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SimBiology[®] Reference

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Functions

sbioabstractkineticlaw

Create kinetic law definition

Syntax

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

Arguments

	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 <i>kineticlaw0bj</i> .
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 3-170 property, and the parameter variables are defined in the ParameterVariables on page 3-128 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 (AbstractKineticLaw)	
	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
Туре	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.

See Also

addkineticlaw | addparameter | addreaction | sbiomodel

Introduced in R2006a

sbioaccelerate

Prepare model object for accelerated simulations

Syntax

```
sbioaccelerate(model0bj)
sbioaccelerate(model0bj,cs0bj)
sbioaccelerate(model0bj,dv0bj)
```

```
sbioaccelerate(model0bj,cs0bj,dv0bj)
```

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 dv0bj as variants, the function uses the specified variants and active doses. Any other variants are ignored.

If you specify dv0bj 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(model0bj,cs0bj,dv0bj) uses a configset object cs0bj and doses or variants
specified by dv0bj.

If you set cs0bj 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 dv0bj to variants, the function uses the specified variants and active doses. Any other variants are ignored.

If you set dv0bj 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 cs0bj 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')
```

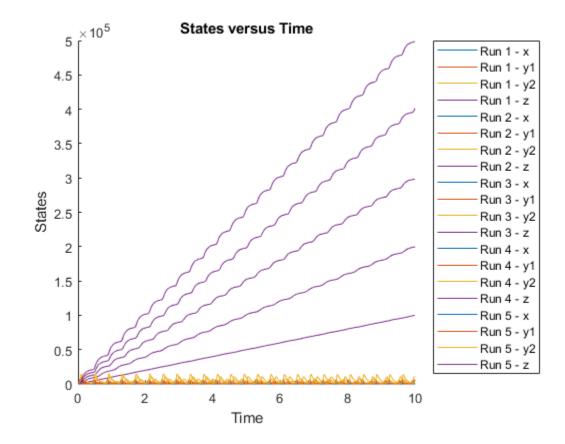
Prepare the model for accelerated simulation.

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.

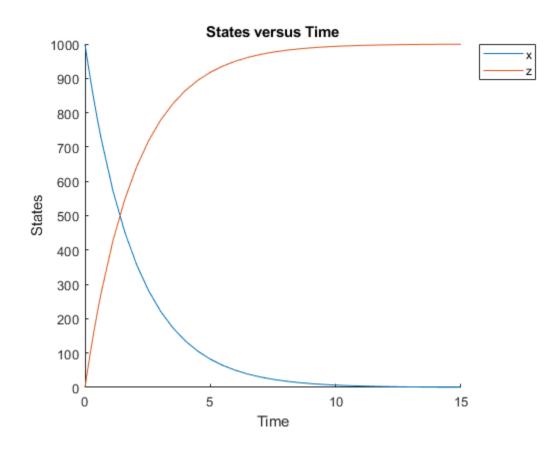
csObj = addconfigset(m1, 'newStopTimeConfigSet'); csObj.StopTime = 15;

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

```
sbioaccelerate(m1,cs0bj);
```

Simulate the model using the same configset object.

```
sim = sbiosimulate(m1,cs0bj);
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.

```
d0bj1 = adddose(m1,'d1','schedule');
d0bj1.Amount = 100;
d0bj1.AmountUnits = 'molecule';
d0bj1.TimeUnits = 'second';
d0bj1.Time = 2;
d0bj1.TargetName = 'unnamed.x';
d0bj2 = adddose(m1,'d2','schedule');
d0bj2.Amount = 100;
d0bj2.AmountUnits = 'molecule';
d0bj2.TimeUnits = 'second';
d0bj2.Time = 4;
d0bj2.TargetName = 'unnamed.x';
```

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

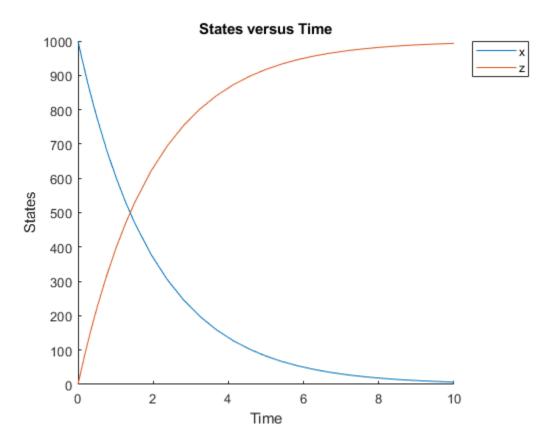
```
sbioaccelerate(m1,[d0bj1,d0bj2]);
```

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

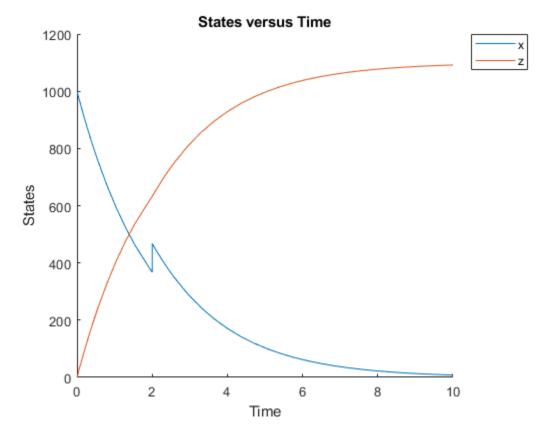
```
sim1 = sbiosimulate(m1);
sim2 = sbiosimulate(m1,d0bj1);
sim3 = sbiosimulate(m1,d0bj2);
sim4 = sbiosimulate(m1,[d0bj1,d0bj2]);
```

Plot the results.

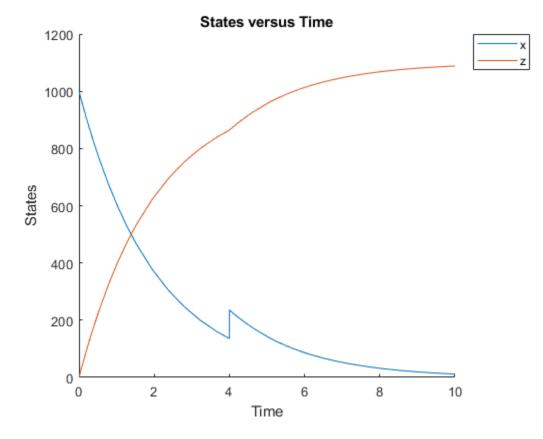
sbioplot(sim1);



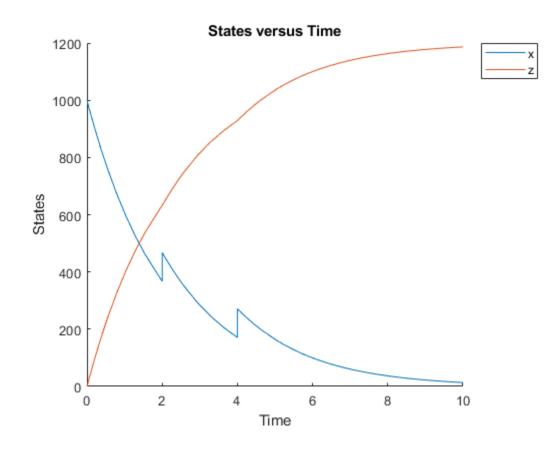
sbioplot(sim2);



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.

```
d0bj = adddose(m1, 'd1', 'schedule');
d0bj.Amount = 100;
d0bj.AmountUnits = 'molecule';
d0bj.TimeUnits = 'second';
d0bj.Time = 2;
d0bj.TargetName = 'unnamed.x';
```

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

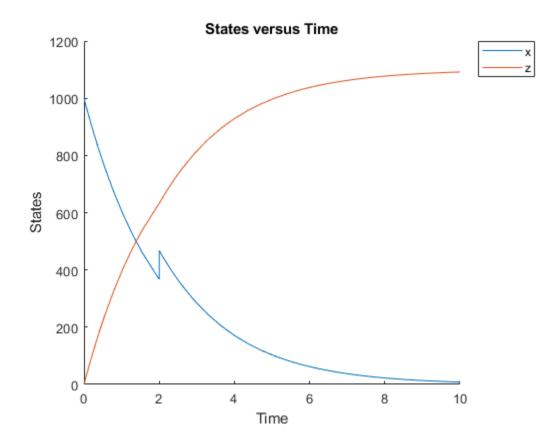
sbioaccelerate(m1,defaultConfigSet,d0bj);

Simulate the model using the same configset and dose objects.

```
sim = sbiosimulate(m1,defaultConfigSet,d0bj);
```

```
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.

```
d0bj = adddose(m1, 'd1', 'schedule');
d0bj.Amount = 100;
d0bj.AmountUnits = 'molecule';
d0bj.TimeUnits = 'second';
d0bj.Time = 2;
d0bj.TargetName = 'unnamed.x';
```

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

```
v0bj = addvariant(m1,'v1');
addcontent(v0bj,{'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.

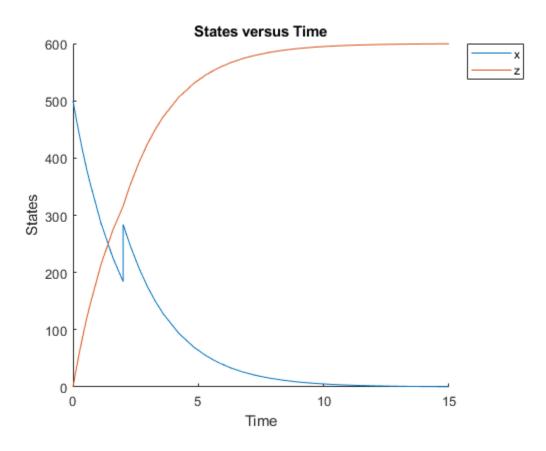
```
sbioaccelerate(m1,cs0bj,v0bj,d0bj);
```

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

```
sim = sbiosimulate(m1,cs0bj,v0bj,d0bj);
```

Plot the result.

sbioplot(sim);



Input Arguments

model0bj — 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.

cs0bj — Configuration set object

configset object | []

Configuration set object, specified as a configset object that stores simulation-specific information. When you specify cs0bj as[], sbioaccelerate uses the currently active configset.

dv0bj – 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.

variant0bj — 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.

dose0bj — 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.

See Also

SimFunction object | sbiosimulate

Topics

"Accelerating Model Simulations and Analyses"

Introduced in R2010a

sbioaddtolibrary

Add to user-defined library

Syntax

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

Arguments

abstkineticlaw0bj	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 <i>kineticlawObj</i> . For more information about creating <i>kineticlawObj</i> , see sbioabstractkineticlaw.
unitObj	Specify the user-defined unit to add to the library. For more information about creating <i>unitObj</i> , see sbiounit.
unitprefix0bj	Specify the user-defined unit prefix to add to the library. For more information about creating <i>unitprefixObj</i> , see sbiounitprefix.

Description

The function **sbioaddtolibrary** adds kinetic law definitions, units, and unit prefixes to the userdefined 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.

See Also

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

Introduced in R2006a

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 <i>G</i> 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 <i>G</i> . 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.	
model0bj	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'.	
Н	Cell array of character vectors containing the conserved moieties.	
р	Prints the output according to the format defined by <i>FormatArg</i> .	
FormatArg	Specifies formatting for the output <i>H</i> . <i>FormatArg</i> 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.	
LO	Link matrix relating SI and SD. The link matrix <i>LO</i> satisfies ND = LO*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. <i>LO</i> 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.	

Reduced stoichiometry matrices containing one row for each dependent species. The concatenated matrix [<i>NR</i> ; <i>ND</i>] is a row-permuted version of the full stoichiometry matrix of <i>modelObj</i> .
<i>ND</i> 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] = sbioconsmolety(modelObj, alg) provides an algorithm specification. For alg, specify 'qr', 'rreduce', or 'semipos'.

- When you specify 'qr', sbioconsmolety 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', sbioconsmolety 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 = sbioconsmolety(modelObj, alg, 'p') returns a cell array of character vectors H
containing the conserved quantities in modelObj.

H = sbioconsmolety(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*, *LO*, *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.

2

Example 2

'c'

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'
```

See Also

getstoichmatrix

Topics "Conserved Moiety Determination"

Introduced in R2006a

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

See Also

sbioshowunits

Topics sbioshowunits

Introduced in R2006a

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:
 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
```

See Also

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

Introduced in R2006a

sbiodesktop

(To be removed) Open SimBiology desktop for modeling and simulation

Note sbiodesktop will be removed in a future release. Use simBiologyModelBuilder instead.

Syntax

```
sbiodesktop
sbiodesktop(model0bj)
sbiodesktop(File)
```

Input Arguments

model0bj	SimBiology model object or an array of model objects.
	String specifying a file name or path and file name of an sbproj file. If you specify only a file name, that file must be on the MATLAB search path or in the MATLAB Current Folder.

Description

sbiodesktop opens the SimBiology desktop, which lets you:

- Build a SimBiology model by representing reaction pathways and entering kinetic data for the reactions.
- Import or export SimBiology models to and from the MATLAB workspace or from a Systems Biology Markup Language (SBML) file.
- Modify an existing SimBiology model.
- Simulate a SimBiology model through individual or ensemble runs.
- View results from the simulation.
- Perform analysis tasks such as sensitivity analysis, parameter and species scans, and calculation of conserved moieties.
- Create and/or modify user-defined units and unit prefixes.
- Create and/or modify user-defined kinetic laws.

sbiodesktop(modelObj) opens the SimBiology desktop with modelObj, a SimBiology model
object. If there is a project open in the SimBiology desktop, this command adds modelObj to the
project.

sbiodesktop(File) opens the project specified by File in the SimBiology desktop. File is a
string specifying a file name or path and file name of an sbproj file. If you specify only a file name,
that file must be on the MATLAB search path or in the MATLAB Current Folder. If a project is open in
the desktop, the software replaces it with the new project, after prompting you to save any changes.

The Parent property of a SimBiology model object is 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, changes you make to the model at the command line are reflected in the desktop, and vice versa.

Note The sbioreset command removes all models from the root object. Therefore, this command also removes all models from the SimBiology desktop.

Examples

Create a SimBiology model in the MATLAB workspace, and then open the SimBiology desktop with the model:

```
modelObj = sbiomodel('cell');
sbiodesktop(modelObj)
```

Compatibility Considerations

sbiodesktop will be removed Not recommended starting in R2020b

sbiodesktop will be removed in a future release. Use simBiologyModelBuilder instead.

See Also SimBiology Model Builder | sbiofittool | sbioroot | simbiology

Introduced before R2006a

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 (dl.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'};

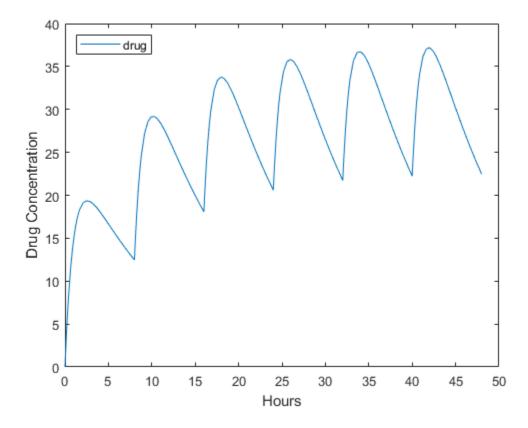
Simulate the model using the dosing schedule defined by the |d1 |dose object.

[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 (dl.StartTime = 0).

Simulate the Model

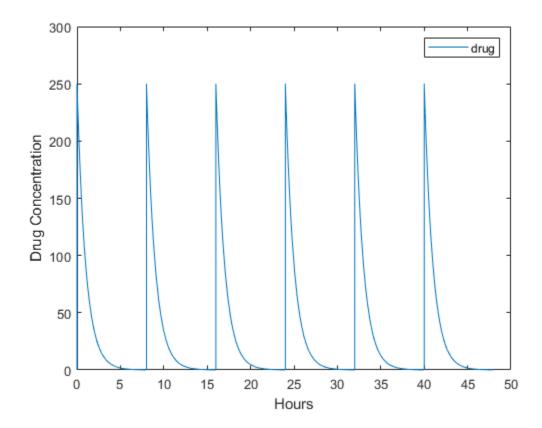
Change the simulation stop time to 48 hours to match the dosing schedule defined by the d1 dose object.

```
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';
```

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

Simulate the Model

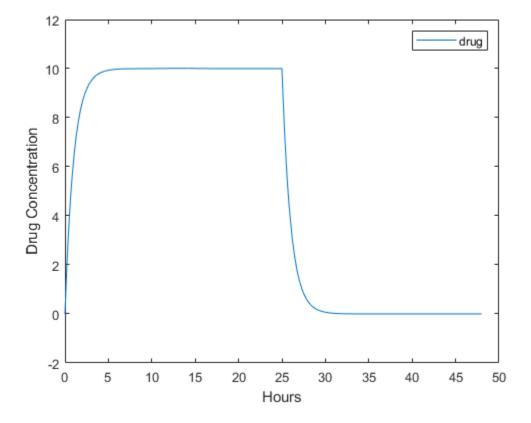
Change the simulation stop time to 48 hours to see the complete time profile. Apply the dosing schedule defined by d1 to the model during simulation.

```
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.

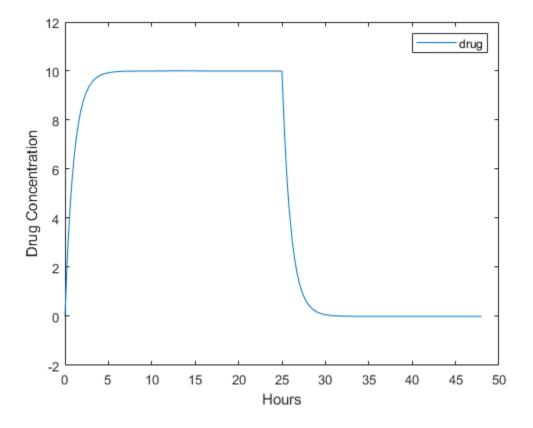
cs = getconfigset(m1); cs.StopTime = 48;

```
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.

See Also

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

Topics Model "Doses in SimBiology Models"

Introduced in R2010a

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 <i>simdataObj</i> object using the function sbioensemblerun. All elements of <i>simdataOb</i> 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 <i>Time</i> is not an element of the time vectors in <i>simdataObj</i> , then the function resamples <i>simdataObj</i> 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'});
```

See Also

sbioensemblerun | sbioensemblestats | sbiomodel

Introduced in R2006a

sbioensemblerun

Multiple stochastic ensemble runs of SimBiology model

Syntax

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

Arguments

simdata0bj	An array of SimData objects containing simulation data generated by sbioensemblerun. All elements of <i>simdataObj</i> contain data for the same states in the same model.		
model0bj	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.		
configset0bj	Specify the configuration set object to use in the ensemble simulation. For more information about configuration sets, see Configset object.		
variant0bj	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);
```

See Also

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

Introduced in R2006a

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 <i>simDataObj</i> must contain data for the same states in the same model. When the time vectors of the elements of <i>simDataObj</i> are not identical, <i>simDataObj</i> is first resampled onto a common time vector (see <i>interpolation</i> 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 <i>m</i> and <i>v</i> , respectively. The number of elements i is the same as the number of columns of <i>m</i> and <i>v</i> . The order of names in corresponds to the order of columns of <i>m</i> and <i>v</i> .		
names	Character vector, string, string vector, string array, or cell array of character vectors. <i>names</i> 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 <i>simDataObj</i> .		
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'});
```

See Also

sbioensembleplot | sbioensemblerun | sbiomodel

Introduced in R2006a

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 $k_e = Cl/V$.

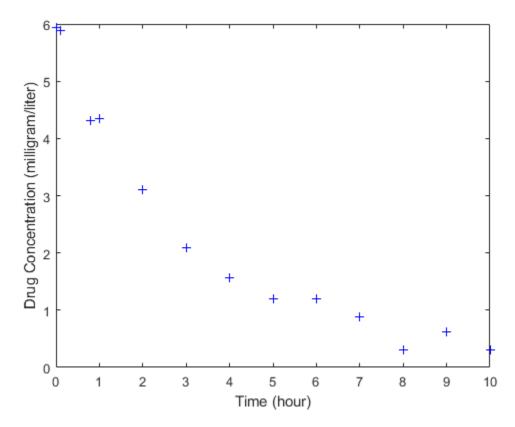
The synthetic data in this example was generated using the following model, parameters, and dose:

- 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.

```
clear all
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".

<pre>= sbiodose('dose');</pre>
<pre>= 'Drug_Central';</pre>
= 0;
= 10;
<pre>= 'milligram';</pre>
<pre>= 'hour';</pre>

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);

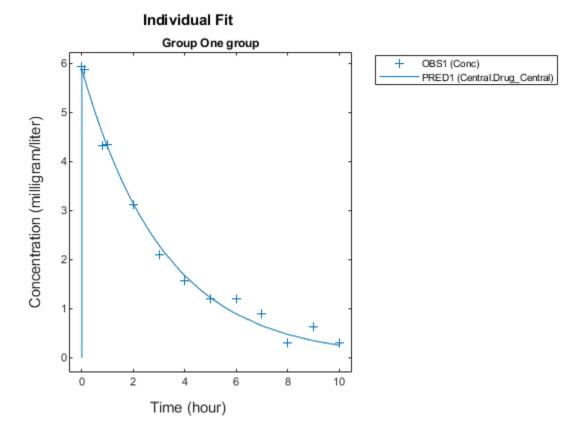
Display Estimated Parameters and Plot Results

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	Boun	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).

```
'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 combined error model	1.1984 3.9163	1.6032 -3.8326	2.7331 -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 a 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')

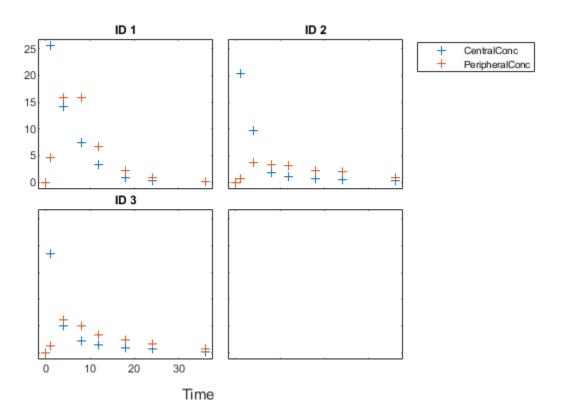
Convert the data set to a groupedData object which is the required data format for the fitting function sbiofit for later use. A groupedData object also lets you set independent variable and group variable names (if they exist). Set the units of the ID, Time, CentralConc, and PeripheralConc variables. 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 =
```

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);
                     = getconfigset(model);
configset
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]);
```

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)

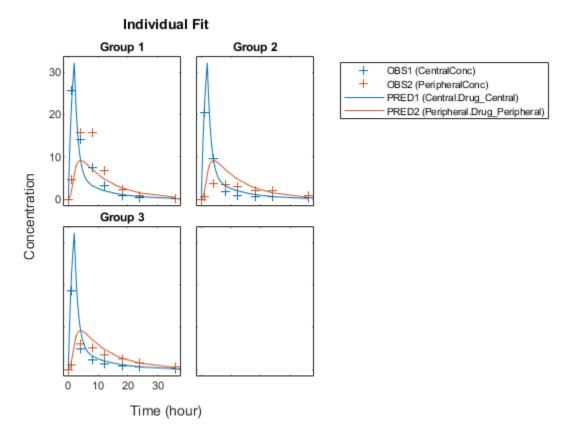
```
pooledFit =
```

```
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}
EstimatedParameterNames: {'Central'
                                     'Peripheral' 'Q12' 'Cl_Central'}
         ErrorModelInfo: [1x3 table]
     EstimationFunction: 'lsgnonlin'
```

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);

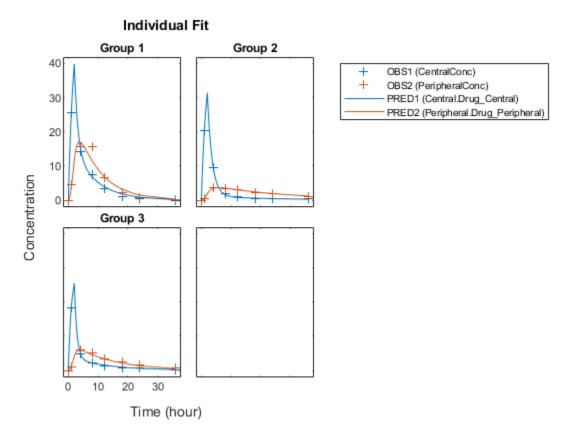


Estimate one set of parameters for each individual and see if there is any improvement in the parameter estimates. In this example, since there are three individuals, three sets of parameters are estimated.

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);



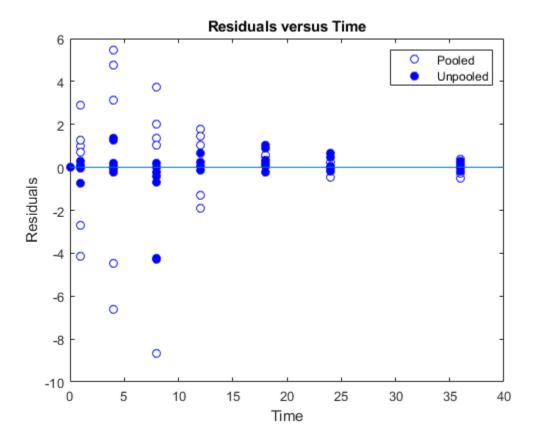
Display the fitted results of the first individual. The MSE was lower than that of the pooled fit. This is also true for the other two individuals.

```
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}
   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.

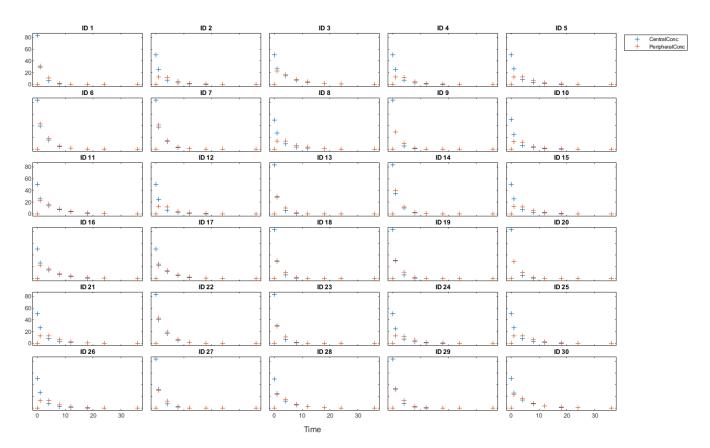
```
gData = groupedData(data);
gData.Properties.VariableUnits = {'', 'hour', 'milligram/liter', 'milligram/liter', '', ''};
gData.Properties
```

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;
                                         = addCompartment(pkmd, 'Peripheral');
pkc2
model
                                         = construct(pkmd);
                                         = getconfigset(model);
configset
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

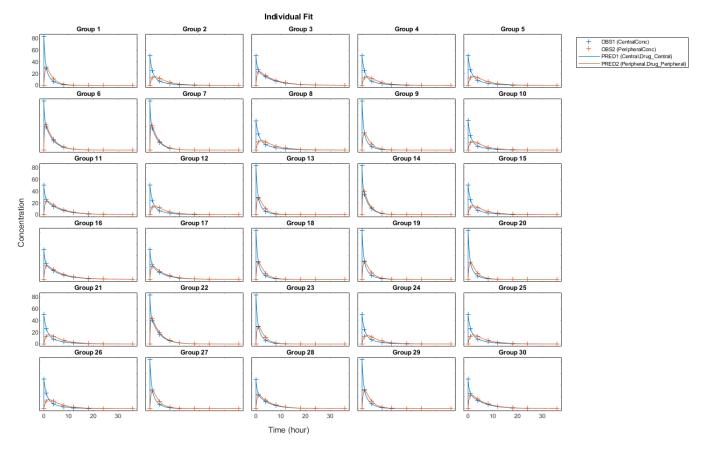
Estimate one set of parameters for each individual by setting the '**Pooled**' name-value pair argument to false.

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

Display Results

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

```
t = plot(unpooledFit);
% Resize the figure.
t.hFig.Position(:) = [100 100 1280 800];
```



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'}));

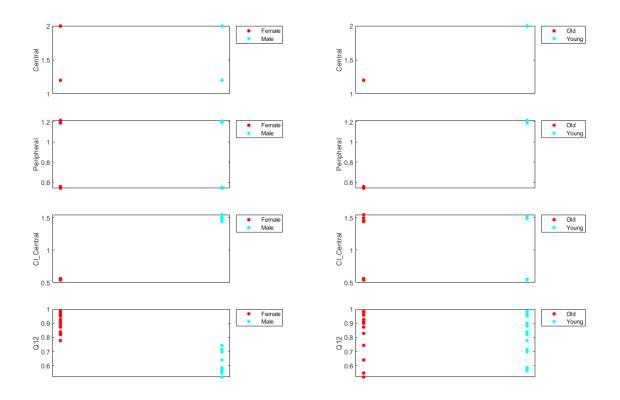
Add variables to the table containing each parameter's estimate.

```
allParamValues = vertcat(unpooledFit.ParameterEstimates);
catParamValues.Central = allParamValues.Estimate(strcmp(allParamValues.Name, 'Central'));
catParamValues.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 ToolboxTM. If you do not have it, use other alternative plotting functions such as plot.

```
h = figure;
ylabels = {'Central', 'Peripheral', 'Cl\_Central', 'Q12'};
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);
   ах
                = gca;
    ax.XTick
                = [1];
   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);
   ах
                = 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 higher 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.

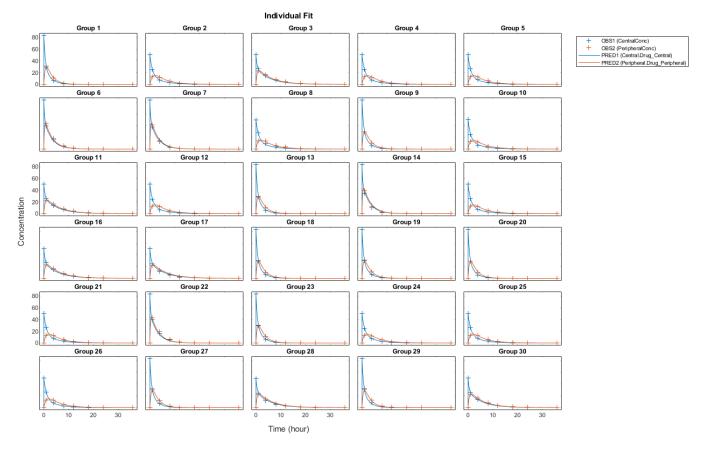
```
estimatedParam(1).CategoryVariableName = 'Age';
estimatedParam(2).CategoryVariableName = 'Age';
estimatedParam(3).CategoryVariableName = 'Sex';
estimatedParam(4).CategoryVariableName = 'Sex';
categoryFit = sbiofit(model,gData,responseMap,estimatedParam,dose)
categoryFit =
  OptimResults with properties:
                   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}
                                         'Peripheral' 'Q12' 'Cl Central'}
    EstimatedParameterNames: {'Central'
             ErrorModelInfo: [1x3 table]
         EstimationFunction: 'lsgnonlin'
```

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.

```
t = plot(categoryFit);
% Resize the figure.
t.hFig.Position(:) = [100 100 1280 800];
```



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).

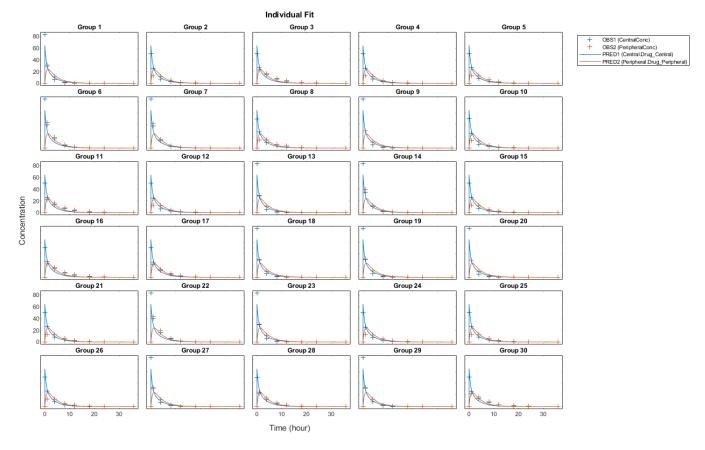
```
pooledFit = sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',true);
```

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

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).

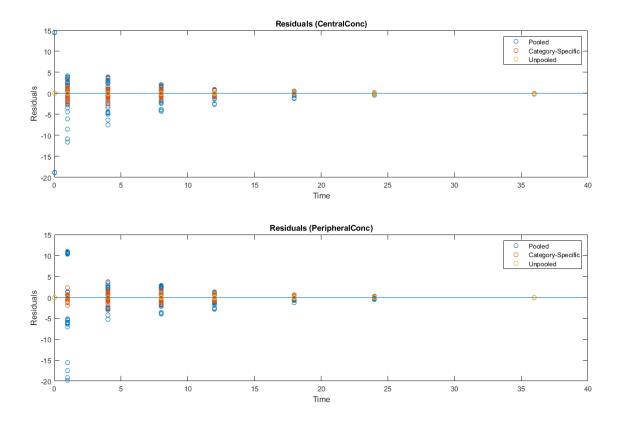
```
t = plot(pooledFit);
% Resize the figure.
t.hFig.Position(:) = [100 100 1280 800];
```



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 a Parameter from the Yeast G Protein 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]';

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.

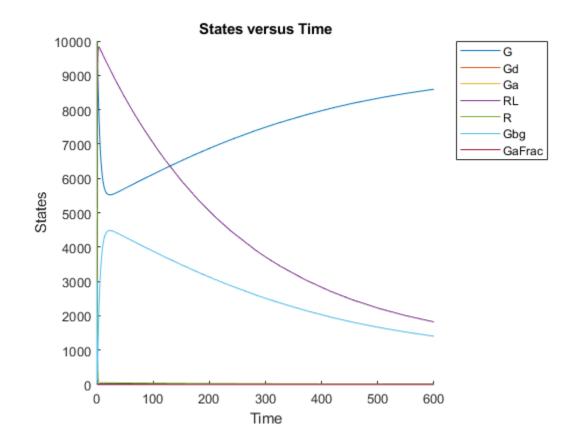
fitResult.ParameterEstimates

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

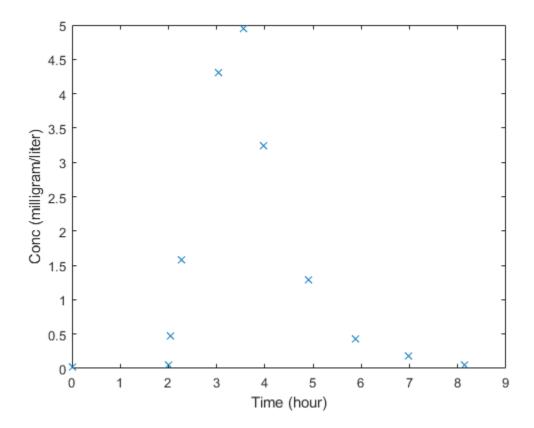
This example shows how to estimate the time lag before a bolus dose was administered and the duration of the dose using a one-compartment model.

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');
                         =
                           'Bolus';
pkc1.DosingType
                        =
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')
```

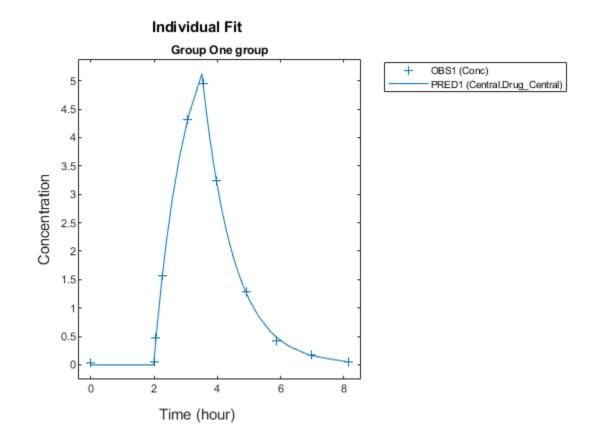
```
fitResults =
 OptimResults with properties:
                   ExitFlag: 1
                      Output: [1x1 struct]
                  GroupName: One group
                        Beta: [2x4 table]
         ParameterEstimates: [2x4 table]
                           J: [11x2 double]
                        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}
    EstimatedParameterNames: {'lagP' 'durP'}
             ErrorModelInfo: [1x3 table]
         EstimationFunction: 'fminsearch'
```

Display the result.

fitResults.ParameterEstimates

ans=2×4 table Name	Estimate	StandardError	Bou	nds
{'lagP'} {'durP'}	1.986 1.527	0.0051568 0.012956	1 1	5 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 "boundValues" 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

Dosing information, specified as an empty array, or 2-D matrix of dose objects (ScheduleDose object or RepeatDose object).

- If empty, no doses are applied during simulation, even if the model has active doses.
- If not empty, the matrix must have a single row or one row per group in the input data. If it has a single row, 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. All doses in a column must reference the same components in the model. For example, doses in the same column must have the same dose target (TargetName). If you parameterize any property of a dose, then all doses within the column must have this property parameterized to the same parameter. If some groups require more doses than others, then fill in the matrix with default (dummy) doses.
- A default dose has default values for all properties, except for the Name property. Create a default dose as follows.

d1 = sbiodose('d1');

• In addition to manually constructing dose objects using sbiodose, if grpData 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 1-80

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 1-78 for more details and default options associated with each estimation function.

variants — Variants

[] | vector of variant objects

Variants, specified as an empty array or vector of variant objects. If empty, no variants are used even if the model has active variants.

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: '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 *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 the responseMap argument.

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

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*.

- '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 are using 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 may 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 1-76.

Weights - Weights

matrix | function handle

Weights used for estimation, specified as a 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 function uses the constant error model with equal weights.

Pooled — Fit option flag

false (default) | true

Fit option flag, specifying whether to fit each individual (false) or pool all individual data (true).

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

When false, the function 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 (default) | true

Flag to enable parallelization, specified as true or 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 1-84.

SensitivityAnalysis — Flag to use parameter sensitivities to determine gradients of the objective function

true | false

Flag to use parameter sensitivities to determine gradients of the objective function, specified as true or false. By default, it is true for fmincon, fminunc, lsqnonlin, and lsqcurvefit methods. Otherwise, it is false. If it is true, SimBiology always uses the sundials solver, regardless of what you have selected as the SolverType property in the Configset object.

SimBiology 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 (default) | true

Flag to show the progress of parameter estimation, specified as true or false. If true, a new figure opens containing plots that show the log-likelihood, termination criteria, and estimated parameters for each iteration. This option is not supported for the nlinfit method.

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.

When '**Pooled**' is set to false, 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.

When 'Pooled' is set to true, the function performs fitting for all individuals or groups simultaneously using the same parameter estimates, and fitResults is a scalar results object.

When 'Pooled' is not used, and CategoryVariableName values of estiminfo are all <none>, fitResults is a single result object. This is the same behavior as setting 'Pooled' to true.

When 'Pooled' is not used, and CategoryVariableName values of estiminfo are all <GroupVariableName>, fitResults is a vector of results objects. This is the same behavior as setting 'Pooled' to false.

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 <code>lsqnonlin</code> and <code>lsqcurvefit</code>. 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
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
<i>y</i> _i	The <i>i</i> th experimental observation
f_i	Predicted value of the <i>i</i> th observation
σ_i	Standard deviation of the <i>i</i> th observation.
	• For the constant error model, $\sigma_i = a$
	• For the proportional error model, $\sigma_i = b f_i $
	• For the combined error model, $\sigma_i = a + b f_i $
f _{gm}	$f_{gm} = \left(\prod_{i}^{N} f_i \right)^{1/N}$
Wi	The weight of the <i>i</i> th 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
$constant : y_i = f_i + ae$	$a^{2} = \frac{1}{N} \sum_{i}^{N} (y_{i} - f_{i})^{2}$
'exponent ial': $y_i = f_i \exp(ae)$	$a^{2} = \frac{1}{N} \sum_{i}^{N} (\ln y_{i} - \ln f_{i})^{2}$
'proporti onal': $y_i = f_i$ $+ b f_i e$	$b^2 = \frac{1}{N} \sum_{i}^{N} \left(\frac{y_i - f_i}{f_i} \right)^2$
'combined ': $y_i = f_i$ + $(a + b f_i)e$	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
	<pre>sbiofit uses the default options structure associated with nlinfit, except for: FunValCheck = 'off' DerivStep = max(eps^(1/3), min(1e-4,SolverOptions.RelativeTolerance)), where SolverOptions property corresponds to the model's active configset object.</pre>

Function	Default Options
fmincon	<pre>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 objective function. OptimalityTolerance = 1e-6*abs(f0), where f0 is the initial value of 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 SolverOptions property corresponds to the model active configset object. TypicalX = 1e-6*x0, where x0 is an array of transformed initial estimates.</pre>
fminunc	<pre>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 objective function. OptimalityTolerance = 1e-6*abs(f0), where f0 is the initial value of 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 SolverOptions property corresponds to the model active configset object. TypicalX = 1e-6*x0, where x0 is an array of transformed initial estimates.</pre>
fminsearch	<pre>sbiofit uses the default options structure associated with fminsearch, except for: Display = 'off' TolFun = le-6*abs(f0), where f0 is the initial value of objective function.</pre>

Function	Default Options
lsqcurvefit, lsqnonlin	Requires Optimization Toolbox.
	<pre>sbiofit uses the default options structure associated with lsqcurvefit and lsqnonlin, except for: Display = 'off'</pre>
	FunctionTolerance = $1e-6*norm(f0)$, where f0 is the initial value of objective function.
	<pre>OptimalityTolerance = 1e-6*norm(f0), where f0 is the initial value of objective function. FiniteDifferenceStepSize =</pre>
	<pre>max(eps^(1/3),min(le-4,SolverOptions.RelativeTolerance)), where SolverOptions property corresponds to the model active configset object.</pre>
	TypicalX = $1e-6*x0$, where x0 is an array of transformed initial estimates.
patternsearch	Requires Global Optimization Toolbox.
	<pre>sbiofit uses the default options object (optimoptions) associated with patternsearch, except for: Display = 'off'</pre>
	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.
	<pre>sbiofit uses the default options object (optimoptions) associated with ga, except for: Display = 'off'</pre>
	FunctionTolerance = $1e-6*abs(f0)$, where f0 is the initial value of objective function.
nanti clocularm	MutationFcn = @mutationadaptfeasible
particleswarm	Requires Global Optimization Toolbox. <pre>sbiofit uses the following default options for the particleswarm algorithm, except for: Display = 'off'</pre>
	FunctionTolerance = 1e-6*abs(f0), where f0 is the initial value of objective function.
	<pre>InitialSwarmSpan = 2000 or 8; 2000 for estimated parameters with no transform; 8 for estimated parameters with log, logit, or probit transforms.</pre>
scattersearch	See "Scatter Search Algorithm" on page 1-80.

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
	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
CreationFc n	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.
FractionIn itialBest	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.
FunctionTo lerance	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.
InitialPoi ntMatrix	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 <i>M</i> < NumInitialPoints, then scattersearch creates more points so that the total number of rows is NumInitialPoints.
	<pre>If M > NumInitialPoints, then scattersearch uses the first NumInitialPoints rows.</pre>
	Default is the initial transformed values of estimated parameters stored in the InitialTransformedValue property of the EstimatedInfo object, that is, [estiminfo.InitialTransformedValue].

Option	Description
LocalOptio ns	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 1-78. 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
LocalSearc hInterval	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.
	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.
LocalSolve r	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.
MaxIterati ons	Positive integer. Default is the character vector 'auto' representing $20*N$, where N is the number of estimated parameters.
MaxStallIt erations	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.
MaxStallTi me	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.
NumInitial Points	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.
NumTrialPo ints	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 $n^2 - n \ge 10 * N$, where N is the number of estimated parameters.
ObjectiveL imit	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.
TrialStall Limit	Positive integer, with default value of 22. If a particular trial point does not improve after TrialStallLimit iterations, it is replaced with another point.
UseParalle l	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 fit runs in parallel. For a pooled fit, parallelization happens at the solver level if the solver supports it. That is, sbiofit sets the parallel option of the corresponding estimation method (solver) to true, and the objection function evaluations are performed in parallel. For instance, gradients are computed in parallel for gradient-based methods. If you are performing a pooled fit with multiple groups using a solver that does not have the parallel option, the simulations run in parallel for each group during optimization (maximum likelihood estimation on page 1-76).

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(pool0bj);

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.

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

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 for sbiofit"

"Supported Methods for Parameter Estimation in SimBiology"

"Sensitivity Analysis in SimBiology"

"Progress Plot"

"Importing Data - Supported Files and Data Types"

"Create Data File with SimBiology Definitions"

Introduced in R2014a

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,opt)
fitResults = sbiofitmixed(sm,grpData,responseMap,covEstiminfo,dosing,
functionName,opt,variants)
fitResults = sbiofitmixed(_,'UseParallel',tf_parallel)
fitResults = sbiofitmixed(_,'ProgressPlot',tf_progress)
[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(_,'UseParallel',tf_parallel) specifies whether to estimate
parameters in parallel if Parallel Computing Toolbox is available.

fitResults = sbiofitmixed(_,'ProgressPlot',tf_progress) specifies whether to show the progress of parameter estimation.

[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
```

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 = 1x1 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 = 2x1 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 = 1x1 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.

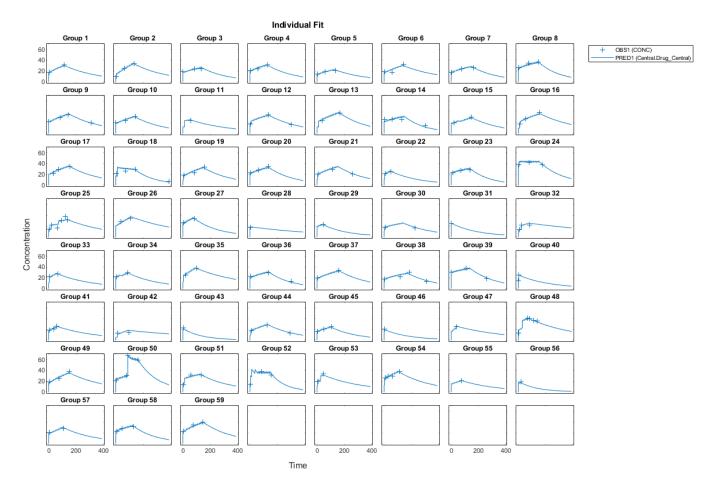
[nlmeResults,simI,simP] = sbiofitmixed(onecomp,data,responseMap,estimatedParams,doses,'nlmefit')

Visualize the fitted results using individual-specific parameter estimates.

fig1 = plot(nlmeResults, 'ParameterType', 'individual');

```
% Resize the figure.
```

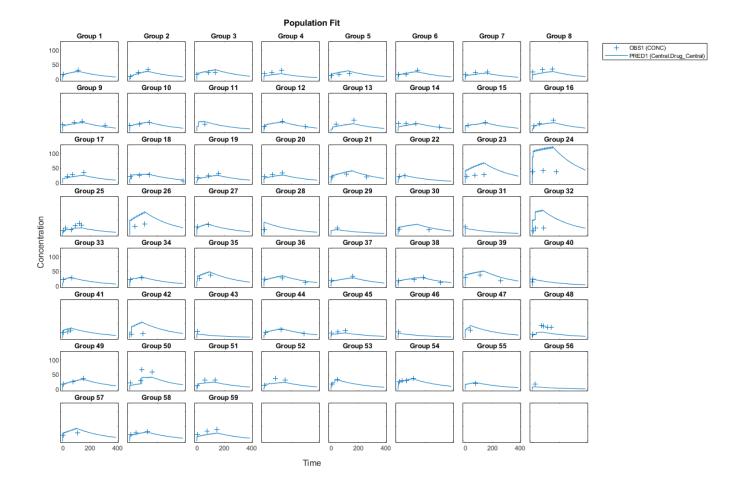
fig1.hFig.Position(:) = [100 100 1200 800];



Visualize the fitted results using population parameter estimates.

fig2 = plot(nlmeResults, 'ParameterType', 'population');

```
% Resize the figure.
fig2.hFig.Position(:) = [100 100 1200 800];
```



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';

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 object

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

Dosing information, specified as an empty array or 2-D matrix of dose objects (ScheduleDose object or RepeatDose object).

- If empty, no doses are applied during simulation, even if the model has active doses.
- If not empty, the matrix must have a single row or one row per group in the input data. If it has a single row, 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. All doses in a column must reference the same components in the model. For example, doses in the same column must have the same dose target (TargetName). If you parameterize any property of a dose, then all doses within the column must have this property parameterized to the same parameter. If some groups require more doses than others, then fill in the matrix with default (dummy) doses.
- A default dose has default values for all properties, except for the Name property. Create a default dose as follows.

d1 = sbiodose('d1');

• In addition to manually constructing dose objects using sbiodose, if grpData 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 contains fields and default values that are the name-value pair 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 covEstiminfo is a vector of estimatedInfo objects.

Use the statset function only to set the 'Options' field of the opt structure as follows.

opt.Options = statset('Display','iter','TolX',1e-3,'TolFun',1e-3);

For other supported name-value pair 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 vector of variant objects. If empty, no variants are used even if the model has active variants.

tf_parallel — 'UseParallel' option

false (default) | true

'UseParallel' option, specified as true or false. If true, and Parallel Computing Toolbox is available, the function performs parameter estimation in parallel.

tf_progress — 'ProgressPlot' option

false (default) | true

'ProgressPlot' option, specified as true or false. If true, a new figure opens containg plots that show the progress of parameter estimation. Specifically, 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".

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.

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

CovariateModel object | EstimatedInfo object | NLMEResults object | groupedData | nlmefit | nlmefitsa | sbiofit | sbiofitstatusplot

Topics

"Modeling 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"
"Importing Data — Supported Files and Data Types"
"Create Data File with SimBiology Definitions"

Introduced in R2014a

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

See Also

```
nlmefit | sbiofitmixed | sbionlinfit | sbionlmefit | sbionlmefitsa
```

Topics "Progress Plot"

Introduced in R2009b

sbiofittool

Open SimBiology desktop for population fitting

Note sbiofittool will be removed in a future release. Use simBiologyModelBuilder to open the SimBiology Model Builder app. Use simBiologyModelAnalyzer to open the SimBiology Model Analyzer app.

Syntax

sbiofittool

Description

sbiofittool opens the SimBiology desktop in a state designed for:

- Importing and plotting data for fitting
- Selecting from a library of pharmacokinetic models
- Performing population fit tasks using sbionlmefit or sbionlmefitsa
- Performing individual fit tasks using sbionlinfit

sbiofittool opens a simplified configuration of the SimBiology desktop. However, all desktop
functionality is available.

If you opened the SimBiology desktop using the simbiology function, then sbiofittool changes the desktop layout to optimize it for population fitting.

See Also

simbiology

Introduced in R2011a

sbiogetmodel

Get model object that generated simulation data

Syntax

modelObj = sbiogetmodel(simDataObj)

Arguments

	SimData object returned by the function sbiosimulate or by sbioensemblerun.
model0bj	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
```

See Also

sbiosimulate

Introduced before R2006a

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:

Туре	'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);
```

See Also

sbiolastwarning|verify

Topics

sbioroot on page 1-202

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:

Туре	'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).

See Also sbiolasterror | verify

Topics sbioroot on page 1-202

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.

See Also

sbioaddtolibrary | sbioremovefromlibrary | sbiosaveproject | sbiowhos

Topics

sbiosaveproject on page 1-218 sbiowhos on page 1-284 sbioaddtolibrary on page 1-16 sbioremovefromlibrary on page 1-198

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.
	Property name for a Model object from "Property Summary" on page 1-110.
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 2-41, addparameter on page 2-65, addreaction on page 2-73, addrule on page 2-78, and addspecies on page 2-89.

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
	5 G5

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
Туре	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(model0bj)

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.

model0bj

```
SimBiology Model - cell
Model Components:
Models: 0
Parameters: 0
Reactions: 0
Rules: 0
Species: 0
```

See Also

addcompartment|addconfigset|addevent|addkineticlaw|addparameter|addreaction |addrule|addspecies|copyobj|get|model object|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(simdata,samples,classifiers)
mpgsaResults = sbiompgsa(____,Name,Value)
```

Description

mpgsaResults = sbiompgsa(modelObj,params,classifiers) performs a multiparametric global sensitivity analysis (MPGSA on page 1-121) [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(simdata,samples,classifiers) uses model simulation data simdata to perform a multiparametric global sensitivity analysis of classifiers.

mpgsaResults = sbiompgsa(_____, Name, Value) uses additional options specified by one or more name-value pair arguments. Available name-value pairs differ depending on which syntax you are using.

Examples

Perform Multiparametric Global Sensitivity Analysis (MPGSA)

Load the "Target-Mediated Drug Disposition (TMDD) Model".

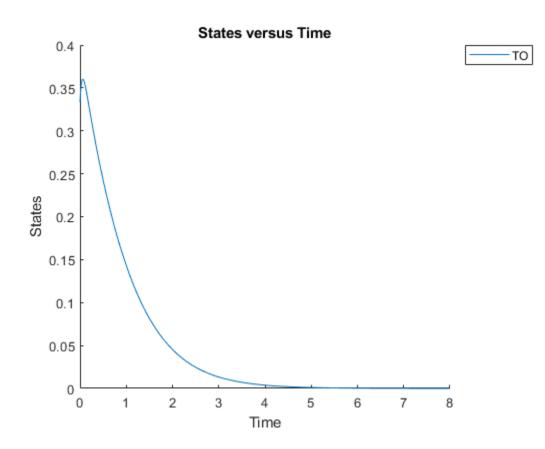
sbioloadproject tmdd_with_T0.sbproj

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 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,T0) <= 0.1';</pre>

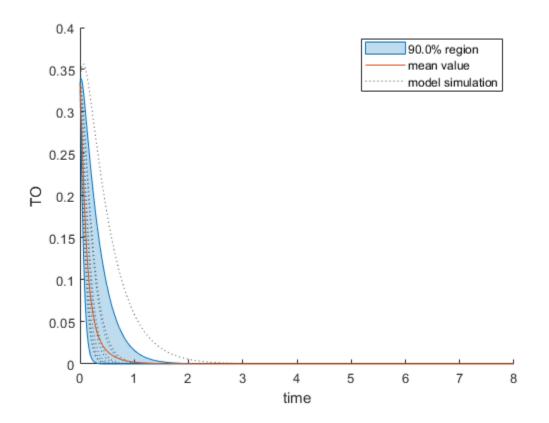
Perform MPGSA to find sensitive parameters with respect to the TO. Vary the parameter values between predefined bounds to generate 10,000 parameter samples.

```
% 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,T0) <= 0.1'}</pre>
    KolmogorovSmirnovStatistics: [4x1 table]
                        ECDFData: {4x4 cell}
              SignificanceLevel: 0.0500
                         PValues: [4x1 table]
              SupportHypothesis: [10000x1 table]
                     Observables: {'TO'}
                ParameterSamples: [10000x4 table]
```

```
SimulationInfo: [1x1 struct]
```

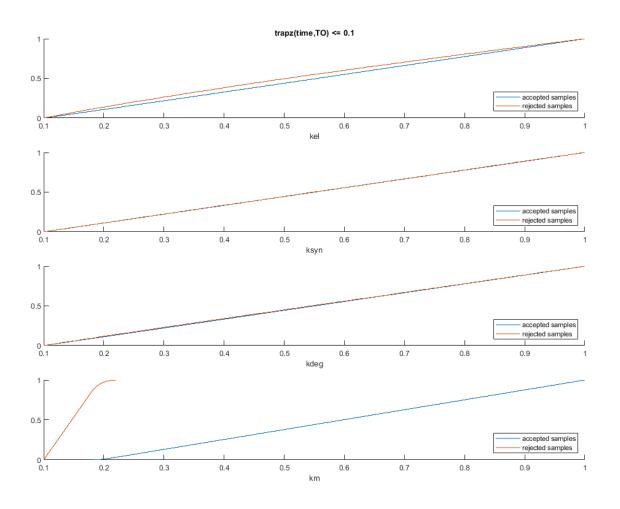
Plot the quantiles of the simulated model response.

plotData(mpgsaResults);



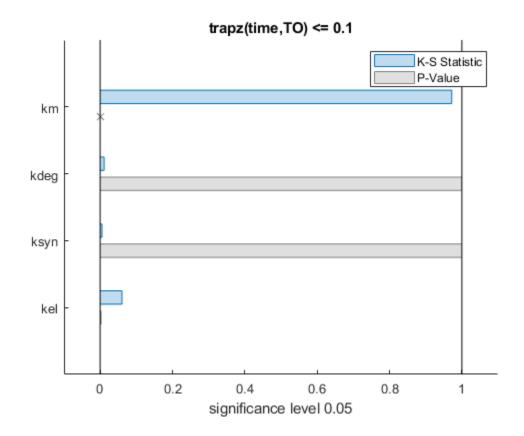
Plot the empirical cumulative distribution functions (eCDFs) of the accepted and rejected samples. Except for km, none of the parameters shows a significant difference in the eCDFs for the accepted and rejected samples. The km plot shows a large Kolmogorov-Smirnov (K-S) distance between the eCDFs of 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)



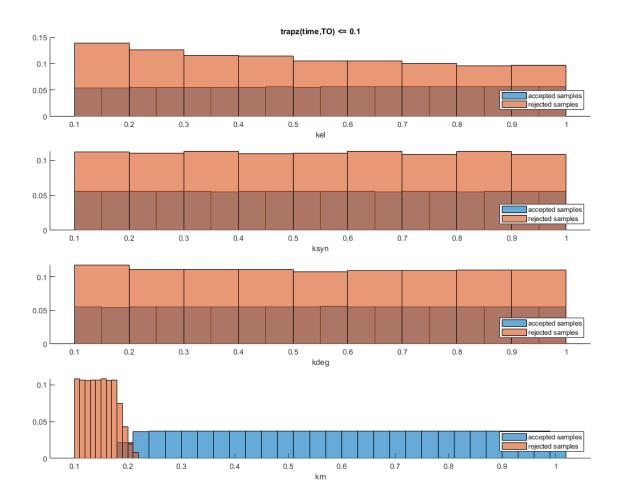
The bar plot shows two bars for each parameter: one for the K-S distance (K-S statistic) and another for the corresponding p-value. You reject the null hypothesis if the p-value is less than the significance level. A cross (x) is shown for any p-value that is almost 0. You can see the exact p-value corresponding to each parameter.

[mpgsaResults.ParameterSamples.Properties.VariableNames',mpgsaResults.PValues]

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 histograms 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

model0bj — 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.

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. For details, see "Multiparametric Global Sensitivity Analysis (MPGSA)" on page 1-121.

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.

Example: "max(Central.Drug(time > 1,:),[],1) <= 7"</pre>

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 the comma-separated pair consisting of 'Bounds' and 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 $\pm 10\%$ 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 the comma-separated pair consisting of 'SamplingMethod' and 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

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 the comma-separated pair consisting of 'Doses' and 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 the comma-separated pair consisting of 'Variants' and a variant object or vector of variant objects.

When there are multiple variants and 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.

StopTime — Simulation stop time

nonnegative scalar

Simulation stop time, specified as the comma-separated pair consisting of 'StopTime' and 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 the comma-separated pair consisting of 'UseParallel' and true or false.

Data Types: logical

Accelerate — Flag to turn on model acceleration

true (default) | false

Flag to turn on model acceleration, specified as the comma-separated pair consisting of 'Accelerate' and 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

"interplq" (default) | character vector | string

Method for interpolation of model simulations to new output times, specified as the comma-separated pair consisting of 'InterpolationMethod' and a character vector or string. The valid options follow.

- "interplq" Use the interplq 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

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.

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

Observable | SimBiology.gsa.MPGSA | ecdf | kstest2 | sbiosobol

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.

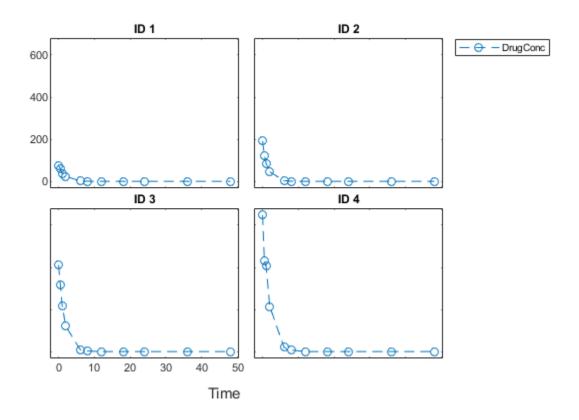
load data1.mat

Set the dose amounts to NaN at time points when no dose was administered.

```
datal.Dose(datal.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 ID	table doseSchedule	administrationRoute	Lambda_Z	R2	adjusted_R2	Num_point:
1	{'Single'}	{'IVBolus'}	0.57893	0.99991	0.9999	11
2	{'Single'}	{'IVBolus'}	0.66798	0.99998	0.99998	11
3 4	{'Single'} {'Single'}	{'IVBolus'} {'IVBolus'}	0.62124 0.58011	0.99999 0.99995	0.99999 0.99995	11 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<sup>3</sup> ×
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".

See Also

sbioncaoptions

Topics

"Noncompartmental Analysis" "Importing Data — Supported Files and Data Types" "Create Data File with SimBiology Definitions"

Introduced in R2017b

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.

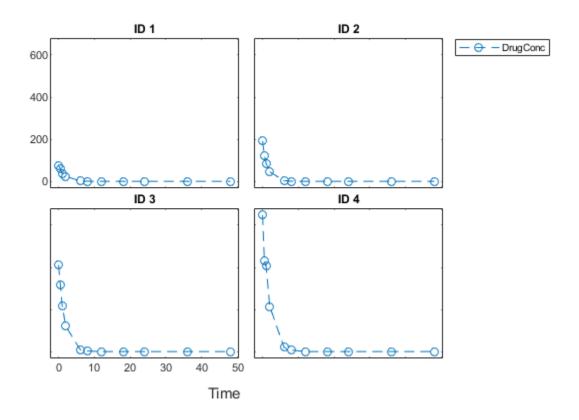
load data1.mat

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 ID	table doseSchedule	administrationRoute	Lambda_Z	R2	adjusted_R2	Num_point:
1	{'Single'}	{'IVBolus'}	0.57893	0.99991	0.9999	11
2	{'Single'}	{'IVBolus'}	0.66798	0.99998	0.99998	11
3 4	{'Single'} {'Single'}	{'IVBolus'} {'IVBolus'}	0.62124 0.58011	0.99999 0.99995	0.99999 0.99995	11 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<sup>3</sup> ×
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 NCA options object

Options to calculate NCA parameters, returned as an NCA options object. The properties of the object are classified into two groups, data classification options and parameter calculation 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, then you must also specify groupColumnName.
infusionRateColumnName	Name of the data column that contains the infusion rates.

Data Classification Options

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.

See Also

sbionca

Topics

"Noncompartmental Analysis" "Importing Data — Supported Files and Data Types" "Create Data File with SimBiology Definitions"

Introduced in R2017b

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

model0bj

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 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.

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*abs(f)*e
- 'combined': *y* = *f* + (*a*+*b**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 *pkData0bj*. 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 *i*th time point and the *j*th 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

$$J(i, j, k) = \frac{\partial y_k}{\partial \beta_j} \bigg|_{t_i}$$

where t_i is the *i*th time point, β_j is the *j*th estimated parameter in the transformed space, and y_k is the *k*th 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 twoelement 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.

See Also

Model object | PKData object | PKModelDesign object | PKModelDesign object |
PKModelMap object | nlinfit | sbionlmefit | sbionlmefitsa

Topics

"Perform Data Fitting with PK/PD Models"

sbionImefit

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 1-137.

[*results*, *SimDataI*, *SimDataP*] = sbionlmefit(...) returns simulation data of the SimBiology model, modelObj, using the estimated values of the parameters.

Input Arguments

model0bject

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 2-345 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).

CovModel0bj

CovariateModel object that defines the relationship between parameters and covariates. For details, see CovariateModel object.

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 1-139.

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 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.

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.

See Also

Model object | PKData object | PKModelDesign object | PKModelMap object | SimData
object | nlmefit | sbiofitstatusplot | sbionlinfit | sbionlmefitsa

Topics

"Perform Data Fitting with PK/PD Models"

Introduced in R2009a

sbionImefitsa

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 1-142.

[*results*, *SimDataI*, *SimDataP*] = sbionlmefitsa(...) returns simulation data of the SimBiology model, *modelObj*, using the estimated values of the parameters.

Input Arguments

model0bject

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).

CovModel0bj

CovariateModel object that defines the relationship between parameters and covariates. For details, see CovariateModel object.

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 1-144.

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 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.

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 namevalue 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.

See Also

Model object | PKData object | PKModelDesign object | PKModelMap object | SimData
object | nlmefitsa | sbiofitstatusplot | sbionlinfit | sbionlmefit

Topics

"Perform Data Fitting with PK/PD Models"

Introduced in R2010a

sbionmfiledef

NONMEM file definition object for sbionmimport

Syntax

```
nmdef0bj = sbionmfiledef
nmdef0bj = sbionmfiledef('PropertyName', PropertyValue)
```

Description

nmdef0bj = 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.

nmdef0bj = sbionmfiledef('PropertyName', PropertyValue) accepts one or more commaseparated 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: ''

Туре

Identifies the object as 'NMFileDef', (Read-only).

Output Arguments

nmdef0bj

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';
                                  = 'II';
       def.DoseIntervalLabel
       def.DoseRepeatLabel
                                 = 'ADDL';
                                 = 'ID';
       def.GroupLabel
                                 = 'TIME';
       def.TimeLabel
       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".

See Also

sbionmimport

Topics

"Importing Data" "Support for Importing NONMEM Formatted Files"

Introduced in R2010a

sbionmimport

Import NONMEM-formatted data

Syntax

```
data = sbionmimport('Filename')
data = sbionmimport(nmds)
data = sbionmimport('Filename', nmdef0bj)
data = sbionmimport(_,'ParameterName',ParameterValue)
data = sbionmimport(nmds,nmdef0bj)
[data, PKData0bj] = 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', nmdef0bj) 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 nmdef0bj.

data = sbionmimport(_,'ParameterName', ParameterValue) accepts one or more commaseparated 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,nmdef0bj) 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.

nmdef0bj

nmdef0bj defines the meanings of the file column headings. nmdef0bj 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

PkData0bj

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.

```
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);

See Also

sbionmfiledef

Topics

"Importing Data" "Support for Importing NONMEM Formatted Files"

Introduced in R2010a

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 object or OptimResults object 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.

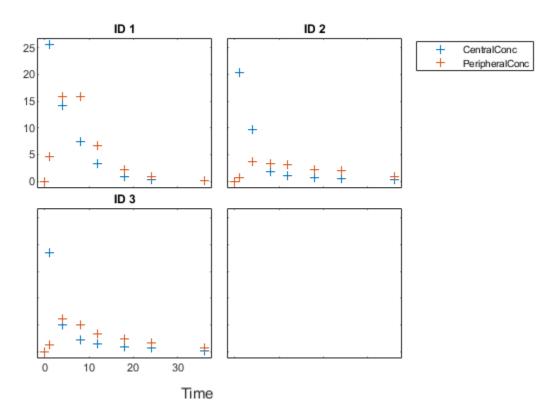
Examples

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.

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 2-448.

ci2table(ciParamUnpooled)

ans =

12x7 table

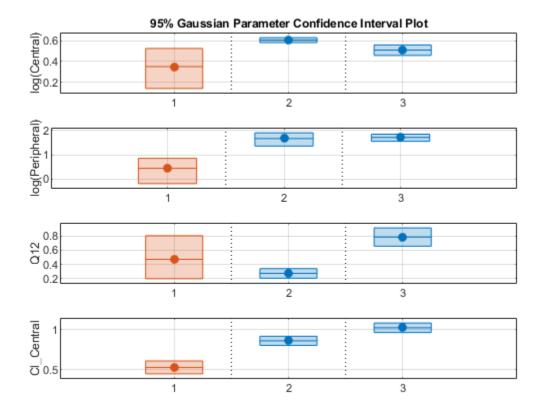
Group	Name	Estimate	te ConfidenceInterval		Туре	Alpha	Status	
1	{'Central' }	1.422	1.1533	1.6906	Gaussian	0.05	estimable	
1	{'Peripheral'}	1.5629	0.83143	2.3551	Gaussian	0.05	constrained	
1	{'Q12' }	0.47159	0.20093	0.80247	Gaussian	0.05	constrained	
1	{'Cl Central'}	0.52898	0.44842	0.60955	Gaussian	0.05	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 Estim
```

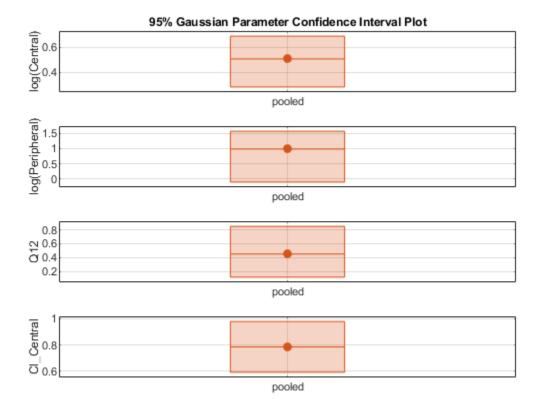
Estimate ConfidenceInterval

Type Alpha

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

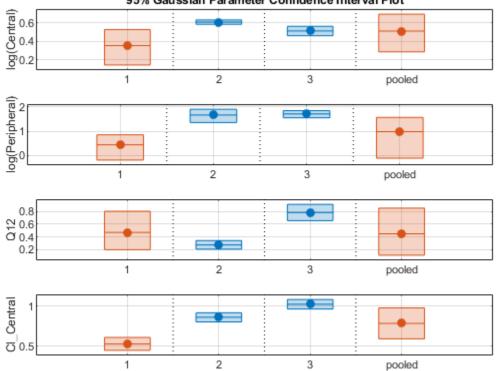
Plot the confidence intervals. The group name is labeled as "pooled" to indicate such fit.

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.

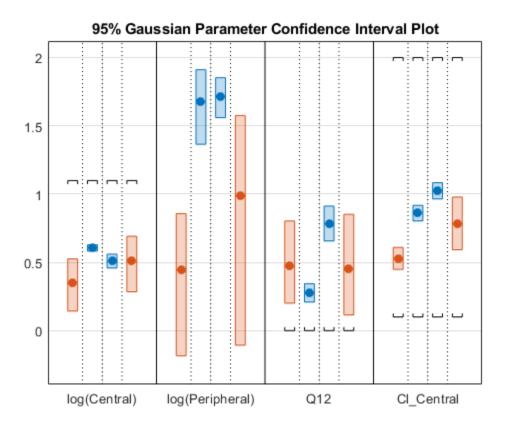
ciAll = [ciParamUnpooled;ciParamPooled]; plot(ciAll)



95% Gaussian Parameter Confidence Interval Plot

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

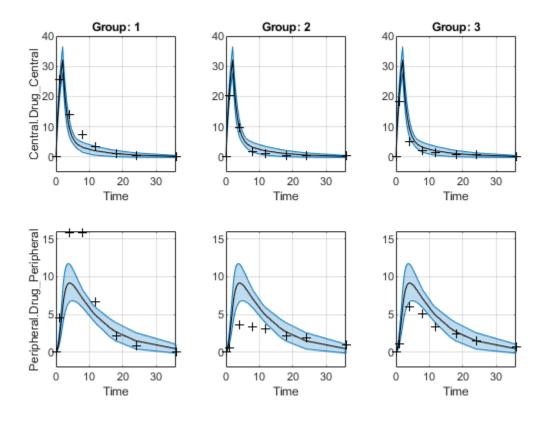
Calculate 95% confidence intervals for the model predictions, that is, simulation results using the estimated parameters.

