Curve Fitting Toolbox

For Use with MATLAB®

- Computation
- Visualization
- Programming

User's Guide

Version 1

The MathWorks

Curve Fitting Toolbox User's Guide

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Contents

Getting Started with the Curve Fitting Toolbox

This chapter describes a particular example in detail to help you get started with the Curve Fitting Toolbox. In this example, you will fit census data to several toolbox library models, find the best fit, and extrapolate the best fit to predict the US population in future years. In doing so, the basic steps involved in any curve fitting scenario are illustrated. These steps include

What Is the Curve Fitting Toolbox?

The Curve Fitting Toolbox is a collection of graphical user interfaces (GUIs) and M-file functions built on the MATLAB® technical computing environment. The toolbox provides you with these main features:

- Data preprocessing such as sectioning and smoothing
- Parametric and nonparametric data fitting:
  - You can perform a parametric fit using a toolbox library equation or using a custom equation. Library equations include polynomials, exponentials, rationals, sums of Gaussians, and so on. Custom equations are equations that you define to suit your specific curve fitting needs.
  - You can perform a nonparametric fit using a smoothing spline or various interpolants.
- Standard linear least squares, nonlinear least squares, weighted least squares, constrained least squares, and robust fitting procedures
- Fit statistics to assist you in determining the goodness of fit
- Analysis capabilities such as extrapolation, differentiation, and integration
- A graphical environment that allows you to:
  - Explore and analyze data sets and fits visually and numerically
  - Save your work in various formats including M-files, binary files, and workspace variables

The Curve Fitting Toolbox consists of two different environments:

- The Curve Fitting Tool, which is a graphical user interface (GUI) environment
- The MATLAB command line environment

You can explore the Curve Fitting Tool by typing

```
cftool
```

Click the GUI Help buttons to learn how to proceed. Additionally, you can follow the examples in the tutorial sections of this guide, which are all GUI oriented.

To explore the command line environment, you can list the toolbox functions by typing

```
help curvefit
```

To view the code for any function, type

```
type function_name
```

To view the help for any function, type

```
help function_name
```

You can change the way any toolbox function works by copying and renaming the M-file, and then modifying your copy. However, these changes will not be reflected in the graphical environment.

You can also extend the toolbox by adding your own M-files, or by using it in combination with other products such as the Statistics Toolbox or the Optimization Toolbox.

Differences Between the Curve Fitting Tool and Command-Line Environments

Although the Curve Fitting Tool and the command-line environments are functionally equivalent, you generally cannot mix the two when performing a given curve fitting task. For example, you cannot generate a fit at the command line and then import that fit into the Curve Fitting Tool. However, you can create a fit in the Curve Fitting Tool and then generate an associated M-file. You can then recreate the fit from the command line and modify the M-file according to your needs. For this reason, as well as for the enhanced data analysis and exploration tools that are available, we recommend that you use the Curve Fitting Tool for most tasks.

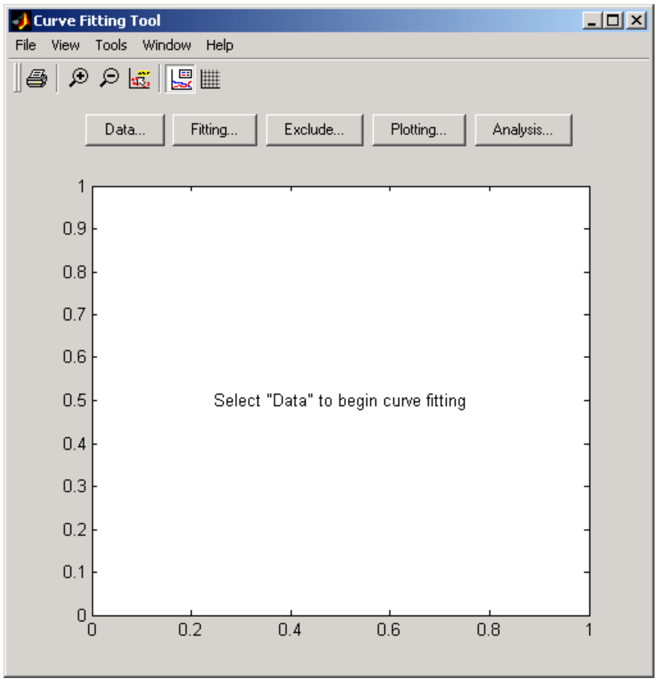
Opening the Curve Fitting Tool

The Curve Fitting Tool is a graphical user interface (GUI) that allows you to

- Visually explore one or more data sets and fits as scatter plots.
- Graphically evaluate the goodness of fit using residuals and prediction bounds.
- Access additional interfaces for
  - Importing, viewing, and smoothing data
  - Fitting data, and comparing fits and data sets
  - Marking data points to be excluded from a fit
  - Selecting which fits and data sets are displayed in the tool
  - Interpolating, extrapolating, differentiating, or integrating fits

You open the Curve Fitting Tool with the `cftool` command.

```
cftool
```


Curve Fitting Tool
File View Tools Window Help
Data... Fitting... Exclude... Plotting... Analysis...
Select "Data" to begin curve fitting
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
0 0.2 0.4 0.6 0.8 1

Importing the Data

Before you can import data into the Curve Fitting Tool, the data variables must exist in the MATLAB workspace. For this example, the data is stored in the file `census.mat`, which is provided with MATLAB.

```
load census
```

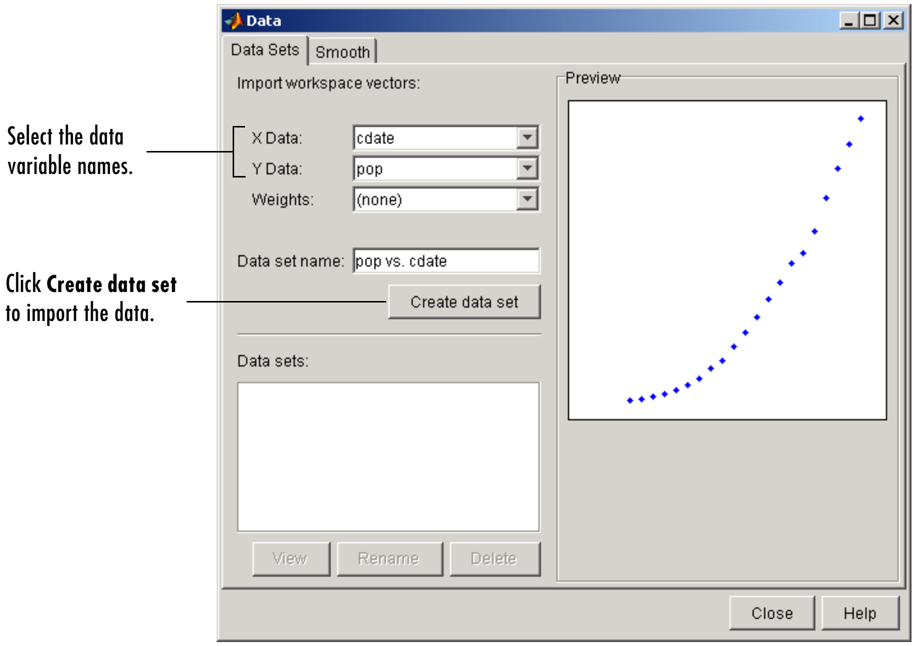
The workspace now contains two new variables, `cdate` and `pop`:

- `cdate` is a column vector containing the years 1790 to 1990 in 10-year increments.
- `pop` is a column vector with the US population figures that correspond to the years in `cdate`.

You can import data into the Curve Fitting Tool with the Data GUI. You open this GUI by clicking the **Data** button on the Curve Fitting Tool. As shown below, the Data GUI consists of two panes: Data sets and Smooth. The Data Sets pane allows you to

- Import predictor (X) data, response (Y) data, and weights. If you do not import weights, then they are assumed to be 1 for all data points.
- Specify the name of the data set.
- Preview the data.

To load `cdate` and `pop` into the Curve Fitting Tool, select the appropriate variable names from the **X Data** and **Y Data** lists. The data is then displayed in the **Preview** window. Click the **Create data set** button to complete the data import process.


Select the data variable names.
Click **Create data set** to import the data.
Data
Data Sets
Smooth
Import workspace vectors:
Preview
Create data set
Data sets:
View
Rename
Delete
Close
Help

X Data: cdate
Y Data: pop
Weights: (none)
Data set name: pop vs. cdate

The Smooth pane is described in Chapter 2, “Importing, Viewing, and Preprocessing Data.”

Fitting the Data

You fit data with the Fitting GUI. You open this GUI by clicking the **Fitting** button on the Curve Fitting Tool. The Fitting GUI consists of two parts: the **Fit Editor** and the **Table of Fits**. The **Fit Editor** allows you to

- Specify the fit name, the current data set, and the exclusion rule.
- Explore various fits to the current data set using a library or custom equation, a smoothing spline, or an interpolant.
- Override the default fit options such as the coefficient starting values.
- Compare fit results including the fitted coefficients and goodness of fit statistics.

The **Table of Fits** allows you to

- Keep track of all the fits and their data sets for the current session.
- Display a summary of the fit results.
- Save or delete the fit results.

The Data Fitting Procedure

For this example, begin by fitting the census data with a second degree polynomial. Then continue fitting the data using polynomial equations up to sixth degree, and a single-term exponential equation.

The data fitting procedure follows these general steps:

1 From the **Fit Editor**, click **New Fit**.

   Note that this action always defaults to a linear polynomial fit type. You use **New Fit** at the beginning of your curve fitting session, and when you are exploring different fit types for a given data set.

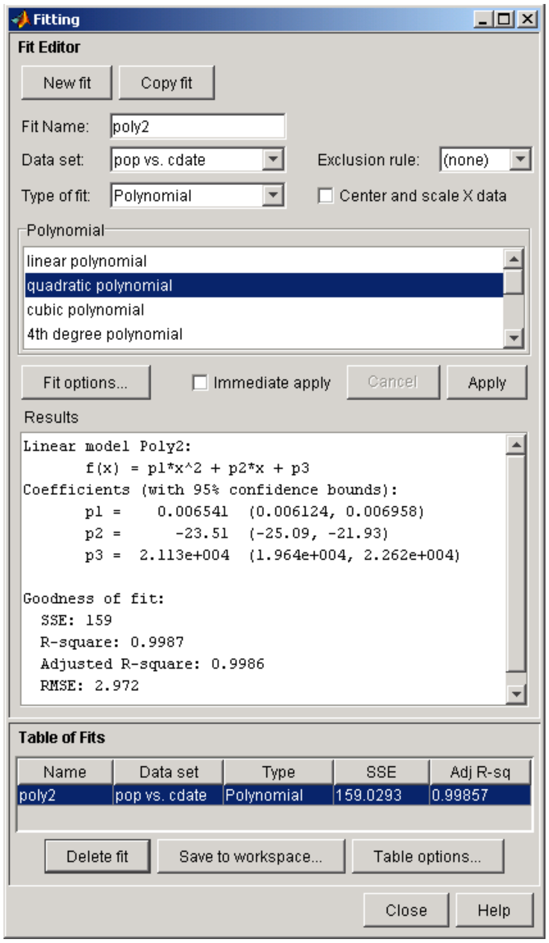
2 Because the initial fit uses a second degree polynomial, select **quadratic polynomial** from the **Polynomial** list. Name the fit `poly2`.

3 Click the **Apply** button or select the **Immediate apply** check box. The library model, fitted coefficients, and goodness of fit statistics are displayed in the **Results** area.

4 Fit the additional library equations.

For fits of a given type (for example, polynomials), you should use **Copy Fit** instead of **New Fit** because copying a fit retains the current fit type state thereby requiring fewer steps than creating a new fit each time.

The Fitting GUI is shown below with the results of fitting the census data with a quadratic polynomial.



Fit Name: poly2
Data set: pop vs. cdate
Exclusion rule: (none)
Type of fit: Polynomial
Center and scale X data: [ ]

Polynomial:
- linear polynomial
- quadratic polynomial
- cubic polynomial
- 4th degree polynomial

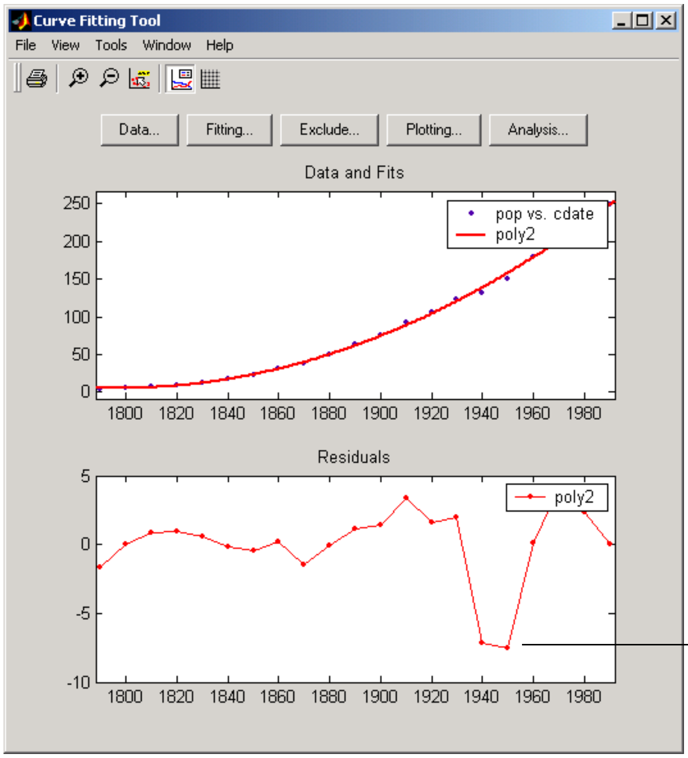
```
Linear model Poly2:
       f(x) = p1*x^2 + p2*x + p3
Coefficients (with 95% confidence bounds):
       p1 =    0.006541  (0.006124, 0.006958)
       p2 =      -23.51  (-25.09, -21.93)
       p3 =  2.113e+004  (1.964e+004, 2.262e+004)

Goodness of fit:
  SSE: 159
  R-square: 0.9987
  Adjusted R-square: 0.9986
  RMSE: 2.972
```

Name	Data set	Type	SSE	Adj R-sq
poly2	pop vs. cdate	Polynomial	159.0293	0.99857

The **Fit Editor** allows you to select a data set and a fit name, and to explore and compare various library and custom fits.

The **Table of Fits** allows you to keep track of all the fits, their data sets, and fit results for the current session.

The data, fit, and residuals are shown below. You display the residuals as a line plot by selecting the menu item **View->Residuals->Line plot** from the Curve Fitting Tool.



These residuals indicate that a better fit may be possible.

The residuals indicate that a better fit may be possible. Therefore, you should continue fitting the census data following the procedure outlined in the beginning of this section.

The residuals from a good fit should look random with no apparent pattern. A pattern, such as a tendency for consecutive residuals to have the same sign, can be an indication that a better model exists.

When you fit higher degree polynomials, the **Results** area displays this warning:

```
Equation is badly conditioned. Remove repeated data points
or try centering and scaling.
```

The warning arises because the fitting procedure uses the `cdate` values as the basis for a matrix with very large values. The spread of the `cdate` values results in scaling problems. To address this problem, you can normalize the `cdate` data. Normalization is a process of scaling the predictor data to improve the accuracy of the subsequent numeric computations. A way to normalize `cdate` is to center it at zero mean and scale it to unit standard deviation.

```
(cdate - mean(cdate))./std(cdate)
```

To normalize data with the Curve Fitting Tool, select the **Center and scale X data** check box.

Note Because the predictor data changes after normalizing, the values of the fitted coefficients also change when compared to the original data. However, the functional form of the data and the resulting goodness of fit statistics do not change. Additionally, the data is displayed in the Curve Fitting Tool using the original scale.

Determining the Best Fit

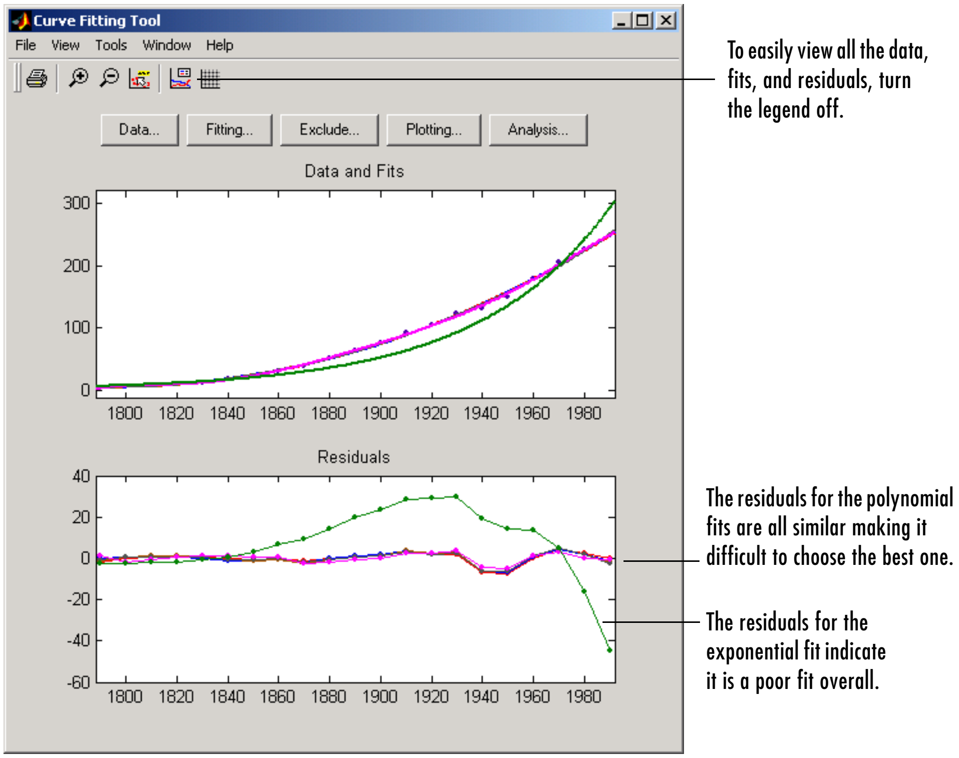
To determine the best fit, you should examine both the graphical and numerical fit results.

Examining the Graphical Fit Results

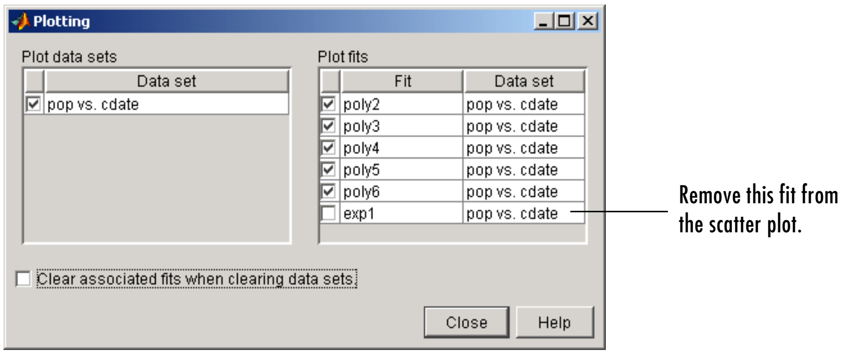
Your initial approach in determining the best fit should be a graphical examination of the fits and residuals. The graphical fit results shown below indicate that

- The fits and residuals for the polynomial equations are all similar, making it difficult to choose the best one.

- The fit and residuals for the single-term exponential equation indicate it is a poor fit overall. Therefore, it is a poor choice for extrapolation.


Curve Fitting Tool
File View Tools Window Help
Data... Fitting... Exclude... Plotting... Analysis...
Data and Fits
Residuals
To easily view all the data, fits, and residuals, turn the legend off.
The residuals for the polynomial fits are all similar making it difficult to choose the best one.
The residuals for the exponential fit indicate it is a poor fit overall.

Use the Plotting GUI to remove exp1 from the scatter plot display.



Plot data sets

	Data set
✓	pop vs. cdate

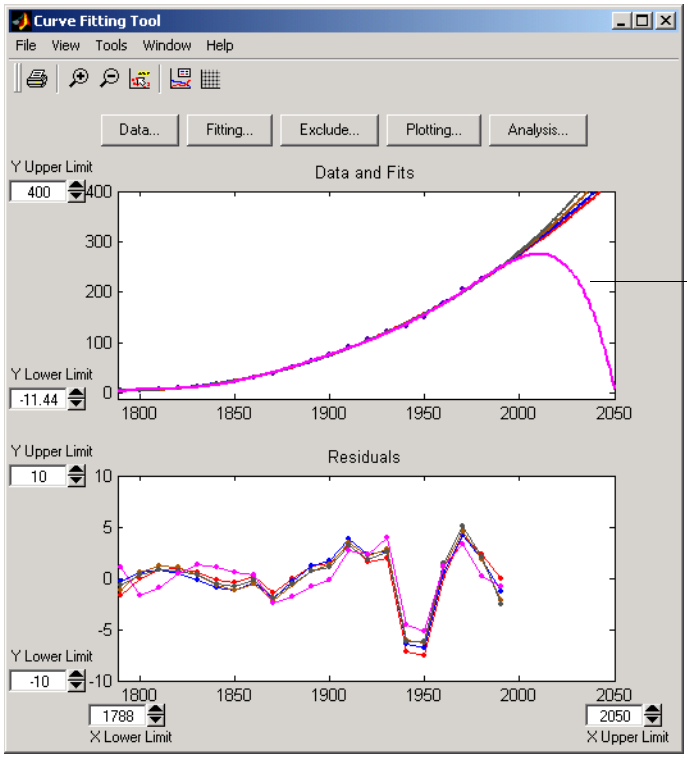
Plot fits

	Fit	Data set
✓	poly2	pop vs. cdate
✓	poly3	pop vs. cdate
✓	poly4	pop vs. cdate
✓	poly5	pop vs. cdate
✓	poly6	pop vs. cdate
	exp1	pop vs. cdate

☐ Clear associated fits when clearing data sets

Because the goal of fitting the census data is to extrapolate the best fit to predict future population values, you should explore the behavior of the fits up to the year 2050. You can change the axes limits of the Curve Fitting Tool by selecting the menu item **Tools->Axes Limit Control**.

The census data and fits are shown below for an upper abscissa limit of 2050. The behavior of the sixth degree polynomial fit beyond the data range makes it a poor choice for extrapolation.



The sixth degree polynomial fit beyond the data range makes it a poor choice for extrapolation.

Change the upper abscissa limit to 2050.

As you can see, you should exercise caution when extrapolating with polynomial fits because they can diverge wildly outside the data range.

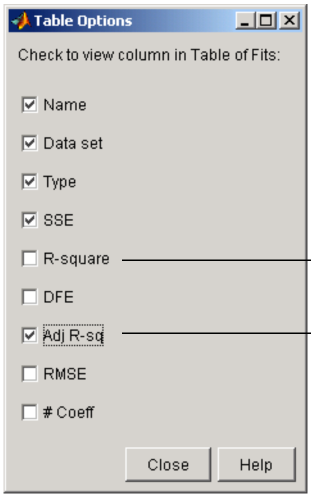
Examining the Numerical Fit Results

Because you can no longer eliminate fits by examining them graphically, you should examine the numerical fit results. There are two types of numerical fit results displayed in the Fitting GUI: goodness of fit statistics and confidence intervals on the fitted coefficients. The goodness of fit statistics help you determine how well the curve fits the data. The confidence intervals on the coefficients determine their accuracy.

Some goodness of fit statistics are displayed in the **Results** area of the **Fit Editor** for a single fit. All goodness of fit statistics are displayed in the **Table of Fits** for all fits, which allows for easy comparison.

In this example, the sum of squares due to error (SSE) and the adjusted R-square statistics are used to help determine the best fit. As described in "Goodness of Fit Statistics" on page 3-29, the SSE statistic is the least squares error of the fit, with a value closer to zero indicating a better fit. The adjusted R-square statistic is generally the best indicator of the fit quality when you add additional coefficients to your model.

You can modify the information displayed in the **Table of Fits** with the Table Options GUI. You open this GUI by clicking the **Table options** button on the Fitting GUI. As shown below, select the adjusted R-square statistic and clear the R-square statistic.



Check to view column in Table of Fits:

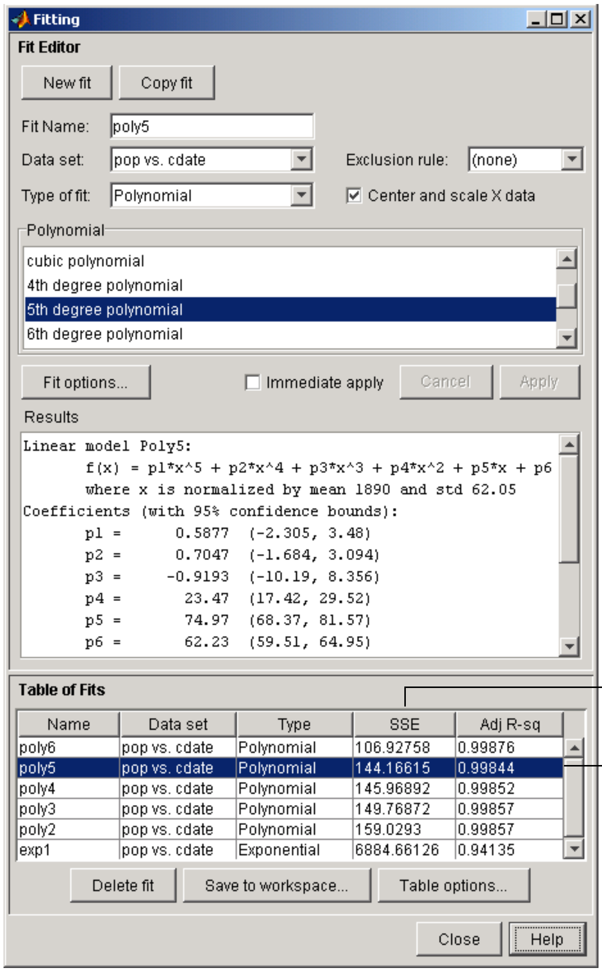
- [✓] Name
- [✓] Data set
- [✓] Type
- [✓] SSE
- [ ] R-square
- [ ] DFE
- [✓] Adj R-sq
- [ ] RMSE
- [ ] # Coeff

Do not display the R-square statistic in the **Table of Fits**.

Display the adjusted R-square statistic in the **Table of Fits**.

The numerical fit results are shown below. You can click the **Table of Fits** column headings to sort by statistics results.

The SSE for `exp1` indicates it is a poor fit, which was already determined by examining the fit and residuals. The lowest SSE value is associated with `poly6`. However, the behavior of this fit beyond the data range makes it a poor choice for extrapolation. The next best SSE value is associated with the fifth degree polynomial fit, `poly5`, suggesting it may be the best fit. However, the SSE and adjusted R-square values for the remaining polynomial fits are all very close to each other. Which one should you choose?



Fit Name: poly5
Data set: pop vs. cdate
Exclusion rule: (none)
Type of fit: Polynomial
☑ Center and scale X data

Polynomial: cubic polynomial / 4th degree polynomial / **5th degree polynomial** / 6th degree polynomial

```
Linear model Poly5:
      f(x) = p1*x^5 + p2*x^4 + p3*x^3 + p4*x^2 + p5*x + p6
      where x is normalized by mean 1890 and std 62.05
Coefficients (with 95% confidence bounds):
      p1 =      0.5877  (-2.305, 3.48)
      p2 =      0.7047  (-1.684, 3.094)
      p3 =     -0.9193  (-10.19, 8.356)
      p4 =       23.47  (17.42, 29.52)
      p5 =       74.97  (68.37, 81.57)
      p6 =       62.23  (59.51, 64.95)
```

Table of Fits

Name	Data set	Type	SSE	Adj R-sq
poly6	pop vs. cdate	Polynomial	106.92758	0.99876
poly5	pop vs. cdate	Polynomial	144.16615	0.99844
poly4	pop vs. cdate	Polynomial	145.96892	0.99852
poly3	pop vs. cdate	Polynomial	149.76872	0.99857
poly2	pop vs. cdate	Polynomial	159.0293	0.99857
exp1	pop vs. cdate	Exponential	6884.66126	0.94135

The confidence bounds for the p1-p3 coefficients suggest that a fifth degree polynomial overfits the census data.

