the model object (`modelObj`).

```
parameterObj1 = addparameter(modelObj, 'K1', 0.5, 'ValueUnits', '1/second')
```

MATLAB returns:

```
SimBiology Parameter Array

Index:    Name:    Value:    ValueUnits:
 1         K1       0.5       1/second
```

See Also

`addparameter`, `sbioconvertunits`, `sbioshowunits`

ZeroOrderDurationParameter

Zero-order dose absorption duration

Description

`ZeroOrderDurationParameter` is a property of the `PKModelMap` object. It specifies the name(s) of parameter object(s) that represent the duration of absorption when the `DosingType` property is `ZeroOrder`.

Specify the name(s) of parameter object(s) that are:

- Scoped to a model
- Constant, that is, their `ConstantValue` property is `true`

When dosing multiple compartments, a one-to-one relationship must exist between the number and order of elements in the `ZeroOrderDurationParameter` property and the `DosingType` property. For a dose that is not dosed with zero-order kinetics, use `''` (an empty character vector).

Characteristics

Applies to	Object: `PKModelMap`
Data type	Character vector or cell array of character vectors **Tip** If you are not using any zero-order doses, you can set this property to a cell array of empty character vectors, or simply an empty cell array.
Data values	Name of a parameter object or empty. Default is an empty cell array. The parameter object(s) must be: • Scoped to a model • Constant, that is, have a `ConstantValue` property set to `true`
Access	Read/write

See Also

DosingType, `PKModelMap object`