```
% For the pooled fit
ciPredPooled = sbiopredictionci(pooledFit);
% For the unpooled fit
ciPredUnpooled = sbiopredictionci(unpooledFit);
```

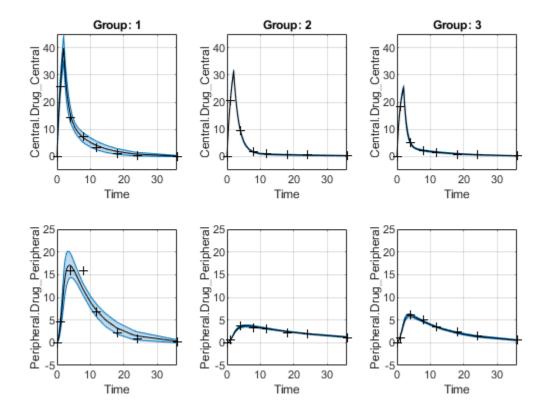
Plot Confidence Intervals for Model Predictions

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 object, OptimResults object, or a vector of objects for unpooled fits that were returned from the same sbiofit call.

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: '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 (\checkmark) 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	r	v	r	V
"'Type'" on page 1-0	r	v	r	V
"'Display'" on page 1-0	v	v	v	v
"'UseParallel' " on page 1- 0	~	V	V	V
"'NumSamples'" on page 1-0				V
"'Tolerance'" on page 1-0		v	V	v
"'Parameters'" on page 1-0		v	V	
"'MaxStepSize' " on page 1- 0		V	V	
"'UseIntegrati on'" on page 1-0		V	V	
"'Integration0 ptions'" on page 1-0			V	

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 1-167 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 1-167.

Note This type is not supported for parameter estimates from hierarchical models, that is, estimated results from fitting different categories on page 1-57 (such as age or sex). In other words, if you set the CategoryVariableName property of the EstimatedInfo object 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 1-169.

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 1-167.

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 1-169.

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 1-167.

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 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, $i \pm \sqrt{Si}, i * Tinv(1 - \frac{Alpha}{2})$, 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 $PL(Pi) = \max_{\substack{Pj, j \neq i}} LH(P1, ..., Pi, ..., Pn)$, 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: $\log(L) - \log(PL(P_i)) \le \frac{chiinv(1, 1 - alpha)}{2}$.

Equivalently, $\log(PL(P_i)) \ge \log(L) - \frac{chiinv(1, 1 - alpha)}{2}$, 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, $k = 1, 2, 3, \dots$ and $k = -1, -2, -3, \dots$
- **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 $PL(Pi) = \max_{\substack{Pj, j \neq i}} LH(P1, ..., Pi, ..., Pn)$ by integrating the differential equations derived from the Lagrange equations

$$-\nabla_{\vec{p}} L(\vec{p}(c)) + \lambda(c)\vec{e}_i = 0$$
$$\vec{p}_i(c) = c$$

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.

$$\begin{pmatrix} -\nabla_{\overrightarrow{p}}^{2}L(\overrightarrow{p}(c)) & \overrightarrow{e}_{i} \\ \pm \overrightarrow{e}_{i}^{T} & 0 \end{pmatrix} \begin{vmatrix} \dot{\overrightarrow{p}}(c) \\ \dot{\overrightarrow{\lambda}}(c) \end{vmatrix} = \begin{pmatrix} 0 \\ 1 \\ \ddots \end{pmatrix}$$

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:

$$\begin{pmatrix} -I & \overrightarrow{e}_i \\ \overrightarrow{p}(c) \\ \pm \overrightarrow{e}_i^T & 0 \end{pmatrix} \begin{vmatrix} \dot{\overrightarrow{p}}(c) \\ \dot{\lambda}(c) \end{vmatrix} = \begin{pmatrix} -\gamma \nabla_{\overrightarrow{p}} L(\overrightarrow{p}(c)) \\ 1 \end{pmatrix}$$

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.

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

ConfidenceInterval | ParameterConfidenceInterval | sbiofit | sbiopredictionci

Introduced in R2017b

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.
model0bj	SimBiology model object.
tspan	<i>n</i> -by-1 vector representing the time span of the target data xtarget.
xtarget	<i>n</i> -by- <i>m</i> matrix, where <i>n</i> is the number of time samples and <i>m</i> 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 <i>compartmentName.speciesName</i> or <i>reactionName.parameterName</i> . 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 <i>compartmentName.speciesName</i> or <i>reactionName.parameterName</i> . 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.

	either of the following:	ng the estimation process, specified by					
	Character vector (or string) spec	• 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 sbiopa see the Function Descriptions ta	ramestim uses the previous functions,					
	functions, and the second eleme	first element being one of the previous nt being an options structure or object. cture or object for each method listed					
	Method	Outline Churchard an Ohlis at					
	Method	Options Structure or Object					
	'fminsearch'	optimset					
	'fminsearch' 'fmincon'	optimset					
	'fminsearch' 'fmincon' 'lsqcurvefit' 'lsqnonlin'	optimset optimoptions					
	'fminsearch' 'fmincon' 'lsqcurvefit' 'lsqnonlin' 'particleswarm'	optimset optimoptions					
	'fminsearch' 'fmincon' 'lsqcurvefit' 'lsqnonlin' 'particleswarm' 'particleswarm_hybrid'	optimset optimoptions					
	<pre>'fminsearch' 'fmincon' 'lsqcurvefit' 'lsqnonlin' 'particleswarm' 'particleswarm_hybrid' 'patternsearch'</pre>	optimset optimoptions					
	<pre>'fminsearch' 'fmincon' 'lsqcurvefit' 'lsqnonlin' 'particleswarm' 'particleswarm_hybrid' 'patternsearch' 'patternsearch_hybrid'</pre>	optimset optimoptions					

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	<pre>sbioparamestim uses the default options structure associated with fminsearch, except for: Display = 'off' TolFun = 1e-6* (Initial value of objective function)</pre>
	Note 'fminsearch' is an unconstrained optimization method, which can result in negative values for parameters.
lsqcurvefit	Requires Optimization Toolbox.
	<pre>sbioparamestim uses the default options structure associated with lsqcurvefit, except for: Display = 'off'</pre>
	<pre>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)</pre>
lsqnonlin	Requires Optimization Toolbox.
	<pre>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)</pre>
fmincon	Requires Optimization Toolbox.
	<pre>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)</pre>
patternsearch	Requires Global Optimization Toolbox.
	<pre>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</pre>

Function	Description
	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 = le-6*[Initial objective function value] SwarmSize = 10; MaxIter = 30;

Function	Description
rid	Requires Global Optimization Toolbox. <pre>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.</pre>
	Display = 'off'; FunctionTolerance = 1e-6*[Initial objective function valu 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:

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.

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

optimset | sbiomodel

Introduced in R2006a

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 object or OptimResults object 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.

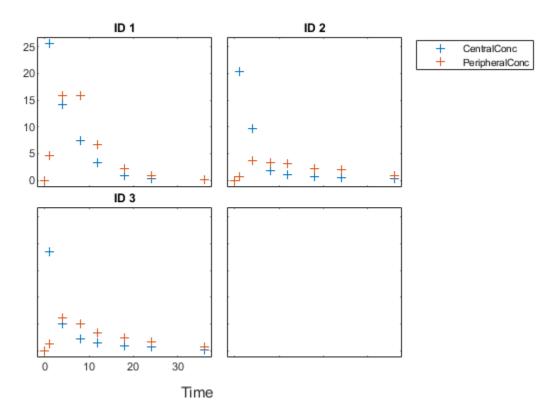
Examples

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.

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 2-448.

ci2table(ciParamUnpooled)

ans =

12x7 table

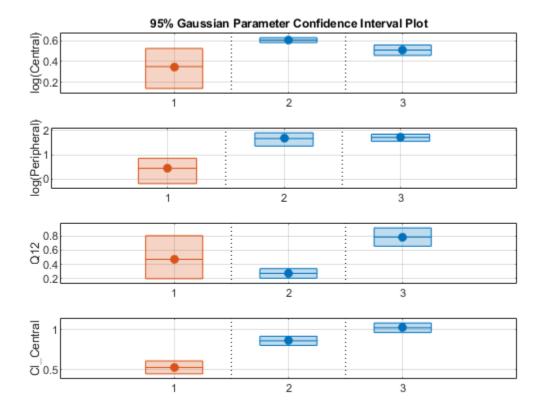
Group	Name	Estimate	Confidenc	eInterval	Туре	Alpha	Status
1	{'Central' }	1.422	1.1533	1.6906	Gaussian	0.05	estimable
1	{'Peripheral'}	1.5629	0.83143	2.3551	Gaussian	0.05	constrained
1	{'Q12' }	0.47159	0.20093	0.80247	Gaussian	0.05	constrained
1	{'Cl Central'}	0.52898	0.44842	0.60955	Gaussian	0.05	estimable
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

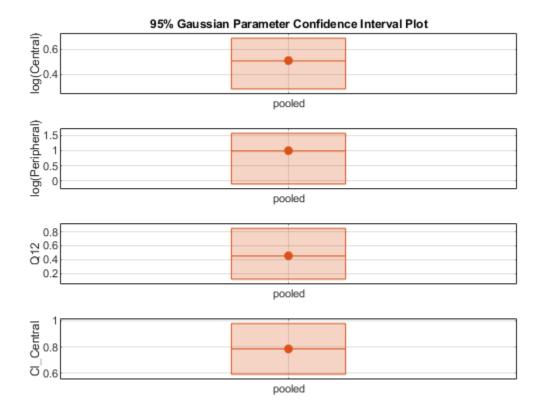
Туре Alpha

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

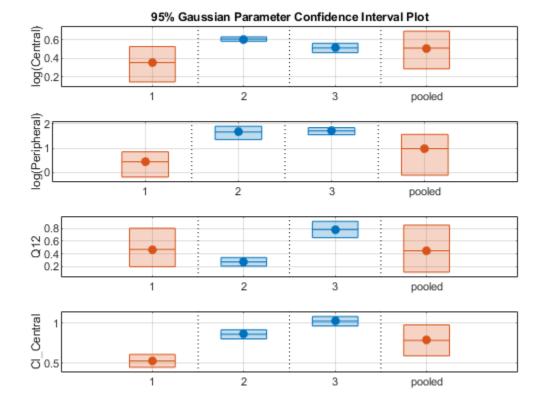
Plot the confidence intervals. The group name is labeled as "pooled" to indicate such fit.

plot(ciParamPooled)



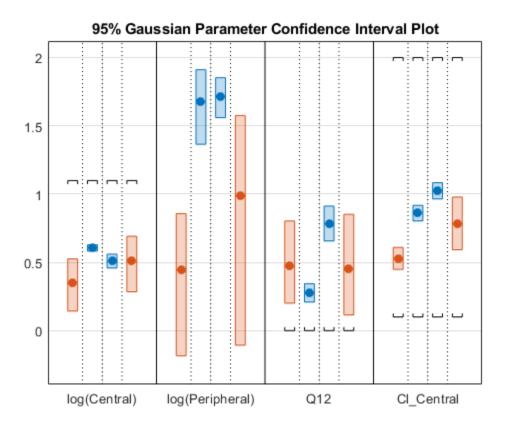
Plot all the confidence interval results together. By default, the confidence interval for each parameter estimate is plotted on a separate axes. Vertical lines group confidence intervals of parameter estimates that were computed in a common fit.

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

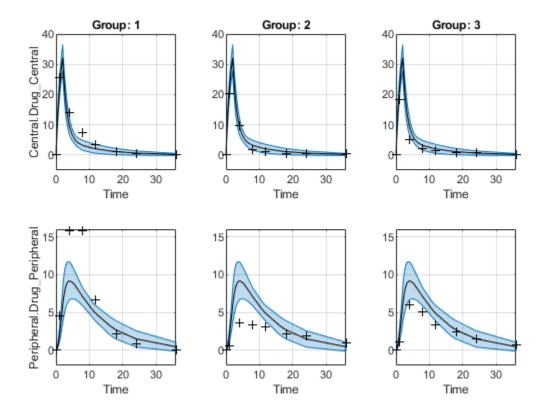
Calculate 95% confidence intervals for the model predictions, that is, simulation results using the estimated parameters.

```
% For the pooled fit
ciPredPooled = sbiopredictionci(pooledFit);
% For the unpooled fit
ciPredUnpooled = sbiopredictionci(unpooledFit);
```

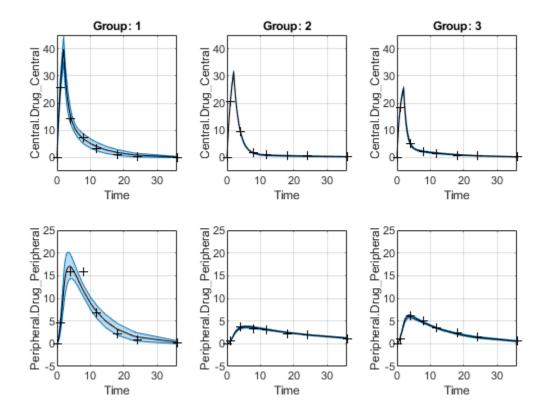
Plot Confidence Intervals for Model Predictions

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 object, OptimResults object, or a vector of objects for unpooled fits that were returned from the same sbiofit call.

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: '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 1-190 of the distribution of the linearized model responses around the parameter estimates.
- 'bootstrap'- Compute confidence intervals using the bootstrap method on page 1-190.

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.

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

ParameterConfidenceInterval | PredictionConfidenceInterval | sbiofit |
sbioparameterci

Introduced in R2017b

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.

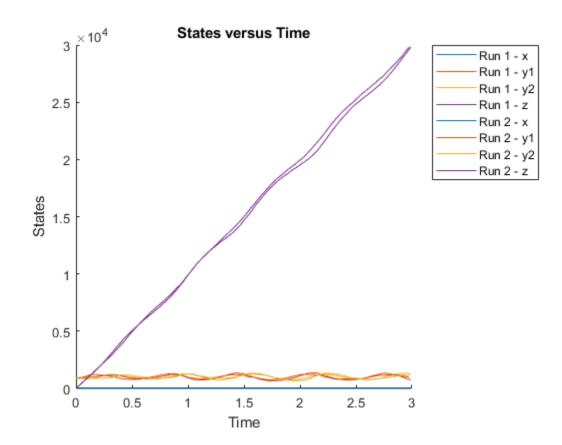
```
sbioloadproject lotka;
cs = getconfigset(m1);
cs.SolverType = 'SSA';
cs.StopTime = 3;
rng('default') % For reproducibility
```

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.

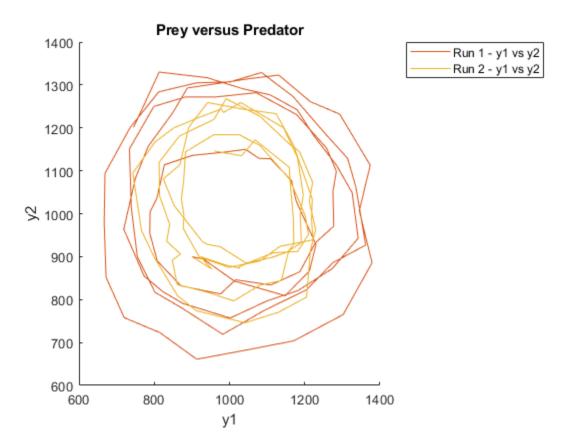
sbioplot(sd);



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 1-192.

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 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: '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

Compatibility Considerations

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

Introduced in R2008a

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', 'mylawl');

See Also

sbioabstractkineticlaw|sbioaddtolibrary|sbiounit|sbiounitprefix

Introduced in R2006a

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 root0bj 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 Usesbioreset 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

See Also

sbioaddtolibrary|sbioroot|sbiounit|sbiounitprefix

Topics sbioroot on page 1-202

Introduced before R2006a

sbioroot

Return SimBiology root object

Syntax

rootObj = sbioroot

Arguments

root0bj	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
Туре	Display SimBiology object type
UserDefinedLibrary	Library of user-defined components

See Also

Unit object | UnitPrefix object | addkineticlaw | sbiomodel | sbioreset

Topics

sbiomodel on page 1-108 addkineticlaw on page 2-41 sbioreset on page 1-200

Introduced in R2006a

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

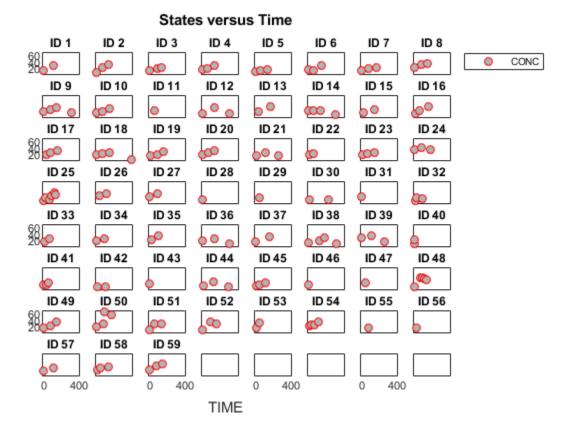
This example uses data collected on 59 preterm infants given phenobarbital during the first 16 days after birth. Each infant received an initial dose followed by one or more sustaining doses by intravenous bolus administration. A total of between 1 and 6 concentration measurements were obtained from 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, θ s (thetas) are fixed effects, η (eta) represents random effects, and WEIGHT is the covariate.

```
covM = CovariateModel;
covM.Expression = {'Central = exp(thetal+theta2*WEIGHT+etal)'};
```

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.

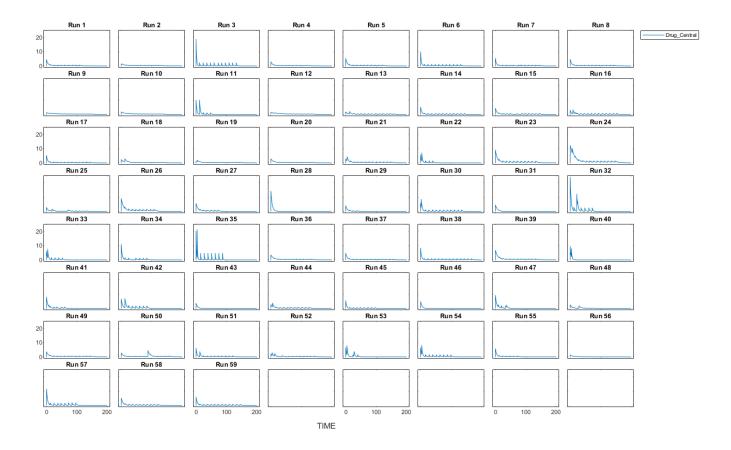
```
f = createSimFunction(onecomp,covM.ParameterNames,'Drug_Central','Drug_Central');
```

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 object to learn more about covariate expressions.

thetas — Fixed effects

table | dataset | numeric vector

Fixed effects, specified as a table, 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.

- 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({'theta0ne','theta2','theta3'})
ans =
1×3 cell array
{'theta2'} {'theta3'} {'theta0ne'}
```

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 | dataset | matrix

Covariance matrix of random effects, specified as a table, 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'})
```

- 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({'etal','eta2','eta3'})
ans =
   1×3 cell array
   {'eta1'} {'eta2'} {'eta3'}
```

ds – Covariate data

dataset | table

Covariate data, specified as a dataset or table containing the covariate data for all groups.

ds must have a column named 'Group' or 'GROUP' specifying the group labels as well as a column each for all covariates 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.

Compatibility Considerations

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

CovariateModel object | SimFunction object | createSimFunction | sbiosampleerror

Introduced in R2014a

sbiosampleerror

Sample error based on error model and add noise to simulation data

Syntax

sdN = sbiosampleerror(sd,errormodel,errorparam)

Description

sdN = sbiosampleerror(sd,errormodel,errorparam) adds noise to the simulation data sd
using one or more error models errormodel and error parameters errorparam.

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.

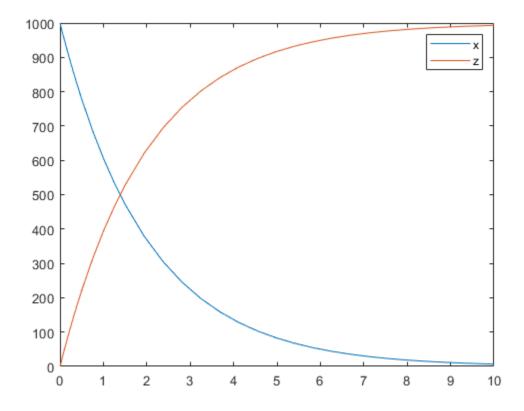
```
sbioloadproject radiodecay;
```

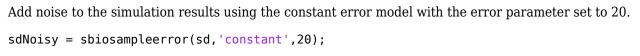
Simulate the model.

[t,sd,names] = sbiosimulate(m1);

Plot the simulation results.

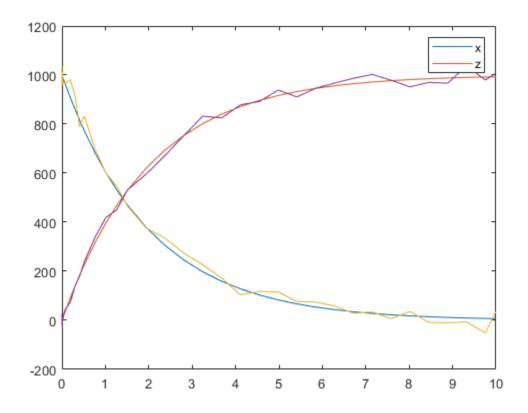
```
plot(t,sd);
legend(names,'AutoUpdate','off');
hold on
```





Plot the noisy simulation data.

plot(t,sdNoisy);



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

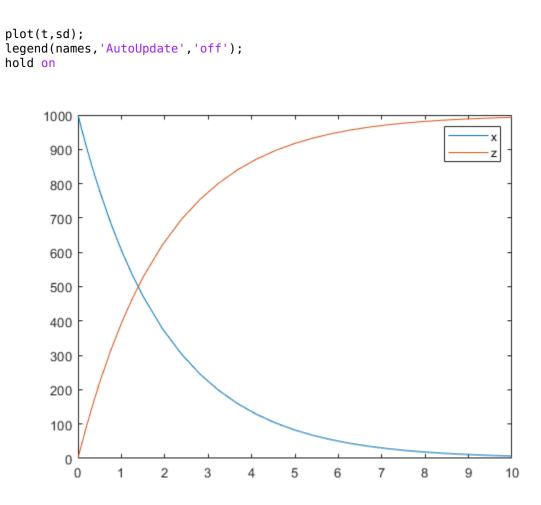
Define a function handle that represents the error model.

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.

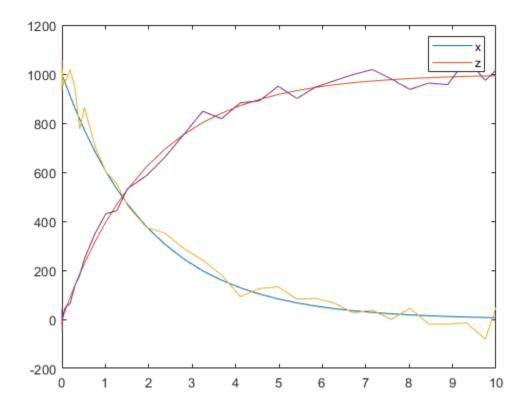


Sample the error using the previously defined custom function with two parameters set to 0.5 and 30, respectively.

sdNoisy = sbiosampleerror(sd,em,{0.5,30});

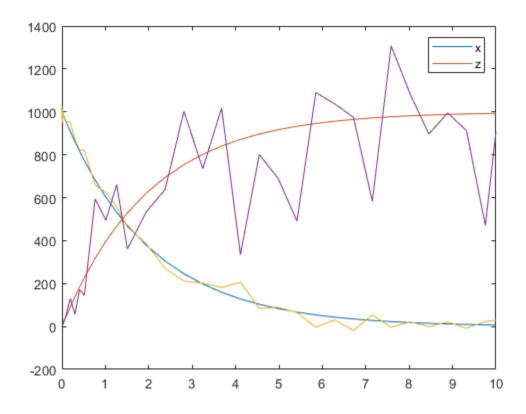
Plot the noisy simulation data.

plot(t,sdNoisy);



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
sdNoisy = sbiosampleerror(sd, {em, 'proportional'}, {{0.5,30}, 0.3});
plot(t,sd);
legend(names, 'AutoUpdate', 'off');
hold on
plot(t,sdNoisy);
```



Input Arguments

sd — Simulation results

SimData object | matrix

Simulation results, specified as a SimData object or 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 sd, and each error model is applied to the corresponding column in sd. If it is a single character vector, string, or function handle, the same error model is applied to all columns in sd.

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 sd 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 sd, 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

sdN — Simulation results with added noise

vector of SimData objects | matrix

Simulation results with added noise, returned as a vector of SimData objects or numeric matrix. If sd is a vector of SimData objects, sdN is also a vector of SimData objects, and the error is added to each column in the sd.Data property. If sd is specified as a matrix, sdN is a matrix, and the error is added to each column in the matrix.

See Also

SimFunction object | createSimFunction | sbiosampleparameters

Introduced in R2014a

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
```

See Also

sbioaddtolibrary | sbioloadproject | sbioremovefromlibrary | sbiowhos

Topics

sbioloadproject on page 1-107 sbiowhos on page 1-284 sbioaddtolibrary on page 1-16 sbioremovefromlibrary on page 1-198 Introduced in R2006a

sbioselect

Search for objects with specified constraints

Syntax

```
Out = sbioselect('PropertyName', PropertyValue)
Out = sbioselect('Where', 'PropertyName', 'Condition', 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. <i>Out</i> might contain a mixture of object types (for example, species and parameters), depending on the selection you specify.
	If <i>PropertyValue</i> is a cell array, then the function returns all objects with the property ' <i>PropertyName</i> ' that matches any element of <i>PropertyValue</i> .
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 <i>PropertyValue</i> 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 1-221 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 <i>PropertyNameCondition</i> .
DepthValue	Specify the depth number to search. Valid numbers are positive integer values and inf. If <i>DepthValue</i> is inf, sbioselect searches <i>Obj</i> and all of its children. If <i>DepthValue</i> is 1, sbioselect only searches <i>Obj</i> and not its children. By default, <i>DepthValue</i> 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.
	<pre>parameterObj = sbioselect (modelObj, 'Where', 'Value', '==', 0.5)</pre>
	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).
	<pre>parameterObj = sbioselect (modelObj, 'Where', 'ConstantValue', '==', false)</pre>
~=	Search in the model object (modelObj), and return parameter objects that do not have Value equal to 0.5.
	<pre>parameterObj = sbioselect (modelObj, 'Where', 'Value', '~=', 0.5)</pre>
>,<,>=,<=	Search in the model object (modelObj), and return species objects that have an initial amount (InitialAmount) greater than 50.
	<pre>species0bj = sbioselect (model0bj, 'Where', 'InitialAmount', '>', 50)</pre>
	Search in the model object (modelObj), and return species objects that have an initial amount (InitialAmount) less than or equal to 50.
	<pre>species0bj = sbioselect (model0bj, 'Where', 'InitialAmount', '<=', 50)</pre>
between	Search in the model object (modelObj), and return species objects that have an initial amount (InitialAmount) between 200 and 300.
	<pre>species0bj = sbioselect (model0bj, 'Where', 'InitialAmount', 'between', [200 300])</pre>
~between	Search in the model object (modelObj), and return species objects that have an initial amount (InitialAmount) that is not between 200 and 300.
	<pre>species0bj = sbioselect (model0bj, 'Where', 'InitialAmount', '~between', [200 300])</pre>

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.)
	<pre>zeroObj = sbioselect(modelObj, 'Where', '*', 'equal_and_same_type', 0);</pre>
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 ' \sim =' would also select objects containing a property with a value of true.)
	<pre>nonzeroObj = sbioselect(modelObj, 'Where', '*', 'unequal_and_same_type', 0);</pre>

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'.
	<pre>species0bj = sbioselect (model0bj, 'Type', 'species', 'Where', 'Name', '==', 'Glucose')</pre>
~=	<pre>Search in the model object (modelObj), and return species objects that are not named 'Glucose'. speciesObj = sbioselect (modelObj,</pre>
	'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.
	<pre>species0bj = sbioselect (model0bj, 'Type', 'species', 'Where', 'Name', '~=i', 'glucose')</pre>

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.
	<pre>Obj = sbioselect (modelObj, 'Where', 'Name', 'regexp', '[ea]se')</pre>
	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.
	<pre>Obj = sbioselect (modelObj, 'Where', 'Name', '~regexp', 'kinase')</pre>
~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*.
	<pre>Obj = sbioselect (modelObj, 'Where', 'Name', '~wildcard', 'kin*')</pre>
~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.
	<pre>Out = sbioselect(modelObj, 'Where', 'Stoichiometry', 'function', @(x)any(x>2))</pre>
	Select all objects with a numeric value that is even.
	<pre>iseven = @(x) isnumeric(x) && isvector(x) && mod(x, 2) == 0; evenValuedObj = sbioselect(modelObj, 'where', 'Value', 'function', iseven);</pre>

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'	<pre>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))</pre>

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.

Compound expressions with multiple boolean operators are supported. Precedence of the operators follows the order of operations for boolean algebra $not \rightarrow and \rightarrow xor \rightarrow or$.

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
                                рΑ
                                               100
                                рΒ
   2
              unnamed
                                               (\cdot)
   3
                                pA_0pB1
                                               0
              unnamed
   4
                                pB_0pC1
                                               0
              unnamed
   5
                                pA_0pB_pA
                                               20
              unnamed
   6
              unnamed
                                pA OpB2
                                               0
   7
              unnamed
                                pB 0pC2
                                               0
   8
              unnamed
                                pB OpC pB
                                               0
```

Find a cell array. Note how cell array values must be specified inside another cell array.

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', '');
```

See Also

regexp

Introduced before R2006a

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 <i>Name</i> to the base unit. For example, the multiplier in picomole is 10e-12.
Builtin	An array of logical values. If <i>Builtin</i> is true for a unit prefix, the unit prefix is built in. If <i>Builtin</i> 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');
```

See Also

sbioconvertunits|sbioshowunits|sbiounitprefix

Introduced in R2006a

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 <i>Name</i> . For example, molarity is mole/liter.
Multiplier	The numerical value that defines the relationship between the unit <i>Name</i> and the base or derived unit as a product of the <i>Multiplier</i> and the base unit or derived unit. For example, 1 mole is 6.0221e23*molecule. The <i>Multiplier</i> is 6.0221e23.
Builtin	An array of logical values. If <i>Builtin</i> is true for a unit, the unit is built in. If <i>Builtin</i> 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');

Compatibility Considerations

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.

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.

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

Introduced in R2006a

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 dv0bj to empty [], the function uses the active configset, active variants, and active doses.

If you specify dv0bj as variants, the function uses the specified variants and active doses. Any other variants are ignored.

If you specify dv0bj 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 cs0bj 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 dv0bj as variants, the function uses the specified variants and active doses. Any other variants are ignored.

If you specify dv0bj 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.

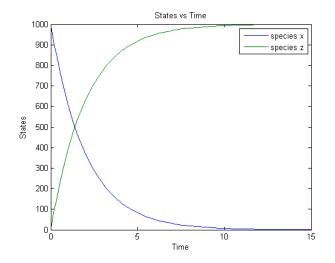
csObj = getconfigset(m1, 'active'); set(csObj, 'Stoptime', 15);

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')
```

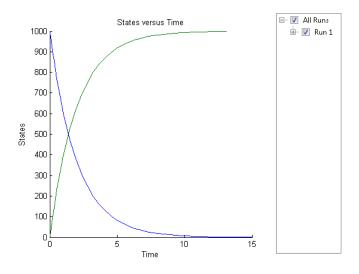


You can also return the results to a SimData object.

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.

```
d0bj1 = adddose(m1,'d1','schedule');
d0bj1.Amount = 100;
d0bj1.AmountUnits = 'molecule';
```

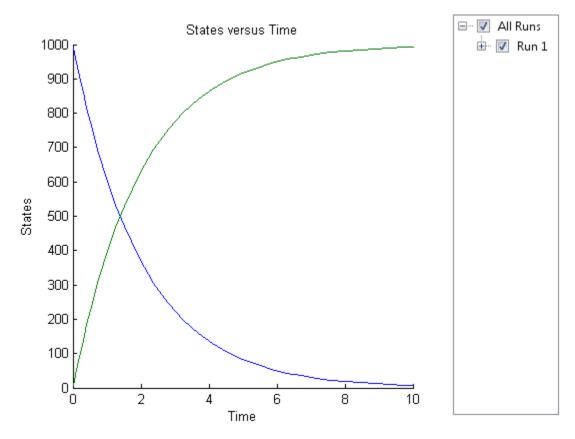
```
d0bj1.TimeUnits = 'second';
d0bj1.Time = 2;
d0bj1.TargetName = 'unnamed.x';
d0bj2 = adddose(m1,'d2','schedule');
d0bj2.Amount = 100;
d0bj2.AmountUnits = 'molecule';
d0bj2.TimeUnits = 'second';
d0bj2.Time = 4;
d0bj2.TargetName = 'unnamed.x';
```

Simulate the model using no dose or any subset of the dose array.

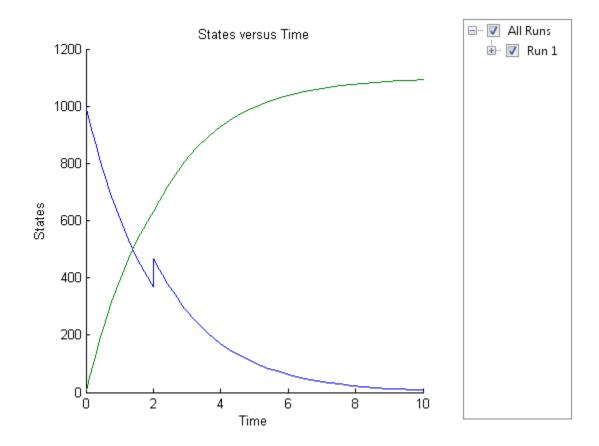
```
sim1 = sbiosimulate(m1);
sim2 = sbiosimulate(m1,d0bj1);
sim3 = sbiosimulate(m1,d0bj2);
sim4 = sbiosimulate(m1,[d0bj1,d0bj2]);
```

Plot the results.

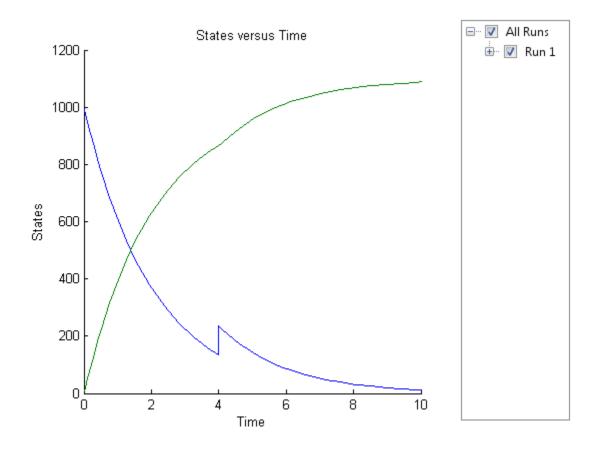
sbioplot(sim1)



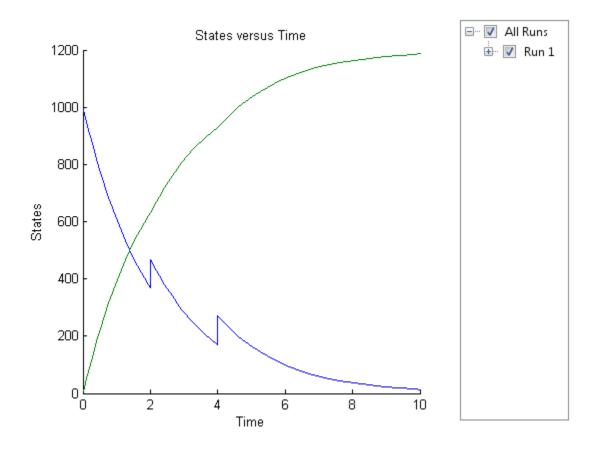
sbioplot(sim2)



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.

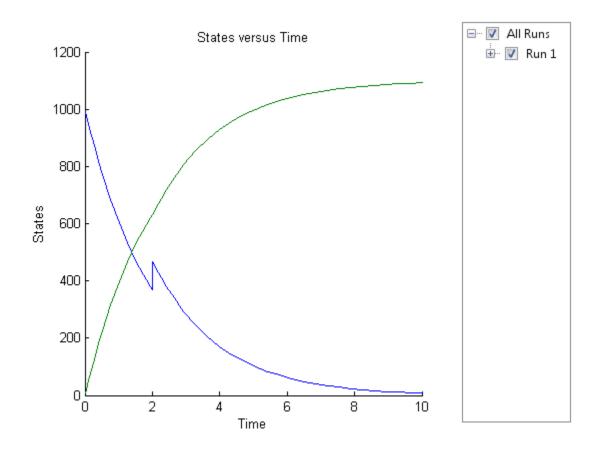
```
d0bj = adddose(m1, 'd1', 'schedule');
d0bj.Amount = 100;
d0bj.AmountUnits = 'molecule';
d0bj.TimeUnits = 'second';
d0bj.Time = 2;
d0bj.TargetName = 'unnamed.x';
```

Simulate the model using configset and dose objects.

sim = sbiosimulate(m1,defaultConfigSet,d0bj);

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.

```
d0bj = adddose(m1,'d1','schedule');
d0bj.Amount = 100;
d0bj.AmountUnits = 'molecule';
d0bj.TimeUnits = 'second';
d0bj.Time = 2;
d0bj.TargetName = 'unnamed.x';
```

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

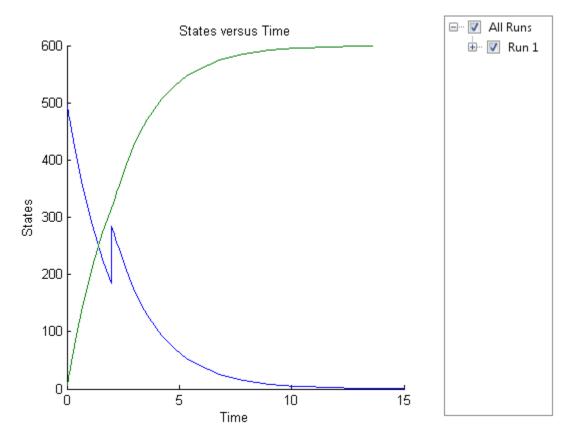
```
v0bj = addvariant(m1,'v1');
addcontent(v0bj,{'species','x','InitialAmount',500});
```

Simulate the model using the same configset, variant, and dose objects. Use the same order of input arguments as shown next.

sim = sbiosimulate(m1,cs0bj,v0bj,d0bj);

Plot the result.

sbioplot(sim);



Input Arguments

model0bj — SimBiology model

SimBiology model object

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

cs0bj — 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.

dv0bj - 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.

variant0bj — 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.

dose0bj — 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.

See Also

Configset object | Model object | RepeatDose object | ScheduleDose object | SimData object | Variant object | addconfigset | getconfigset | sbioaccelerate | sbiomodel | setactiveconfigset

Topics

"Model Simulation" "Deriving ODEs from Reactions"

Introduced before R2006a

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,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,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.

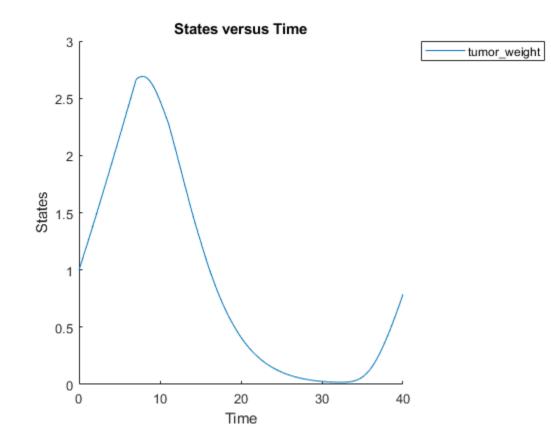
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

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].

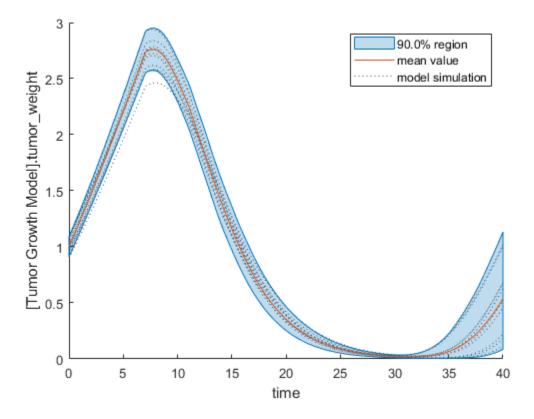
sobolResults = sbiosobol(m1,modelParamNames,outputName,'Variants',v,'Doses',d,'ShowWaitBar',true

```
sobolResults =
   Sobol with properties:
        Time: [444x1 double]
        SobolIndices: [5x1 struct]
        Variance: [444x1 table]
        Observables: {'[Tumor Growth Model].tumor_weight'}
   ParameterSamples: [1000x5 table]
        SimulationInfo: [1x1 struct]
```

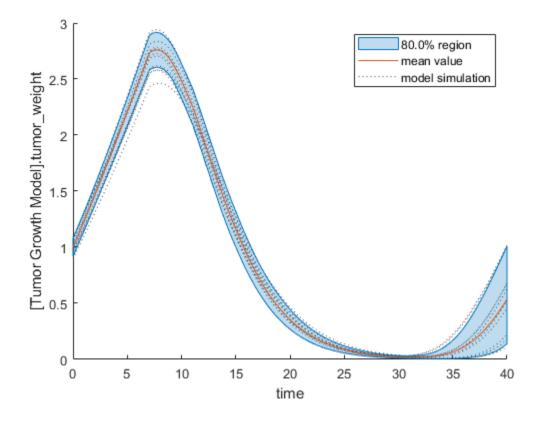
You can change the number of samples by specifying the 'NumberSamples' name-value pair argument. The function requires a total of (number of input parameters + 2) * NumberSamples model simulations.

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

plotData(sobolResults);

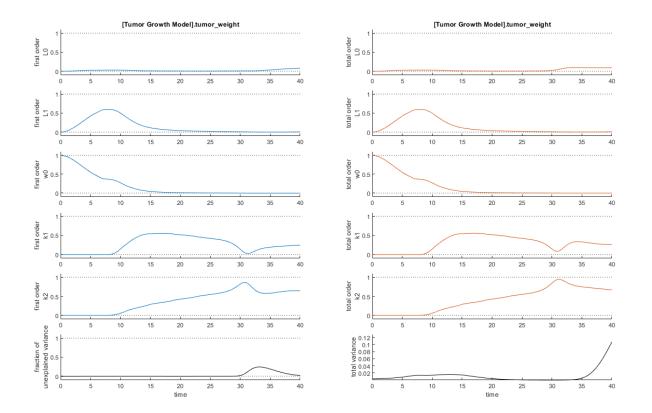


plotData(sobolResults, 'Alphas',0.1);



Plot the time course of the first- and total-order Sobol indices.

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

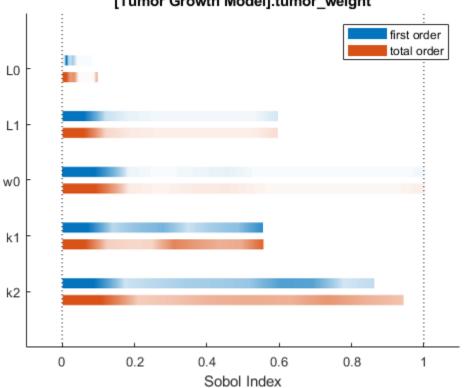


The first-order Sobol index of an input parameter gives the fraction of the overall response variance that can be attributed to variations in the input parameter alone. The total-order index gives the fraction of the overall response variance that can be attributed to any joint parameter variations that 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.

bar(sobolResults)



[Tumor Growth Model].tumor_weight

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: ModelName: DataCount: Name: 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

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.

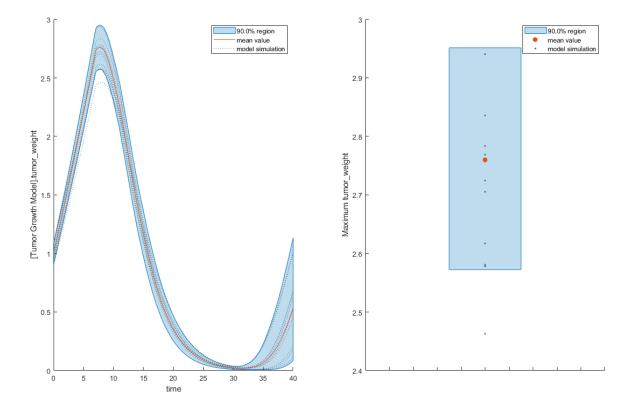
```
[samplesUsed,sd,validruns] = getSimulationResults(sobolResults,4);
```

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);
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

model0bj — 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 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: sobolResults =
sbiosobol(modelObj,params,observables,'ShowWaitbar',true) specifies to show a
simulation progress bar.

Bounds — Parameter bounds

numeric matrix

Parameter bounds, specified as the comma-separated pair consisting of 'Bounds' and 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 $\pm 10\%$ 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 the comma-separated pair consisting of 'Doses' and 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 the comma-separated pair consisting of 'Variants' and a variant object or vector of variant objects.

When there are multiple variants and 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.

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

SamplingMethod — Method to generate parameter samples

'Sobol' (default) | character vector | string

Method to generate parameter samples, specified as the comma-separated pair consisting of 'SamplingMethod' and 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

StopTime — Simulation stop time

nonnegative scalar

Simulation stop time, specified as the comma-separated pair consisting of 'StopTime' and 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 the comma-separated pair consisting of 'UseParallel' and true or false.

Data Types: logical

Accelerate — Flag to turn on model acceleration

true (default) | false

Flag to turn on model acceleration, specified as the comma-separated pair consisting of 'Accelerate' and true or false.

Data Types: logical

InterpolationMethod — Method for interpolation of model simulations

"interplq" (default) | character vector | string

Method for interpolation of model simulations to new output times, specified as the comma-separated pair consisting of 'InterpolationMethod' and a character vector or string. The valid options follow.

- "interplq" Use the interplq 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

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 commaseparated 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.

$$S_{Ti} = 1 - \frac{V_{X_{\sim i}}(E_{Xi}(Y|X_{\sim i}))}{V(Y)} = \frac{E_{X_{\sim i}}(V_{Xi}(Y|X_{\sim i}))}{V(Y)}$$

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 *i*th column, which is from B for i = 1, 2, ..., params.

$$\boldsymbol{A}_{B}^{i} = \begin{pmatrix} X_{11} \ X_{12} \ \dots \ X_{1i}^{i} \ \dots \ X_{1k} \\ X_{21} \ X_{22} \ \dots \ X_{2i}^{i} \ \dots \ X_{2k} \\ \dots \ \dots \ \dots \ \dots \ \dots \\ X_{n1} \ X_{n2} \ \dots \ X_{ni}^{i} \ \dots \ X_{nk} \end{pmatrix}$$

The formulas to approximate the first- and total-order Sobol indices are as follows.

$$\widehat{S}_{i} = \frac{\frac{1}{n} \sum_{j=1}^{n} f(B)_{j} \left(f\left(\boldsymbol{A}_{B}^{i}\right)_{j} - f(A)_{j} \right)}{V(Y)}$$
$$\widehat{S}_{Ti} = \frac{\frac{1}{2n} \sum_{j=1}^{n} \left(f(A)_{j} - f\left(\boldsymbol{A}_{B}^{i}\right)_{j} \right)^{2}}{V(Y)}$$

f(A), f(B), and $f(A_B^i)_j$ 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 *i*th index (A_B^i) from the SimulationInfo.SimData array.

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

Observable | SimBiology.gsa.Sobol | sbiompgsa

Topics "Sensitivity Analysis in SimBiology"

Introduced in R2020a

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 non-constant 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 SimBiology variant object, variant_in, to the model before trying to find
the steady-state values.

[success, variant_out] = sbiosteadystate(model, variant_in, scheduleDose)
applies a SimBiology schedule dose object on page 2-553, scheduleDose, or a vector of schedule
doses 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:
                                           Value:
                                                     Units:
                            Name:
                                                     molecule
  1
            unnamed
                            DNA
                                           50
  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
2	species	DNA	InitialAmount	8.79024
3	species	DNA_protein	InitialAmount	41.2098
4	species	mRNA	InitialAmount	1.17203
5	species	protein	InitialAmount	23.4406
6	parameter	Transcription.k1	Value	0.2
7	parameter	Translation.k2	Value	20
8	parameter	[Binding/Unbin	Value	0.2
9	parameter	[Binding/Unbin	Value	1
10	parameter	[mRNA Degradat	Value	1.5
11	parameter	[Protein Degra	Value	1

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
   2
                                                     InitialAmount
                                                                          12.7876
                      species
                                   DNA
   3
                                                                          87.2124
                      species
                                   DNA protein
                                                     InitialAmount
   4
                                                                          1.70502
                     species
                                   mRNA
                                                     InitialAmount
   5
                                   protein
                                                     InitialAmount
                                                                          34.1003
                     species
   6
                                   Transcription.k1 Value
                                                                          0.2
                     parameter
   7
                                   Translation.k2
                                                     Value
                                                                          20
                     parameter
   8
                                   [Binding/Unbin... Value
                                                                          0.2
                     parameter
   9
                                   [Binding/Unbin... Value
                     parameter
                                                                          1
                                   [mRNA Degradat... Value
                                                                          1.5
   10
                     parameter
                                   [Protein Degra... Value
   11
                     parameter
                                                                          1
m2 =
   SimBiology Model - cell
   Model Components:
     Compartments:
                         1
     Events:
                         0
     Parameters:
                        6
                        5
     Reactions:
                        0
     Rules:
     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
                              DNA protein
                                             87.2124
                                                         molecule
             unnamed
   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

SimBiology variant, specified as a Variant object. The alternate quantity values stored in the variant are applied to the model before finding the steady state.

scheduleDose — Dosing information

SimBiology schedule dose object

Dosing information, specified as a SimBiology schedule dose object on page 2-553. 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 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: '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 1-260.

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 1-260.

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 1-260.

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:

 $\left(\left\|\frac{d\vec{S}}{dt}\right\| < AbsTol\right) or \left(\left\|\frac{d\vec{S}}{dt}\right\| < RelTol * \|\vec{S}\|\right), \text{ where } \vec{S} \text{ is a vector of nonconstant species, parameters,} \right)$

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
$$\left(\left\| \frac{d\vec{S}}{dt} \right\| < AbsTol \right) or \left(\left\| \frac{d\vec{S}}{dt} \right\| < RelTol * \|\vec{S}\| \right)$$
, 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

 $\label{eq:sbiosteadystate} simulates the model until MaxStopTime on page 1-0 \quad . During the simulation, the function approximates the gradient using finite differencing (forward difference) over time to detect a steady state.$

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.

See Also

Model object | ScheduleDose object | Variant object | commit | sbioaccelerate | sbiomodel | sbiosimulate | sbiovariant

Introduced in R2016a

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.

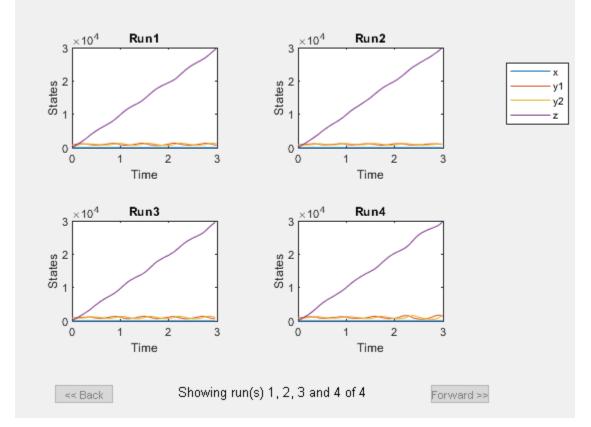
```
sbioloadproject lotka;
cs = getconfigset(m1);
cs.SolverType = 'SSA';
cs.StopTime = 3;
rng('default') % For reproducibility
```

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.

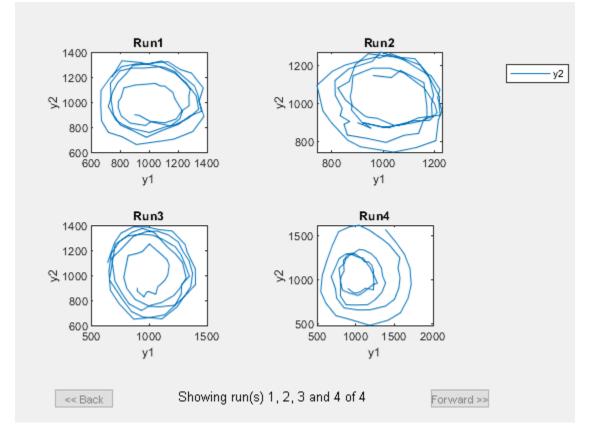
sbiosubplot(sd);



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 1-262.

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 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 Namel, Valuel, ..., NameN, ValueN.

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

See Also sbioplot | SimData

Introduced in R2008a

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.

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.

Examples

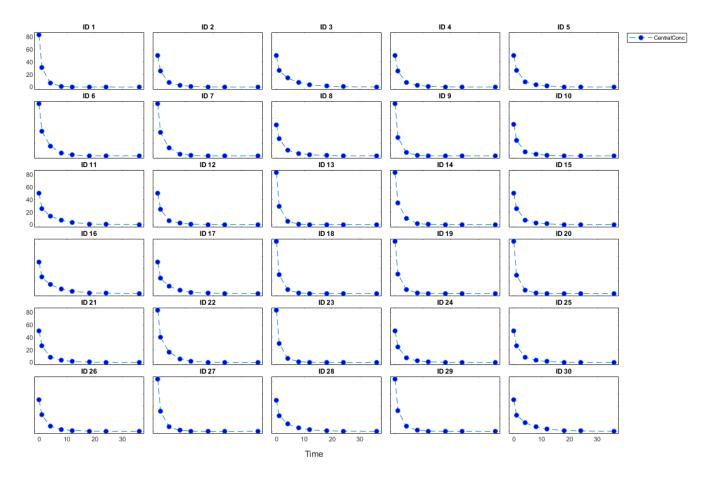
Create a Trellis Plot for Grouped Data

Load a sample dataset. The data contains measurements of drug concentration in the central and peripheral compartments for 30 subjects.

```
load('sd5 302RAgeSex.mat');
```

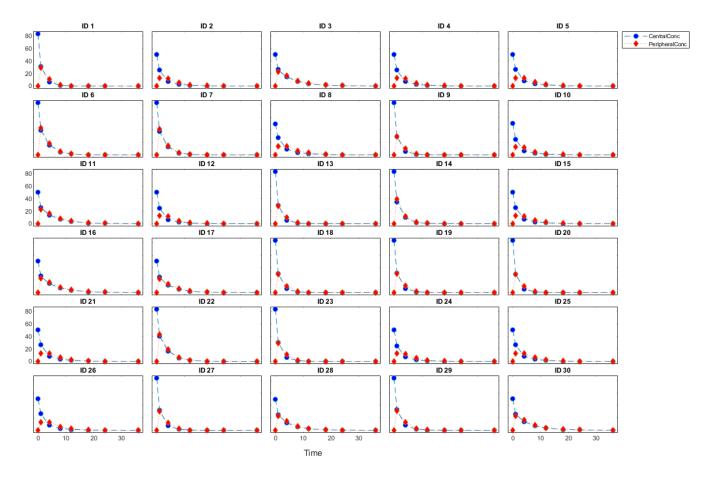
Create a trellis plot of the Central concentrations for each subject.

```
t = sbiotrellis(data, 'ID', 'Time', 'CentralConc',...
'Marker', 'o','LineStyle','--','MarkerFaceColor','b');
% Resize the figure.
t.hFig.Position(:) = [100 100 1200 800];
```



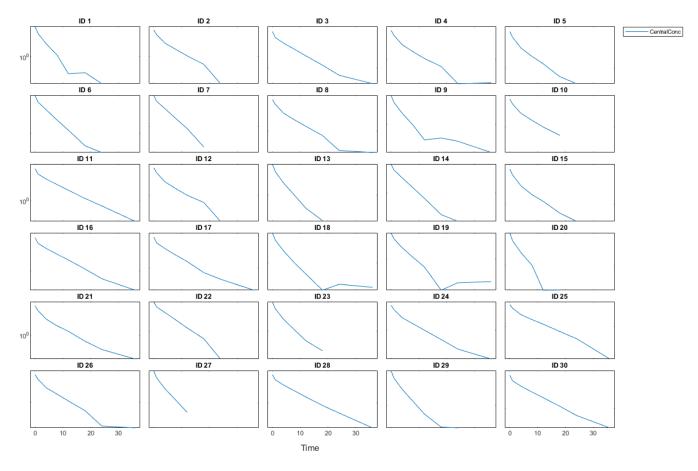
Use the **plot** method of the sbiotrellis object to overlay the peripheral concentration data on the same plot.

```
plot(t,data,'ID','Time','PeripheralConc','Marker','d',...
'LineStyle',':','MarkerFaceColor','r');
```

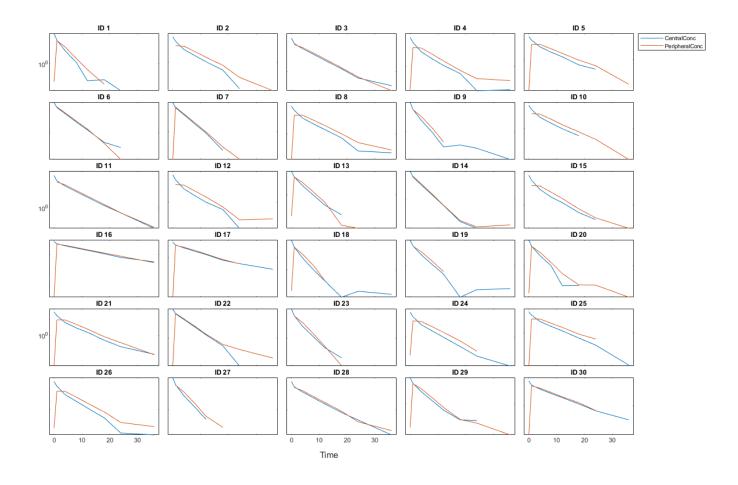


Specify the function handle @semilogy to change the y-axis to log scale.

t2 = sbiotrellis(data,@semilogy,'ID','Time','CentralConc'); %Resize the figure t2.hFig.Position(:) = [100 100 1200 800];



plot(t2,data,@semilogy,'ID','Time','PeripheralConc');



See Also sbioplot | sbiosubplot

Introduced in R2009a

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. <i>NameValue</i> must begin with characters and can contain characters, underscores, or numbers. <i>NameValue</i> can be any valid MATLAB variable name.
CompositionValue	Shows the combination of base and derived units that defines the unit <i>NameValue</i> . 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 <i>NameValue</i> and the base unit as a product of the <i>MultiplierValue</i> and the base unit. For example, 1 mole is 6.0221e23*molecule. The <i>MultiplierValue</i> is 6.0221e23.
PropertyName	Name of the unit object property, for example, 'Notes'.
PropertyValue	Value of the unit object property, for example, ' <i>New unit for GPCR model</i> '.

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

Compatibility Considerations

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.

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

Introduced in R2008a

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)

See Also

sbioshowunits

Introduced in R2006a

sbiounitprefix

Create user-defined unit prefix

Syntax

```
unitprefixObject = sbiounitprefix('NameValue')
unitprefixObject = sbiounitprefix('NameValue', 'ExponentValue')
unitprefixObject = sbiounitprefix('NameValue', ...'PropertyName',
PropertyValue ...)
```

Arguments

NameValue	Name of the user-defined unit prefix. <i>NameValue</i> must begin with characters and can contain characters, underscores, or numbers. <i>NameValue</i> can be any valid MATLAB variable name.
ExponentValue	Shows the value of 10 ^{Exponent} that defines the relationship of the unit <i>Name</i> to the base unit. For example, for the unit picomole, Exponent is – 12.
PropertyName	Name of the unit prefix object property. For example, 'Notes'.
PropertyValue	Value of the unit prefix object property. For example, ' <i>New unitprefix for GPCR model</i> '.

Description

unitprefixObject = sbiounitprefix('NameValue') constructs a SimBiology unit prefix
object with the name NameValue. Valid names must begin with a letter, and be followed by letters,
underscores, or numbers.

```
unitprefixObject = sbiounitprefix('NameValue', 'ExponentValue') creates a unit-
prefix object with a multiplicative factor of 10<sup>^</sup>ExponentValue'.
```

unitprefixObject = sbiounitprefix('NameValue', ...'PropertyName', PropertyValue ...) defines optional properties. The property name/property value pairs can be in any format supported by the function set.

In order to use *unitprefixObject*, you must add it to the user-defined library with the **sbioaddtolibrary** function. To get the unit-prefix object into the user-defined library, use the following command:

```
sbioaddtolibrary(unitprefixObject);
```

You can view additional *unitprefixObject* properties with the get command. You can modify additional properties with the set command.

Use the sbioshowunitprefixes function to list the units available in the user-defined library.

Examples

This example shows how to create a user-defined unit prefix, add it to the user-defined library, and query the library.

1 Create a unit prefix.

unitprefixObj1 = sbiounitprefix('peta', 15);

2 Add the unit prefix to the user-defined library.

sbioaddtolibrary(unitprefix0bj1);

3 Query the user-defined library in the root object.

```
rootObj = sbioroot;
```

rootObj.UserDefinedLibrary.UnitPrefixes

Unit Prefix Array

Index: Library: Name: Exponent:

1 UserDefined peta 15

Alternatively, use the **sbiowhos** command.

sbiowhos -userdefined -unitprefix

SimBiology UserDefined Unit Prefixes

Index:	Name:	Multiplier:
1	peta	1.000000e+015

See Also

sbioaddtolibrary|sbioshowunits|sbiounit|sbiowhos

Topics

sbioshowunits on page 1-229

Introduced in R2008a

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 namevalue 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 0.004

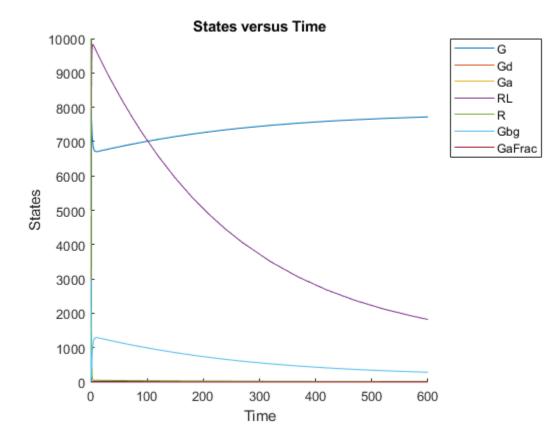
Create another variant with the kGd value of 0.5, and initial amount of 5000 for the G species.

```
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	0.5
2	species	G	InitialAmount	5000

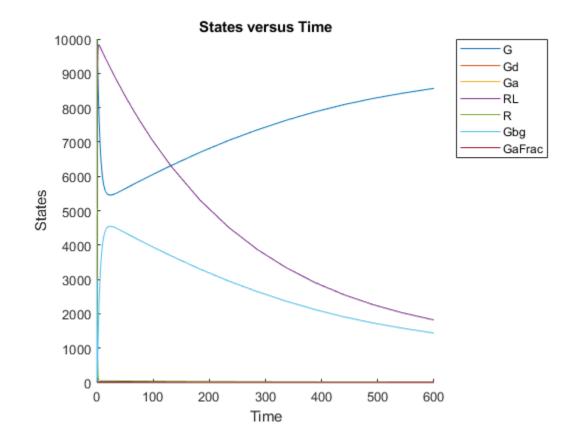
Simulate the model using the initial conditions specified in v2.

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

variant0bj — Variant with alternate model values

variant object

Variant with alternate model values, specified as a Variant object.

See Also

addvariant|delete|get|getvariant|set

Topics

"Simulate Biological Variability of the Yeast G Protein Cycle Using the Wild-Type and Mutant Strains" "Simulate Model of Glucose-Insulin Response with Different Initial Conditions" "Variants in SimBiology Models"

Introduced in R2008a

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

See Also

whos

Introduced in R2006a

sbmlexport

Export SimBiology model to SBML file

Syntax

```
sbmlexport(model0bj)
sbmlexport(model0bj, 'FileName')
```

Arguments

model0bj	Model object. Enter a variable name for a model object.
	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(model0bj,'gene_regulation.xml');

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

"Exporting a SimBiology Model to SBML Format"

"SBML Support" sbiomodel on page 1-108 sbiosaveproject on page 1-218

Introduced before R2006a

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');
```

Compatibility Considerations

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.

Support for URL schemes other than HTTP and HTTPS will be removed

Not recommended starting in R2021a

Support for passing in a URL that is not HTTP and HTTPS will be 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

DimensionalAnalysis | get | sbiosimulate | sbmlexport | set

Topics "SBML Support"

"Importing from SBML Files"

Introduced before R2006a

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 "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

Compatibility Considerations

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

Model | SimBiology Model Analyzer | SimBiology Model Builder | sbioreset | sbioroot

Introduced in R2009a

SimBiology.export.Dose class

Superclasses: matlab.mixin.Heterogeneous

Exported SimBiology model dose object

Description

SimBiology.export.Dose is the superclass for modifiable export dose objects. An export dose is either of subclass SimBiology.export.RepeatDose or SimBiology.export.ScheduleDose.

Construction

Export dose objects are created by the export method 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.

export (model) Export SimBiology models for deployment and standalone applications

Properties

Amount

Amount of dose, a nonnegative scalar value. This property is read-only if it is parameterized in the export model.

AmountUnits

Dose amount units. This property is read-only.

DurationParameterName

Parameter specifying length of time to administer a dose. This property is read-only.

EventMode

Determine how events that change dose parameters affect in-progress dosing. This property is readonly.

LagParameterName

Parameter specifying time lag for the dose. This property is read-only.

Name

Name of dose object. This property is read-only.

Notes

Text describing dose object. This property is read-only.

Parent

Name of the parent export model. This property is read-only.

Rate

Rate of dose, 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. This property is read-only.

TargetName

Species receiving dose. This property is read-only.

TimeUnits

Time units for dosing. This property is read-only.

Copy Semantics

Handle. To learn how handle classes affect copy operations, see Copying Objects.

Examples

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.

See Also

SimBiology.export.RepeatDose | SimBiology.export.ScheduleDose | export

Topics "PK/PD Modeling and Simulation to Guide Dosing Strategy for Antibiotics" "Deploy a SimBiology Model"

SimBiology.export.ExplicitTauSimulationOptions class

Superclasses: SimBiology.export.StochasticSimulationOptions

Settings for explicit tau-leaping solver of exported SimBiology model

Description

SimBiology.export.ExplicitTauSimulationOptions is the class of simulation options associated with the explicit tau-leaping solver of an export model.

Construction

Explicit tau simulation options are created by the export method for SimBiology models with a stochastic SolverType set to 'expltau'.

export (model) Export SimBiology models for deployment and standalone applications

Properties

ErrorTolerance

Error tolerance, a scalar value in the range (0,1).

LogDecimation

Frequency to log stochastic simulation output, a positive integer value.

MaximumNumberofLogs

Maximum number of logs criterion to stop simulation, a positive scalar value.

MaximumWallClock

Maximum elapsed wall clock time criterion to stop simulation, a positive scalar value.

RandomState

Random number generator, a positive integer value.

SolverType

Character vector indicating solver type to use for simulation, 'expltau'. This property is read only.

StopTime

Simulation time criterion to stop simulation, a nonnegative scalar value.

TimeUnits

Time units for simulation. This property is read only.

Copy Semantics

Handle. To learn how handle classes affect copy operations, see Copying Objects.

See Also

```
SimBiology.export.ImplicitTauSimulationOptions |
SimBiology.export.ODESimulationOptions | SimBiology.export.SimulationOptions |
SimBiology.export.StochasticSimulationOptions | export
```

SimBiology.export.ImplicitTauSimulationOptions class

Superclasses: SimBiology.export.StochasticSimulationOptions

Settings for implicit tau-leaping stochastic simulation of exported SimBiology model

Description

SimBiology.export.ImplicitTauSimulationOptions is the class of simulation options associated with the implicit tau-leaping solver of an export model.

Construction

Implicit tau-leaping simulation options are created by the export method for SimBiology models with a stochastic SolverType set to 'impltau'.

export (model) Export SimBiology models for deployment and standalone applications

Properties

ErrorTolerance

Error tolerance, a scalar value in the range (0,1).

LogDecimation

Frequency to log stochastic simulation output, a positive integer value.

MaxIterations

Nonlinear solver maximum number of iterations, a positive integer value.

MaximumNumberofLogs

Maximum number of logs criterion to stop simulation, a positive scalar value.

MaximumWallClock

Maximum elapsed wall clock time criterion to stop simulation, a positive scalar value.

RandomState

Random number generator, a positive integer value.

SolverType

 $Character\ vector\ indicating\ solver\ type\ to\ use\ for\ simulation,\ \verb'impltau'.\ This\ property\ is\ read\ only.$

StopTime

Simulation time criterion to stop simulation, a nonnegative scalar value.

TimeUnits

Time units for simulation. This property is read only.

Copy Semantics

Handle. To learn how handle classes affect copy operations, see Copying Objects.

See Also

```
SimBiology.export.ExplicitTauSimulationOptions |
SimBiology.export.ODESimulationOptions | SimBiology.export.SimulationOptions |
SimBiology.export.StochasticSimulationOptions | export
```

SimBiology.export.Model class

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^M.

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.

Construction

Use the export method to export a SimBiology model.

export (model) Export SimBiology models for deployment and standalone applications

Properties

DependentFiles

Function files the model depends on. This property is read only.

ExportNotes

Text with additional information associated with the exported model. This property is read only.

ExportTime

Creation time of the exported model. This property is read only.

InitialValues

Vector of initial values for modifiable species, compartments, and parameters.

Name

Name of the exported model. This property is read only.

Notes

HTML text describing the exported model object. This property is read only.

SimulationOptions

SimBiology.export.SimulationOptions object specifying simulation options.

ValueInfo

Array of SimBiology.export.ValueInfo objects of modifiable species, parameters, and compartments.

Methods

accelerate	Prepare exported SimBiology model for acceleration
getdose	Return exported SimBiology model dose object
getIndex	Get indices into ValueInfo and InitialValues properties
isAccelerated	Determine whether an exported SimBiology model is accelerated
simulate	Simulate exported SimBiology model

Copy Semantics

Handle. To learn how handle classes affect copy operations, see Copying Objects.

Examples

Export SimBiology Model Object

Load a sample SimBiology model object, and export.

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
Columns 1 through 7
{'unnamed'} {'x'} {'y1'} {'y2'} {'z'} {'c1'} {'c2'}
Column 8
{'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'
```

See Also

SimBiology.export.Dose | SimBiology.export.SimulationOptions |
SimBiology.export.ValueInfo | export

Topics

"PK/PD Modeling and Simulation to Guide Dosing Strategy for Antibiotics" "Deploy a SimBiology Model" Class Attributes Property Attributes

SimBiology.export.ODESimulationOptions class

Superclasses: SimBiology.export.SimulationOptions

Settings for deterministic, ordinary differential equation simulation of exported SimBiology model

Description

SimBiology.export.ODESimulationOptions is the class of simulation options associated with determinist, ordinary differential equation (ODE) solvers.