Click this column heading to sort the fits by the SSE values.

The SSE and adjusted R-square values suggest that the fifth degree polynomial fit is the best one.

To resolve this issue, examine the confidence bounds for the remaining fits. By default, 95% confidence bounds are calculated. You can change this level by selecting the menu item **View->Confidence Level** from the Curve Fitting Tool.

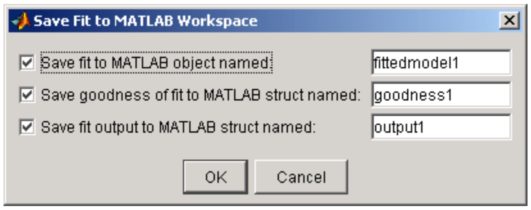
The `p1`, `p2`, and `p3` coefficients for the fifth degree polynomial suggest that it overfits the census data. However, the confidence bounds for the quadratic fit, `poly2`, indicate that the fitted coefficients are known fairly accurately. Therefore, after examining both the graphical and numerical fit results, it appears that you should use `poly2` to extrapolate the census data.

Note The fitted coefficients associated with the constant, linear, and quadratic terms are nearly identical for each polynomial equation. However, as the polynomial degree increases, the coefficient bounds associated with the higher degree terms increase, which suggests overfitting.

For more information about confidence bounds, refer to "Confidence and Prediction Bounds" on page 3-32.

Saving the Fit Results

By clicking the **Save to workspace** button, you can save the selected fit and the associated fit results to the MATLAB workspace. The fit is saved as a MATLAB object and the associated fit results are saved as structures. This example saves all the fit results for the best fit, `poly2`.



Save Fit to MATLAB Workspace

☑ Save fit to MATLAB object named: fittedmodel1
☑ Save goodness of fit to MATLAB struct named: goodness1
☑ Save fit output to MATLAB struct named: output1

`fittedmodel1` is saved as a Curve Fitting Toolbox `cfit` object.

```
whos fittedmodel1

  Name                 Size                       Bytes  Class
  fittedmodel1         1x1                         6178  cfit object

Grand total is 386 elements using 6178 bytes
```

The cfit object display includes the model, the fitted coefficients, and the confidence bounds for the fitted coefficients.

```
fittedmodel1

fittedmodel1 =
     Linear model Poly2:
       fittedmodel1(x) = p1*x^2 + p2*x + p3
     Coefficients (with 95% confidence bounds):
       p1 =    0.006541  (0.006124, 0.006958)
       p2 =      -23.51  (-25.09, -21.93)
       p3 =  2.113e+004  (1.964e+004, 2.262e+004)
```

The goodness1 structure contains goodness of fit results.

```
goodness1

goodness1 =
           sse: 159.0293
       rsquare: 0.9987
           dfe: 18
    adjrsquare: 0.9986
          rmse: 2.9724
```

The output1 structure contains additional information associated with the fit.

```
output1

output1 =
       numobs: 21
     numparam: 3
    residuals: [21x1 double]
     Jacobian: [21x3 double]
     exitflag: 1
    algorithm: 'QR factorization and solve'
```

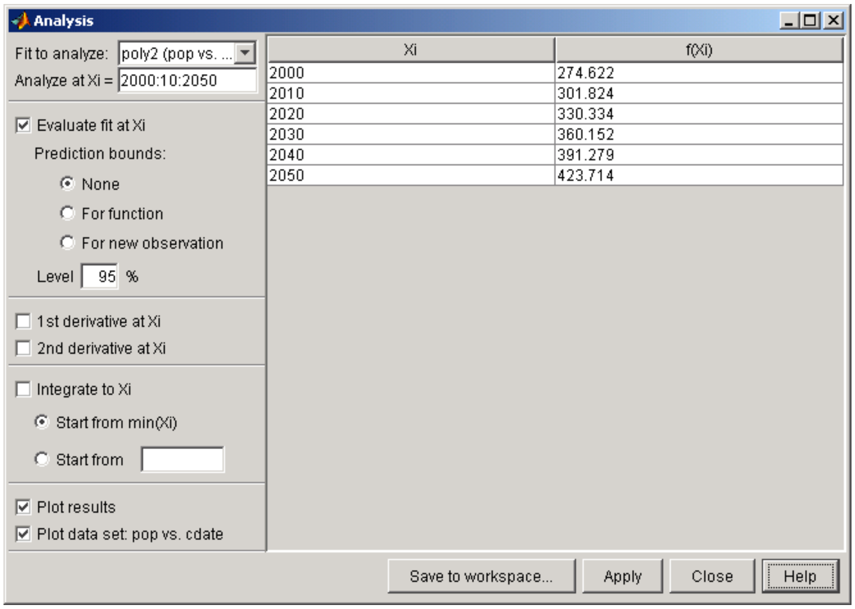
Analyzing the Fit

You can evaluate (interpolate or extrapolate), differentiate, or integrate a fit over a specified data range with the Analysis GUI. You open this GUI by clicking the **Analysis** button on the Curve Fitting Tool.

For this example, you will extrapolate the quadratic polynomial fit to predict the US population from the year 2000 to the year 2050 in 10 year increments, and then plot both the analysis results and the data. To do this:

- Enter the appropriate MATLAB vector in the **Analyze at Xi** field.
- Select the **Evaluate fit at Xi** check box.
- Select the **Plot results** and **Plot data set** check boxes.
- Click the **Apply** button.

The numerical extrapolation results are shown below.



Specify the fit and data to analyze.

Fit to analyze: poly2 (pop vs. ...

Analyze at Xi = 2000:10:2050

Select this check box to extrapolate.

☑ Evaluate fit at Xi

Prediction bounds: (● None) ○ For function ○ For new observation

Level 95 %

☐ 1st derivative at Xi

☐ 2nd derivative at Xi

☐ Integrate to Xi

(● Start from min(Xi)) ○ Start from

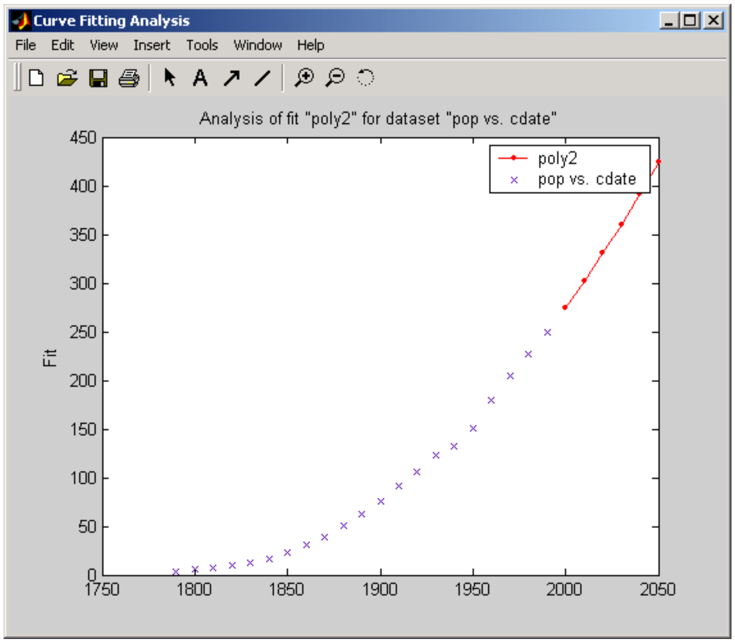
Plot both the analysis results and the data.

☑ Plot results

☑ Plot data set: pop vs. cdate

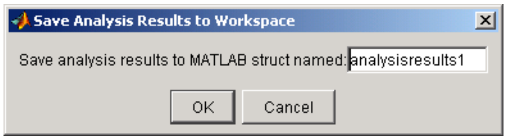
Xi	f(Xi)
2000	274.622
2010	301.824
2020	330.334
2030	360.152
2040	391.279
2050	423.714

The extrapolated values and the census data set are displayed together in a new figure window.



Saving the Analysis Results

By clicking the **Save to workspace** button, you can save the extrapolated values as a structure to the MATLAB workspace.



Save analysis results to MATLAB struct named: analysisresults1

The resulting structure is shown below.

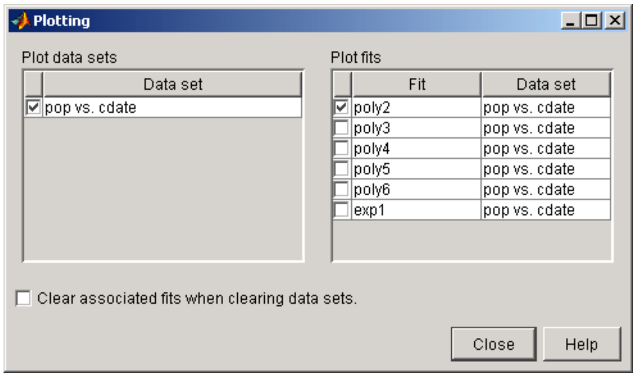
```
analysisresults1

analysisresults1 =
       xi: [6x1 double]
     yfit: [6x1 double]
```

Saving Your Work

The Curve Fitting Toolbox provides you with several options for saving your work. For example, as described in “Saving the Fit Results” on page 1-15, you can save one or more fits and the associated fit results as variables to the MATLAB workspace. You can then use this saved information for documentation purposes, or to extend your data exploration and analysis. In addition to saving your work to MATLAB workspace variables, you can

- Save the session.
- Generate an M-file.

Before performing any of these tasks, you may want to remove unwanted data sets and fits from the Curve Fitting Tool display. An easy way to do this is with the Plotting GUI. The Plotting GUI shown below is configured to display only the census data and the best fit, `poly2`.



	Data set
✓	pop vs. cdate

	Fit	Data set
✓	poly2	pop vs. cdate
☐	poly3	pop vs. cdate
☐	poly4	pop vs. cdate
☐	poly5	pop vs. cdate
☐	poly6	pop vs. cdate
☐	exp1	pop vs. cdate

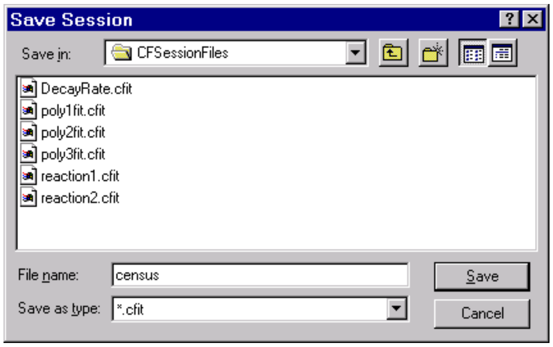
☐ Clear associated fits when clearing data sets.

Clear the remaining fits associated with the census data except the best fit.

Saving the Session

The curve fitting session is defined as the current collection of fits for all data sets. You may want to save your session so that you can continue data exploration and analysis at a later time using the Curve Fitting Tool without losing any current work.

Save the current curve fitting session by selecting the menu item **File->Save Session** from the Curve Fitting Tool. The **Save Session** dialog is shown below.



The session is stored in binary form in a `cfit` file, and contains this information:

- All data sets and associated fits
- The state of the Fitting GUI, including **Table of Fits** entries and exclusion rules
- The state of the Plotting GUI

To avoid saving unwanted data sets, you should delete them from the Curve Fitting Tool. You delete data sets using the Data Sets pane of the Data GUI. If there are fits associated with the unwanted data sets, they are deleted as well.

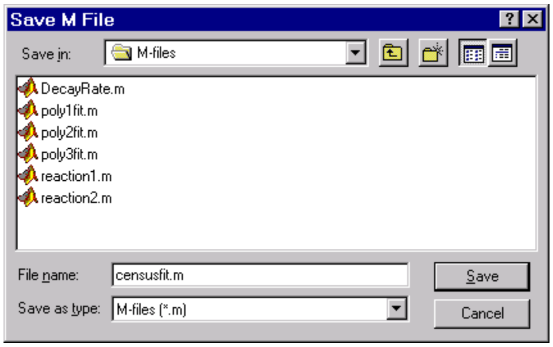
You can load a saved session by selecting the menu item **File->Load Session** from the Curve Fitting Tool. When the session is loaded, the saved state of the Curve Fitting Tool display is reproduced, and may display the data, fits, residuals, and so on. If you open the Fitting GUI, then the loaded fits are displayed in the **Table of Fits**. Select a fit from this table to continue your curve fitting session.

Generating an M-File

You may want to generate an M-file so that you can continue data exploration and analysis from the MATLAB command line. You can run the M-file without modification to recreate the fits and results that you created with the Curve Fitting Tool, or you can edit and modify the file as needed. For detailed descriptions of the functions provided by the toolbox, refer to Chapter 4, "Function Reference."

If you have many data sets to fit and you want to automate the fitting process, you should use the Curve Fitting Tool to select the appropriate model and fit options, generate an M-file, and then run the M-file in batch mode.

Save your work to an M-file by selecting the menu item **File->Save M-file** from the Curve Fitting Tool. The **Save M-File** dialog is shown below.



File name: censusfit.m

Save as type: M-files (*.m)

The M-file can capture this information from the Curve Fitting Tool:

- All data set variable names, associated fits, and residuals
- Fit options such as whether the data should be normalized, the fit starting points, and the fitting method

You can recreate the saved fits in a new figure window by typing the name of the M-file at the MATLAB command line. Note that you must provide the appropriate data variables as inputs to the M-file. These variables are given in the M-file help.

For example, the help for the `censusfit` M-file indicates that the variables `cdate` and `pop` are required to recreate the saved fit.

```
help censusfit

 CENSUSFIT    Create plot of datasets and fits
    CENSUSFIT(CDATE,POP)
    Creates a plot, similar to the plot in the main curve fitting
    window, using the data that you provide as input.  You can
    apply this function to the same data you used with cftool
    or with different data.  You may want to edit the function to
    customize the code and this help message.

    Number of datasets:  1
    Number of fits:  6
```

Importing, Viewing, and Preprocessing Data

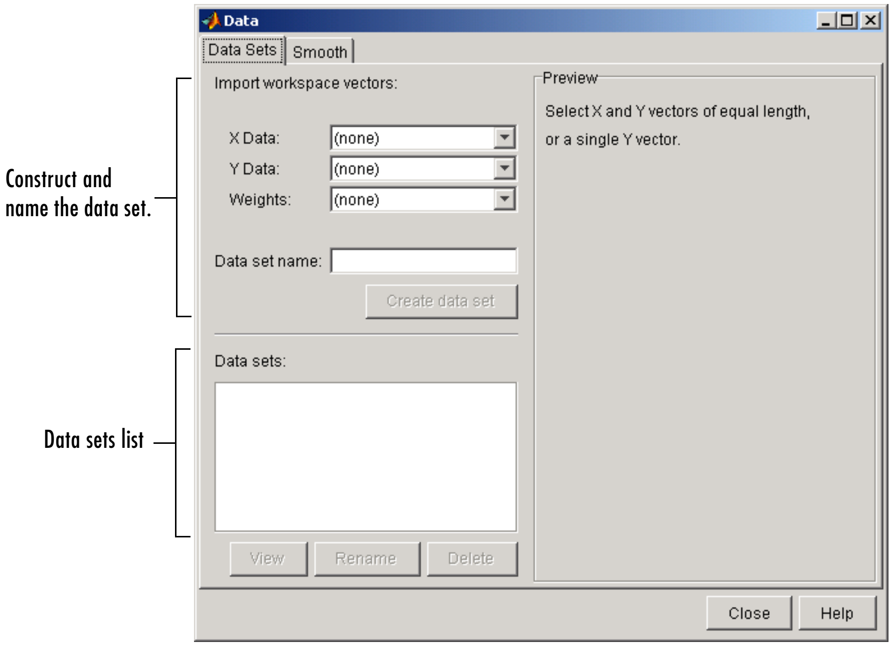
This chapter describes how to import, view, and preprocess data with the Curve Fitting Toolbox. You import data with the Data GUI, and view data graphically as a scatter plot using the Curve Fitting Tool. The main preprocessing steps are smoothing, and excluding and sectioning data. You smooth data with the Data GUI, and exclude and section data with the Exclude GUI. The sections are as follows.

Importing Data Sets

You import data sets into the Curve Fitting Tool with the Data Sets pane of the Data GUI. Using this pane, you can

- Select workspace variables that compose a data set
- Display a list of all imported data sets
- View, delete, or rename one or more data sets

The Data Sets pane is shown below followed by a description of its features.



Construct and Name the Data Set

- **Import workspace vectors** — All selected variables must be the same length. You can import only vectors, not matrices or scalars. `Infs` and `NaNs` are ignored because you cannot fit data containing these values, and only the real part of a complex number is used. To perform any curve-fitting task, you must select at least one vector of data:
  - **X data** — Select the predictor data.
  - **Y data** — Select the response data.
  - **Weights** — Select the weights associated with the response data. If weights are not imported, they are assumed to be 1 for all data points.
- **Preview** — The selected workspace vectors are displayed graphically in the preview window. Weights are not displayed.
- **Data set name** — The name of the imported data set. The toolbox automatically creates a unique name for each imported data set. You can change the name by editing this field. Click the **Create data set** button to complete the data import process.

Data Sets List

- **Data sets** — Lists all data sets added to the Curve Fitting Tool. The data sets can be created from workspace variables, or from smoothing an existing imported data set. When you select a data set, you can perform these actions:
  - Click **View** to open the View Data Set GUI. Using this GUI, you can view a single data set both graphically and numerically. Additionally, you can display data points to be excluded in a fit by selecting an exclusion rule.
  - Click **Rename** to change the name of a single data set.
  - Click **Delete** to delete one or more data sets. To select multiple data sets, you can use the **Ctrl** key and the mouse to select data sets one by one, or you can use the **Shift** key and the mouse to select a range of data sets.

Example: Importing Data

This example imports the ENSO data set into the Curve Fitting Toolbox using the Data Sets pane of the Data GUI. The first step is to load the data from the file `enso.mat` into the MATLAB workspace.

```
load enso
```

The workspace contains two new variables, `pressure` and `month`:

- `pressure` is the monthly averaged atmospheric pressure differences between Easter Island and Darwin, Australia. This difference drives the trade winds in the southern hemisphere.
- `month` is the relative time in months.

Alternatively, you can import data by specifying the variable names as arguments to the `cftool` function.

```
cftool(month,pressure)
```

In this case, the Data GUI is not opened.

Data Import Process

The data import process is described below:

1. Select workspace variables.

   The predictor and response data are displayed graphically in the **Preview** window. Weights and data points containing `Infs` or `NaNs` are not displayed.

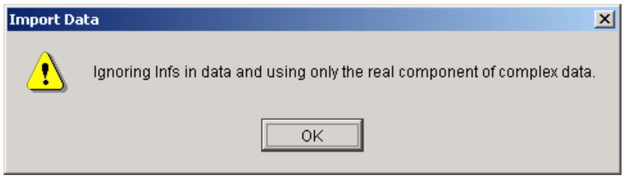
2. Specify the data set name.

   You should specify a meaningful name when you import multiple data sets. If you do not specify a name, the default name, which is constructed from the selected variable names, is used.

3 Click the **Create data set** button.

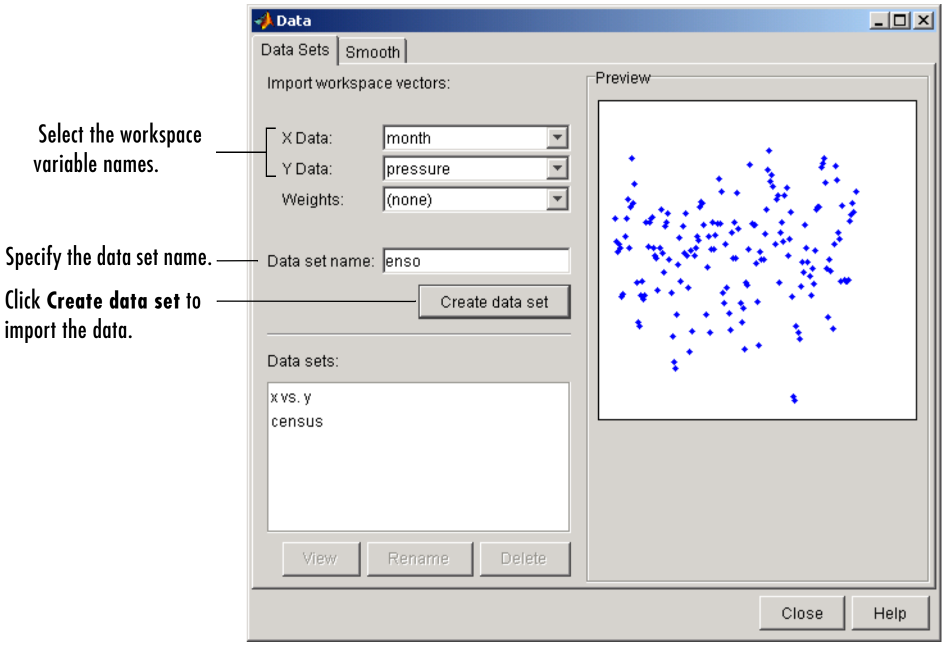
The **Data sets** list box displays all the data sets added to the toolbox. Note that you can construct data sets from workspace variables, or by smoothing an existing data set.

If your data contains `Infs` or complex values, a warning message such as the message shown below is displayed.


Import Data

Ignoring Infs in data and using only the real component of complex data.

The Data Sets pane shown below displays the imported ENSO data in the **Preview** window. After you click the **Create data set** button, the data set `enso` is added to the **Data sets** list box. You can then view, rename, or delete `enso` by selecting it in the list box and clicking the appropriate button.


Select the workspace variable names.
Specify the data set name.
Click **Create data set** to import the data.
Data
Data Sets
Smooth
Import workspace vectors:
Preview
Create data set
Data sets:
View
Rename
Delete
Close
Help

X Data: month
Y Data: pressure
Weights: (none)
Data set name: enso

Data sets:
x vs. y
census

Viewing Data

The Curve Fitting Toolbox provides two ways to view imported data:

- Graphically in a scatter plot
- Numerically in a table

Viewing Data Graphically

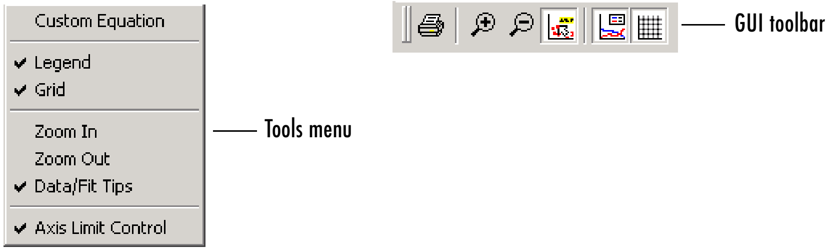
After you import a data set, it is automatically displayed as a scatter plot in the Curve Fitting Tool. The response data is plotted on the vertical axis and the predictor data is plotted on the horizontal axis.

The scatter plot is a powerful tool because it allows you to view the entire data set at once, and it can easily display a wide range of relationships between the two variables. You should examine the data carefully to determine whether preprocessing is required, or to deduce a reasonable fitting approach. For example, it's typically very easy to identify outliers in a scatter plot, and to determine whether you should fit the data with a straight line, a periodic function, a sum of Gaussians, and so on.

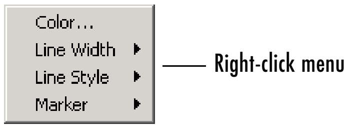
Enhancing the Graphical Display

The Curve Fitting Toolbox provides several tools for enhancing the graphical display of a data set. These tools are available through the **Tools** menu, the GUI toolbar, and right-click menus.

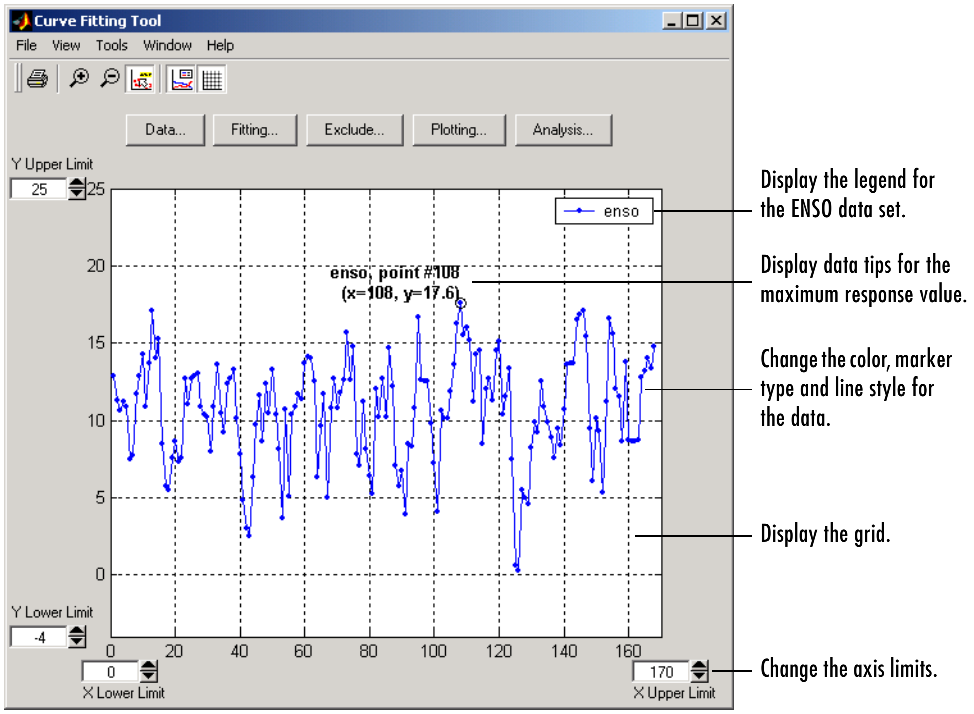
You can zoom in, zoom out, display data and fit tips, and so on using the **Tools** menu and the GUI toolbar shown below.



You can change the color, line width, line style, and marker type of the displayed data points using the right-click menu shown below. You activate this menu by placing your mouse over a data point and right-clicking. Note that a similar menu is available for fitted curves.

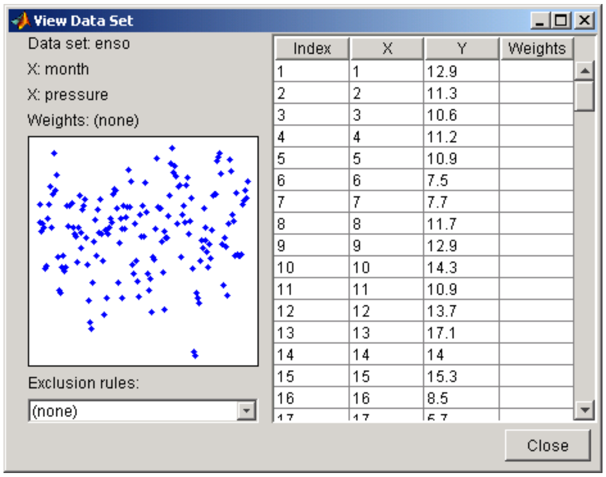


The ENSO data is shown below after the display has been enhanced using several of these tools.


Curve Fitting Tool
File View Tools Window Help
Data... Fitting... Exclude... Plotting... Analysis...
Y Upper Limit
25
Y Lower Limit
-4
X Lower Limit
0
X Upper Limit
170
enso
enso, point #108
(x=108, y=17.6)
25
20
15
10
5
0
0
20
40
60
80
100
120
140
160
Display the legend for the ENSO data set.
Display data tips for the maximum response value.
Change the color, marker type and line style for the data.
Display the grid.
Change the axis limits.

Viewing Data Numerically

You can view the numerical values of a data set, as well as data points to be excluded from subsequent fits, with the View Data Set GUI. You open this GUI by selecting a name in the **Data sets** list box of the Data GUI and clicking the **View** button. The View Data Set GUI for the ENSO data set is shown below, followed by a description of its features.