Construction

Deterministic simulation options are created by the export method for SimBiology models with a deterministic SolverType (for example, sundials or ode15s).

export (model) Export SimBiology models for deployment and standalone applications

Properties

AbsoluteTolerance

Absolute error tolerance applied to state value during simulation, a positive scalar value.

AbsoluteToleranceScaling

Control scaling of absolute error tolerance, a logical value.

AbsoluteToleranceStepSize

Initial guess for time step size for scaling of absolute error tolerance, [] or a scalar value.

MaximumNumberofLogs

Maximum number of logs criterion to stop simulation, a positive scalar value.

MaximumWallClock

Maximum elapsed wall clock time criterion to stop simulation, a positive scalar value.

MaxStep

Upper bound on ODE solver step size, [] or a positive scalar value.

OutputTimes

Times to log in simulation output, a vector of sorted nonnegative values.

RelativeTolerance

Allowable error tolerance relative to state value during simulation, a scalar value in the range (0,1).

SolverType

Character vector indicating solver type to use for simulation. Possible deterministic solver types are:

- 'sundials'
- 'ode15s'
- 'ode23t'
- 'ode45'

StopTime

Simulation time criterion to stop simulation, a nonnegative scalar value.

TimeUnits

Time units for simulation. This property is read only.

Copy Semantics

Handle. To learn how handle classes affect copy operations, see Copying Objects.

See Also

```
SimBiology.export.SimulationOptions |
SimBiology.export.StochasticSimulationOptions | export
```

SimBiology.export.RepeatDose class

Superclasses: SimBiology.export.Dose

Repeated doses for exported SimBiology model

Description

SimBiology.export.RepeatDose is the class for export repeat doses.

Construction

Export repeat dose objects are created by the export method 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.

export (model) Export SimBiology models for deployment and standalone applications

Properties

Amount

Amount of dose, 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. This property is read-only.

DurationParameterName

Parameter specifying length of time to administer a dose. This property is read-only.

EventMode

Determine how events that change dose parameters affect in-progress dosing. This property is readonly.

Interval

Time between doses, 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. This property is read-only.

Name

Name of dose object. This property is read-only.

Notes

Text describing dose object. This property is read-only.

Parent

Name of the parent export model. This property is read-only.

Rate

Rate of dose, 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.

RateUnits

Units for dose rate. This property is read-only.

RepeatCount

Dose repetitions, a nonnegative integer value or the name (string or character vector) of a modelscoped parameter. This property is read-only if it is parameterized in the export model.

StartTime

Start time for initial dose, 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. This property is read-only.

TimeUnits

Time units for dosing. This property is read-only.

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.

Copy Semantics

Handle. To learn how handle classes affect copy operations, see Copying Objects.

See Also

SimBiology.export.Dose | SimBiology.export.ScheduleDose | export

SimBiology.export.ScheduleDose class

Superclasses: SimBiology.export.Dose

Schedule dose for exported SimBiology model

Description

SimBiology.export.ScheduleDose is the class for export schedule doses.

Construction

Export schedule dose objects are created by the export method 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.

export (model) Export SimBiology models for deployment and standalone applications

Properties

Amount

Amount of dose, a nonnegative scalar value.

AmountUnits

Dose amount units. This property is read-only.

DurationParameterName

Parameter specifying length of time to administer a dose. This property is read-only.

EventMode

Determine how events that change dose parameters affect in-progress dosing. This property is readonly.

LagParameterName

Parameter specifying time lag for the dose. This property is read-only.

Name

Name of dose object. This property is read-only.

Notes

Text describing dose object. This property is read-only.

Parent

Name of the parent export model. This property is read-only.

Rate

Rate of dose, 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.

RateUnits

Units for dose rate. This property is read-only.

TargetName

Species receiving dose. This property is read-only.

Time

Schedule dose times, a vector of nonnegative values.

TimeUnits

Time units for dosing. This property is read-only.

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.

Copy Semantics

Handle. To learn how handle classes affect copy operations, see Copying Objects.

See Also

SimBiology.export.Dose | SimBiology.export.RepeatDose | export

SimBiology.export.SimulationOptions class

Simulation settings for exported SimBiology model

Description

SimBiology.export.SimulationOptions is the superclass of simulation options for exported models. Simulation options are either of subclass SimBiology.export.ODESimulationOptions for deterministic solvers, or SimBiology.export.StochasticSimulationOptions for stochastic solvers.

Construction

Simulation options are created by the export method for SimBiology models.

export (model) Export SimBiology models for deployment and standalone applications

Properties

MaximumNumberofLogs

Maximum number of logs criterion to stop simulation, a positive scalar value.

MaximumWallClock

Maximum elapsed wall clock time criterion to stop simulation, a positive scalar value.

StopTime

Simulation time criterion to stop simulation, a nonnegative scalar value.

TimeUnits

Time units for simulation. This property is read only.

Copy Semantics

Handle. To learn how handle classes affect copy operations, see Copying Objects.

See Also

```
SimBiology.export.ODESimulationOptions |
SimBiology.export.StochasticSimulationOptions | export
```

SimBiology.export.StochasticSimulationOptions class

Superclasses: SimBiology.export.SimulationOptions

Settings for stochastic simulation of exported SimBiology model

Description

```
SimBiology.export.StochasticSimulationOptions is the superclass of simulation options
associated with stochastic solvers. The subclasses of
SimBiology.export.StochasticSimulationOptions are
SimBiology.export.ExplicitTauSimulationOptions and
SimBiology.export.ImplicitTauSimulationOptions.
```

Construction

Stochastic simulation options are created by the export method for SimBiology models with a stochastic SolverType (ssa, expltau, or impltau).

export (model) Export SimBiology models for deployment and standalone applications

Properties

LogDecimation

Frequency to log stochastic simulation output, a positive integer value.

MaximumNumberofLogs

Maximum number of logs criterion to stop simulation, a positive scalar value.

MaximumWallClock

Maximum elapsed wall clock time criterion to stop simulation, a positive scalar value.

RandomState

Random number generator, a positive integer value.

SolverType

Character vector indicating solver type to use for simulation. This property is read only. The stochastic solver type is one of:

- 'ssa'
- 'expltau'
- 'impltau'

StopTime

Simulation time criterion to stop simulation, a nonnegative scalar value.

TimeUnits

Time units for simulation. This property is read only.

Copy Semantics

Handle. To learn how handle classes affect copy operations, see Copying Objects.

See Also

```
SimBiology.export.ExplicitTauSimulationOptions |
SimBiology.export.ImplicitTauSimulationOptions |
SimBiology.export.ODESimulationOptions | SimBiology.export.SimulationOptions |
export
```

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.

ml.Species

ans = Sim	Biology Species Ar	ray		
Ind	lex: Compartment	: Name:	Value:	Units:
1	unnamed	Х	1	
2	unnamed	y1	900	
3	unnamed	y2	900	
4	unnamed	Z	Θ	

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.

```
ml.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:
                     1
    Compartments:
                      0
    Events:
    Parameters:
                      3
    Reactions:
                      3
                      2
    Rules:
    Species:
                      4
    Observables:
                      0
```

In order to remove order dependencies, SimBiology updated the initial assignment expression x = z t 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 2-310 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.
	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 2-339 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.

See Also

Model on page 2-310 | Parameter on page 2-339

Topics "Evaluation Order of Rules"

Introduced in R2017b

SimBiology.export.ValueInfo class

Modifiable species, compartments, or parameters in exported SimBiology model

Description

SimBiology.export.ValueInfo is the class that describes the modifiable value components in a
SimBiology.export.Model, including species, parameters, and compartments.

Construction

ValueInfo objects are created by the export method for SimBiology models. By default, all model species, parameters, and compartments are ValueInfo objects, but you can specify which value components to export using the optional editvals input argument to export.

export (model) Export SimBiology models for deployment and standalone applications

Properties

Constant

Display whether value is constant or time-varying. This property is read only.

InitialValue

Initial value for the component, a scalar value.

Name

Name of species, compartment, or parameter. This property is read only.

Parent

Name of parent model, compartment, or reaction. This property is read only.

QualifiedName

Qualified name of species, compartment, or parameter. This property is read only.

- 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. This property is read only.

Туре

Type of value (species, parameter, or compartment). This property is read only.

Units

Value units. This property is read only

Copy Semantics

Handle. To learn how handle classes affect copy operations, see Copying Objects.

See Also

SimBiology.export.Model|export

simbio.diagram.getBlock

Package: simbio.diagram

Get SimBiology diagram block properties

Syntax

```
SV = simbio.diagram.getBlock(s0bj)
SV = simbio.diagram.getBlock(species0bj,expr0bj)
QV = simbio.diagram.getBlock(s0bj,propertyNames)
QV = simbio.diagram.getBlock(species0bj,expr0bj,propertyNames)
simbio.diagram.getBlock(____)
```

Description

SV = simbio.diagram.getBlock(s0bj) returns the names and current values of the block properties of a SimBiology object s0bj as a structure SV.

Note 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 the 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(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
                             Х
                                       1
   2
             unnamed
                              y1
                                       900
                             у2
   3
                                       900
             unnamed
   4
             unnamed
                                       0
                              7
```

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 *m*1.

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.

Unpin the cloned block and move it to another position.

simbio.diagram.setBlock(Gbg,r2,'Pin',false,'Position',[391 340 30 15])

Input Arguments

s0bj — 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
Connection s	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' For details, see ColorSpec (Color Specification).
Expression Lines	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.

Property Name	Description			
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' 			
	For details, see ColorSpec (Color Specification).			
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'			
0bject	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.			

Property Name	Description
Shape	Block shape, specified as a character vector or string. Valid options are:
	 'rounded rectangle' 'rectangle' 'oval' 'triangle' 'hexagon' 'chevron'
	 'parallellogram' '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' For details, see ColorSpec (Color Specification).
TextLocati on	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.

Example: 'Position'

Data Types: double | char | string | cell

species0bj — Species object

Species object

Species object, specified as a SimBiology Species object. speciesObj must be scalar.

expr0bj — 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 s0bj is an array of objects, SV is an array of structures. The function returns one structure per block. If s0bj has multiple cloned blocks, SV contains a structure for each cloned block.

See Also

SimBiology Model Builder | simbio.diagram.getLine | simbio.diagram.joinBlock | simbio.diagram.setBlock | 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"

Introduced in R2021a

simbio.diagram.getLine

Package: simbio.diagram

Get SimBiology diagram line properties

Syntax

```
SV = simbio.diagram.getLine(s0bj)
SV = simbio.diagram.getLine(obj1,obj2)
QV = simbio.diagram.getLine(s0bj,propertyNames)
QV = simbio.diagram.getLine(obj1,obj2,propertyNames)
simbio.diagram.getLine(____)
```

Description

SV = simbio.diagram.getLine(s0bj) returns the names and current values of all properties of all lines connected to a SimBiology object s0bj as a structure SV.

Note 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 the 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(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:
                                        Value:
                                                   Units:
                               Name:
   1
             unnamed
                               Х
                                         1
   2
             unnamed
                               y1
                                         900
   3
             unnamed
                               y2
                                         900
   4
             unnamed
                                         0
                               Ζ
```

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.

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.

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

s0bj — 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 		
	For details, see ColorSpec (Color Specification).		
Connection s	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 s0bj or if s0bj is an array of objects, SV is an array of structures. The function returns one structure per line.

See Also

SimBiology Model Builder | simbio.diagram.getBlock | simbio.diagram.joinBlock | simbio.diagram.setBlock | 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"

Introduced in R2021a

simbio.diagram.joinBlock

Package: simbio.diagram

Combine all copies of SimBiology species blocks in diagram

Syntax

```
simbio.diagram.joinBlock(species0bj)
simbio.diagram.joinBlock(species0bj,expr0bj)
simbio.diagram.joinBlock(species0bj,expr0bj1,expr0bj2)
```

Description

simbio.diagram.joinBlock(speciesObj) combines all copies of the SimBiology species
speciesObj blocks into one block in the model diagram. speciesObj must be scalar.

Note 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 the 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,exprObj) combines all copies of the species
speciesObj blocks 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	Θ	
4	unnamed	RL	Θ	
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

species0bj — Species object

Species object

Species object, specified as a SimBiology Species object. speciesObj must be scalar.

expr0bj — 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.

expr0bj1 — 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.

expr0bj2 — 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.

See Also

SimBiology Model Builder | simbio.diagram.getBlock | simbio.diagram.getLine | simbio.diagram.setBlock | 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"

Introduced in R2021a

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,propertyName)
simbio.diagram.setBlock(speciesObj,exprObj, ____)
simbio.diagram.setBlock(speciesObj,exprObj)
```

Description

simbio.diagram.setBlock(s0bj,propertyNames,propertyValues) sets the values of specified block properties of a SimBiology object or array of objects s0bj.

Note 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 the 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(s0bj,S) sets the property values of s0bj 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(s0bj) displays the names and possible values of configurable block
properties of a SimBiology object s0bj. s0bj must be scalar.

outStruct = simbio.diagram.setBlock(s0bj) returns a structure outStruct containing the names and possible values of configurable block properties of a SimBiology object s0bj. s0bj must be scalar.

CV = simbio.diagram.setBlock(s0bj,propertyName) returns a cell array of possible values CV for the block property propertyName. s0bj 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: unnamed 1 Х 1 2 900 unnamed y1 3 unnamed y2 900 4 unnamed 0 7

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' }
{'triangle' }
{'hexagon' }
{'chevron' }
{'parallelogram' }
}
```

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 =

SimBiolo	gy Species Array	1		
Index:	Compartment:	Name:	Value:	Units:
1	unnamed	G	7000	
2	unnamed	Gd	3000	
3	unnamed	Ga	Θ	
4	unnamed	RL	Θ	
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

s0bj — 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
Connection s	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' For details, see ColorSpec (Color Specification).
Expression Lines	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' For details, see ColorSpec (Color Specification).

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'				
0bject	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'				
	• 'parallellogram'				
	• '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' For details, see ColorSpec (Color Specification).
TextLocati on	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.

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* so 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 s0bj.

Data Types: structure

species0bj — Species object Species object

Species object, specified as a SimBiology Species object. speciesObj must be scalar.

expr0bj — 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.

See Also

SimBiology Model Builder | simbio.diagram.getBlock | simbio.diagram.getLine | simbio.diagram.joinBlock | 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"

Introduced in R2021a

simbio.diagram.setLine

Package: simbio.diagram

Set SimBiology diagram line properties

Syntax

```
simbio.diagram.setLine(s0bj,propertyNames,propertyValues)
simbio.diagram.setLine(s0bj,S)
simbio.diagram.setLine(s0bj,Name,Value)
simbio.diagram.setLine(s0bj)
outStruct = simbio.diagram.setLine(s0bj,propertyName)
simbio.diagram.setLine(obj1,obj2,____)
simbio.diagram.setLine(obj1,obj2)
```

Description

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.

Note 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 the 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(s0bj,S) sets the property values of s0bj 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(s0bj) displays the names and possible values of configurable
properties of a line connected to a SimBiology object s0bj. This syntax requires that only one line is
connected to s0bj. If there are multiple lines connected to s0bj, 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. s0bj 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:
                                       Value:
                                                 Units:
                             Name:
             unnamed
   1
                             Х
                                       1
   2
             unnamed
                                       900
                              y1
   3
             unnamed
                             y2
                                       900
   4
             unnamed
                                       0
                              Ζ
```

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 = ml.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.

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

s0bj — 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' For details, see ColorSpec (Color Specification).
Connection s	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 s0bj 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 s0bj.

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.

See Also

SimBiology Model Builder | simbio.diagram.getBlock | simbio.diagram.getLine |
simbio.diagram.joinBlock | simbio.diagram.setBlock | simbio.diagram.splitBlock

Topics

"Create Model of Receptor-Ligand Kinetics"

"Incorporate SGLT2 Inhibition into Physiologically Based Glucose-Insulin Model Using SimBiology Model Builder"

Introduced in R2021a

simbio.diagram.splitBlock

Package: simbio.diagram

Split SimBiology species block in diagram

Syntax

expr = simbio.diagram.splitBlock(speciesObj)

Description

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.

Note 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 the 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.

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	Θ	
4	unnamed	RL	Θ	
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 ($G + RL \rightarrow Ga + Gbg + RL$). Note that the order of reactions returned in expr can change.

```
simbio.diagram.joinBlock(Gbg,expr(2))
```

Input Arguments

species0bj — 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.

See Also

SimBiology Model Builder | simbio.diagram.getBlock | simbio.diagram.getLine | simbio.diagram.joinBlock | simbio.diagram.setBlock | simbio.diagram.setLine

Topics

"Create Model of Receptor-Ligand Kinetics" "Incorporate SGLT2 Inhibition into Physiologically Based Glucose-Insulin Model Using SimBiology Model Builder" Introduced in R2021a

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 pharamacokinetic/pharmacodynamic (PK/PD) models of drugs. It provides several methods to analyze models and various plots to visualize the results.

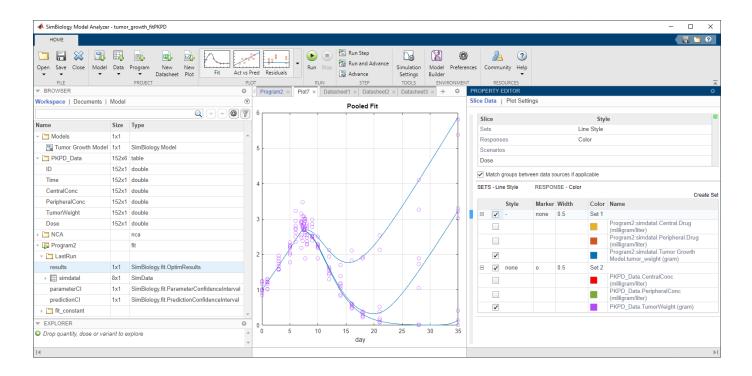
Using the app, you can:

- 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



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 App"
- "Find Important Parameters with Sensitivity Analysis Using SimBiology Model Analyzer App"
- "Model Biological Variability with Virtual Patients Using SimBiology Model Analyzer App"
- "Scan Dosing Regimens Using SimBiology Model Analyzer App"

Programmatic Use

simBiologyModelAnalyzer opens the SimBiology Model Analyzer app.

simBiologyModelAnalyzer(m1) opens the SimBiology model m1 in the SimBiology Model
Analyzer 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.

simBiologyModelAnalyzer(prjFile) opens the project file prjFile in the SimBiology Model
Analyzer app. file 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 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.

Compatibility Considerations

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

sbiofit | sbionca | sbioparameterci | sbiopredictionci | sbiosimulate |
sbiosteadystate

Topics

"Calculate NCA Parameters and Fit Model to PK/PD Data Using SimBiology Model Analyzer App" "Find Important Parameters with Sensitivity Analysis Using SimBiology Model Analyzer App" "Model Biological Variability with Virtual Patients Using SimBiology Model Analyzer App" "Scan Dosing Regimens Using SimBiology Model Analyzer App" "Model Simulation" "Noncompartmental Analysis" "Sensitivity Analysis in SimBiology" "Nonlinear Regression" "Nonlinear Mixed-Effects Modeling"

Introduced in R2019b

SimBiology Model Builder

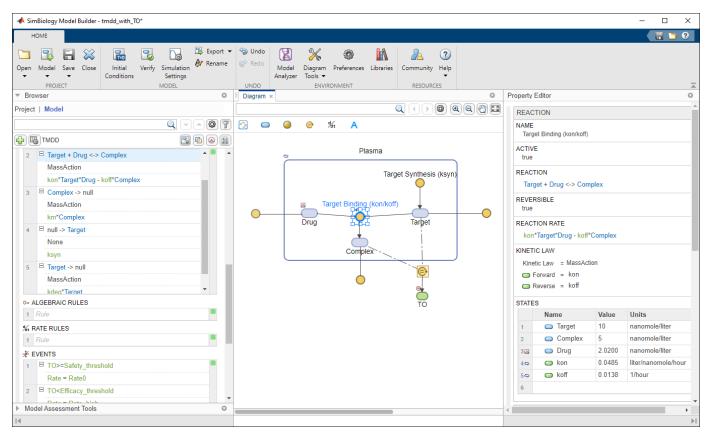
Build QSP, PK/PD, and mechanistic systems biology models interactively

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 simbiology.

Examples

- "Create Model of Receptor-Ligand Kinetics"
- "Incorporate SGLT2 Inhibition into Physiologically Based Glucose-Insulin Model Using SimBiology Model Builder"

Programmatic Use

simBiologyModelBuilder opens the app.

simBiologyModelBuilder(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.

simBiologyModelBuilder(prjFile) opens the project file prjFile in the SimBiology Model Builder app. prjFile 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 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.

Compatibility Considerations

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

sbiodose | sbioloadproject | sbiomodel | sbioreset | sbiovariant | sbmlimport

Topics

"Create Model of Receptor-Ligand Kinetics"

"Incorporate SGLT2 Inhibition into Physiologically Based Glucose-Insulin Model Using SimBiology Model Builder"

"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"

Introduced in R2020b

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.cl', 'Reaction2.c2'},{'y1', 'y2'}, [])
```

f =

SimFunction

Parameters:

Name	Value	Туре
'Reaction1.c1' 'Reaction2.c2'	10	'parameter'
Reactionz.cz	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

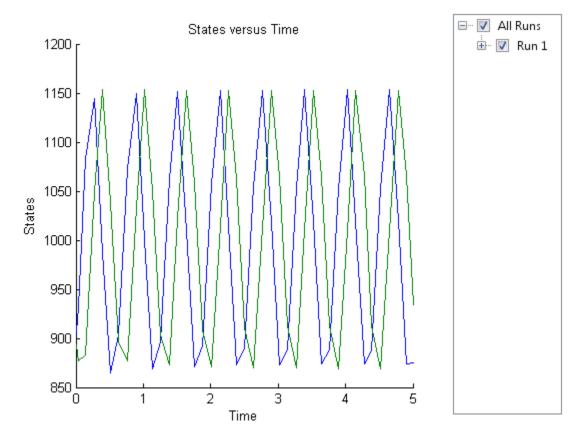
ans = 0

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

References

[1] Gillespie D.T. "Exact Stochatic Simulation of Coupled Chemical Reactions," (1977) The Journal of Physical Chemistry, 81(25), 2340-2361.

Introduced in R2014a

accelerate

Class: SimBiology.export.Model

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.

Input Arguments

model

SimBiology.export.Model object.

Examples

Accelerate Exported SimBiology Model

Load a sample SimBiology model object, and export.

Accelerate the exported model.

```
accelerate(em);
em.isAccelerated
```

```
ans = logical
1
```

The logical value 1 indicates that the exported model is accelerated.

See Also

SimBiology.export.Model|export|isAccelerated

Topics

"PK/PD Modeling and Simulation to Guide Dosing Strategy for Antibiotics" "Deploy a SimBiology 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(root0bj.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 desktop.

Create kinetic law definition

Constructor Summary

sbioabstractkineticlaw

Method Summary	
delete	Delete SimBiology object
display	Display summary of SimBiology object
findUsages (AbstractKineticLaw)	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
Туре	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

Introduced in R2006b

add

Add quantity values, doses, or variants to SimBiology.Scenarios object

Syntax

```
s0bj = add(s0bj,combination,name,content)
s0bj = add(s0bj,combination,quantityNames,probDist,Name,Value)
s0bj = add(s0bj,combination,s0bj2)
```

Description

s0bj = add(s0bj,combination,name,content) adds an entry on page 2-550 to the SimBiology.Scenarios object s0bj. 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 s0bj.

s0bj = add(s0bj,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.

s0bj = add(s0bj,combination,s0bj2) adds entries from the SimBiology.Scenarios object s0bj2 to s0bj. The function combines the entries from s0bj2 with the existing entries from s0bj 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 "Simulating 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.

```
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(s0bj)
```

```
scenariosTbl=5×2 table
variants dose
[1x1 SimBiology.Variant]
```

Change the entry name of the first entry.

```
rename(s0bj,1,'Insulin Impairements')
```

ans = Scenarios (5 scenarios)

	ľ	Name	Conte	ent	Number
Entry 1 x Entry 2	Insulin I dose	Impairements	SimBiology SimBiology		5 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:

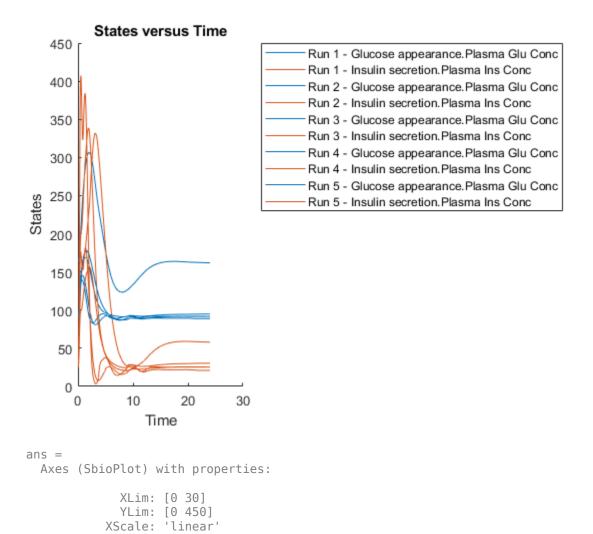
Name	Value	Туре	Units
{'Plasma Volume (Glu)' }	1.88	{'parameter'}	{'deciliter'
{ 'k1' }	0.065	{'parameter'}	{'1/minute'
{ 'k2 ' }	0.079	{'parameter'}	{'1/minute'
{'Plasma Volume (Ins)' }	0.05	{'parameter'}	{'liter'
{'m1' }	0.19	{'parameter'}	{'1/minute'
{'m2' }	0.484	{'parameter'}	{'1/minute'
{'m4' }	0.1936	{'parameter'}	{'1/minute'
{'m5' }	0.0304	{'parameter'}	{'minute/picomole'
{'m6' }	0.6469	{'parameter'}	{ 'dimensionless '
{'Hepatic Extraction' }	0.6	{'parameter'}	<pre>{'dimensionless'</pre>
{'kmax' }	0.0558	{'parameter'}	<pre>{'1/minute'</pre>
{'kmin' }	0.008	{'parameter'}	{'1/minute'
{'kabs' }	0.0568	{'parameter'}	{'1/minute'
{'kgri' }	Θ	{'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'
{'Stomach Glu After Dosing'}	78	{'parameter'}	{'gram'
{'kp1' }	2.7	{'parameter'}	{'milligram/minute'
{ 'kp2 ' }	0.0021	{'parameter'}	{'1/minute'
{'kp3' }	0.009	{'parameter'}	{'(milligram/minute)/(picomole/li
{'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/li
{ '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/de
{'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		Туре	Units
	{'[Plasma Glu {'[Plasma Ins			{'milligram/deciliter'} {'picomole/liter' }
Dose	ed:			
	TargetName	TargetD	imension	
	{'Dose'}	{'Mass (e.	g., gram)'}	

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(s0bj,24); sbioplot(sd)



YScale: 'linear'

```
GridLineStyle: '-'
Position: [0.0920 0.1100 0.2956 0.8150]
Units: 'normalized'
Show all properties
```

If you have Statistics and Machine Learning ToolboxTM, 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 distribution 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 s0bj.

Add an entry that defines the joint probability distribution with a rank correlation matrix.

add(s0bj,'cartesian',["Vmx","kp3"],[pd_Vmx, pd_kp3],'RankCorrelation',[1,0.5;0.5,1])

```
ans =
 Scenarios (2 scenarios)
                                                          Number
                    Name
                                    Content
                             SimBiology dose
   Entry 1
                    dose
                                                        1
   x (Entrv 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(s0bj,2,'Number',50)
```

```
ans =
 Scenarios (50 scenarios)
                                    Content
                                                        Number
                    Name
                             SimBiology dose
    Entry 1
                    dose
                                                          1
   x (Entry 2.1
                    Vmx
                             Lognormal distribution
                                                          50
    + Entry 2.2)
                             Lognormal distribution
                    kp3
                                                          50
```

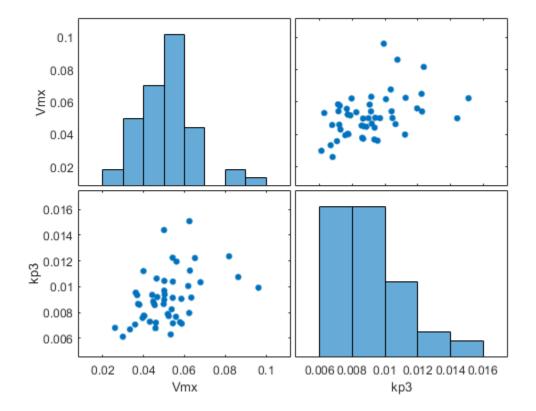
See also Expression property.

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(s0bj,m1)

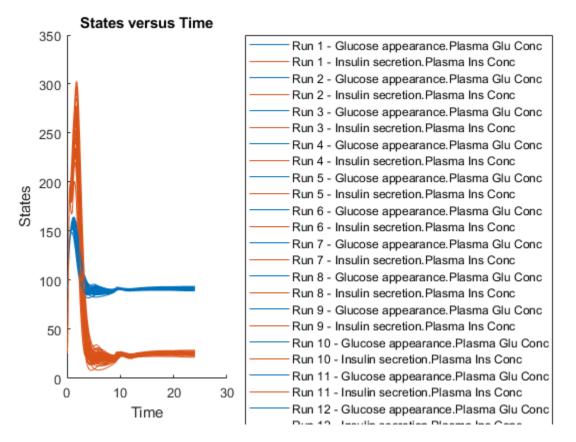
Generate the simulation scenarios. Plot the sample values using plotmatrix. You can see the value of Vmx is varied around its model value 0.047 and that of kp3 around 0.009.

```
sTbl = generate(s0bj);
[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(s0bj,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(s0bj,2)

entry2struct.SamplingMethod = 'lhs'

You can now use the updated structure to modify entry 2.

```
updateEntry(s0bj,2,entry2struct)
```

```
ans =
Scenarios (50 scenarios)
Name Content
```

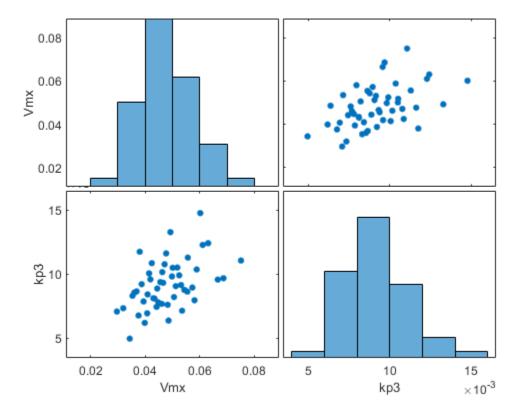
Entry 1	dose	SimBiology dose	1
x (Entry 2.1	Vm×	Lognormal distribution	50
+ Entry 2.2)	kp3	Lognormal distribution	50

Number

See also Expression property.

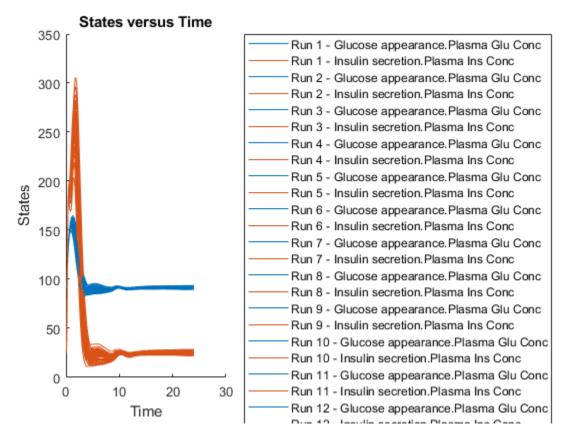
Visualize the sample values.

```
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(s0bj,24); sbioplot(sd3);



Restore warning settings.

warning(warnSettings);

Input Arguments

s0bj — Simulation scenarios

SimBiology.Scenarios object

Simulation scenarios, specified as a SimBiology.Scenarios object.

s0bj2 — 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 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'

Output Arguments

s0bj — Simulation scenarios

Scenarios object

Simulation scenarios, returned as a Scenarios object.

See Also

SimBiology.Scenarios | SimFunction object | createSimFunction (model)

Topics "SimBiology.Scenarios Terminology" on page 2-550 "Combine Simulation Scenarios in SimBiology"

Introduced in R2019b

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

model0bj	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 <i>PropertyName</i> . 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,	Create comportment shipst
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 (species, parameter,	
compartment)	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 $% \left({{{\left({{{{\bf{n}}}} \right)}_{i}}}_{i}} \right)$
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
Туре	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.

```
compl.Capacity = 2;
compl.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

See Also

model object, addproduct, addreactant, addreaction, addspecies

Introduced in R2007b

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

C	PKModelDesign object to which you want to add a compartment
	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

Introduced in R2009a

addconfigset (model)

Create configuration set object and add to model object

Syntax

```
configsetObj = addconfigset(modelObj, 'NameValue')
configsetObj = addconfigset(..., 'PropertyName', PropertyValue, ...)
```

Arguments

model0bj	Model object. Enter a variable name.
	Descriptive name for a configuration set object. Reserved words 'active' and 'default' are not allowed.
configset0bj	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. *configset0bj* is not automatically set to active. Use the function setactiveconfigset to define the active configset for model0bj.

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
SolverOptions	Specify model solver options
SolverType	Select solver type for simulation
StopTime	Simulation time criteria to stop simulation
TimeUnits	Show time units for dosing and simulation
Туре	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.

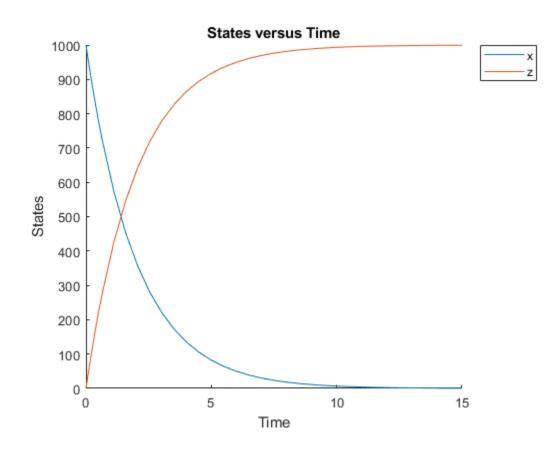
```
configsetObj.StopTime = 15;
```

Set the configset object to be active so that its settings are used during simulation.

```
setactiveconfigset(m1,configset0bj);
```

Simulate the model and plot results.

```
simdata = sbiosimulate(m1);
sbioplot(simdata);
```



See Also

model object, configset object, getconfigset, removeconfigset, setactiveconfigset

Introduced in R2006a

addcontent (variant)

Append content to variant object

Syntax

addcontent(variant0bj, contents)

addcontent(variant0bj1, variant0bj2)

Arguments

variant0bj	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, 'compl');
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

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

model0bj	odel object to which you add a dose object.	
	Name of a dose object to construct and add to a model object. <i>DoseName</i> 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'.	
dose0bj	Dose object to add to a model object. Created with the constructor sbiodose.	

Outputs

ScheduleDose object or RepeatDose object. A RepeatDose or ScheduleDose object defines an increase (dose) to a species amount during a simulation.
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

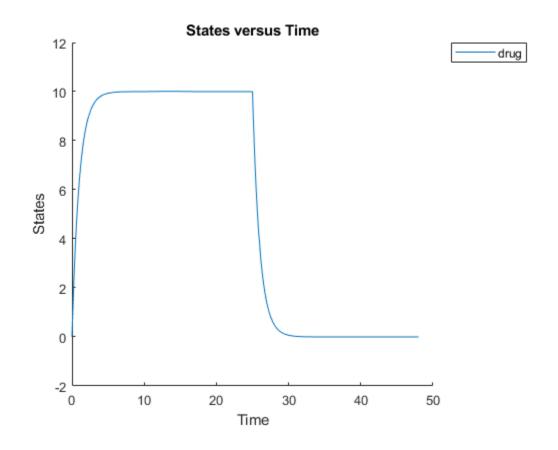
Change the simulation stop time to 48 hours to see the complete time course.

```
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);
```



See Also

RepeatDose object|ScheduleDose object|getdose|model object|removedose|
sbiodose

Topics

"Doses in SimBiology Models"

Introduced in R2010a

addevent (model)

Add event object to model object

Syntax

event0bj = addevent(model0bj, 'TriggerValue', 'EventFcnsValue')

```
event0bj = addevent(...'PropertyName', PropertyValue...)
```

Arguments

model0bj	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 ' <i>objectname</i> = <i>expression</i> ', where <i>objectname</i> 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 2-39.
PropertyValue	Property value. For more information on property values, see the property reference for each property listed in "Property Summary" on page 2-39.

Description

event0bj = addevent(model0bj, 'TriggerValue', 'EventFcnsValue') creates an Event
object(event0bj) and adds the event to the model(model0bj). 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 (model0bj) 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
Туре	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 \rightarrow B, where A and B are species. Also add the reaction rate parameter, p1, with the parameter value of 0.5.

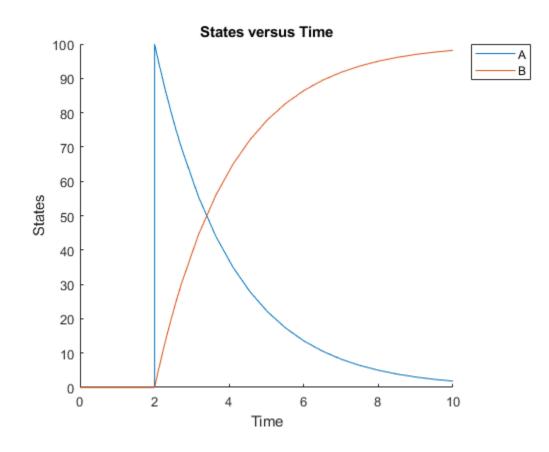
```
model = sbiomodel('example');
r1 = addreaction(model,'A -> B');
kl = addkineticlaw(r1,'MassAction');
p1 = addparameter(model,'p1',0.5);
kl.ParameterVariableNames = 'p1';
```

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 \geq = 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);
```



See Also

Topics

"Deterministic Simulation of a Model Containing a Discontinuity" "Events in SimBiology Models"

Introduced in R2007b

addkineticlaw (reaction)

Create kinetic law object and add to reaction object

Syntax

kineticlawObj = addkineticlaw(reactionObj, 'KineticLawNameValue')

kineticlawObj= addkineticlaw(..., 'PropertyName', PropertyValue, ...)

Arguments

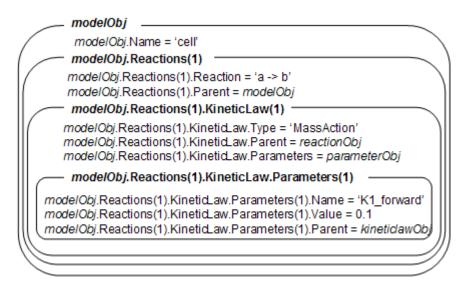
reaction0bj	Reaction object. Enter a variable name for a reaction object.
KineticLawNameValue	Property to select the type of kinetic law object to create. For built- in kinetic law, valid values are:
	<pre>'Unknown', 'MassAction', 'Henri-Michaelis-Menten', 'Henri-Michaelis-Menten-Reversible', 'Hill-Kinetics', '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</pre>
	<pre>rootObj.UserDefinedLibrary.KineticLaws. sbiowhos -kineticlaw lists kinetic laws in the SimBiology root, which includes kinetic laws from both the BuiltInLibrary and</pre>
	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 3-71 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 2-42.

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 3-142.

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
Туре	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

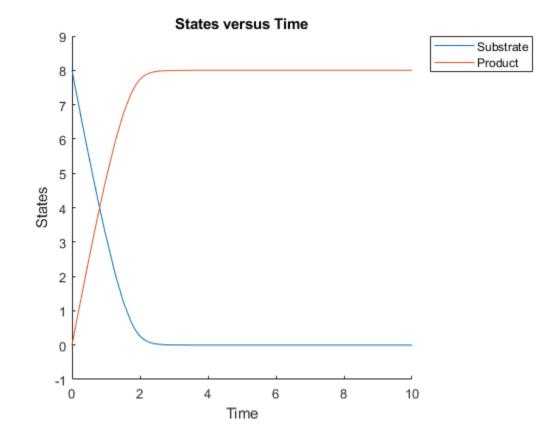
```
ans =
'Vm_param*Substrate/(Km_param+Substrate)'
```

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

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 2-331.

Examples

Calculate Statistics After Model Simulation Using Observables

Load the "Target-Mediated Drug Disposition (TMDD) Model".

sbioloadproject tmdd_with_T0.sbproj

Set the target occupancy (T0) as a response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'T0';
```

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,'T0',d)
```

```
f =
SimFunction
```

Parameters:

	Name	Value	Туре	Units		
	{'AmountParam'}	1	{'parameter'}	{'nanomole'}		
Obse	ervables:					
	Name T	уре	Units			
	{'T0'} {'par	ameter'}	{'dimensionless'}			
Dose	ed:					
	TargetName		TargetDimension		Amount	AmountValue
	{'Plasma.Drug'}	{'Amour	nt (e.g., mole or m	olecule)'}	{'AmountParam'}	1

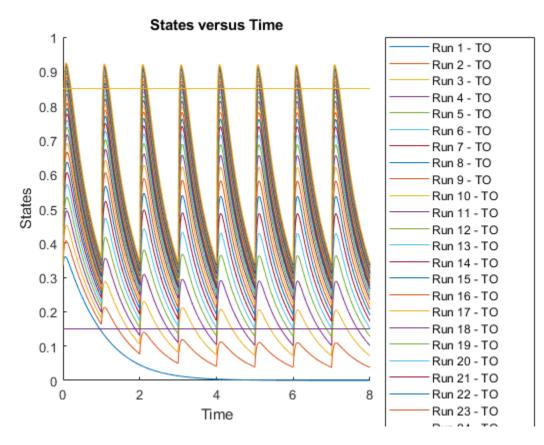
warning('on','SimBiology:SimFunction:DOSES_NOT_EMPTY');

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 T0 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,'statl','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
```

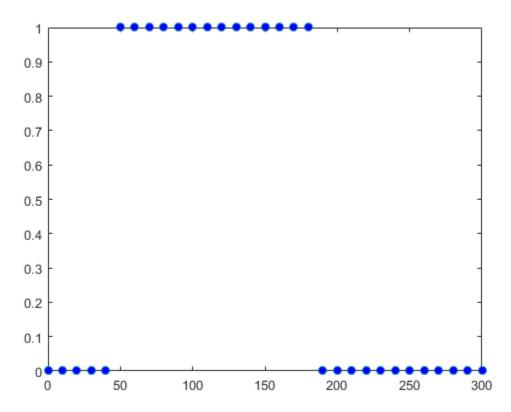
The addobservable function evaluates the new observable expression for each SimData in sd and returns the evaluated results as a new SimData array, newSD, which now has the added observable (stat1).

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 TO 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(TO) < 0.75 \& min(TO) > 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

model0bj — 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

obs0bj — Observable object

Observable object

Observable object, returned as an observable object.

See Also

```
Observable | addobservable(SimData) | renameobservable(SimData) |
updateobservable(SimData)
```

Introduced in R2020a

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_T0.sbproj
```

Set the target occupancy (T0) as a response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'T0';
```

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,'T0',d)
```

f =
SimFunction

Name	э	Value	Туре	Units		
{'AmountF	Param'}	1	{'parameter'}	{'nanomole'}		
oservables:						
Name	Тур	e	Units			
{'T0'}	{'param	<pre>ieter'}</pre>	{'dimensionless'}			
osed:						
Target	Vame		TargetDimension		Amount	AmountValue

warning('on','SimBiology:SimFunction:DOSES_NOT_EMPTY');

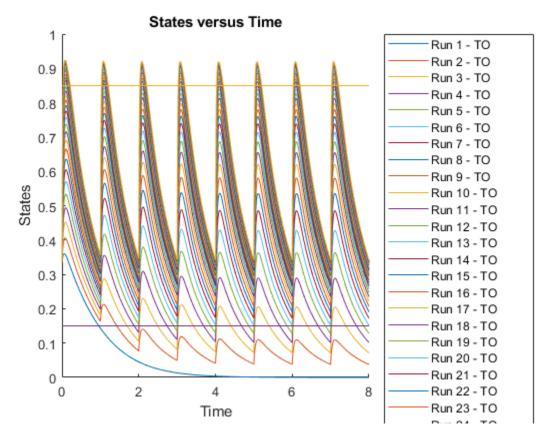
Simulate the model using the dose amounts generated by the Scenarios object. In this case, the object generates 31 different doses; hence the model is simulated 31 times and generates a SimData array.

```
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 T0 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,'statl','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
```

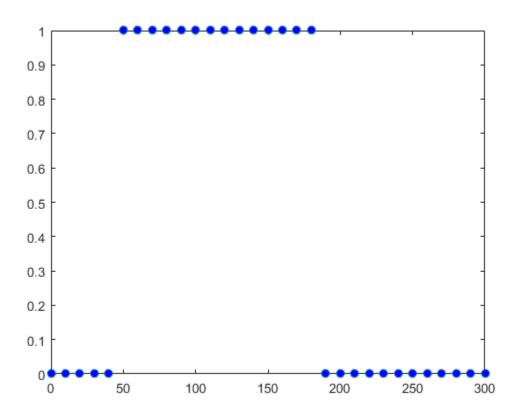
The addobservable function evaluates the new observable expression for each SimData in sd and returns the evaluated results as a new SimData array, newSD, which now has the added observable (stat1).

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 TO 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.

See Also

SimData | renameobservable | updateobservable

Introduced in R2020a

addobservable

Compute Sobol indices for new observable expression

Syntax

```
results = addobservable(sobolObj,obsNames,obsExpressions)
results = addobservable(sobolObj,obsNames,obsExpressions,'Units',units)
```

Description

results = addobservable(sobolObj,obsNames,obsExpressions) computes Sobol indices
for the new observables specified by obsNames with the corresponding expressions
obsExpressions.

results = addobservable(sobolObj,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.

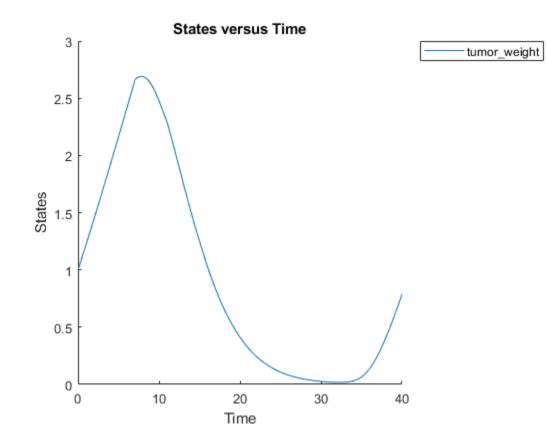
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

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].

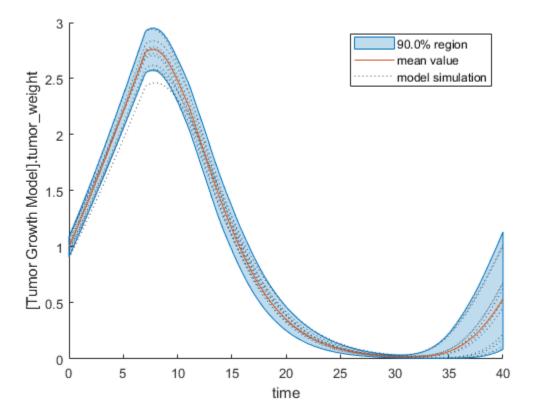
sobolResults = sbiosobol(m1,modelParamNames,outputName,'Variants',v,'Doses',d,'ShowWaitBar',true

```
sobolResults =
   Sobol with properties:
        Time: [444x1 double]
        SobolIndices: [5x1 struct]
        Variance: [444x1 table]
        Observables: {'[Tumor Growth Model].tumor_weight'}
   ParameterSamples: [1000x5 table]
        SimulationInfo: [1x1 struct]
```

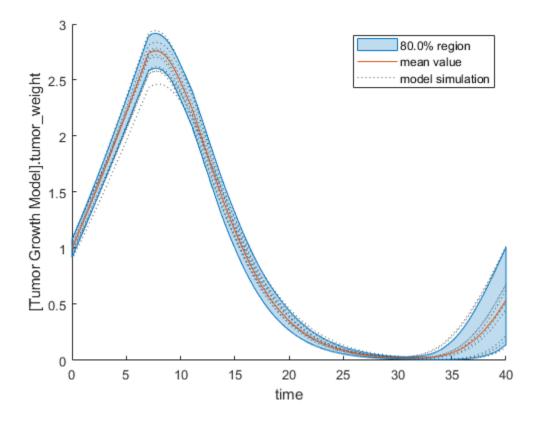
You can change the number of samples by specifying the 'NumberSamples' name-value pair argument. The function requires a total of (number of input parameters + 2) * NumberSamples model simulations.

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

plotData(sobolResults);

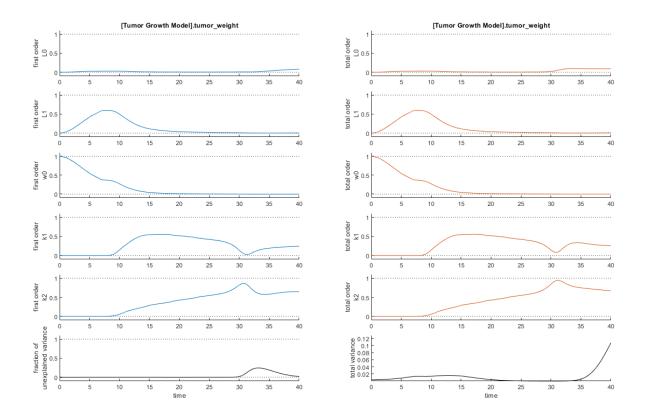


plotData(sobolResults, 'Alphas',0.1);



Plot the time course of the first- and total-order Sobol indices.

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

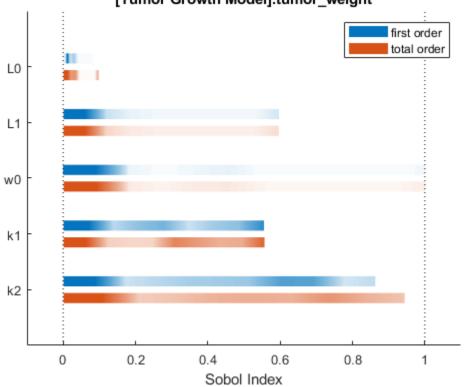


The first-order Sobol index of an input parameter gives the fraction of the overall response variance that can be attributed to variations in the input parameter alone. The total-order index gives the fraction of the overall response variance that can be attributed to any joint parameter variations that 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.

bar(sobolResults)



[Tumor Growth Model].tumor_weight

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-7Index:Name:ModelName:DataCount:1-Tumor Growth Model 12-Tumor Growth Model 13-Tumor Growth Model 1...-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

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.

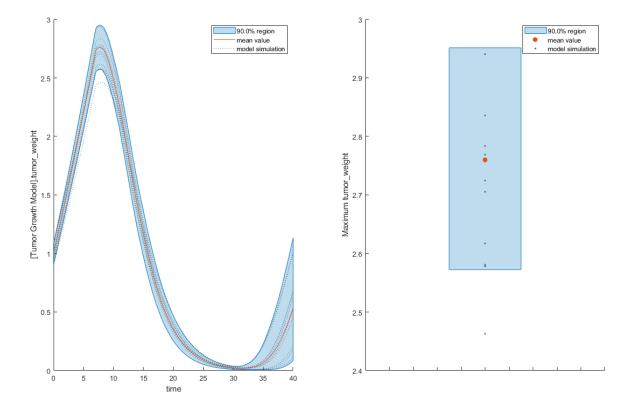
```
[samplesUsed,sd,validruns] = getSimulationResults(sobolResults,4);
```

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);
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

sobol0bj — Results containing Sobol indices

SimBiology.gsa.Sobol object

Results containing the first- and total-order Sobol indices, specified as a SimBiology.gsa.Sobol 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 for observables

SimBiology.gsa.Sobol

Computed Sobol indices for added observables, returned as a SimBiology.gsa.Sobol object.

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

Introduced in R2020a

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

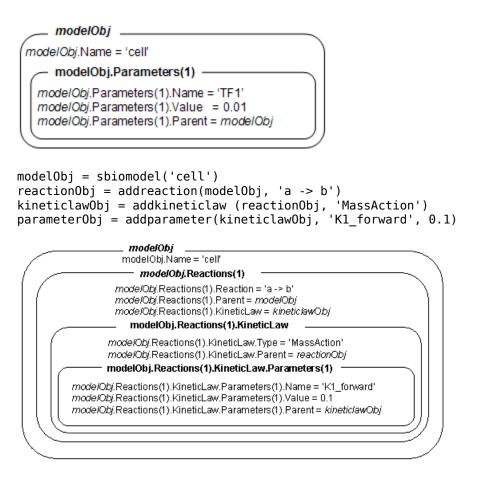
Obj	Model object or kineticlaw object. Enter a variable name for the object.
NameValue	 Property for a parameter object. Enter a unique character vector. Since objects can use this property to reference a parameter, a parameter object must have a unique name at the level it is created. For example, a 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)
```



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 (species, parameter, compartment)	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	e 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	
Туре	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
                             ValueUnits:
Index:
          Name:
                   Value:
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
                              ValueUnits:
Index:
           Name:
                    Value:
   1
             K2
                      1
```

See Also

model object, kineticlaw object, addreaction

Introduced in R2006a

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

reaction0bj	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 1-220 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 <i>NameValue</i> or <i>speciesObj</i> .

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 2-89.

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 \rightarrow U to A + C \rightarrow U + 2 H.

```
speciesObj = addproduct(reactionObj, 'H', 2);
```

See Also

addspecies

Introduced in R2006a

addreactant (reaction)

Add species object as reactant to reaction object

Syntax

```
speciesObj = addreactant(reactionObj, 'NameValue')
addreactant(reactionObj, speciesObj, StoichCoefficient)
addreactant(reactionObj, 'NameValue', StoichCoefficient)
```

Arguments

reaction0bj	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 1-220 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 <i>NameValue</i> or <i>species0bj</i> .

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 2-89.

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.

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

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...)
```

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 <i>compartmentName.speciesName</i> to qualify the species name.
	<pre>Examples are 'cytoplasm.A -> cytoplasm.B', 'cytoplasm.A -> nucleus.A', and 'cytoplasm.A + cytoplasm.B -> nucleus.AB'.</pre>
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 <i>ReactantsValue</i> .
PStoichCoefficients	Stoichiometric coefficients for products, length of array equal to length of <i>ProductsValue</i> .

Arguments

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')
```

modelObj	~
(mode/Obj.Name = 'cell'	
modelObj.Reactions(1)	
mode/Obj.Reactions(1).Reaction = 'a -> b' mode/Obj.Parameters(1).Parent = mode/Obj	

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 3-175. 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
Туре	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)
```

See Also

model object, addkineticlaw, addproduct, addreactant, rmproduct, rmreactant

Introduced in R2006a

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

model0bj	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	<pre>Character vector specifying the type of rule. Choices are: 'algebraic' 'initialAssignment' 'repeatedAssignment' 'rate' For more information, see RuleType</pre>

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 2-135, or delete a rule object from a model with the function delete on page 2-167.

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
Туре	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: ''
Parent: [1x1 SimBiology.Model]
Rule: 'c = k*(a+b)'
RuleType: 'rate'
Tag: ''
Type: 'rule'
UserData: []
```

See Also

model object, copyobj, delete, sbiomodel

Introduced in R2006a

addsamples

Add additional samples to Sobol indices

Syntax

```
results = addsamples(sobolObj,numSamples)
results = addobservable(sobolObj,numSamples,'ShowWaitbar',tf)
```

Description

results = addsamples(sobolObj,numSamples) adds the specified number of new samples to increase the accuracy of the variance decomposition (Sobol indices). The function simulates the model numSamples * (2 + number of parameters) times. To learn more, see "Saltelli Method to Compute Sobol Indices" on page 2-627 [1].

results = addobservable(sobol0bj,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.

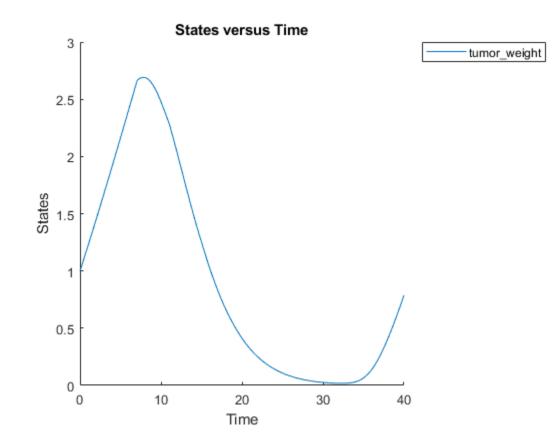
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

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';
```

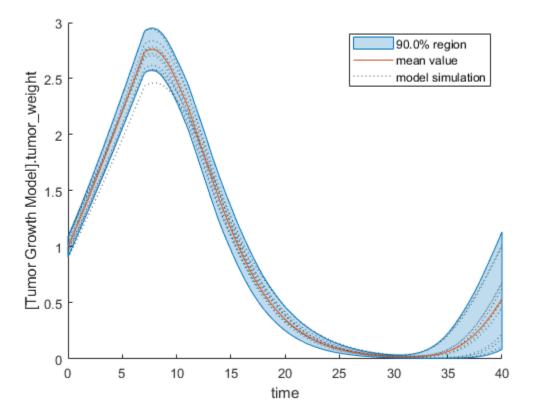
Then perform GSA by computing the first- and total-order Sobol indices using sbiosobol. Set 'ShowWaitBar' to true to show the simulation progress. By default, the function uses 1000 parameter samples to compute the Sobol indices [1].

sobolResults = sbiosobol(m1,modelParamNames,outputName,'Variants',v,'Doses',d,'ShowWaitBar',true

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.

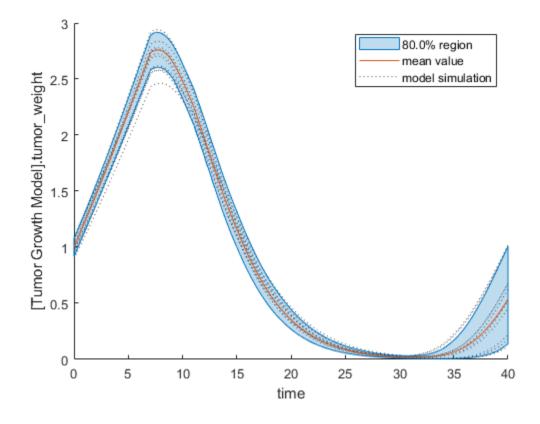
Show the mean model response, the simulation results, and a shaded region covering 90% of the simulation results.

plotData(sobolResults);



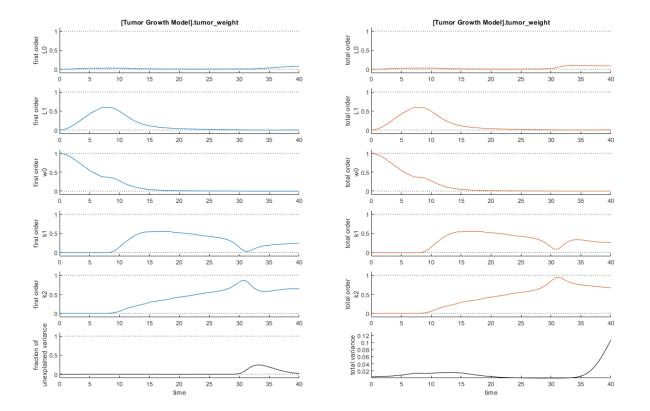
You can adjust the quantile region to a different percentage by specifying 'Alphas' for the lower and upper quantiles of all model responses. For instance, an alpha value of 0.1 plots a shaded region between the $100 \times 100 \times (1 - alpha)$ quantiles of all simulated model responses.

plotData(sobolResults, 'Alphas',0.1);



Plot the time course of the first- and total-order Sobol indices.

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

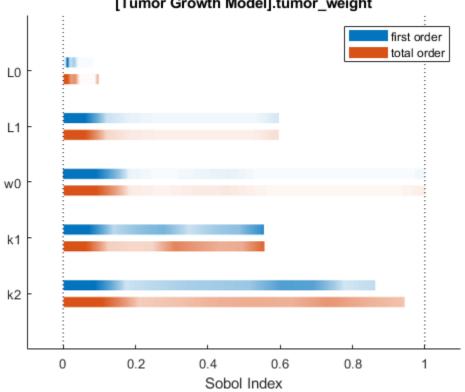


The first-order Sobol index of an input parameter gives the fraction of the overall response variance that can be attributed to variations in the input parameter alone. The total-order index gives the fraction of the overall response variance that can be attributed to any joint parameter variations that 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.

bar(sobolResults)



[Tumor Growth Model].tumor_weight

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: ModelName: DataCount: Name: 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

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.

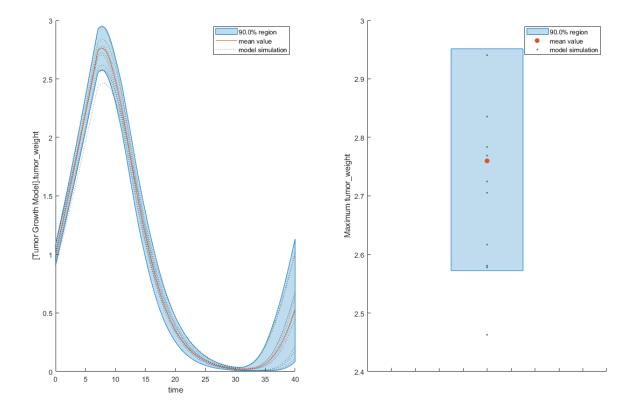
```
[samplesUsed,sd,validruns] = getSimulationResults(sobolResults,4);
```

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);
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

sobol0bj — Results containing Sobol indices

SimBiology.gsa.Sobol object

Results containing the first- and total-order Sobol indices, specified as a SimBiology.gsa.Sobol 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 for observables

SimBiology.gsa.Sobol object

Computed Sobol indices for added observables, returned as a SimBiology.gsa.Sobol object.

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

Introduced in R2020a

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

comp0bj	Compartment object.
model0bj	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 1-220 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 2-91.
PropertyValue	Enter the value for the property specified in <i>PropertyName</i> . 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 2-71 and addproduct on page 2-69.

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 H20. However, another compartment can have a species named H20.

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 (species, parameter, compartment)	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
Initial Amount Units	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
Туре	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, ...
```

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: 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
InitialAmountUnits: ''
Name: 'glucose_6_phosphate'
Notes: ''
Parent: [1x1 SimBiology.Compartment]
Tag: ''
Type: 'species'
UserData: []
```

See Also

Model object, Compartment object, addcompartment, addproduct, addreactant, addreaction, get, set

Introduced in R2006a

addvariant (model)

Add variant to model

Syntax

```
variantObj = addvariant(modelObj, 'NameValue')
variantObj2 = addvariant(modelObj, variantObj)
```

Arguments

model0bj	Specify the Model object to which you want add a variant.
variant0bj	Variant object to create and add to the model object.
	Name of the variant object. <i>NameValue</i> 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, 'compl');
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

Model object, Variant object, addcontent, commit, copyobj, delete, getvariant

Introduced in R2007b

bar

Create bar plot of multiparametric global sensitivity analysis statistics

Syntax

```
h = bar(mpgsa0bj)
h = bar(mpgsa0bj,Name,Value)
```

Description

h = bar(mpgsa0bj) 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".

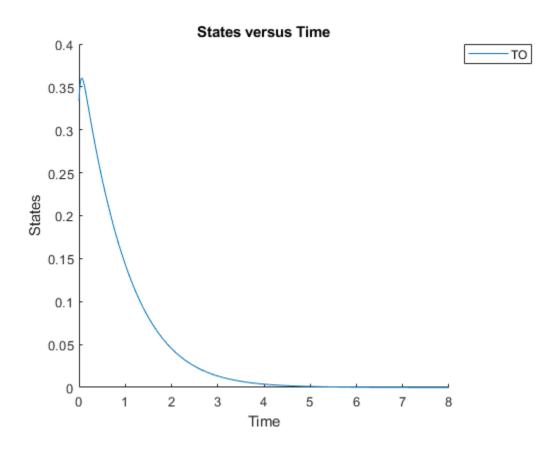
sbioloadproject tmdd_with_T0.sbproj

Get the active configset and set the target occupancy (T0) as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = '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,T0) <= 0.1';</pre>
```

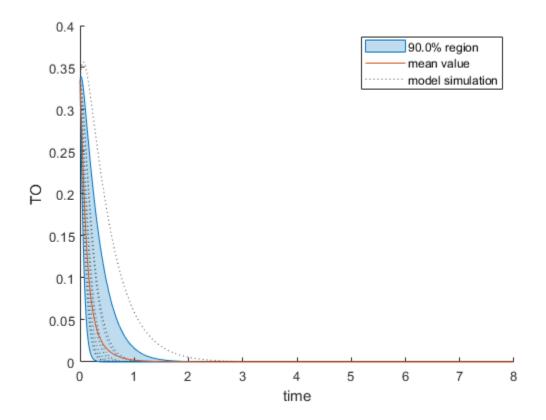
Perform MPGSA to find sensitive parameters with respect to the TO. Vary the parameter values between predefined bounds to generate 10,000 parameter samples.

```
% 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,T0) <= 0.1'}</pre>
    KolmogorovSmirnovStatistics: [4x1 table]
                        ECDFData: {4x4 cell}
              SignificanceLevel: 0.0500
                         PValues: [4x1 table]
              SupportHypothesis: [10000x1 table]
                     Observables: {'TO'}
                ParameterSamples: [10000x4 table]
```

SimulationInfo: [1x1 struct]

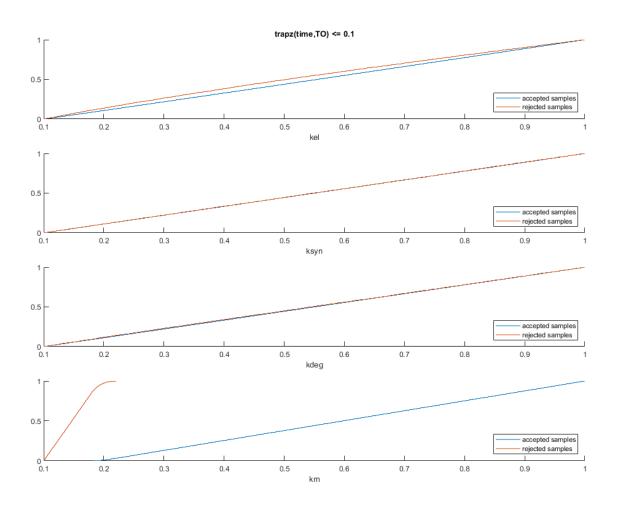
Plot the quantiles of the simulated model response.

plotData(mpgsaResults);



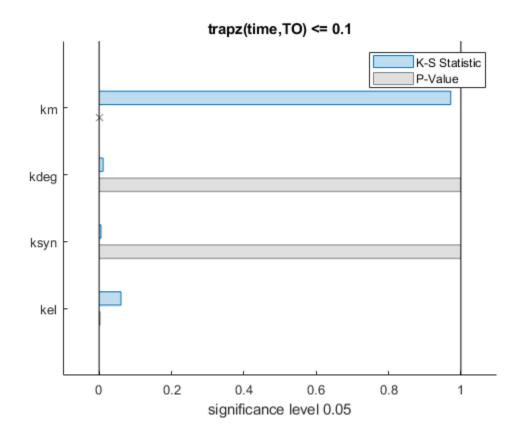
Plot the empirical cumulative distribution functions (eCDFs) of the accepted and rejected samples. Except for km, none of the parameters shows a significant difference in the eCDFs for the accepted and rejected samples. The km plot shows a large Kolmogorov-Smirnov (K-S) distance between the eCDFs of 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)



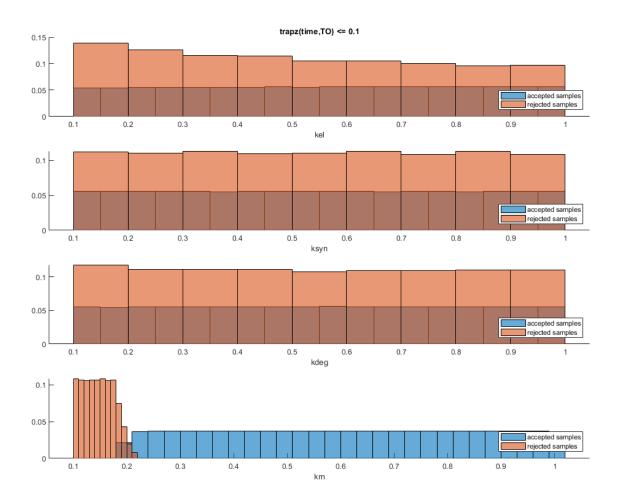
The bar plot shows two bars for each parameter: one for the K-S distance (K-S statistic) and another for the corresponding p-value. You reject the null hypothesis if the p-value is less than the significance level. A cross (x) is shown for any p-value that is almost 0. You can see the exact p-value corresponding to each parameter.

[mpgsaResults.ParameterSamples.Properties.VariableNames',mpgsaResults.PValues]

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 histograms 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

mpgsa0bj — 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 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: 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 the comma-separated pair consisting of 'Parameters' and a character vector, string, string vector, cell array of character vectors, or a vector of positive integers indexing into the columns of the mpgsa0bj.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 the comma-separated pair consisting of 'Classifiers' and 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

Color of Kolmogorov-Smirnov statistic (K-S Statistic), specified as the comma-separated pair consisting of 'Color' and a three-element row vector. 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.

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

Color of *p*-values, specified as the comma-separated pair consisting of '**PValueColor**' and a threeelement row vector. The default color is gray [0.5,0.5,0.5].

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.

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 | bar | ecdf | histogram | kstest2 | plotData | sbiompgsa

Introduced in R2020a

bar

Create bar plot of first- and total-order Sobol indices

Syntax

```
h = bar(sobol0bj)
h = bar(sobol0bj,Name,Value)
```

Description

h = bar(sobol0bj) plots the first- and total-order Sobol indices as a bar plot and returns the figure handle h.

h = bar(sobol0bj,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.

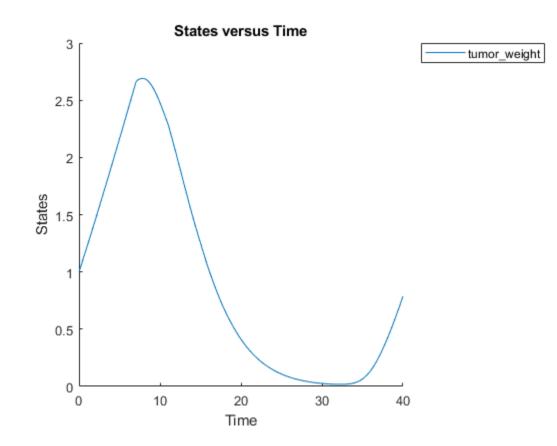
v = getvariant(m1); d = getdose(m1,'interval_dose');

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].

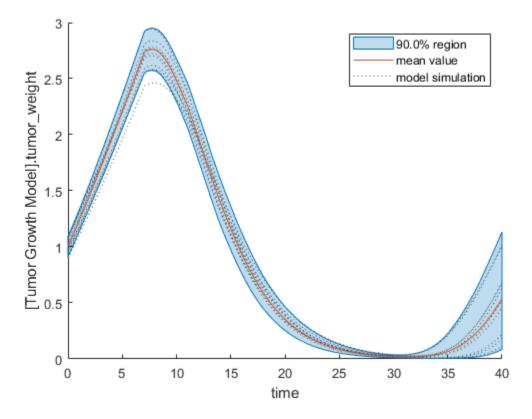
sobolResults = sbiosobol(m1,modelParamNames,outputName,'Variants',v,'Doses',d,'ShowWaitBar',true

```
sobolResults =
   Sobol with properties:
        Time: [444x1 double]
        SobolIndices: [5x1 struct]
        Variance: [444x1 table]
        Observables: {'[Tumor Growth Model].tumor_weight'}
   ParameterSamples: [1000x5 table]
        SimulationInfo: [1x1 struct]
```

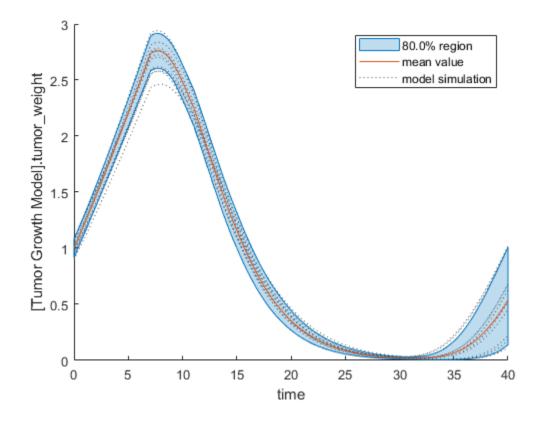
You can change the number of samples by specifying the 'NumberSamples' name-value pair argument. The function requires a total of (number of input parameters + 2) * NumberSamples model simulations.

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

plotData(sobolResults);

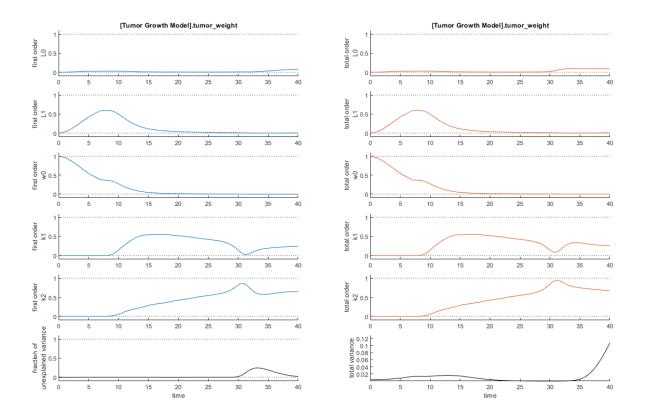


plotData(sobolResults, 'Alphas',0.1);



Plot the time course of the first- and total-order Sobol indices.

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

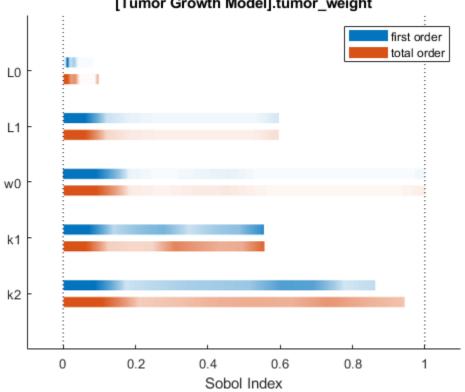


The first-order Sobol index of an input parameter gives the fraction of the overall response variance that can be attributed to variations in the input parameter alone. The total-order index gives the fraction of the overall response variance that can be attributed to any joint parameter variations that 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.

bar(sobolResults)



[Tumor Growth Model].tumor_weight

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: ModelName: DataCount: Name: 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.

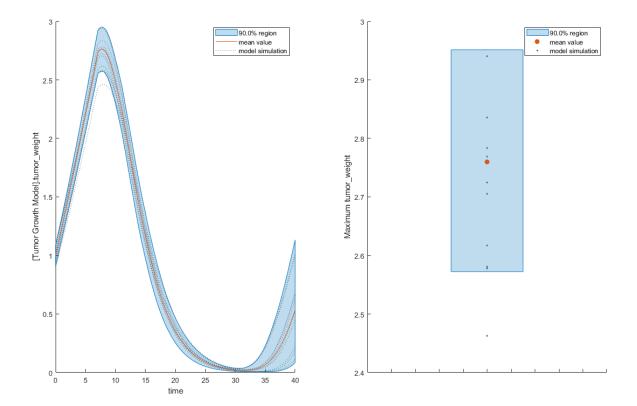
```
[samplesUsed,sd,validruns] = getSimulationResults(sobolResults,4);
```

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);
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 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: 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 the comma-separated pair consisting of 'Parameters' and a character vector, string, string vector, cell array of character vectors, or vector of positive integers indexing into the columns of the sobolObj.ParameterSamples table. Use this name-value pair argument to select parameters and plot their corresponding Sobol indices.

Example: 'Parameters', 'k1'

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 the comma-separated pair consisting of 'Observables and a character vector, string, string vector, cell array of character vectors, or vector of positive integers indexing into resultsObj.Observables.

Example: 'Observables', 'tumor_weight'

Data Types: double | char | string | cell

FirstOrderColor — Color first-order Sobol indices

three-element row vector

Color of the first-order Sobol indices, specified as the comma-separated pair consisting of 'FirstOrderColor' and a three-element row vector. 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.

Example: 'FirstOrderColor',[0.4,0.3,0.2]

Data Types: double

TotalOrderColor — Color of total-order Sobol indices

three-element row vector

Color of the total-order Sobol indices, specified as the comma-separated pair consisting of 'TotalOrderColor' and a three-element row vector. 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.

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.

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 | plot | plotData | sbiosobol

Introduced in R2020a

boxplot(LeastSquaresResults,OptimResults,NLINR esults)

Create box plot showing the variation of estimated SimBiology model parameters

Syntax

boxplot(results0bj)

Description

boxplot(results0bj) creates a box plot showing the variation of the estimated SimBiology model
parameters.

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.

See Also

NLINResults object | OptimResults object | sbiofit

Introduced in R2014a

boxplot(NLMEResults)

Create box plot showing the variation of estimated SimBiology model parameters

Syntax

boxplot(results0bj)

Description

boxplot(results0bj) 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.

See Also

NLMEResults object | sbiofitmixed

Introduced in R2014a

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.

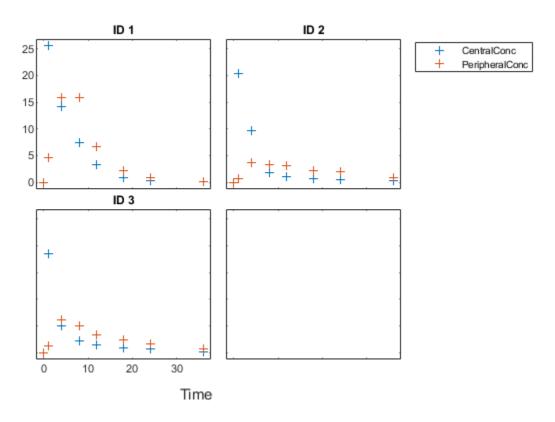
Examples

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.

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 2-448.

ci2table(ciParamUnpooled)

ans =

12x7 table

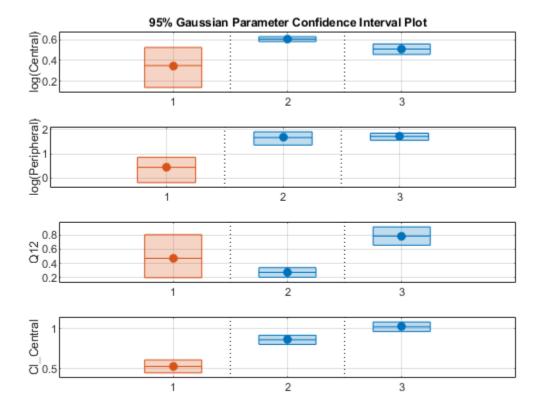
Group	Name	Estimate	Confidenc	eInterval	Туре	Alpha	Status
1	{'Central' }	1.422	1.1533	1.6906	Gaussian	0.05	estimable
1	{'Peripheral'}	1.5629	0.83143	2.3551	Gaussian	0.05	constrained
1	{'Q12' }	0.47159	0.20093	0.80247	Gaussian	0.05	constrained
1	{'Cl Central'}	0.52898	0.44842	0.60955	Gaussian	0.05	estimable
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
```

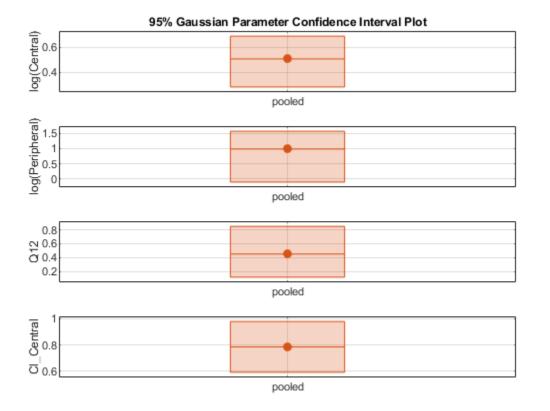
ConfidenceInterval

Туре Alpha

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

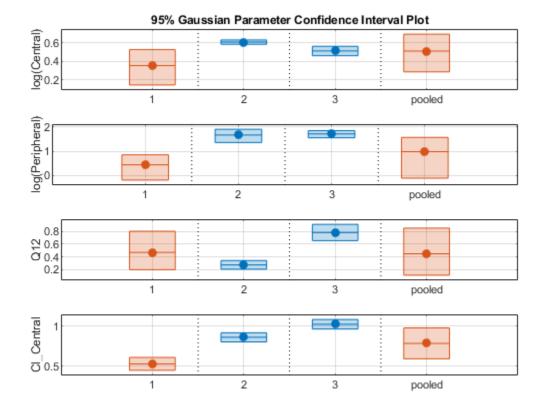
Plot the confidence intervals. The group name is labeled as "pooled" to indicate such fit.

plot(ciParamPooled)



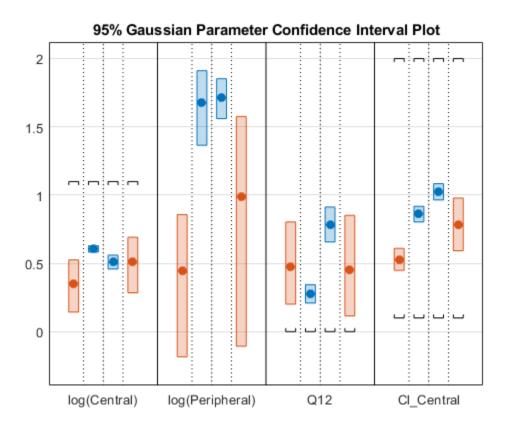
Plot all the confidence interval results together. By default, the confidence interval for each parameter estimate is plotted on a separate axes. Vertical lines group confidence intervals of parameter estimates that were computed in a common fit.

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

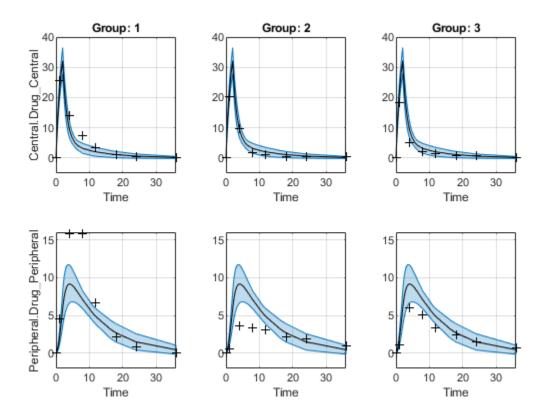
Calculate 95% confidence intervals for the model predictions, that is, simulation results using the estimated parameters.

```
% For the pooled fit
ciPredPooled = sbiopredictionci(pooledFit);
% For the unpooled fit
ciPredUnpooled = sbiopredictionci(unpooledFit);
```

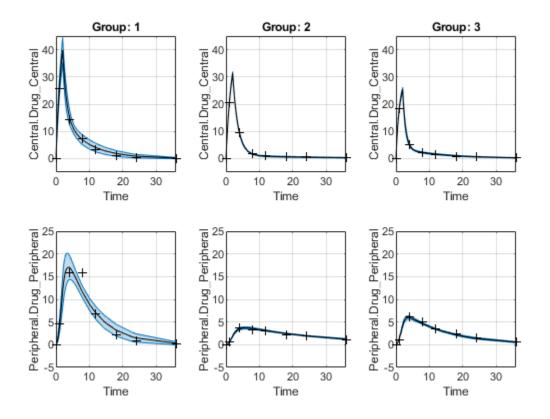
Plot Confidence Intervals for Model Predictions

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
Туре	Confidence interval type

Column Name	Description
Alpha	Confidence level
	Confidence interval estimation status (for details, see "Parameter Confidence Interval Estimation Status" on page 2-448)

See Also

ParameterConfidenceInterval|sbioparameterci

Introduced in R2017b

commit (variant)

Commit variant contents to model

Syntax

commit(variantObj, modelObj)

Arguments

model0bj	Specify the model object to which you want to commit a variant.
variant0bj	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 (*variant0bj*).

```
commit (variantObj, modelObj);
```

See Also

addvariant, Variant object

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 2-126 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 (species, parameter,	
compartment)	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 $% \left({{{\left({{{{\bf{n}}}} \right)}_{i}}_{i}}} \right)$
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
Туре	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

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 [].

See Also

ParameterConfidenceInterval | PredictionConfidenceInterval | sbioparameterci | sbiopredictionci

Introduced in R2017b

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 2-131 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
SolverOptions	Specify model solver options
SolverType	Select solver type for simulation
StopTime	Simulation time criteria to stop simulation
TimeUnits	Show time units for dosing and simulation
Туре	Display SimBiology object type

See Also

AbstractKineticLaw object,KineticLaw object,Model object,Parameter object, Reaction object,Root object,Rule object,Species object

Introduced in R2006b

construct (PKModelDesign)

Construct SimBiology model from PKModelDesign object

Syntax

```
[model0bj, pkModelMap0bject] = construct(pkModelDesign0bject)
[model0bj, pkModelMap0bject, CovModel0bj] = construct(pkModelDesign0bject)
```

Arguments

modelObj	SimBiology model object specifying a pharmacokinetic model.
	Defines the roles of the components in <i>modelObj</i> . For details, see PKModelMap object.
	Defines the relationship between parameters and covariates. For details, see CovariateModel object.

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(thetal + etal) (without covariate dependencies), where thetal is a fixed effect, and etal is a random effect. You can modify the expressions to add covariate dependencies. For details, see CovariateModel on page 2-137 object.

See Also

CovariateModel object | PKModelDesign object | PKModelMap object

Topics

"Create a Pharmacokinetic Model Using the Command Line" "Modeling the Population Pharmacokinetics of Phenobarbital in Neonates" "Specify a Covariate Model" Introduced in R2009a

constructDefaultFixedEffectValues (covmodel)

Create initial estimate vector needed for fit

Syntax

FEInitEstimates = constructDefaultFixedEffectValues(CovModelObj)

Description

FEInitEstimates = constructDefaultFixedEffectValues(CovModelObj) creates
FEInitEstimates, a structure containing the initial estimates for the fixed effects in CovModelObj,
a CovariateModel object. These initial estimates are set to a default of zero, but you can edit these
estimates. 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 3-69 property of
CovModelObj.

Tip After creating the *FEInitEstimates* structure, you can edit it and use it to change the FixedEffectValues property of *CovModelObj*, before using the object as an input argument to sbionlmefit or sbionlmefitsa.

See Also

CovariateModel on page 2-137 | Expression on page 3-69 | FixedEffectValues on page 3-76 | sbionlmefit | sbionlmefitsa

Topics

"Modeling the Population Pharmacokinetics of Phenobarbital in Neonates" "Specify a Covariate Model"

Introduced in R2011b

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.		
parent0bj	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	
model0bj	Model object to be copied.		
copied0bj	Output returned by the copyobj method with the parent set as specified in input argument (<i>parent0bj</i>).		

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

Introduced in R2006a

CovariateModel object

Define relationship between parameters and covariates

Description

CovariateModel defines the relationship between estimated parameters and covariates.

Tip 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** on page 3-76 property to specify the initial estimates for the fixed effects.

Construction

CovModelObj = CovariateModel creates an empty CovariateModel object.

CovModelObj = CovariateModel(*Expression*) creates a CovariateModel object with its Expression property set to *Expression*, a character vector, string, string vector, or cell array of character vectors, where each character vector or string represents the relationship between a parameter being estimated and one or more covariates. *Expression* must denote fixed effects with the prefix theta, and random effects with the prefix eta. Each character vector or string in *Expression* must be in the form:

parameterName = relationship

This example of an expression defines the relationship between a parameter (volume) and a covariate (weight), with fixed effects, but no random effects: Expression = {'volume = theta1 + theta2*weight'};

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.

Parameter-Covariate Relationship	Expression Format
Linear with random effect	Cl = theta1 + theta2*WEIGHT + eta1
Exponential without random effect	<pre>Cl = exp(theta_Cl + theta_Cl_WT*WEIGHT)</pre>
Exponential, WEIGHT centered by mean, has random effect	<pre>Cl = exp(thetal + theta2*(WEIGHT - mean(WEIGHT)) + etal)</pre>
Exponential, log(WEIGHT), which is equivalent to power model	<pre>Cl = exp(thetal + theta2*log(WEIGHT) + etal)</pre>
Exponential, dependent on WEIGHT and AGE, has random effect	Cl = exp(thetal + theta2*WEIGHT + theta3*AGE + etal)

This table illustrates expression formats for some common parameter-covariate relationships.

Parameter-Covariate Relationship	Expression Format
Inverse of probit, dependent on WEIGHT and AGE, has random effect	<pre>Cl = probitinv(thetal + theta2*WEIGHT + theta3*AGE + etal)</pre>
Inverse of logit, dependent on WEIGHT and AGE, has random effect	<pre>Cl = logitinv(thetal + theta2*WEIGHT + theta3*AGE + etal)</pre>

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.

Method Summary

constructDefaultFixedEffectValues (covmodel)	
	Create initial estimate vector needed for fit
verify (covmodel)	Check covariate model for errors

Property Summary

CovariateLabels (CovariateModel)	Labels for covariates in CovariateModel object
Expression (CovariateModel)	Define relationship between parameters and covariates
FixedEffectDescription (CovariateModel)	Descriptions of fixed effects in CovariateModel object
FixedEffectNames (CovariateModel)	Names of fixed effects in CovariateModel object
FixedEffectValues (CovariateModel)	Values for initial estimates of fixed effects in CovariateModel object
ParameterNames (CovariateModel)	Names of parameters in CovariateModel object
RandomEffectNames (CovariateModel)	Names of random effects in CovariateModel object

Examples

Create a CovariateModel object and set the Expression property to define the relationship between two parameters (clearance and volume) and two covariates (weight and age) using fixed effects (thetas) and random effects (etas):

covModelObj = CovariateModel covModelObj.Expression = {'CL = theta1 + theta2*WT + eta1', 'V = theta3 + theta4*AGE + eta2'};

See Also

PKData object | PKModelDesign object | construct | getCovariateData on page 2-228 |
sbionlmefit | sbionlmefitsa

Topics

"Modeling the Population Pharmacokinetics of Phenobarbital in Neonates" "Specify a Covariate Model"

Introduced in R2011b

covariateModel(NLMEResults)

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 mixedeffects estimation using sbiofitmixed. The model describes the relationship between SimBiology model parameters, fixed effects, random effects, and covariates.

See Also

NLMEResults object | sbiofitmixed

Introduced in R2014a

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.

See Also

RepeatDose object|ScheduleDose object|groupedData|table

Introduced in R2014a

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 2-595.

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 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: '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 timedependent 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:

Nan	ie	Value	Туре	Units
{'Reacti	Lonl.c'}	0.5	{'parameter'}	{'1/second'}
Observables:				
Name	Туре		Units	
{ ' X ' }	{'species	;'} {	'molecule'}	

Dosed: None

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	Туре	
{'Reaction1.c'}	0.5	{'parameter'}	

Observables:

Name	Туре
{'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:

Nam	е	Value	Туре	Units
'Reacti	onl.c'	0.5	'parameter'	'1/second'
Observables	:			
Name	Туре		Units	

'molecule'

'molecule'

Dosed:

' X '

'z'

'species'

'species'

TargetName	TargetDimension			
' X '	'Amount(e.g. mole or molecule)'			
DurationParame	eterName	DurationParameterValue		
'dp'		1		
DurationParame	eterUnits	LagParameterName		
'second'		'lp'		
LagParameterVa	alue Lag	ParameterUnits		

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	Туре	
<pre>{'Reaction1.c1'} {'Reaction2.c2'}</pre>	10 0.01	{'parameter'} {'parameter'}	

Observables:

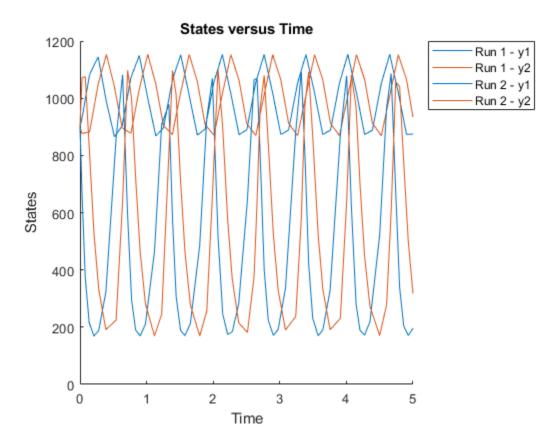
Dosed: None

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];

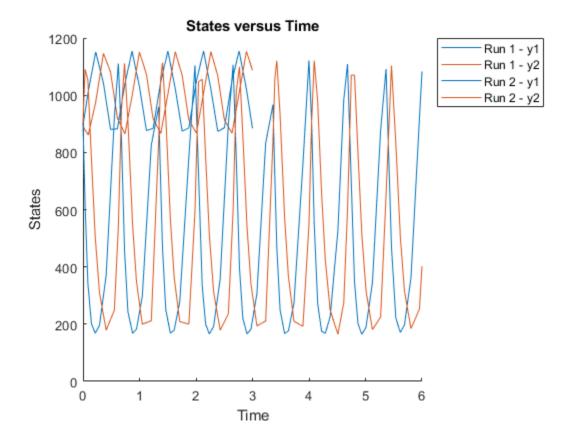
Run simulations until the stop time is 5 and plot the simulation results.

sbioplot(f(phi, 5));



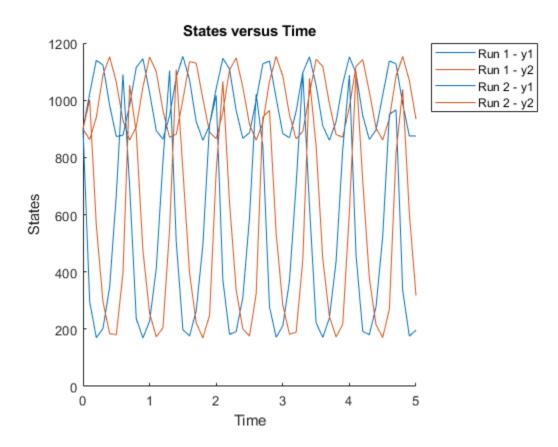
You can also specify a vector of different stop times for each simulation.

t_stop = [3;6]; sbioplot(f(phi, t_stop));



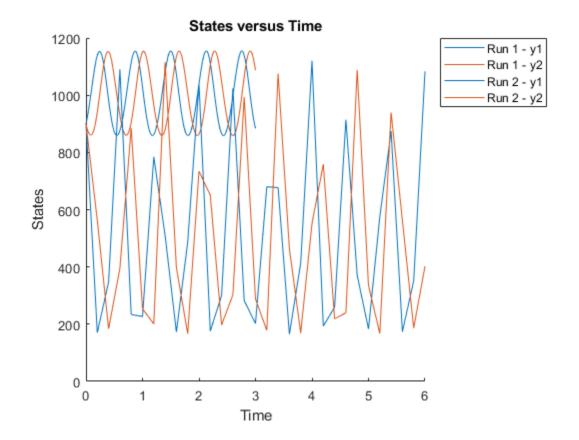
Next, specify the output times as a vector.

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 Sensitivities Using SimFunctionSensitivity Object

This example shows how to calculate the 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	Туре	
{'Reaction1.c1'}	10	{'parameter'}	
{'Reaction2.c2'}	0.01	{'parameter'}	

Observables:

Name	Туре		
{'y1'}	{'species'}		
{'y2'}	{'species'}		

Dosed: None

Sensitivity Input Factors:

Name	Туре	
{'Reaction1.c1'} {'Reaction2.c2'}	{'parameter'} {'parameter'}	
Sensitivity Output Fact	ors:	

Name Type

{'y1'}	{'species'}
{'y2'}	{'species'}
l y∠ j	[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.

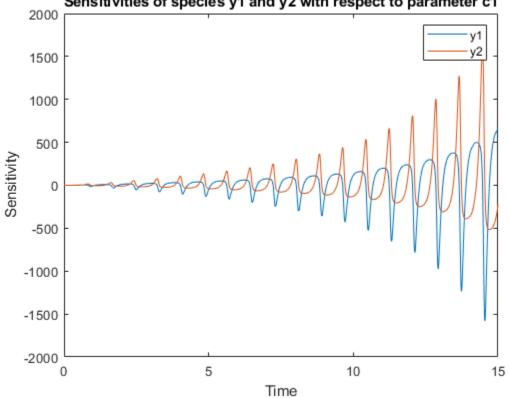
sd = f([10, 0.1], 15);

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');
```

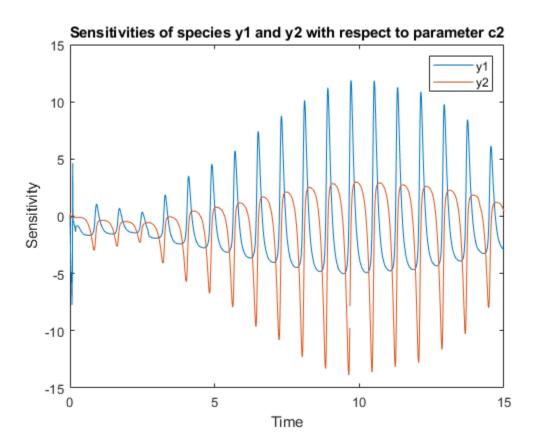


Sensitivities of species y1 and y2 with respect to parameter c1

Plot the sensitivities of species y1 and y2 with respect to c2.

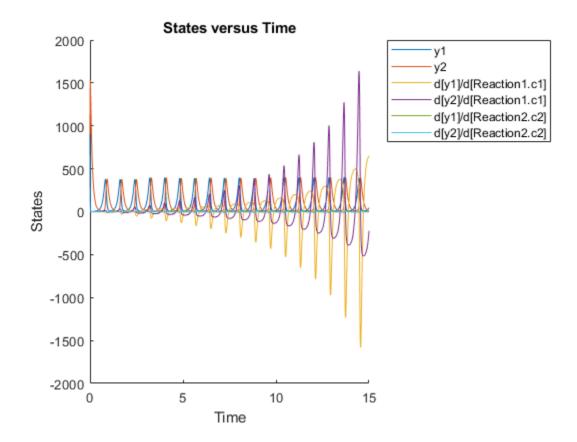
figure; plot(t,y(:,:,2));

```
legend(outputs);
title('Sensitivities of species y1 and y2 with respect to parameter c2');
xlabel('Time');
ylabel('Sensitivity');
```



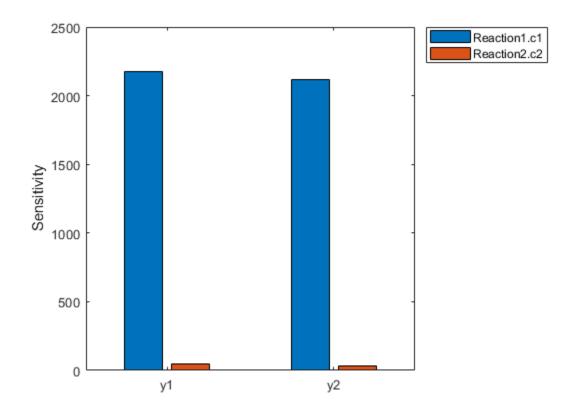
Alternatively, you can use sbioplot.

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 "Simulating 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 Vari	lant - Type 2 d	iabetic (inactive)		
ContentIndex:	Type:	Name:	Property:	Value:
1	parameter	Plasma Volume	Value	1.49
2	parameter	k1	Value	0.042
3	parameter	k2	Value	0.071

4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 27	parameter parameter	<pre>m1 m2 m4 m5 m6 Hepatic Extrac kmax kmin kabs kgri f a b c d Stomach Glu Af kp1 kp2 kp3 kp4 ki [Ins Ind Glu U Vm0 Vmx Km p2U K alpha beta gamma ke1 ke2</pre>	Value Value	0.04 0.379 0.673 0.269 0.0526 0.8118 0.6 0.0465 0.0076 0.023 0.0465 0.9 6e-05 0.68 0.00023 0.09 125 3.09 0.0007 0.005 0.0786 0.0007 0.005 0.0786 0.004 1 4.65 0.034 466.21 0.084 0.99 0.013 0.05 0.5 0.0007 269
36 37 38	parameter parameter parameter		Value	269 164.18 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.

Parameters:

Observables:

Name	Туре	Units	
{'[Plasma Glu Conc]'} {'[Plasma Ins Conc]'}		{'milligram/deciliter'} {'picomole/liter' }	
sed ·			

Dosed:

TargetName	Targ	TargetDimension		
{'Dose'}	{'Macc		gram)'}	
{ Dose }	1 Mdss	(e.g.,	graii) }	

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)'}
```

Select a dose that represents a single meal of 78 grams of glucose at the start of the simulation.

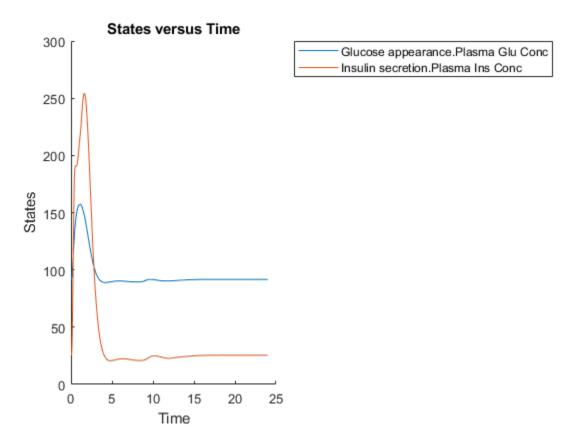
```
singleMeal = sbioselect(m1,'Name','Single Meal');
```

Convert the dosing information to the table format.

mealTable = getTable(singleMeal);

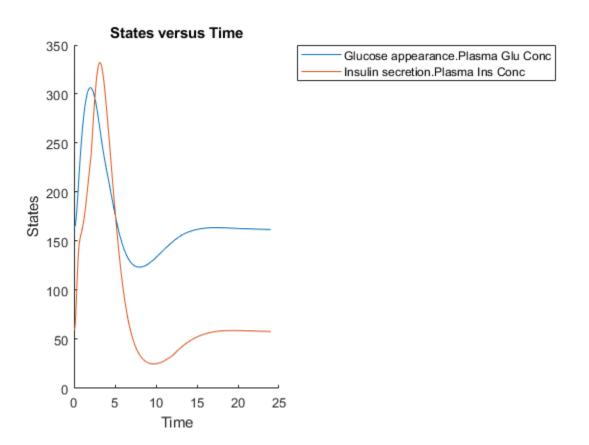
Simulate the glucose-insulin response for a normal subject for 24 hours.

```
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 Varia	ant - Low insu	lin sensitiv	ity (inactive)	
ContentIndex:	Type:	Name:	Property:	Value:
1	parameter	Vmx	Value	0.0235
2	parameter	kp3	Value	0.0045

varToScan(2)

```
ans =
   SimBiology Variant - High insulin sensitivity (inactive)
```

ContentIndex:	Type:	Name:	Property:	Value:
1	parameter	Vm×	Value	0.094
2	parameter	kp3	Value	0.018

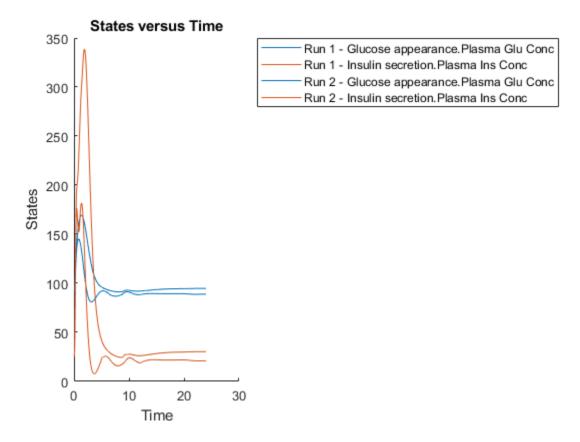
Both variants store alternate values for Vmx and kp3 parameters. You need to specify them as input parameters when you create a SimFunction object.

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);

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 | SimFunction object | SimFunctionSensitivity object | model
object | sbiosampleerror | sbiosampleparameters

Topics

"Model Simulation"

Introduced in R2014a

delete

Delete SimBiology object

Syntax

delete(sobj)

Description

delete(sobj) removes the SimBiology object sobj from its parent on page 3-129 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
                       3.32e-18
             kRL
   3
            kRdo
                       0.0004
            kRs
   4
                       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.

See Also

SimData|set

Introduced in R2006a

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.

See Also SimData|set

Introduced in R2006a

EstimatedInfo object

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.

Construction

estimInfo = estimatedInfo creates an empty estimatedInfo object.

estimInfoArray = estimatedInfo(transformedNames) creates an array 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(____, 'InitialTransformedValue',itValues) defines
the initial transformed values of model quantities specified by itValues. You cannot specify this
name-value pair along with the 'InitialValue' name-value pair.

estimInfoArray = estimatedInfo(_____, 'InitialValue', iValues) defines the initial values
of model quantities specified by iValues. You cannot specify this name-value pair along with the
'InitialTransformedValue' name-value pair.

estimInfoArray = estimatedInfo(_____, 'Bounds', boundValues) defines the lower and upper bounds for parameter estimation specified by boundValues. You cannot specify this namevalue pair along with the 'TransformedBounds' name-value pair. All methods support parameter bounds in sbiofit (that is, fminsearch, nlinfit, fminunc, fmincon, lsqcurvefit, lsqnonlin, patternsearch, ga, particleswarm, and scattersearch on page 1-80). 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 illconditioned or not being able to estimate if the final result is too close to the bounds. sbiofitmixed does not support parameter bounds.

estimInfoArray = estimatedInfo(____, 'TransformedBounds',tBoundValues) defines the transformed bounds for parameter estimation specified by tBoundValues. You cannot specify this name-value pair along with the 'Bounds' name-value pair.

estimInfoArray = estimatedInfo(____, 'CategoryVariableName',groups) defines which
groups in the data have separate estimated values for parameters. In other words, this allows you to
estimate parameter values specific for each group or category. For example, you can estimate
parameters based on individuals' age or sex.

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. 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".

itValues — 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 [].

iValues — 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 [].

boundValues — Bound constraints for estimated parameters

[] (default) | matrix | cell array

Bound constraints for estimated parameters, specified as a matrix or cell array. If **boundValues** is a matrix, it 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 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.

You cannot specify this name-value pair along with the 'TransformedBounds' name-value pair.

tBoundValues — Transformed bound constraints for estimated parameters

[] (default) | matrix | cell array

Transformed bound constraints for estimated parameters, 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 pair along with the 'Bounds' name-value pair.

groups — 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.

Property Summary

Name	Character vector indicating the name of an estimated model
	quantity. Changing this property also updates the
	TransformedName property.

Transform	Character vector indicating whether the quantity value is transformed during estimation. Valid names are '', 'log', 'logit', and '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	Read-only character vector that combines the transform name (such as 'log') and the quantity name (such as 'Central') into an expression (such as 'log(Central)').
InitialValue	Empty matrix [] or real, finite, scalar value specifying the initial values of model quantities used for estimation. 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	Empty matrix [] or scalar value specifying the initial transformed values of model quantities used for estimation. 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	Empty matrix [] or 1-by-2 vector of real, finite value specifying the lower and upper bound for an estimated parameter. 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	Empty matrix [] or 1-by-2 vector of real, finite value specifying the lower and upper bound for an estimated parameter. 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	Character vector or cell array of character vectors specifying which groups in the data have separate estimated values for the parameter. 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 pair argument (to either true or false) when you run sbiofit, then the function ignores this variable. sbiofitmixed always ignores this property.</none></groupvariablename></none></groupvariablename>

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])
```

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 $k_e = Cl/V$.

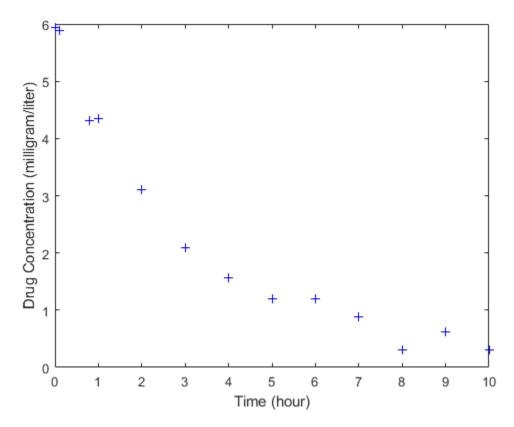
The synthetic data in this example was generated using the following model, parameters, and dose:

- 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.

```
clear all
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	<pre>= sbiodose('dose');</pre>
dose.TargetName	<pre>= 'Drug_Central';</pre>
dose.StartTime	= 0;
dose.Amount	= 10;
dose.AmountUnits	<pre>= 'milligram';</pre>
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);

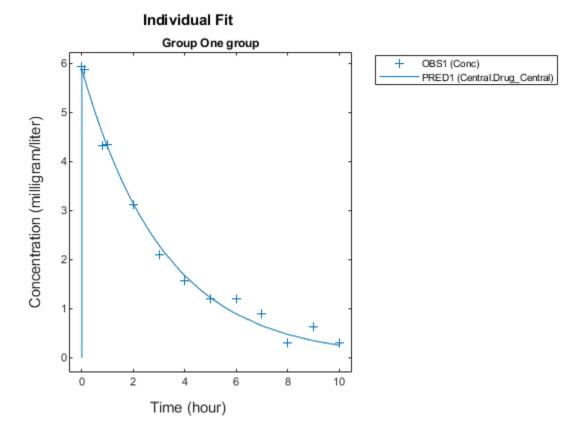
Display Estimated Parameters and Plot Results

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	Boun	ds
{'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).

```
'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.

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 combined error model	1.1984 3.9163	1.6032 -3.8326	2.7331 -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.

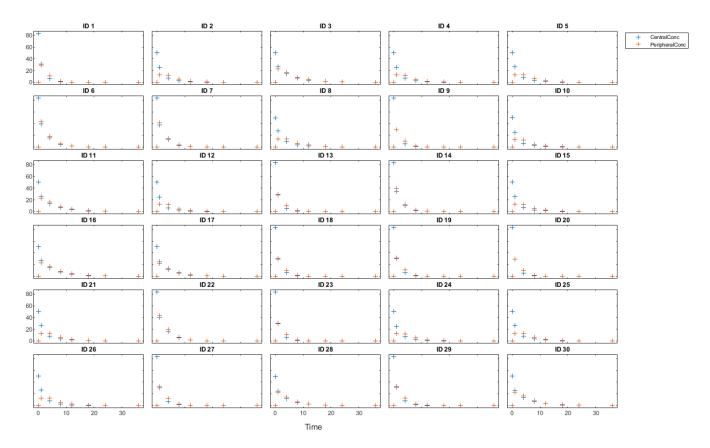
```
gData = groupedData(data);
gData.Properties.VariableUnits = {'','hour','milligram/liter','milligram/liter',''};
gData.Properties
```

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	<pre>= PKModelDesign;</pre>
pkc1	<pre>= addCompartment(pkmd, 'Central');</pre>
pkc1.DosingType	= 'Bolus';
pkc1.EliminationType	<pre>= 'linear-clearance';</pre>
pkc1.HasResponseVariable	= true;
pkc2	<pre>= addCompartment(pkmd, 'Peripheral');</pre>
model	<pre>= construct(pkmd);</pre>
configset	<pre>= getconfigset(model);</pre>
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

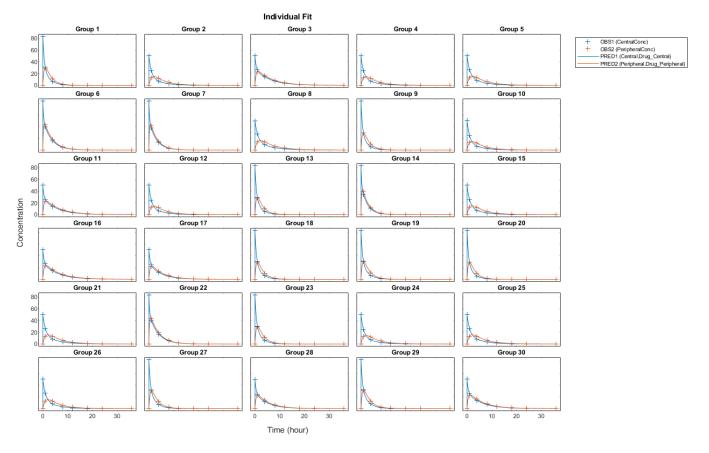
Estimate one set of parameters for each individual by setting the '**Pooled**' name-value pair argument to false.

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

Display Results

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

```
t = plot(unpooledFit);
% Resize the figure.
t.hFig.Position(:) = [100 100 1280 800];
```



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.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 ToolboxTM. If you do not have it, use other alternative plotting functions such as plot.

```
h = figure;
ylabels = {'Central', 'Peripheral', 'Cl\_Central', 'Q12'};
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);
   ах
                = gca;
    ax.XTick
                = [1];
   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);
   ах
                = 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 higher 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.

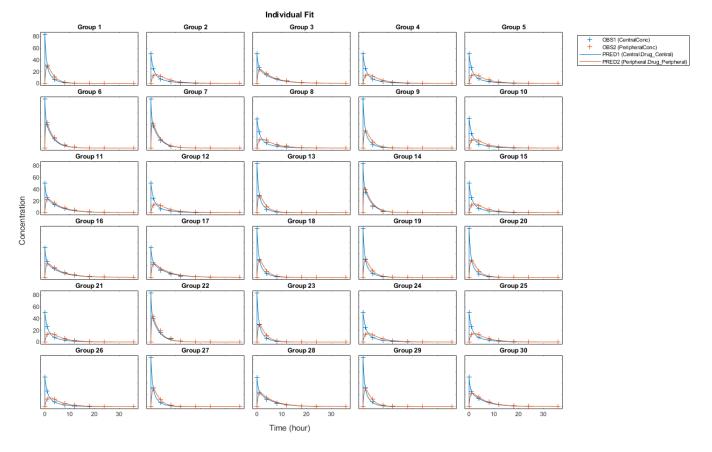
```
estimatedParam(1).CategoryVariableName = 'Age';
estimatedParam(2).CategoryVariableName = 'Age';
estimatedParam(3).CategoryVariableName = 'Sex';
estimatedParam(4).CategoryVariableName = 'Sex';
categoryFit = sbiofit(model,gData,responseMap,estimatedParam,dose)
categoryFit =
  OptimResults with properties:
                   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}
                                         'Peripheral' 'Q12' 'Cl Central'}
    EstimatedParameterNames: {'Central'
             ErrorModelInfo: [1x3 table]
         EstimationFunction: 'lsgnonlin'
```

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.

```
t = plot(categoryFit);
% Resize the figure.
t.hFig.Position(:) = [100 100 1280 800];
```



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).

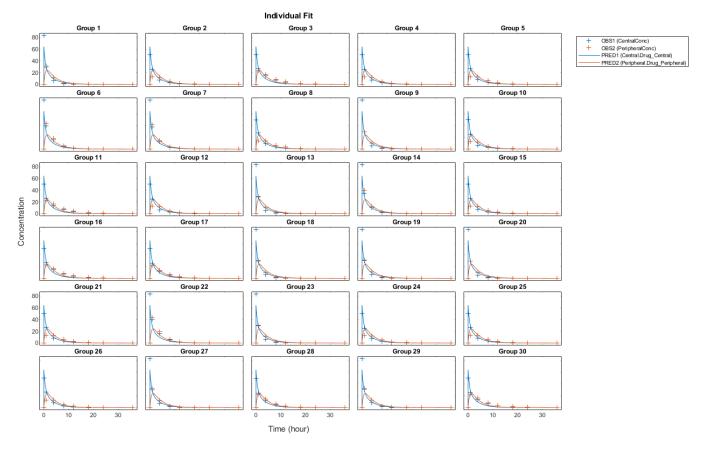
```
pooledFit = sbiofit(model,gData,responseMap,estimatedParam,dose,'Pooled',true);
```

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

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).

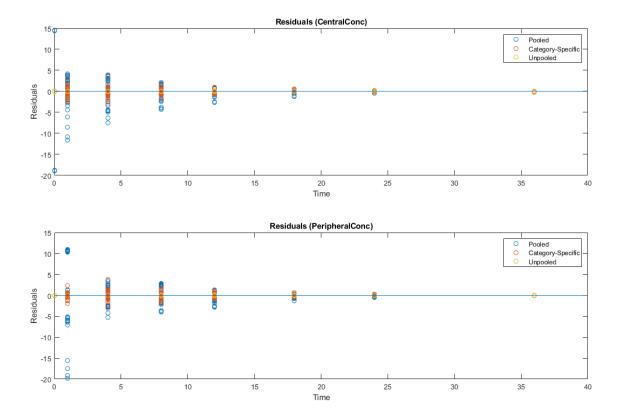
```
t = plot(pooledFit);
% Resize the figure.
t.hFig.Position(:) = [100 100 1280 800];
```



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.

See Also

CovariateModel object | groupedData object | sbiofit | sbiofitmixed

Topics

"Fit a Two-Compartment Model to PK Profiles of Multiple Individuals" on page 1-50

"Estimate a Parameter from the Yeast G Protein Model" on page 1-65

"Parameter Transformations"

"Nonlinear Regression"

Introduced in R2014a

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 2-191 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
Туре	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

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
getdose	Return exported SimBiology model dose object
getIndex	Get indices into ValueInfo and InitialValues properties
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: '23-Feb-2021 17:27:58'
ExportNotes: ''
```

Display the editable values (compartments, species, and parameters) information for the exported model object.

{exportedModel.ValueInfo.Name}

```
ans = 1x8 cell
Columns 1 through 7
{'unnamed'} {'x'} {'y1'} {'y2'} {'z'} {'c1'} {'c2'}
Column 8
{'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'}
```

See Also

Compartment object | Model object | Parameter object | SimBiology.export.Model | Species object

Topics

"PK/PD Modeling and Simulation to Guide Dosing Strategy for Antibiotics" "Deploy a SimBiology Model"

Introduced in R2012b

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)
```

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
```

See Also

Model object|findUsages(AbstractKineticLaw)|
findUsages(species,parameter,compartment)|findUsages(unit,unitprefix)

Topics

"Component Usage"

Introduced in R2016b

findUsages (species, parameter, compartment)

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.

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.

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.

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' }

See Also

Compartment object | Parameter object | Species object | findUnusedComponents |
findUsages(AbstractKineticLaw) | findUsages(unit, unitprefix)

Topics

"Component Usage"

Introduced in R2016b

findUsages (AbstractKineticLaw)

Find out how an AbstractKineticLaw object is used

Syntax

rxnList= findUsages(akl0bj,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".

Input Arguments

akl0bj — 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 akl0bj

vector

List of reactions that use aklObj, returned as a vector of reaction objects.

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,ml)
```

```
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
```

See Also

```
abstractkineticlaw object | findUnusedComponents |
findUsages(species,parameter,compartment) | findUsages(unit,unitprefix) |
kineticlaw object | reaction object
```

Topics

"Component Usage"

Introduced in R2016b

findUsages

Find out how observable object is used in SimBiology model

Syntax

```
[componentList,usageTable] = findUsages(obsObj)
```

Description

[componentList,usageTable] = findUsages(obs0bj) returns a vector of components that use the observable object obs0bj 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_T0.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 T0 profile.

```
obs1 = addobservable(m1, 'Max_T0', 'max(T0)');
```

Add another observable that references the first observable.

```
obs2 = addobservable(m1, 'Max_Square', 'Max_T0.^2');
```

Find usages of the first observable.

```
[c,t] = findUsages(obs1)
C =
   SimBiology Observable Array
   Index:
             Name:
                           Expression:
                                           Active:
                                                      Units:
             Max Square
                           Max T0.^2
   1
                                           true
t=1×3 table
             Component
                                       Property
                                                           Usage
    [1x1 SimBiology.Observable]
                                    {'Expression'}
                                                       {'Max T0.^2'}
```

Input Arguments

obs0bj — 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.

See Also

Observable

Topics "Component Usage"

Introduced in R2020a

findUsages (unit, unitprefix)

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.

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.

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
```

See Also

Compartment object | Parameter object | Species object | findUnusedComponents |
findUsages(AbstractKineticLaw) | findUsages(species,parameter,compartment)

Topics

"Component Usage"

Introduced in R2016b

fitted(LeastSquaresResults,OptimResults,NLINRes ults)

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.

Input Arguments

results0bj — 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.

Examples

Estimate a Parameter from the Yeast G Protein 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]';
```

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

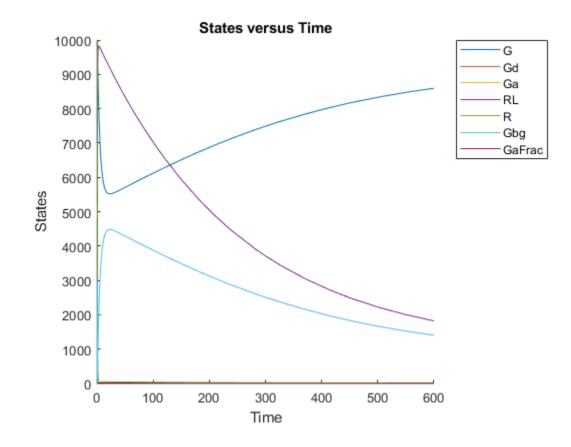
ans=1×3 table Name Estimate StandardError ('kGd'} 0.11307 3.4439e-05

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);



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

Introduced in R2014a

fitted(NLMEResults)

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'.

See Also

NLMEResults object | sbiofitmixed

Introduced in R2014a

generate

Generate scenarios from SimBiology. Scenarios object and return table

Syntax

```
scenariosTable = generate(s0bj)
scenariosTable = generate(s0bj,n)
scenariosTable = generate(____,'StandardizedOutput',tf)
```

Description

scenariosTable = generate(s0bj) generates scenarios from the SimBiology.Scenarios
object s0bj and returns a table, where each row represents a scenario and each column represents
an entry.

scenariosTable = generate(sObj,n) returns only the specified nth 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 "Simulating 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.

```
s0bj = SimBiology.Scenarios;
add(s0bj,'cartesian','variants',variants);
add(s0bj,'cartesian','dose',singleMeal)
ans =
  Scenarios (5 scenarios)
                                                     Number
                   Name
                                    Content
                             SimBiology variants
    Entry 1
                 variants
                                                        5
    x Entry 2
                             SimBiology dose
                                                       1
                 dose
```

```
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(s0bj)
```

```
scenariosTbl=5×2 table
variants dose
[1x1 SimBiology.Variant]
```

Change the entry name of the first entry.

ans =

```
rename(sObj,1,'Insulin Impairements')
```

```
      Scenarios (5 scenarios)
      Name
      Content
      Number

      Insulin Impairements
      SimBiology variants
      5

      X Entry 2
      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,s0bj,{'[Plasma Glu Conc]','[Plasma Ins Conc]'},[])

f = SimFunction

Parameters:

Name	Value	Туре	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'
{'Stomach Glu After Dosing'}	78	{'parameter'}	{'gram'
{'kp1' }	2.7	{'parameter'}	{'milligram/minute'
{'kp2' }	0.0021	{'parameter'}	{'1/minute'
{'kp3' }	0.009	{'parameter'}	{'(milligram/minute)/(picomole/li
{'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/li
{'Km' }	225.59	{'parameter'}	{ 'milligram'
{ 'p2U' }	0.0331	{ parameter } { 'parameter'}	{ mittigram {'1/minute'
{ 'K' }	2.28	{ parameter } {'parameter'}	{ 'picomole/(milligram/deciliter)'
{`alpha'}	0.05	{ parameter } {'parameter'}	{ picomote/(mittigram/decititer) {'1/minute'
{ beta }	0.11 0.5	{'parameter'}	{'(picomole/minute)/(milligram/de
{'gamma' }	0.0005	{'parameter'}	{'1/minute'
{ 'ke1' }		{'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:

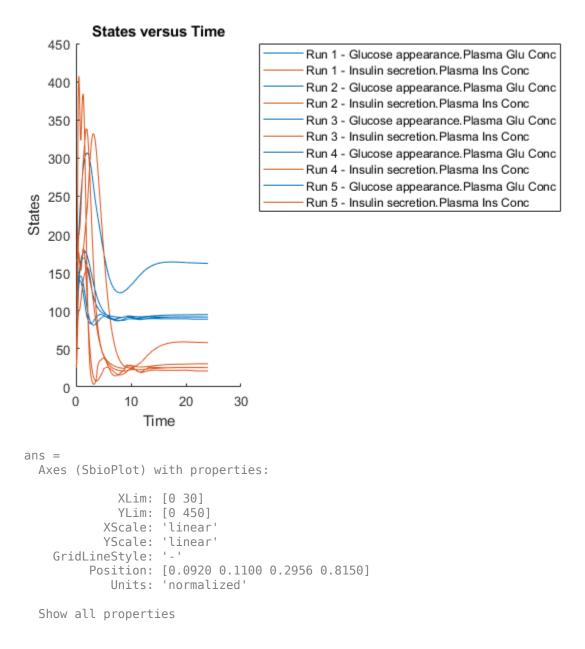
Name	Туре	Units
{'[Plasma Glu Conc]'}	{'species'}	{'milligram/deciliter'}
{'[Plasma Ins Conc]'}	{'species'}	{'picomole/liter' }

Dosed:

TargetName	TargetDimension		
{'Dose'}	{'Mass (e.g., gram)'}		

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(s0bj,24);
sbioplot(sd)
```



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 distribution 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 s0bj.

remove(s0bj,1)

ans = Scenarios (1	scenar	ios)	
	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(s0bj,'cartesian',["Vmx","kp3"],[pd_Vmx, pd_kp3],'RankCorrelation',[1,0.5;0.5,1])

```
ans =
 Scenarios (2 scenarios)
                   Name
                                  Content
                                                       Number
                           SimBiology dose
   Entry 1
                   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(s0bj,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.

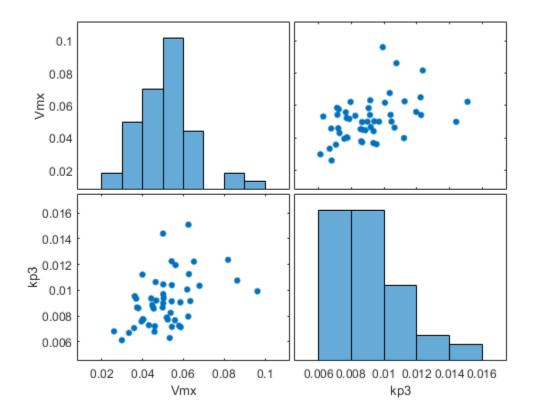
Verify that the Scenarios object can be simulated with the model. The verify function throws an error if any entry does not resolve uniquely to an object in the model or the entry contents have inconsistent lengths (sample sizes). The function throws a warning if multiple entries resolve to the same object in the model.

verify(s0bj,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.

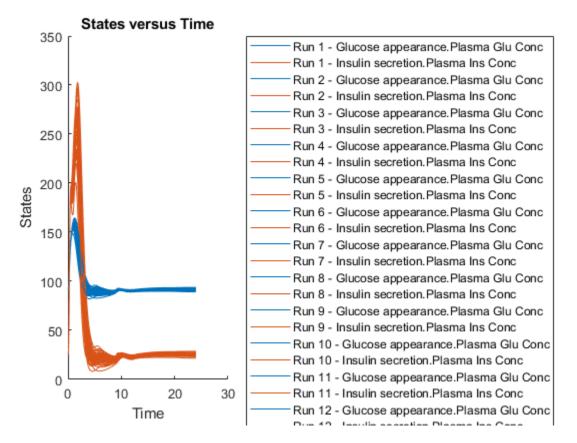
sTbl = generate(s0bj); [s,ax,bigax,h,hax] = plotmatrix([sTbl.Vmx,sTbl.kp3]);

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(s0bj,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(s0bj,2)

entry2struct.SamplingMethod = 'lhs'

You can now use the updated structure to modify entry 2.

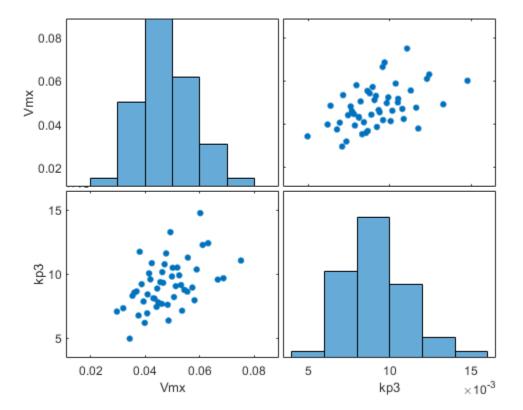
```
updateEntry(s0bj,2,entry2struct)
```

```
ans =
  Scenarios (50 scenarios)
                    Name
                                    Content
                                                       Number
                             SimBiology dose
    Entry 1
                    dose
                                                          1
    x (Entry 2.1
                             Lognormal distribution
                                                          50
                    Vmx
                    kp3
    + Entry 2.2)
                            Lognormal distribution
                                                          50
```

See also Expression property.

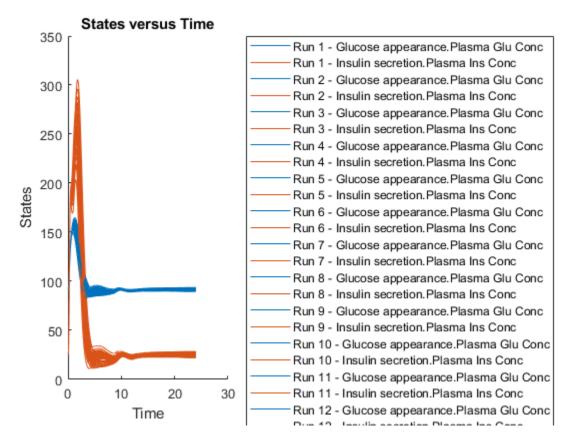
Visualize the sample values.

```
sTbl2 = generate(s0bj);
[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(s0bj,24); sbioplot(sd3);



Restore warning settings.

warning(warnSettings);

Input Arguments

s0bj — 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.

See Also

SimBiology.Scenarios | SimFunction object | createSimFunction (model)

Topics

"SimBiology.Scenarios Terminology" on page 2-550 "Combine Simulation Scenarios in SimBiology"

Introduced in R2019b

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.

See Also

SimData|set

Introduced in R2008b

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

Μ	Adjacency matrix for modelObj.		
model0bj	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 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 inm1, 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

Compatibility Considerations

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.

Introduced in R2006a

getconfigset (model)

Get configuration set object from model object

Syntax

```
configsetObj = getconfigset(modelObj, 'NameValue')
configsetObj = getconfigset(modelObj)
configsetObj = getconfigset(modelObj,'active')
```

Arguments

model0bj	Model object. Enter a variable name for a model object.
NameValue	Name of the configset object.
configset0bj	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: odel5s
StopTime: 10
SolverOptions:
AbsoluteTolerance: 1.000000e-06
RelativeTolerance: 1.000000e-03
SensitivityAnalysis: false
```

```
RuntimeOptions:
         StatesToLog:
                                        all
       CompileOptions:
         UnitConversion:
                                        false
         DimensionalAnalysis:
                                        true
       SensitivityAnalysisOptions:
                                        0
         Inputs:
         Outputs:
                                        0
2 Configure the SolverType to ssa.
    set(configset0bj, 'SolverType', 'ssa')
    get(configset0bj)
                             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

Introduced in R2006a

getCovariateData (pkdata)

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.

Tip Use the getCovariateData method to view the covariate data when writing equations for the Expression on page 3-69 property of a CovariateModel on page 2-137 object.

See Also

CovariateModel on page 2-137 | Expression on page 3-69 | PKData on page 2-342

Topics

"Modeling the Population Pharmacokinetics of Phenobarbital in Neonates" "Specify a Covariate Model"

Introduced in R2011b

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

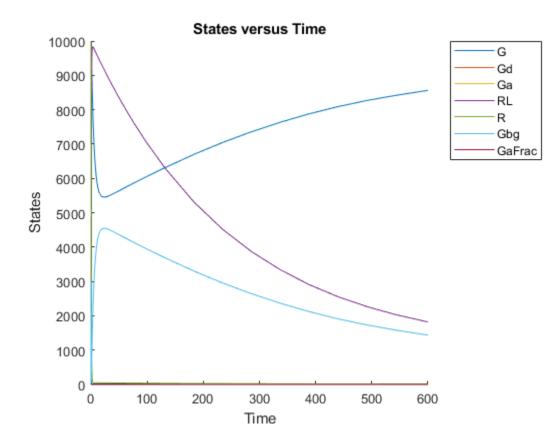
Extract Data from SimData Object

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.

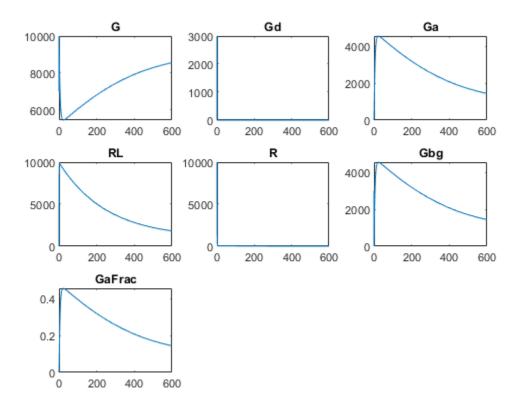
[time,data,names] = getdata(sd0bj);

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.

See Also SimData|get|set

Introduced in R2008b

getdose

Class: SimBiology.export.Model

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.

Input Arguments

model

SimBiology.export.Model object.

doseName

String containing a dose name to match against the Name property of the export dose objects in model.

Default: All dose objects.

Output Arguments

doses

Export dose objects in model, or the export dose object with Name property 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'
```

See Also

SimBiology.export.Dose | SimBiology.export.Model | export

Topics

"PK/PD Modeling and Simulation to Guide Dosing Strategy for Antibiotics" "Deploy a SimBiology Model"

getdose (model)

Return SimBiology dose object

Syntax

```
doseObj = getdose(modelObj)
doseObj = getdose(modelObj, 'DoseName')
```

Arguments

model0bj	Selects a model object that contains a dose object.
	Name of a dose object contained in a model object. <i>DoseName</i> is from the dose object property, Name.

Outputs

-	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');
doselObj = adddose(modelObj, 'dosel');
```

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

Introduced in R2012b

getEntry

Get entry contents from SimBiology.Scenarios object

Syntax

```
entryStruct = getEntry(s0bj,entryNameOrIndex)
entryStruct = getEntry(s0bj,entryIndex,subIndex)
```

Description

entryStruct = getEntry(s0bj,entryNameOrIndex) returns a structure containing the contents of the entry (or subentry on page 2-550) specified by entryNameOrIndex.

entryStruct = getEntry(s0bj,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 "Simulating 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.

```
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(s0bj)
```

```
scenariosTbl=5×2 table
variants dose
[1x1 SimBiology.Variant]
```

Change the entry name of the first entry.

See also Expression property.

dose

x Entry 2

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.

SimBiology dose

Number

5

1

f = createSimFunction(m1,s0bj,{'[Plasma Glu Conc]','[Plasma Ins Conc]'},[])

f = SimFunction

Parameters:

Name	Value	Туре	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'}	<pre>{'dimensionless'</pre>
{'kmax' }	0.0558	{'parameter'}	{'1/minute'
{'kmin' }	0.008	{'parameter'}	{'1/minute'
{ 'kabs' }	0.0568	{'parameter'}	{'1/minute'
{'kgri' }	Θ	{'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'
{'Stomach Glu After Dosing'}	78	{'parameter'}	{'gram'
{'kp1' }	2.7	{'parameter'}	{'milligram/minute'
{'kp2' }	0.0021	{'parameter'}	{'1/minute'
{'kp3' }	0.009	{'parameter'}	{'(milligram/minute)/(picomole/li
{'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/li
{'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'}	<pre>{'(picomole/minute)/(milligram/de</pre>
{'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	Туре	Units	
{'[Plasma Glu Conc]'}	{'species'}	{'milligram/deciliter'}	
{'[Plasma Ins Conc]'}	{'species'}	{'picomole/liter' }	

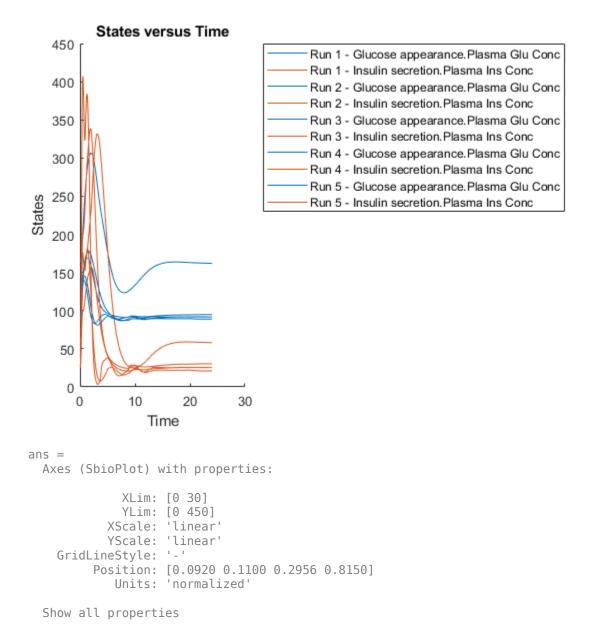
Dosed:

TargetName TargetDimension

{'Dose'} {'Mass (e.g., gram)'}

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(s0bj,24); sbioplot(sd)



If you have Statistics and Machine Learning Toolbox^m, 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 distribution 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 s0bj.

```
remove(s0bj,1)
ans =
   Scenarios (1 scenarios)
```

	Name	Content	Number
Entry 1	dose	SimBiology dose	1
See also Ex	pression	property.	