View Data Set

Data set: enso
X: month
X: pressure
Weights: (none)

Exclusion rules: (none)

Index	X	Y	Weights
1	1	12.9	
2	2	11.3	
3	3	10.6	
4	4	11.2	
5	5	10.9	
6	6	7.5	
7	7	7.7	
8	8	11.7	
9	9	12.9	
10	10	14.3	
11	11	10.9	
12	12	13.7	
13	13	17.1	
14	14	14	
15	15	15.3	
16	16	8.5	

- **Data set** — Lists the names of the viewed data set and the associated variables. The data is displayed graphically below this list.

  The index, predictor data (**X**), response data (**Y**), and weights (if imported) are displayed numerically in the table. If the data contains `Inf`s or `NaN`s, those values are labeled "ignored." If the data contains complex numbers, only the real part is displayed.

- **Exclusion rules** — Lists all the exclusion rules that are compatible with the viewed data set. When you select an exclusion rule, the data points marked for exclusion are grayed in the table, and are identified with an "x" in the graphical display. To exclude the data points while fitting, you must select the exclusion rule in the Fitting GUI.

  An exclusion rule is compatible with the viewed data set if their lengths are the same, or if it is created by sectioning only.

Smoothing Data

If your data is noisy, you might need to apply a smoothing algorithm to expose its features, and to provide a reasonable starting approach for parametric fitting. The two basic assumptions that underlie smoothing are

- The relationship between the response data and the predictor data is smooth.
- The smoothing process results in a smoothed value that is a better estimate of the original value because the noise has been reduced.

  The smoothing process attempts to estimate the average of the distribution of each response value. The estimation is based on a specified number of neighboring response values.

You can think of smoothing as a local fit because a new response value is created for each original response value. Therefore, smoothing is similar to some of the nonparametric fit types supported by the toolbox, such as smoothing spline and cubic interpolation. However, this type of fitting is not the same as parametric fitting, which results in a global parameterization of the data.

Note You should not fit data with a parametric model after smoothing, because the act of smoothing invalidates the assumption that the errors are normally distributed. Instead, you should consider smoothing to be a data exploration technique.

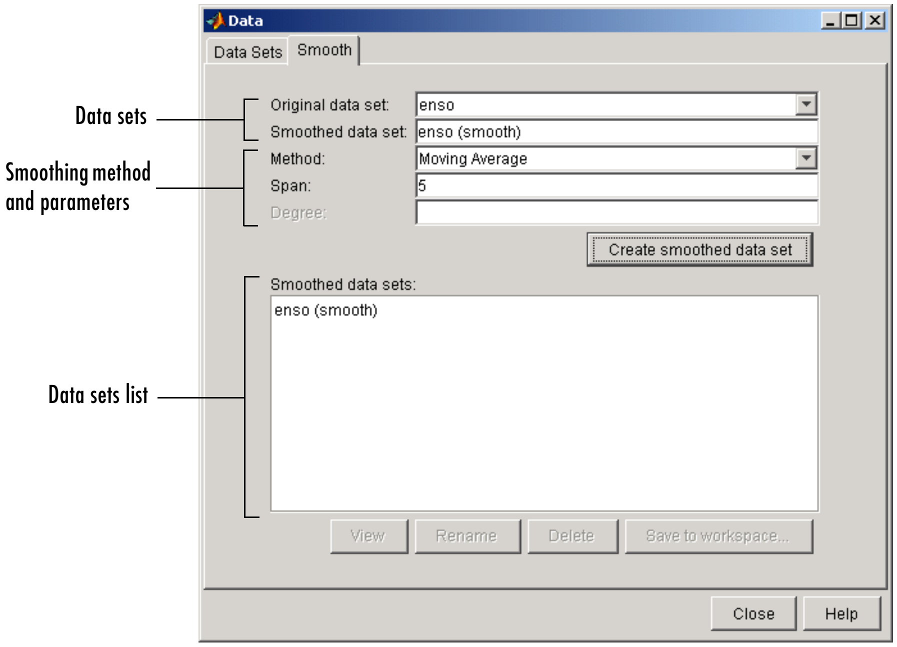
There are two common types of smoothing methods: filtering (averaging) and local regression. Each smoothing method requires a *span*. The span defines a window of neighboring points to include in the smoothing calculation for each data point. This window moves across the data set as the smoothed response value is calculated for each predictor value. A large span increases the smoothness but decreases the resolution of the smoothed data set, while a small span decreases the smoothness but increases the resolution of the smoothed data set. The optimal span value depends on your data set and the smoothing method, and usually requires some experimentation to find.

The Curve Fitting Toolbox supports these smoothing methods:

- Moving average filtering — Lowpass filter that takes the average of neighboring data points.
- Lowess and loess — Locally weighted scatter plot smooth. These methods use linear least squares fitting, and a first-degree polynomial (lowess) or a second-degree polynomial (loess). Robust lowess and loess methods that are resistant to outliers are also available.
- Savitzky-Golay filtering — A generalized moving average where you derive the filter coefficients by performing an unweighted linear least squares fit using a polynomial of the specified degree.

Note that you can also smooth data using a smoothing spline. Refer to "Nonparametric Fitting" on page 3-68 for more information.

You smooth data with the Smooth pane of the Data GUI. The pane is shown below followed by a description of its features.



Original data set: enso
Smoothed data set: enso (smooth)
Method: Moving Average
Span: 5
Degree:
Smoothed data sets:
enso (smooth)

Data Sets

- **Original data set** — Select the data set you want to smooth.
- **Smoothed data set** — Specify the name of the smoothed data set. Note that the process of smoothing the original data set always produces a new data set containing smoothed response values.

Smoothing Method and Parameters

- **Method** — Select the smoothing method. Each response value is replaced with a smoothed value that is calculated by the specified smoothing method.
  - **Moving average** — Filter the data by calculating an average.
  - **Lowess** — Locally weighted scatter plot smooth using linear least squares fitting and a first-degree polynomial.
  - **Loess** — Locally weighted scatter plot smooth using linear least squares fitting and a second-degree polynomial.
  - **Savitzky-Golay** — Filter the data with an unweighted linear least squares fit using a polynomial of the specified degree.
  - **Robust Lowess** — Lowess method that is resistant to outliers.
  - **Robust Loess** — Loess method that is resistant to outliers.
- **Span** — The number of data points used to compute each smoothed value.

  For the moving average and Savitzky-Golay methods, the span must be odd. For all locally weighted smoothing methods, if the span is less than 1, it is interpreted as the percentage of the total number of data points.
- **Degree** — The degree of the polynomial used in the Savitzky-Golay method. The degree must be smaller than the span.

Data Sets List

- **Smoothed data sets** — Lists all the smoothed data sets. You add a smoothed data set to the list by clicking the **Create smoothed data set** button. When you select a data set from the list, you can perform these actions:
  - Click **View** to open the View Data Set GUI. Using this GUI, you can view a single data set both graphically and numerically. Additionally, you can display data points to be excluded in a fit by selecting an exclusion rule.
  - Click **Rename** to change the name of a single data set.

- Click **Delete** to delete one or more data sets. To select multiple data sets, you can use the **Ctrl** key and the mouse to select data sets one by one, or you can use the **Shift** key and the mouse to select a range of data sets.
- Click **Save to workspace** to save a single data set to a structure.

Moving Average Filtering

A moving average filter smooths data by replacing each data point with the average of the neighboring data points defined within the span. This process is equivalent to lowpass filtering with the response of the smoothing given by the difference equation

$$y_s(i) = \frac{1}{2N+1}(y(i+N)+y(i+N-1)+\ldots+y(i-N))$$

where $y_s(i)$ is the smoothed value for the `i`th data point, N is the number of neighboring data points on either side of $y_s(i)$, and $2N+1$ is the span.

The moving average smoothing method used by the Curve Fitting Toolbox follows these rules:

- The span must be odd.
- The data point to be smoothed must be at the center of the span.
- The span is adjusted for data points that cannot accommodate the specified number of neighbors on either side.
- The end points are not smoothed because a span cannot be defined.

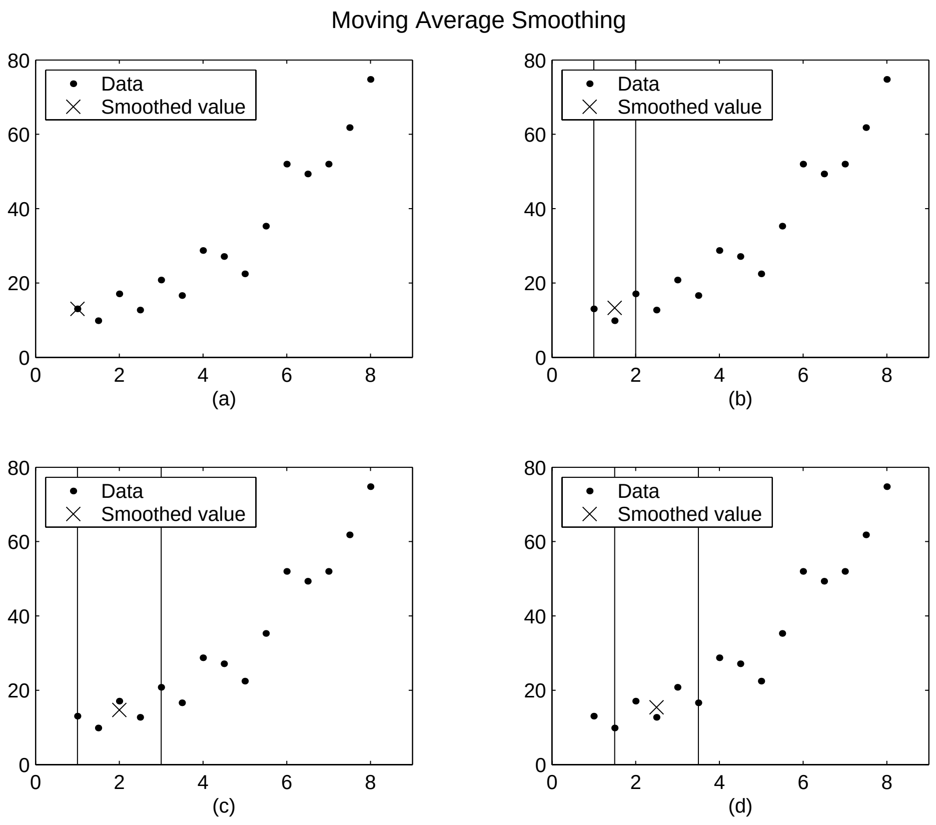
Note that you can use `filter` function to implement difference equations such as the one shown above. However, because of the way that the end points are treated, the toolbox moving average result will differ from the result returned by `filter`. Refer to “Difference Equations and Filtering” in the MATLAB documentation for more information.

For example, suppose you smooth data using a moving average filter with a span of 5. Using the rules described above, the first four elements of y_s are given by

```
ys(1) = y(1)
ys(2) = (y(1)+y(2)+y(3))/3
ys(3) = (y(1)+y(2)+y(3)+y(4)+y(5))/5
ys(4) = (y(2)+y(3)+y(4)+y(5)+y(6))/5
```

Note that `ys(1)`, `ys(2)`, ... ,`ys(end)` refer to the order of the data after sorting, and not necessarily the original order.

The smoothed values and spans for the first four data points of a generated data set are shown below.



Plot `(a)` indicates that the first data point is not smoothed because a span cannot be constructed. Plot `(b)` indicates that the second data point is smoothed using a span of three. Plots `(c)` and `(d)` indicate that a span of five is used to calculate the smoothed value.

Lowess and Loess: Local Regression Smoothing

The names "lowess" and "loess" are derived from the term "locally weighted scatter plot smooth," as both methods use locally weighted linear regression to smooth data.

The smoothing process is considered local because, like the moving average method, each smoothed value is determined by neighboring data points defined within the span. The process is weighted because a regression weight function is defined for the data points contained within the span. In addition to the regression weight function, you can use a robust weight function, which makes the process resistant to outliers. Finally, the methods are differentiated by the model used in the regression: lowess uses a linear polynomial, while loess uses a quadratic polynomial.

The local regression smoothing methods used by the Curve Fitting Toolbox follow these rules:

- The span can be even or odd.
- You can specify the span as a percentage of the total number of data points in the data set. For example, a span of 0.1 uses 10% of the data points.

The regression smoothing and robust smoothing procedures are described in detail below.

Local Regression Smoothing Procedure

The local regression smoothing process follows these steps for each data point:

1 Compute the *regression weights* for each data point in the span. The weights are given by the tricube function shown below.

$$w_i = \left(1 - \left|\frac{x - x_i}{d(x)}\right|^3\right)^3$$

x is the predictor value associated with the response value to be smoothed, x_i are the nearest neighbors of x as defined by the span, and $d(x)$ is the distance along the abscissa from x to the most distant predictor value within the span. The weights have these characteristics:

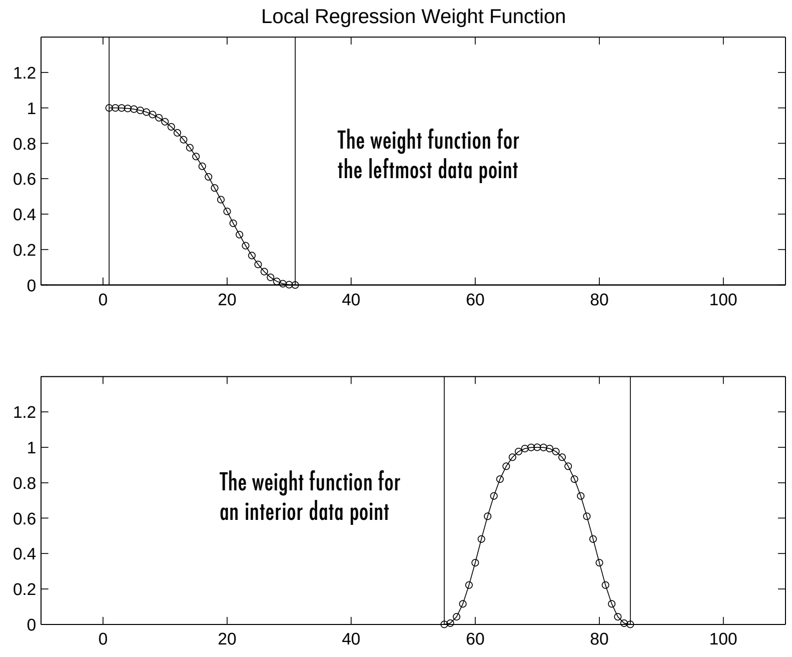
- The data point to be smoothed has the largest weight and the most influence on the fit.
- Data points outside the span have zero weight and no influence on the fit.

2 A weighted linear least squares regression is performed. For lowess, the regression uses a first degree polynomial. For loess, the regression uses a second degree polynomial.

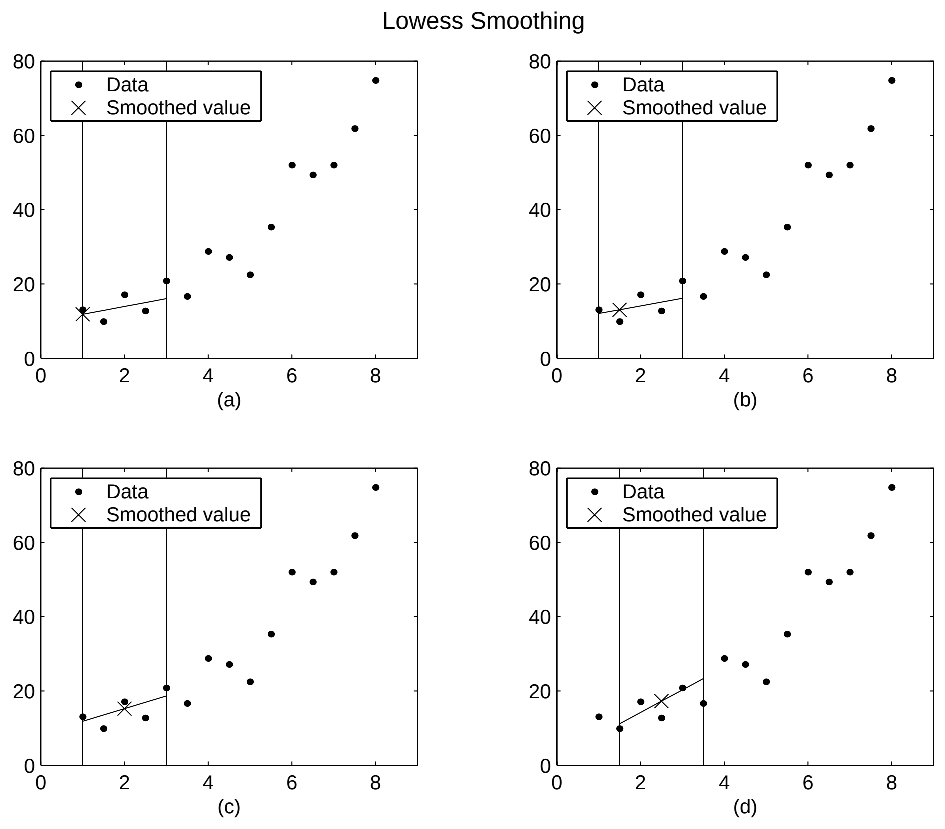
3 The smoothed value is given by the weighted regression at the predictor value of interest.

If the smooth calculation involves the same number of neighboring data points on either side of the smoothed data point, the weight function is symmetric. However, if the number of neighboring points is not symmetric about the smoothed data point, then the weight function is not symmetric. Note that unlike the moving average smoothing process, the span never changes. For example, when you smooth the data point with the smallest predictor value, the shape of the weight function is truncated by one half, the leftmost data point in the span has the largest weight, and all the neighboring points are to the right of the smoothed value.

The weight function for an end point and for an interior point is shown below for a span of 31 data points.



Using the lowess method with a span of five, the smoothed values and associated regressions for the first four data points of a generated data set are shown below.



Notice that the span does not change as the smoothing process progresses from data point to data point. However, depending on the number of nearest neighbors, the regression weight function might not be symmetric about the data point to be smoothed. In particular, plots `(a)` and `(b)` use an asymmetric weight function, while plots `(c)` and `(d)` use a symmetric weight function.

For the loess method, the graphs would look the same except the smoothed value would be generated by a second-degree polynomial.

Robust Smoothing Procedure

If your data contains outliers, the smoothed values can become distorted, and not reflect the behavior of the bulk of the neighboring data points. To overcome this problem, you can smooth the data using a robust procedure that is not influenced by a small fraction of outliers. For a description of outliers, refer to “Marking Outliers” on page 2-27.

The Curve Fitting Toolbox provides a robust version for both the lowess and loess smoothing methods. These robust methods include an additional calculation of robust weights, which is resistant to outliers. The robust smoothing procedure follows these steps:

1 Calculate the residuals from the smoothing procedure described in the previous section.

2 Compute the *robust weights* for each data point in the span. The weights are given by the bisquare function shown below.

$$w_i = \begin{cases} (1-(r_i/6MAD)^2)^2 & |r_i| < 6MAD \\ 0 & |r_i| \geq 6MAD \end{cases}$$

r_i is the residual of the `ith` data point produced by the regression smoothing procedure, and *MAD* is the median absolute deviation of the residuals:

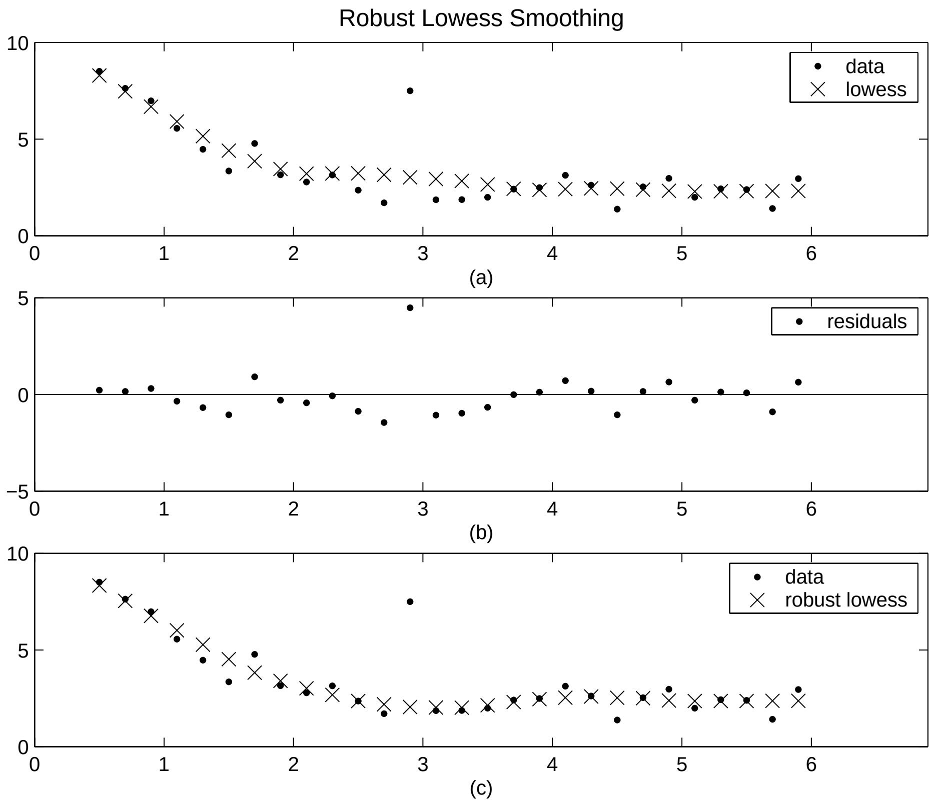
$$MAD = \text{median}(|r|)$$

The median absolute deviation is a measure of how spread out the residuals are. If r_i is small compared to 6*MAD*, then the robust weight is close to 1. If r_i is greater than 6*MAD*, the robust weight is 0 and the associated data point is excluded from the smooth calculation.

3 Smooth the data again using the robust weights. The final smoothed value is calculated using both the local regression weight and the robust weight.

4 Repeat the previous two steps for a total of five iterations.

The smoothing results of the lowess procedure are compared below to the results of the robust lowess procedure for a generated data set that contains a single outlier. The span for both procedures is 11 data points.



Plot `(a)` shows that the outlier influences the smoothed value for several nearest neighbors. Plot `(b)` suggests that the residual of the outlier is greater than six median absolute deviations. Therefore, the robust weight is zero for this data point. Plot `(c)` shows that the smoothed values neighboring the outlier reflect the bulk of the data.

Savitzky-Golay Filtering

Savitzky-Golay filtering can be thought of as a generalized moving average. You derive the filter coefficients by performing an unweighted linear least squares fit using a polynomial of a given degree. For this reason, a Savitzky-Golay filter is also called a digital smoothing polynomial filter or a least squares smoothing filter. Note that a higher degree polynomial makes it possible to achieve a high level of smoothing without attenuation of data features.

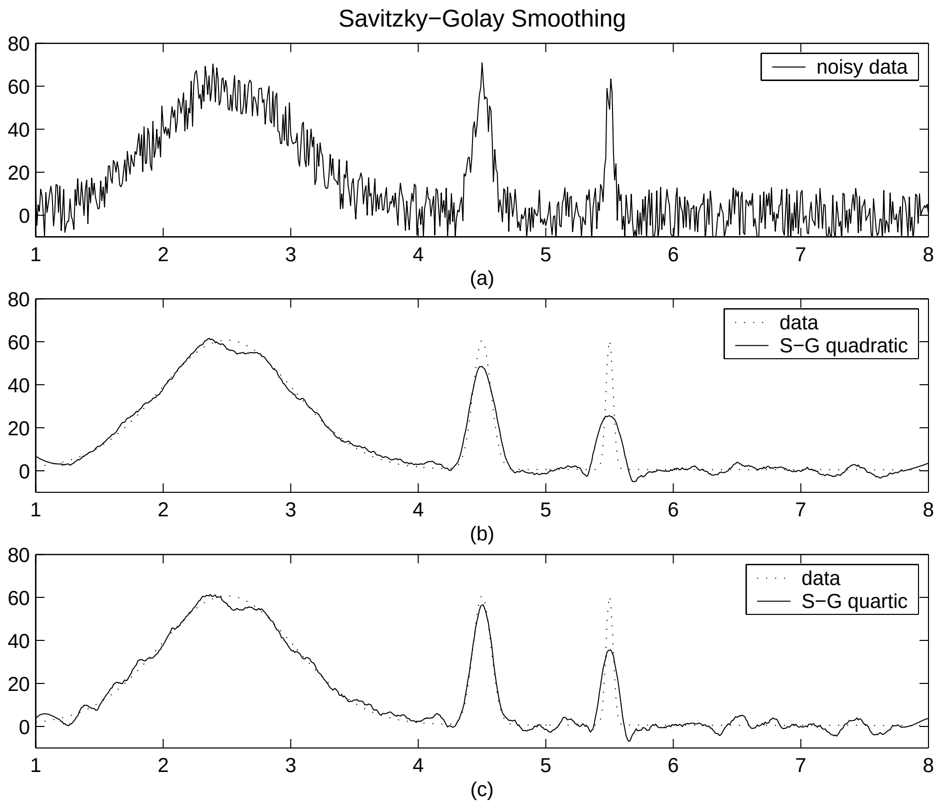
The Savitzky-Golay filtering method is often used with frequency data or with spectroscopic (peak) data. For frequency data, the method is effective at preserving the high-frequency components of the signal. For spectroscopic data, the method is effective at preserving higher moments of the peak such as the line width. By comparison, the moving average filter tends to filter out a significant portion of the signal's high-frequency content, and it can only preserve the lower moments of a peak such as the centroid. However, Savitzky-Golay filtering can be less successful than a moving average filter at rejecting noise.

The Savitzky-Golay smoothing method used by the Curve Fitting Toolbox follows these rules:

- The span must be odd.
- The polynomial degree must be less than the span.
- The data points are not required to have uniform spacing.

  Normally, Savitzky-Golay filtering requires uniform spacing of the predictor data. However, the algorithm provided by the Curve Fitting Toolbox supports nonuniform spacing. Therefore, you are not required to perform an additional filtering step to create data with uniform spacing.

The plot shown below displays generated Gaussian data and several attempts at smoothing using the Savitzky-Golay method. The data is very noisy and the peak widths vary from broad to narrow. The span is equal to 5% of the number of data points.

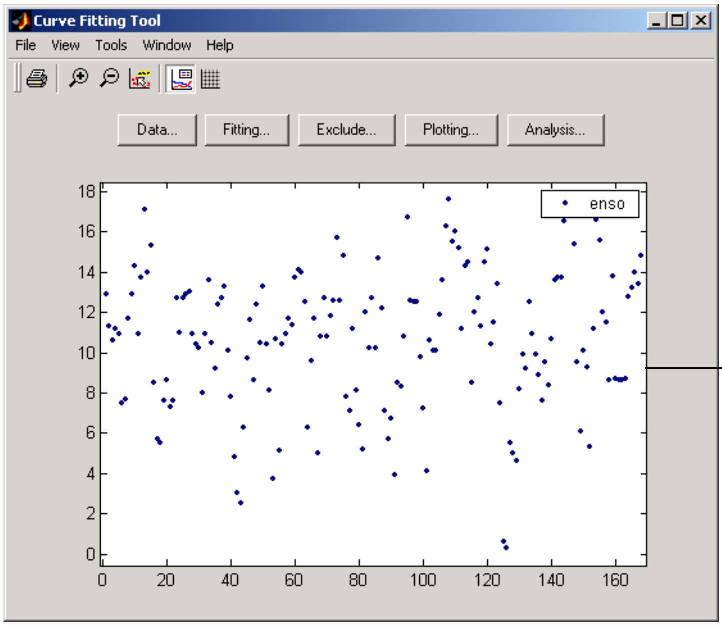


Plot `(a)` shows the noisy data. To more easily compare the smoothed results, plots `(b)` and `(c)` show the data without the added noise.

Plot `(b)` shows the result of smoothing with a quadratic polynomial. Notice that the method performs poorly for the narrow peaks. Plot `(c)` shows the result of smoothing with a quartic polynomial. In general, higher degree polynomials can more accurately capture the heights and widths of narrow peaks, but can do poorly at smoothing wider peaks.