Add an entry that defines the joint probability distribution with a rank correlation matrix.

add(s0bj,'cartesian',["Vmx","kp3"],[pd_Vmx, pd_kp3],'RankCorrelation',[1,0.5;0.5,1])

```
ans =
 Scenarios (2 scenarios)
                                                          Number
                    Name
                                    Content
   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(s0bj,2,'Number',50)
```

```
ans =
 Scenarios (50 scenarios)
                                    Content
                                                        Number
                     Name
    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.

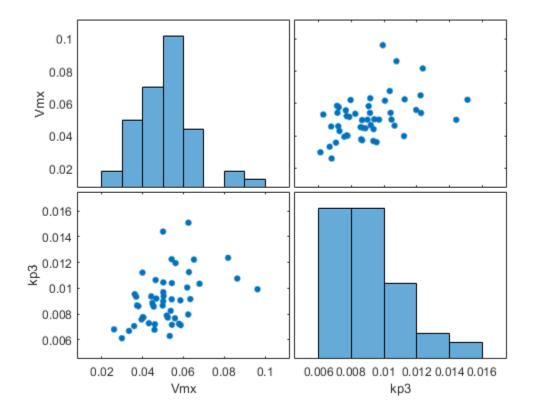
Verify that the Scenarios object can be simulated with the model. The verify function throws an error if any entry does not resolve uniquely to an object in the model or the entry contents have inconsistent lengths (sample sizes). The function throws a warning if multiple entries resolve to the same object in the model.

verify(s0bj,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.

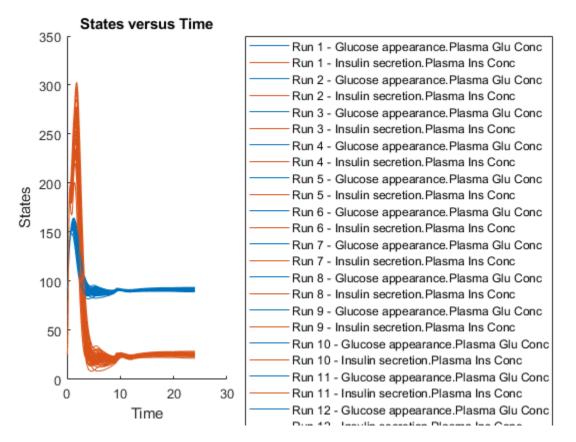
```
sTbl = generate(s0bj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl.Vmx,sTbl.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
```

```
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(s0bj,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(s0bj,2)
```

entry2struct.SamplingMethod = 'lhs'

You can now use the updated structure to modify entry 2.

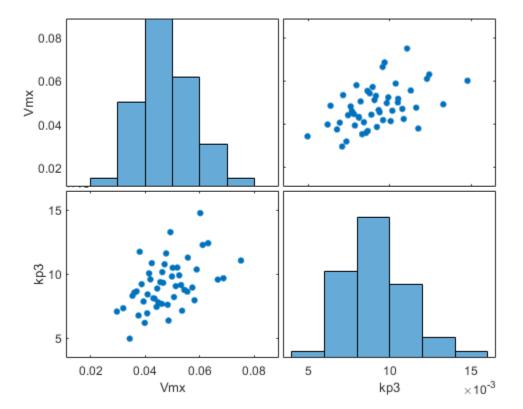
```
updateEntry(s0bj,2,entry2struct)
```

```
ans =
  Scenarios (50 scenarios)
                    Name
                                    Content
                                                       Number
                             SimBiology dose
    Entry 1
                    dose
                                                          1
    x (Entry 2.1
                             Lognormal distribution
                                                          50
                    Vmx
                    kp3
    + Entry 2.2)
                            Lognormal distribution
                                                          50
```

See also Expression property.

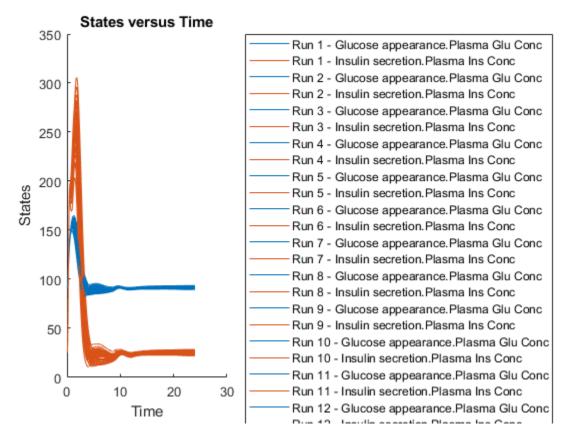
Visualize the sample values.

```
sTbl2 = generate(s0bj);
[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(s0bj,24); sbioplot(sd3);



Restore warning settings.

warning(warnSettings);

Input Arguments

s0bj — 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 — Simulation scenarios

Scenarios object

Simulation scenarios, returned as a Scenarios object.

The output 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

See Also

SimBiology.Scenarios | SimFunction object | createSimFunction (model)

Topics

"SimBiology.Scenarios Terminology" on page 2-550 "Combine Simulation Scenarios in SimBiology"

Introduced in R2019b

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 2-310 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 2-130 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 2-655 class.

Default: [] (Empty, which specifies no variant object)

doseobj

Object or array of objects of the RepeatDose on page 2-508 or ScheduleDose on page 2-553 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:

```
mlequations = getequations(model1)
```

```
mleguations =
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
y^2 = 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:

ml_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
y^2 = 900
z = 0
x = 1
Doses:
Variable
                               Туре
                                                   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

Configset object | Model object | RepeatDose object | ScheduleDose object | Variant
object

Topics

"Show Model Equations and Initial Conditions"

getIndex

Class: SimBiology.export.Model

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.

Input Arguments

model

SimBiology.export.Model object.

name

Character vector containing a name to match against the QualifiedName, then Name, properties of the ValueInfo objects in model.

type

Character vector containing a name to match against the Type property of the ValueInfo objects in model.

Default: All types.

Output Arguments

indices

Vector of indices indicating which ValueInfo objects in a SimBiology.export.Model object match on the specified name and type.

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.

Display the type of value.

em.ValueInfo(ix).Type

ans =

species

The name y1 corresponds to an editable species.

See Also

SimBiology.export.Model | SimBiology.export.ValueInfo | export

Topics

"PK/PD Modeling and Simulation to Guide Dosing Strategy for Antibiotics" "Deploy a SimBiology Model"

getNumberScenarios

Return number of scenarios from SimBiology.Scenarios object

Syntax

numScenarios = getNumberScenarios(s0bj)

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.

s0bj = 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(s0bj,'cartesian','s1',[2.7; 3.1; 3.4]);

Get the number of simulation sceanarios that the object has after combining the entries.

```
n = getNumberScenarios(s0bj)
```

n = 6

Input Arguments

s0bj — 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.

See Also

SimBiology.Scenarios | SimFunction object | createSimFunction (model)

Topics "SimBiology.Scenarios Terminology" on page 2-550 "Combine Simulation Scenarios in SimBiology"

Introduced in R2019b

getparameters (kineticlaw)

Get specific parameters in kinetic law object

Syntax

```
parameterObj = getparameters(kineticlawObj)
parameterObj = getparameters(kineticlawObj, 'ParameterVariablesValue')
```

Arguments

kineticlaw0bj	Retrieve parameters used by the kinetic law object.
	Retrieve parameters used by the kinetic law object corresponding to the specified parameter in the ParameterVariables property of the kinetic law object.

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 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.

```
parameter0bj1 = addparameter(kineticlaw0bj,'Va');
parameter0bj2 = addparameter(kineticlaw0bj,'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:

```
parameter0bj3 = getparameters(kineticlaw0bj, 'Vm')
MATLAB returns:
SimBiology Parameter Array
Index: Name: Value: ValueUnits:
1 Va 1
parameter0bj4 = getparameters (kineticlaw0bj, 'Km')
```

See Also

addparameter, getspecies, setparameter

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 Sensitivities Using SimFunctionSensitivity Object

This example shows how to calculate the 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.

Value

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:
```

Paralleters:

Name

Туре

{'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 Туре

{'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.

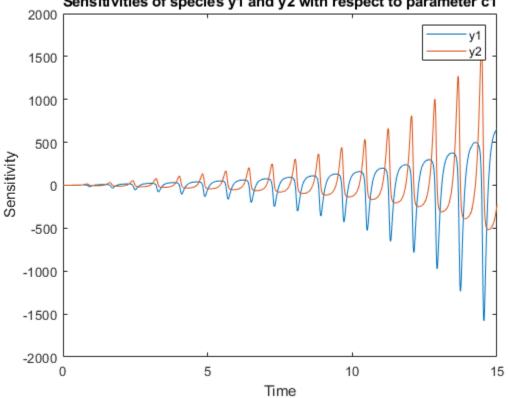
sd = f([10, 0.1], 15);

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');
```

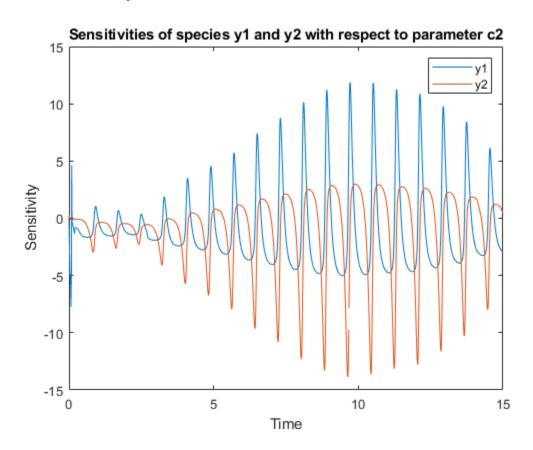


Sensitivities of species y1 and y2 with respect to parameter c1

Plot the sensitivities of species y1 and y2 with respect to c2.

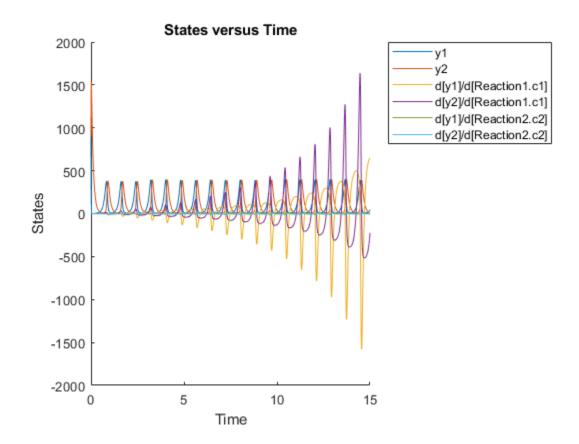
figure; plot(t,y(:,:,2));

```
legend(outputs);
title('Sensitivities of species y1 and y2 with respect to parameter c2');
xlabel('Time');
ylabel('Sensitivity');
```



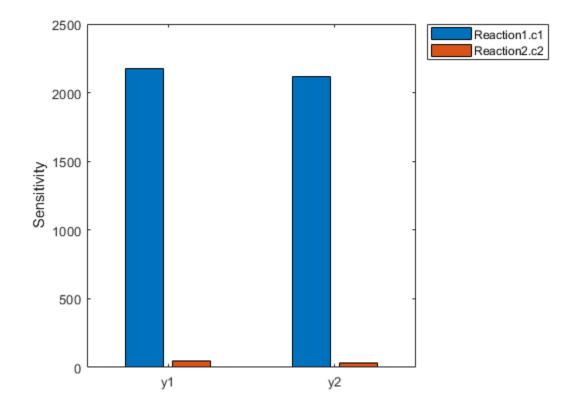
Alternatively, you can use sbioplot.

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)".

See Also

SimData | SimFunctionSensitivity object | sbiosimulate

Topics

"Local Sensitivity Analysis (LSA)" "Calculate Local Sensitivities Using sbiosimulate" "Calculate Local Sensitivities Using SimFunctionSensitivity object"

Introduced in R2008b

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.

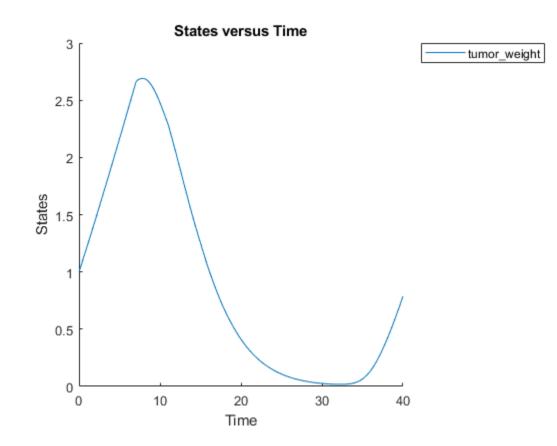
v = getvariant(m1); d = getdose(m1,'interval_dose');

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].

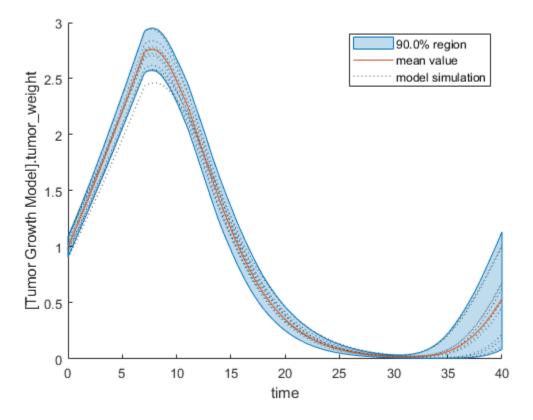
sobolResults = sbiosobol(m1,modelParamNames,outputName,'Variants',v,'Doses',d,'ShowWaitBar',true

```
sobolResults =
   Sobol with properties:
        Time: [444x1 double]
        SobolIndices: [5x1 struct]
        Variance: [444x1 table]
        Observables: {'[Tumor Growth Model].tumor_weight'}
   ParameterSamples: [1000x5 table]
        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.

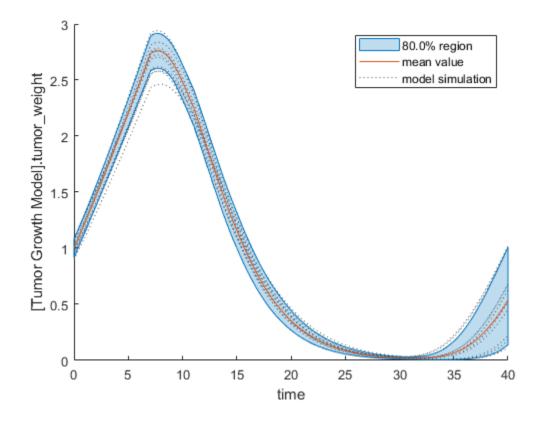
Show the mean model response, the simulation results, and a shaded region covering 90% of the simulation results.

plotData(sobolResults);



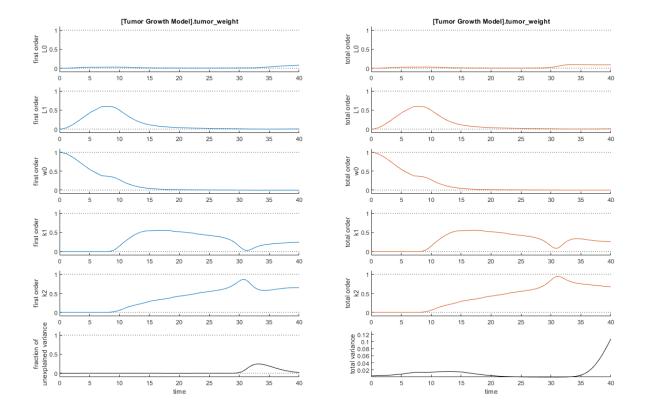
You can adjust the quantile region to a different percentage by specifying 'Alphas' for the lower and upper quantiles of all model responses. For instance, an alpha value of 0.1 plots a shaded region between the $100 \times 100 \times (1 - alpha)$ quantiles of all simulated model responses.

plotData(sobolResults, 'Alphas',0.1);



Plot the time course of the first- and total-order Sobol indices.

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

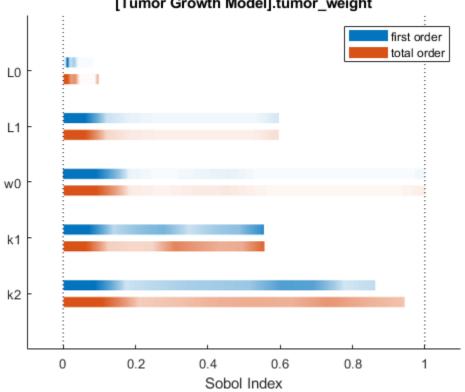


The first-order Sobol index of an input parameter gives the fraction of the overall response variance that can be attributed to variations in the input parameter alone. The total-order index gives the fraction of the overall response variance that can be attributed to any joint parameter variations that 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.

bar(sobolResults)



[Tumor Growth Model].tumor weight

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: ModelName: DataCount: Name: 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

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.

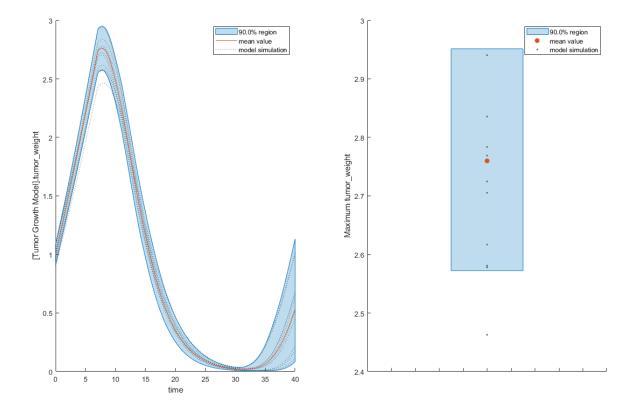
```
[samplesUsed,sd,validruns] = getSimulationResults(sobolResults,4);
```

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);
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 2-272.

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 ith 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 1-252, A and B are sample matrices. A_B^i is a matrix where all columns are from A except the *i*th 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 $A^{1} + A^{2} = A^{params}$

correspond to $A_B^1, A_B^2, ..., A_B^{params}$. In other words, you can consider the following:

sobolObj.SimulationInfo.SimData =
$$\left[SimData(A), SimData(B), SimData(A_B^1), SimData(A_B^2), ..., SimData(A_B^{params})\right]$$

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(sobol0bj,3) returns:

samplesTable (first output), which is $A^1_{\scriptscriptstyle B}$.

- - 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 *i*th column of sobolObj.SimulationInfo.ValidSample on page 2-0 .

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|bar|plot|plotData|sbiosobol

Introduced in R2020a

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.
	Retrieve species used by the kinetic law object corresponding to the specified species in the SpeciesVariables property of the kinetic law object.

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 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.

```
species0bj = getspecies (kineticlaw0bj, 'S')
```

MATLAB returns:

SimBiology Species Array

See Also

addspecies, getparameters, setparameter, setspecies

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

Μ	Stoichiometry matrix for <i>model0bj</i> .			
modelObj	Specify the model object.			
objSpecies	Return the list of <i>modelObj</i> 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 <i>modelObj</i> 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 \rightarrow 3 C and B + 3 D \rightarrow 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"

Compatibility Considerations

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.

Introduced in R2006a

getTable(ScheduleDose,RepeatDose)

Return data from SimBiology dose object as table

Syntax

tbl = getTable(dose0bj)

Description

tbl = getTable(doseObj) returns dosing data from the dose object doseObj as a table tbl.

Input Arguments

dose0bj — 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.

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.

See Also

RepeatDose object | ScheduleDose object | setTable

Introduced in R2014a

getvariant (model)

Get variant from model

Syntax

variantObj = getvariant(modelObj)

variantObj = getvariant(modelObj, 'NameValue')

Arguments

variant0bj	Variant object returned by the getvariant method.		
model0bj	Model object from which to get the variant.		
'NameValue'	Name of the variant to get from the model object <i>modelObj</i> .		

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.

```
v0bjs = getvariant(model0bj)
```

SimBiology Variant Array Index: Name: Active: 1 v1 false 2 v2 false 3 Get the variant object named 'v2' from the model.

```
v0bjv2 = getvariant(model0bj, 'v2');
```

See Also

Model object, Variant object, addvariant, removevariant

Introduced in R2007b

groupedData

Table-like collection of data and metadata

Description

The groupedData object is the required data format to store data needed for fitting using 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 two additional methods that let you create doses from data set containing dosing data 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 every function of table and provides the following additional functions. createDoses Create dose 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

GroupVariableName and IndpendentVariableName have been automatically assigned to 'ID' and 'Time', respectively.

See Also

sbiofit | sbiofitmixed | table

Topics

"Importing Data" "Importing Data — Supported Files and Data Types" "Create Data File with SimBiology Definitions"

Introduced in R2014a

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

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 ID	table TIME	DOSE	WEIGHT	APGAR	CONC
1	Θ	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.

See Also

groupedData|sbiofit|sbiofitmixed|table

Introduced in R2014a

histogram

Plot histogram of multiparametric global sensitivity analysis results

Syntax

```
h = histogram(mpgsa0bj)
h = histogram(mpgsa0bj,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 namevalue pair arguments.

Examples

Perform Multiparametric Global Sensitivity Analysis (MPGSA)

Load the "Target-Mediated Drug Disposition (TMDD) Model".

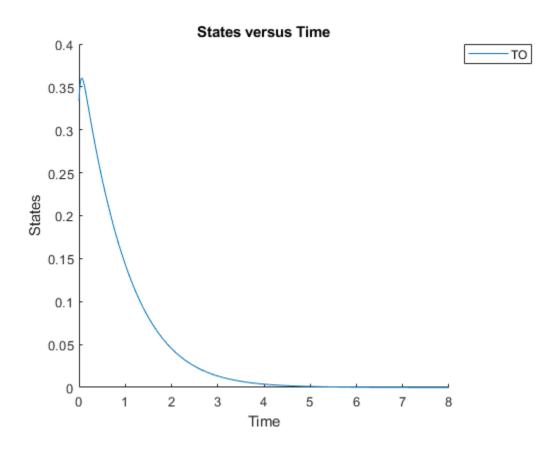
```
sbioloadproject tmdd_with_T0.sbproj
```

Get the active configset and set the target occupancy (T0) as the response.

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

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.

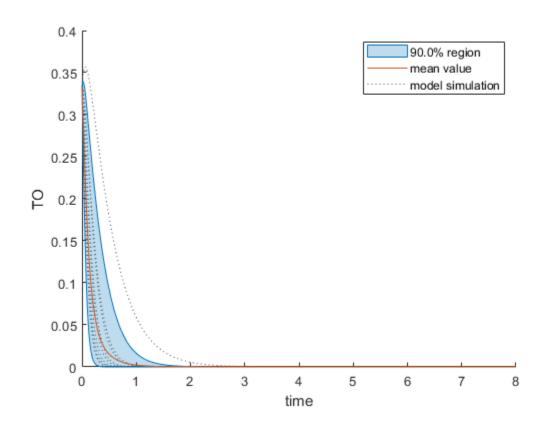
```
classifier = 'trapz(time,T0) <= 0.1';</pre>
```

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,T0) <= 0.1'}</pre>
    KolmogorovSmirnovStatistics: [4x1 table]
                        ECDFData: {4x4 cell}
              SignificanceLevel: 0.0500
                         PValues: [4x1 table]
              SupportHypothesis: [10000x1 table]
                     Observables: {'TO'}
                ParameterSamples: [10000x4 table]
```

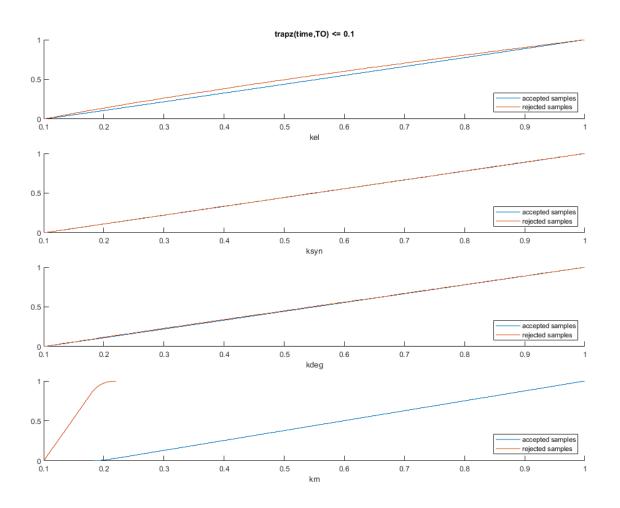
```
SimulationInfo: [1x1 struct]
```

Plot the quantiles of the simulated model response.
plotData(mpgsaResults);



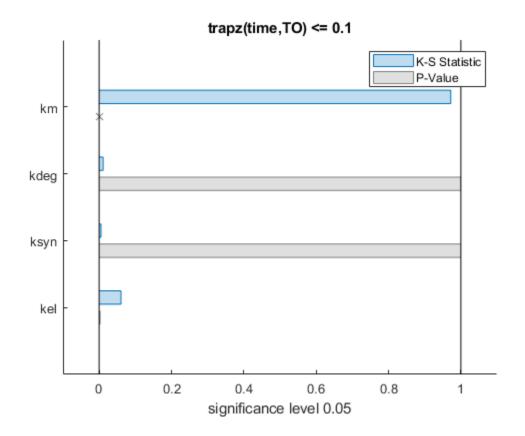
Plot the empirical cumulative distribution functions (eCDFs) of the accepted and rejected samples. Except for km, none of the parameters shows a significant difference in the eCDFs for the accepted and rejected samples. The km plot shows a large Kolmogorov-Smirnov (K-S) distance between the eCDFs of 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)



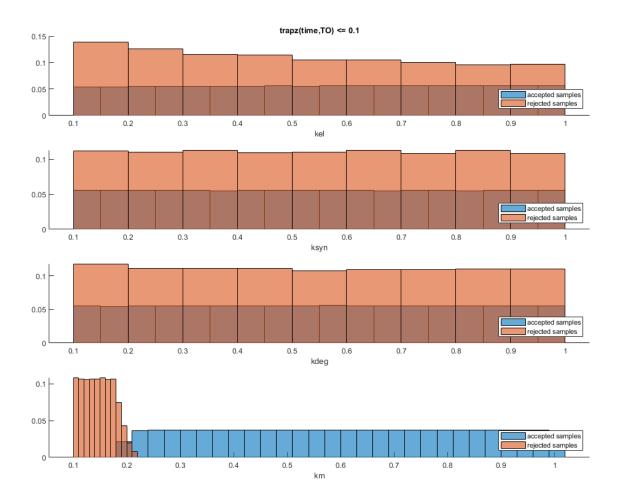
The bar plot shows two bars for each parameter: one for the K-S distance (K-S statistic) and another for the corresponding p-value. You reject the null hypothesis if the p-value is less than the significance level. A cross (x) is shown for any p-value that is almost 0. You can see the exact p-value corresponding to each parameter.

[mpgsaResults.ParameterSamples.Properties.VariableNames',mpgsaResults.PValues]

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 histograms 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

mpgsa0bj — 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 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: 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 the comma-separated pair consisting of 'Parameters' and a character vector, string, string vector, cell array of character vectors, or a vector of positive integers indexing into the columns of the mpgsa0bj.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 the comma-separated pair consisting of 'Classifiers' and 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 eCDFs of accepted samples

three-element row vector

Color of eCDFs of accepted samples, specified as the comma-separated pair consisting of 'AcceptedSamplesColor' and a three-element row vector. 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.

Example: 'AcceptedSamplesColor',[0.4,0.3,0.2]

Data Types: double

RejectedSamplesColor — Color of eCDFs of rejected samples

three-element row vector

Color of eCDFs of rejected samples, specified as the comma-separated pair consisting of 'RejectedSamplesColor' and a three-element row vector. By default, the function uses the second 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.

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.

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 | bar | ecdf | histogram | kstest2 | plotData | sbiompgsa

Introduced in R2020a

isAccelerated(SimFunction)

Determine if SimFunction object is accelerated

Syntax

```
tf = isaccelerated(F)
tf = isaccelerated(F,computerType)
```

Arguments

SimFunction object created by the createSimFunction method of a SimBiology model.	
 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:

Ν	ame	Value	Туре
	ion1.c1' ion2.c2'	10 0.01	'parameter' 'parameter'
Observable	S:		
Name	Туре		
'y1' 'y2'	'species' '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 =

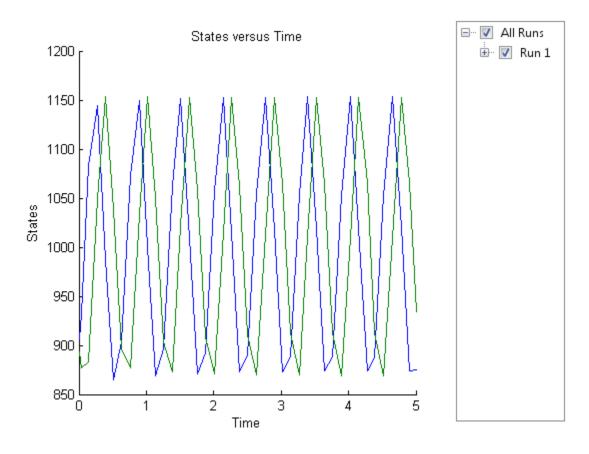
0

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

References

[1] Gillespie D.T. "Exact Stochatic Simulation of Coupled Chemical Reactions," (1977) The Journal of Physical Chemistry, 81(25), 2340-2361.

Introduced in R2012b

isAccelerated

Class: SimBiology.export.Model

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.

Input Arguments

model

SimBiology.export.Model object.

computerType

String specifying a computer type. You can specify any valid archstr supported by the function computer.

Output Arguments

tf

Logical value true if model is accelerated for the current computer type, or computer type specified by computerType. Logical value false if the exported model is not 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.

See Also

```
SimBiology.export.Model|accelerate|computer
```

Topics

"PK/PD Modeling and Simulation to Guide Dosing Strategy for Antibiotics" "Deploy a SimBiology 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 3-71 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 2-303.

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 2-301.

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 2-303.

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 expressionused to determine thereaction 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
Туре	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)

Introduced in R2006b

LeastSquaresResults object

Results object containing estimation results from least-squares regression

Description

The LeastSquaresResults object is a superclass of two results objects: NLINResults object and OptimResults object. These objects contain estimation results from fitting a SimBiology model to data using sbiofit with any supported algorithm.

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.

Method Summary

boxplot(LeastSquaresResults,OptimResults,NLINResults)	
	Create box plot showing the variation of estimated SimBiology model parameters
fitted (Least Squares Results, Optim Results, NLINR esults)	
	Return simulation results of SimBiology model fitted using least-squares regression
plot(LeastSquaresResults,OptimResults,NLINResults)	
	Compare simulation results to the training data, creating a time- course subplot for each group
plotActual Versus Predicted (Least Squares Results, Optim Results, NLIN Results)	
	Compare predictions to actual data, creating a subplot for each response
plotResiduals(LeastSquaresResults,OptimResults,NLINResults)	
	Plot residuals for each response, using time, group, or prediction as <i>x</i> -axis
plot Residual Distribution (Least Squares Results, Optim Results, NLIN Results)	Plot the distribution of the residuals
predict(LeastSquaresResults,OptimResults,NLINResults)	
	Simulate and evaluate fitted SimBiology model
random (Least Squares Results, Optim Results, NLIN Results)	
	Simulate SimBiology model, adding variations by sampling error model
summary (Least Squares Results, Optim Results, NLIN Results)	
	Plot a summary figure that contains estimated values and estimation statistics

Property Summary

GroupName	Categorical variable representing the name of the group associated with the results, or [] if the 'Pooled' name-value pair argument was set to true when you ran sbiofit.
Beta	Table of estimated parameters where the <i>j</i> th row represents the <i>j</i> th estimated parameter β_j . It contains transformed values of parameter estimates if any parameter transform is specified.
	<pre>Standard errors of these parameter estimates (StandardError) are calculated as: sqrt(diag(COVB)).</pre>
	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 where the <i>j</i> th row represents the <i>j</i> th estimated parameter β_j . This table contains untransformed values of parameter estimates.
	<pre>Standard errors of these parameter estimates (StandardError) are calculated as: sqrt(diag(CovarianceMatrix)).</pre>
	It can also contain the following variables:
	• Bounds — the values of 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, with respect to an estimated parameter, that is,
	$J(i, j, k) = \frac{\partial y_k}{\partial \beta_j} \Big _{t_i}$
	where t_i is the <i>i</i> th time point, β_j is the <i>j</i> th estimated parameter in the transformed space, and y_k is the <i>k</i> th response in the group of data.

СОУВ	Estimated covariance matrix for Beta, which is calculated as: COVB = inv(J'*J)*MSE.
CovarianceMatrix	<pre>Estimated covariance matrix for ParameterEstimates, which is calculated as: CovarianceMatrix = T'*COVB*T, where T = diag(JInvT(Beta)).</pre>
	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 where R_{ij} is the residual for the <i>i</i> th time point and the <i>j</i> th response in the group of data.
LogLikelihood	Maximized loglikelihood for the fitted model.
AIC	Akaike Information Criterion (AIC), calculated as $AIC = 2^{*}(-LogLikelihood + P)$, where P is the number of parameters.
BIC	Bayes Information Criterion (BIC), 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, calculated as $DFE = N-P$, where N is the number of observations and P is the number of parameters.
MSE	Mean squared error.
SSE	Sum of squared (weighted) errors or residuals.
Weights	Matrix of weights with one column per response and one row per observation.
EstimatedParameterNames	Cell array of character vectors specifying estimated parameter names.

ErrorModelInfo	 Table describing the error models and estimated error model parameters. It 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 <i>e</i>, the function value <i>f</i>, and one or two parameters <i>a</i> and <i>b</i>. In SimBiology, the function <i>f</i> represents simulation results from a SimBiology model. 'constant': <i>y</i> = <i>f</i> + <i>ae</i> 'proportional': <i>y</i> = <i>f</i> + <i>b</i> <i>f</i> <i>e</i> 'combined': <i>y</i> = <i>f</i> + <i>b</i> <i>f</i> <i>e</i>
	• 'combined': $y = f + (a + b f)e$
	• 'exponential': $y = f * \exp(ae)$
EstimationFunction	Name of the estimation function.
DependentFiles	File names to include for deployment.

Note Loglikelihood, AIC, and BIC properties are empty for LeastSquaresResults objects that were obtained before R2016a.

See Also

NLINResults object | OptimResults object | sbiofit | sbiofitmixed

Introduced in R2014a

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 2-312 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,	Create compartment object
compartment) addconfigset (model)	Create configuration set object and add to model object
adddose (model)	Add dose object to model
	5
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
Туре	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

Introduced in R2006b

move

Move SimBiology species or parameter object to new parent

Syntax

```
spObj = move(spObj,parentObj)
spObj = move(spObj,parentObj,conflictOption)
```

Description

sp0bj = move(sp0bj,parent0bj) moves a SimBiology species or parameter object sp0bj to a new parent SimBiology object parent0bj. The function automatically updates the corresponding expressions, observables, variants, and parameterized dose properties that reference sp0bj. Expressions include reactions, kinetic laws, rules, and events.

sp0bj = move(sp0bj,parent0bj,conflict0ption) specifies how to handle naming conflicts if
parent0bj is already the parent of another object with the same name as sp0bj.

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:
                         2
    Compartments:
                         0
     Events:
     Parameters:
                         1
     Reactions:
                         1
                         0
     Rules:
     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.

Input Arguments

sp0bj — SimBiology species or parameter

species object | parameter object

SimBiology species or parameter, specified as a species object or parameter object.

If sp0bj 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.

parent0bj — 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.

See Also

Compartment | Species | Parameter | Model | Reaction | KineticLaw | Observable | copyobj | move

Introduced in R2020b

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.

c1.0wner

Input Arguments

comp0bj — 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.

See Also

Compartment | Species | Parameter | Model | Reaction | KineticLaw | Observable | copyobj | move

Introduced in R2020b

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 2-326.

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 or sbiompgsa. 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

plotDataPlot quantile summary of model simulations from global sensitivity analysis (requires
Statistics and Machine Learning Toolbox)plotPlot empirical CDF of multiparametric global sensitivity analysis
Create bar plot of multiparametric global sensitivity analysis statisticshistogramPlot histogram of multiparametric global sensitivity analysis results

Examples

Perform Multiparametric Global Sensitivity Analysis (MPGSA)

Load the "Target-Mediated Drug Disposition (TMDD) Model".

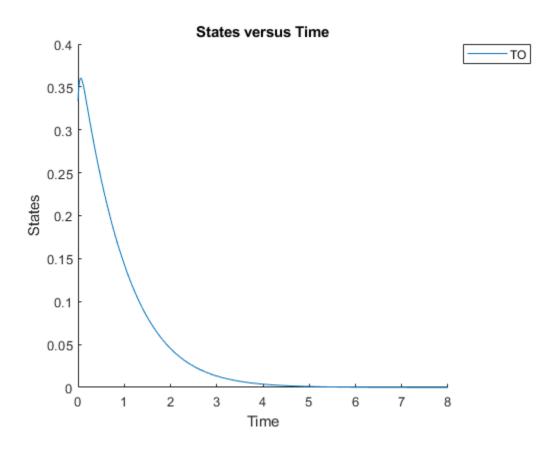
sbioloadproject tmdd_with_T0.sbproj

Get the active configset and set the target occupancy (T0) as the response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = '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,T0) <= 0.1';</pre>
```

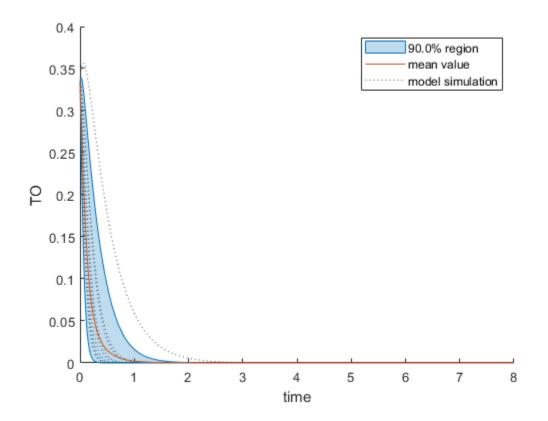
Perform MPGSA to find sensitive parameters with respect to the TO. Vary the parameter values between predefined bounds to generate 10,000 parameter samples.

```
% 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,T0) <= 0.1'}</pre>
    KolmogorovSmirnovStatistics: [4x1 table]
                        ECDFData: {4x4 cell}
              SignificanceLevel: 0.0500
                         PValues: [4x1 table]
              SupportHypothesis: [10000x1 table]
                     Observables: {'TO'}
                ParameterSamples: [10000x4 table]
```

SimulationInfo: [1x1 struct]

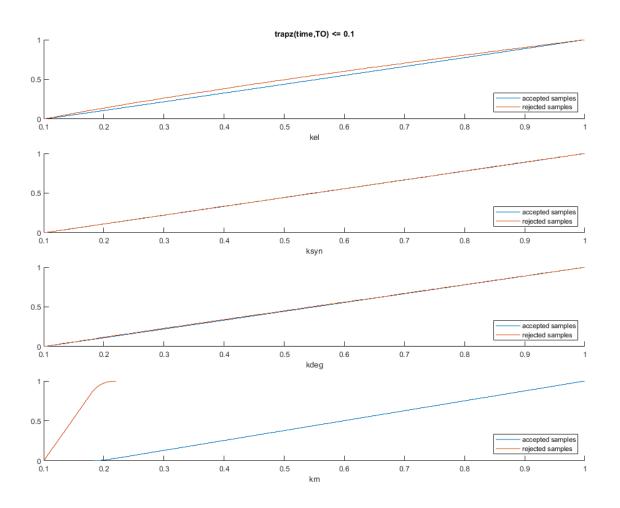
Plot the quantiles of the simulated model response.

plotData(mpgsaResults);



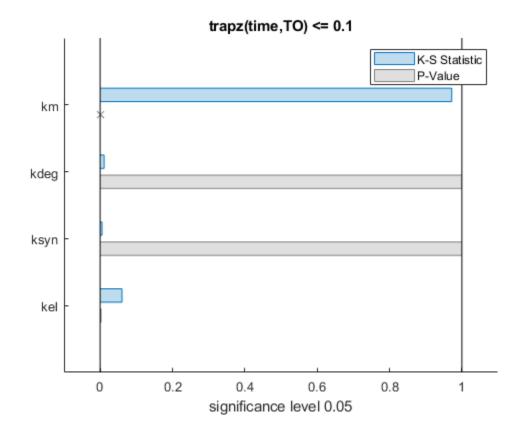
Plot the empirical cumulative distribution functions (eCDFs) of the accepted and rejected samples. Except for km, none of the parameters shows a significant difference in the eCDFs for the accepted and rejected samples. The km plot shows a large Kolmogorov-Smirnov (K-S) distance between the eCDFs of 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.

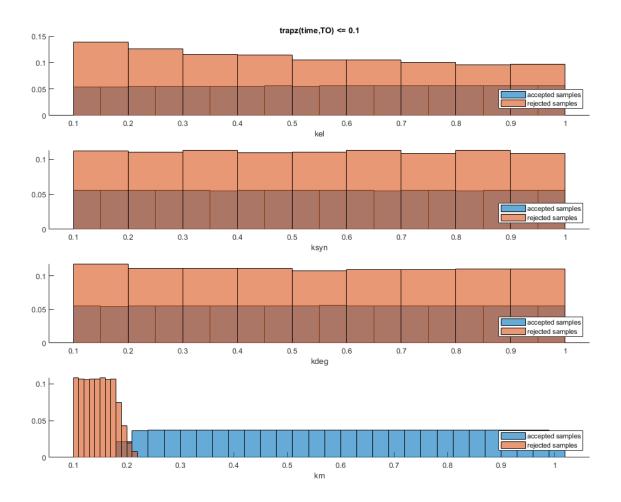
[mpgsaResults.ParameterSamples.Properties.VariableNames',mpgsaResults.PValues]

ans=4×2 table Varl	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 histograms 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.

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

Observable | ecdf | kstest2 | sbiompgsa | sbiosobol

Topics

"Sensitivity Analysis in SimBiology"

NLINResults object

Estimation results object, subclass of LeastSquaresResults

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.

Method Summary

The NLINResults object shares all methods of the LeastSquaresResults object.

Property Summary

The NLINResults object shares all properties of the LeastSquaresResults object.

See Also

LeastSquaresResults object | OptimResults object | sbiofit | sbiofitmixed

Introduced in R2014a

NLMEResults object

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.

Method Summary

boxplot(NLMEResults)	Create box plot showing the variation of estimated SimBiology model parameters
covariateModel(NLMEResults)	Return a copy of the covariate model that was used for the nonlinear mixed-effects estimation using sbiofitmixed
fitted(NLMEResults)	Return the simulation results of a fitted nonlinear mixed- effects model
plot(NLMEResults)	Compare simulation results to the training data, creating a time-course subplot for each group
plotActualVersusPredicted(NLMEResults))
	Compare predictions to actual data, creating a subplot for each response
plotResiduals(NLMEResults)	Plot the residuals for each response, using the time, group, or prediction as the x-axis
plotResidualDistribution(NLMEResults)	
-	Plot the distribution of the residuals
predict(NLMEResults)	Simulate and evaluate fitted SimBiology model
random(NLMEResults)	Simulate a SimBiology model, adding variations by sampling the error model

Property Summary

FixedEffects	Table of the estimated fixed effects and their standard errors.
RandomEffects	Table of the estimated random effects for each group.
IndividualParameterEstima tes	Table of estimated parameter values, including fixed and random effects.
PopulationParameterEstima tes	Table of estimated parameter values, including only fixed effects.
RandomEffectCovarianceMat rix	Table of the covariance matrix of the random effects.
stats	Struct of statistics returned by the nlmefit and nlmefitsa algorithm.

CovariateNames	Cell array of character vectors specifying covariate names.
EstimatedParameterNames	Cell array of character vectors specifying estimated parameter names.
ErrorModelInfo	Table describing the error models and estimated error model parameters.
	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 which must be either 'nlmefit' or 'nlmefitsa'.
LogLikelihood	Maximized loglikelihood for the fitted model.
AIC	Akaike Information Criterion (AIC), calculated as AIC = 2*(- LogLikelihood + P), where <i>P</i> is the number of parameters. For details, see nlmefit.
BIC	Bayes Information Criterion (BIC), 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, 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);

See Also

nlmefit | nlmefitsa | sbiofit | sbiofitmixed

Introduced in R2014a

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 $A \cdot / (A+B)$ 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_T0.sbproj

Set the target occupancy (T0) as a response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'T0';
```

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,'T0',d)
```

f = SimFunction

Parameters:

aram'} 1	{'parameter'}	{'nanomole'}		
Туре	Units			
{'parameter'}	{'dimensionless'}			
ame	TargetDimension		Amount	AmountValue
_	{'parameter'} ame	<pre>{'parameter'} {'dimensionless'} ame TargetDimension</pre>	{'parameter'} {'dimensionless'} ame TargetDimension	{'parameter'} {'dimensionless'} ame TargetDimension Amount

```
warning('on','SimBiology:SimFunction:DOSES_NOT_EMPTY');
```

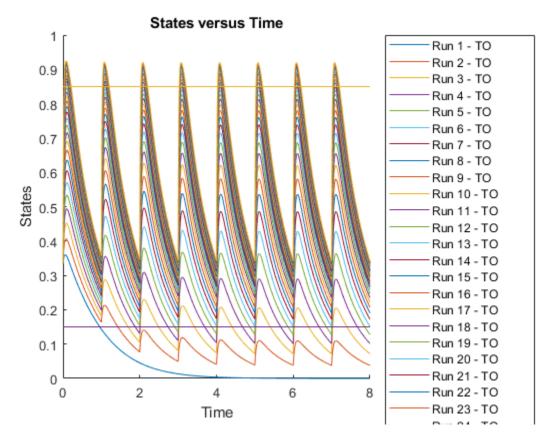
Simulate the model using the dose amounts generated by the Scenarios object. In this case, the object generates 31 different doses; hence the model is simulated 31 times and generates a SimData array.

```
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 T0 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,'statl','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
```

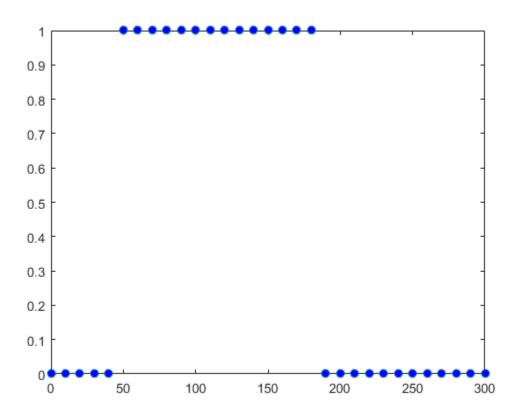
The addobservable function evaluates the new observable expression for each SimData in sd and returns the evaluated results as a new SimData array, newSD, which now has the added observable (stat1).

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 TO 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');
```

See Also

addobservable(SimData) | addobservable(model) | renameobservable(SimData) |
updateobservable(SimData)

OptimResults object

Estimation results object, subclass of LeastSquaresResults

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.

Method Summary

The OptimResults object shares all methods of the LeastSquaresResults object.

Property Summary

The OptimResults object shares all properties of the LeastSquaresResults object and has the following additional properties.

ExitFlag	An exit flag specific to the estimation function.
Output	A struct of additional outputs specific to the estimation function.

Note See the reference page of the specific algorithm to get more information on the values of ExitFlag and the Output structure.

See Also

LeastSquaresResults object | NLINResults object | sbiofit | sbiofitmixed

Introduced in R2014a

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 2-340 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

Copy SimBiology object and its children
Delete SimBiology object
Display summary of SimBiology object
Find out how a species, parameter, or compartment is used in a model
Get SimBiology object properties
Move SimBiology species or parameter object to new parent
Rename object and update expressions
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
Туре	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

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

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

ete	Delete SimBiology object
play	Display summary of SimBiology object
	Get SimBiology object properties
CovariateData (pkdata)	Create design matrix needed for fit
	Set SimBiology object properties
play CovariateData (pkdata)	Display summary of SimBiology object Get SimBiology object properties Create design matrix needed for fit

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

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
delete display get	Delete SimBiology object Display summary of SimBiology object Get SimBiology object properties

Property Summary

PKCompartments	Hold compartments in PK model
----------------	-------------------------------

See Also

"Create Pharmacokinetic Models" in the SimBiology User's Guide, PKCompartment object

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

plot(LeastSquaresResults,OptimResults,NLINResul ts)

Compare simulation results to the training data, creating a time-course subplot for each group

Syntax

plot(results0bj)

Description

plot(results0bj) returns a figure displaying the comparison between simulation results to the training data, with a time-course subplot for each group.

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.

See Also

NLINResults object | OptimResults object | sbiofit

Introduced in R2014a

plot(NLMEResults)

Compare simulation results to the training data, creating a time-course subplot for each group

Syntax

```
plot(resultsObj)
plot(resultsObj,'ParameterType',value)
```

Description

plot(results0bj) 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'.

See Also

NLMEResults object | sbiofitmixed

Introduced in R2014a

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.

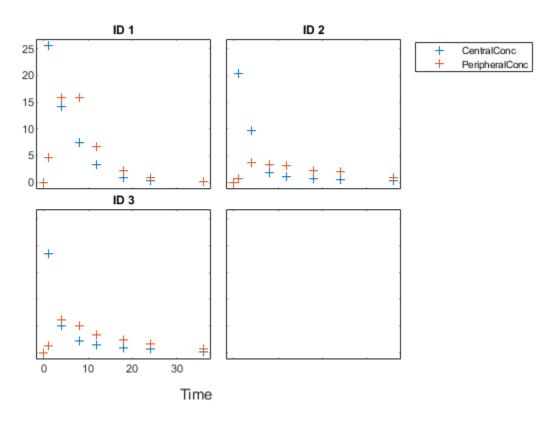
Examples

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.

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

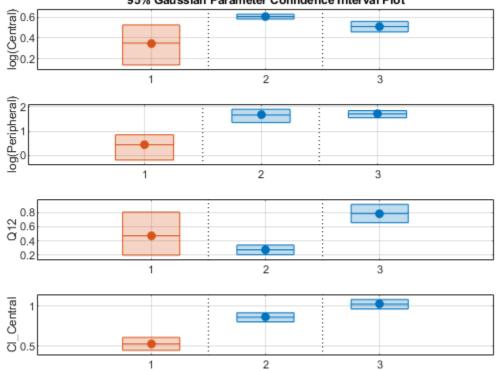
Compute 95% confidence intervals for each estimated parameter in the unpooled fit using the Gaussian approximation.

```
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.

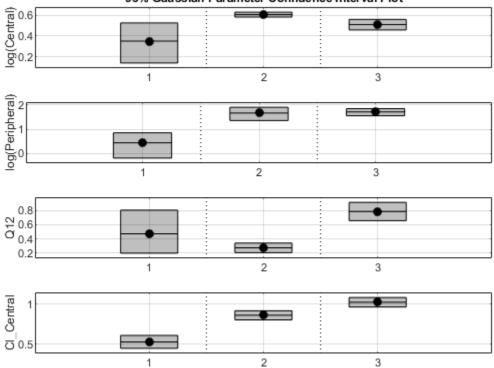
plot(ciParamUnpooled)



95% Gaussian Parameter Confidence Interval Plot

Plot using a single color.

plot(ciParamUnpooled, 'Color',[0 0 0])

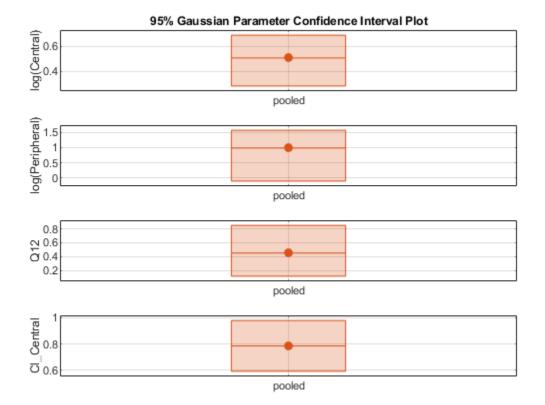


95% Gaussian Parameter Confidence Interval Plot

Compute the confidence intervals for the pooled fit.

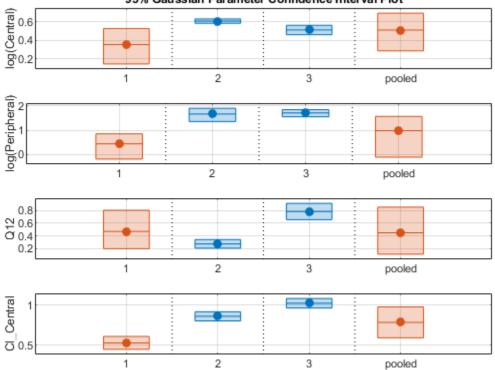
ciParamPooled = sbioparameterci(pooledFit);

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).

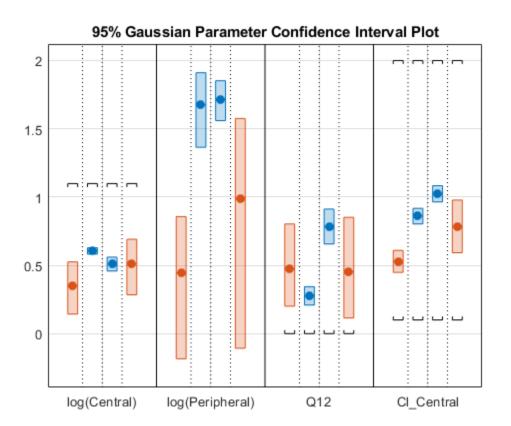
ciAll = [ciParamUnpooled;ciParamPooled];
plot(ciAll)



95% Gaussian Parameter Confidence Interval Plot

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.

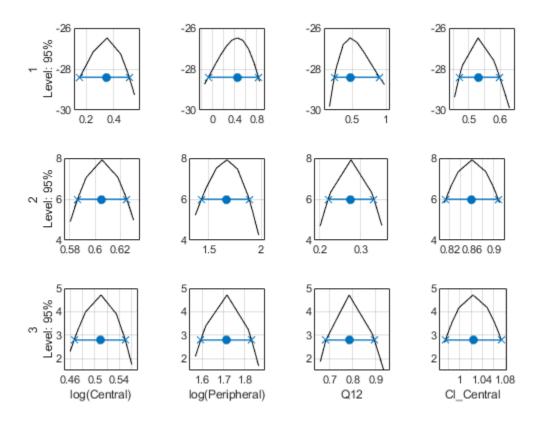
ciParamUnpooledProf = sbioparameterci(unpooledFit, 'Type', 'profilelikelihood');

Compute the confidence intervals for the pooled fit.

```
ciParamPooledProf = sbioparameterci(pooledFit, 'Type', 'profilelikelihood');
```

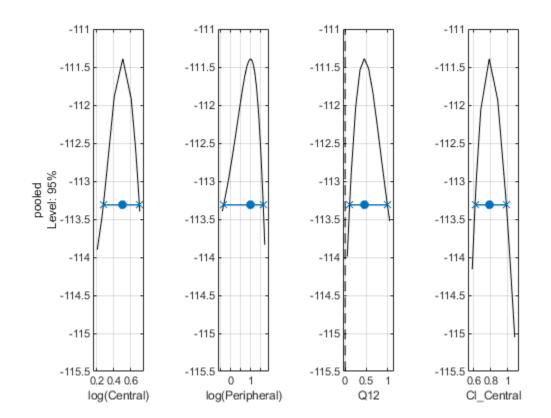
Plot the profile likelihood curves for the unpooled fit. The parameter bounds defined in the original fit are displayed by vertical dotted lines (if visible in the parameter range being plotted). The confidence interval is indicated by two crosses and a line in between them. The center dot denotes the 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);

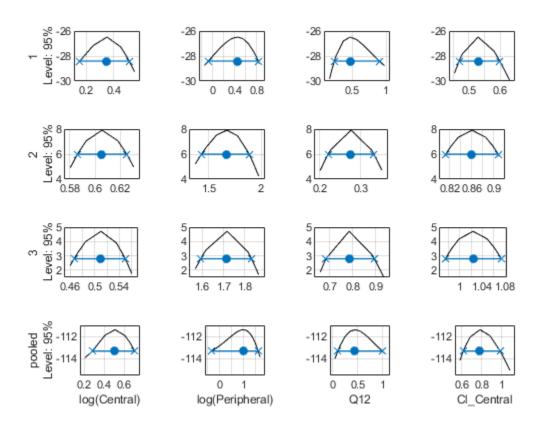


Each group is plotted in a separate row, and each parameter is plotted in a separate column. Plot the curves for the pooled fit.

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 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: '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.

See Also

ParameterConfidenceInterval | sbioparameterci

Introduced in R2017b

plot

Package: SimBiology.fit

Plot confidence interval results for model predictions

Syntax

fh = plot(predCI)

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.

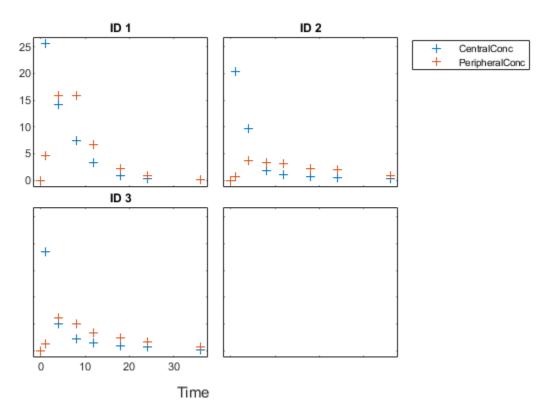
Examples

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.

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

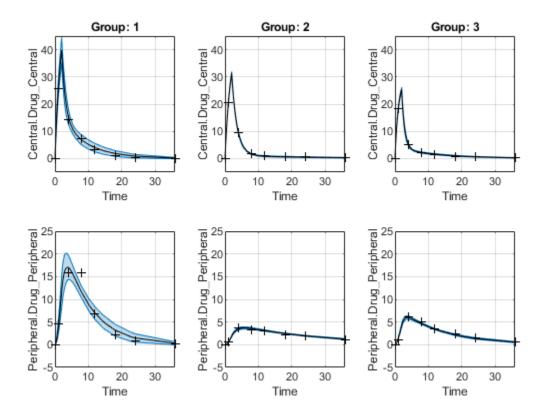
Compute 95% confidence intervals for predicted model responses in the unpooled fit using the Gaussian approximation.

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').

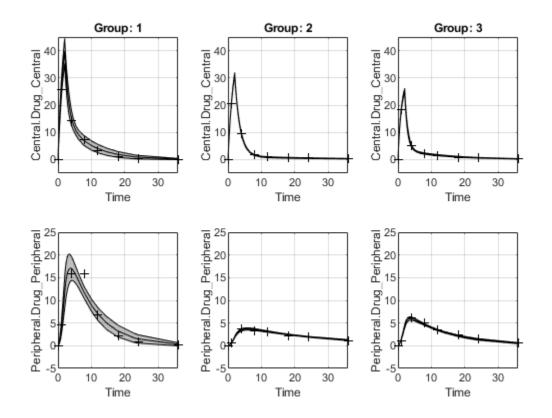
Each group is displayed in each column, from left to right, in the same order that they appear in the GroupNames property of the object, which is used to label each column.

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.

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: 'Color', [0 0 0] specifies to plot using only the color black.

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 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]

Output Arguments

fh — Figure handle handle

Figure handle of the plot, returned as a figure handle.

See Also

ParameterConfidenceInterval | PredictionConfidenceInterval | sbioparameterci |
sbiopredictionci

Introduced in R2017b

plot

Plot empirical CDF of multiparametric global sensitivity analysis

Syntax

h = plot(mpgsaObj) h = plot(mpgsaObj,Name,Value)

Description

h = plot(mpgsa0bj) 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".

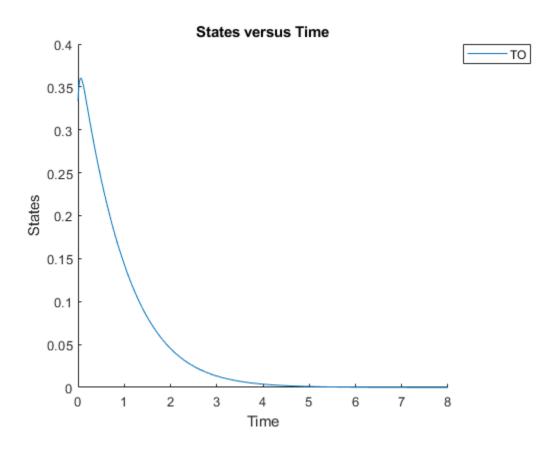
```
sbioloadproject tmdd_with_T0.sbproj
```

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 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,T0) <= 0.1';</pre>
```

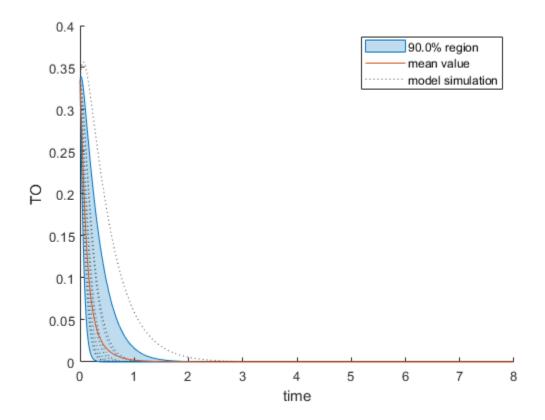
Perform MPGSA to find sensitive parameters with respect to the TO. Vary the parameter values between predefined bounds to generate 10,000 parameter samples.

```
% 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,T0) <= 0.1'}</pre>
    KolmogorovSmirnovStatistics: [4x1 table]
                        ECDFData: {4x4 cell}
              SignificanceLevel: 0.0500
                         PValues: [4x1 table]
              SupportHypothesis: [10000x1 table]
                     Observables: {'TO'}
                ParameterSamples: [10000x4 table]
```

SimulationInfo: [1x1 struct]

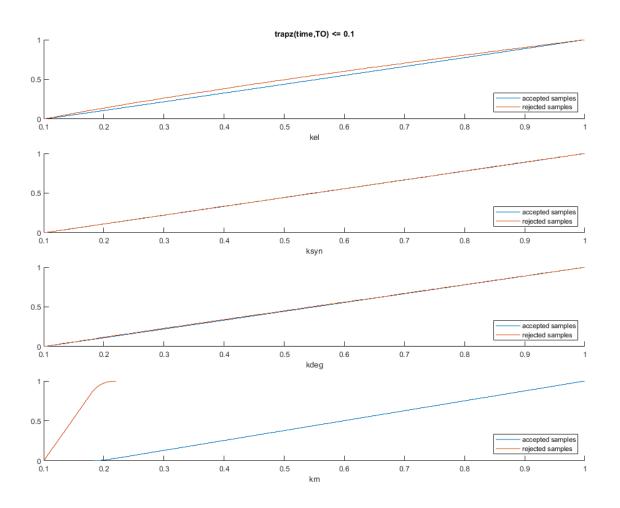
Plot the quantiles of the simulated model response.

plotData(mpgsaResults);



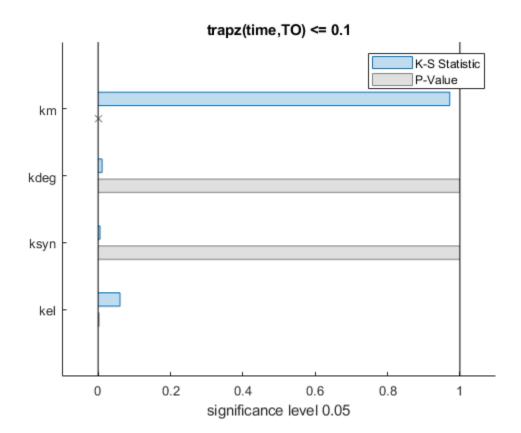
Plot the empirical cumulative distribution functions (eCDFs) of the accepted and rejected samples. Except for km, none of the parameters shows a significant difference in the eCDFs for the accepted and rejected samples. The km plot shows a large Kolmogorov-Smirnov (K-S) distance between the eCDFs of 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)



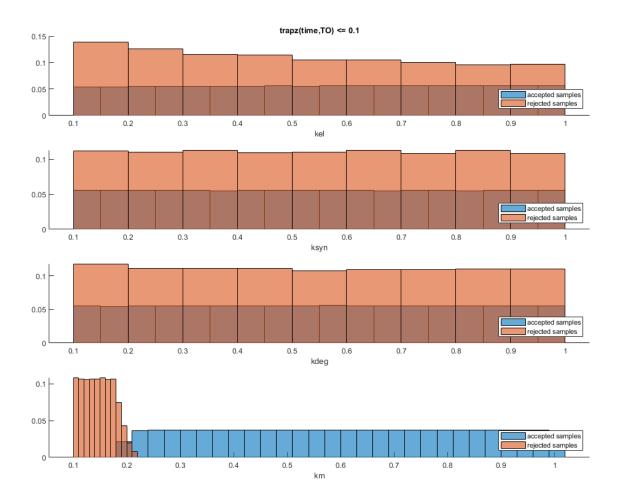
The bar plot shows two bars for each parameter: one for the K-S distance (K-S statistic) and another for the corresponding p-value. You reject the null hypothesis if the p-value is less than the significance level. A cross (x) is shown for any p-value that is almost 0. You can see the exact p-value corresponding to each parameter.

[mpgsaResults.ParameterSamples.Properties.VariableNames',mpgsaResults.PValues]

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 histograms 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

mpgsa0bj — 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 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: 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 the comma-separated pair consisting of 'Parameters' and a character vector, string, string vector, cell array of character vectors, or a vector of positive integers indexing into the columns of the mpgsa0bj.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 the comma-separated pair consisting of 'Classifiers' and 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 eCDFs of accepted samples

three-element row vector

Color of eCDFs of accepted samples, specified as the comma-separated pair consisting of 'AcceptedSamplesColor' and a three-element row vector. 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.

Example: 'AcceptedSamplesColor',[0.4,0.3,0.2]

Data Types: double

RejectedSamplesColor — Color of eCDFs of rejected samples

three-element row vector

Color of eCDFs of rejected samples, specified as the comma-separated pair consisting of 'RejectedSamplesColor' and a three-element row vector. By default, the function uses the second 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.

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.

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 | bar | ecdf | histogram | kstest2 | plotData | sbiompgsa

Introduced in R2020a

plot

Plot first- and total-order Sobol indices and variances

Syntax

h = plot(sobolObj) h = plot(sobolObj,Name,Value)

Description

h = plot(sobol0bj) plots the variance decomposition in the form of the first- and total-order Sobol indices and returns the figure handle h.

h = plot(sobol0bj,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.

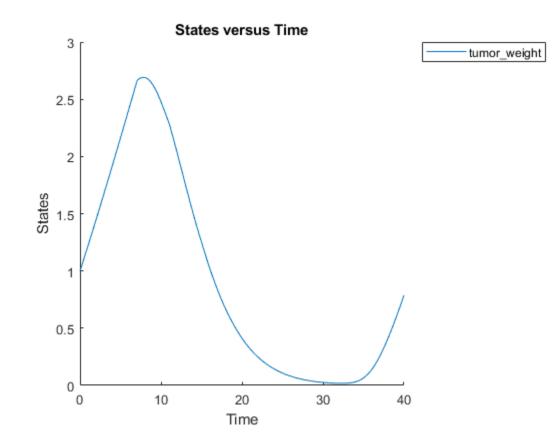
v = getvariant(m1); d = getdose(m1,'interval_dose');

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].

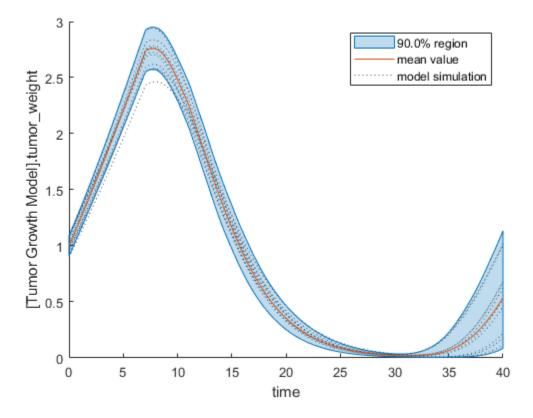
sobolResults = sbiosobol(m1,modelParamNames,outputName,'Variants',v,'Doses',d,'ShowWaitBar',true

```
sobolResults =
   Sobol with properties:
        Time: [444x1 double]
        SobolIndices: [5x1 struct]
        Variance: [444x1 table]
        Observables: {'[Tumor Growth Model].tumor_weight'}
   ParameterSamples: [1000x5 table]
        SimulationInfo: [1x1 struct]
```

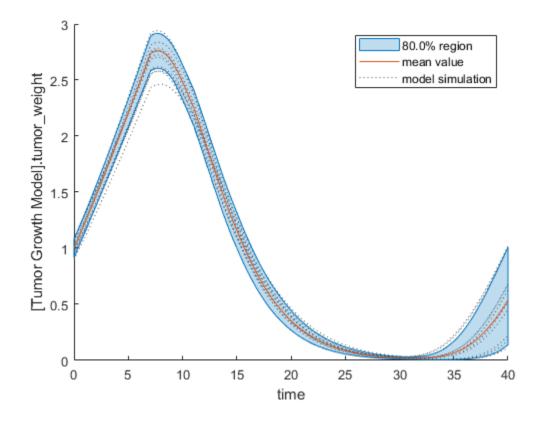
You can change the number of samples by specifying the 'NumberSamples' name-value pair argument. The function requires a total of (number of input parameters + 2) * NumberSamples model simulations.

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

plotData(sobolResults);

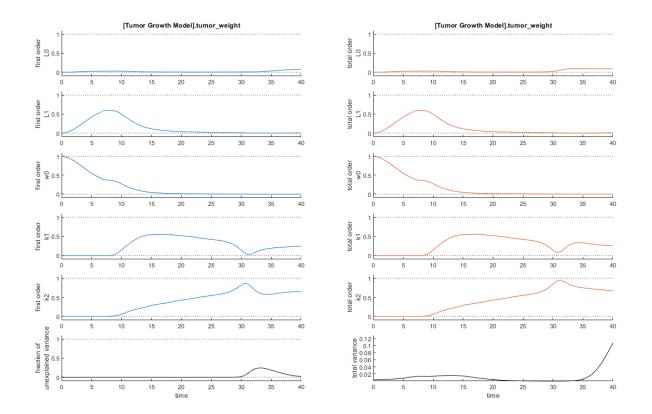


plotData(sobolResults, 'Alphas',0.1);



Plot the time course of the first- and total-order Sobol indices.

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

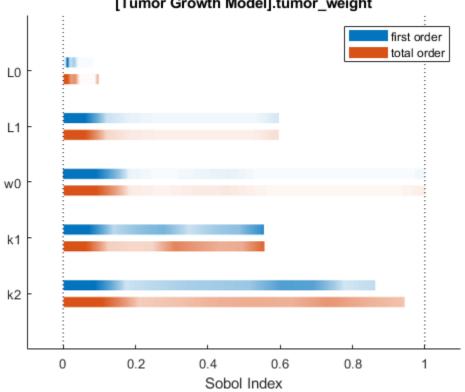


The first-order Sobol index of an input parameter gives the fraction of the overall response variance that can be attributed to variations in the input parameter alone. The total-order index gives the fraction of the overall response variance that can be attributed to any joint parameter variations that 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.

bar(sobolResults)



[Tumor Growth Model].tumor_weight

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: ModelName: DataCount: Name: 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.

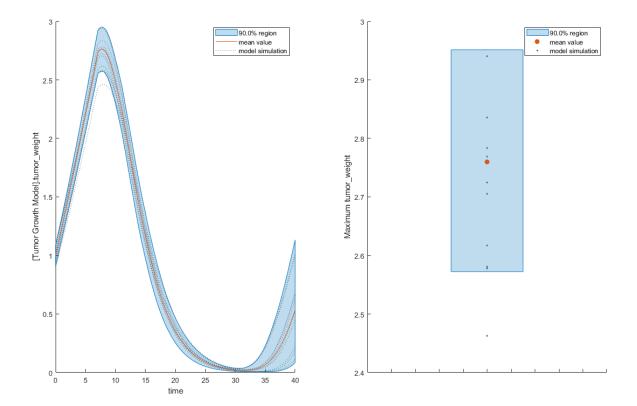
```
[samplesUsed,sd,validruns] = getSimulationResults(sobolResults,4);
```

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);
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 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: 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 the comma-separated pair consisting of 'Parameters' and a character vector, string, string vector, cell array of character vectors, or vector of positive integers indexing into the columns of the sobolObj.ParameterSamples table. Use this name-value pair argument to select parameters and plot their corresponding Sobol indices.

Example: 'Parameters', 'k1'

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 the comma-separated pair consisting of 'Observables and a character vector, string, string vector, cell array of character vectors, or vector of positive integers indexing into resultsObj.Observables.

Example: 'Observables', 'tumor_weight'

Data Types: double | char | string | cell

Color – Color of first- and total-order Sobol indices

three-element row vector

Color of the first- and total-order Sobol indices, specified as the comma-separated pair consisting of 'Color' and a three-element row vector. 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.

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

Color of the total and unexplained variances, specified as the comma-separated pair consisting of 'VarianceColor' and a three-element row vector. By default, the function uses the color black [0,0,0].

Example: 'VarianceColor',[0.2,0.5,0.8]

Data Types: double

DelimiterColor — Color of delimiting lines

[0,0,0] (default) | three-element row vector

Color of the total and unexplained variances, specified as a comma-separated pair consisting of 'DelimiterColor' and a three-element row vector. By default, the function uses the color black [0,0,0].

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.

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|bar|plotData|sbiosobol

Introduced in R2020a

plotActualVersusPredicted(LeastSquaresResults,O ptimResults,NLINResults)

Compare predictions to actual data, creating a subplot for each response

Syntax

plotActualVersusPredicted(resultsObj)

Description

plotActualVersusPredicted(results0bj) returns a figure displaying the comparison between
predictions to the actual data, with a subplot for each response.

Input Arguments

results0bj — 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.

See Also

NLINResults object | OptimResults object | sbiofit

Introduced in R2014a

plotActualVersusPredicted(NLMEResults)

Compare predictions to actual data, creating a subplot for each response

Syntax

plotActualVersusPredicted(results0bj)

Description

plotActualVersusPredicted(results0bj) 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.

See Also

NLMEResults object | sbiofitmixed

Introduced in R2014a

plotData

Plot quantile summary of model simulations from global sensitivity analysis (requires Statistics and Machine Learning Toolbox)

Syntax

```
h = plotData(results0bj)
h = plotData(results0bj,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 namevalue 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.

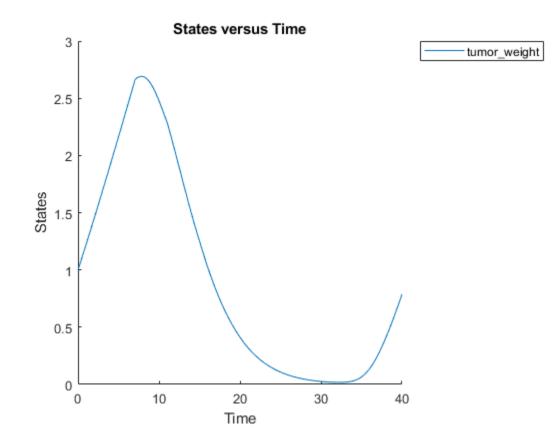
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

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';
```

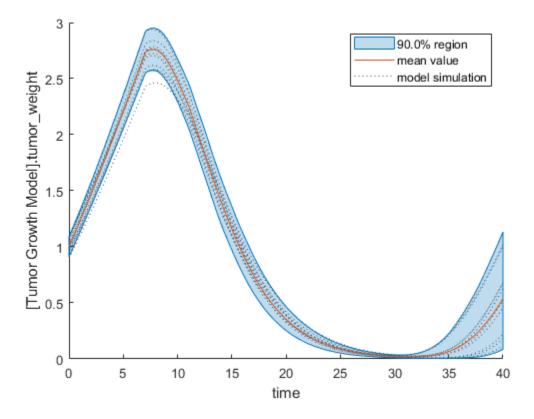
Then perform GSA by computing the first- and total-order Sobol indices using sbiosobol. Set 'ShowWaitBar' to true to show the simulation progress. By default, the function uses 1000 parameter samples to compute the Sobol indices [1].

sobolResults = sbiosobol(m1,modelParamNames,outputName,'Variants',v,'Doses',d,'ShowWaitBar',true

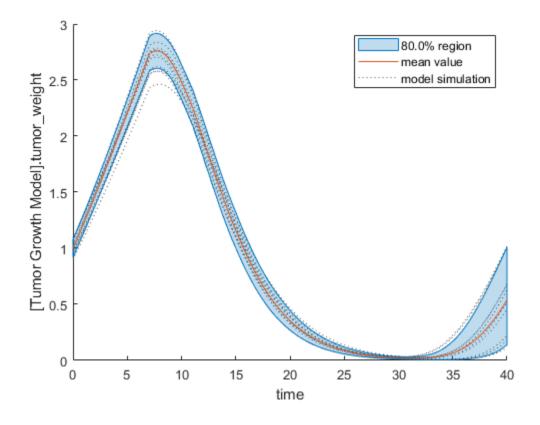
You can change the number of samples by specifying the 'NumberSamples' name-value pair argument. The function requires a total of (number of input parameters + 2) * NumberSamples model simulations.

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

plotData(sobolResults);

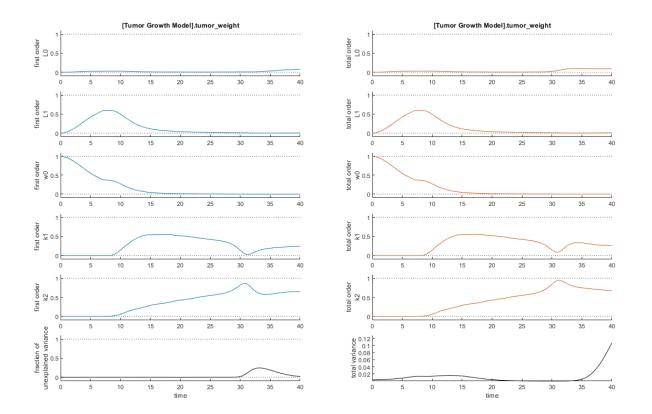


plotData(sobolResults, 'Alphas',0.1);



Plot the time course of the first- and total-order Sobol indices.

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

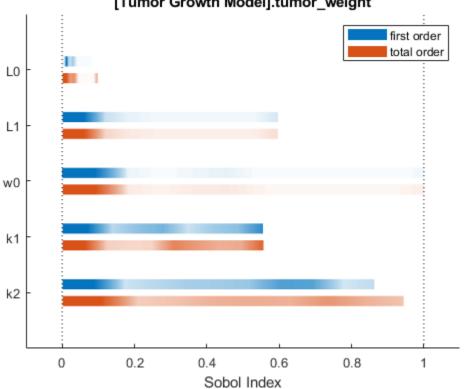


The first-order Sobol index of an input parameter gives the fraction of the overall response variance that can be attributed to variations in the input parameter alone. The total-order index gives the fraction of the overall response variance that can be attributed to any joint parameter variations that 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.

bar(sobolResults)



[Tumor Growth Model].tumor_weight

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: ModelName: DataCount: Name: 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

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.

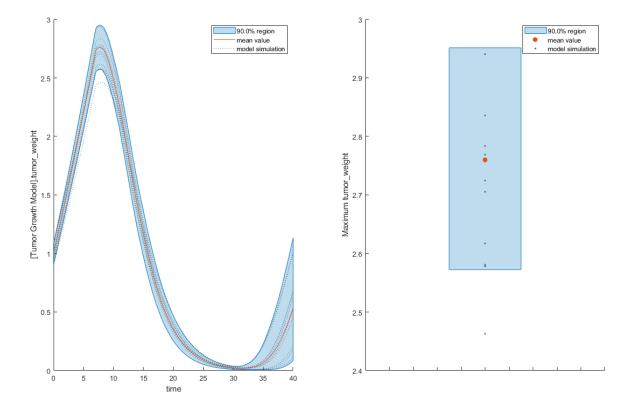
```
[samplesUsed,sd,validruns] = getSimulationResults(sobolResults,4);
```

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);
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".

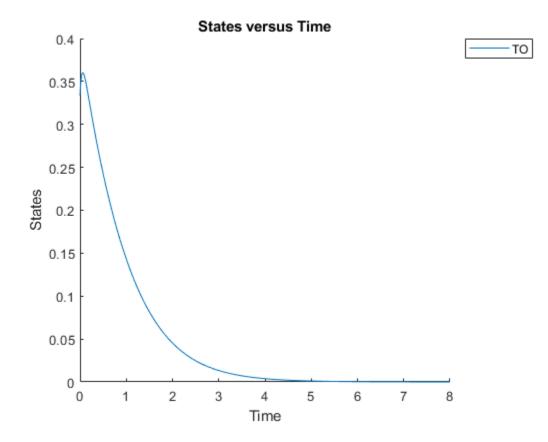
```
sbioloadproject tmdd_with_T0.sbproj
```

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));



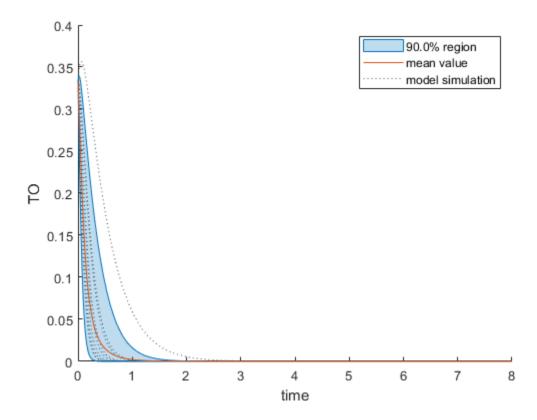
Define an exposure (area under the curve of the TO profile) threshold for the target occupancy.
classifier = 'trapz(time,TO) <= 0.1';</pre>

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;
            0.1, 1];
mpgsaResults = sbiompgsa(m1,params,classifier,'Bounds',bounds,'NumberSamples',10000)
mpgsaResults =
  MPGSA with properties:
                        Classifiers: {'trapz(time,T0) <= 0.1'}</pre>
    KolmogorovSmirnovStatistics: [4x1 table]
                           ECDFData: {4x4 cell}
                 SignificanceLevel: 0.0500
                            PValues: [4x1 table]
                 SupportHypothesis: [10000x1 table]
                        Observables: {'TO'}
                  ParameterSamples: [10000x4 table]
                    SimulationInfo: [1x1 struct]
```

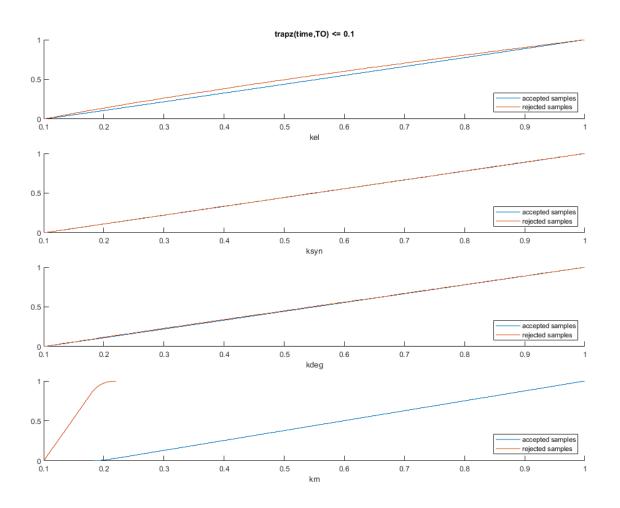
Plot the quantiles of the simulated model response.

plotData(mpgsaResults);



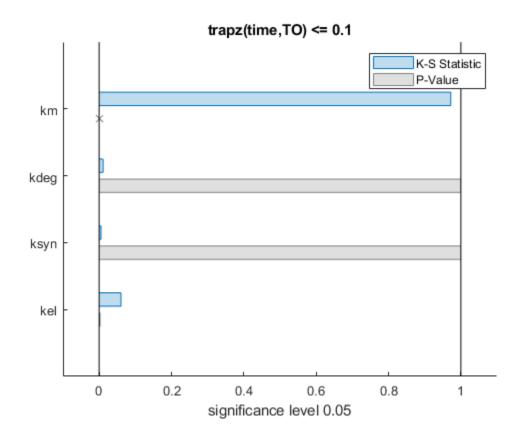
Plot the empirical cumulative distribution functions (eCDFs) of the accepted and rejected samples. Except for km, none of the parameters shows a significant difference in the eCDFs for the accepted and rejected samples. The km plot shows a large Kolmogorov-Smirnov (K-S) distance between the eCDFs of 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)



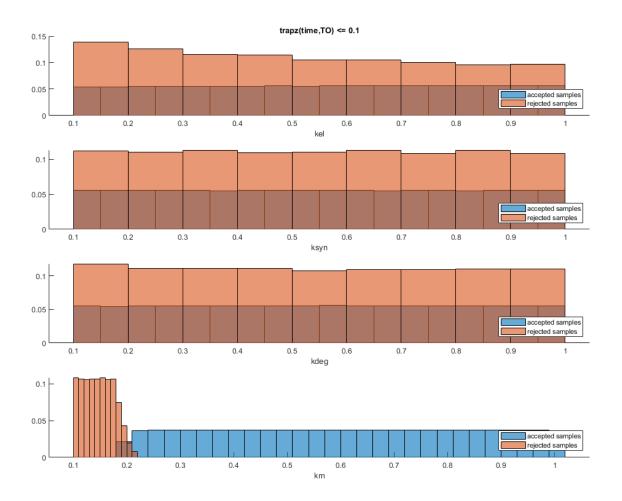
The bar plot shows two bars for each parameter: one for the K-S distance (K-S statistic) and another for the corresponding p-value. You reject the null hypothesis if the p-value is less than the significance level. A cross (x) is shown for any p-value that is almost 0. You can see the exact p-value corresponding to each parameter.

[mpgsaResults.ParameterSamples.Properties.VariableNames',mpgsaResults.PValues]

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 histograms 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

results0bj — Global sensitivity analysis results

SimBiology.gsa.Sobol object | SimBiology.gsa.MPGSA object

Global sensitivity analysis results, specified as a SimBiology.gsa.Sobol or SimBiology.gsa.MPGSA object.

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: h = plotData(results, 'ResponseLeap', 10) specifies to plot 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 the comma-separated pair consisting of 'Observables and a character vector, string, string vector, cell array of character vectors, or vector of positive integers indexing into resultsObj.Observables.

Example: 'Observables', 'tumor weight'

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 the comma-separated pair consisting of 'Alphas' and a positive scalar between 0 and 1 or numeric vector. The percentage of a region is calculated as $100 \times (1 - 2 \times Alpha)$. 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.

Example: 'Alphas',0.1

Data Types: double

FaceColor — Color of shaded regions

three-element row vector

Color of the shaded regions, specified as the comma-separated pair consisting of 'FaceColor' and a three-element row vector. 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.

Example: 'FaceColor', [0.4 0.3 0.2]

Data Types: double

MeanColor — Color of mean model response

three-element row vector

Color of the mean model response, specified as the comma-separated pair consisting of 'MeanColor' and a three-element row vector. 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.

Example: 'MeanColor', [0.2 0.5 0.8]

Data Types: double

ResponseColor — Color of model responses

[0.3 0.3 0.3] (default) | three-element row vector

Color of model responses or simulations, specified as a comma-separated pair consisting of 'ResponseColor' and a three-element row vector. By default, the function uses the color gray [0.3 0.3 0.3].

Example: 'MeanColor', [0.4 0.3 0.3]

Data Types: double

ResponseLeap — Every *n*th response to plot

positive integer

Every *n*th response to plot, specified as the comma-separated pair consisting of 'ResponseLeap' and a positive integer. By default, the function plots 10% of all model responses.

Example: 'ResponseLeap', 15

Data Types: double

Output Arguments

h — Handle figure handle

Handle to the figure, specified as a figure handle.

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|bar|plot|sbiosobol

Introduced in R2020a

plotResiduals(LeastSquaresResults,OptimResults, NLINResults)

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 predictions as the x-axis as specified by the argument type.

Input Arguments

results0bj — 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'.

See Also

NLINResults object | OptimResults object | sbiofit

plotResiduals(NLMEResults)

Plot the residuals for each response, using the time, group, or prediction as the x-axis

Syntax

plotResiduals(results0bj,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'.

See Also

NLMEResults object | sbiofitmixed

plotResidualDistribution(LeastSquaresResults,Opti mResults,NLINResults)

Plot the distribution of the residuals

Syntax

plotResidualDistribution(resultsObj)

Description

plotResidualDistribution(results0bj) plots the distribution of the residuals.

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.

See Also

NLINResults object | OptimResults object | sbiofit

plotResidualDistribution(NLMEResults)

Plot the distribution of the residuals

Syntax

plotResidualDistribution(results0bj)

Description

plotResidualDistribution(results0bj) 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.

See Also

NLMEResults object | sbiofitmixed

predict(LeastSquaresResults,OptimResults,NLINRe sults)

Simulate and evaluate fitted SimBiology model

Syntax

```
[ynew,parameterEstimates]= predict(resultsObj)
[ynew,parameterEstimates]= predict(resultsObj,data,dosing)
```

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.

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 results0bj.

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 SimBiology dose objects

Dosing information, specified as an empty array [] or 2-D matrix of SimBiology dose objects (ScheduleDose object or RepeatDose object). If dosing is a matrix of dose objects, the matrix must contain default doses or be consistent with the original dosing data used with sbiofit. That is, dose objects in dosing 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.

- If empty, no doses are applied during simulation, even if the model has active doses.
- If not empty, the matrix 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. If some groups (or time vectors) require more doses than others, then fill in the matrix with default (dummy) doses.
- Multiple columns are allowed so that you can apply multiple dose objects to each group or time vector. All doses in a column must be default doses or must reference the same components in the model (for instance, the doses must have the same dose target TargetName) and must have consistent parameterized properties as in the original dosing data used with sbiofit. For example, if 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 dosing must have the Amount property parameterized to 'A'.
- A default dose has default values for all properties, except for the Name property. Create a default dose as follows.

d1 = sbiodose('d1');

• In addition to manually constructing dose objects using sbiodose, if the input data is a groupedData object and has dosing information, you can use the createDoses method to construct doses from it.

The number of rows in the dosing matrix 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.

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.
Ν	0, that is, dosing is empty []	The total number of SimData objects in ynew is N.
		No doses are applied during simulation.
Ν	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. The predict method uses these parameter values during 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.

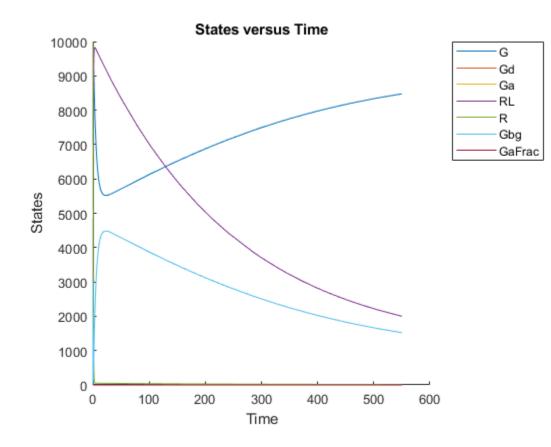
T = [0; 10; 50; 80; 100; 150; 300; 350; 400; 450; 500; 550];

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.

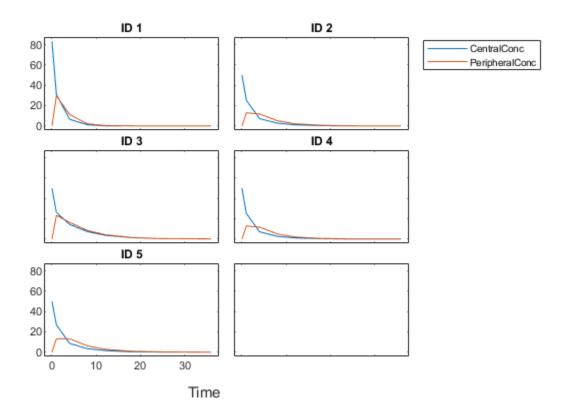
```
gData.Properties
```

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:
                                          =
                                           addCompartment(pkmd, 'Peripheral');
pkc2
model
                                           construct(pkmd);
                                          =
confiaset
                                          = 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]);
```

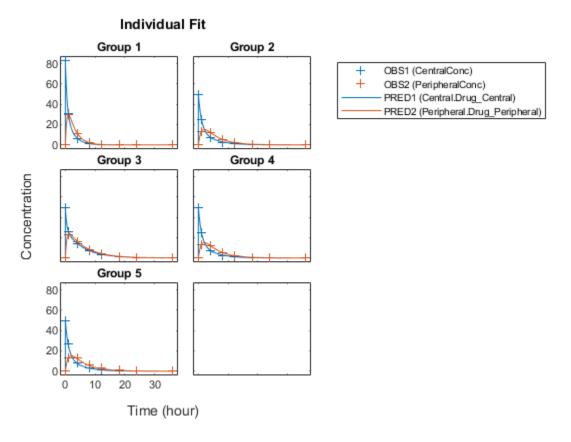
Use the 'CategoryVariableName' property of the estimatedInfo object to specify which category to use during fitting. Use 'Sex' as the group to fit for the clearance Cl_Central and Q12 parameters. Use 'Age' as the group to fit for the Central and Peripheral parameters.

```
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}
    EstimatedParameterNames: {'Central'
ErrorModelInfo: [1x3 table]
                                          'Peripheral' 'Q12' 'Cl Central'}
         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);



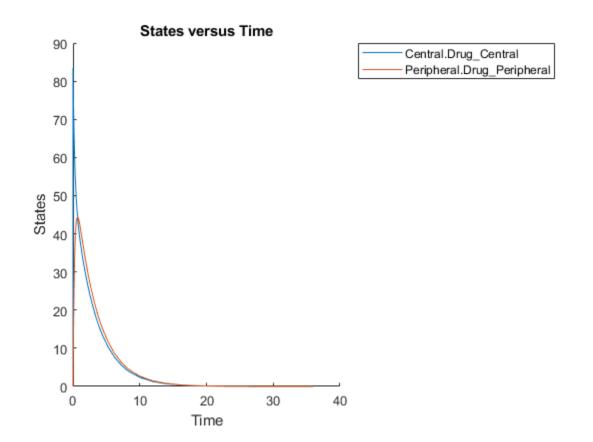
As for testing purposes, simulate the responses of the 6th individual who is an old male. Since you have estimated one set of parameters for the Age category (young versus old), and another set for Sex category (male versus female), you can simulate the responses of an old male even though there is no such individual in the training data.

Use the predict method to simulate the responses. ynew contains simulation data and parametrim contains parameter estimates used during simulation.

[ynew,paramestim] = predict(categoryFit,testData,dose);

Plot the simulated responses of the old male.

sbioplot(ynew);



The parameterin 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.

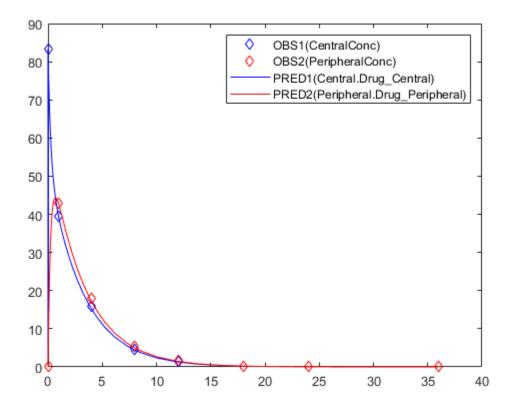
paramestim

paramestim=4×6 table Name	Estimate	StandardError	Group	CategoryVariableName	CategoryValue
{'Central' } {'Peripheral'} {'012' }	1.1993 0.55195 1.4969	0.0046483 0.015098 0.074321	6 6 6	{'Age'} {'Age'} {'Sex'}	Old Old 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)'});
```



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(NLMEResults)

Simulate and evaluate fitted SimBiology model

Syntax

```
[ynew,parameterEstimates] = predict(resultsObj)
[ynew,parameterEstimates] = predict(resultsObj,data,dosing)
[ynew,parameterEstimates] = predict(____,'ParameterType',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(____, 'ParameterType',value) returns simulation results ynew from evaluating the fitted SimBiology model using either individual or population parameter estimates. The two choices for value are 'individual' (default) or 'population'.

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,:)

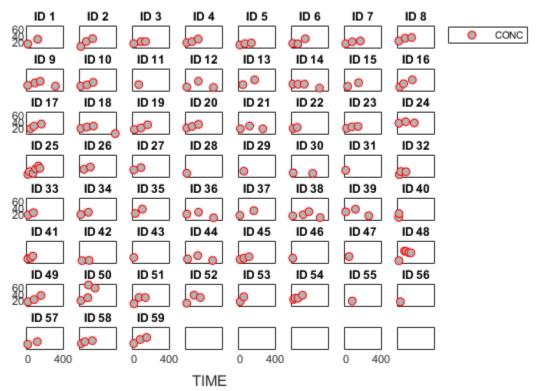
```
ans =
```

5×6 groupedData

ID	TIME	DOSE	WEIGHT	APGAR	CONC
1 1 1 1	0 2 12.5 24.5	25 NaN 3.5 3.5	1.4 1.4 1.4 1.4	7 7 7 7	NaN 17.3 NaN NaN
1	37	3.5	1.4	7	NaN

Visualize Data

Display the data in a trellis plot.



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

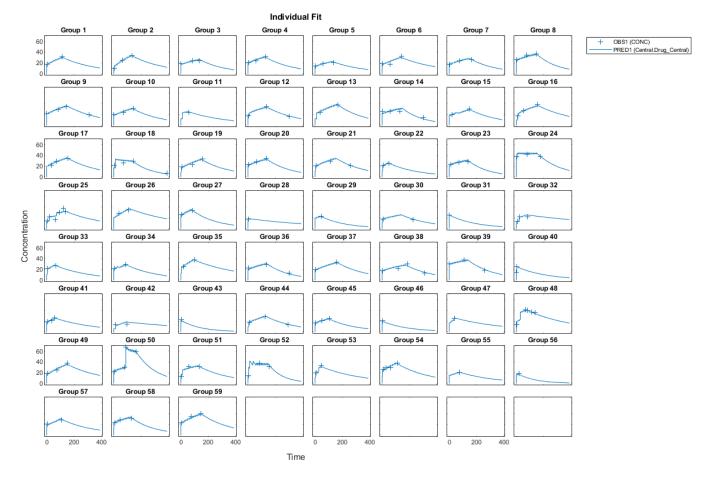
Use sbiofitmixed to fit the one-compartment model to the data.

```
nlmeResults = sbiofitmixed(onecomp,data,responseMap,estimatedParams,doses,'nlmefit');
```

Visualize Results

Visualize the fitted results using individual-specific parameter estimates.

```
fig1 = plot(nlmeResults,'ParameterType','individual');
% Resize the figure.
fig1.hFig.Position(:) = [100 100 1200 800];
```



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;
```

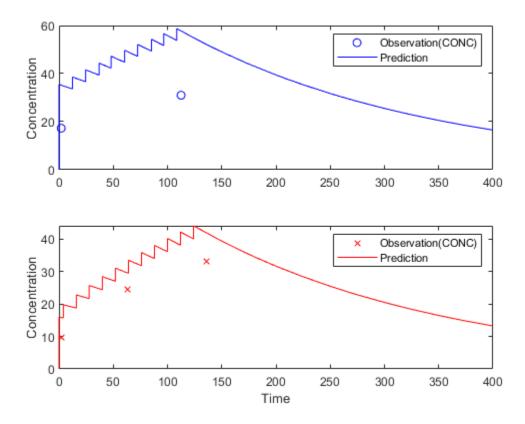
Use the predict function to evaluate the fitted model using the new dosing data. If you want response predictions at particular times, provide the new output time vector. Use the 'ParameterType' option to specify individual or population parameters to use. By default, predict uses the population parameters 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.

```
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(thetal + theta2*WEIGHT + etal)',...
'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 = 4×1 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
{'thetal'} {'theta3'} {'theta2'} {'theta2'}	{'Central' {'Cl_Central' {'Central/WEIGHT' {'Cl_Central/WEIGHT'	} } }	-0.45664 -5.9519 0.52948 0.61954	0.078933 0.1177 0.047342 0.071386

disp('Estimated Covariance Matrix:');

Estimated Covariance Matrix:

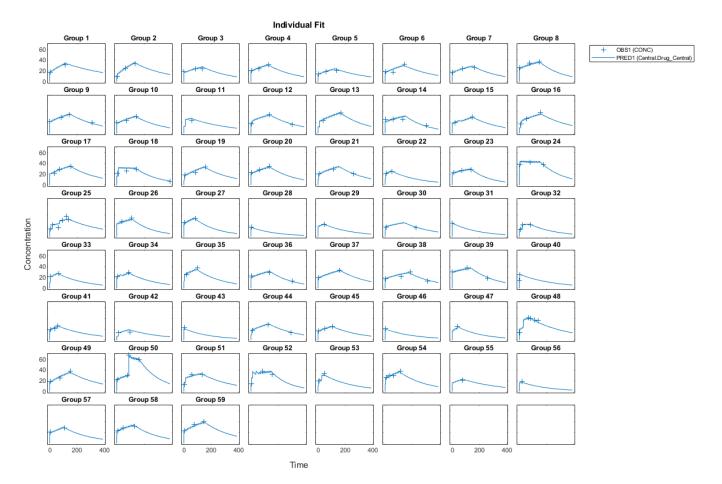
disp(nlmeResults_cov.RandomEffectCovarianceMatrix);

	etal	eta2
etal	0.046503	Θ
eta2	Θ	0.041609

Visualize Results

Visualize the fitted results using individual-specific parameter estimates.

```
fig2 = plot(nlmeResults_cov,'ParameterType','individual');
% Resize the figure.
fig2.hFig.Position(:) = [100 100 1200 800];
```



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 Group	s=4×3 table Name	Estimate
1	{'Central' }	2.5596
1	{'Cl_Central'}	0.0065965
2	{'Central' }	1.7123
2	{'Cl_Central'}	0.0064806

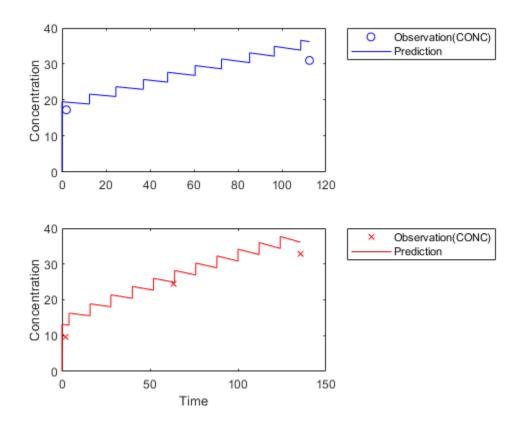
Compare to the estimated values from the original fit using the old covariate data.

```
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.

```
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 mixedeffects 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 covariate model on page 2-137.

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 SimBiology dose objects

Dosing information, specified as an empty array [] or 2-D matrix of SimBiology dose objects (ScheduleDose object or RepeatDose object). If dosing is a matrix of dose objects, the matrix must contain default doses or be consistent with the original dosing data used with sbiofitmixed. That is, dose objects in dosing 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 first column targets species x and the second column targets species y. Then dosing must have doses in the first column targeting species x and doses in the second column targeting species y.

- If empty, no doses are applied during simulation, even if the model has active doses.
- If not empty, the matrix 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. If some groups (or time vectors) require more doses than others, then fill in the matrix with default (dummy) doses.
- Multiple columns are allowed so that you can apply multiple dose objects to each group or time vector. All doses in a column must be default doses or must reference the same components in the model (for instance, the doses must have the same TargetName) and must have consistent parameterized properties as in the original dosing data used with sbiofitmixed. For example, if 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 dosing must have the Amount property parameterized to 'A'.
- A default dose has default values for all properties, except for the Name property. Create a default dose as follows.

d1 = sbiodose('d1');

• In addition to manually constructing dose objects using sbiodose, if the input data is a groupedData object and has dosing information, you can use the createDoses method to construct doses from it.

The number of rows in the dosing matrix 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.

value — 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 (θ s) 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 (θ s) and random effects (η s). 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.

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.
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.
Ν	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.

See Also

CovariateModel object | NLMEResults object | sbiofitmixed | sbiosampleerror | sbiosampleparameters

Topics

"Modeling the Population Pharmacokinetics of Phenobarbital in Neonates" "Nonlinear Mixed-Effects Modeling"

random(LeastSquaresResults,OptimResults,NLINR esults)

Simulate SimBiology model, adding variations by sampling error model

Syntax

```
[ynew,parameterEstimates] = random(resultsObj)
[ynew,parameterEstimates] = random(resultsObj,data,dosing)
```

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.

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. If there is a separate error model for each response, the noise is added to each response separately using the corresponding error model.

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 results0bj.

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 SimBiology dose objects

Dosing information, specified as an empty array [] or 2-D matrix of SimBiology dose objects (ScheduleDose object or RepeatDose object). If dosing is a matrix of dose objects, the matrix must contain default doses or be consistent with the original dosing data used with sbiofit. That is, dose objects in dosing 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.

- If empty, no doses are applied during simulation, even if the model has active doses.
- If not empty, the matrix 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. If some groups (or time vectors) require more doses than others, then fill in the matrix with default (dummy) doses.
- Multiple columns are allowed so that you can apply multiple dose objects to each group or time vector. All doses in a column must be default doses or must reference the same components in the model (for instance, the doses must have the same dose target TargetName) and must have consistent parameterized properties as in the original dosing data used with sbiofit. For example, if 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 dosing must have the Amount property parameterized to 'A'.
- A default dose has default values for all properties, except for the Name property. Create a default dose as follows.

d1 = sbiodose('d1');

• In addition to manually constructing dose objects using sbiodose, if the input data is a groupedData object and has dosing information, you can use the createDoses method to construct doses from it.

The number of rows in the dosing matrix 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.

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.
М	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.

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 more 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
```

Enter the experimental data containing the time course for the fraction of active G protein, as reported in the reference paper [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 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 pair 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 =

Name	Estimate	StandardError
'kGd'	0.11	0.00064116

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.

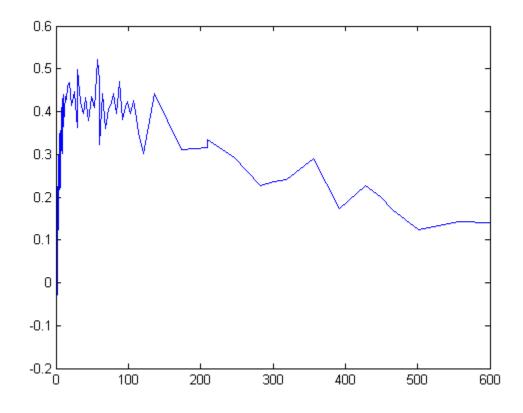
[ynew,paramEstim] = random(fitResult);

Select the simulation data for the GaFrac parameter.

GaFracNew = select(ynew,{'Name','GaFrac'});

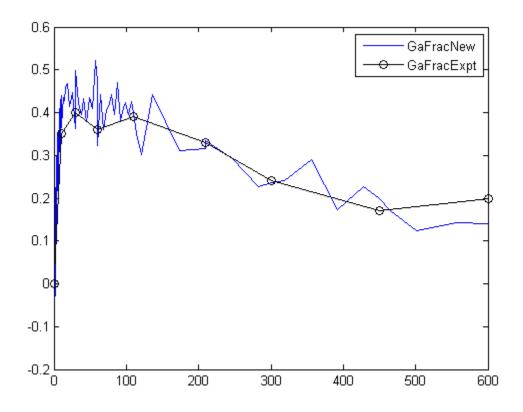
Plot the simulation results.

```
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')



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

Introduced in R2014a

random(NLMEResults)

Simulate a SimBiology model, adding variations by sampling the error model

Syntax

```
[ynew,parameterEstimates,randomEffects]= random(results0bj)
[ynew,parameterEstimates]= random(results0bj,data,dosing)
[ynew,parameterEstimates,randomEffects]= random(_,'ParameterType',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(_,'ParameterType',value) adds noise to simulation results that are simulated using either individual or population parameter estimates. The two choices for value are 'population' or 'individual' (default).

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.

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.

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.

For both cases, new parameter values are calculated using sbiosampleparameters with the covariate model returned by resultsObj.covariateModel, the fixed effect estimates (resultsObj.FixedEffects), and random effect covariance matrix (resultsObj.RandomEffectCovarianceMatrix).

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 SimBiology dose objects

Dosing information, specified as an empty array [] or 2-D matrix of SimBiology dose objects (ScheduleDose object or RepeatDose object). If dosing is a matrix of dose objects, the matrix must contain default doses or be consistent with the original dosing data used with sbiofitmixed. That is, dose objects in dosing 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 first column targets species x and the second column targets species y. Then dosing must have doses in the first column targeting species x and doses in the second column targeting species y.

- If empty, no doses are applied during simulation, even if the model has active doses.
- If not empty, the matrix 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. If some groups (or time vectors) require more doses than others, then fill in the matrix with default (dummy) doses.
- Multiple columns are allowed so that you can apply multiple dose objects to each group or time vector. All doses in a column must be default doses or must reference the same components in the model (for instance, the doses must have the same TargetName) and must have consistent parameterized properties as in the original dosing data used with sbiofitmixed. For example, if 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 dosing must have the Amount property parameterized to 'A'.
- A default dose has default values for all properties, except for the Name property. Create a default dose as follows.

d1 = sbiodose('d1');

• In addition to manually constructing dose objects using sbiodose, if the input data is a groupedData object and has dosing information, you can use the createDoses method to construct doses from it.

The number of rows in the dosing matrix 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.

value — Parameter type

'individual' (default) | 'population'

Parameter type, specified as 'population' or 'individual' (default). If value is 'population', the method returns the simulation results with noise using the 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.

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

(resultsubj.RandomEffectCovarianceMatrix). Parameter estimates and random effects are resampled for all groups.

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.
Ν	0, that is, dosing is empty []	The total number of SimData objects in ynew is N .
		No doses are applied during simulation.
Ν	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
Ν	N	The total number of SimData objects in ynew is <i>N</i> .
		Each row of dosing is applied to a separate group, in the same order that groups appear in data.
М	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.

See Also

NLMEResults object | sbiofitmixed | sbiosampleerror | sbiosampleparameters

Introduced in R2014a

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 <i>CategoryVariableName</i>
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 2-448)

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

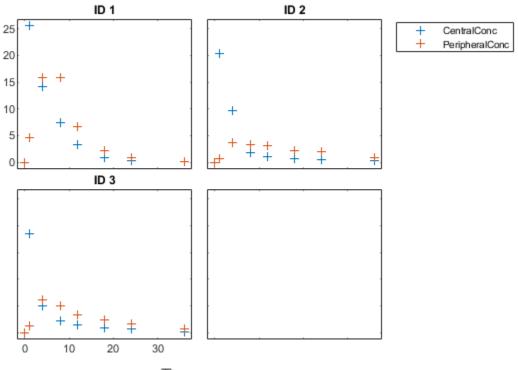
Examples

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');
```



Time

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 2-448.

```
ci2table(ciParamUnpooled)
```

```
ans =
```

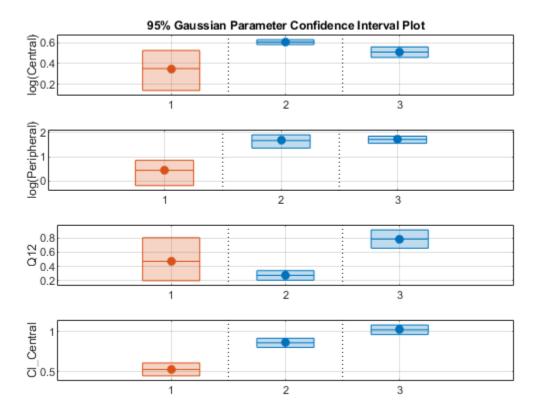
12x7 table

Group	Name	Estimate	Confidenc	eInterval	Туре	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	constraine
1	{'Q12' }	0.47159	0.20093	0.80247	Gaussian	0.05	constraine
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.

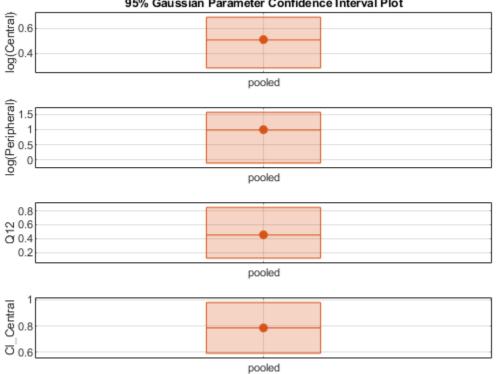
ci2table(ciParamPooled)

ans = 4x7 table

Group	Name	Estimate	Confidenc	eInterval	Туре	Alpha	Status
pooled pooled pooled pooled	{'Central' } {'Peripheral'} {'Q12' } {'Cl_Central'}	1.6626 2.687 0.44956 0.78493	1.3287 0.89848 0.11445 0.59222	1.9965 4.8323 0.85152 0.97764	Gaussian Gaussian Gaussian Gaussian	0.05 0.05 0.05 0.05 0.05	estimable constraine constraine estimable

Plot the confidence intervals. The group name is labeled as "pooled" to indicate such fit.

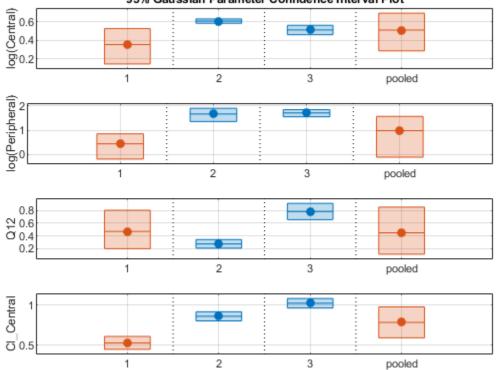
plot(ciParamPooled)



95% Gaussian Parameter Confidence Interval Plot

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.

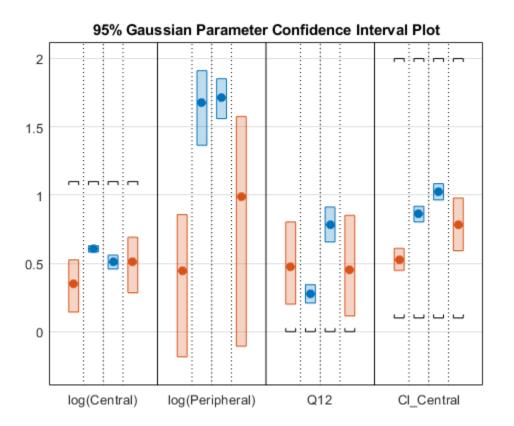
ciAll = [ciParamUnpooled;ciParamPooled]; plot(ciAll)



95% Gaussian Parameter Confidence Interval Plot

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

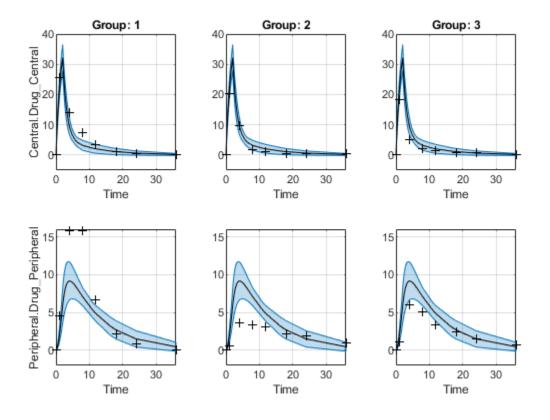
Calculate 95% confidence intervals for the model predictions, that is, simulation results using the estimated parameters.

```
% For the pooled fit
ciPredPooled = sbiopredictionci(pooledFit);
% For the unpooled fit
ciPredUnpooled = sbiopredictionci(unpooledFit);
```

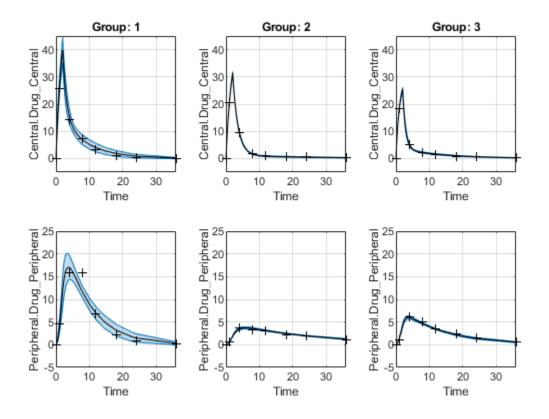
Plot Confidence Intervals for Model Predictions

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 1-167.

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 1-167.

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 1-169.

See Also

PredictionConfidenceInterval|sbioparameterci|sbiopredictionci

Introduced in R2017b

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 1-190 and "Bootstrap Confidence Interval Calculation" on page 1-190.

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

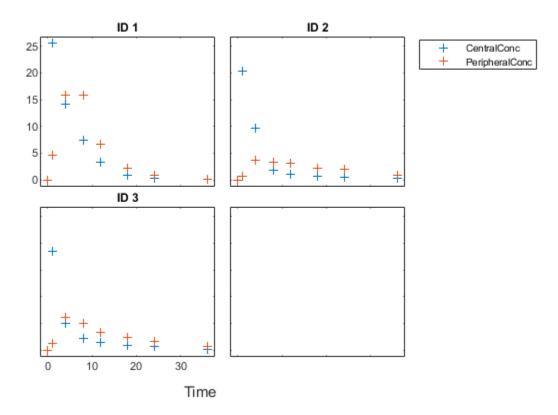
Examples

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; pkcl = 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 2-448.

```
ci2table(ciParamUnpooled)
```

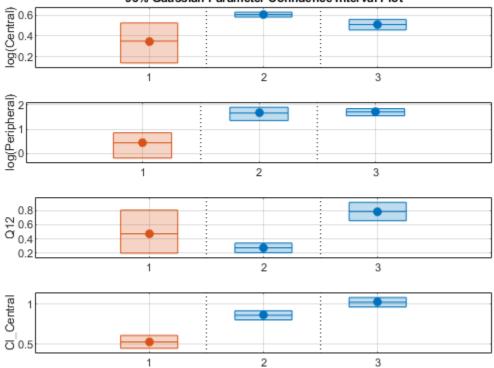
```
ans =
12x7 table
```

Group	Name	Estimate	Confidenc	eInterval	Туре	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	constraine
1	{'Q12' }	0.47159	0.20093	0.80247	Gaussian	0.05	constraine
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)



95% Gaussian Parameter Confidence Interval Plot

Compute the confidence intervals for the pooled fit.

ciParamPooled = sbioparameterci(pooledFit);

```
Display the confidence intervals.
```

```
ci2table(ciParamPooled)
```

ans =

4x7 table

Group	Name	Estimate	Confidenc	eInterval	Туре	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

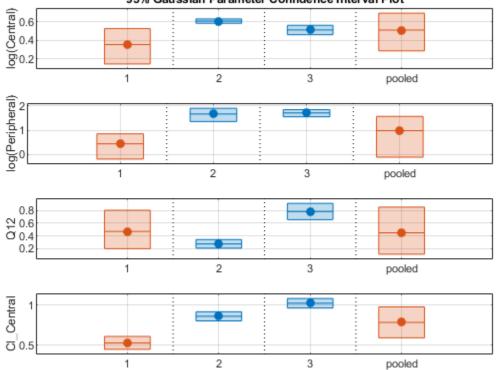
Plot the confidence intervals. The group name is labeled as "pooled" to indicate such fit.

```
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.

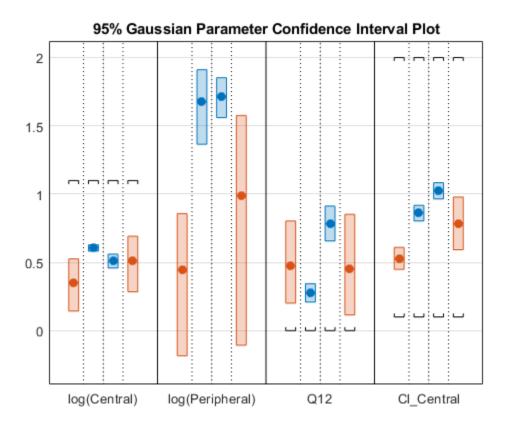
ciAll = [ciParamUnpooled;ciParamPooled]; plot(ciAll)



95% Gaussian Parameter Confidence Interval Plot

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

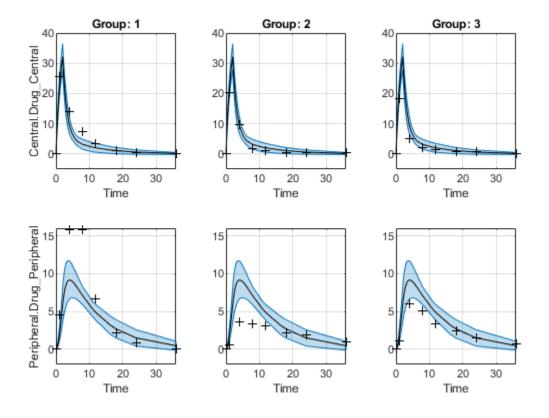
Calculate 95% confidence intervals for the model predictions, that is, simulation results using the estimated parameters.

```
% For the pooled fit
ciPredPooled = sbiopredictionci(pooledFit);
% For the unpooled fit
ciPredUnpooled = sbiopredictionci(unpooledFit);
```

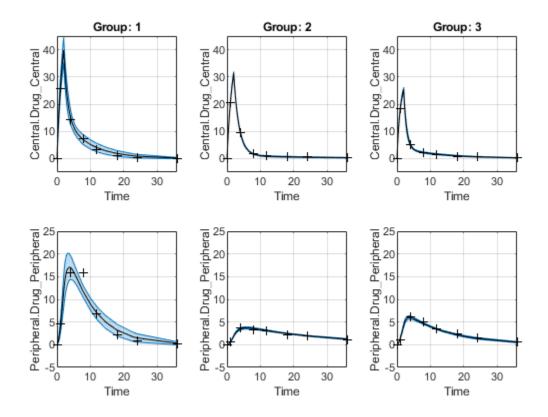
Plot Confidence Intervals for Model Predictions

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)



See Also ParameterConfidenceInterval|sbioparameterci|sbiopredictionci

Introduced in R2017b

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 H20

Spaces are required before and after species names and stoichiometric values.

See "Property Summary" on page 2-462 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
Туре	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

Introduced in R2006b

remove

Remove entries from SimBiology.Scenarios object

Syntax

s0bj = remove(s0bj,entryNameOrIndex) s0bj = remove(s0bj,entryIndex,subIndex)

Description

s0bj = remove(s0bj,entryNameOrIndex) removes the entry (or subentry on page 2-550)
entryNameorIndex from the SimBiology.Scenarios object s0bj.

s0bj = remove(s0bj,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 "Simulating 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.

```
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(s0bj)
```

```
scenariosTbl=5×2 table
variants dose
[1x1 SimBiology.Variant]
```

Change the entry name of the first entry.

```
rename(sObj,1,'Insulin Impairements')
ans =
Scenarios (5 scenarios)

Name
Content
Entry 1 Insulin Impairements SimBiology variants
x Entry 2 dose
SimBiology dose
```

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.

Number

5

1

f = createSimFunction(m1,sObj,{'[Plasma Glu Conc]','[Plasma Ins Conc]'},[])

f = SimFunction

Parameters:

Name	Value	Туре	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' }	Θ	{'parameter'}	{'1/minute'
{'f' }	0.9	{'parameter'}	{'dimensionless'
{'a' }	Θ	{'parameter'}	{'1/milligram'
{'b' }	0.82	{'parameter'}	{ 'dimensionless '
{'c' }	0	{'parameter'}	{'1/milligram'
{'d' }	0.01	{'parameter'}	{ 'dimensionless '
{'Stomach Glu After Dosing'}	78	{'parameter'}	{'gram'
{'kp1' }	2.7	{'parameter'}	{'milligram/minute'
{'kp2' }	0.0021	{'parameter'}	{'1/minute'
{'kp3' }	0.009	{'parameter'}	{ '(milligram/minute)/(picomole/li
{'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/li
{'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/de
{'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	Туре	Units
{'[Plasma Glu Conc]'}	{'species'}	{'milligram/deciliter'}
{'[Plasma Ins Conc]'}	{'species'}	{'picomole/liter' }

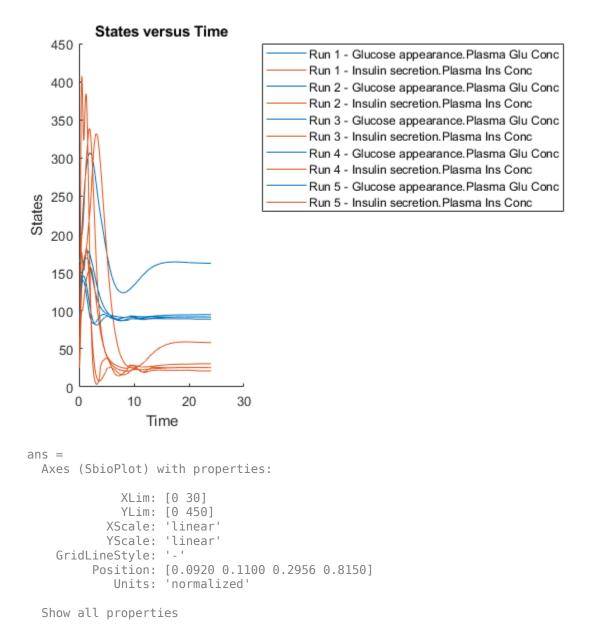
Dosed:

TargetName TargetDimension

{'Dose'} {'Mass (e.g., gram)'}

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(s0bj,24); sbioplot(sd)



If you have Statistics and Machine Learning ToolboxTM, 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 distribution 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 s0bj.

```
remove(s0bj,1)
ans =
   Scenarios (1 scenarios)
```

	Name	Content	Number
Entry 1	dose	SimBiology dose	1
See also Ex	pression	property.	

Add an entry that defines the joint probability distribution with a rank correlation matrix.

add(s0bj,'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(s0bj,2,'Number',50)
```

```
ans =
 Scenarios (50 scenarios)
                                    Content
                                                        Number
                    Name
    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.

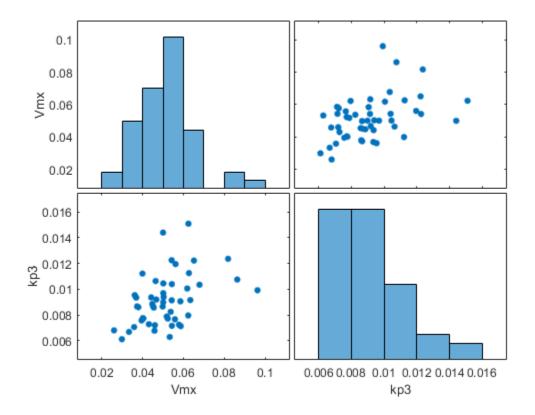
Verify that the Scenarios object can be simulated with the model. The verify function throws an error if any entry does not resolve uniquely to an object in the model or the entry contents have inconsistent lengths (sample sizes). The function throws a warning if multiple entries resolve to the same object in the model.

verify(s0bj,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.

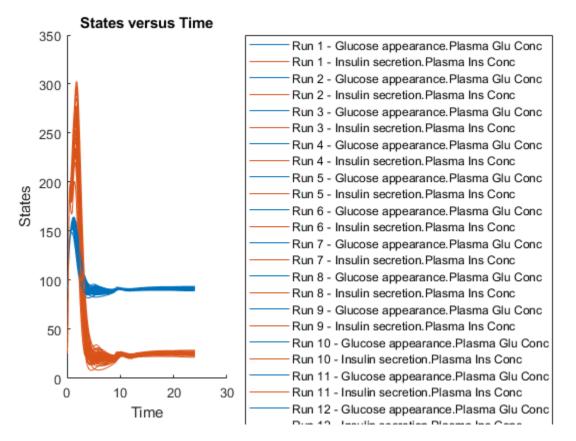
```
sTbl = generate(s0bj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl.Vmx,sTbl.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
```

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(s0bj,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(s0bj,2)
```

entry2struct.SamplingMethod = 'lhs'

You can now use the updated structure to modify entry 2.

```
updateEntry(s0bj,2,entry2struct)
```

```
ans =
 Scenarios (50 scenarios)
                    Name
                                    Content
                                                       Number
                            SimBiology dose
   Entry 1
                    dose
   x (Entry 2.1
                            Lognormal distribution
                    Vmx
                    kp3
   + Entry 2.2)
                            Lognormal distribution
```

1

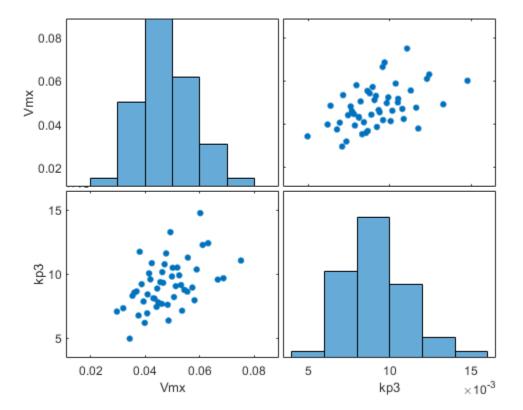
50

50

See also Expression property.

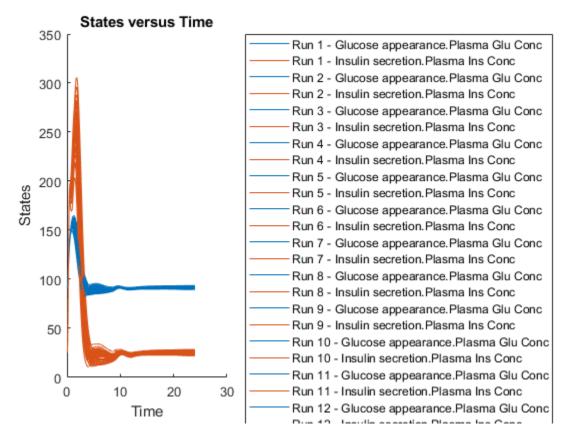
Visualize the sample values.

```
sTbl2 = generate(s0bj);
[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(s0bj, 24);sbioplot(sd3);



Restore warning settings.

warning(warnSettings);

Input Arguments

s0bj — 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

s0bj — Simulation scenarios

Scenarios object

Simulation scenarios, returned as a Scenarios object.

See Also

SimBiology.Scenarios | SimFunction object | createSimFunction (model)

Topics

"SimBiology.Scenarios Terminology" on page 2-550 "Combine Simulation Scenarios in SimBiology"

Introduced in R2019b

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.
configset0bj	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

Introduced in R2006a

removedose (model)

Remove dose object from model

Syntax

```
doseObj2 = removedose(modelObj, 'DoseName')
doseObj2 = removedose(modelObj, doseObj)
```

Arguments

model0bj	Model object from which you remove a dose object.
	Name of the dose object to remove from a model object. <i>DoseName</i> is the value of the dose object property Name.
dose0bj	Dose object to remove from a model object.

Outputs

dose0bj2	ScheduleDose or RepeatDose object.
3	1 5

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');
doselObj = adddose(modelObj, 'dosel');
```

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

Introduced in R2010a

removeobservable

Remove Sobol indices of observables

Syntax

results = removeobservable(sobol0bj,obsNames)

Description

results = removeobservable(sobolObj,obsNames) removes the Sobol indices computed for the specified observables obsNames from sobolObj.

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.

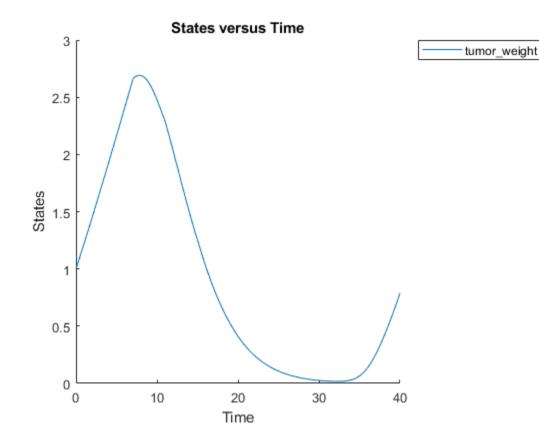
```
v = getvariant(m1);
d = getdose(m1,'interval_dose');
```

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';
```

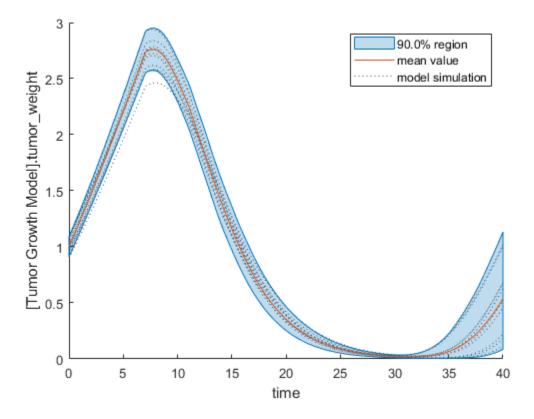
Then perform GSA by computing the first- and total-order Sobol indices using sbiosobol. Set 'ShowWaitBar' to true to show the simulation progress. By default, the function uses 1000 parameter samples to compute the Sobol indices [1].

sobolResults = sbiosobol(m1,modelParamNames,outputName,'Variants',v,'Doses',d,'ShowWaitBar',true

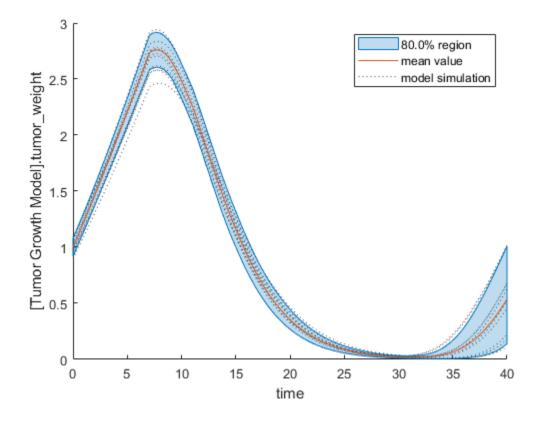
You can change the number of samples by specifying the 'NumberSamples' name-value pair argument. The function requires a total of (number of input parameters + 2) * NumberSamples model simulations.

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

plotData(sobolResults);

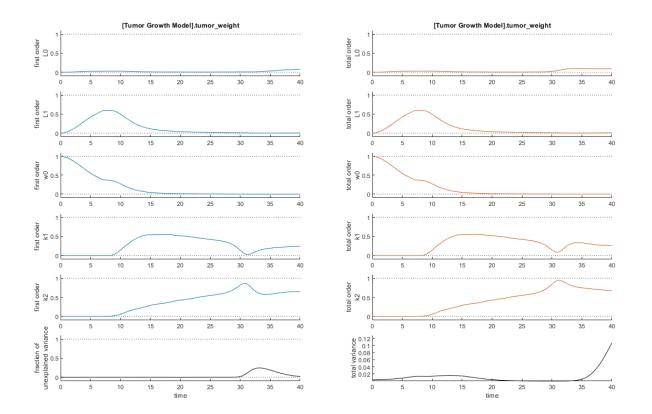


plotData(sobolResults, 'Alphas',0.1);



Plot the time course of the first- and total-order Sobol indices.

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

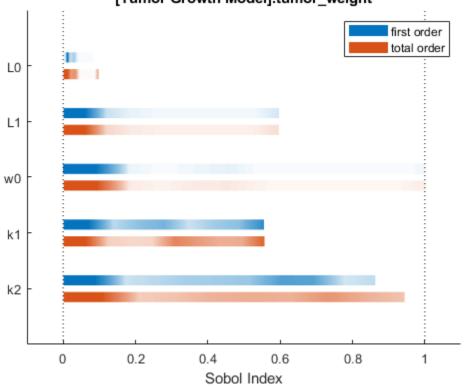


The first-order Sobol index of an input parameter gives the fraction of the overall response variance that can be attributed to variations in the input parameter alone. The total-order index gives the fraction of the overall response variance that can be attributed to any joint parameter variations that 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.

bar(sobolResults)



[Tumor Growth Model].tumor_weight

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-7Index:Name:ModelName:DataCount:1-Tumor Growth Model 12-Tumor Growth Model 13-Tumor Growth Model 1...-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

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.

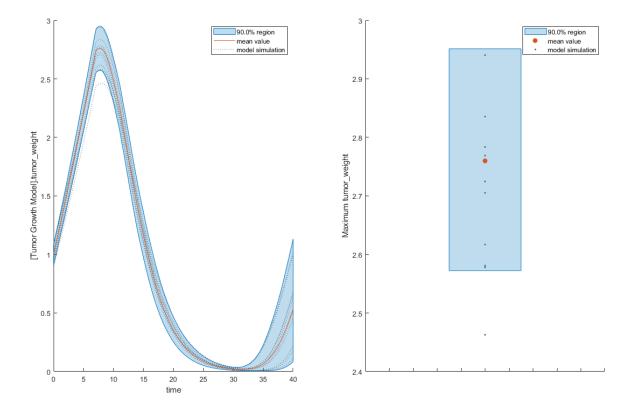
```
[samplesUsed,sd,validruns] = getSimulationResults(sobolResults,4);
```

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);
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

sobol0bj — Results containing Sobol indices

SimBiology.gsa.Sobol object

Results containing the first- and total-order Sobol indices, specified as a SimBiology.gsa.Sobol 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

Updated results after removal of the Sobol indices for specified observables, returned as a SimBiology.gsa.Sobol object.

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

Introduced in R2020a

removevariant (model)

Remove variant from model

Syntax

```
variantObj = removevariant(modelObj, 'NameValue')
```

```
variantObj = removevariant(modelObj, variantObj)
```

Arguments

-	Specify the Model object from which you want to remove the variant.
variant0bj	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(model0bj, 'v1');

- **3** Remove a variant object using its index number.
 - **a** Get the index number of the variant in the model.

v0bjs = getvariant(model0bj)

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

Introduced in R2007b

rename

Rename object and update expressions

Syntax

rename(Obj, 'NewNameValue')

Arguments

	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

Introduced in R2008b

rename

Rename entry from SimBiology.Scenarios object

Syntax

- s0bj = rename(s0bj,entryNameOrIndex,newName)
- s0bj = rename(s0bj,entryIndex,subIndex,newName)

Description

s0bj = rename(s0bj,entryNameOrIndex,newName) renames the entry (or subentry on page 2-550) entryNameorIndex to newName.

s0bj = rename(s0bj,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 "Simulating 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.

```
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(s0bj)
```

```
scenariosTbl=5×2 table
variants dose
[1x1 SimBiology.Variant]
```

Change the entry name of the first entry.

```
rename(sObj,1,'Insulin Impairements')
ans =
Scenarios (5 scenarios)

Name
Content
Number
Entry 1 Insulin Impairements
x Entry 2 dose
SimBiology variants
5
1
Soc also Expression property
```

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	Туре	Units
<pre>{'Plasma Volume (Glu)' {'k1' {'k2' {'Plasma Volume (Ins)' {'m1' {'m2' {'m4' {'m5' {'m6' }{'m6' }{'Hepatic Extraction' {'kmax' {'kmin' {'kabs' {'kgri' {'f' {'a' {'b' {'c' }{'d' {'Stomach Glu After Dosing'} {'kp1'</pre>	<pre> } 1.88 } 0.065 } 0.079 } 0.05 } 0.19 } 0.484 } 0.1936 } 0.6469 } 0.6469 } 0.66469 } 0.6558 } 0.008 } 0.0558 } 0.0568 } 0 } 0.9 } 0.9 } 0.9 } 0.82 } 0 } 0.01 } 78 } 2.7</pre>	<pre>{'parameter'} {'parameter'} {'parameter</pre>	<pre>{'deciliter' {'1/minute' {'1/minute' {'liter' {'1/minute' {'1/minute' {'1/minute' {'dimensionless' {'dimensionless' {'dimensionless' {'1/minute' {'1/minute' {'1/minute' {'1/minute' {'1/minute' {'1/minute' {'dimensionless' {'1/milligram' {'dimensionless' {'1/milligram' {'dimensionless' {'gram' {'milligram/minute'</pre>
<pre>{'kp2' {'kp3' {'kp4' } {'ki' } {'[Ins Ind Glu Util]' } {'Vm0' } {'Vmx' } {'Km' } {'p2U' } {'K' } {'alpha' } {'beta' } {'beta' } {'ke1' } {'ke2' } {'Basal Plasma Glu Conc'</pre>	<pre>} 0.0021 } 0.009 } 0.0618 } 0.0079 } 1 } 2.5129 } 0.047 } 225.59 } 0.0331 } 2.28 } 0.05 } 0.11 } 0.5 } 0.0005 } 339 } 91.76 } 25.49</pre>	<pre>{'parameter'} {'parameter'} }</pre>	<pre>{'1/minute' {'(milligram/minute)/(picomole/li' {'(milligram/minute)/picomole' {'1/minute' {'milligram/minute' {'milligram/minute)/(picomole/li' {'milligram' {'1/minute' {'picomole/(milligram/deciliter)' {'1/minute' {'(picomole/minute)/(milligram/deo {'1/minute' {'picomole/minute)/(milligram/deo {'1/minute' {'milligram'</pre>

Observables:

Name	Туре	Units
{'[Plasma Glu Conc]'}	{'species'}	{'milligram/deciliter'}
{'[Plasma Ins Conc]'}	{'species'}	{'picomole/liter' }

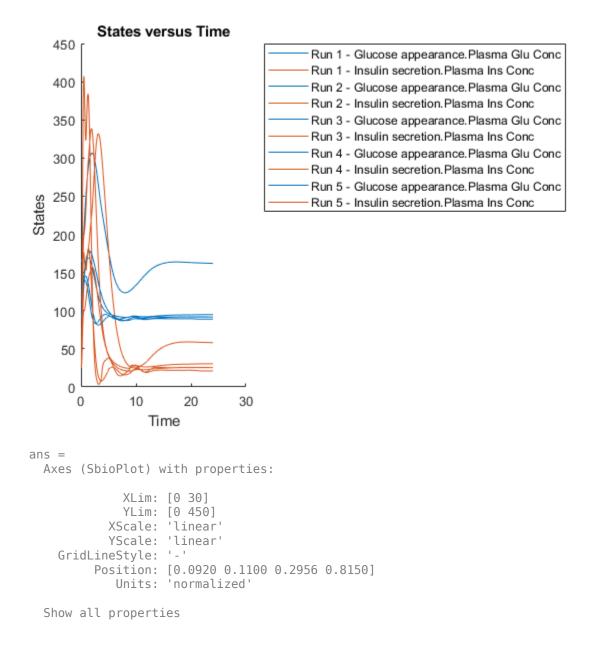
Dosed:

TargetName TargetDimension

{'Dose'} {'Mass (e.g., gram)'}

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(s0bj,24); sbioplot(sd)



If you have Statistics and Machine Learning ToolboxTM, 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 distribution 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 s0bj.