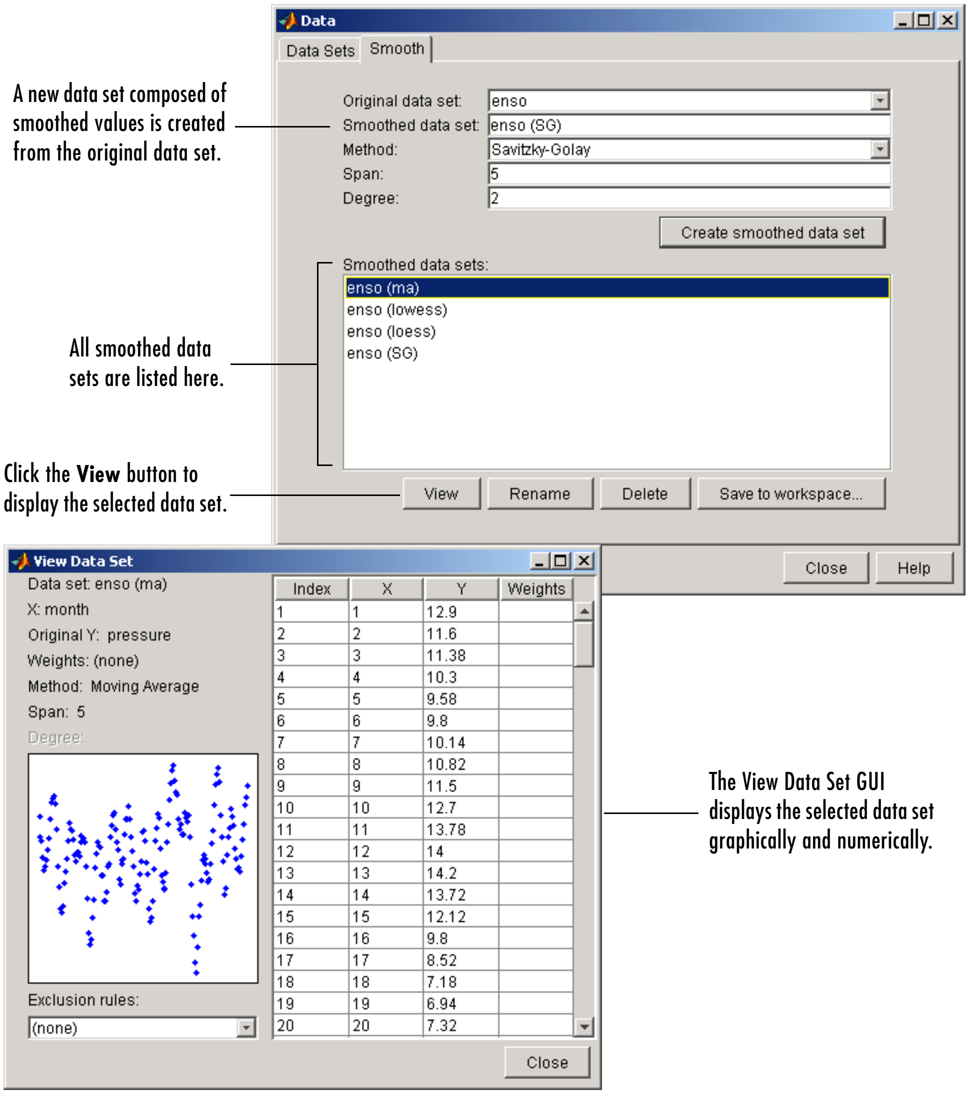
Example: Smoothing Data

This example smooths the ENSO data set using the moving average, lowess, loess, and Savitzky-Golay methods with the default span. As shown below, the data appears noisy. Smoothing might help you visualize patterns in the data, and provide insight toward a reasonable approach for parametric fitting.



Because the data appears noisy, smoothing might help uncover its structure.

The Smooth pane shown below displays all the new data sets generated by smoothing the original ENSO data set. Whenever you smooth a data set, a new data set of smoothed values is created. The smoothed data sets are automatically displayed in the Curve Fitting Tool. You can also display a single data set graphically and numerically by clicking the **View** button.



A new data set composed of smoothed values is created from the original data set.

All smoothed data sets are listed here.

Click the **View** button to display the selected data set.

The View Data Set GUI displays the selected data set graphically and numerically.

Original data set: enso
Smoothed data set: enso (SG)
Method: Savitzky-Golay
Span: 5
Degree: 2

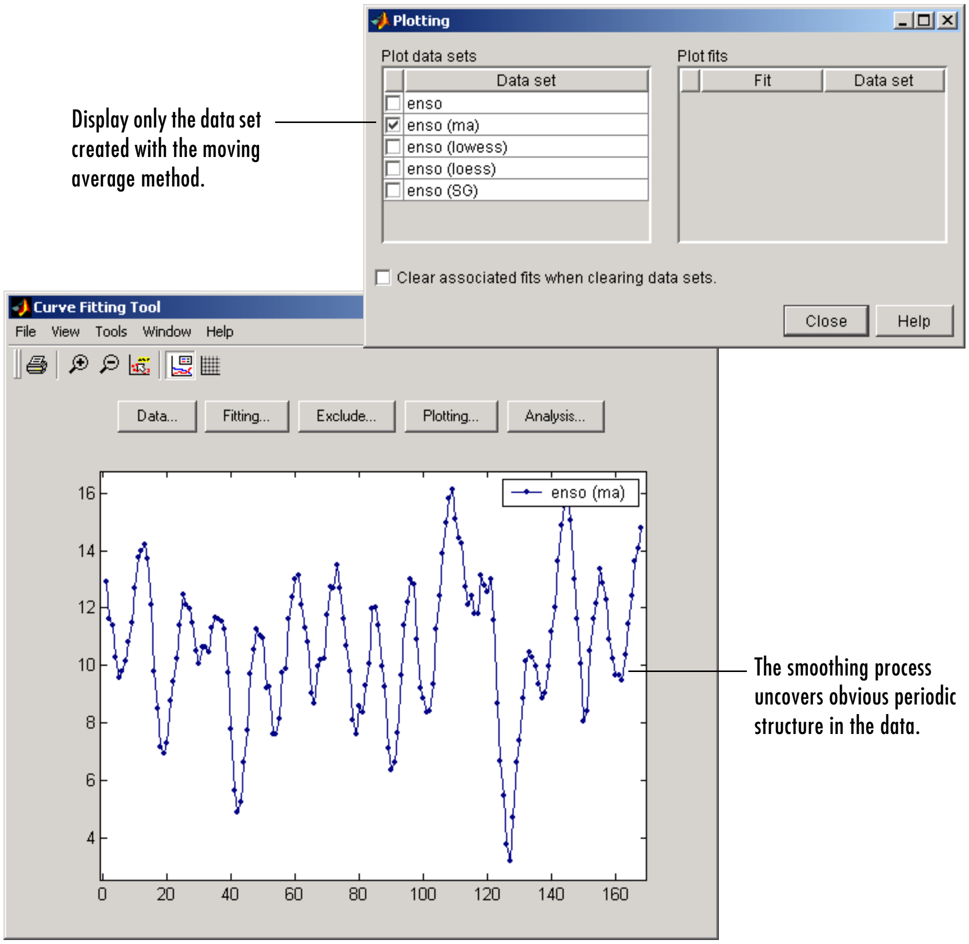
Smoothed data sets:
enso (ma)
enso (lowess)
enso (loess)
enso (SG)

Data set: enso (ma)
X: month
Original Y: pressure
Weights: (none)
Method: Moving Average
Span: 5
Degree:

Exclusion rules: (none)

Index	X	Y	Weights
1	1	12.9	
2	2	11.6	
3	3	11.38	
4	4	10.3	
5	5	9.58	
6	6	9.8	
7	7	10.14	
8	8	10.82	
9	9	11.5	
10	10	12.7	
11	11	13.78	
12	12	14	
13	13	14.2	
14	14	13.72	
15	15	12.12	
16	16	9.8	
17	17	8.52	
18	18	7.18	
19	19	6.94	
20	20	7.32	

Use the Plotting GUI to display only the data sets of interest. As shown below, the periodic structure of the ENSO data set becomes apparent when it is smoothed using a moving average filter with the default span. Not surprisingly, the uncovered structure is periodic, which suggests that a reasonable parametric model should include trigonometric functions.


Plotting
Curve Fitting Tool
File View Tools Window Help
Data... Fitting... Exclude... Plotting... Analysis...
enso (ma)
Close Help

Display only the data set created with the moving average method.

Plot data sets

	Data set
☐	enso
✓	enso (ma)
☐	enso (lowess)
☐	enso (loess)
☐	enso (SG)

Plot fits

	Fit	Data set

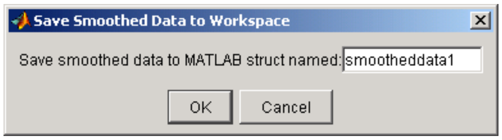
☐ Clear associated fits when clearing data sets.

The smoothing process uncovers obvious periodic structure in the data.

Refer to “General Equation: Fourier Series Fit” on page 3-52 for an example that fits the ENSO data using a sum of sine and cosine functions.

Saving the Results

By clicking the **Save to workspace** button, you can save a smoothed data set as a structure to the MATLAB workspace. This example saves the moving average results contained in the `enso (ma)` data set.



Save smoothed data to MATLAB struct named: smootheddata1

The saved structure contains the original predictor data `x` and the smoothed data `y`.

```
smootheddata1

smootheddata1 =
    x: [168x1 double]
    y: [168x1 double]
```

Excluding and Sectioning Data

If there is justification, you might want to exclude part of a data set from a fit. Typically, you exclude data so that subsequent fits are not adversely affected. For example, if you are fitting a parametric model to measured data that has been corrupted by a faulty sensor, the resulting fit coefficients will be inaccurate.

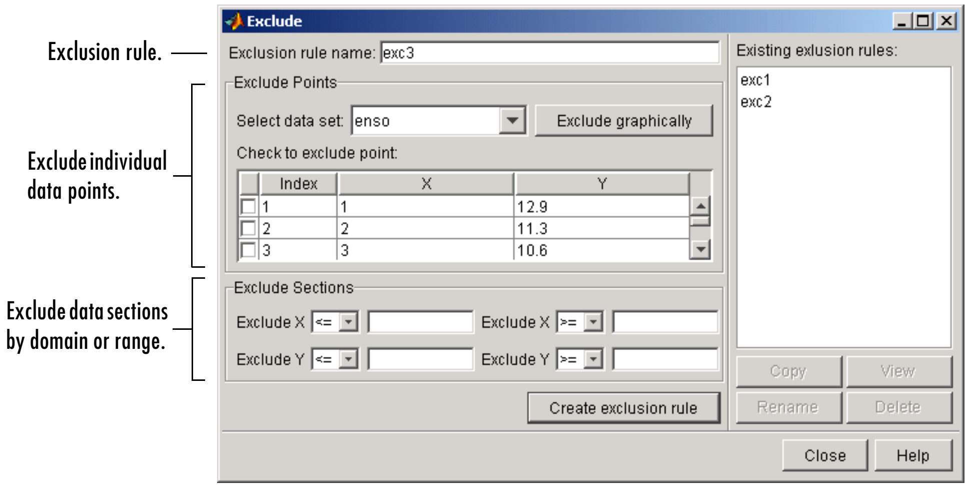
The Curve Fitting Toolbox provides two methods to exclude data:

- Marking Outliers — Outliers are defined as individual data points that you exclude because they are inconsistent with the statistical nature of the bulk of the data.
- Sectioning — Sectioning excludes a window of response or predictor data. For example, if many data points in a data set are corrupted by large systematic errors, you might want to section them out of the fit.

For each of these methods, you must create an *exclusion rule*, which captures the range, domain, or index of the data points to be excluded.

To exclude data while fitting, you use the Fitting GUI to associate the appropriate exclusion rule with the data set to be fit. Refer to “Example: Robust Fit” on page 3-61 for more information about fitting a data set using an exclusion rule.

You mark data to be excluded from a fit with the **Exclude** GUI, which you open from the Curve Fitting Tool. The GUI is shown below followed by a description of its features.



Exclusion rule name: exc3

Select data set: enso

Index	X	Y
1	1	12.9
2	2	11.3
3	3	10.6

Exclude X <= Exclude X >=

Exclude Y <= Exclude Y >=

Existing exlusion rules: exc1, exc2

Exclusion Rule

- **Exclusion rule name** — Specify the name of the exclusion rule that identifies the data points to be excluded from subsequent fits.
- **Existing exclusion rules** — Lists the names of all exclusion rules created during the current session. When you select an existing exclusion rule, you can perform these actions:
  - Click **Copy** to copy the exclusion rule. The exclusions associated with the original exclusion rule are recreated in the GUI. You can modify these exclusions and then click **Create exclusion rule** to save them to the copied rule.
  - Click **Rename** to change the name of the exclusion rule.
  - Click **Delete** to delete the exclusion rule. To select multiple exclusion rules, you can use the **Ctrl** key and the mouse to select exclusion rules one by one, or you can use the **Shift** key and the mouse to select a range of exclusion rules.
  - Click **View** to display the exclusion rule graphically. If a data set is associated with the exclusion rule, the data is also displayed.

Exclude Individual Data Points

- **Select data set** — Select the data set from which data points will be marked as excluded. You must select a data set to exclude individual data points.
- **Exclude graphically** — Open a GUI that allows you to exclude individual data points graphically.

  Individually excluded data points are marked by an "x" in the GUI, and are automatically identified in the **Check to exclude point** table.
- **Check to exclude point** — Select individual data points to exclude. You can sort this table by clicking on any of the column headings.

Exclude Data Sections by Domain or Range

- **Section** — Specify a vertical window, a horizontal window, or a box of data points to include. The excluded data lie outside these windows. You do not need to select a data set to create an exclusion rule by sectioning.
  - **Exclude X** — Section the predictor data by specifying the domain outside of which data is excluded.
  - **Exclude Y** — Section the response data by specifying the range outside of which data is excluded.

Marking Outliers

Outliers are defined as individual data points that you exclude from a fit because they are inconsistent with the statistical nature of the bulk of the data, and will adversely affect the fit results. Outliers are often readily identified by a scatter plot of response data versus predictor data.

Marking outliers with the Curve Fitting Toolbox follows these rules:

- You must specify a data set before creating an exclusion rule.

  In general, you should use the exclusion rule only with the specific data set it was based on. However, the toolbox does not prevent you from using the exclusion rule with another data set provided the size is the same.
- Using the Exclude GUI, you can exclude outliers either graphically or numerically.

As described in "Parametric Fitting" on page 3-4, one of the basic assumptions underlying curve fitting is that the data is statistical in nature and is described by a particular distribution, which is often assumed to be Gaussian. The statistical nature of the data implies that it contains random variations along with a deterministic component.

data = deterministic component + random component

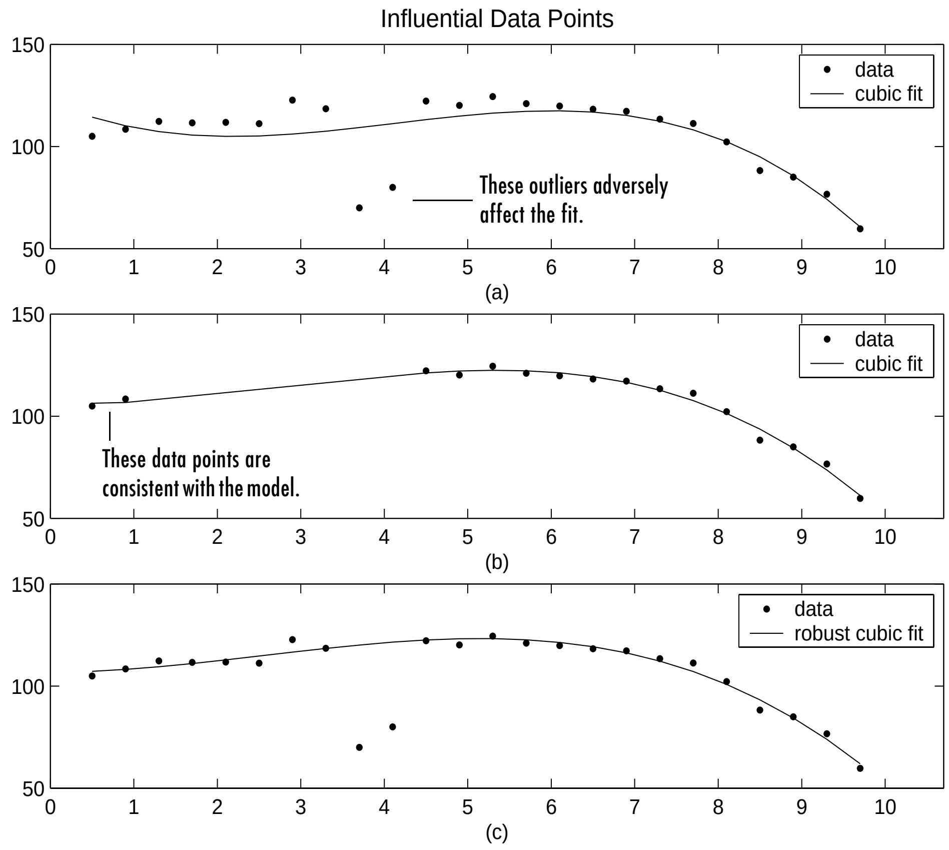
However, your data set might contain one or more data points that are nonstatistical in nature, or are described by a different statistical distribution. These data points might be easy to identify, or they might be buried in the data and difficult to identify.

A nonstatistical process can involve the measurement of a physical variable such as temperature or voltage in which the random variation is negligible compared to the systematic errors. For example, if your sensor calibration is inaccurate, the data measured with that sensor will be systematically inaccurate. In some cases, you might be able to quantify this nonstatistical data component and correct the data accordingly. However, if the scatter plot reveals that a handful of response values are far removed from neighboring response values, these data points are considered outliers and should be excluded from the fit. Outliers are usually difficult to explain away. For example, it might be that your sensor experienced a power surge or someone wrote down the wrong number in a log book.

If you decide there is justification, you should mark outliers to be excluded from subsequent fits — particularly parametric fits. Removing these data points can have a dramatic effect on the fit results because the fitting process minimizes the square of the residuals. If you do not exclude outliers, the resulting fit will be poor for a large portion of your data. Conversely, if you do exclude the outliers and choose the appropriate model, the fit results should be reasonable.

Because outliers can have a significant effect on a fit, they are considered *influential data*. However, not all influential data points are outliers. For example, your data set can contain valid data points that are far removed from the rest of the data. The data is valid because it is well described by the model used in the fit. The data is influential because its exclusion will dramatically affect the fit results.

Two types of influential data points are shown below for generated data. Also shown are cubic polynomial fits and a robust fit that is resistant to outliers.



Plot (a) shows that the two influential data points are outliers and adversely affect the fit. Plot (b) shows that the two influential data points are consistent with the model and do not adversely affect the fit. Plot (c) shows that a robust fitting procedure is an acceptable alternative to marking outliers for exclusion. Robust fitting is described in “Robust Least Squares” on page 3-11.

Sectioning

Sectioning involves specifying a range of response data or a range of predictor data to exclude. You might want to section a data set because different parts of the data set are described by different models or many contiguous data points are corrupted by noise, large systematic errors, and so on.

Sectioning data with the Curve Fitting Toolbox follows these rules:

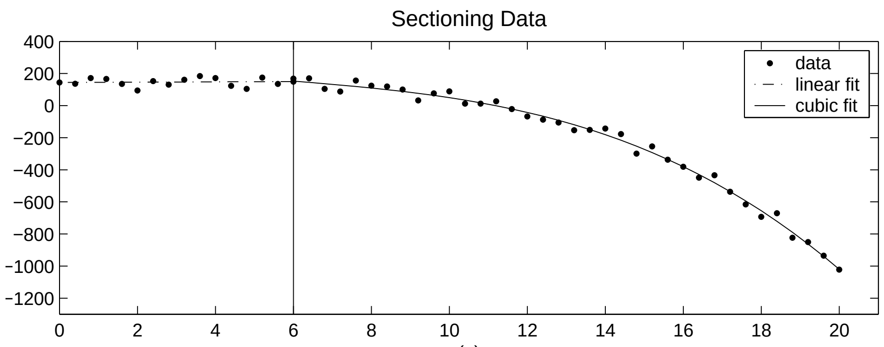
- If you are only sectioning data and not excluding individual data points, then you can create an exclusion rule without specifying a data set name.

  Note that you can associate the exclusion rule with any data set provided that the range or domain of the exclusion rule overlaps with the range or domain of the data set. This is useful if you have multiple data sets from which you want to exclude data points using the same range or domain.
- Using the Exclude GUI, you specify a range or domain of data to *include*. The excluded data lies outside this specification.

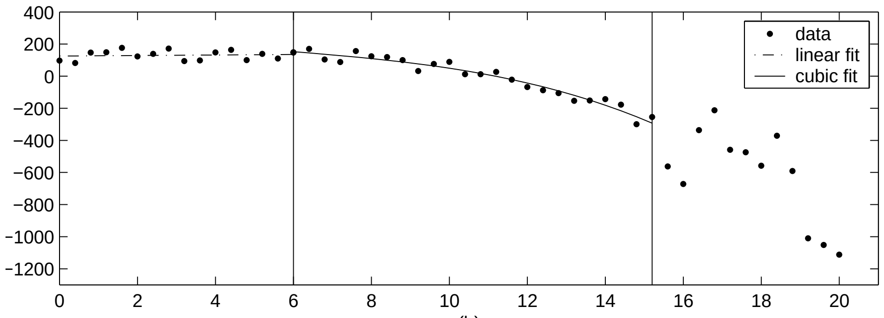
  Additionally, you can specify only a single range, domain, or box (range and domain) of included data points. Therefore, at most, you can define two vertical strips, two horizontal strips, or a border of excluded data. Refer to "Example: Excluding and Sectioning Data" on page 2-32 for an example.

  To exclude multiple sections of data, you can use the `excludedata` function from the MATLAB command line.

Two examples of sectioning by domain are shown below for generated data.



(a)



(b)

Plot `(a)` shows the data set sectioned by fit type. The left section is fit with a linear polynomial, while the right section is fit with a cubic polynomial. Plot `(b)` shows the data set sectioned by fit type and by valid data. Here, the rightmost section is not part of any fit because the data is corrupted by noise. Note that reproducing these plots using the toolbox is a multistep process. For example, to reproduce plot (a), the steps are

1. Create an exclusion rule by sectioning the predictor data such that the data points described by the linear polynomial are excluded.

2. Create a different exclusion rule by sectioning the predictor data such that the data points described by the cubic polynomial are excluded.

3. Fit the data twice (once for each exclusion rule) using the appropriate model.

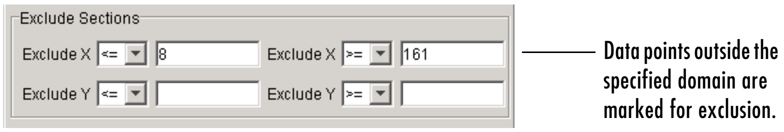
Example: Excluding and Sectioning Data

This example modifies the ENSO data set to illustrate excluding and sectioning data. First, copy the ENSO response data to a new variable and add two outliers that are far removed from the bulk of the data.

```
rand('state',0)
yy = pressure;
yy(ceil(length(month)*rand(1))) = mean(pressure)*2.5;
yy(ceil(length(month)*rand(1))) = mean(pressure)*3.0;
```

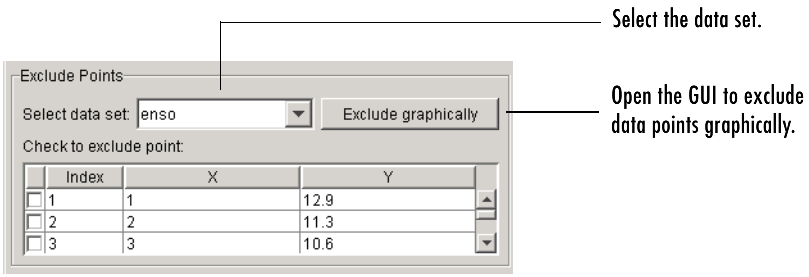
Import the variables `month` and `yy` as the new data set `enso1`, and open the Exclude GUI.

Assume that the first and last eight months of the data set are unreliable, and should be excluded from subsequent fits. The simplest way to exclude these data points is to section the predictor data. To do this, specify the range of data you want to include in the **Exclude X outside of** field of the **Section** pane.


Exclude Sections
Exclude X <=
Exclude X >=
Exclude Y <=
Exclude Y >=
Data points outside the specified domain are marked for exclusion.

Exclude X <= 8, Exclude X >= 161

There are two ways to exclude individual data points: using the **Check to exclude point** table or graphically. For this example, the simplest way to exclude the outliers is graphically. To do this, select the data set name and click the **Exclude graphically** button, which opens the Select Points for Exclusion Rule GUI.

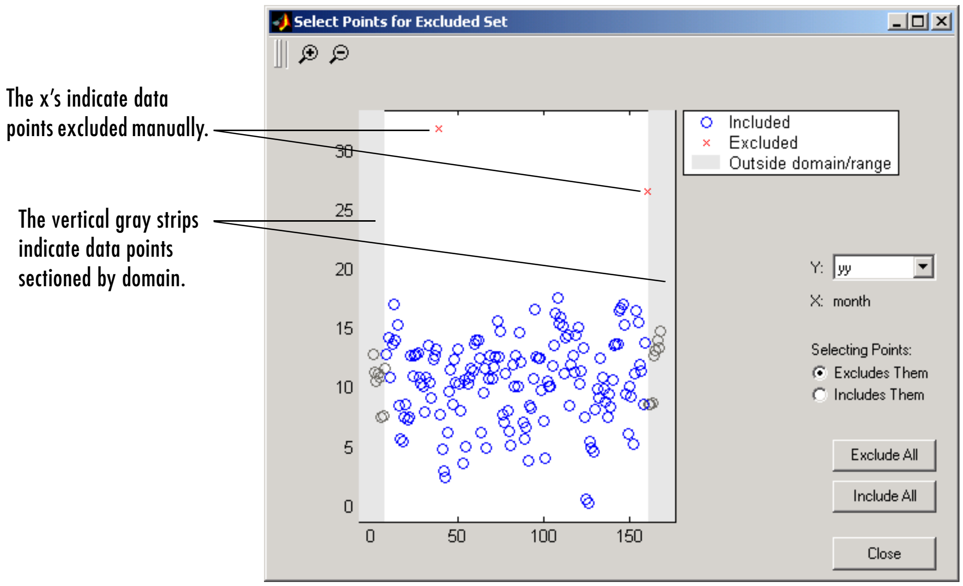


Select data set: enso

	Index	X	Y
☐	1	1	12.9
☐	2	2	11.3
☐	3	3	10.6

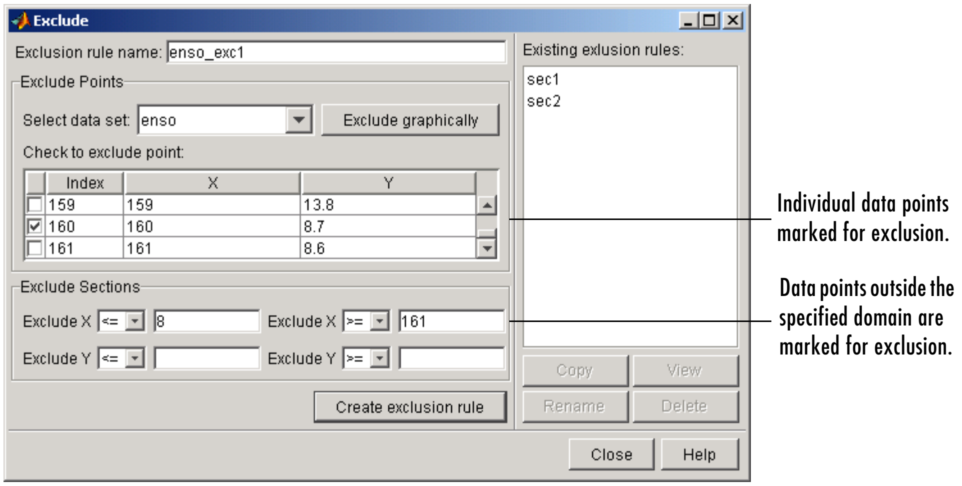
To mark data points for exclusion in the GUI, place the mouse cursor over the data point and left-click. The excluded data point is marked with a red X. To include an excluded data point, right-click the data point or select the **Include Them** radio button and left-click. Included data points are marked with a blue circle. To select multiple data points, click the left mouse button and drag the selection rubber band so that the rubber band box encompasses the desired data points. Note that the GUI identifies sectioned data with gray strips. You cannot graphically include sectioned data.