```
remove(s0bj,1)
ans =
   Scenarios (1 scenarios)
```

	Name	Content	Number
Entry 1	dose	SimBiology dose	1
See also Ex	pression	property.	

Add an entry that defines the joint probability distribution with a rank correlation matrix.

add(s0bj,'cartesian',["Vmx","kp3"],[pd_Vmx, pd_kp3],'RankCorrelation',[1,0.5;0.5,1])

```
ans =
 Scenarios (2 scenarios)
                                                          Number
                    Name
                                    Content
   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(s0bj,2,'Number',50)
```

```
ans =
 Scenarios (50 scenarios)
                                    Content
                                                        Number
                    Name
    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.

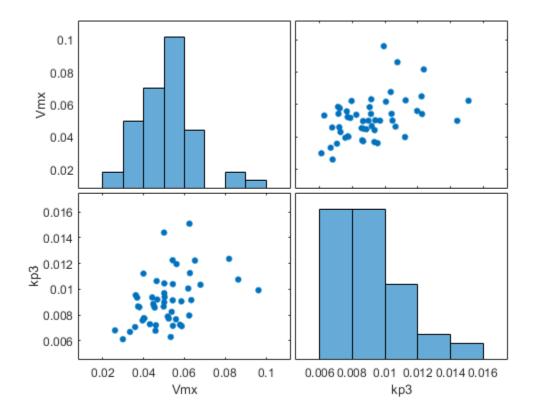
Verify that the Scenarios object can be simulated with the model. The verify function throws an error if any entry does not resolve uniquely to an object in the model or the entry contents have inconsistent lengths (sample sizes). The function throws a warning if multiple entries resolve to the same object in the model.

verify(s0bj,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.

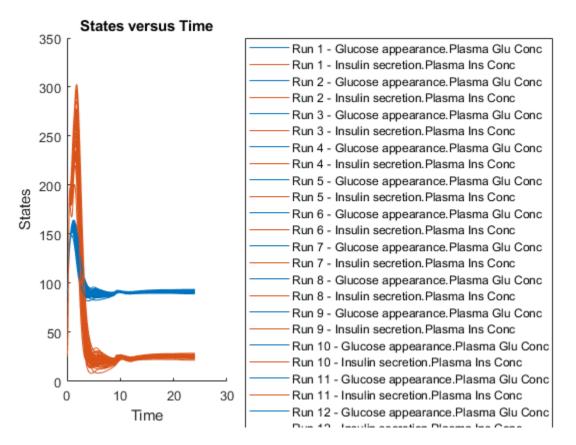
```
sTbl = generate(s0bj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl.Vmx,sTbl.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
```

```
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(s0bj,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(s0bj,2)

entry2struct.SamplingMethod = 'lhs'

You can now use the updated structure to modify entry 2.

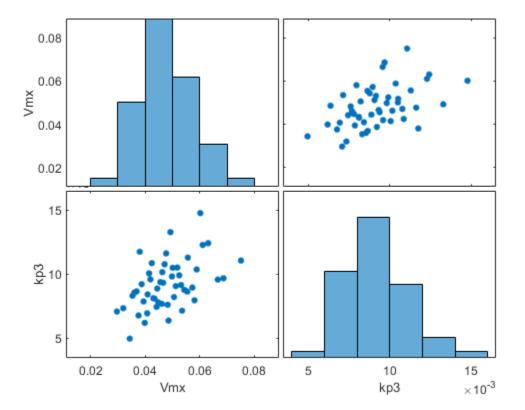
```
updateEntry(s0bj,2,entry2struct)
```

```
ans =
  Scenarios (50 scenarios)
                    Name
                                    Content
                                                        Number
                             SimBiology dose
    Entry 1
                    dose
                                                          1
                             Lognormal distribution
    x (Entry 2.1
                    Vmx
                                                          50
                    kp3
    + Entry 2.2)
                            Lognormal distribution
                                                          50
```

See also Expression property.

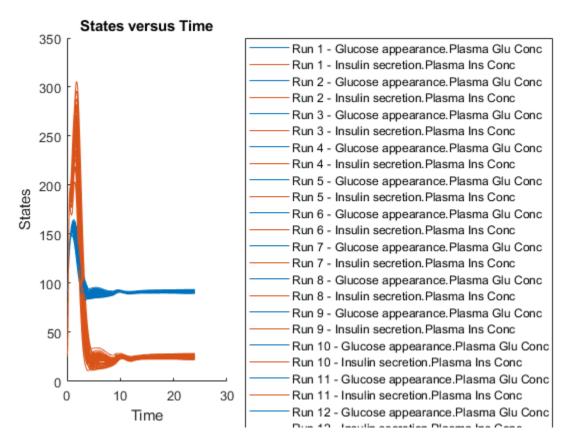
Visualize the sample values.

```
sTbl2 = generate(s0bj);
[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(s0bj,24); sbioplot(sd3);



Restore warning settings.

warning(warnSettings);

Input Arguments

s0bj — 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

s0bj — Simulation scenarios

Scenarios object

Simulation scenarios, returned as a Scenarios object.

See Also

SimBiology.Scenarios | SimFunction object | createSimFunction (model)

Topics

"SimBiology.Scenarios Terminology" on page 2-550 "Combine Simulation Scenarios in SimBiology"

Introduced in R2019b

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_T0.sbproj
```

Set the target occupancy (T0) as a response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'T0';
```

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,'T0',d)
f =
SimFunction
Parameters:
Name Value Type Units
```

{'AmountF	Param'}	1	{'parameter'}	{'nanomole'}		
)bservables:						
Name	Туре		Units			
{'T0'}	{'paramet	ter'}	{'dimensionless'}			
osed:						
TargetName TargetDimension			Amount	AmountValue		
			nt (e.g., mole or m		{'AmountParam'}	1

warning('on','SimBiology:SimFunction:DOSES_NOT_EMPTY');

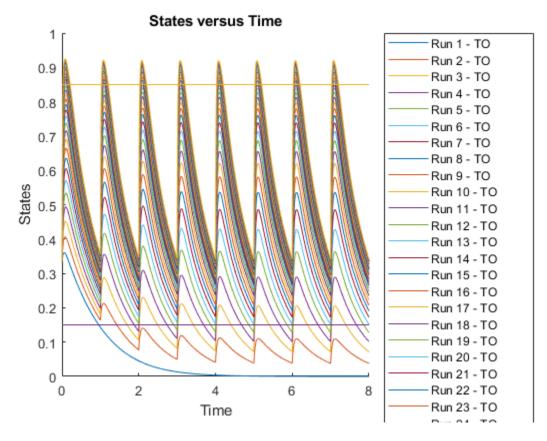
Simulate the model using the dose amounts generated by the Scenarios object. In this case, the object generates 31 different doses; hence the model is simulated 31 times and generates a SimData array.

```
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 T0 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,'statl','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
```

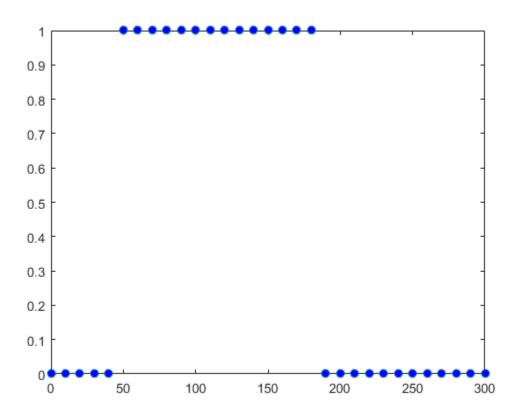
The addobservable function evaluates the new observable expression for each SimData in sd and returns the evaluated results as a new SimData array, newSD, which now has the added observable (stat1).

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 TO 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.

See Also

SimData | addobservable | updateobservable

Introduced in R2020a

reorder (model, compartment, kinetic law)

Reorder component lists

Syntax

modelObj = reorder(Obj,NewOrder)

Input Arguments

Obj	Model, compartment, or kinetic law object.
New0rder	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

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
```

See Also

Compartment object | KineticLaw object | Model object

Introduced in R2007b

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		
Туре	Display SimBiology object type		
UserData	Specify data to associate with object		
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
             А
                      50
                                 milligram
```

Create a dose with its Amount property set to the amount parameter 'A'.

dose	<pre>= adddose(model,'adaptive dose','</pre>	<pre>repeat');</pre>
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.

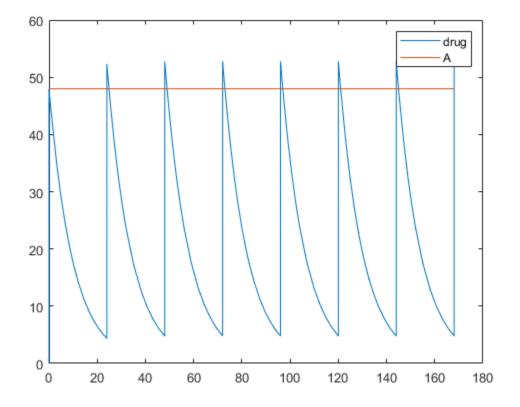
```
weightParam = addparameter(model,'weight', 80);
weightParam.ValueUnits = 'kilogram';
```

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.

```
= sbiomodel('simple model');
model
compartment
                           = addcompartment(model, 'Central',1);
compartment.CapacityUnits
                           = 'liter';
                            = addspecies(model,'drug');
species
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 rateParam.Va	alueUnits		dparameter(model,'R',10); illigram/hour'
rateParam = SimBiolog	gy Paramet	er 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	<pre>= adddose(model,'adaptive dose','repeat');</pre>
dose.Amount	= 'A';
dose.Rate	= 'R';

Set other dose properties.

dose.TargetName	= 'drug';
dose.StartTime	= 0;
dose.TimeUnits	<pre>= 'hour';</pre>
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 .

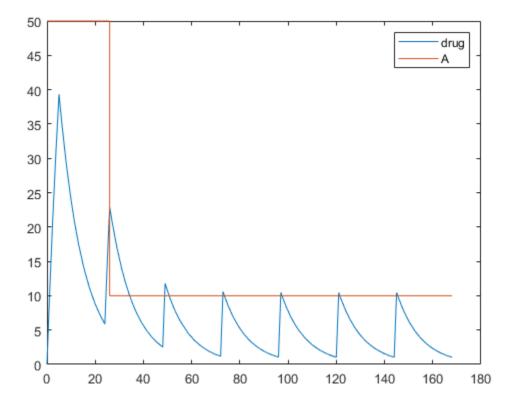
event = addevent(model,'time >= 26','A = 10');

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');
```

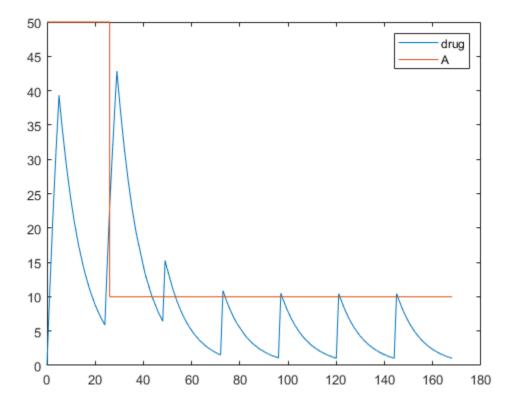


Alternatively, you can allow the ongoing dose event to finish before applying the new dose amount by setting EventMode to 'continue'.

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

Model object | ScheduleDose object | sbiodose | sbiosimulate

Topics

"Parameterized and Adaptive Doses"

Introduced in R2010a

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

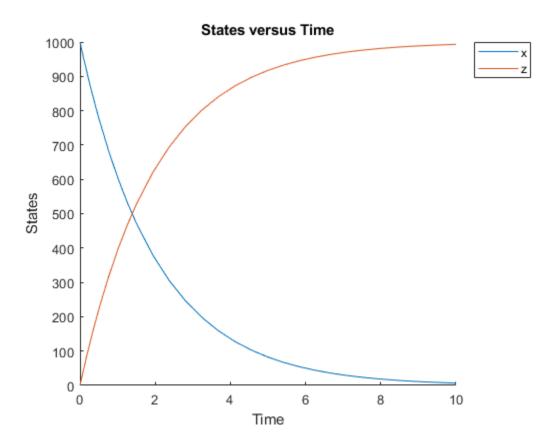
Resample Simulation Data

Load the radioactive decay model.

sbioloadproject('radiodecay');

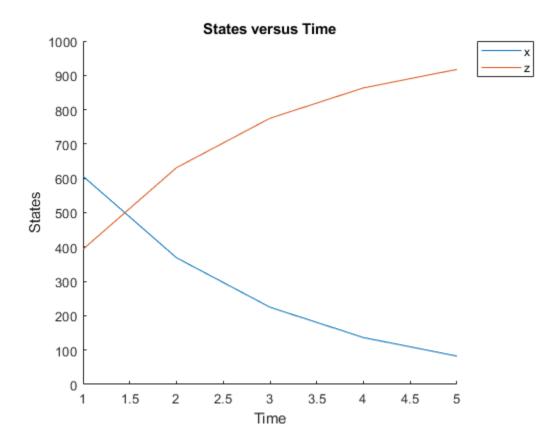
Simulate the model.

```
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

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 and throws a warning. 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

'interplq' (default) | character vector | string

Interpolation method for resampling, specified as a character vector or string. The valid choices follow.

- 'interplq' Use the interplq 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.

See Also SimData|sbiosimulate

Introduced in R2007b

resample

Resample Sobol indices to new time vector

Syntax

```
results = resample(sobol0bj,timeVector)
results = resample(sobol0bj,timeVector,method)
```

Description

results = resample(sobolObj,timeVector) resamples model evaluations to a vector of new time points. By default, the function uses the interplq interpolation method.

results = resample(sobolObj,timeVector,method) specifies the interpolation method.

Examples

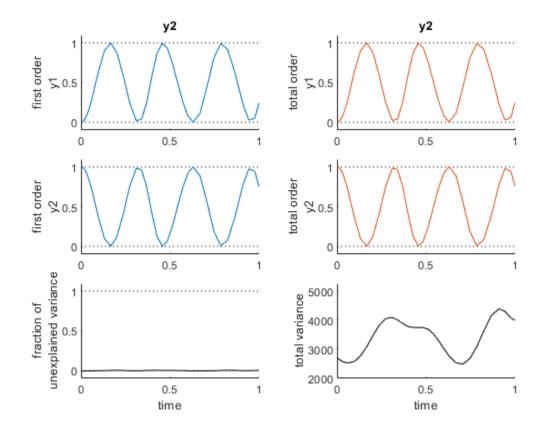
Resample Sobol Indices to New Time Points

Load the lotka model.

```
m = sbmlimport("lotka");
```

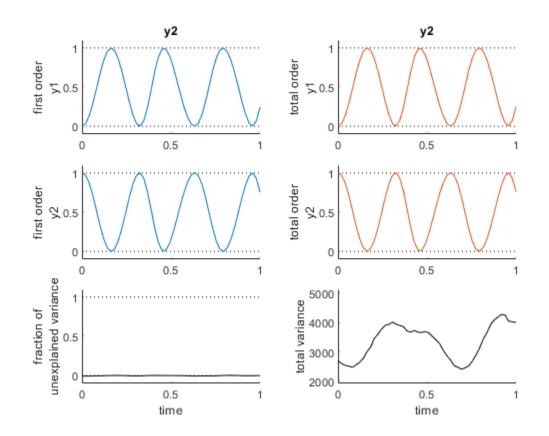
Decompose the variance of predators y2 into attributions of the initial values of the prey y1 and predators.

```
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

sobol0bj — Results containing Sobol indices

SimBiology.gsa.Sobol object

Results containing the first- and total-order Sobol indices, specified as a SimBiology.gsa.Sobol 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 sobol0bj, 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

'interplq' (default) | string | character vector

Interpolation method, specified as a string or character vector. The valid options follows.

- 'interplq' Use the interplq function.
- Use the interpl 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

Resampled simulation results with Sobol indices computed at new time points, returned as a SimBiology.gsa.Sobol object.

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

Introduced in R2020a

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 1-200.

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

Introduced in R2006a

rmcontent (variant)

Remove contents from variant object

Syntax

rmcontent(variantObj, contents)

rmcontent(variant0bj, idx)

Arguments

variant0bjSpecify the variant object from which you want to property is modified to remove the new data.				e data. The Content	
contents		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 {'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'	
	'specie	S '	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'	
	'parame	ter'	If the parameter scope is a model, specify the parameter name. If the parameter scope is a kinetic law, specify [reactionName.parameterName].	'Value'	
	'compar	tment'	Name of the compartment.	'Capacity'	
			the ContentIndex or indices of the data to be removed. To display the tIndex, enter the object name and press Enter.		

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, 'compl');
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)

1 spe	ecies A ecies C	Property: InitialAmount InitialAmount	Value: 5 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

Introduced in R2007b

rmproduct (reaction)

Remove species object from reaction object products

Syntax

```
rmproduct(reactionObj, SpeciesName)
rmproduct(reactionObj, speciesObj)
```

Arguments

reactionObj	Reaction object.
	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

Introduced in R2006a

rmreactant (reaction)

Remove species object from reaction object reactants

Syntax

```
rmreactant(reactionObj, SpeciesName)
rmreactant(reactionObj, speciesObj)
```

Arguments

reactionObj	Reaction object.
	Name for a species object. Enter a species name or a cell array of species names.
species0bj	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');
```

See Also

delete, rmproduct

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 2-532 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
Туре	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 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 2-534 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
Туре	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

Introduced in R2006b

summary(LeastSquaresResults,OptimResults,NLIN Results)

Plot a summary figure that contains estimated values and estimation statistics

Syntax

stats = summary(results0bj)

Description

stats = summary(resultsObj) returns a structure array stats that contains estimated values
and estimation statistics.

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

Compatibility Considerations

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

Introduced in R2014a

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
```

```
s0bj = SimBiology.Scenarios(name,content)
```

```
s0bj = SimBiology.Scenarios(quantityNames,probDist,Name,Value)
```

Description

sObj = SimBiology.Scenarios returns a Scenarios object sObj that contains no entries on page 2-550.

s0bj = SimBiology.Scenarios(name,content) returns a Scenarios object s0bj 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.

s0bj = 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'

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: $(k1 + k2 + k3) \times doses'$

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 2³² | 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 quantity values, doses, or variants to SimBiology.Scenarios object
Get entry contents from SimBiology.Scenarios object
Update entry contents from SimBiology.Scenarios object
Rename entry from SimBiology.Scenarios object
Remove entries from SimBiology.Scenarios object
Verify SimBiology.Scenarios object
Generate scenarios from SimBiology.Scenarios object and return table
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 "Simulating 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.

```
s0bj = SimBiology.Scenarios;
add(s0bj,'cartesian','variants',variants);
add(s0bj,'cartesian','dose',singleMeal)
```

```
ans =
 Scenarios (5 scenarios)
                    Name
                                     Content
                                                       Number
   Entry 1
                 variants
                              SimBiology variants
                                                         5
                                                         1
   x Entry 2
                 dose
                              SimBiology dose
```

```
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(s0bj)
```

```
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.RepeatDose] [1x1 SimBiology.Variant] [1x1 SimBiology.Variant] [1x1 SimBiology.RepeatDose]

Change the entry name of the first entry.

```
rename(s0bj,1,'Insulin Impairements')
```

ans =

Scenarios (5 scenarios)

	Name		Content		Number
Entry 1 x Entry 2	Insulin dose	Impairements	SimBiology SimBiology		5 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.

Туре

Units

```
f = createSimFunction(m1,s0bj,{'[Plasma Glu Conc]','[Plasma Ins Conc]'},[])
f =
SimFunction
Parameters:
                Name
                                    Value
```

{'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' }	Θ	{'parameter'}	{'l/minute'
{'f' }	0.9	{'parameter'}	{'dimensionless'
{'a' }	\odot	{'parameter'}	{'1/milligram'
{'b' }	0.82	{'parameter'}	{'dimensionless'
{'c' }	Θ	{'parameter'}	{'1/milligram'
{'d' }	0.01	{'parameter'}	{'dimensionless'
<pre>{'Stomach Glu After Dosing'}</pre>	78	{'parameter'}	{'gram'
{'kp1' }	2.7	{'parameter'}	{'milligram/minute'
{'kp2' }	0.0021	{'parameter'}	{'1/minute'
{'kp3' }	0.009	{'parameter'}	{ '(milligram/minute)/(picomole/li
{'kp4' }	0.0618	{'parameter'}	{'(milligram/minute)/picomole'
{'ki' }	0.0079	{'parameter'}	{'1/minute'
{'[Ins Ind Glu Util]' }	1	{'parameter'}	{'milligram/minute'
{'VmO' }	2.5129	{'parameter'}	{'milligram/minute'
{'Vmx' }	0.047	{'parameter'}	{ '(milligram/minute)/(picomole/li
{'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		{ '(picomole/minute)/(milligram/de
{'gamma' }	0.5	{'parameter'} {'parameter'}	{ (promote/minute)/(mittigram/de {'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'

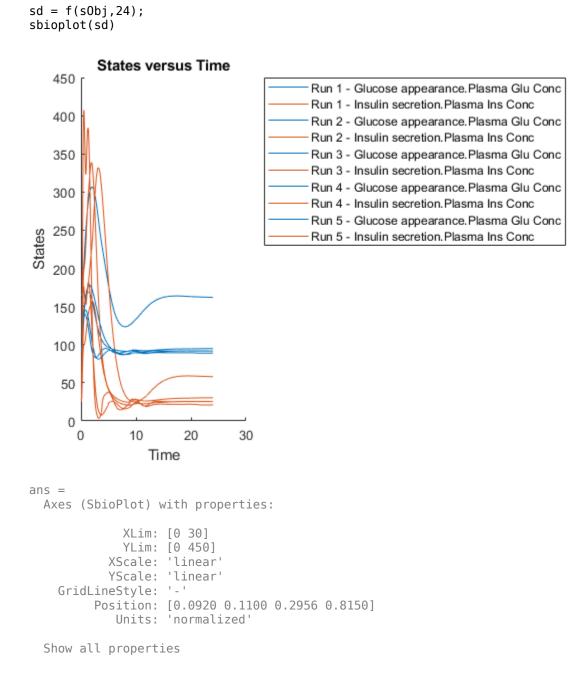
Observables:

Name	Туре	Units
{'[Plasma Glu Conc]'}	{'species'}	{'milligram/deciliter'}
{'[Plasma Ins Conc]'}	{'species'}	{'picomole/liter' }

Dosed:

TargetName	TargetDimension		
{'Dose'}	{'Mass (e.g., gram)'}		

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.



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 distribution 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
```

0.2

sigma =

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 s0bj.

```
remove(s0bj,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(s0bj,'cartesian',["Vmx","kp3"],[pd_Vmx, pd_kp3],'RankCorrelation',[1,0.5;0.5,1])

```
ans =
```

Scenarios (2 scenarios)

	Name	Content	Number
Entry 1 x (Entry 2.1	dose Vmx	SimBiology dose Lognormal distribution	1 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(s0bj,2,'Number',50)
```

```
ans =
 Scenarios (50 scenarios)
                                    Content
                                                       Number
                    Name
   Entry 1
                    dose
                            SimBiology dose
                                                         1
   x (Entry 2.1
                    Vmx
                            Lognormal distribution
                                                         50
   + Entry 2.2)
                    kp3
                            Lognormal distribution
                                                         50
```

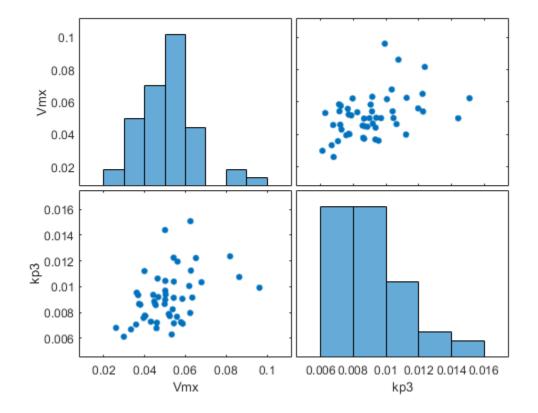
See also Expression property.

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(s0bj,m1)

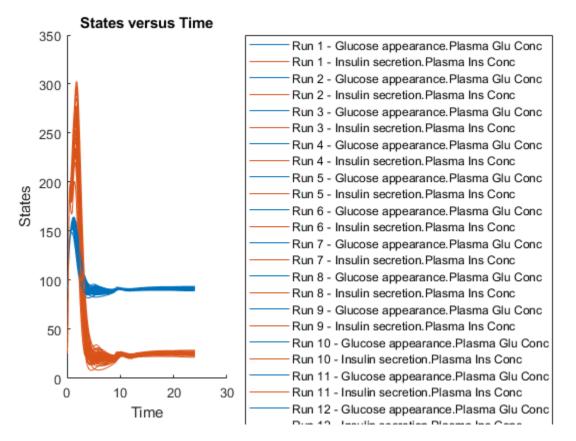
Generate the simulation scenarios. Plot the sample values using plotmatrix. You can see the value of Vmx is varied around its model value 0.047 and that of kp3 around 0.009.

```
sTbl = generate(s0bj);
[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(s0bj,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(s0bj,2)
```

entry2struct.SamplingMethod = 'lhs'

You can now use the updated structure to modify entry 2.

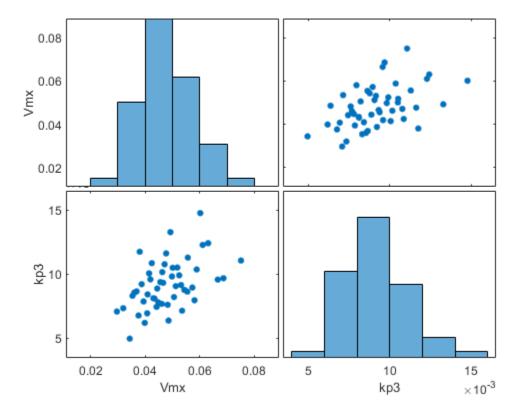
```
updateEntry(s0bj,2,entry2struct)
```

```
ans =
  Scenarios (50 scenarios)
                    Name
                                    Content
                                                        Number
                             SimBiology dose
    Entry 1
                    dose
                                                          1
    x (Entry 2.1
                             Lognormal distribution
                                                          50
                    Vmx
                    kp3
    + Entry 2.2)
                            Lognormal distribution
                                                          50
```

See also Expression property.

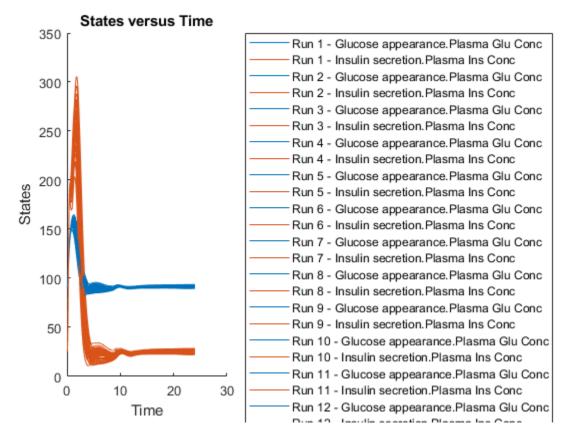
Visualize the sample values.

```
sTbl2 = generate(s0bj);
[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(s0bj,24); sbioplot(sd3);



Restore warning settings.

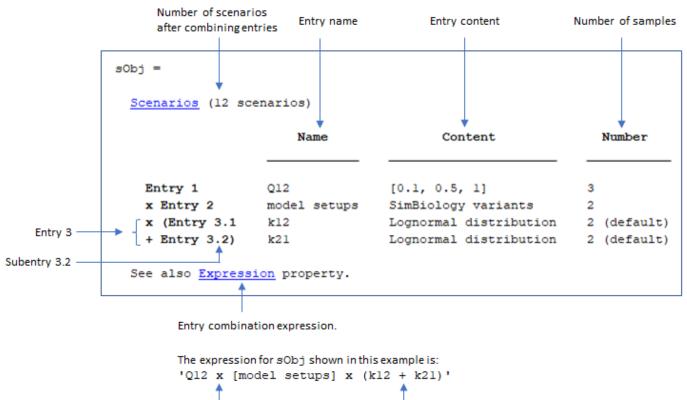
warning(warnSettings);

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.



cartesian combination elementwise combination

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.

inconsistent s the Diagnosis	ample sizes. Look at column to fix.)iagnosiscolumn w uggested sample si
bj2 =				
Scenarios (incon	♥ sistent)			
	Name	Content	Number	Diagnosis
(Entry 1	Q12	[0.1, 0.5, 1]	3	consistent
x Entry 2	model setups	SimBiology variants	2	consistent
x (Entry 3.1	k12	Lognormal distribution	2 (default)	consistent
+ Entry 3.2))	k21	Lognormal distribution	2 (default)	consistent
+ Entry 4	ka_Central	[0.1, 1.2, 2.3, 3.4, 4.5, 5.6, 6.7, 7.8, 8.9, 10]	10	expected 1
				↑

The number of samples for Entry 4 is expected to be 12 so that the entries can be combined.

The Diagnosis column suggests which entries to fix to have the correct number of samples. Use updateEntry, rename, and remove to edit the entries.

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"

Introduced in R2019b

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
Туре	Display SimBiology object type
UserData	Specify data to associate with object

See Also

Model object, RepeatDose object, sbiodose, sbiosimulate

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 "Simulating the Glucose-Insulin Response".

sbioloadproject('insulindemo.sbproj','m1');

Suppress an information warning that is issued during simulations.

warnSettings = warning('off', 'SimBiology:DimAnalysisNotDone_MatlabFcn_Dimensionless');

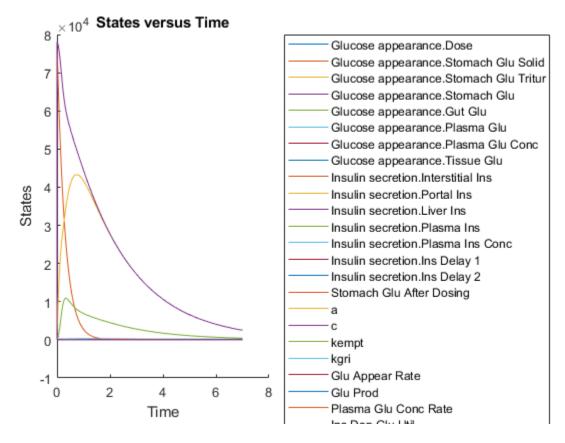
Simulate a single meal for a normal subject for 7 hours.

```
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 SystemLogged Data:5Species:15Compartment:0Parameter:24Sensitivity:0Observable: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'
                                             3
    {'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

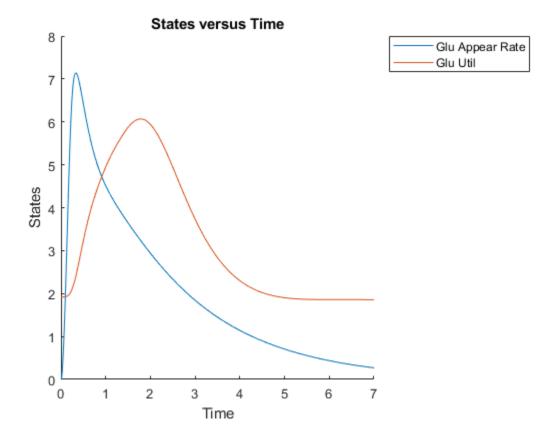
Compartment: 0

Parameter: 2

Sensitivity: 0

Observable: 0
```

sbioplot(newsd);



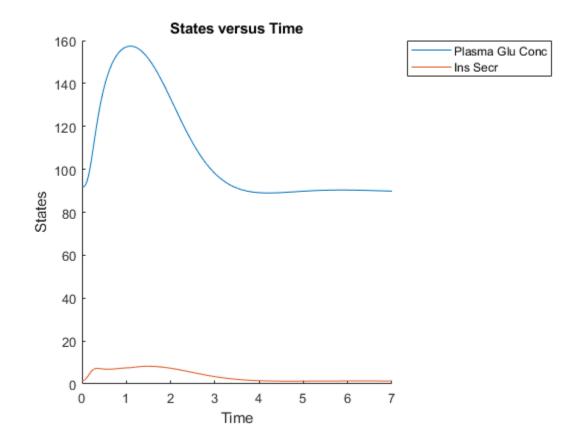
Compare data for the plasma glucose concentration (the species named Plasma Glu Conc) and insulin secretion rate (the parameter named *Ins Secr*). Use selectbyname to extract data by specifying the corresponding names.

```
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 SystemLogged Data:7Species:7Compartment:0Parameter:11Sensitivity:0Observable: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.

See Also SimData|get|set

Introduced in R2007b

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 "Simulating the Glucose-Insulin Response".

sbioloadproject('insulindemo.sbproj','m1');

Suppress an information warning that is issued during simulations.

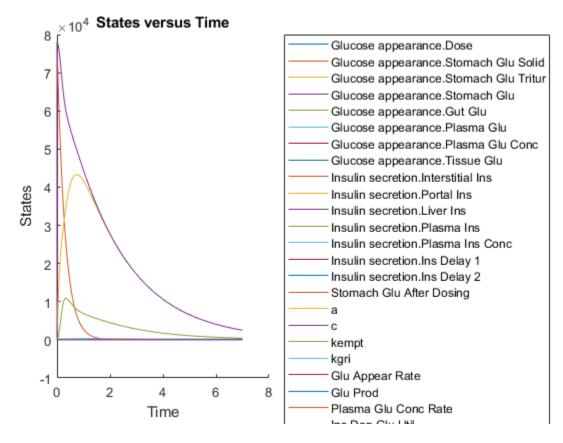
warnSettings = warning('off', 'SimBiology:DimAnalysisNotDone_MatlabFcn_Dimensionless');

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

```
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'
                                             3
    {'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

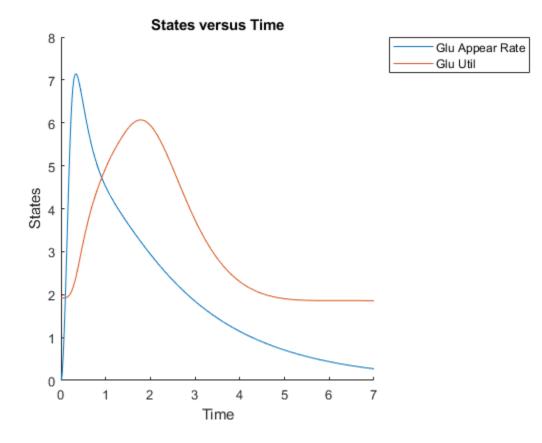
Compartment: 0

Parameter: 2

Sensitivity: 0

Observable: 0
```

sbioplot(newsd);



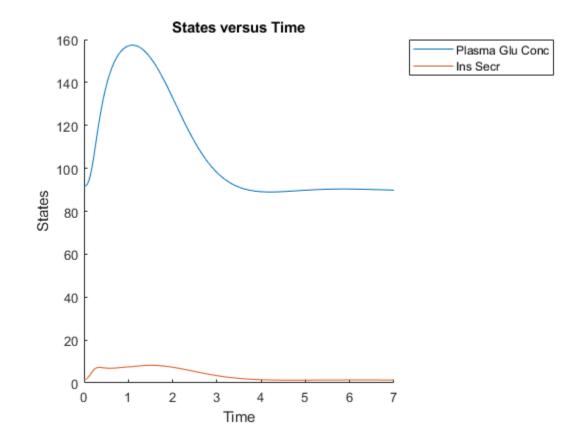
Compare data for the plasma glucose concentration (the species named Plasma Glu Conc) and insulin secretion rate (the parameter named *Ins Secr*). Use selectbyname to extract data by specifying the corresponding names.

```
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 SystemLogged Data:7Species:7Compartment:0Parameter:11Sensitivity:0Observable: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.

See Also SimData|get|set Introduced in R2007b

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 namevalue 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: ''
		Tgpe: '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

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.

See Also

SimData|get

Introduced in R2008b

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

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

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.
	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

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.
	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

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

dose0bj — 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);
```

See Also

RepeatDose object | ScheduleDose object | getTable

Introduced in R2014a

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 three 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

mx0 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.

Туре	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

Туре	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

$\ensuremath{\mathsf{Vector0bservables}}$ — Results from vector-valued observable expressions $\ensuremath{\mathsf{table}}$

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
updateobservable	Update observable expressions or units in SimData
renameobservable	Rename observables in SimData
getdata	Get simulation data from SimData object
getsensmatrix	Get 3-D sensitivity matrix from SimData object
select	Select simulation data from SimData object using expressions
selectbyname	Select simulation data by name from SimData object
resample	Resample simulation data onto new time vector
get	Get SimBiology object properties
set	Set SimBiology object properties
delete	Delete SimBiology object
display	Display summary of SimBiology object

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
                                         Value:
                                                       Units:
   Index:
              Compartment:
                               Name:
   1
              unnamed
                               G
                                         7000
   2
                               Gd
                                         3000
             unnamed
   3
             unnamed
                               Ga
                                         0
   4
                               RL
                                         0
             unnamed
   5
                                         6.022e+17
             unnamed
                               1
   6
             unnamed
                               R
                                         10000
   7
                               Gbg
             unnamed
                                         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);
v0bj = addvariant(m1,'initCond');
for i = 1:numSpecies
    addcontent(v0bj,{'species',info{i}.Name,'Value',finalData(i)});
end
commit(v0bj,m1);
```

Verify the species initial amounts.

m1.Species

```
ans =
   SimBiology Species Array
   Index:
             Compartment:
                              Name:
                                        Value:
                                                      Units:
   1
             unnamed
                              G
                                        8562.5
   2
                              Gd
                                        0.109565
             unnamed
   3
                              Ga
                                        1437.39
             unnamed
   4
             unnamed
                              RL
                                        1820.54
                                        6.022e+17
   5
             unnamed
                              L
```

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_T0.sbproj

Set the target occupancy (T0) 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,'T0',d)
```

```
f =
SimFunction
```

Parameters:

_	Name		Value	Туре	Units
{	{'AmountPa	aram'}	1	{'parameter'}	{'nanomole'}
0bser	rvables:				
	Name	Туре	9	Units	
-	{'T0'}	{'parame	eter'}	{'dimensionless'}	
Dosec	: t				
	TargetNa	ame		TargetDimension	

{'Plasma.Drug'} {'Amount (e.g., mole or molecule)'} {'AmountParam'} 1

```
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

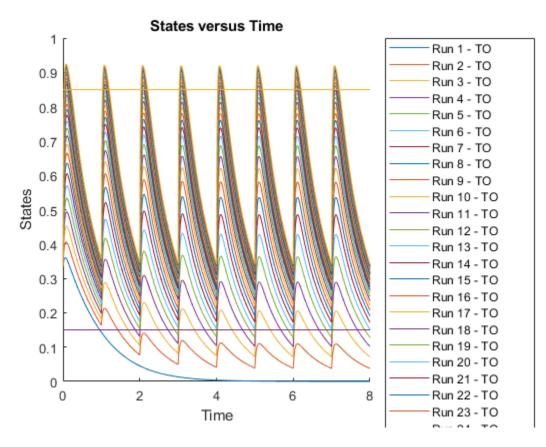
Parameter: 1

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 T0 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,'statl','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
```

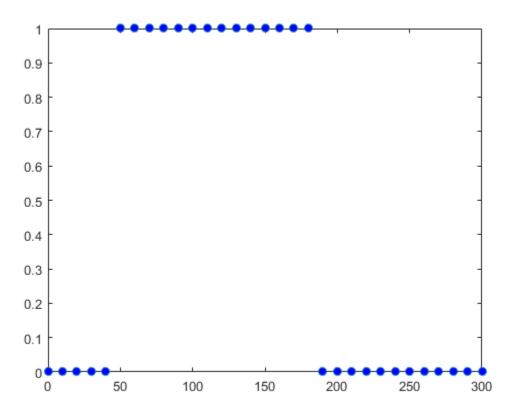
The addobservable function evaluates the new observable expression for each SimData in sd and returns the evaluated results as a new SimData array, newSD, which now has the added observable (stat1).

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 TO 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(TO) < 0.75 \& min(TO) > 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');
```

See Also

Compartment | Model | Parameter | Reaction | Species

Introduced in R2007b

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.

Т

Cell array containing a numeric vector of size S \times 1. S is the number of simulations. The ith element of T contains the time point from the ith simulation.

Υ

Cell array of 2-D numeric matrices. The ith element of Y contains data from the ith 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'(on	ly if UnitConve	ersion is turned	l 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 varia	ables named:			
	• 'Name'				
	• 'Type'				
	• 'Units'(on	ly if UnitConve	rsion is turned	l on)	
	This table contai or parameters) t 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 <i>Value (PropertyNameValue)</i> , and the value is the default value of the parameter. If the UnitConversion is on, the unit column is also added with the name <i>PropertyNameUnits</i> . Suppose the Amount property of a repeat dose targeting the <i>Drug</i> 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 TargetDimen Amount AmountValue AmountUnits				
		sion	AmountDara	10	lmillignom
	'Drug'	'Mass (e.g., gram)'	'AmountPara m'	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.

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 "Simulating 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)
```

SimBiology Variant - Type 2 diabetic (inactive)

ContentIndex:	Type:	Name:	Property:	Value:
1	parameter	Plasma Volume	. Value	1.49
2	parameter	k1	Value	0.042
3	parameter	k2	Value	0.071
4	parameter	Plasma Volume	. Value	0.04

5parameterm16parameterm27parameterm48parameterm59parameterm610parameterHep11parameterkma12parameterkma13parameterkab14parameterkgr15parameterf16parametera17parameterb18parameterc	n Value s Value	0.379 0.673 0.269 0.0526 0.8118 0.6 0.0465 0.0076 0.023 0.0465 0.9 6e-05 0.68 0.00023
19parameterd20parameterStol	Value mach Glu Af Value	0.09 125
21 parameter kp1	Value	3.09
22 parameter kp2		0.0007
23 parameter kp3		0.005
24 parameter kp4		0.0786
25 parameter ki	Value	0.0066
	s Ind Glu U Value	1
27 parameter Vm0		4.65
28 parameter Vmx	Value	0.034
29 parameter Km	Value	466.21
30 parameter p2U	Value	0.084
31 parameter K	Value	0.99
32 parameter alp	ha Value	0.013
33 parameter bet		0.05
34 parameter gam		0.5
35 parameter kel		0.0007
36 parameter ke2		269
l l	al Plasma G Value al Plasma I Value	164.18 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		Туре	Units
	Plasma Glu Plasma Ins		<pre>{'species'} {'species'}</pre>	{'milligram/deciliter'} {'picomole/liter' }
Dosed:				
Tar	getName	TargetD:	imension	
{ '	Dose'}	{'Mass (e.e	g., gram)'}	

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]'}
                                             {'picomole/liter'
                              {'species'}
                                                                    }
Dosed:
```

```
TargetName
                 TargetDimension
 {'Dose'}
              {'Mass (e.g., gram)'}
```

Select a dose that represents a single meal of 78 grams of glucose at the start of the simulation.

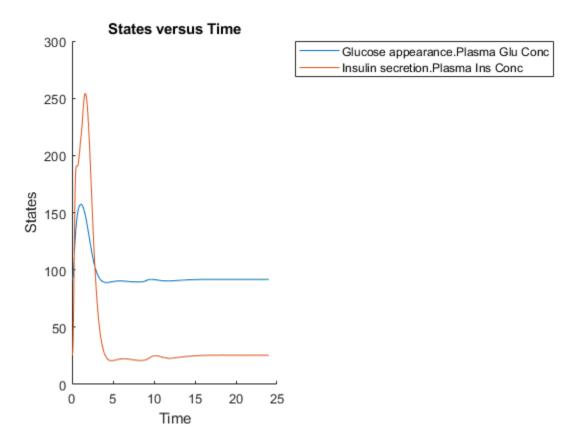
```
singleMeal = sbioselect(m1, 'Name', 'Single Meal');
```

Convert the dosing information to the table format.

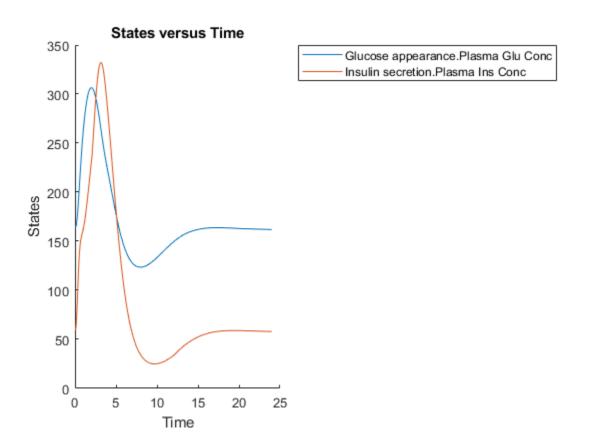
mealTable = getTable(singleMeal);

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	0.0235
2	parameter	kp3	Value	0.0045

varToScan(2)

```
ans =
   SimBiology Variant - High insulin sensitivity (inactive)
```

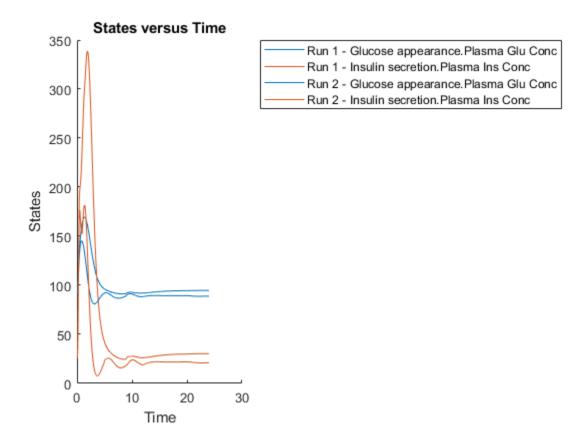
ContentIndex:	Type:	Name:	Property:	Value:
1	parameter	Vmx	Value	0.094
2	parameter	kp3	Value	0.018

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	Туре	Units
{ ' × ' }	1000	{'species'}	{'molecule'}
Observables:			
Namo	Tupo	Unite	

Name	Туре	Units
{'x'} {'z'}	{'species'} {'species'}	{'molecule'} {'molecule'}

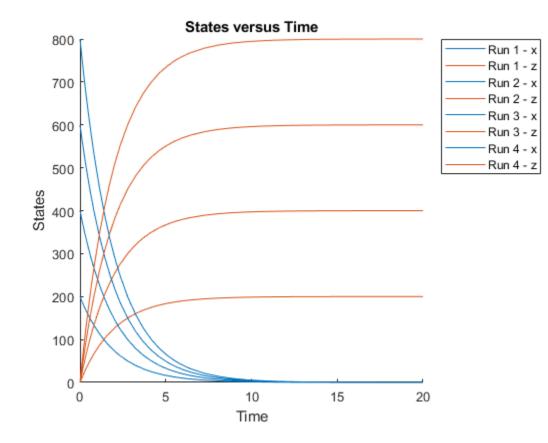
Dosed: None

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'});

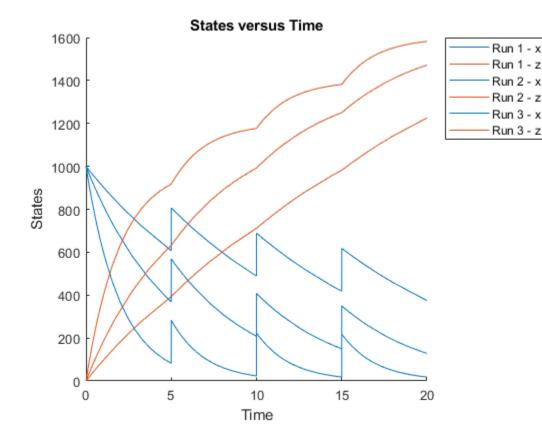
Define a scalar dose of amount 200 molecules given at three time points (5, 10, and 15 seconds).

```
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.



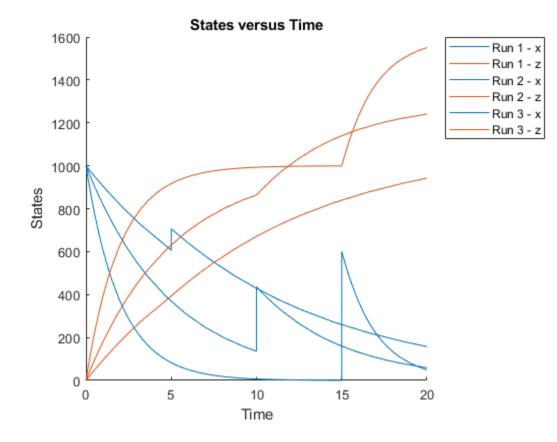
sbioplot(f(phi,20,u));

You can also specify different dose amounts at different times.

```
d1 = table(5, 100);
dl.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}));

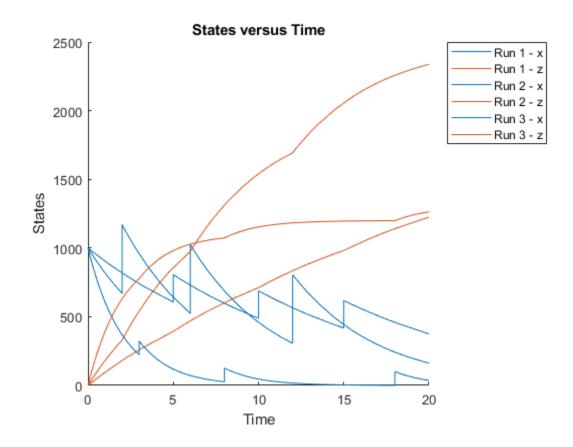


You can also define a cell array of dose tables.

```
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));



References

[1] Gillespie, D.T. (1977). Exact Stochastic Simulation of Coupled Chemical Reactions. The Journal of Physical Chemistry. 81(25), 2340–2361.

See Also

RepeatDose object | ScheduleDose object | SimBiology.Scenarios | SimFunctionSensitivity object | createSimFunction | sbiosampleerror | sbiosampleparameters

Topics

"PK/PD Modeling and Simulation to Guide Dosing Strategy for Antibiotics" "Model Simulation"

Introduced in R2014a

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.

SensitivityOutp table with variables named:

uts

- '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.

SensitivityInpu table with variables named:

ts

- '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.

SensitivityNorm	Character vector specifying the normalization method for calculated		
alization	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.

```
\Big(\frac{1}{x(t)}\Big)\Big(\frac{\partial x(t)}{\partial k}\Big)
```

• 'Full' — Full dedimensionalization

(k)	$\left(\frac{\partial x(t)}{\partial k}\right)$
$\left(\overline{x(t)}\right)$	$\left(\frac{\partial k}{\partial k} \right)$

Examples

Calculate Sensitivities Using SimFunctionSensitivity Object

This example shows how to calculate the 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	Туре
<pre>{'Reaction1.c1'} {'Reaction2.c2'}</pre>	10 0.01	{'parameter'} {'parameter'}

```
Observables:
```

Name Туре {'y1'} {'species'} { 'y2 ' } {'species'} Dosed: None Sensitivity Input Factors: Name Туре {'parameter'} {'Reaction1.c1'} {'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.

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.

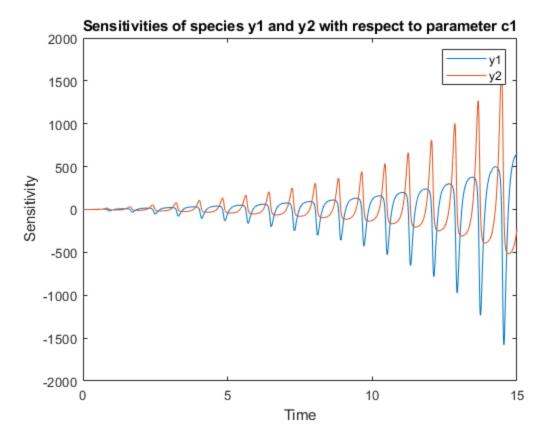
sd = f([10, 0.1], 15);

Retrieve the calculated sensitivities from the SimData object sd.

[t,y,outputs,inputs] = getsensmatrix(sd);

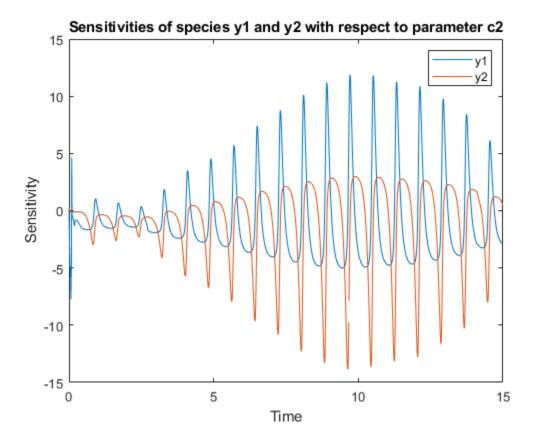
Plot the sensitivities of species y1 and y2 with respect to c1.

```
figure;
plot(t,y(:,:,1));
legend(outputs);
title('Sensitivities of species y1 and y2 with respect to parameter c1');
xlabel('Time');
ylabel('Sensitivity');
```



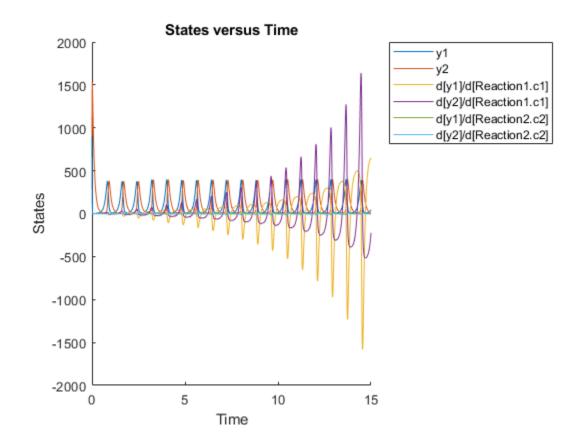
Plot the sensitivities of species y1 and y2 with respect to c2.

```
figure;
plot(t,y(:,:,2));
legend(outputs);
title('Sensitivities of species y1 and y2 with respect to parameter c2');
xlabel('Time');
ylabel('Sensitivity');
```



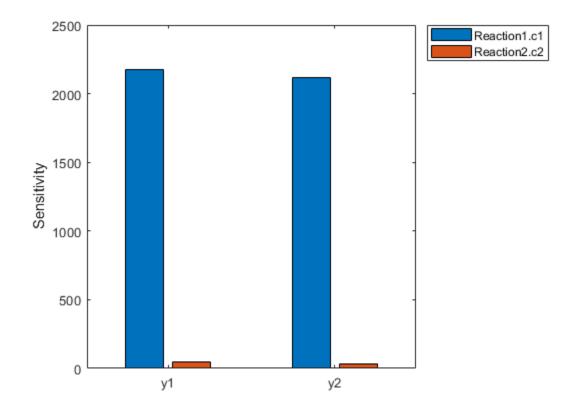
Alternatively, you can use **sbioplot**.

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');
```



See Also

SimFunction object|createSimFunction|sbiosampleerror|sbiosampleparameters

Topics

"Sensitivity Analysis in SimBiology"

Introduced in R2015a

simulate

Class: SimBiology.export.Model

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.

Input Arguments

model

SimBiology.export.Model object.

initialValues

Vector of values for simulate to use as the initial values of the simulation. initialValues must have the same number of elements as model.InitialValues.

Default: Values specified in model.InitialValues.

doses

Vector of dose objects specifying the doses used for simulation. The input dose objects must be a subset of the doses in the exported model, as returned by getdose.

Default: All dose objects in the exported model.

Output Arguments

t

n-by-1 vector of time samples from the simulation, where *n* is the number of time samples.

Х

n-by-*m* matrix of simulation data, 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

m-by-1 cell array of character vectors with names labeling the rows and columns of x, respectively.

simDataObj

SimData object containing simulation time and state data, as well as metadata, such as the types and names for the reported states.

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'});
```

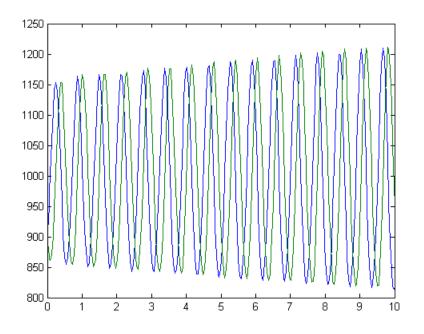
Export the model object.

```
em = export(model0bj);
```

Simulate the exported model.

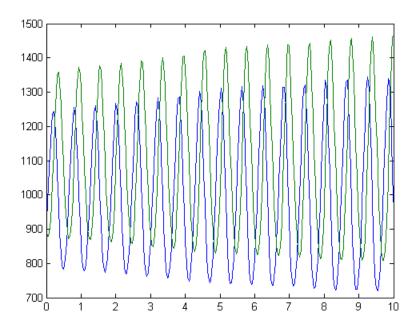
[t,y] = simulate(em);

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)
```



See Also

SimBiology.export.Model|SimBiology.export.SimulationOptions| SimBiology.export.ValueInfo|SimData object|export|getdose

Topics

"PK/PD Modeling and Simulation to Guide Dosing Strategy for Antibiotics" "Deploy a SimBiology 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 2-627.

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 2-627.

- 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 or sbiompgsa. 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 2-627.

Data Types: struct

Object Functions

Resample Sobol indices to new time vector
Compute Sobol indices for new observable expression
Remove Sobol indices of observables
Retrieve model simulation results and sample values used for computing
Sobol indices
Add additional samples to Sobol indices
Plot quantile summary of model simulations from global sensitivity analysis
(requires Statistics and Machine Learning Toolbox)
Plot first- and total-order Sobol indices and variances
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.

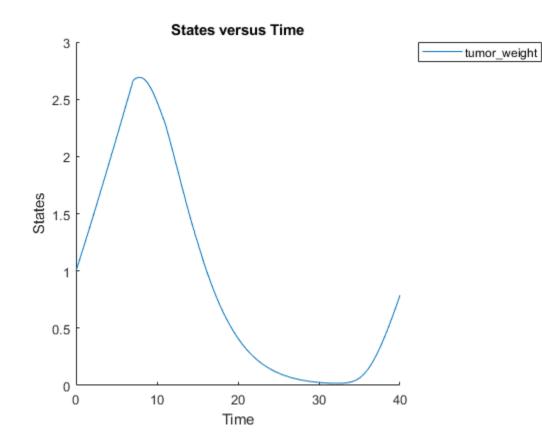
v = getvariant(m1); d = getdose(m1,'interval_dose');

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].

sobolResults = sbiosobol(m1,modelParamNames,outputName,'Variants',v,'Doses',d,'ShowWaitBar',true

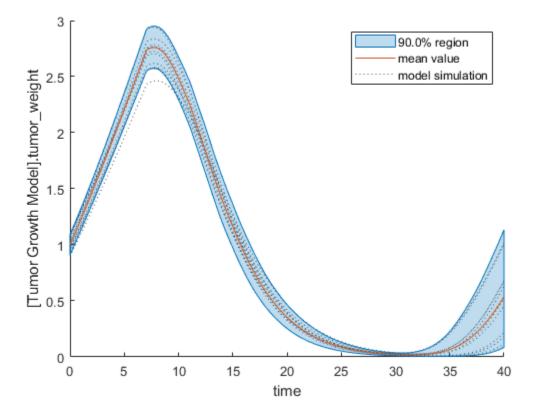
```
sobolResults =
   Sobol with properties:
        Time: [444x1 double]
        SobolIndices: [5x1 struct]
        Variance: [444x1 table]
```

```
Observables: {'[Tumor Growth Model].tumor_weight'}
ParameterSamples: [1000x5 table]
SimulationInfo: [1x1 struct]
```

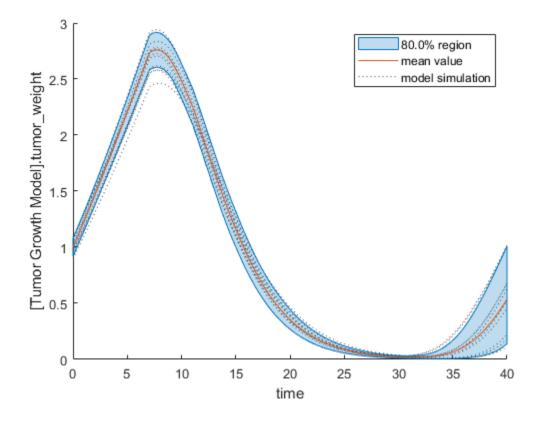
You can change the number of samples by specifying the 'NumberSamples' name-value pair argument. The function requires a total of (number of input parameters + 2) * NumberSamples model simulations.

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

plotData(sobolResults);

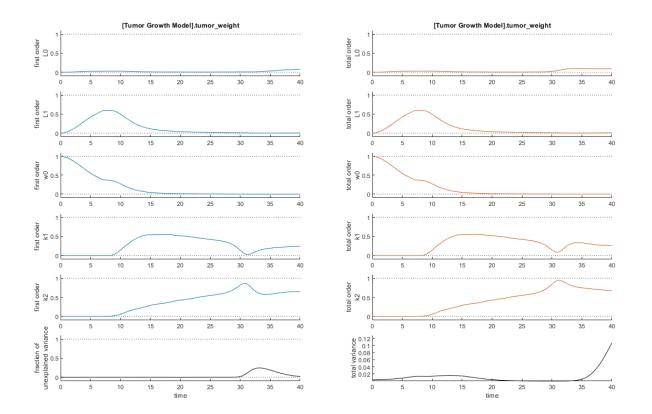


plotData(sobolResults, 'Alphas',0.1);



Plot the time course of the first- and total-order Sobol indices.

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

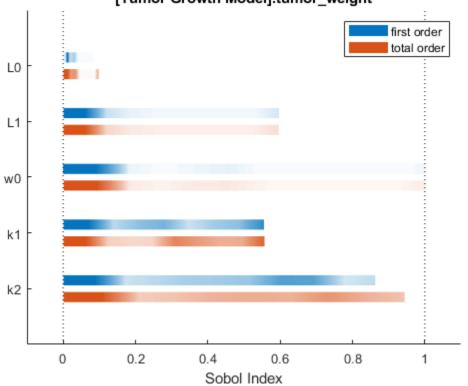


The first-order Sobol index of an input parameter gives the fraction of the overall response variance that can be attributed to variations in the input parameter alone. The total-order index gives the fraction of the overall response variance that can be attributed to any joint parameter variations that 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.

bar(sobolResults)



[Tumor Growth Model].tumor_weight

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

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.

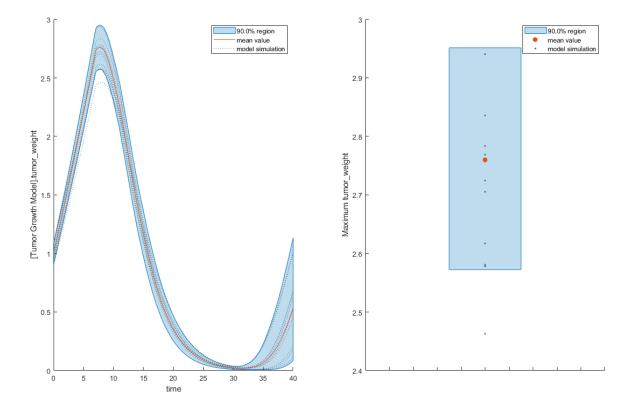
```
[samplesUsed,sd,validruns] = getSimulationResults(sobolResults,4);
```

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);
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.

$$S_i = \frac{V_{X_i}(E_{X_{\sim i}}(Y|X_i))}{V(Y)}$$

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.

$$S_{Ti} = 1 - \frac{V_{X_{\sim i}}(E_{X_i}(Y|X_{\sim i}))}{V(Y)} = \frac{E_{X_{\sim i}}(V_{X_i}(Y|X_{\sim i}))}{V(Y)}$$

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 *i*th 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.

$$\widehat{S}_{i} = \frac{\frac{1}{n} \sum_{j=1}^{n} f(B)_{j} \left(f\left(\boldsymbol{A}_{B}^{i}\right)_{j} - f(A)_{j} \right)}{V(Y)}$$
$$\widehat{S}_{Ti} = \frac{\frac{1}{2n} \sum_{j=1}^{n} \left(f(A)_{j} - f\left(\boldsymbol{A}_{B}^{i}\right)_{j} \right)^{2}}{V(Y)}$$

f(A), f(B), and $f(A_B^i)_j$ 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 *i*th index (A_B^i) from the SimulationInfo.SimData

Tips

array.

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.

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

Observable | sbiompgsa | sbiosobol

Topics

"Sensitivity Analysis in SimBiology"

Introduced in R2020a

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 2-630 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 (species, parameter, compartment)	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 $% \left({{{\left({{{{\bf{n}}}} \right)}_{i}}_{i}}} \right)$
ConstantAmount	Specify variable or constant species amount
InitialAmount	Species initial amount
Initial Amount Units	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
Туре	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

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 2-632 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 SimBiology object
Display summary of SimBiology object
Find out how a unit or unit prefix is used
Get SimBiology object properties
Rename object and update expressions
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
Туре	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

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 2-634 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 SimBiology object
Display summary of SimBiology object
Find out how a unit or unit prefix is used
Get SimBiology object properties
Rename object and update expressions
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
Туре	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 Introduced in R2008a

updateEntry

Update entry contents from SimBiology.Scenarios object

Syntax

```
s0bj = updateEntry(s0bj,entryNameOrIndex,Name,Value)
```

s0bj = updateEntry(s0bj,entryIndex,subIndex,Name,Value)

Description

s0bj = updateEntry(s0bj,entryNameOrIndex,Name,Value) updates the contents of the entry
(or subentry on page 2-550) entryNameOrIndex as specified by one or more name-value pair
arguments. You must specify at least one name-value pair argument.

s0bj = updateEntry(s0bj,entryIndex,subIndex,Name,Value) updates the contents of the subentry subIndex as specified by one or more name-value pair 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 "Simulating 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.

```
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(s0bj)
```

```
scenariosTbl=5×2 table
variants dose
[1x1 SimBiology.Variant]
```

Change the entry name of the first entry.

```
rename(sObj,1,'Insulin Impairements')
ans =
Scenarios (5 scenarios)

Name
Content
Number
Entry 1
Insulin Impairements
X Entry 2
dose
SimBiology variants
5
SimBiology dose
1
Content
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	Туре	Units
	} 1.88	{'parameter'}	{'deciliter'
	} 0.065	{'parameter'}	{'1/minute'
	} 0.079	{'parameter'}	{'1/minute'
{'Plasma Volume (Ins)'	} 0.05	{'parameter'}	{'liter'
{'m1'	} 0.19	{'parameter'}	{'1/minute'
	} 0.484	{'parameter'}	{'1/minute'
	} 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'
	} 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'
{'Stomach Glu After Dosing'		{'parameter'}	{'gram'
{'kpl'	} 2.7	{'parameter'}	{'milligram/minute'
{ ' kp2 '	} 0.0021	{'parameter'}	{'l/minute'
{'kp3'	} 0.009	{'parameter'}	{'(milligram/minute)/(picomole/li
{ ' 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'
{ 'Vm×'	} 0.047	{'parameter'}	{'(milligram/minute)/(picomole/li
{'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/de
{'gamma'	} 0.5	{'parameter'}	{'1/minute'
{'kel'	} 0.0005	{'parameter'}	{'1/minute'
{ ' ke2 '	} 339	{'parameter'}	{'milligram'
	} 91.76	{'parameter'}	{'milligram/deciliter'
-	} 25.49	{'parameter'}	{'picomole/liter'

Observables:

Name Type		Units	
{'[Plasma Glu Conc]'}	{'species'}	{'milligram/deciliter'}	
{'[Plasma Ins Conc]'}	{'species'}	{'picomole/liter' }	

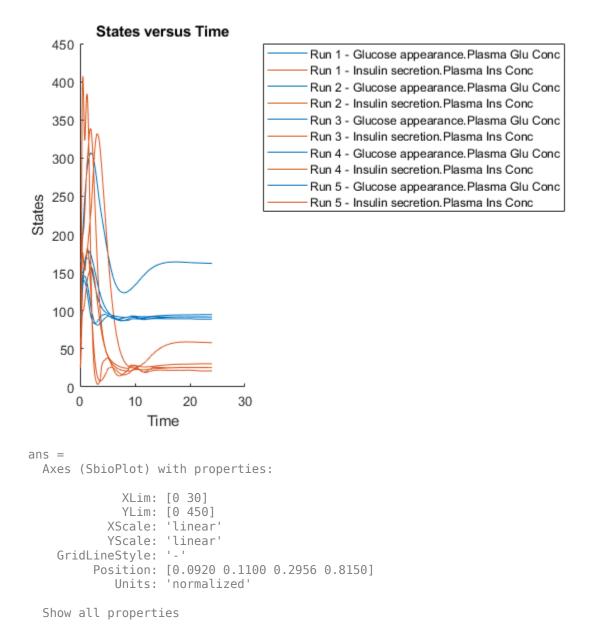
Dosed:

TargetName TargetDimension

{'Dose'} {'Mass (e.g., gram)'}

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(s0bj,24); sbioplot(sd)



If you have Statistics and Machine Learning ToolboxTM, 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 distribution 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 s0bj.

```
remove(s0bj,1)
ans =
   Scenarios (1 scenarios)
```

	Name	Content	Number
Entry 1	dose	SimBiology dose	1
See also Ex	pression	property.	

Add an entry that defines the joint probability distribution with a rank correlation matrix.

add(s0bj,'cartesian',["Vmx","kp3"],[pd_Vmx, pd_kp3],'RankCorrelation',[1,0.5;0.5,1])

```
ans =
 Scenarios (2 scenarios)
                                    Content
                                                          Number
                    Name
   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(s0bj,2,'Number',50)
```

```
ans =
 Scenarios (50 scenarios)
                                    Content
                                                        Number
                    Name
                             SimBiology dose
    Entry 1
                    dose
                                                          1
   x (Entry 2.1
                    Vmx
                             Lognormal distribution
                                                          50
    + Entry 2.2)
                    kp3
                             Lognormal distribution
                                                          50
```

See also Expression property.

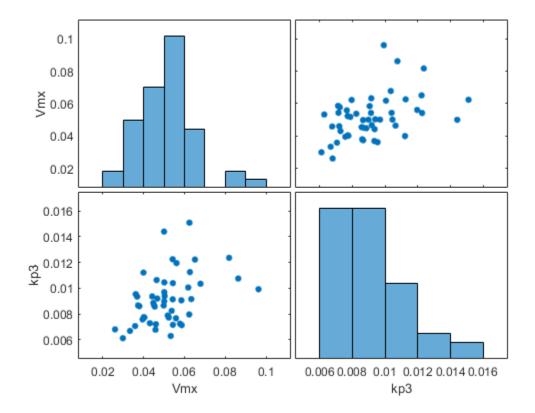
Verify that the Scenarios object can be simulated with the model. The verify function throws an error if any entry does not resolve uniquely to an object in the model or the entry contents have inconsistent lengths (sample sizes). The function throws a warning if multiple entries resolve to the same object in the model.

verify(s0bj,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.

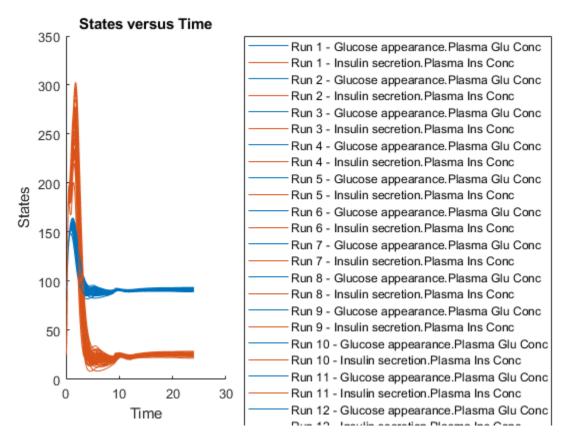
```
sTbl = generate(s0bj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl.Vmx,sTbl.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
```

```
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(s0bj,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(s0bj,2)

entry2struct.SamplingMethod = 'lhs'

You can now use the updated structure to modify entry 2.

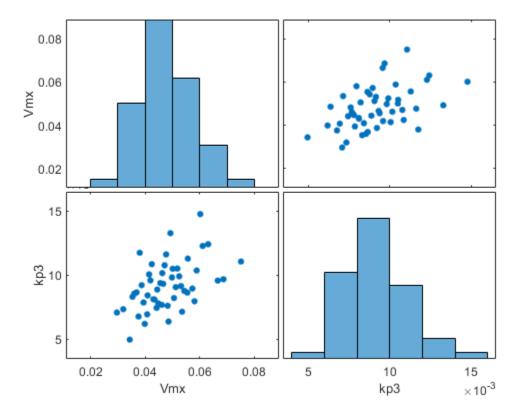
```
updateEntry(s0bj,2,entry2struct)
```

```
ans =
  Scenarios (50 scenarios)
                    Name
                                    Content
                                                        Number
                             SimBiology dose
    Entry 1
                    dose
                                                          1
                             Lognormal distribution
    x (Entry 2.1
                    Vmx
                                                          50
                    kp3
    + Entry 2.2)
                            Lognormal distribution
                                                          50
```

See also Expression property.

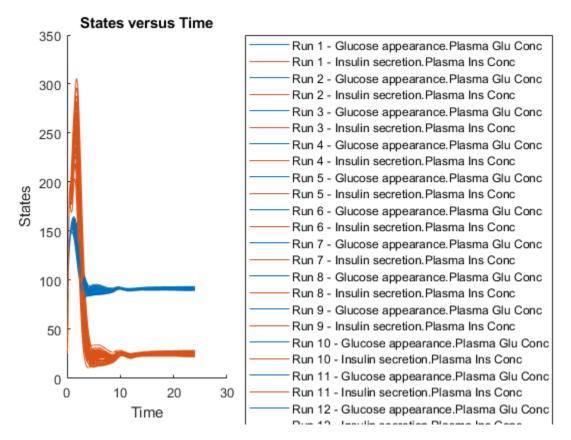
Visualize the sample values.

```
sTbl2 = generate(s0bj);
[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(s0bj,24); sbioplot(sd3);



Restore warning settings.

warning(warnSettings);

Input Arguments

s0bj — 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 pair argument.

Instead of using name-value pair 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'

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

s0bj — Simulation scenarios

Scenarios object

Simulation scenarios, returned as a Scenarios object.

See Also

SimBiology.Scenarios | SimFunction object | createSimFunction (model)

Topics

"SimBiology.Scenarios Terminology" on page 2-550 "Combine Simulation Scenarios in SimBiology"

Introduced in R2019b

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_T0.sbproj
```

Set the target occupancy (T0) as a response.

```
cs = getconfigset(m1);
cs.RuntimeOptions.StatesToLog = 'T0';
```

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,'T0',d)
```

```
f =
SimFunction
```

Parameters:

Nam	е	Value	Туре	Units	
{'Amount	Param'}	1	{'parameter'}	{'nanomole'}	
Observables:					
Name	Тур	е	Units		
{'T0'}	{'param	eter'}	{'dimensionless'}		
Dosed:					
Target	Name		TargetDimension		Δm

TargetName	TargetDimension	Amount	AmountValue
{'Plasma.Drug'}	{'Amount (e.g., mole or molecule)'}	{'AmountParam'}	1 .

warning('on','SimBiology:SimFunction:DOSES NOT EMPTY');

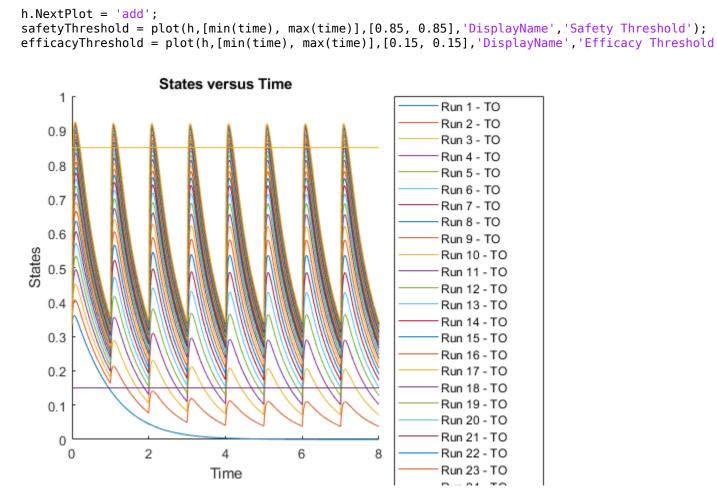
Simulate the model using the dose amounts generated by the Scenarios object. In this case, the object generates 31 different doses; hence the model is simulated 31 times and generates a SimData array.

```
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;
```



Postprocess the simulation results. Find out which dose amounts are effective, corresponding to the T0 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,'statl','max(TO) < 0.85 & min(TO) > 0.15','Units','dimensionless')
```

SimBiology Simulation Data Array: 31-by-1

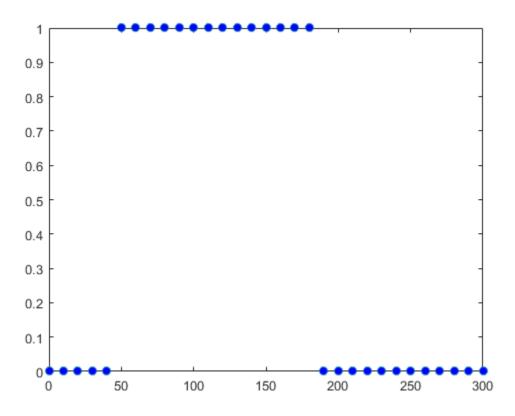
```
ModelName: TMDD
Logged Data:
Species: 0
Compartment: 0
Parameter: 1
Sensitivity: 0
Observable: 1
```

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 TO 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.

See Also

SimData | addobservable | renameobservable

Introduced in R2020a

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 2-656 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
Туре	Display SimBiology object type
UserData	Specify data to associate with object

See Also

Compartment object, Configset object, Model object, Parameter object, Species object

sbiosimulate

Introduced in R2008a

verify (model, variant)

Validate and verify SimBiology model

Syntax

verify(model0bj)
verify(model0bj,cs0bj)
verify(model0bj,dv0bj)

verify(modelObj,csObj,dvObj)

verify(model0bj,cs0bj,variant0bj,dose0bj)

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(model0bj,cs0bj) verifies a model model0bj using the specified configset object cs0bj
and any active variants and active doses. Any other configsets are ignored. If you set cs0bj 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 dv0bj to empty [], the function uses the active configset, active variants, and active doses.

If you specify dv0bj as variants, the function uses the specified variants and active doses. Any other variants are ignored.

If you specify dv0bj 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 cs0bj 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 dv0bj as variants, the function uses the specified variants and active doses. Any other variants are ignored.

If you specify dv0bj as doses, the function uses the specified doses and active variants. Any other doses are ignored.

verify(model0bj,cs0bj,variant0bj,dose0bj) verifies a model model0bj using a configset object cs0bj, variants (variant0bj) and doses (dose0bj). 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

model0bj — SimBiology model

SimBiology model object

SimBiology model, specified as a SimBiology model object.

cs0bj — Configuration set object

configset object

Configuration set object, specified as a Configset object that stores simulation-specific information.

dv0bj - 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.

variant0bj — Variant object

variant object or array of variant objects

Variant object, specified as a Variant object or an array of variant objects.

dose0bj — 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,cs0bj);
```

After verification, check the latest errors and warnings if there is any.

```
sbiolasterror
```

```
ans =
```

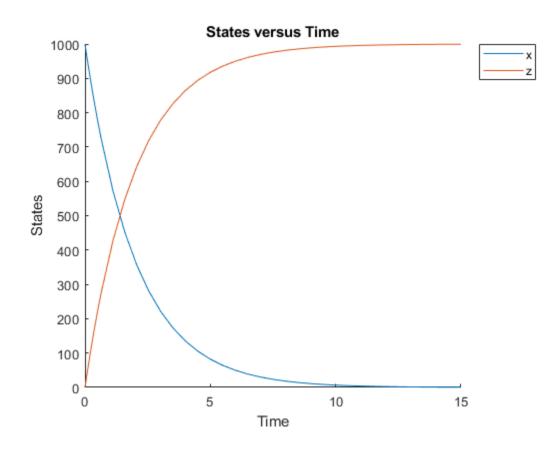
0x1 empty struct array with fields:

Type MessageID Message

sbiolastwarning

Simulate the model.

```
sim = sbiosimulate(m1,cs0bj);
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.

```
d0bj = adddose(m1, 'd1', 'schedule');
d0bj.Amount = 100;
d0bj.AmountUnits = 'molecule';
d0bj.TimeUnits = 'second';
d0bj.Time = 2;
d0bj.TargetName = 'unnamed.x';
```

Verify the model while using the default configset object and added dose object.

verify(m1,defaultConfigSet,d0bj);

After verification, check the latest errors and warnings if there is any.

sbiolasterror

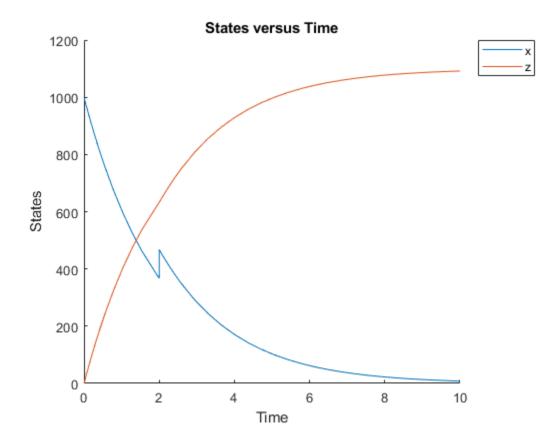
```
ans =
    0x1 empty struct array with fields:
    Type
    MessageID
    Message
sbiolastwarning
```

Simulate the model using the same configset and dose objects.

```
sim = sbiosimulate(m1,defaultConfigSet,d0bj);
```

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.

```
d0bj = adddose(m1, 'd1', 'schedule');
d0bj.Amount = 100;
d0bj.AmountUnits = 'molecule';
d0bj.TimeUnits = 'second';
d0bj.Time = 2;
d0bj.TargetName = 'unnamed.x';
```

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

```
v0bj = addvariant(m1,'v1');
addcontent(v0bj,{'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,cs0bj,v0bj,d0bj);

After verification, check the latest errors and warnings if there is any.

```
sbiolasterror
```

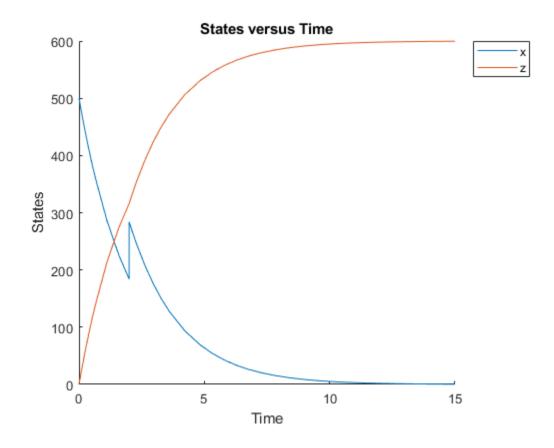
sbiolastwarning

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

```
sim = sbiosimulate(m1,cs0bj,v0bj,d0bj);
```

Plot the result.

sbioplot(sim);



See Also

sbiolasterror, sbiolastwarning

Introduced in R2006a

verify

Verify SimBiology.Scenarios object

Syntax

verify(s0bj,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 "Simulating 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.

```
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(s0bj)
```

```
scenariosTbl=5×2 table
variants dose
[1x1 SimBiology.Variant]
```

Change the entry name of the first entry.

```
rename(sObj,1,'Insulin Impairements')
ans =
Scenarios (5 scenarios)

Name
Content
Number
Entry 1
Insulin Impairements
X Entry 2
dose
SimBiology variants
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	Туре	Units
<pre>{'Plasma Volume (Glu)' {'k1' {'k2' {'Plasma Volume (Ins)' {'m1' {'m2' {'m4' {'m5' {'m6' }{'m6' }{'Hepatic Extraction' {'kmax' {'kmin' {'kabs' {'kgri' {'f' {'a' {'b' {'c' {'d' {'Stomach Glu After Dosing'} {'kp1'</pre>	<pre> } 1.88 } 0.065 } 0.079 } 0.05 } 0.19 } 0.484 } 0.1936 } 0.6469 } 0.6469 } 0.66469 } 0.6558 } 0.008 } 0.0558 } 0.0568 } 0 } 0.9 } 0.9 } 0.9 } 0.82 } 0 } 0.01 } 78 } 2.7</pre>	<pre>{'parameter'} {'parameter'} {'parameter</pre>	<pre>{'deciliter' {'1/minute' {'1/minute' {'liter' {'1/minute' {'1/minute' {'1/minute' {'dimensionless' {'dimensionless' {'dimensionless' {'1/minute' {'1/minute' {'1/minute' {'1/minute' {'1/minute' {'1/minute' {'dimensionless' {'1/milligram' {'dimensionless' {'1/milligram' {'dimensionless' {'gram' {'milligram/minute'</pre>
<pre>{'kp2' {'kp3' {'kp4' } {'ki' } {'[Ins Ind Glu Util]' } {'Vm0' } {'Vmx' } {'Km' } {'p2U' } {'K' } {'alpha' } {'beta' } {'gamma' } {'ke1' } {'ke2' } {'Basal Plasma Glu Conc'</pre>	<pre>} 0.0021 } 0.009 } 0.0618 } 0.0079 } 1 } 2.5129 } 0.047 } 225.59 } 0.0331 } 2.28 } 0.05 } 0.11 } 0.5 } 0.0005 } 339 } 91.76 } 25.49</pre>	<pre>{'parameter'} {'parameter'} }</pre>	<pre>{'1/minute' {'(milligram/minute)/(picomole/li' {'(milligram/minute)/picomole' {'1/minute' {'milligram/minute' {'(milligram/minute)/(picomole/li' {'milligram' {'1/minute' {'picomole/(milligram/deciliter)' {'1/minute' {'(picomole/minute)/(milligram/deo {'1/minute' {'picomole/minute)/(milligram/deo {'1/minute' {'milligram'</pre>

Observables:

Name	Туре	Units
{'[Plasma Glu Conc]'}	{'species'}	{'milligram/deciliter'}
{'[Plasma Ins Conc]'}	{'species'}	{'picomole/liter' }

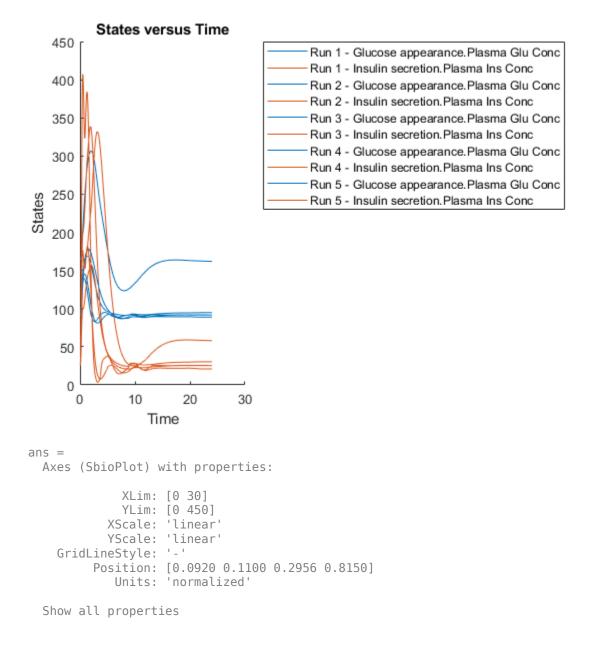
Dosed:

TargetName TargetDimension

{'Dose'} {'Mass (e.g., gram)'}

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(s0bj,24); sbioplot(sd)



If you have Statistics and Machine Learning ToolboxTM, 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 distribution 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 s0bj.

```
remove(s0bj,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(s0bj,'cartesian',["Vmx","kp3"],[pd_Vmx, pd_kp3],'RankCorrelation',[1,0.5;0.5,1])

```
ans =
 Scenarios (2 scenarios)
                                                          Number
                    Name
                                    Content
   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(s0bj,2,'Number',50)
```

```
ans =
 Scenarios (50 scenarios)
                                    Content
                                                        Number
                     Name
    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.

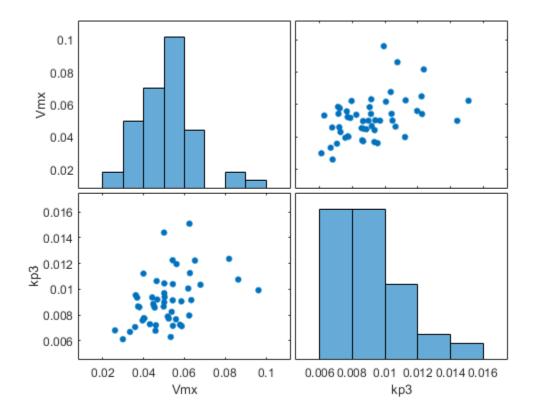
Verify that the Scenarios object can be simulated with the model. The verify function throws an error if any entry does not resolve uniquely to an object in the model or the entry contents have inconsistent lengths (sample sizes). The function throws a warning if multiple entries resolve to the same object in the model.

verify(s0bj,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.

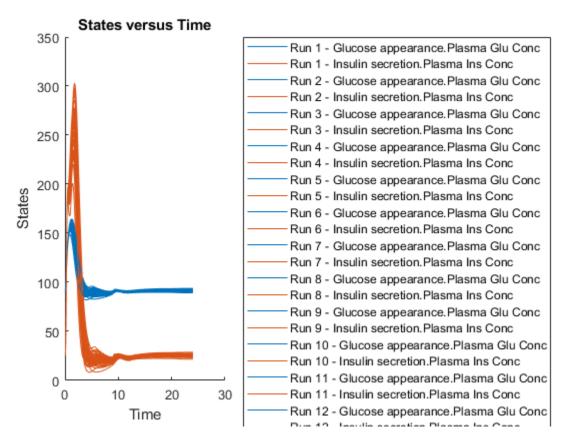
```
sTbl = generate(s0bj);
[s,ax,bigax,h,hax] = plotmatrix([sTbl.Vmx,sTbl.kp3]);
ax(1,1).YLabel.String = "Vmx";
ax(2,1).YLabel.String = "kp3";
```

```
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(s0bj,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(s0bj,2)

entry2struct.SamplingMethod = 'lhs'

You can now use the updated structure to modify entry 2.

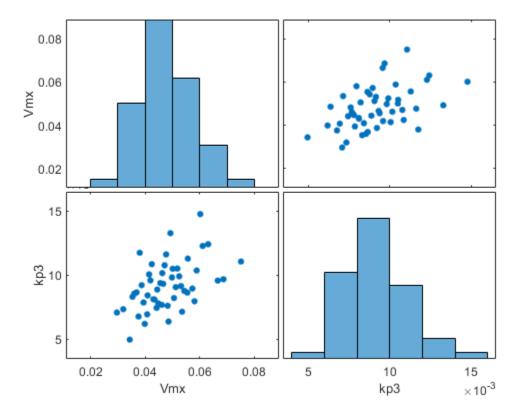
```
updateEntry(s0bj,2,entry2struct)
```

```
ans =
  Scenarios (50 scenarios)
                    Name
                                    Content
                                                        Number
                             SimBiology dose
    Entry 1
                    dose
                                                          1
                             Lognormal distribution
                                                          50
    x (Entry 2.1
                    Vmx
                    kp3
    + Entry 2.2)
                            Lognormal distribution
                                                          50
```

See also Expression property.

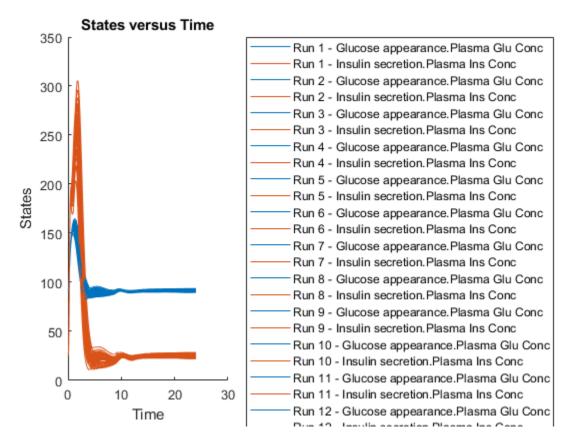
Visualize the sample values.

```
sTbl2 = generate(s0bj);
[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(s0bj,24); sbioplot(sd3);



Restore warning settings.

warning(warnSettings);

Input Arguments

s0bj — 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

s0bj — Simulation scenarios

Scenarios object

Simulation scenarios, returned as a Scenarios object.

See Also

SimBiology.Scenarios | SimFunction object | createSimFunction (model)

Topics

"SimBiology.Scenarios Terminology" on page 2-550 "Combine Simulation Scenarios in SimBiology"

Introduced in R2019b

verify (covmodel)

Check covariate model for errors

Syntax

verify(CovModelObj)

Description

verify(CovModelObj) verifies that the following are true about the Expression on page 3-69
property of CovModelObj, a CovariateModel object:

- 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.

If the previous requirements are true, then verify returns nothing.

See Also

CovariateModel on page 2-137 | Expression on page 3-69 | PKModelDesign object | construct

Topics

"Modeling the Population Pharmacokinetics of Phenobarbital in Neonates" "Specify a Covariate Model"

Introduced in R2011b

Properties

AbsoluteTolerance

Absolute error tolerance applied to state value during simulation

Description

AbsoluteTolerance is a property of a SolverOptions object, which is a property of a Configset object. It 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".

Characteristics

Applies to	Object: SolverOptions
Data type	double
Data values	Positive scalar. Default is 1e-6.
Access	Read/write

Examples

This example shows how to change AbsoluteTolerance.

1 Retrieve the configset object from the modelObj.

```
modelObj = sbiomodel('cell');
configsetObj = getconfigset(modelObj)
```

2 Change the AbsoluteTolerance to 1e-8.

```
set(configsetObj.SolverOptions, 'AbsoluteTolerance', 1.0e-8);
get(configsetObj.SolverOptions, 'AbsoluteTolerance')
```

ans =

1.0000e-008

See Also

AbsoluteToleranceScaling, AbsoluteToleranceStepSize, RelativeTolerance, MassUnits, AmountUnits, Configset object

See Also

Topics "Model Simulation" "Choosing a Simulation Solver" "Ordinary Differential Equations"

AbsoluteToleranceScaling

Control scaling of absolute error tolerance during simulation

Description

AbsoluteToleranceScaling is a property of a SolverOptions object, which is a property of a Configset object. It is available for the ode solvers (ode15s, ode23t, ode45, and sundials).

AbsoluteToleranceScaling controls how the software determines the largest allowable absolute error at any step in a simulation. For details, see "Selecting Absolute Tolerance and Relative Tolerance for Simulation".

Characteristics

Applies to	Object: SolverOptions
Data type	logical
Data values	1, 0, true, or false. Default is true.
Access	Read/write

See Also

AbsoluteTolerance, AbsoluteToleranceStepSize, RelativeTolerance

AbsoluteToleranceStepSize

Initial guess for time step size for scaling of absolute error tolerance

Description

AbsoluteToleranceStepSize is a property of a SolverOptions object, which is a property of a Configset object. It is available for the ode solvers (ode15s, ode23t, ode45, and sundials).

When the AbsoluteToleranceScaling property is enabled, you can set the AbsoluteToleranceStepSize property to specify the initial guess for time step size for scaling. For details, "Selecting Absolute Tolerance and Relative Tolerance for Simulation".

Tip Use AbsoluteToleranceStepSize when a simulation is unsuccessful and generates numerically unstable solutions, and other corrective actions such as checking the model's kinetics do not work. You might encounter unstable solutions if you have very stiff systems in which state values change rapidly at the beginning of a simulation. To solve this, iteratively decrease AbsoluteToleranceStepSize and simulate to find the optimal setting. As a starting point, try setting this property to AbsoluteTolerance * StopTime * 0.1.

Characteristics

Applies to	Object: SolverOptions
Data type	double
Data values	Scalar in units specified by TimeUnits property. Default is [].
Access	Read/write

See Also

AbsoluteTolerance, AbsoluteToleranceScaling, RelativeTolerance

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 modelscoped 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 0×1 empty double column vector (ScheduleDose).
Access	Read/write.

Compatibility Considerations

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 0×1 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 10⁶) 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>.</automatic>
Access	Read/write for properties of Configset

See Also

Configset object, MassUnits

Annotation

(Removed) Store link to URL or file

Note The Annotation property has been removed. Use the Notes property instead.

Description

The Annotation property stores the URL or file name linking to information about a model.

Characteristics

	SimBiology objects: abstract kinetic law, configuration set, compartment, event, kinetic law, model, observable, parameter, reaction, RepeatDose, rule, ScheduleDose, species, or unit
Data type	char string,URL
Data values	Character string with a directory path and filename or a URL
Access	Read/write

Compatibility Considerations

Annotation property has been removed

Errors starting in R2021a

The Annotation property has been removed. Use the Notes property instead to add additional information about the object.

See Also

Notes

BoundaryCondition

Indicate species boundary condition

Description

The BoundaryCondition property indicates whether a species object has a boundary condition.

When the BoundaryCondition of a species is false (default), the species quantity is modified by reactions, rules, events, and doses. If the BoundaryCondition is true, the species quantity is modified by rules, events, and doses, but not by reactions.

Set the BoundaryCondition to true when you want the species to participate in a reaction, but do not want any reactions to modify its quantity.

All SimBiology species are state variables regardless of the BoundaryCondition or ConstantAmount on page 3-29 property.

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 3-17]. 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 dexamethas one (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 3-29 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
```

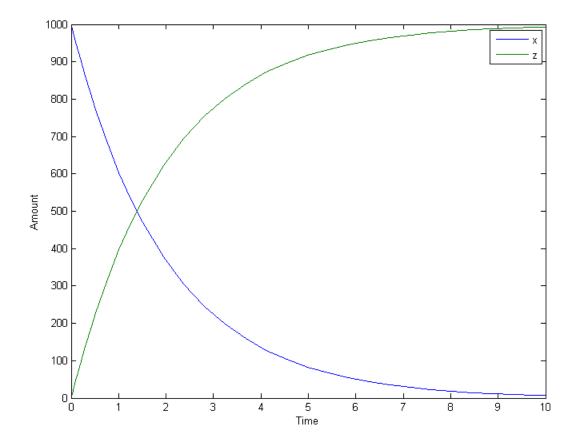
A SimBiology model named m1 is loaded to the MATLAB Workspace. The model is a simple radioactive decay model in which two species (x and z) are modified by the following reaction.

ml.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.

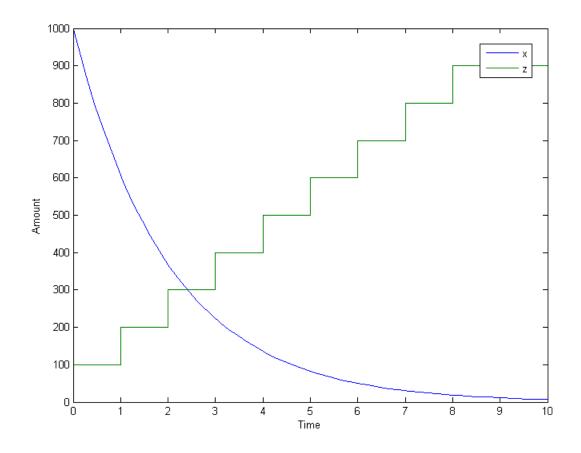
set(m1.species(2), 'BoundaryCondition', true);

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 3-71 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

CapacityUnits | ConstantCapacity | Value | addcompartment | addspecies

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 3-23.

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(compartment0bj2, 'Compartments')
```

```
SimBiology Compartment - matrix
```

Compartment Components:

Capacity:1CapacityUnits:0Compartments:0ConstantCapacity:trueOwner:mitochondrionSpecies: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	Perform dimensional analysis on model
Туре	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(unit0bj);
```

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	

See Also

BoundaryCondition | ConstantAmount | ConstantCapacity | ConstantValue | StatesToLog | addspecies

Topics

"Model Simulation" "Conservation of Amounts During Simulation"

Introduced in R2019b

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 3-32 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.

species0bj = addspecies (model0bj, 'glucose');
get (species0bj, '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

ConstantAmount | ConstantValue | addcompartment

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:

 $\begin{array}{l} A spartic \text{ acid } \xrightarrow{\text{aspartate kinase}} \beta - A spartylpho sphate \\ \beta - A spartylpho sphate \rightarrow Threonine \end{array}$

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

Value:

5

10

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
variant0bj
SimBiology Variant - v1 (inactive)
   ContentIndex:
                       Type:
                                      Name:
                                                          Property:
                                                          InitialAmount
                       species
                                      А
   1
                       species
                                      R
                                                          InitialAmount
Append data to the Content property.
addcontent(variantObj, {'species', 'C', 'InitialAmount', 15});
SimBiology Variant - v1 (inactive)
```

ContentIndex:	Type:	Name:	Property:	Value:
1 2	species species	A B	InitialAmount InitialAmount	5 10
3	species	C	InitialAmount	15

4 Remove a species from the Content property.

rmcontent(variant0bj, 3);

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 3-42 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

CovariateLabels (CovariateModel)

Labels for covariates in CovariateModel object

Description

The **CovariateLabels** property is a cell array of character vectors specifying the labels for the covariates in the **Expression** on page 3-69 property of a **CovariateModel** object.

Characteristics

Applies to	Object: CovariateModel on page 2-137
Data type	Cell array of character vectors
	Labels for the covariates in the Expression on page 3-69 property
Access	Read only

See Also

CovariateModel on page 2-137 | Expression on page 3-69

Data

Store simulation data

Description

The Data property contains the simulation data stored in the SimData object.

This property contains all data logged during a simulation, including species amounts, parameter values, and sensitivities. The property is an $m \times n$ array, where m is the number of time steps in the simulation and n is the number of quantities logged. The rows of the array are labeled by the time points in the Time property, and the columns are labeled by the metadata in the DataInfo property.

Characteristics

Applies to	Object: SimData
Data type	double
Data values	Default value is [] (empty).
Access	Read-only

See Also

DataInfo, ModelName

DataCount

Numbers of species, parameters, sensitivities

Description

The DataCount property shows how many species, parameters, and sensitivities are logged in a SimData object. It is a MATLAB structure with the fields Species, Parameter, and Sensitivity. The information in this property is redundant with the DataInfo property and is there to give you a convenient means to access the information.

Characteristics

Applies to	Object: SimData
Data type	struct
Data values	Default value for each field is 0.
Access	Read-only

See Also

StopTime

DataInfo

Metadata labels for simulation data

Description

The DataInfo property contains the metadata that label the columns of the SimData object array. It is an $n \times 1$ cell array of structures. The ith cell contains metadata labeling the ith column of the SimData object array.

The possible types of structures are as follows.

Туре	Fields	
Species	Type: species Name: Compartment: Units:	
Parameter	Type: parameter Name: Reaction: <name a="" is="" of="" parameter="" reaction="" scoped="" that="" to,<br="">or '' if parameter is scoped to model> Units:</name>	
Sensitivity	Units:	

Characteristics

Applies to	Object: SimData
Data type	n x 1 cell array of structs
Data values	Default value is 0×1 cell array.
Access	Read-only

See Also

StopTime

DataNames

Show names in SimData object

Description

The DataNames property holds the names that label the columns of the data matrix in the Data property. The property contains an n-by-1 cell array of character vectors. The software provides this information for your convenience.

Characteristics

Applies to	Object: SimData
Data type	Cell array of character vectors
Data values	Default value is 0×1 cell array.
Access	Read-only

See Also

StopTime

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 3-42 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 1-229 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

Perform dimensional analysis on model

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
Retrieve the configset object of the model
```

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

get, getconfigset, sbiosimulate, set

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 3-42. 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 1-229 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.
	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

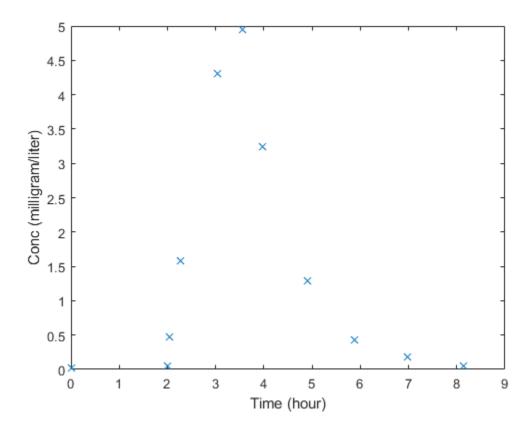
This example shows how to estimate the time lag before a bolus dose was administered and the duration of the dose using a one-compartment model.

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');
                         =
                           'Bolus';
pkc1.DosingType
                         =
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')
```

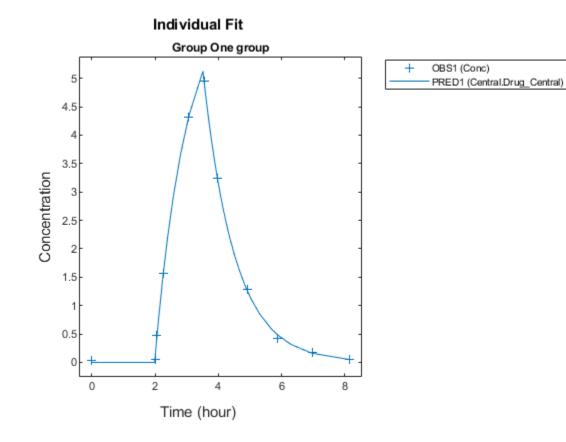
```
fitResults =
  OptimResults with properties:
                    ExitFlag: 1
                      Output: [1x1 struct]
                   GroupName: One group
                        Beta: [2x4 table]
         ParameterEstimates: [2x4 table]
                           J: [11x2 double]
                        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}
    EstimatedParameterNames: {'lagP' 'durP'}
             ErrorModelInfo: [1x3 table]
         EstimationFunction: 'fminsearch'
```

Display the result.

fitResults.ParameterEstimates

ans=2×4 table Name	Estimate	StandardError	Bou	nds
{'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 adrug 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

ErrorTolerance

Specify explicit or implicit tau error tolerance

Description

The ErrorTolerance property specifies the error tolerance for the explicit tau and implicit tau stochastic solvers. It is a property of the SolverOptions object. SolverOptions is a property of the configset object. 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 % to 5 %.

Characteristics

Applies to	Object: SolverOptions
Data type	double
Data values	>0, <1. The default is 3e-2.
Access	Read/write

Examples

This example shows how to change ErrorTolerance settings.

1 Retrieve the configset object from the modelObj and change the SolverType to expltau.

```
modelObj = sbiomodel('cell');
configsetObj = getconfigset(modelObj);
set(configsetObj, 'SolverType', 'expltau')
```

2 Change the ErrorTolerance to 1e-8.

```
set(configsetObj.SolverOptions, 'ErrorTolerance', 5.0e-2);
get(configsetObj.SolverOptions, 'ErrorTolerance')
```

ans =

5.000000e-002

See Also

LogDecimation, RandomState

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.

Applies to	Object: PKModelMap
Data type	Character vector or cell array of character vectors
	Name of a species, compartment, or parameter object or empty. Default is an empty cell array.
Access	Read/write

Characteristics

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(event0bj, 'EventFcns', {'pA = 0pA', 'mA = pol'});

3 Get the EventFcns property.

```
get(event0bj, '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
                           = addparameter(model, 'A', 50);
amountParam
amountParam.ConstantValue = false;
amountParam.ValueUnits
                           = 'milligram'
amountParam =
   SimBiology Parameter Array
   Index:
             Name:
                      Value:
                                 Units:
   1
             А
                      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	<pre>= adddose(model,'adaptive dose','repeat');</pre>
dose.Amount	= 'A';
dose.Rate	= 'R';

Set other dose properties.

dose.TargetName	<pre>= 'drug';</pre>
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 .

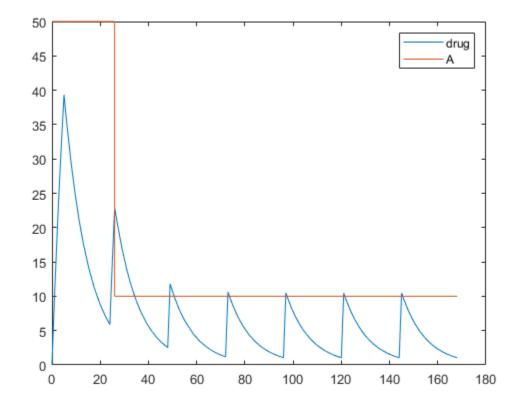
```
event = addevent(model,'time >= 26','A = 10');
```

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');
```

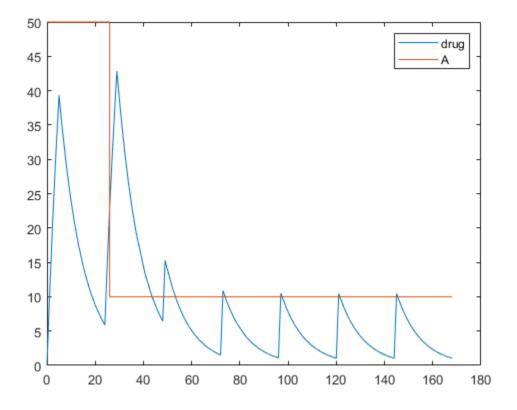


Alternatively, you can allow the ongoing dose event to finish before applying the new dose amount by setting EventMode to 'continue'.

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(event0bj)

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(unitprefix0bj1);

3 Query the Exponent property.

```
get(unitprefix0bj1, 'Exponent')
```

ans =

15

See Also

get, sbioaddtolibrary, sbiounitprefix, set, UnitPrefix object

Expression (CovariateModel)

Define relationship between parameters and covariates

Description

The Expression property is a character vector or cell array of character vectors, where each character vector represents the relationship between a parameter and one or more covariates. The Expression property denotes fixed effects with the prefix theta, and random effects with the prefix eta.

Each expression must be in the form:
parameterName = relationship

This example of an expression defines the relationship between a parameter (volume) and a covariate (weight), with fixed effects, but no random effects: CovModelObj.Expression = { 'volume = thetal + theta2*weight'};

Parameter-Covariate Relationship	Expression Format
Linear with random effect	Cl = theta1 + theta2*WEIGHT + eta1
Exponential without random effect	<pre>Cl = exp(theta_Cl + theta_Cl_WT*WEIGHT)</pre>
Exponential, WEIGHT centered by mean, has random effect	<pre>Cl = exp(thetal + theta2*(WEIGHT - mean(WEIGHT)) + etal)</pre>
Exponential, log(WEIGHT), which is equivalent to power model	<pre>Cl = exp(theta1 + theta2*log(WEIGHT) + eta1)</pre>
Exponential, dependent on WEIGHT and AGE, has random effect	Cl = exp(thetal + theta2*WEIGHT + theta3*AGE + etal)
Inverse of probit, dependent on WEIGHT and AGE, has random effect	<pre>Cl = probitinv(thetal + theta2*WEIGHT + theta3*AGE + etal)</pre>
Inverse of logit, dependent on WEIGHT and AGE, has random effect	<pre>Cl = logitinv(theta1 + theta2*WEIGHT + theta3*AGE + eta1)</pre>

This table illustrates expression formats for some common parameter-covariate relationships.

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.

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.

Tip Use the getCovariateData on page 2-228 method to view the covariate data when writing equations for the Expression property of a CovariateModel object.

Tip Use the verify on page 2-675 method to check that the Expression property of a CovariateModel object meets the conditions described previously.

Characteristics

Applies to	Object: CovariateModel on page 2-137	
Data type	Character vector or cell array of character vectors	
Data values	<pre>parameterName = relationship</pre>	
Access	Read/write	

See Also

CovariateModel on page 2-137 | getCovariateData on page 2-228 | verify on page 2-675

Topics

"Modeling the Population Pharmacokinetics of Phenobarbital in Neonates" "Specify a Covariate Model"

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 3-141 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 3-92. 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 3-170 property, and the parameter variables are defined in the ParameterVariables on page 3-128 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 3-168 to SpeciesVariables and ParameterVariableNames on page 3-126 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 \rightarrow 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

$$r = k \prod_{i=1}^{nr} [Si]^m$$

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 1-284). 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 reactionObjis 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

FixedEffectDescription (CovariateModel)

Descriptions of fixed effects in CovariateModel object

Description

The FixedEffectDescription property is a cell array of character vectors describing the fixed effects in the Expression on page 3-69 property of a CovariateModel object. Each character vector describes the role of a fixed effect in the expression equation. For example, in the following expression equation:

```
Cl = exp(theta1 + theta2*WEIGHT + theta3*AGE + eta1)
```

The description for the fixed effect thetal 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.

Characteristics

Applies to	Object: CovariateModel on page 2-137
Data type	Cell array of character vectors
	Description of the roles of the fixed effects in the Expression on page 3-69 property
Access	Read only

See Also

CovariateModel on page 2-137 | Expression on page 3-69 | FixedEffectNames on page 3-75 | FixedEffectValues on page 3-76

FixedEffectNames (CovariateModel)

Names of fixed effects in CovariateModel object

Description

The FixedEffectNames property is a cell array of character vectors specifying the names of the fixed effects in the Expression on page 3-69 property of a CovariateModel object. Names of fixed effects are denoted with the prefix theta.

Characteristics

Applies to	Object: CovariateModel on page 2-137
Data type	Cell array of character vectors
	Names of the fixed effects in the Expression on page 3-69 property. These name are denoted with the prefix theta.
Access	Read only

See Also

CovariateModel on page 2-137 | Expression on page 3-69 | FixedEffectDescription on page 3-74 | FixedEffectValues on page 3-76

FixedEffectValues (CovariateModel)

Values for initial estimates of fixed effects in CovariateModel object

Description

The FixedEffectValues property is a structure containing one field for each fixed effect in the Expression on page 3-69 property of a CovariateModel object. Each field contains the value of the initial estimate for a fixed effect.

Tip You must set this property before using the CovariateModel object as input to sbionlmefit or sbionlmefitsa. Use the constructDefaultFixedEffectValues on page 2-134 method to create a structure of fixed-effect initial estimate values, set to a default of zero. Then edit the structure and use it to modify this property.

Characteristics

Applies to	Object: CovariateModel on page 2-137
Data type	Structure with one field for each fixed effect
	Each field contains a double specifying the value of the initial estimate for a fixed effect in the CovariateModel object
Access	Read/write

See Also

CovariateModel on page 2-137 | Expression on page 3-69 | FixedEffectDescription on page 3-74 | FixedEffectNames on page 3-75 | constructDefaultFixedEffectValues on page 2-134

Topics

"Modeling the Population Pharmacokinetics of Phenobarbital in Neonates" "Specify a Covariate Model"

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 3-42 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 3-42 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 3-42 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 1-229 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

Valueaddspecies, 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 1-229 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 meter², then species must be amount/meter² 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	С	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 modelscoped 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.
	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 2-41 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 3-168 and ParameterVariableNames on page 3-126. 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 3-71 for more information.

You can find the KineticLawName list in the kinetic law library by using the command sbiowhos - kineticlaw (sbiowhos on page 1-284). 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.

```
model0bj = sbiomodel ('my_model');
reaction0bj = addreaction (model0bj, 'a + b -> c + d');
kineticlaw0bj = addkineticlaw(reaction0bj, '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.
	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

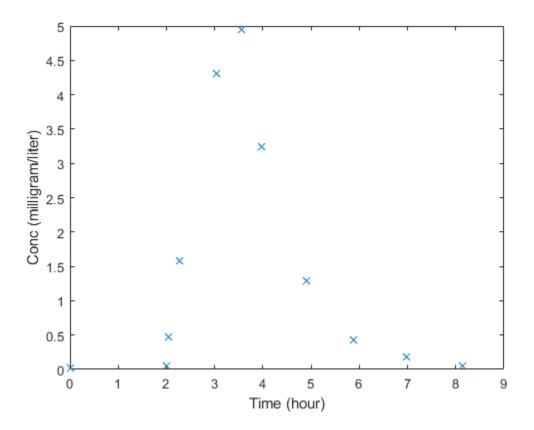
This example shows how to estimate the time lag before a bolus dose was administered and the duration of the dose using a one-compartment model.

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');
                         =
                           'Bolus';
pkc1.DosingType
                        =
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')
```

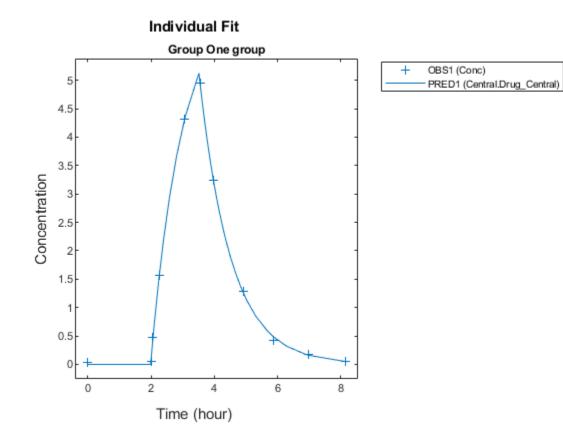
```
fitResults =
 OptimResults with properties:
                   ExitFlag: 1
                     Output: [1x1 struct]
                  GroupName: One group
                        Beta: [2x4 table]
         ParameterEstimates: [2x4 table]
                           J: [11x2 double]
                        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}
    EstimatedParameterNames: {'lagP' 'durP'}
             ErrorModelInfo: [1x3 table]
         EstimationFunction: 'fminsearch'
```

Display the result.

fitResults.ParameterEstimates

ans=2×4 table Name	Estimate	StandardError	Bou	nds
{'lagP'} {'durP'}	1.986 1.527	0.0051568 0.012956	1 1	5 5

plot(fitResults)



See Also

RepeatDose object | ScheduleDose object

Topics

"Parameterized and Adaptive Doses"

LogDecimation

Specify frequency to log stochastic simulation output

Description

LogDecimation is a property of the SolverOptions property, which is a property of a configset object. This property defines how often stochastic simulation data is recorded. LogDecimation 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.

Characteristics

Applies to	Object: SolverOptions
Data type	int
Data values	>0. Default is 1.
Access	Read/write

Examples

This example shows how to change LogDecimation settings.

1 Retrieve the configset object from the modelObj, and change the SolverType to expltau.

```
model0bj = sbiomodel('cell');
configset0bj = getconfigset(model0bj);
set(configset0bj, 'SolverType', 'expltau')
```

2 Change the LogDecimation to 10.

```
set(configsetObj.SolverOptions, 'LogDecimation', 10);
get(configsetObj.SolverOptions, 'LogDecimation')
ans =
10
```

See Also

ErrorTolerance, RandomState

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>.</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(configset0bj)
```

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 $50 \log s$ 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(configset0bj, 'MaximumWallClock', 20)
```

View the properties of configsetObj.

```
get(configset0bj)
```

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

MaxIterations

Specify nonlinear solver maximum iterations in implicit tau

Description

The MaxIterations property specifies the maximum number of iterations for the nonlinear solver in impltau. It is a property of the SolverOptions object. SolverOptions is a property of the configset object.

The implicit tau solver in SimBiology software 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. The default value of MaxIterations is 15.

Characteristics

Applies to	Object: SolverOptions
Data type	int
Data values	>0. Default is 15.
Access	Read/write

Examples

This example shows how to change MaxIterations settings.

1 Retrieve the configset object from the modelObj, and change the SolverType to impltau.

```
modelObj = sbiomodel('cell');
configsetObj = getconfigset(modelObj);
set(configsetObj, 'SolverType', 'impltau');
```

2 Change the MaxIterations to 25.

```
set(configsetObj.SolverOptions, 'MaxIterations', 25);
get(configsetObj.SolverOptions, 'MaxIterations')
```

```
ans =
```

25

See Also

ErrorTolerance, LogDecimation, RandomState

MaxStep

Specify upper bound on ODE solver step size

Description

MaxStep is a property of the SolverOptions property, which is a property of a configset object. This property specifies the bounds on the size of the time steps. MaxStep is available only for ODE solvers (ode15s, ode23t, ode45, and sundials).

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 on MaxStep, see odeset.

Characteristics

Applies to	Object: SolverOptions
Data type	Positive scalar or empty
Data values	Default value is [] (empty), which is equivalent to setting MaxStep to infinity.
Access	Read/write

See Also

SimBiology property RelativeTolerance

MATLAB function odeset

ModelName

Name of model simulated

Description

The ${\tt ModelName}$ property shows the name of the model for which the SimData object contains the simulation data.

Characteristics

Applies to	Object: SimData
Data type	Character vector
Data values	Default value is ' ' (empty).
Access	Read-only

See Also

Data, DataInfo

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.

	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

Characteristics

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-P04]

3 Set the reaction Name and verify.

```
set (reactionObj, 'Name', 'Aspartate kinase reaction');
get (reactionObj, 'Name')
```

MATLAB returns:

ans =

Aspartate kinase reaction

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.

$$\Big(\frac{1}{x(t)}\Big)\Big(\frac{\partial x(t)}{\partial k}\Big)$$

• '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

	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, 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

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
	Name of a species or parameter object or empty. Default is an empty cell array.
Access	Read/write

See Also

Dosed, Estimated, PKModelMap object

Offset

(Removed) Unit composition modifier

Note The Offset property has been removed. Use an absolute unit that does not require an offset instead.

Description

The Offset is the numerical value by which the unit composition is modified from the base unit. For example, °Celsius = (5/9)*(°Fahrenheit-32); Multiplier is 5/9 and Offset is -32.

Characteristics

Applies to	Object: Unit
Data type	double
Data values	Real number. Default is 0.
Access	Read/write

See Also

Composition, get, Multiplier, sbioaddtolibrary, sbioshowunits, sbiounit, set

Compatibility Considerations

Offset property has been removed

Errors starting in R2021a

The Offset property has been removed. Use an absolute unit that does not require an offset. For example, use kelvin instead of Celsius or Fahrenheit.

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.

See Also

 $Inputs, \verb+sbioselect, SensitivityAnalysis, SensitivityAnalysisOptions$

OutputTimes

Specify times to log deterministic simulation output

Description

OutputTimes is a property of the SolverOptions property, which is a property of a Configset object. This property specifies the times during a deterministic (ODE) simulation that data is recorded. Time units are specified by the TimeUnits property of the Configset object. OutputTimes is available only for ODE solvers (ode15s, ode23t, ode45, and sundials).

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.

Characteristics

Applies to	Object: SolverOptions
Data type	double
	Vector of nonnegative, monotonically increasing values, or [], an empty vector. Default is [], which results in data being logged every time the simulation solver takes a step.
Access	Read/write

Examples

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.

```
set(configsetObj.SolverOptions, 'OutputTimes', [1:10])
get(configsetObj.SolverOptions, '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.

See Also

MaximumNumberOfLogs, MaximumWallClock, SolverOptions, StopTime, TimeUnits, MassUnits, AmountUnits

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.

compartment0bj3 = addcompartment(compartment0bj2, 'matrix');

4 Display the Owner property in the compartment objects.

get(compartment0bj3, '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

ParameterNames (CovariateModel)

Names of parameters in CovariateModel object

Description

The ParameterNames property is a cell array of character vectors specifying the names of the parameters in the Expression on page 3-69 property of a CovariateModel object.

Characteristics

Applies to	Object: CovariateModel on page 2-137
Data type	Cell array of character vectors
	Names of the parameters in the Expression on page 3-69 property
Access	Read only

See Also

CovariateModel on page 2-137 | Expression on page 3-69

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 2-65 and delete it with the method delete on page 2-135.

You can view parameter object properties with the **get** command and configure properties with the **set** command.

Applies to	Objects: model, kineticlaw	
Data type	Array of parameter objects	
Data values	Parameter objects. Default value is [] (empty).	
Access	Read-only	

Characteristics

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 3-141 equation in the reaction object. Use setparameter on page 2-573 to assign ParameterVariableNames. When you assign species to ParameterVariableNames, SimBiology software maps these parameter names to ParameterVariables on page 3-128 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 3-71. 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 3-71 property of the abstract kinetic law object. Use this property to specify the parameters in the ReactionRate on page 3-141 equation. Use the method set to assign ParameterVariables to a kinetic law definition. For more information, see "Kinetic Law Definition" on page 3-71.

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

	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 2-69 function. You can remove product species from the reaction with rmproduct on page 2-528. 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

RandomEffectNames (CovariateModel)

Names of random effects in CovariateModel object

Description

The RandomEffectNames property is a cell array of character vectors specifying the names of the random effects in the Expression on page 3-69 property of a CovariateModel object. Names of random effects are denoted with the prefix eta.

Characteristics

Applies to	Object: CovariateModel on page 2-137
Data type	Cell array of character vectors
	Names of the random effects in the Expression on page 3-69 property. These name are denoted with the prefix eta.
Access	Read only

See Also

CovariateModel on page 2-137 | Expression on page 3-69

RandomState

Set random number generator

Description

The RandomState property sets the random number generator for the stochastic solvers. It is a property of the SolverOptions object. SolverOptions is a property of the configset object.

SimBiology software uses a pseudorandom number generator. The sequence of numbers generated is determined by the state of the generator, which can be specified by the integer RandomState. If RandomState is set to 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 software resets the state at startup. The default value of RandomState is [].

Characteristics

Applies to	Objects: SolverOptions for SSA, expltau, impltau
Data type	int
Data values	Default is [] (empty).
Access	Read/write

Examples

This example shows how to change RandomState settings.

1 Retrieve the configset object from the modelObj and change the SolverType to expltau.

```
modelObj = sbiomodel('cell');
configsetObj = getconfigset(modelObj);
set(configsetObj, 'SolverType', 'expltau')
```

2 Change the Randomstate to 5.

```
set(configsetObj.SolverOptions, 'RandomState', 5);
get(configsetObj.SolverOptions, 'RandomState'))
```

ans =

5

See Also

ErrorTolerance, LogDecimation, MaxIterations

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 modelscoped 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.

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 0×1 empty double column vector (ScheduleDose), that is, the dose is interpreted as a bolus (instantaneous) dose.
Access	Read/write.

Characteristics

Compatibility Considerations

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 3-42 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 2-71 method.

You can remove reactant species from the reaction with the rmreactant on page 2-530 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 reaction0bj.

```
get(reactionObj, 'Reactants')
```

MATLAB returns:

SimBiology Species Array

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 \rightarrow 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
	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
	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', '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 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.

```
rl.ReactionRate = 'Vm / ( (Kh/a)^n + 1 )';
kl.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)

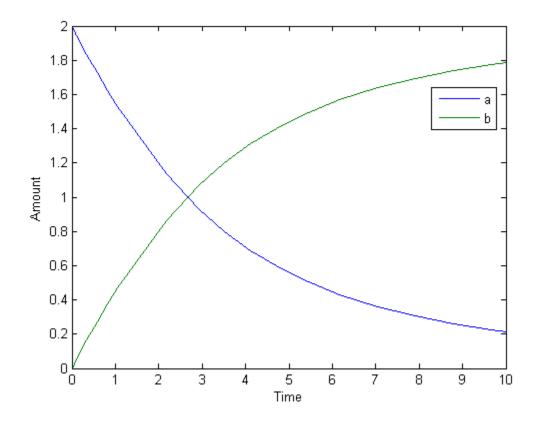
You no longer see the error message.

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 2-73, and you can remove a reaction from the model object with the method delete on page 2-135.

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.

```
model0bj = sbiomodel ('my_model');
reaction0bj = addreaction (model0bj, '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

RelativeTolerance

Allowable error tolerance relative to state value during a simulation

Description

RelativeTolerance is a property of the SolverOptions object, which is a property of a Configset object. It is available 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.

If you set the RelativeTolerance at 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".

Characteristics

Applies to	Object: SolverOptions
Data type	double
Data values	Positive scalar that is <1. Default is 1e-3.
Access	Read/write

Examples

This example shows how to change AbsoluteTolerance.

1 Retrieve the configset object from the modelObj.

```
modelObj = sbiomodel('cell');
configsetObj = getconfigset(modelObj)
```

2 Change the AbsoluteTolerance to 1e-8.

```
set(configsetObj.SolverOptions, 'RelativeTolerance', 1.0e-6);
get(configsetObj.SolverOptions, 'RelativeTolerance')
ans =
```

1.0000e-006

See Also

AbsoluteTolerance, MassUnits, AmountUnits, Configset object

See Also

Topics "Model Simulation" "Choosing a Simulation Solver" "Ordinary Differential Equations"

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 modelscoped 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.
	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 3-194 when the rule is evaluated.

You can add a rule to a model object with the addrule on page 2-78 method and remove the rule with the delete on page 2-135 method. For more information on rules, see addrule on page 2-78 and RuleType on page 3-153.

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
	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 3-194 when the rule is evaluated.

You can add a rule to a model object with the addrule on page 2-78 method and remove the rule with the delete on page 2-135 method. For more information on rules, see addrule on page 2-78.

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	<pre>'initialAssignment', 'repeatedAssignment''algebraic', 'rate'. Default value is 'initialAssignment'.</pre>
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 \rightarrow 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: ''
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

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 2-78 method and remove the rule with the delete on page 2-135 method. For more information on rules, see addrule and RuleType on page 3-153.

Characteristics

Applies to	Object: model
Data type	Array of rule objects
Data values	Rule object
Access	Read-only

Examples

2

1 Create a model object, and then add a reaction object.

```
modelObj = sbiomodel ('my_model');
reactionObj = addreaction (modelObj, 'a + b -> c + d');
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"

RunInfo

Information about simulation

Description

The RunInfo property contains information describing the simulation run that yielded the data in the SimData object.

The following information is stored:

- **Configset** A struct form of the configuration set used during simulation. This would typically be the model's active configset.
- Variant A struct form of the variant(s) used during simulation.
- SimulationDate The date/time of simulation.
- SimulationType Either 'single run' or 'ensemble run', depending on whether the data object was created using the function sbiosimulate or the function sbioensemblerun.

Characteristics

Applies to	Object: SimData
Data type	struct
Data values	Default values are as follows: ConfigSet: [] SimulationDate: '' SimulationType: '' Variant: [] In practice, the ConfigSet, SimulationDate, and SimulationType fields are rarely empty, since they are populated after simulation.
Access	Read-only

See Also

StopTime

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
Туре	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

SensitivityAnalysis

Enable or disable sensitivity analysis

Description

SensitivityAnalysis is a property of the SolverOptions property, which is a property of a configset object. 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.

Note Models containing the following active components do not support sensitivity analysis:

- Nonconstant compartments
- Algebraic rules
- Events

For more information on setting up sensitivity analysis, see SensitivityAnalysisOptions . For a description of sensitivity analysis calculations, see "Sensitivity Analysis in SimBiology".

Characteristics

Applies to	Object: SolverOptions
Data type	logical
Data values	1, 0, true, false. Default is false.
Access	Read/write

Examples

This example shows how to enable SensitivityAnalysis.

1 Retrieve the configset object from the modelObj.

```
modelObj = sbiomodel('cell');
configsetObj = getconfigset(modelObj);
```

2 Enable SensitivityAnalysis.

See Also

 $Sensitivity Analysis Options, \ Solver Options, \ Solver Type, \ States To Log$

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 3-160.

When sensitivity analysis is enabled, the following command

```
[t,x,names] = sbiosimulate(model0bj)
```

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 3-161.

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 3-6 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
	SensitivityAnalysisOptions properties as summarized in "Property Summary" on page 3-160.
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 =

6 Simulate and return the results to three output variables. See "Description" on page 3-160 for more information.

[t,x,names] = sbiosimulate(model0bj);

7 Display the names.

```
names
names =
    'x'
    'z'
    'd[z]/d[z]_0'
    'd[z]/d[Reaction1.c]'
```

Display state values x.

х

The display follows the column order shown in ${\tt names}$ for the values in x. The rows correspond to ${\tt t}.$

See Also

addconfigset, getconfigset, SensitivityAnalysis

SolverOptions

Specify model solver options

Description

The SolverOptions property is an object that holds the model solver options in the configset object. Changing the property SolverType changes the options specified in the SolverOptions object.

Properties of SolverOptions are summarized in "Property Summary" on page 3-163.

Property Summary

AbsoluteTolerance	Absolute error tolerance applied to state value during simulation
AbsoluteToleranceScaling	Control scaling of absolute error tolerance during simulation
AbsoluteToleranceStepSize	Initial guess for time step size for scaling of absolute error tolerance
ErrorTolerance	Specify explicit or implicit tau error tolerance
LogDecimation	Specify frequency to log stochastic simulation output
MaxIterations	Specify nonlinear solver maximum iterations in implicit tau
MaxStep	Specify upper bound on ODE solver step size
OutputTimes	Specify times to log deterministic simulation output
RandomState	Set random number generator
RelativeTolerance	Allowable error tolerance relative to state value during a simulation
SensitivityAnalysis	Enable or disable sensitivity analysis
Туре	Display SimBiology object type

Characteristics

Applies to	Object: configset
Data type	Object
	Solver options depending on SolverType. Default is SolverOptions for default SolverType (ode15s).
Access	Read-only

Examples

This example shows the changes in SolverOptions for various SolverType settings.

1 Retrieve the configset object from the modelObj.

```
modelObj = sbiomodel('cell');
configsetObj = getconfigset(modelObj);
```

2 Configure the SolverType to ode45.

```
set(configsetObj, 'SolverType', 'ode45');
get(configsetObj, 'SolverOptions')
```

Solver Settings: (ode)

AbsoluteTolerance:	1.000000e-006
RelativeTolerance:	1.000000e-003

3 Configure the SolverType to ssa.

```
set(configsetObj, 'SolverType', 'ssa');
get(configsetObj, 'SolverOptions')
```

Solver Settings: (ssa) LogDecimation:

LogDecimation: 1 RandomState: []

4 Configure the SolverType to impltau.

```
set(configsetObj, 'SolverType', 'impltau');
get(configsetObj, 'SolverOptions')
```

Solver Settings: (impltau)

ErrorTolerance:	3.000000e-002
LogDecimation:	1
AbsoluteTolerance:	1.000000e-002
RelativeTolerance:	1.000000e-002
MaxIterations:	15
RandomState:	[]

5 Configure the SolverType to expltau.

```
set(configsetObj, 'SolverType', 'expltau');
get(configsetObj, 'SolverOptions')
```

Solver Settings: (expltau)

ErrorTolerance:	3.000000e-002
LogDecimation:	1
RandomState:	[]

See Also

addconfigset, getconfigset

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	<pre>'ode15s', 'ode23t', 'ode45', 'sundials', 'ssa', 'expltau', 'impltau'. Default is 'ode15s'.</pre>
	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: RelativeTolerance: SensitivityAnalysis:	1.000000e-006 1.000000e-003 false	
	RuntimeOptions: StatesToLog:	all	
	CompileOptions: UnitConversion: DimensionalAnalysis:	false true	
	SensitivityAnalysisOptions: Inputs: Outputs:	0 0	
2	Configure the SolverType to ode45.		
	<pre>set(configsetObj, 'SolverType', ' configsetObj</pre>	ode45')	
Configuration Settings - defa SolverType: StopTime:		ault (active) ode45 10.000000	
	SolverOptions: AbsoluteTolerance: RelativeTolerance: SensitivityAnalysis:	1.000000e-006 1.000000e-003 false	
	RuntimeOptions: StatesToLog:	all	
	CompileOptions: UnitConversion: DimensionalAnalysis:	false true	
	SensitivityAnalysisOptions: Inputs: Outputs:	0 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 2-73. A species object can also be added to the Species property with the method addspecies on page 2-89.

If you remove a reaction with the method delete on page 2-167, 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.

Applies to	Object: compartment
Data type	Array of species objects
Data values	Species object. Default is [] (empty).
Access	Read-only

Characteristics

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 3-141 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 3-170 in the kinetic law object.

The ReactionRate property of a reaction object shows the result of a mapping from kinetic law definition on page 3-71. 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 3-71 property of the kinetic law object to determine the ReactionRate on page 3-141 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 3-71.

Characteristics

Applies to	Objects: abstract kinetic law, kineticlaw	
Data type	Cell array of character vectors	
Data values	Defined by abstract kinetic law	
	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 modelscoped 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.
	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.

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

Characteristics

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 = SimBiolo	gy Species Array	7		
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
```

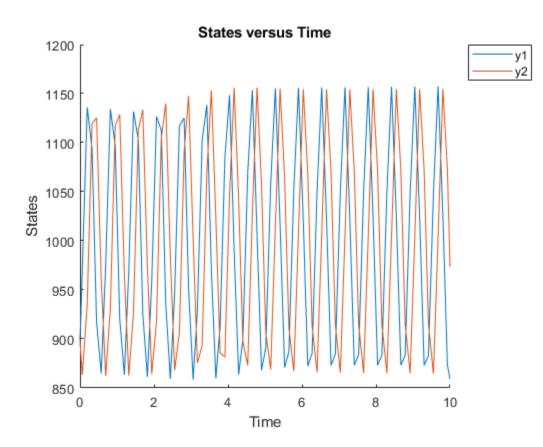
```
ans =
   SimBiology Species Array
Index: Compartment: Name: Value: Units:
   1    unnamed    y1    900
   2    unnamed     y2    900
```

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));
```

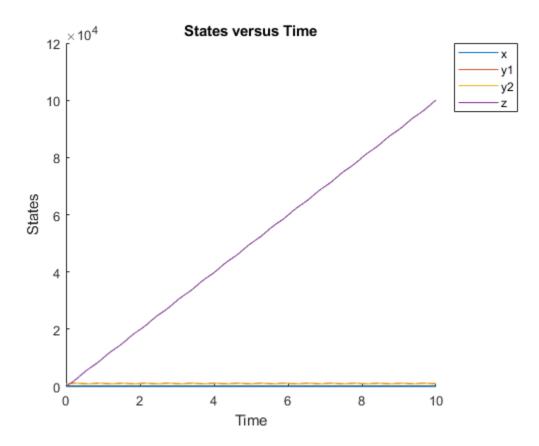


To reset to the default list, set StatesToLog to a string 'all', which means all species objects, all nonconstant compartment objects and all nonconstant parameter objects are logged by default. A nonconstant compartment or parameter means that its Constant property is set to false.

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 2-130, RuntimeOptions on page 3-157

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 2-528 or rmreactant on page 2-530 function. Add a product or reactant and set stoichiometry with methods addproduct on page 2-69 and addreactant on page 2-71.

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
	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
  Note with get that the Reaction property updates automatically.
4
    get (reaction0bj, '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 MaximumNumberOfLogsand 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 ${\tt modelObj}$, 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

	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 $\geq x$. 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.

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

Characteristics

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	<pre>double (SimData), double column (ScheduleDose) .</pre>
	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

Compatibility Considerations

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 0×1 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

Туре

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	<pre>abstract_kinetic_law, compartment, configset, compileoptions, event, kineticlaw, observable parameter, reaction, repeatdose, root, rule, runtimeoptions, sbiomodel, scheduledose, species, solveroptions, unit, unitprefix, and variant</pre>
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 $a + b \rightarrow c$. 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:42Rules:0Species: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
                            1.000000e-003
     RelativeTolerance:
   RuntimeOptions:
     StatesToLog:
                            all
   CompileOptions:
     UnitConversion:
                            false
     DimensionalAnalysis:
                           true
Retrieve the CompileOptions object.
```

```
optionsObj = get(configsetObj,'CompileOptions')
Compile Settings:
```

3

UnitConversion: false DimensionalAnalysis: true

4 Assign a value of false to UnitConversion.

set(options0bj,'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

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 3-71 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 2-65.

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	
	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 1-229 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');
```

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