As shown below, the first and last eight months of data are excluded from the data set by sectioning, and the two outliers are excluded graphically. Note that the graphically excluded data points are identified in the **Check to exclude point** table. If you decide to include an excluded data point using the table, the graph is automatically updated.


The x's indicate data points excluded manually.
The vertical gray strips indicate data points sectioned by domain.
Select Points for Excluded Set
Included
Excluded
Outside domain/range
Y: yy
X: month
Selecting Points:
Excludes Them
Includes Them
Exclude All
Include All
Close

If there are fits associated with the data, you can exclude data points based on the residuals of the fit by selecting the residual data in the **Y** list.

The Exclude GUI for this example is shown below.


Exclude
Exclude Points
Exclude graphically
Exclude Sections
Create exclusion rule
Copy
View
Rename
Delete
Close
Help
Individual data points marked for exclusion.
Data points outside the specified domain are marked for exclusion.

Exclusion rule name: enso_exc1

Select data set: enso

Check to exclude point:

	Index	X	Y
☐	159	159	13.8
✓	160	160	8.7
☐	161	161	8.6

Exclude X <= 8 Exclude X >= 161

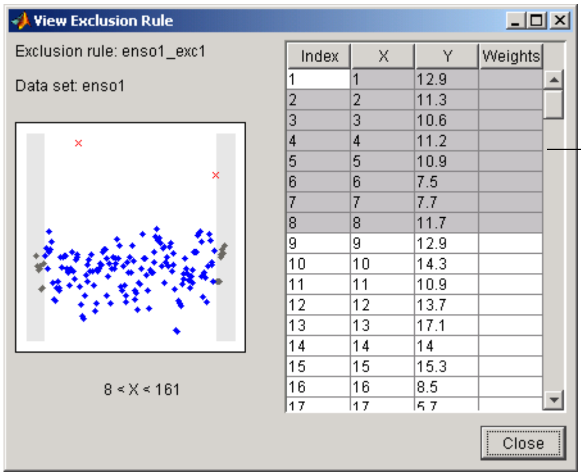
Exclude Y <= Exclude Y >=

Existing exlusion rules:
sec1
sec2

To save the exclusion rule, click the **Create exclusion rule** button. To exclude the data from a fit, you must select the exclusion rule from the Fitting GUI. Because the exclusion rule created in this example uses individually excluded data points, you can use it only with data sets that are the same size as the ENSO data set.

Viewing the Exclusion Rule

To view the exclusion rule, select an existing exclusion rule name and click the **View** button. The View Exclusion Rule GUI shown below displays the modified ENSO data set and the excluded data points, which are grayed in the table.



Exclusion rule: enso1_exc1

Data set: enso1

8 < X < 161

Index	X	Y	Weights
1	1	12.9	
2	2	11.3	
3	3	10.6	
4	4	11.2	
5	5	10.9	
6	6	7.5	
7	7	7.7	
8	8	11.7	
9	9	12.9	
10	10	14.3	
11	11	10.9	
12	12	13.7	
13	13	17.1	
14	14	14	
15	15	15.3	
16	16	8.5	
17	17	5.7	

The excluded data points are grayed in the table.

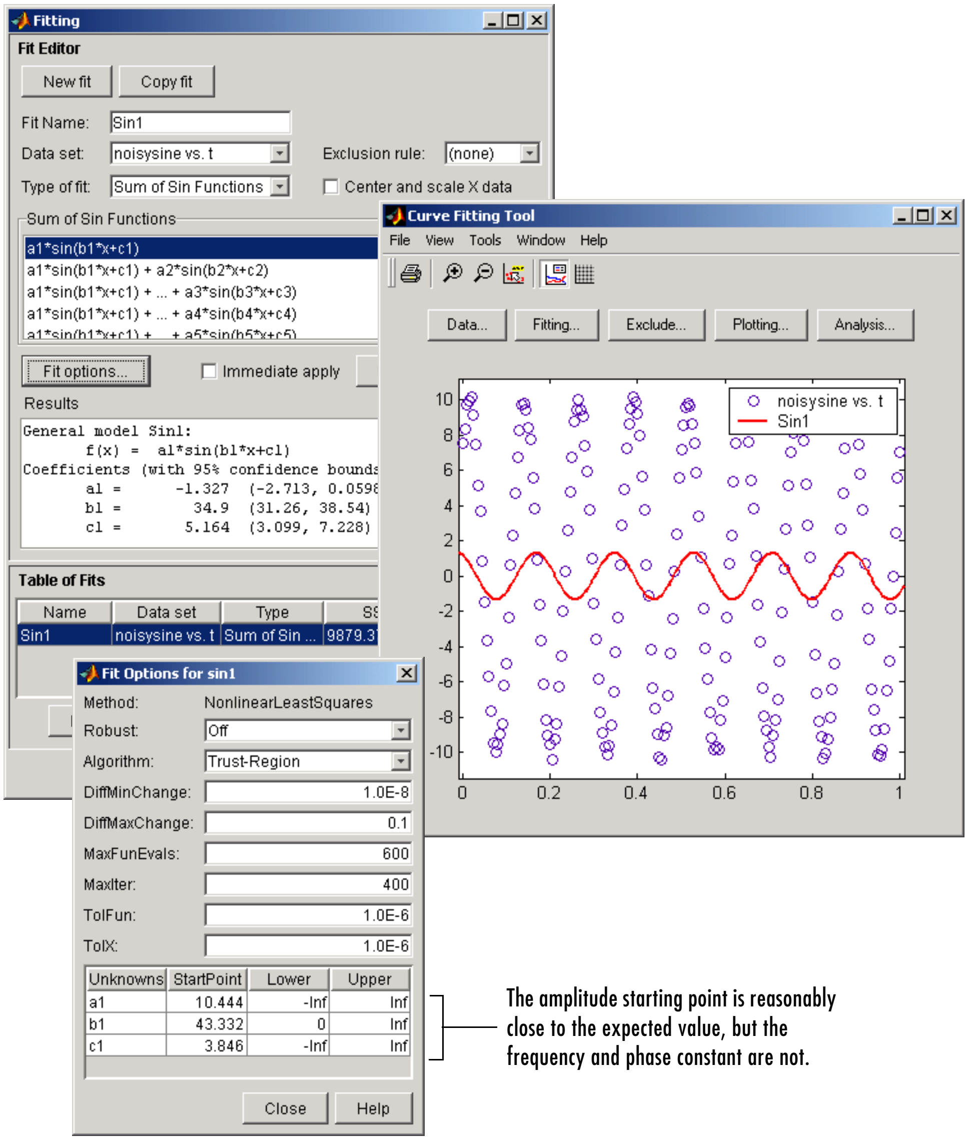
Example: Sectioning Periodic Data

For all parametric equations, the toolbox provides coefficient starting values. For certain types of data sets such as periodic data containing many periods, the starting values may not lead to satisfactory results. In this case, sectioning the data can provide you with improved starting values for the fit.

This example uses generated sine data with noise added. The time vector is given by `t` and the amplitude, frequency, and phase constant of the data are given by the vector `cf`.

```
rand('state',0);
t = [0:0.005:1.0]';
cf = [10 16*pi pi/4];
noisysine = cf(1)*(sin(cf(2)*t+cf(3))) + (rand(size(t))-0.5);
```

Import the variables `t` and `noisysine`, and fit the data with a single-term sine equation. The Fitting GUI, Fit Options GUI, and Curve Fitting Tool are shown below. To display the fit starting values, click the **Fit options** button. Note that the amplitude starting point is reasonably close to the expected value, but the frequency and phase constant are not, which produces a poor fit.


Fitting
Fit Editor
New fit
Copy fit
Sum of Sin Functions
a1*sin(b1*x+c1)
a1*sin(b1*x+c1) + a2*sin(b2*x+c2)
a1*sin(b1*x+c1) + ... + a3*sin(b3*x+c3)
a1*sin(b1*x+c1) + ... + a4*sin(b4*x+c4)
a1*sin(b1*x+c1) + ... + a5*sin(b5*x+c5)
Fit options...
Immediate apply
Results
Table of Fits
Curve Fitting Tool
File View Tools Window Help
Data... Fitting... Exclude... Plotting... Analysis...
noisysine vs. t
Sin1
Fit Options for sin1
Close
Help

Fit Name: Sin1
Data set: noisysine vs. t
Exclusion rule: (none)
Type of fit: Sum of Sin Functions
Center and scale X data

```
General model Sin1:
       f(x) =  a1*sin(b1*x+c1)
Coefficients (with 95% confidence bounds
       a1 =      -1.327  (-2.713, 0.0598
       b1 =        34.9  (31.26, 38.54)
       c1 =       5.164  (3.099, 7.228)
```

Name	Data set	Type	SS
Sin1	noisysine vs. t	Sum of Sin ...	9879.3

Method: NonlinearLeastSquares
Robust: Off
Algorithm: Trust-Region
DiffMinChange: 1.0E-8
DiffMaxChange: 0.1
MaxFunEvals: 600
MaxIter: 400
TolFun: 1.0E-6
TolX: 1.0E-6

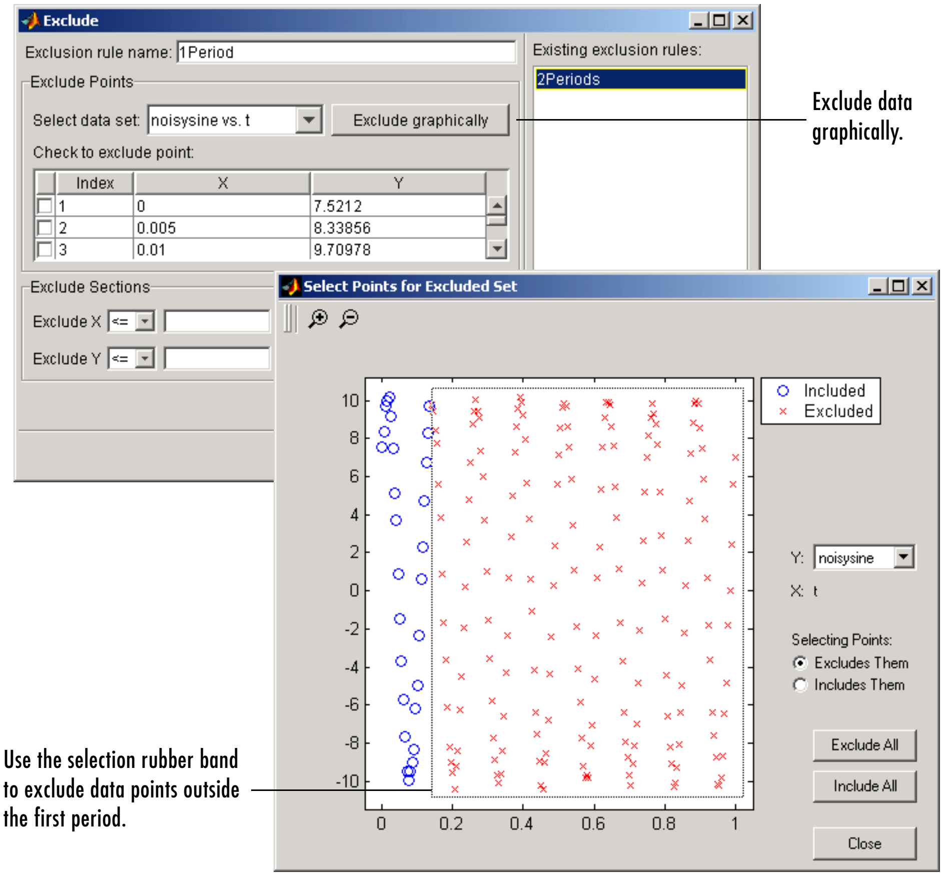
Unknowns	StartPoint	Lower	Upper
a1	10.444	-Inf	Inf
b1	43.332	0	Inf
c1	3.846	-Inf	Inf

The amplitude starting point is reasonably close to the expected value, but the frequency and phase constant are not.

To produce a reasonable fit, follow these steps:

1 Create an exclusion rule that includes one or two periods, and excludes the remaining data.

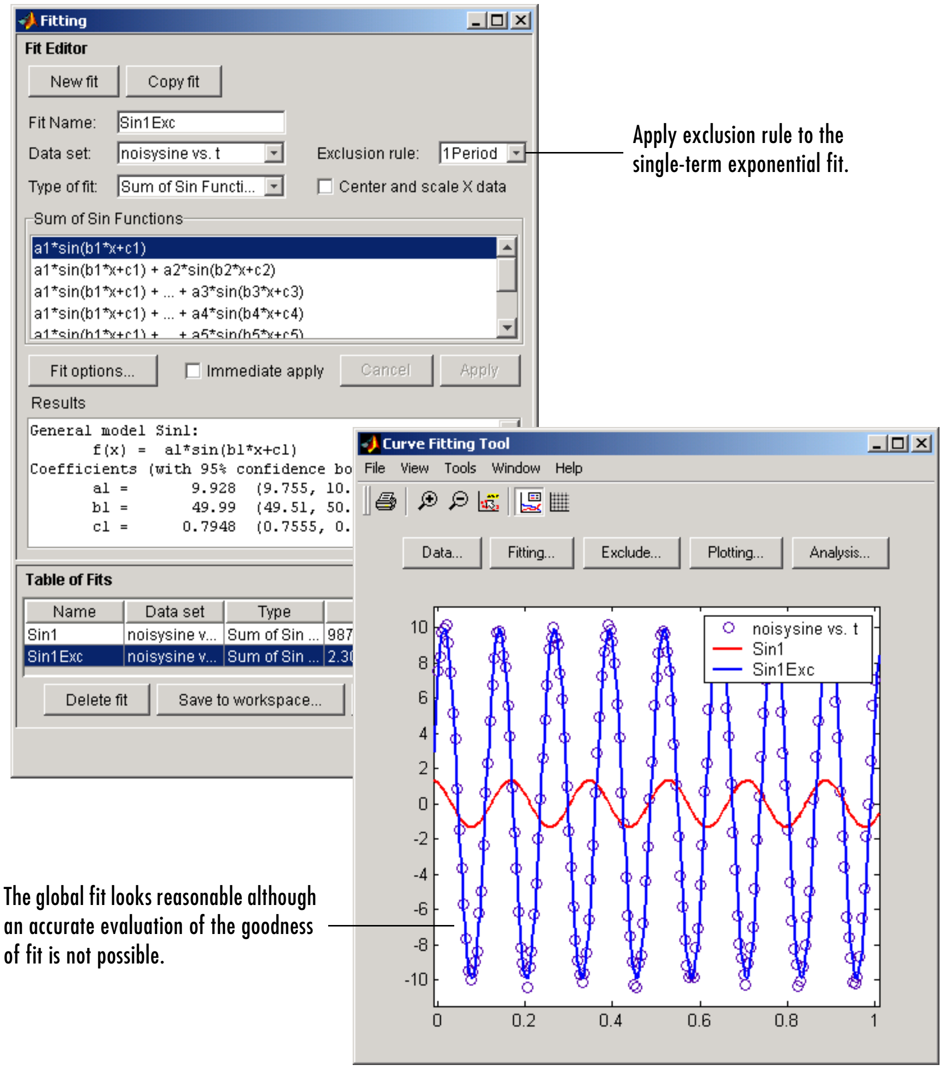
As shown below, an exclusion rule is created graphically by using the selection rubber band to exclude all data points outside the first period. The exclusion rule is named `1Period`.


Exclude
Exclusion rule name: 1Period
Existing exclusion rules:
2Periods
Exclude Points
Select data set: noisysine vs. t
Exclude graphically
Check to exclude point:
Exclude Sections
Exclude X <=
Exclude Y <=
Select Points for Excluded Set
Included
Excluded
Y: noisysine
X: t
Selecting Points:
Excludes Them
Includes Them
Exclude All
Include All
Close
Exclude data graphically.
Use the selection rubber band to exclude data points outside the first period.

	Index	X	Y
☐	1	0	7.5212
☐	2	0.005	8.33856
☐	3	0.01	9.70978

2 Create a new fit using the single-term sine equation with the exclusion rule `1Period` applied.

The fit looks reasonable throughout the entire data set. However, because the global fit was based on a small fraction of data, goodness of fit statistics will not provide much insight into the fit quality.



```
General model Sin1:
       f(x) =  a1*sin(b1*x+c1)
Coefficients (with 95% confidence bo
       a1 =       9.928  (9.755, 10.
       b1 =       49.99  (49.51, 50.
       c1 =      0.7948  (0.7555, 0.
```

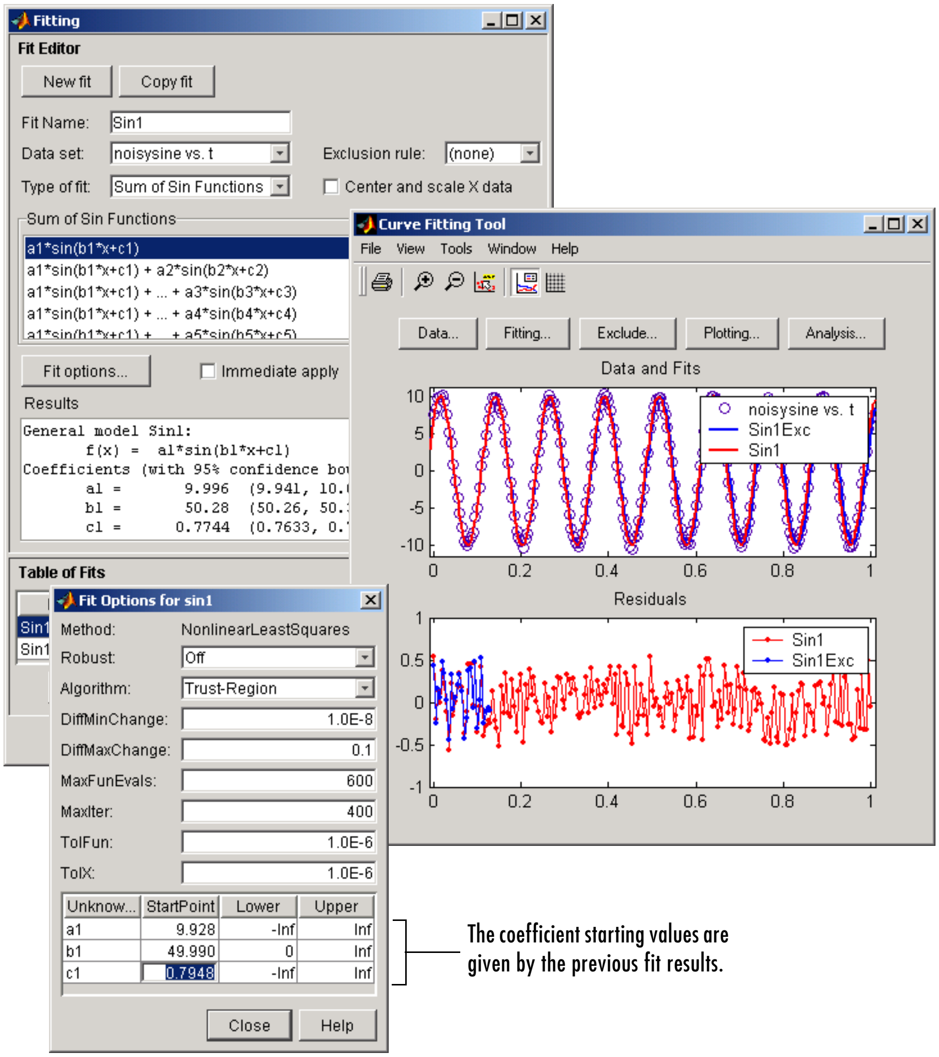
Name	Data set	Type	
Sin1	noisysine v...	Sum of Sin ...	987
Sin1Exc	noisysine v...	Sum of Sin ...	2.30

Apply exclusion rule to the single-term exponential fit.

The global fit looks reasonable although an accurate evaluation of the goodness of fit is not possible.

3 Fit the entire data set using the fitted coefficient values from the previous step as starting values.

The Fitting GUI, Fit Options GUI, and Curve Fitting Tool are shown below. Both the numerical and graphical fit results indicate a reasonable fit.



Fit Name: Sin1
Data set: noisysine vs. t
Exclusion rule: (none)
Type of fit: Sum of Sin Functions
☐ Center and scale X data

Sum of Sin Functions
- a1*sin(b1*x+c1)
- a1*sin(b1*x+c1) + a2*sin(b2*x+c2)
- a1*sin(b1*x+c1) + ... + a3*sin(b3*x+c3)
- a1*sin(b1*x+c1) + ... + a4*sin(b4*x+c4)
- a1*sin(b1*x+c1) + ... + a5*sin(b5*x+c5)

Results

```
General model Sin1:
       f(x) =  a1*sin(b1*x+c1)
Coefficients (with 95% confidence bou
       a1 =       9.996  (9.941, 10.
       b1 =       50.28  (50.26, 50.
       c1 =      0.7744  (0.7633, 0.
```

Method: NonlinearLeastSquares
Robust: Off
Algorithm: Trust-Region
DiffMinChange: 1.0E-8
DiffMaxChange: 0.1
MaxFunEvals: 600
MaxIter: 400
TolFun: 1.0E-6
TolX: 1.0E-6

Unknow...	StartPoint	Lower	Upper
a1	9.928	-Inf	Inf
b1	49.990	0	Inf
c1	0.7948	-Inf	Inf

The coefficient starting values are given by the previous fit results.

Additional Preprocessing Steps

Additional preprocessing steps not available through the Curve Fitting Toolbox GUIs include

- Transforming the response data
- Removing `Inf`s, `NaN`s, and outliers

Transforming the Response Data

In some circumstances, you might want to transform the response data. Common transformations include the logarithm ln(y), and power functions such as $y^{1/2}$, y^{-1}, and so on. Using these transformations, you can linearize a nonlinear model, contract response data that spans one or more orders of magnitude, or simplify a model so that it involves fewer coefficients.

Note You must transform variables at the MATLAB command line, and then import those variables into the Curve Fitting Toolbox. You cannot transform variables using any of the graphical user interfaces.

For example, suppose you want to use the following model to fit your data.

$$y = \frac{1}{ax^2 + bx + c}$$

If you decide to use the power transform y^{-1}, then the transformed model is given by

$$y^{-1} = ax^2 + bx + c$$

As another example, the equation

$$y = ae^{bx}$$

becomes linear if you take the log transform of both sides.

$$\ln(y) = \ln(a) + bx$$

You can now use linear least squares fitting procedures.

There are several disadvantages associated with performing transformations:

- For the log transformation, negative response values cannot be processed.
- For all transformations, the basic assumption that the residual variance is constant is violated. To avoid this problem, you could plot the residuals on the transformed scale. For the power transformation shown above, the transformed scale is given by the residuals

  $$r_i = y_i^{-1} - \hat{y}_i^{-1}$$

  Note that the residual plot associated with the Curve Fitting Tool does not support transformed scales.

Deciding on a particular transformation is not always obvious. However, a scatter plot will often reveal the best form to use. In practice you can experiment with various transforms and then plot the residuals from the command line using the transformed scale. If the errors are reasonable (they appear random with minimal scatter, and don't exhibit any systematic behavior), the transform is a good candidate.

Removing Infs, NaNs, and Outliers

Although the Curve Fitting Toolbox ignores `Infs` and `NaNs` when fitting data, and you can exclude outliers during the fitting process, you might still want to remove this data from your data set. To do so, you modify the associated data set variables from the MATLAB command line.

For example, when using toolbox functions such as `fit` from the command line, you must supply predictor and response vectors that contain finite numbers. To remove `Infs`, you can use the `isinf` function.

```
ind = find(isinf(xx));
xx(ind) = [];
yy(ind) = [];
```

To remove `NaNs`, you can use the `isnan` function. For examples that remove `NaNs` and outliers from a data set, refer to "Data Preprocessing" in the MATLAB documentation.

Selected Bibliography

[1] Cleveland, W.S., “Robust Locally Weighted Regression and Smoothing Scatterplots,” *Journal of the American Statistical Association*, Vol. 74, pp. 829-836, 1979.

[2] Cleveland, W.S. and S.J. Devlin, “Locally Weighted Regression: An Approach to Regression Analysis by Local Fitting,” *Journal of the American Statistical Association*, Vol. 83, pp. 596-610, 1988.

[3] Chambers, J., W.S. Cleveland, B. Kleiner, and P. Tukey, *Graphical Methods for Data Analysis*, Wadsworth International Group, Belmont, CA, 1983.

[4] Press, W.H., S.A. Teukolsky, W.T. Vetterling, and B.P. Flannery, *Numerical Recipes in C, The Art of Scientific Computing*, Cambridge University Press, Cambridge, England, 1993.

[5] Goodall, C., “A Survey of Smoothing Techniques,” *Modern Methods of Data Analysis*, (J. Fox and J.S. Long, eds.), Sage Publications, Newbury Park, CA, pp. 126-176, 1990.

[6] Hutcheson, M.C., “Trimmed Resistant Weighted Scatterplot Smooth,” Master’s Thesis, Cornell University, Ithaca, NY, 1995.

[7] Orfanidis, S.J., *Introduction to Signal Processing*, Prentice-Hall, Englewood Cliffs, NJ, 1996.

Fitting Data

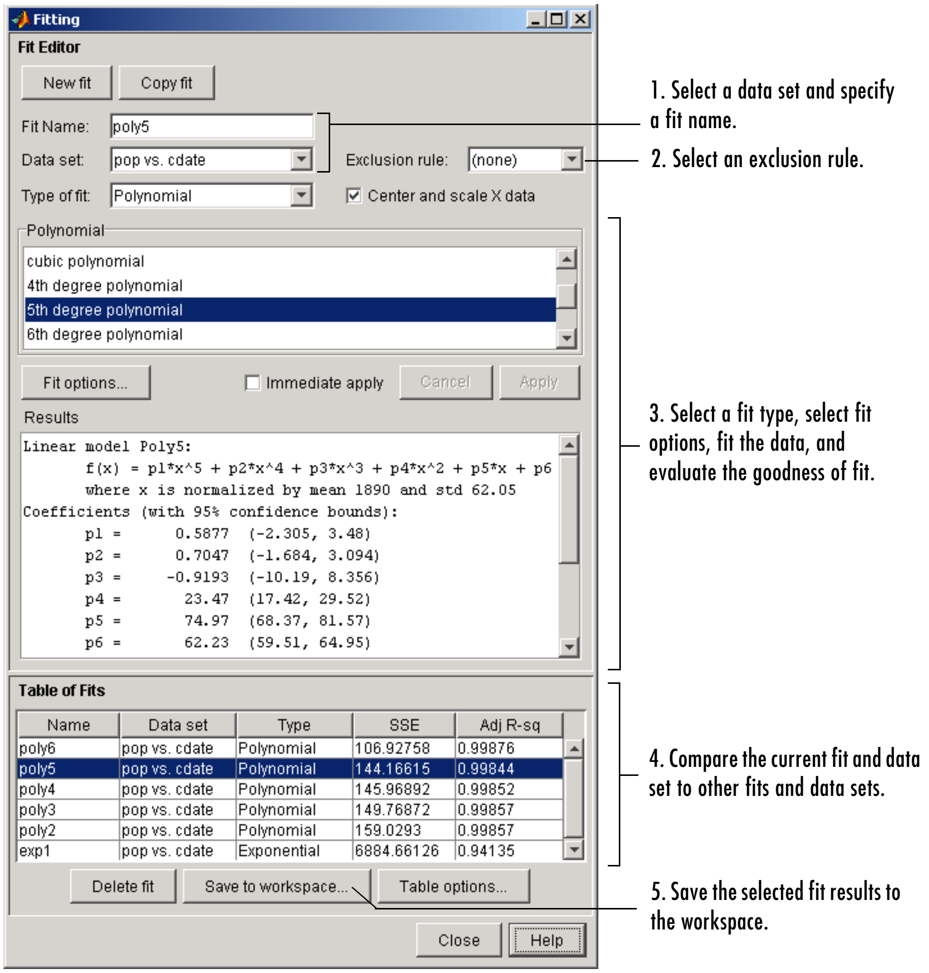
Curve fitting refers to fitting curved lines to data. The curved line comes from regression techniques, a spline calculation, or interpolation. The data can be measured from a sensor, generated from a simulation, historical, and so on. The goal of curve fitting is to gain insight into your data. The insight will enable you to improve data acquisition techniques for future experiments, accept or refute a theoretical model, extract physical meaning from fitted coefficients, and draw conclusions about the data's parent population.

This chapter describes how to fit data and evaluate the goodness of fit with the Curve Fitting Toolbox. The sections are as follows.

The Fitting Process

You fit data using the Fitting GUI. To open the Fitting GUI, click the **Fitting** button from the Curve Fitting Tool.

The Fitting GUI is shown below for the census data described in “Getting Started with the Curve Fitting Toolbox” on page 1-1, followed by the general steps you use when fitting any data set.



Fit Name: poly5
Data set: pop vs. cdate
Exclusion rule: (none)
Type of fit: Polynomial
☑ Center and scale X data

cubic polynomial
4th degree polynomial
5th degree polynomial
6th degree polynomial

```
Linear model Poly5:
       f(x) = p1*x^5 + p2*x^4 + p3*x^3 + p4*x^2 + p5*x + p6
       where x is normalized by mean 1890 and std 62.05
Coefficients (with 95% confidence bounds):
       p1 =      0.5877  (-2.305, 3.48)
       p2 =      0.7047  (-1.684, 3.094)
       p3 =     -0.9193  (-10.19, 8.356)
       p4 =       23.47  (17.42, 29.52)
       p5 =       74.97  (68.37, 81.57)
       p6 =       62.23  (59.51, 64.95)
```

Name	Data set	Type	SSE	Adj R-sq
poly6	pop vs. cdate	Polynomial	106.92758	0.99876
poly5	pop vs. cdate	Polynomial	144.16615	0.99844
poly4	pop vs. cdate	Polynomial	145.96892	0.99852
poly3	pop vs. cdate	Polynomial	149.76872	0.99857
poly2	pop vs. cdate	Polynomial	159.0293	0.99857
exp1	pop vs. cdate	Exponential	6884.66126	0.94135

1. Select a data set and specify a fit name.
2. Select an exclusion rule.
3. Select a fit type, select fit options, fit the data, and evaluate the goodness of fit.
4. Compare the current fit and data set to other fits and data sets.
5. Save the selected fit results to the workspace.

1. Select a data set and fit name.
   - Select the name of the current fit. When you click **New fit** or **Copy fit**, a default fit name is automatically created in the **Fit name** field. You can specify a new fit name by editing this field.
   - Select the name of the current data set from the **Data set** list. All imported and smoothed data sets are listed.

2. Select an exclusion rule.

   If you want to exclude data from a fit, select an exclusion rule from the **Exclusion rule** list. The list contains only exclusion rules that are compatible with the current data set. An exclusion rule is compatible with the current data set if their lengths are identical, or if it is created by sectioning only.

3. Select a fit type and fit options, fit the data, and evaluate the goodness of fit.
   - The fit type can be a library or custom parametric model, a smoothing spline, or an interpolant.
   - Select fit options such as the fitting algorithm, and coefficient starting points and constraints. Depending on your data and model, accepting the default fit options often produces an excellent fit.
   - Fit the data by clicking the **Apply** button or by selecting the **Immediate apply** check box.
   - Examine the fitted curve, residuals, goodness of fit statistics, confidence bounds, and prediction bounds for the current fit.

4. Compare fits.
   - Compare the current fit and data set to previous fits and data sets by examining the goodness of fit statistics.
   - Use the Table Options GUI to modify which goodness of fit statistics are displayed in the **Table of Fits**. You can sort the table by clicking on any column heading.

5. Save the fit results.

   If the fit is good, save the results as a structure to the MATLAB workspace. Otherwise, modify the fit options or select another model.

Parametric Fitting

Parametric fitting involves finding coefficients (parameters) for one or more models that you fit to data. The data is assumed to be statistical in nature and is divided into two components: a deterministic component and a random component.

data = deterministic component + random component

The deterministic component is given by the fit and the random component is often described as error associated with the data.

data = fit + error

The fit is given by a model that is a function of the independent (predictor) variable and one or more coefficients. The error represents random variations in the data that follow a specific probability distribution (usually Gaussian). The variations can come from many different sources, but are always present at some level when you are dealing with measured data. Systematic variations can also exist, but they can be difficult to quantify.

The fitted coefficients often have physical significance. For example, suppose you have collected data that corresponds to a single decay mode of a radioactive nuclide, and you want to find the half-life ($T_{1/2}$) of the decay. The law of radioactive decay states that the activity of a radioactive substance decays exponentially in time. Therefore, the model to use in the fit is given by

$$y = y_0 e^{-\lambda t}$$

where y_0 is the number of nuclei at time $t = 0$, and λ is the decay constant. Therefore, the data can be described by

$$\text{data} = y_0 e^{-\lambda t} + \text{error}$$

Both y_0 and λ are coefficients determined by the fit. Because $T_{1/2} = \ln(2)/\lambda$, the fitted value of the decay constant yields the half-life. However, because the data contains some error, the deterministic component of the equation cannot completely describe the variability in the data. Therefore, the coefficients and half-life calculation will have some uncertainty associated with them. If the uncertainty is acceptable, then you are done fitting the data. If the uncertainty is not acceptable, then you might have to take steps to reduce the error and repeat the data collection process.

Basic Assumptions About the Error

When fitting data that contains random variations, there are two important assumptions that are usually made about the error:

- The error exists only in the response data, and not in the predictor data.
- The errors are random and follow a normal (Gaussian) distribution with zero mean and constant variance, σ^2.

The second assumption is often expressed as

$$\text{error} \sim N(0, \sigma^2)$$

The components of this expression are described below.

Normal Distribution

The errors are assumed to be normally distributed because the normal distribution often provides an adequate approximation to the distribution of many measured quantities. Although the least squares fitting method does not assume normally distributed errors when calculating parameter estimates, the method works best for data that does not contain a large number of random errors with extreme values. The normal distribution is one of the probability distributions in which extreme random errors are uncommon. However, statistical results such as confidence and prediction bounds do require normally distributed errors for their validity.

Zero Mean

If the mean of the errors is zero, then the errors are purely random. If the mean is not zero, then it might be that the model is not the right choice for your data, or the errors are not purely random and contain systematic errors.

Constant Variance

A constant variance in the data implies that the “spread” of errors is constant. Data that has the same variance is sometimes said to be of equal quality.

The assumption that the random errors have constant variance is not implicit to weighted least squares regression. Instead, it is assumed that the weights provided in the fitting procedure correctly indicate the differing levels of quality present in the data. The weights are then used to adjust the amount of influence each data point has on the estimates of the fitted coefficients to an appropriate level.

The Least Squares Fitting Method

The Curve Fitting Toolbox uses the method of least squares when fitting data. The fitting process requires a model that relates the response data to the predictor data with one or more coefficients. The result of the fitting process is an estimate of the "true" but unknown coefficients of the model.

To obtain the coefficient estimates, the least squares method minimizes the summed square of residuals. The residual for the *i*th data point r_i is defined as the difference between the observed response value y_i and the fitted response value $\hat{y}_i$, and is identified as the error associated with the data.

$$r_i = y_i - \hat{y}_i$$

residual = data – fit

The summed square of residuals is given by

$$S = \sum_{i=1}^{n} r_i^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

where n is the number of data points included in the fit and S is the sum of squares error estimate. The supported types of least squares fitting include

- Linear least squares
- Weighted linear least squares
- Robust least squares
- Nonlinear least squares

Linear Least Squares

The Curve Fitting Toolbox uses the linear least squares method to fit a linear model to data. A linear model is defined as an equation that is linear in the coefficients. For example, polynomials are linear but Gaussians are not. To illustrate the linear least squares fitting process, suppose you have n data points that can be modeled by a first-degree polynomial.

$$y = p_1 x + p_2$$

To solve this equation for the unknown coefficients p_1 and p_2, you write S as a system of n simultaneous linear equations in two unknowns. If n is greater than the number of unknowns, then the system of equations is *overdetermined*.

$$S = \sum_{i=1}^{n} (y_i - (p_1 x_i + p_2))^2$$

Because the least squares fitting process minimizes the summed square of the residuals, the coefficients are determined by differentiating S with respect to each parameter, and setting the result equal to zero.

$$\frac{\partial S}{\partial p_1} = -2 \sum_{i=1}^{n} x_i (y_i - (p_1 x_i + p_2)) = 0$$

$$\frac{\partial S}{\partial p_2} = -2 \sum_{i=1}^{n} (y_i - (p_1 x_i + p_2)) = 0$$

The estimates of the true parameters are usually represented by b. Substituting b_1 and b_2 for p_1 and p_2, the previous equations become

$$\sum x_i (y_i - (b_1 x_i + b_2)) = 0$$

$$\sum (y_i - (b_1 x_i + b_2)) = 0$$

where the summations run from i =1 to n. The *normal equations* are defined as

$$b_1 \sum x_i^2 + b_2 \sum x_i = \sum x_i y_i$$

$$b_1 \sum x_i + n b_2 = \sum y_i$$

Solving for b_1

$$b_1 = \frac{n \sum x_i y_i - \sum x_i \sum y_i}{n \sum x_i^2 - (\sum x_i)^2}$$

Solving for b_2 using the b_1 value

$$b_2 = \frac{1}{n}\left(\sum y_i - b_1 \sum x_i\right)$$

As you can see, estimating the coefficients p_1 and p_2 requires only a few simple calculations. Extending this example to a higher degree polynomial is straightforward although a bit tedious. All that is required is an additional normal equation for each linear term added to the model.

In matrix form, linear models are given by the formula

$$y = X\beta + \varepsilon$$

where

- y is an n-by-1 vector of responses.
- β is a m-by-1 vector of coefficients.
- X is the n-by-m design matrix for the model.
- ε is an n-by-1 vector of errors.

For the first-degree polynomial, the n equations in two unknowns are expressed in terms of y, X, and β as

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ . \\ . \\ . \\ y_n \end{bmatrix} = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ x_3 & 1 \\ . & \\ . & \\ . & \\ x_n & 1 \end{bmatrix} \times \begin{bmatrix} p_1 \\ p_2 \end{bmatrix}$$

The least squares solution to the problem is a vector b, which estimates the unknown vector of coefficients β. The normal equations are given by

$$(X^T X)b = X^T y$$

where X^T is the transpose of the design matrix X. Solving for b,

$$b = (X^T X)^{-1} X^T y$$

In MATLAB, you can use the backslash operator to solve a system of simultaneous linear equations for unknown coefficients. Because inverting $X^T X$ can lead to unacceptable rounding errors, MATLAB uses QR decomposition with pivoting, which is a very stable algorithm numerically. Refer to "Arithmetic Operators" in the MATLAB documentation for more information about the backslash operator and QR decomposition.

You can plug b back into the model formula to get the predicted response values, $\hat{y}$.

$$\hat{y} = Xb = Hy$$
$$H = X(X^T X)^{-1} X^T$$

A hat (circumflex) over a letter denotes an estimate of a parameter or a prediction from a model. The projection matrix H is called the hat matrix, because it puts the hat on y.

The residuals are given by

$$r = y - \hat{y} = (1 - H)y$$

Refer to [1] or [2] for a complete description of the matrix representation of least squares regression.

Weighted Linear Least Squares

As described in "Basic Assumptions About the Error" on page 3-5, it is usually assumed that the response data is of equal quality and, therefore, has constant variance. If this assumption is violated, your fit might be unduly influenced by data of poor quality. To improve the fit, you can use weighted least squares regression where an additional scale factor (the weight) is included in the fitting process. Weighted least squares regression minimizes the error estimate

$$S = \sum_{i=1}^{n} w_i (y_i - \hat{y}_i)^2$$

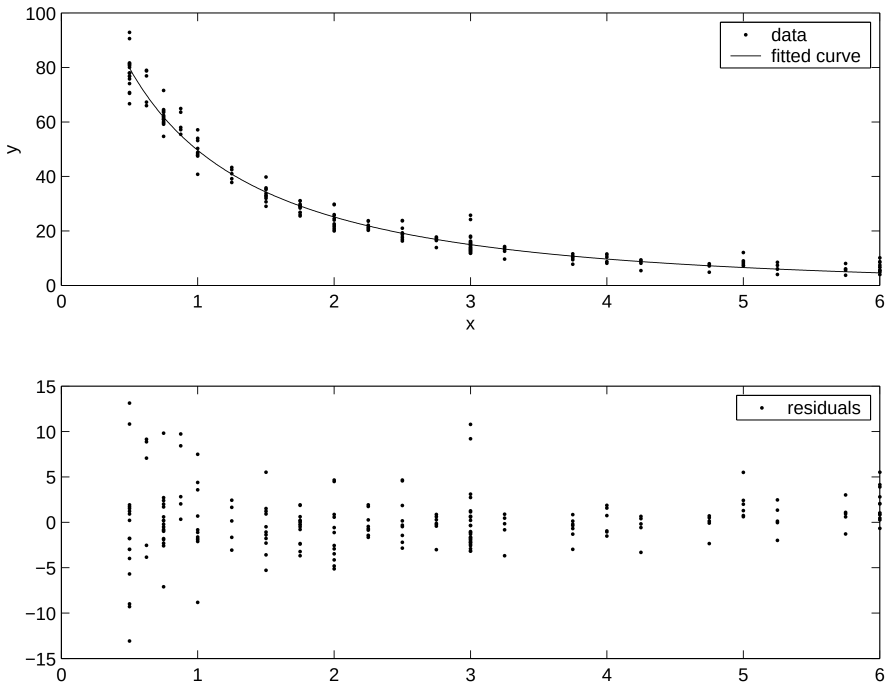
where w_i are the weights. The weights determine how much each response value influences the final parameter estimates. A high-quality data point influences the fit more than a low-quality data point. Weighting your data is recommended if the weights are known, or if there is justification that they follow a particular form.

The weights modify the expression for the parameter estimates b in the following way,

$$b = \hat{\beta} = (X^T W X)^{-1} X^T W y$$

where W is given by the diagonal elements of the weight matrix w.

You can often determine whether the variances are not constant by fitting the data and plotting the residuals. In the plot shown below, the data contains replicate data of various quality and the fit is assumed to be correct. The poor quality data is revealed in the plot of residuals, which has a "funnel" shape where small predictor values yield a bigger scatter in the response values than large predictor values.



The weights you supply should transform the response variances to a constant value. If you know the variances of your data, then the weights are given by

$$w_i = 1/\sigma^2$$

If you don't know the variances, you can approximate the weights using an equation such as

$$w_i = \left(\frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})^2\right)^{-1}$$

This equation works well if your data set contains replicates. In this case, n is the number of sets of replicates. However, the weights can vary greatly. A better approach might be to plot the variances and fit the data using a sensible model. The form of the model is not very important — a polynomial or power function works well in many cases.

Robust Least Squares

As described in "Basic Assumptions About the Error" on page 3-5, it is usually assumed that the response errors follow a normal distribution, and that extreme values are rare. Still, extreme values called *outliers* do occur.

The main disadvantage of least squares fitting is its sensitivity to outliers. Outliers have a large influence on the fit because squaring the residuals magnifies the effects of these extreme data points. To minimize the influence of outliers, you can fit your data using robust least squares regression. The toolbox provides these two robust regression schemes:

- Least absolute residuals (LAR) — The LAR scheme finds a curve that minimizes the absolute difference of the residuals, rather than the squared differences. Therefore, extreme values have a lesser influence on the fit.
- Bisquare weights — This scheme minimizes a weighted sum of squares, where the weight given to each data point depends on how far the point is from the fitted line. Points near the line get full weight. Points farther from

the line get reduced weight. Points that are farther from the line than would be expected by random chance get zero weight.

For most cases, the bisquare weight scheme is preferred over LAR because it simultaneously seeks to find a curve that fits the bulk of the data using the usual least squares approach, and it minimizes the effect of outliers.

Robust fitting with bisquare weights uses an iteratively reweighted least squares algorithm, and follows this procedure:

1 Fit the model by weighted least squares.

2 Compute the *adjusted residuals* and standardize them. The adjusted residuals are given by

$$r_{adj} = \frac{r_i}{\sqrt{1-h_i}}$$

r_i are the usual least squares residuals and h_i are *leverages* that adjust the residuals by downweighting high-leverage data points, which have a large effect on the least squares fit. The standardized adjusted residuals are given by

$$u = \frac{r_{adj}}{Ks}$$

K is a tuning constant equal to 4.685, and s is the robust variance given by $MAD/0.6745$ where MAD is the median absolute deviation of the residuals. Refer to [7] for a detailed description of h, K, and s.

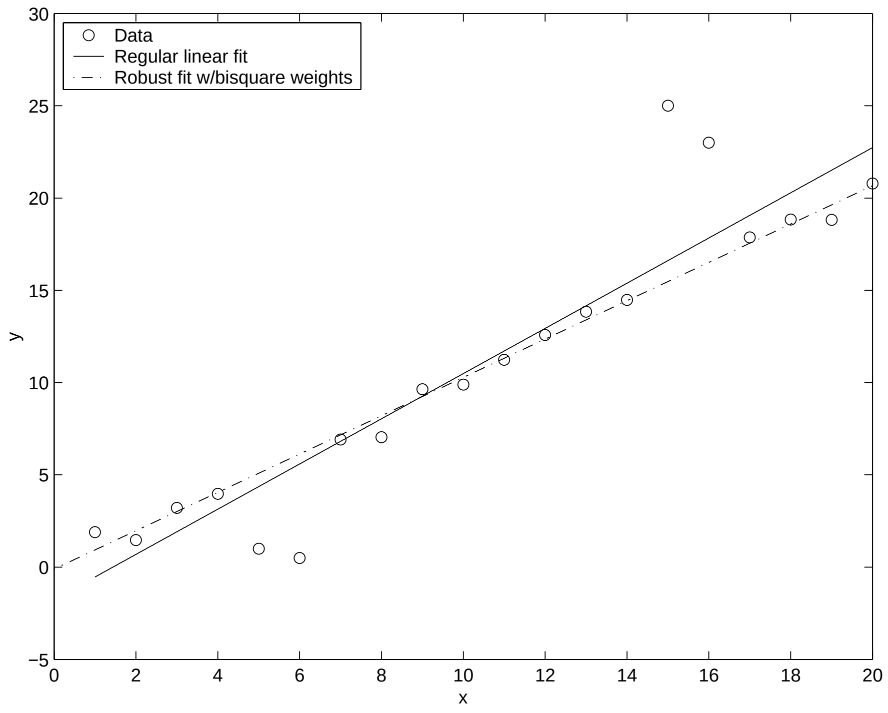
3 Compute the robust weights as a function of u. The bisquare weights are given by

$$w_i = \begin{cases} (1-(u_i)^2)^2 & |u_i| < 1 \\ 0 & |u_i| \ge 1 \end{cases}$$

Note that if you supply your own regression weight vector, the final weight is the product of the robust weight and the regression weight.

4 If the fit converges, then you are done. Otherwise, perform the next iteration of the fitting procedure by returning to the first step.

The plot shown below compares a regular linear fit with a robust fit using bisquare weights. Notice that the robust fit follows the bulk of the data and is not strongly influenced by the outliers.



Instead of minimizing the effects of outliers by using robust regression, you can mark data points to be excluded from the fit. Refer to “Excluding and Sectioning Data” on page 2-25 for more information.

Nonlinear Least Squares

The Curve Fitting Toolbox uses the nonlinear least squares formulation to fit a nonlinear model to data. A nonlinear model is defined as an equation that is nonlinear in the coefficients, or a combination of linear and nonlinear in the coefficients. For example, Gaussians, ratios of polynomials, and power functions are all nonlinear.

In matrix form, nonlinear models are given by the formula

$$y = f(X, \beta) + \varepsilon$$

where

- y is an n-by-1 vector of responses.
- f is a function of β and X.
- β is a m-by-1 vector of coefficients.
- X is the n-by-m design matrix for the model.
- ε is an n-by-1 vector of errors.

Nonlinear models are more difficult to fit than linear models because the coefficients cannot be estimated using simple matrix techniques. Instead, an iterative approach is required that follows these steps:

1. Start with an initial estimate for each coefficient. For some nonlinear models, a heuristic approach is provided that produces reasonable starting values. For other models, random values on the interval [0,1] are provided.

2. Produce the fitted curve for the current set of coefficients. The fitted response value $\hat{y}$ is given by

   $$\hat{y} = f(X, b)$$

   and involves the calculation of the *Jacobian* of $f(X,b)$, which is defined as a matrix of partial derivatives taken with respect to the coefficients.

3. Adjust the coefficients and determine whether the fit improves. The direction and magnitude of the adjustment depend on the fitting algorithm. The toolbox provides these algorithms:
   - Trust-region — This is the default algorithm and must be used if you specify coefficient constraints. It can solve difficult nonlinear problems more efficiently than the other algorithms and it represents an improvement over the popular Levenberg-Marquardt algorithm.
   - Levenberg-Marquardt — This algorithm has been used for many years and has proved to work most of the time for a wide range of nonlinear models and starting values. If the trust-region algorithm does not produce a reasonable fit, and you do not have coefficient constraints, you should try the Levenberg-Marquardt algorithm.
   - Gauss-Newton — This algorithm is potentially faster than the other algorithms, but it assumes that the residuals are close to zero. It's included with the toolbox for pedagogical reasons and should be the last choice for most models and data sets.

   For more information about the trust region algorithm, refer to [4] and to "Trust Region Methods for Nonlinear Minimization" in the Optimization Toolbox documentation. For more information about the Levenberg-Marquardt and Gauss-Newton algorithms, refer to "Nonlinear Least Squares Implementation" in the same guide. Additionally, the Levenberg-Marquardt algorithm is described in [5] and [6].

4. Iterate the process by returning to step 2 until the fit reaches the specified convergence criteria.

You can use weights and robust fitting for nonlinear models, and the fitting process is modified accordingly.

Because of the nature of the approximation process, no algorithm is foolproof for all nonlinear models, data sets, and starting points. Therefore, if you do not achieve a reasonable fit using the default starting points, algorithm, and convergence criteria, you should experiment with different options. Refer to "Specifying Fit Options" on page 3-23 for a description of how to modify the default options. Because nonlinear models can be particularly sensitive to the starting points, this should be the first fit option you modify.

Library Models

The parametric library models provided by the Curve Fitting Toolbox are described below.

Exponentials

The toolbox provides a one-term and a two-term exponential model.

$$y = ae^{bx}$$

$$y = ae^{bx} + ce^{dx}$$

Exponentials are often used when the rate of change of a quantity is proportional to the initial amount of the quantity. If the coefficient associated with e is negative, y represents exponential decay. If the coefficient is positive, y represents exponential growth.

For example, a single radioactive decay mode of a nuclide is described by a one-term exponential. a is interpreted as the initial number of nuclei, b is the decay constant, x is time, and y is the number of remaining nuclei after a specific amount of time passes. If two decay modes exist, then you must use the two-term exponential model. For each additional decay mode, you add another exponential term to the model.

Examples of exponential growth include contagious diseases for which a cure is unavailable, and biological populations whose growth is uninhibited by predation, environmental factors, and so on.

Fourier Series

The Fourier series is a sum of sine and cosine functions that is used to describe a periodic signal. It is represented in either the trigonometric form or the exponential form. The toolbox provides the trigonometric Fourier series form shown below,

$$y = a_0 + \sum_{i=1}^{n} a_i \cos(nwx) + b_i \sin(nwx)$$

where a_0 models any DC offset in the signal and is associated with the $i = 0$ cosine term, w is the fundamental frequency of the signal, n is the number of terms (harmonics) in the series, and $1 \le n \le 8$.

For more information about the Fourier series, refer to “Fourier Analysis and the Fast Fourier Transform” in the MATLAB documentation. For an example that fits the ENSO data to a custom Fourier series model, refer to “General Equation: Fourier Series Fit” on page 3-52.

Gaussian

The Gaussian model is used for fitting peaks, and is given by the equation

$$y = \sum_{i=1}^{n} a_i e^{\left[-\left(\frac{x-b_i}{c_i}\right)^2\right]}$$

where a is the amplitude, b is the centroid (location), c is related to the peak width, n is the number of peaks to fit, and $1 \le n \le 8$.

Gaussian peaks are encountered in many areas of science and engineering. For example, line emission spectra and chemical concentration assays can be described by Gaussian peaks. For an example that fits two Gaussian peaks and an exponential background, refer to “General Equation: Gaussian Fit with Exponential Background” on page 3-57.

Polynomials

Polynomial models are given by

$$y = \sum_{i=1}^{n+1} p_i x^{n+1-i}$$

where $n + 1$ is the *order* of the polynomial, n is the *degree* of the polynomial, and $1 \le n \le 9$. The order gives the number of coefficients to be fit, and the degree gives the highest power of the predictor variable.

In this guide, polynomials are described in terms of their degree. For example, a third-degree (cubic) polynomial is given by

$$y = p_1 x^3 + p_2 x^2 + p_3 x + p_4$$

Polynomials are often used when a simple empirical model is required. The model can be used for interpolation or extrapolation, or it can be used to characterize data using a global fit. For example, the temperature-to-voltage conversion for a Type J thermocouple in the 0^o to 760^o temperature range is described by a seventh-degree polynomial.

Note If you do not require a global parametric fit and want to maximize the flexibility of the fit, piecewise polynomials might provide the best approach. Refer to “Nonparametric Fitting” on page 3-68 for more information.

The main advantages of polynomial fits include reasonable flexibility for data that is not too complicated, and they are linear, which means the fitting process is simple. The main disadvantage is that high-degree fits can become unstable. Additionally, polynomials of any degree can provide a good fit within the data range, but can diverge wildly outside that range. Therefore, you should exercise caution when extrapolating with polynomials. Refer to “Determining the Best Fit” on page 1-10 for examples of good and poor polynomial fits to census data.

Note that when you fit with high-degree polynomials, the fitting procedure uses the predictor values as the basis for a matrix with very large values, which can result in scaling problems. To deal with this, you should normalize the data by centering it at zero mean and scaling it to unit standard deviation. You normalize data by selecting the **Center and scale X data** check box on the Fitting GUI.

Power Series

The toolbox provides a one-term and a two-term power series model.

$$y = ax^b$$

$$y = a + bx^c$$

Power series models are used to describe a variety of data. For example, the rate at which reactants are consumed in a chemical reaction is generally proportional to the concentration of the reactant raised to some power.

Rationals

Rational models are defined as ratios of polynomials and are given by

$$y = \frac{\sum_{i=1}^{n+1} p_i x^{n+1-i}}{x^m + \sum_{i=1}^{m} q_i x^{m-i}}$$

where n is the degree of the numerator polynomial and $0 \le n \le 5$, while m is the degree of the denominator polynomial and $1 \le m \le 5$. Note that the coefficient associated with x^m is always 1. This makes the numerator and denominator unique when the polynomial degrees are the same.

In this guide, rationals are described in terms of the degree of the numerator/the degree of the denominator. For example, a quadratic/cubic rational equation is given by

$$y = \frac{p_1 x^2 + p_2 x + p_3}{x^3 + q_1 x^2 + q_2 x + q_3}$$

Like polynomials, rationals are often used when a simple empirical model is required. The main advantage of rationals is their flexibility with data that has complicated structure. The main disadvantage is that they become unstable when the denominator is around zero. For an example that uses rational polynomials of various degrees, refer to “Example: Rational Fit” on page 3-41.

Sum of Sines

The sum of sines model is used for fitting periodic functions, and is given by the equation

$$y = \sum_{i=1}^{n} a_i \sin(b_i x + c_i)$$

where a is the amplitude, b is the frequency, and c is the phase constant for each sine wave term. n is the number of terms in the series and $1 \le n \le 8$. This equation is closely related to the Fourier series described previously. The main difference is that the sum of sines equation includes the phase constant, and does not include a DC offset term.

Weibull Distribution

The Weibull distribution is widely used in reliability and life (failure rate) data analysis. The toolbox provides the two-parameter Weibull distribution

$$y = abx^{b-1}e^{-ax^b}$$

where a is the scale parameter and b is the shape parameter. Note that there is also a three-parameter Weibull distribution with x replaced by $x - c$ where c is the location parameter. Additionally, there is a one-parameter Weibull distribution where the shape parameter is fixed and only the scale parameter is fitted. To use these distributions, you must create a custom equation.

Note that the Curve Fitting Toolbox does not fit Weibull probability distributions to a sample of data. Instead, it fits curves to response and predictor data such that the curve has the same shape as a Weibull distribution.

Custom Equations

If the toolbox library does not contain the desired parametric equation, you must create your own custom equation. However, if possible, you should use the library equations because they offer the best chance for rapid convergence. This is because

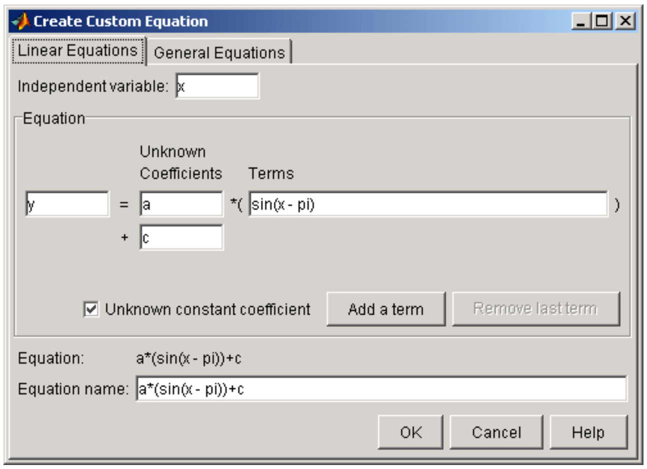
- For most models, optimal default coefficient starting points are calculated. For custom equations, the default starting points are chosen at random on the interval [0,1]. Refer to “Default Coefficient Parameters” on page 3-26 for more information.
- An analytic Jacobian is used instead of finite differencing.
- When using the Analysis GUI, analytic derivatives are calculated as well as analytic integrals if the integral can be expressed in closed form.

Note To save custom equations for later use, you should save the curve-fitting session with the **File-> Save Session** menu item.

You create custom equations with the Create Custom Equation GUI. The GUI contains two panes: a pane for creating linear equations and a pane for creating general (nonlinear) equations. These panes are described below.

Linear Equations

Linear equations are defined as equations that are linear in the parameters. For example, the polynomial library equations are linear. The Linear Equations pane is shown below followed by a description of its parameters.



Independent variable: x

y = a *(sin(x - pi))

+ c

☑ Unknown constant coefficient

Equation: a*(sin(x - pi))+c

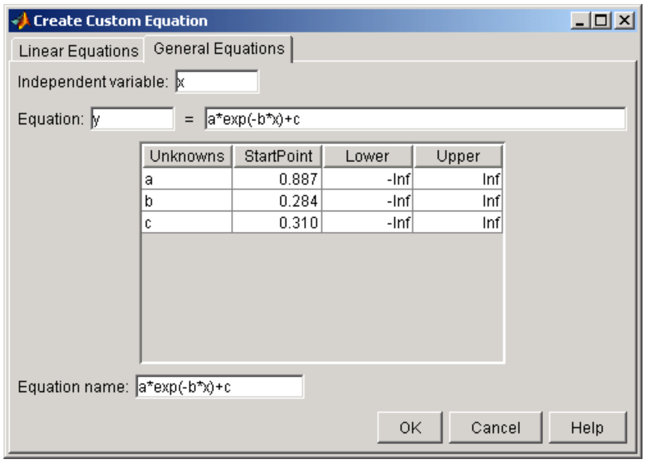
Equation name: a*(sin(x - pi))+c

- **Independent variable** — Symbol representing the independent (predictor) variable. The default symbol is x.
- **Equation** — Symbol representing the dependent (response) variable followed by the linear equation. The default symbol is y.
  - **Unknown Coefficients** — The unknown coefficients to be determined by the fit. The default symbols are a, b, c, and so on.
  - **Terms** — Functions that depend only on the independent variable and constants. Note that if you attempt to define a term that contains a coefficient to be fitted, an error is returned.
  - **Unknown constant coefficient** — If selected, a constant term is included in the equations to be fit. Otherwise, a constant term is not included.
  - **Add a term** — Add a term to the equation. An unknown coefficient is automatically added for each new term.
  - **Remove last term** — Remove the last term added to the equation.

- **Equation** — The custom equation.
- **Equation name** — The name of the equation. By default, the name is automatically updated to be identical to the custom equation given by **Equation**. If you override the default, the name is no longer automatically updated.

General Equations

General (nonlinear) equations are defined as equations that are nonlinear in the parameters, or are a combination of linear and nonlinear in the parameters. For example, the exponential library equations are nonlinear. The General Equations pane is shown below followed by a brief description of its parameters.



Independent variable: x

Equation: y = a*exp(-b*x)+c

Unknowns	StartPoint	Lower	Upper
a	0.887	-Inf	Inf
b	0.284	-Inf	Inf
c	0.310	-Inf	Inf

Equation name: a*exp(-b*x)+c

- **Independent variable** — Symbol representing the independent (predictor) variable. The default symbol is x.
- **Equation** — Symbol representing the dependent (response) variable followed by the general equation. As you type in the terms of the equation, the unknown coefficients, associated starting values, and constraints automatically populate the table. By default, the starting values are randomly selected on the interval [0,1] and are unconstrained.

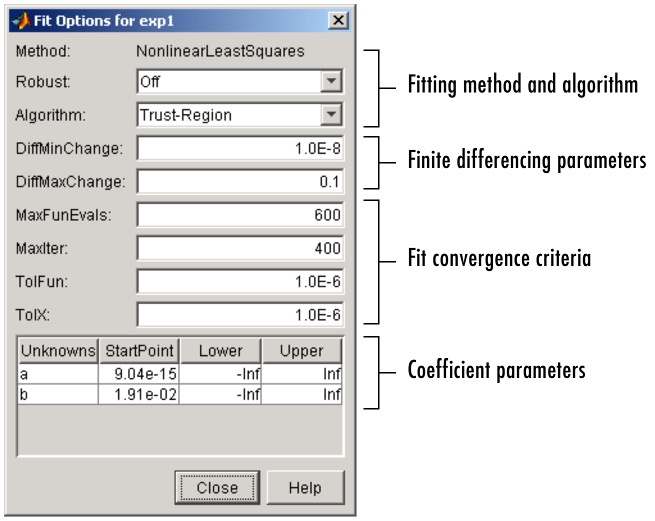
  You can immediately change the default starting values and constraints in this table, or you can change them later using the Fit Options GUI.

- **Equation name** — The name of the equation. By default, the name is automatically updated to be identical to the custom equation given by **Equation**. If you override the default, the name is no longer automatically updated.

Note that even if you define a linear equation, a nonlinear fitting procedure is used. Although this is allowed by the toolbox, it is an inefficient process and can result in less than optimal fitted coefficients. Instead, you should use the **Linear Equations** pane to define the equation.

Specifying Fit Options

You specify fit options with the Fit Options GUI. The fit options for the single-term exponential are shown below. The coefficient starting values and constraints are for the census data.



Method:	NonlinearLeastSquares
Robust:	Off
Algorithm:	Trust-Region
DiffMinChange:	1.0E-8
DiffMaxChange:	0.1
MaxFunEvals:	600
MaxIter:	400
TolFun:	1.0E-6
TolX:	1.0E-6

Unknowns	StartPoint	Lower	Upper
a	9.04e-15	-Inf	Inf
b	1.91e-02	-Inf	Inf

The available GUI options depend on whether you are fitting your data using a linear model, a nonlinear model, or a nonparametric fit type. All the options described below are available for nonlinear models. **Method**, **Robust**, and coefficient constraints (**Lower** and **Upper**) are available for linear models. Interpolants and smoothing splines include **Method**, but no configurable options.

Fitting Method and Algorithm

- **Method** — The fitting method.

  The method is automatically selected based on the library or custom model you use. For linear models, the method is **LinearLeastSquares**. For nonlinear models, the method is **NonlinearLeastSquares**.
- **Robust** — Specify whether to use the robust least squares fitting method. The values are
  - **Off** — Do not use robust fitting (default).
  - **On** — Fit with default robust method (bisquare weights).
  - **LAR** — Fit by minimizing the least absolute residuals (LAR).
  - **Bisquare** — Fit by minimizing the summed square of the residuals, and downweight outliers using bisquare weights. In most cases, this is the best choice for robust fitting.
- **Algorithm** — Algorithm used for the fitting procedure:
  - **Trust-Region** — This is the default algorithm and must be used if you specify coefficient constraints.
  - **Levenberg-Marquardt** — If the trust-region algorithm does not produce a reasonable fit, and you do not have coefficient constraints, you should try the Levenberg-Marquardt algorithm.
  - **Gauss-Newton** — This algorithm is included for pedagogical reasons and should be the last choice for most models and data sets.

Finite Differencing Parameters

- **DiffMinChange** — Minimum change in coefficients for finite difference Jacobians. The default value is 10^{-8}.
- **DiffMaxChange** — Maximum change in coefficients for finite difference Jacobians. The default value is 0.1.

Fit Convergence Criteria

- **MaxFunEvals** — Maximum number of function (model) evaluations allowed. The default value is 600.
- **MaxIter** — Maximum number of fit iterations allowed. The default value is 400.

- **TolFun** — Termination tolerance used on stopping conditions involving the function (model) value. The default value is 10^{-6}.
- **TolX** — Termination tolerance used on stopping conditions involving the coefficients. The default value is 10^{-6}.

Coefficient Parameters

- **Unknowns** — Symbols for the unknown coefficients to be fitted.
- **StartPoint** — The coefficient starting values. The default values depend on the model. For rational, Weibull, and custom models, default values are randomly selected within the range [0,1]. For all other nonlinear library models, the starting values depend on the data set and are calculated heuristically.
- **Lower** — Lower bounds on the fitted coefficients. The bounds are used only with the trust region fitting algorithm. The default lower bounds for most library models are `-Inf`, which indicates that the coefficients are unconstrained. However, a few models have finite default lower bounds. For example, Gaussians have the width parameter constrained so that it cannot be less than 0.
- **Upper** — Upper bounds on the fitted coefficients. The bounds are used only with the trust region fitting algorithm. The default upper bounds for all library models are `Inf`, which indicates that the coefficients are unconstrained.

For more information about these fit options, refer to "Optimization Options Parameters" in the Optimization Toolbox documentation.

Default Coefficient Parameters

The default coefficient starting points and constraints for library and custom models are given below. If the starting points are optimized, then they are calculated heuristically based on the current data set. Random starting points are defined on the interval [0,1] and linear models do not require starting points.

If a model does not have constraints, the coefficients have neither a lower bound nor an upper bound. You can override the default starting points and constraints by providing your own values using the Fit Options GUI.

Table 3-1: Default Starting Points and Constraints

Model	Starting Points	Constraints
Custom linear	N/A	None
Custom nonlinear	Random	None
Exponentials	Optimized	None
Fourier series	Optimized	None
Gaussians	Optimized	$c_i > 0$
Polynomials	N/A	None
Power series	Optimized	None
Rationals	Random	None
Sum of sines	Optimized	$b_i > 0$
Weibull	Random	$a, b > 0$

Note that the sum of sines and Fourier series models are particularly sensitive to starting points, and the optimized values might be accurate for only a few terms in the associated equations. For an example that overrides the default starting values for the sum of sines model, refer to “Example: Sectioning Periodic Data” on page 2-35.

Evaluating the Goodness of Fit

After fitting data with one or more models, you should evaluate the goodness of fit. A visual examination of the fitted curve displayed in the Curve Fitting Tool should be your first step. Beyond that, the toolbox provides these goodness of fit measures for both linear and nonlinear parametric fits:

- Residuals
- Goodness of fit statistics
- Confidence and prediction bounds

You can group these measures into two types: graphical and numerical. The residuals and prediction bounds are graphical measures, while the goodness of fit statistics and confidence bounds are numerical measures.

Generally speaking, graphical measures are more beneficial than numerical measures because they allow you to view the entire data set at once, and they can easily display a wide range of relationships between the model and the data. The numerical measures are more narrowly focused on a particular aspect of the data and often try to compress that information into a single number. In practice, depending on your data and analysis requirements, you might need to use both types to determine the best fit.

Note that it is possible that none of your fits can be considered the best one. In this case, it might be that you need to select a different model. Conversely, it is also possible that all the goodness of fit measures indicate that a particular fit is the best one. However, if your goal is to extract fitted coefficients that have physical meaning, but your model does not reflect the physics of the data, the resulting coefficients are useless. In this case, understanding what your data represents and how it was measured is just as important as evaluating the goodness of fit.

Residuals

The residuals from a fitted model are defined as the differences between the response data and the fit to the response data at each predictor value.

residual = data - fit

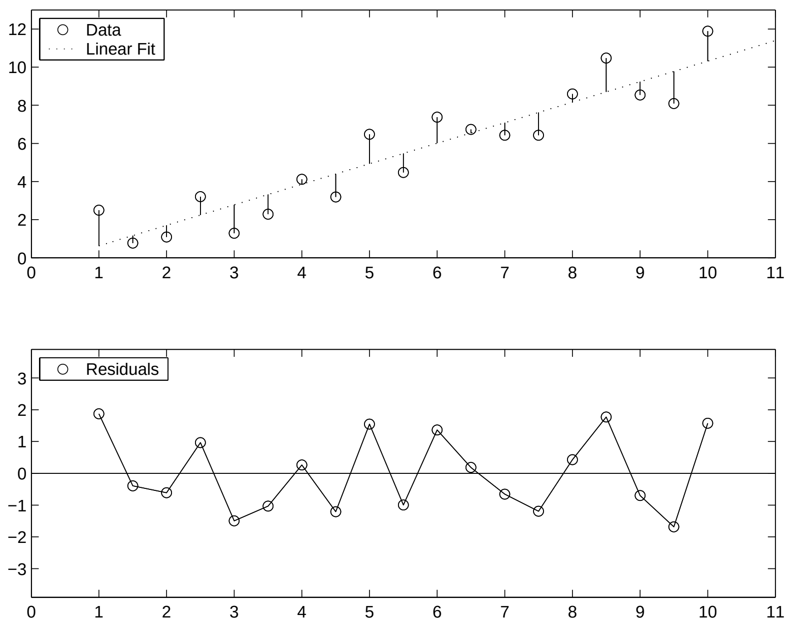
You display the residuals in the Curve Fitting Tool by selecting the menu item **View->Residuals**.

Mathematically, the residual for a specific predictor value is the difference between the response value y and the predicted response value $\hat{y}$.

$$r = y - \hat{y}$$

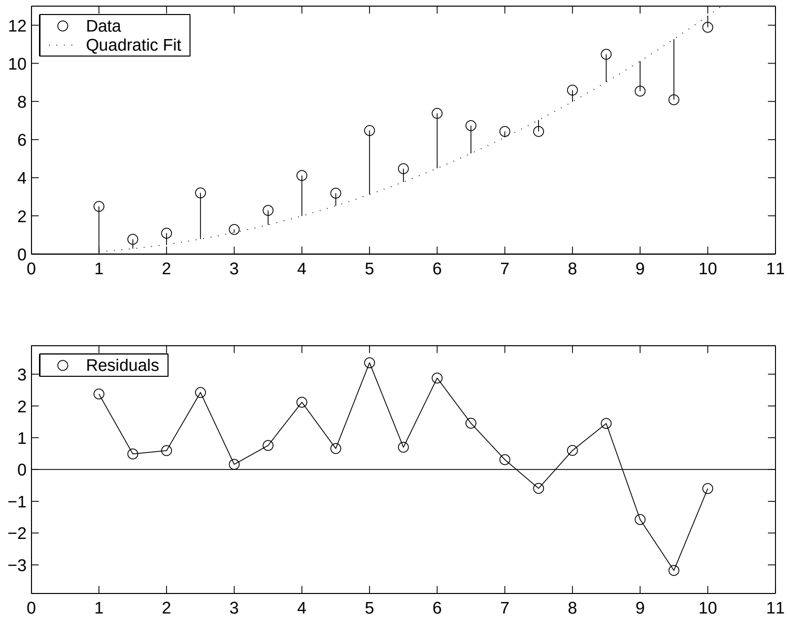
Assuming the model you fit to the data is correct, the residuals approximate the random errors. Therefore, if the residuals appear to behave randomly, it suggests that the model fits the data well. However, if the residuals display a systematic pattern, it is a clear sign that the model fits the data poorly.

A graphical display of the residuals for a first degree polynomial fit is shown below. The top plot shows that the residuals are calculated as the vertical distance from the data point to the fitted curve. The bottom plot shows that the residuals are displayed relative to the fit, which is the zero line.



The residuals appear randomly scattered around zero indicating that the model describes the data well.

A graphical display of the residuals for a second-degree polynomial fit is shown below. The model includes only the quadratic term, and does not include a linear or constant term.



The residuals are systematically positive for much of the data range indicating that this model is a poor fit for the data.

Goodness of Fit Statistics

After using graphical methods to evaluate the goodness of fit, you should examine the goodness of fit statistics. The Curve Fitting Toolbox supports these goodness of fit statistics for parametric models:

- The sum of squares due to error (SSE)
- R-square
- Adjusted R-square
- Root mean squared error (RMSE)

For the current fit, these statistics are displayed in the **Results** list box in the **Fit Editor**. For all fits in the current curve-fitting session, you can compare the goodness of fit statistics in the **Table of fits**.

Sum of Squares Due to Error. This statistic measures the total deviation of the response values from the fit to the response values. It is also called the summed square of residuals and is usually labeled as *SSE*.

$$SSE = \sum_{i=1}^{n} w_i(y_i - \hat{y}_i)^2$$

A value closer to 0 indicates a better fit. Note that the *SSE* was previously defined in "The Least Squares Fitting Method" on page 3-6.

R-Square. This statistic measures how successful the fit is in explaining the variation of the data. Put another way, R-square is the square of the correlation between the response values and the predicted response values. It is also called the square of the multiple correlation coefficient and the coefficient of multiple determination.

R-square is defined as the ratio of the sum of squares of the regression (*SSR*) and the total sum of squares (*SST*). *SSR* is defined as

$$SSR = \sum_{i=1}^{n} w_i(\hat{y}_i - \bar{y})^2$$

SST is also called the sum of squares about the mean, and is defined as

$$SST = \sum_{i=1}^{n} w_i(y_i - \bar{y})^2$$

where $SST = SSR + SSE$. Given these definitions, R-square is expressed as

$$\text{R-square} = \frac{SSR}{SST} = 1 - \frac{SSE}{SST}$$

R-square can take on any value between 0 and 1, with a value closer to 1 indicating a better fit. For example, an R^2 value of 0.8234 means that the fit explains 82.34% of the total variation in the data about the average.

If you increase the number of fitted coefficients in your model, R-square might increase although the fit may not improve. To avoid this situation, you should use the degrees of freedom adjusted R-square statistic described below.

Note that it is possible to get a negative R-square for equations that do not contain a constant term. If R-square is defined as the proportion of variance explained by the fit, and if the fit is actually worse than just fitting a horizontal line, then R-square is negative. In this case, R-square cannot be interpreted as the square of a correlation.

Degrees of Freedom Adjusted R-Square. This statistic uses the R-square statistic defined above, and adjusts it based on the residual degrees of freedom. The residual degrees of freedom is defined as the number of response values n minus the number of fitted coefficients m estimated from the response values.

$$v = n - m$$

v indicates the number of independent pieces of information involving the n data points that are required to calculate the sum of squares. Note that if parameters are bounded and one or more of the estimates are at their bounds, then those estimates are regarded as fixed. The degrees of freedom is increased by the number of such parameters.

The adjusted R-square statistic is generally the best indicator of the fit quality when you add additional coefficients to your model.

$$\text{adjusted R-square} = 1 - \frac{SSE(n-1)}{SST(v)}$$

The adjusted R-square statistic can take on any value less than or equal to 1, with a value closer to 1 indicating a better fit.

Root Mean Squared Error. This statistic is also known as the fit standard error and the standard error of the regression

$$RMSE = s = \sqrt{MSE}$$

where MSE is the mean square error or the residual mean square

$$MSE = \frac{SSE}{v}$$

A $RMSE$ value closer to 0 indicates a better fit.

Confidence and Prediction Bounds

With the Curve Fitting Toolbox, you can calculate confidence bounds for the fitted coefficients, and prediction bounds for new observations or for the fitted function. Additionally, for prediction bounds, you can calculate simultaneous bounds, which take into account all predictor values, or you can calculate nonsimultaneous bounds, which take into account only individual predictor values. The confidence bounds are numerical, while the prediction bounds are displayed graphically.

The available confidence and prediction bounds are summarized below.

Table 3-2: Types of Confidence and Prediction Bounds

Interval Type	Description
Fitted coefficients	Confidence bounds for the fitted coefficients
New observation	Prediction bounds for a new observation (response value)
New function	Prediction bounds for a new function value

Note Prediction bounds are often described as confidence bounds because you are calculating a confidence interval for a predicted response.

Confidence and prediction bounds define the lower and upper values of the associated interval, and define the width of the interval. The width of the interval indicates how uncertain you are about the fitted coefficients, the predicted observation, or the predicted fit. For example, a very wide interval for the fitted coefficients can indicate that you should use more data when fitting before you can say anything very definite about the coefficients.

The bounds are defined with a level of certainty that you specify. The level of certainty is often 95%, but it can be any value such as 90%, 99%, 99.9%, and so on. For example, you might want to take a 5% chance of being incorrect about predicting a new observation. Therefore, you would calculate a 95% prediction interval. This interval indicates that you have a 95% chance that the new observation is actually contained within the lower and upper prediction bounds.

Calculating and Displaying Confidence Bounds. The confidence bounds for fitted coefficients are given by

$$C = b \pm t\sqrt{S}$$

where b are the coefficients produced by the fit, t is the inverse of Student's T cumulative distribution function, and S is a vector of the diagonal elements from the covariance matrix of the coefficient estimates, $(X^T X)^{-1} s^2$. X is the design matrix, X^T is the transpose of X, and s^2 is the mean squared error.

Refer to the `tinv` function, included with the Statistics Toolbox, for a description of t. Refer to "Linear Least Squares" on page 3-6 for more information about X and X^T.

The confidence bounds are displayed in the **Results** list box in the **Fit Editor** using the following format.

```
p1 = 1.275  (1.113, 1.437)
```

The fitted value for the coefficient `p1` is 1.275, the lower bound is 1.113, the upper bound is 1.437, and the interval width is 0.324. By default, the confidence level for the bounds is 95%. You can change this level to any value with the **View->Confidence Level** menu item in the Curve Fitting Tool.

You can calculate confidence intervals at the command line with the `confint` function.

Calculating and Displaying Prediction Bounds. As mentioned previously, you can calculate prediction bounds for a new observation or for the fitted curve. In both cases, the prediction is based on an existing fit to the data. Additionally, the bounds can be simultaneous and measure the confidence for all predictor values, or they can be nonsimultaneous and measure the confidence only for a single predetermined predictor value. If you are predicting a new observation, nonsimultaneous bounds measure the confidence that the new observation lies within the interval given a single predictor value. Simultaneous bounds measure the confidence that a new observation lies within the interval regardless of the predictor value.

The nonsimultaneous prediction bounds for a new observation at the predictor value x are given by

$$P_{n,o} = \hat{y} \pm t\sqrt{s^2 + xSx'}$$

where s^2 is the mean squared error, t is the inverse of Student's T cumulative distribution function, and S is the covariance matrix of the coefficient estimates, $(X^TX)^{-1}s^2$. Note that x is defined as a row vector of the Jacobian evaluated at a specified predictor value.

The simultaneous prediction bounds for a new observation and for all predictor values are given by

$$P_{s,o} = \hat{y} \pm f\sqrt{s^2 + xSx'}$$

where f is the inverse of the F cumulative distribution function. Refer to the `finv` function, included with the Statistics Toolbox, for a description of f.

The nonsimultaneous prediction bounds for the function at a single predictor value x are given by

$$P_{n,f} = \hat{y} \pm t\sqrt{xSx'}$$

The simultaneous prediction bounds for the function and for all predictor values are given by

$$P_{s,f} = \hat{y} \pm f\sqrt{xSx'}$$

You can graphically display prediction bounds two ways: using the Curve Fitting Tool or using the Analysis GUI. With the Curve Fitting Tool, you can display nonsimultaneous prediction bounds for new observations with **View->Prediction Bounds**. By default, the confidence level for the bounds is 95%. You can change this level to any value with **View->Confidence Level**. With the Analysis GUI, you can display nonsimultaneous prediction bounds for the function or for new observations.

You can display numerical prediction bounds of any type at the command line with the `predint` function.

To understand the quantities associated with each type of prediction interval, recall that the data, fit, and residuals (random errors) are related through the formula

data = fit + residuals

Suppose you plan to take a new observation at the predictor value x_{n+1}. Call the new observation $y_{n+1}(x_{n+1})$ and the associated error e_{n+1}. Then $y_{n+1}(x_{n+1})$ satisfies the equation

$$y_{n+1}(x_{n+1}) = f(x_{n+1}) + e_{n+1}$$

where $f(x_{n+1})$ is the true but unknown function you want to estimate at x_{n+1}. The likely values for the new observation or for the estimated function are provided by the nonsimultaneous prediction bounds.

If instead you want the likely value of the new observation to be associated with any predictor value, the previous equation becomes

$$y_{n+1}(x) = f(x) + e$$

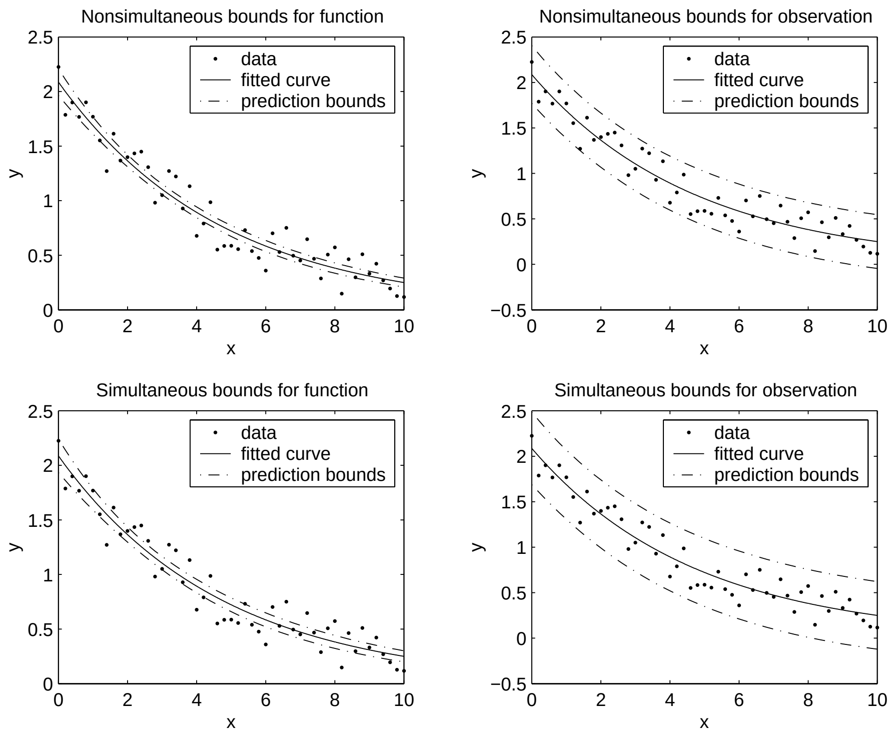
The likely values for this new observation or for the estimated function are provided by the simultaneous prediction bounds.

The types of prediction bounds are summarized below.

Table 3-3: Types of Prediction Bounds

Type of Bound		**Associated Equation**
Observation	Nonsimultaneous	$y_{n+1}(x_{n+1})$
	Simultaneous	$y_{n+1}(x)$, globally for any x
Function	Nonsimultaneous	$f(x_{n+1})$
	Simultaneous	$f(x)$, simultaneously for all x

The nonsimultaneous and simultaneous prediction bounds for a new observation and the fitted function are shown below. Each graph contains three curves: the fit, the lower confidence bounds, and the upper confidence bounds. The fit is a single-term exponential to generated data and the bounds reflect a 95% confidence level. Note that the intervals associated with a new observation are wider than the fitted function intervals because of the additional uncertainty in predicting a new response value (the fit plus random errors).

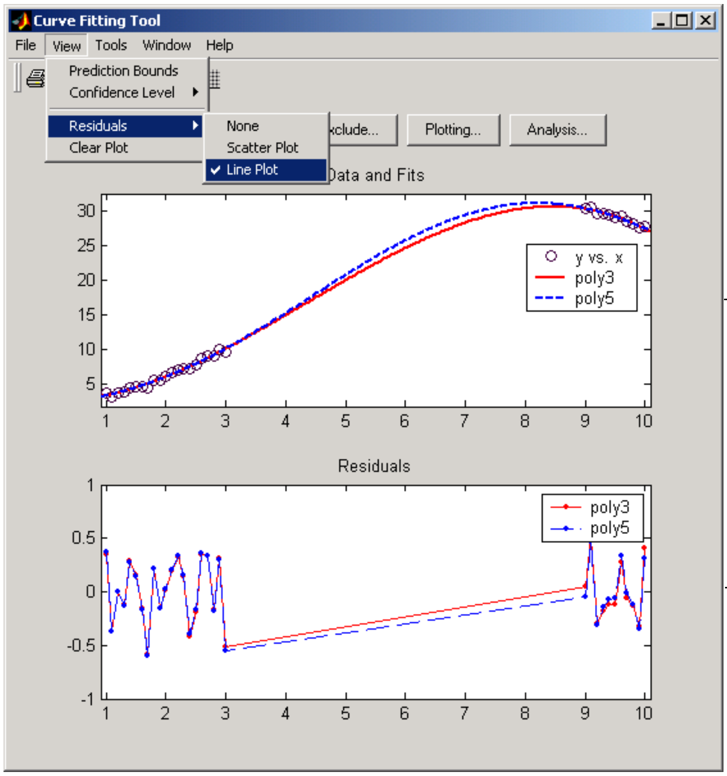


Example: Evaluating the Goodness of Fit

This example fits several polynomial models to generated data and evaluates the goodness of fit. The data is cubic and includes a range of missing values.

```
rand('state',0)
x = [1:0.1:3 9:0.1:10]';
c = [2.5 -0.5 1.3 -0.1];
y =  c(1) + c(2)*x + c(3)*x.^2 + c(4)*x.^3 + (rand(size(x))-0.5);
```

After you import the data, fit it using a cubic polynomial and a fifth degree polynomial. The data, fits, and residuals are shown below. You display the residuals in the Curve Fitting Tool with the **View->Residuals** menu item.

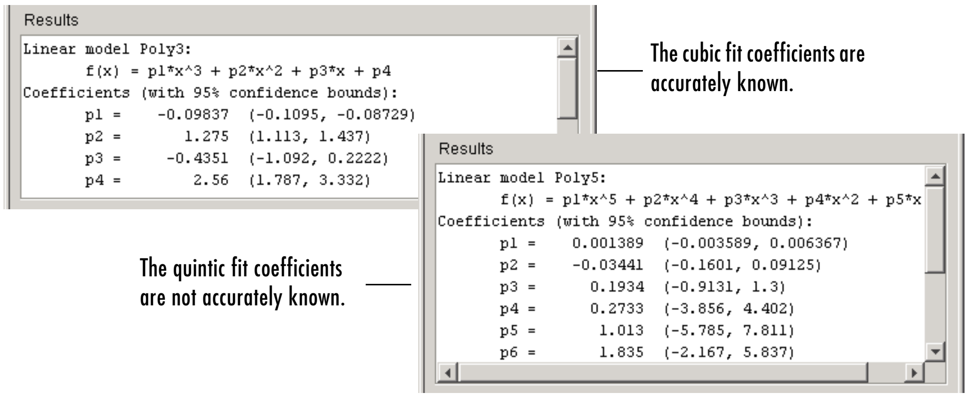


Both fits appear to model the data well.

The residuals for both fits appear to be randomly distributed.

Both models appear to fit the data well, and the residuals appear to be randomly distributed around zero. Therefore, a graphical evaluation of the fits does not reveal any obvious differences between the two equations.

The numerical fit results are shown below.



```
Results
Linear model Poly3:
      f(x) = p1*x^3 + p2*x^2 + p3*x + p4
Coefficients (with 95% confidence bounds):
      p1 =    -0.09837  (-0.1095, -0.08729)
      p2 =       1.275  (1.113, 1.437)
      p3 =     -0.4351  (-1.092, 0.2222)
      p4 =        2.56  (1.787, 3.332)
```

```
Results
Linear model Poly5:
      f(x) = p1*x^5 + p2*x^4 + p3*x^3 + p4*x^2 + p5*x
Coefficients (with 95% confidence bounds):
      p1 =    0.001389  (-0.003589, 0.006367)
      p2 =    -0.03441  (-0.1601, 0.09125)
      p3 =      0.1934  (-0.9131, 1.3)
      p4 =      0.2733  (-3.856, 4.402)
      p5 =       1.013  (-5.785, 7.811)
      p6 =       1.835  (-2.167, 5.837)
```

The cubic fit coefficients are accurately known.
The quintic fit coefficients are not accurately known.

As expected, the fit results for `poly3` are reasonable because the generated data is cubic. The 95% confidence bounds on the fitted coefficients indicate that they are acceptably accurate. However, the 95% confidence bounds for `poly5` indicate that the fitted coefficients are not known accurately.

The goodness of fit statistics are shown below. By default, the adjusted R-square and RMSE statistics are not displayed in the **Table of Fits**. To display these statistics, open the Table Options GUI by clicking the **Table options** button. The statistics do not reveal a substantial difference between the two equations.

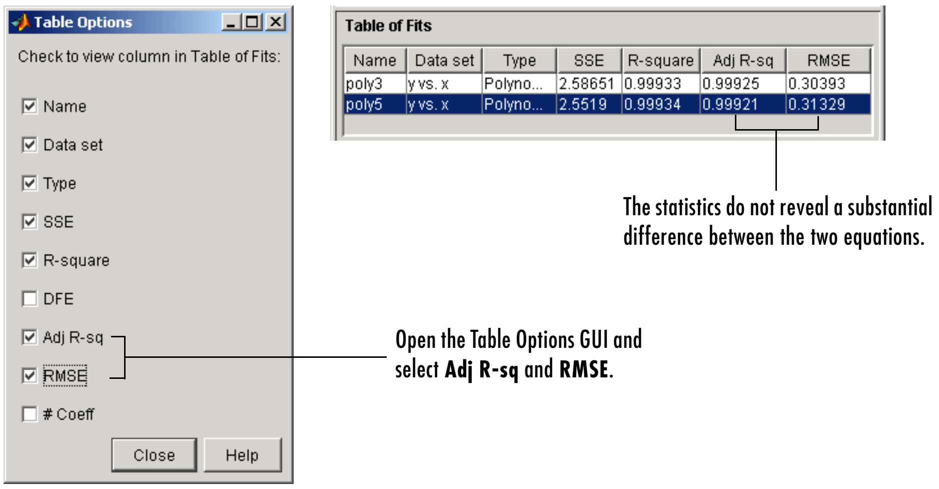
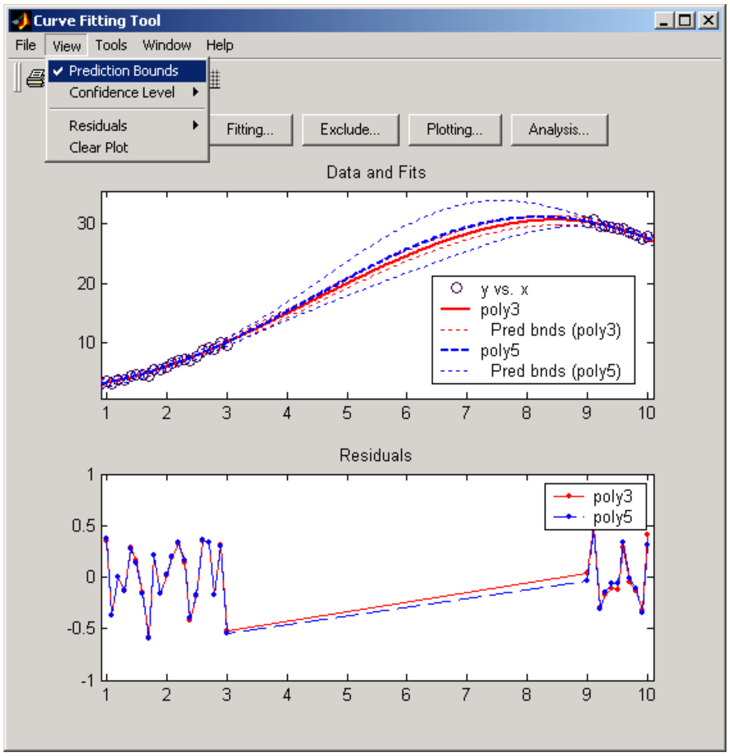


Table Options
Check to view column in Table of Fits:
☑ Name
☑ Data set
☑ Type
☑ SSE
☑ R-square
☐ DFE
☑ Adj R-sq
☑ RMSE
☐ # Coeff
Close
Help
Open the Table Options GUI and select **Adj R-sq** and **RMSE**.
The statistics do not reveal a substantial difference between the two equations.

Table of Fits

Name	Data set	Type	SSE	R-square	Adj R-sq	RMSE
poly3	y vs. x	Polyno...	2.58651	0.99933	0.99925	0.30393
poly5	y vs. x	Polyno...	2.5519	0.99934	0.99921	0.31329

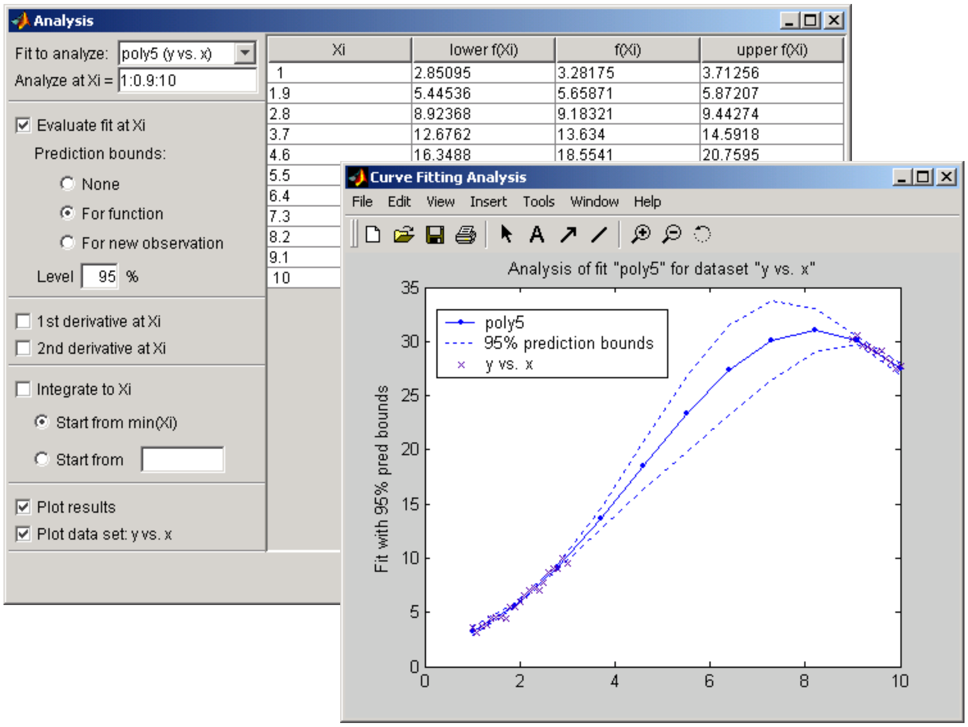
The 95% nonsimultaneous prediction bounds for new observations are shown below. To display prediction bounds in the Curve Fitting Tool, select the **View->Prediction Bounds** menu item. Alternatively, you can view prediction bounds for the function or for new observations using the Analysis GUI.



The prediction bounds for `poly3` indicate that new observations can be predicted accurately throughout the entire data range. This is not the case for `poly5`. It has wider prediction bounds in the area of the missing data, apparently because the data does not contain enough information to estimate the higher degree polynomial terms accurately. In other words, a fifth-degree polynomial overfits the data. You can confirm this by using the Analysis GUI to compute bounds for the functions themselves.

The 95% prediction bounds for `poly5` are shown below. As you can see, the uncertainty in estimating the function is large in the area of the missing data.

Therefore, you would conclude that more data must be collected before you can make accurate predictions using a fifth-degree polynomial.



Fit to analyze: poly5 (y vs. x)
Analyze at Xi = 1:0.9:10

[✓] Evaluate fit at Xi
Prediction bounds:
None [✓ For function] For new observation
Level 95 %

[ ] 1st derivative at Xi
[ ] 2nd derivative at Xi

[ ] Integrate to Xi
[✓ Start from min(Xi)] Start from

[✓] Plot results
[✓] Plot data set: y vs. x

Xi	lower f(Xi)	f(Xi)	upper f(Xi)
1	2.85095	3.28175	3.71256
1.9	5.44536	5.65871	5.87207
2.8	8.92368	9.18321	9.44274
3.7	12.6762	13.634	14.5918
4.6	16.3488	18.5541	20.7595
5.5			
6.4			
7.3			
8.2			
9.1			
10			

In conclusion, you should examine all available goodness of fit measures before deciding on the best fit. A graphical examination of the fit and residuals should always be your initial approach. However, some fit characteristics are revealed only through numerical fit results, statistics, and prediction bounds.

Example: Rational Fit

This example fits measured data using a rational model. The data describes the coefficient of thermal expansion for copper as a function of temperature in degrees Kelvin.

To get started, load the thermal expansion data from the file `hahn1.mat`, which is provided with the toolbox.

```
load hahn1
```

The workspace now contains two new variables, `temp` and `thermex`:

- `temp` is a vector of temperatures in degrees Kelvin.
- `thermex` is a vector of thermal expansion coefficients for copper.

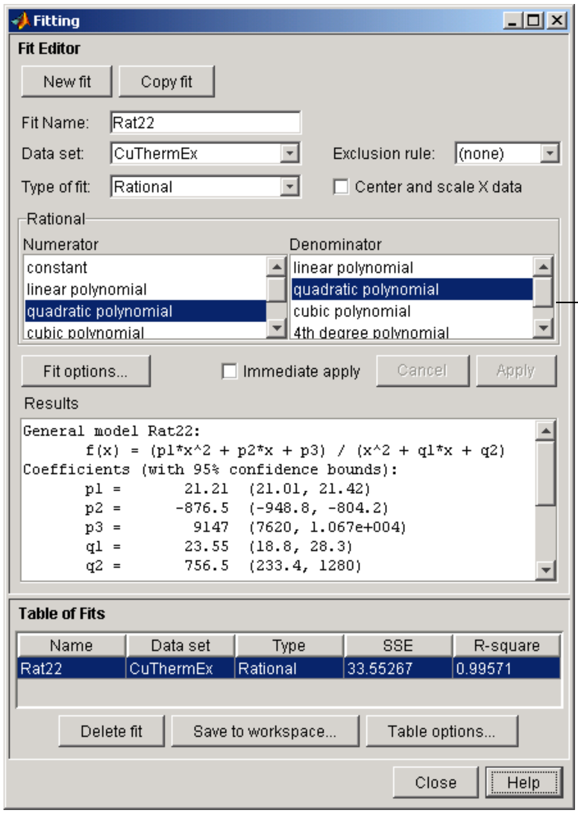
Import these two variables into the Curve Fitting Tool and name the data set `CuThermEx`.

For this data set, you will find the rational equation that produces the best fit. As described in "Library Models" on page 3-16, rational models are defined as a ratio of polynomials

$$y = \frac{p_1 x^n + p_2 x^{n-1} + \ldots + p_{n+1}}{x^m + q_1 x^{m-1} + \ldots + q_m}$$

where n is the degree of the numerator polynomial and m is the degree of the denominator polynomial. Note that the rational equations are not associated with physical parameters of the data. Instead, they provide a simple and flexible empirical model that you can use for interpolation and extrapolation.

As you can see by examining the shape of the data, a reasonable initial choice for the rational model is quadratic/quadratic. The Fitting GUI configured for this equation is shown below.



Fit Name: Rat22

Data set: CuThermEx

Exclusion rule: (none)

Type of fit: Rational

Center and scale X data

Rational

Numerator	Denominator
constant	linear polynomial
linear polynomial	quadratic polynomial
quadratic polynomial	cubic polynomial
cubic polynomial	4th degree polynomial

Results

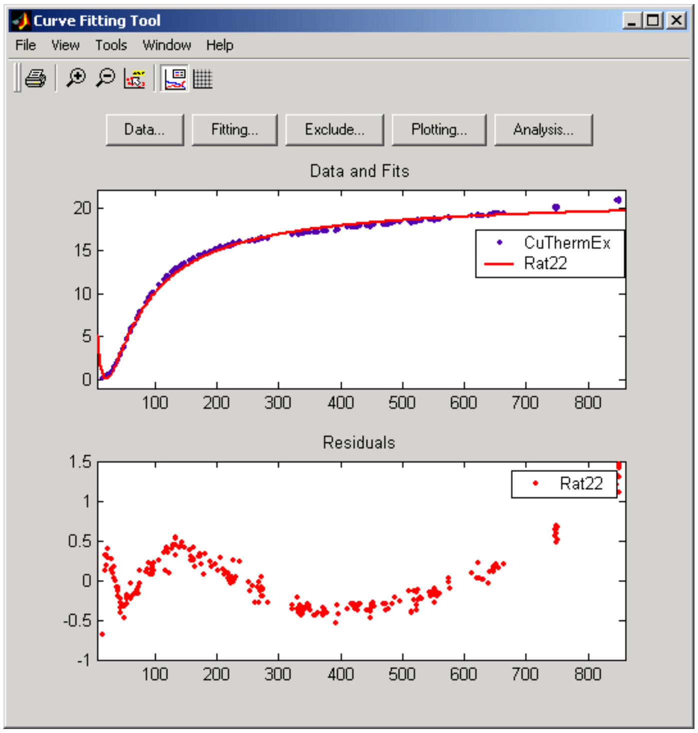
```
General model Rat22:
       f(x) = (p1*x^2 + p2*x + p3) / (x^2 + q1*x + q2)
Coefficients (with 95% confidence bounds):
       p1 =       21.21  (21.01, 21.42)
       p2 =      -876.5  (-948.8, -804.2)
       p3 =        9147  (7620, 1.067e+004)
       q1 =       23.55  (18.8, 28.3)
       q2 =       756.5  (233.4, 1280)
```

Table of Fits

Name	Data set	Type	SSE	R-square
Rat22	CuThermEx	Rational	33.55267	0.99571

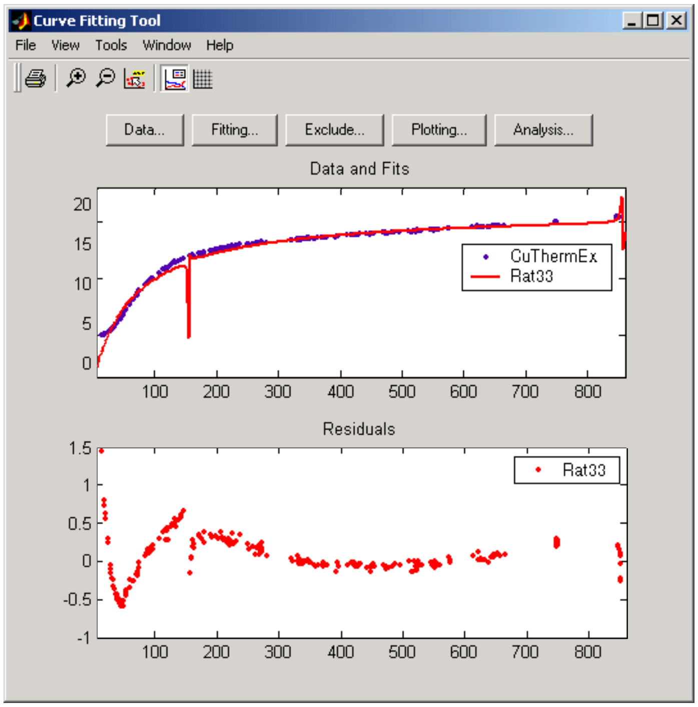
Begin the fitting process with a quadratic/quadratic rational fit.

The data, fit, and residuals are shown below.


Curve Fitting Tool
File View Tools Window Help
Data... Fitting... Exclude... Plotting... Analysis...
Data and Fits
CuThermEx
Rat22
Residuals
Rat22
The fit clearly misses some of the data.
The residuals show a strong pattern indicating a better fit is possible.

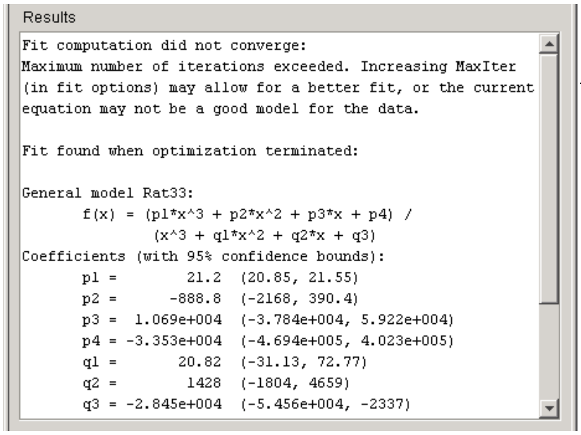
The fit clearly misses the data for the smallest and largest predictor values. Additionally, the residuals show a strong pattern throughout the entire data set indicating that a better fit is possible.

For the next fit, try a cubic/cubic equation. The data, fit, and residuals are shown below.



The fit exhibits several discontinuities around the zeros of the denominator.

The numerical results shown below indicate that the fit did not converge.



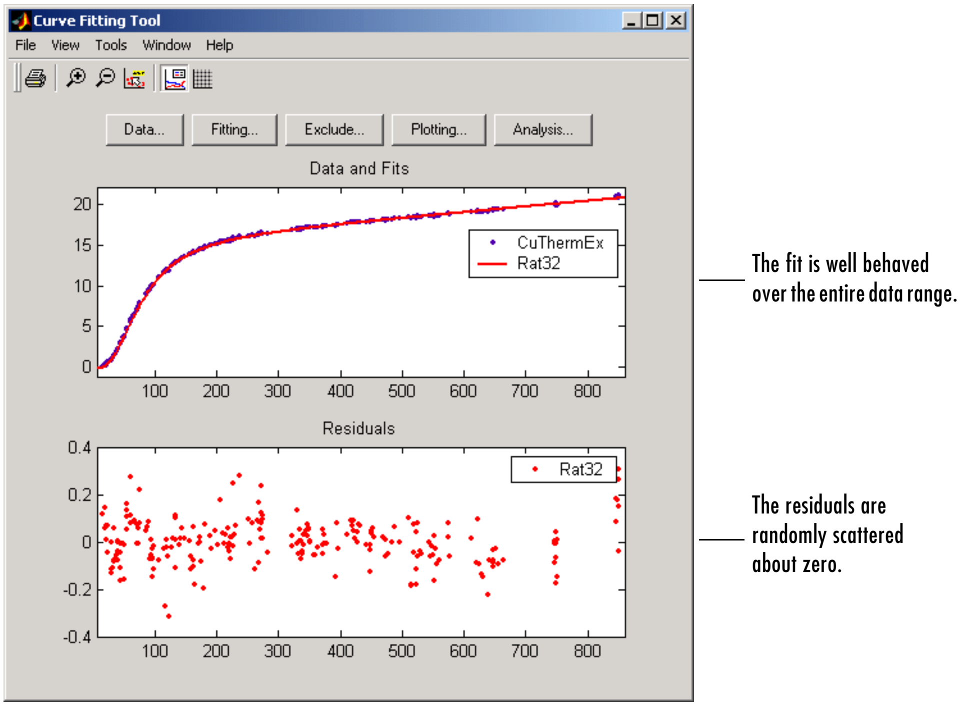
Results

```
Fit computation did not converge:
Maximum number of iterations exceeded. Increasing MaxIter
(in fit options) may allow for a better fit, or the current
equation may not be a good model for the data.

Fit found when optimization terminated:

General model Rat33:
       f(x) = (p1*x^3 + p2*x^2 + p3*x + p4) /
               (x^3 + q1*x^2 + q2*x + q3)
Coefficients (with 95% confidence bounds):
       p1 =        21.2  (20.85, 21.55)
       p2 =      -888.8  (-2168, 390.4)
       p3 =   1.069e+004  (-3.784e+004, 5.922e+004)
       p4 = -3.353e+004  (-4.694e+005, 4.023e+005)
       q1 =       20.82  (-31.13, 72.77)
       q2 =        1428  (-1804, 4659)
       q3 = -2.845e+004  (-5.456e+004, -2337)
```

The fit did not converge, which indicates that the model might be a poor choice for the data.

Although the message in the **Results** window indicates that you might improve the fit if you increase the maximum number of iterations, a better choice at this stage of the fitting process is to use a different rational equation because the current fit contains several discontinuities. These discontinuities are due to the function blowing up at predictor values that correspond to the zeros of the denominator.

As the next try, fit the data using a cubic/quadratic equation. The data, fit, and residuals are shown below.


Curve Fitting Tool
File View Tools Window Help
Data... Fitting... Exclude... Plotting... Analysis...
Data and Fits
CuThermEx
Rat32
Residuals
Rat32
The fit is well behaved over the entire data range.
The residuals are randomly scattered about zero.

The fit is well behaved over the entire data range, and the residuals are randomly scattered about zero. Therefore, you can confidently use this fit for further analysis.

Example: Fitting with Custom Equations

You can define your own equations with the Create Custom Equation GUI. You open this GUI one of two ways:

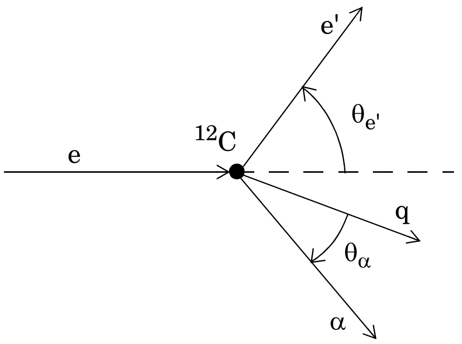
- From the Curve Fitting Tool, select **Tools->Custom Equation**.
- From the Fitting GUI, select **Custom Equations** from the **Type of fit** list, then click the **New Equation** button.

The Create Custom Equation GUI contains two panes: one for creating linear custom equations and one for creating general (nonlinear) custom equations. These panes are described in the following examples.

Linear Equation: Legendre Polynomial Fit

This example fits data using several custom linear equations. The data is generated, and is based on the nuclear reaction $^{12}C(e,e'\alpha)^{8}Be$. The equations use sums of Legendre polynomial terms.

Consider an experiment in which 124 MeV electrons are scattered from ^{12}C nuclei. In the subsequent reaction, alpha particles are emitted and produce the residual nuclei ^{8}Be. By analyzing the number of alpha particles emitted as a function of angle, you can deduce certain information regarding the nuclear dynamics of ^{12}C. The reaction kinematics are shown below.



e is the incident electron.
^{12}C is the carbon target.
q is the momentum transferred to ^{8}Be.
e' is the scattered electron.
α is the emitted alpha particle.
$\theta_{e'}$ is the electron scattering angle.
θ_α is the alpha scattering angle.

The data is collected by placing solid state detectors at values of θ_α ranging from 10^o to 240^o in 10^o increments.

It is sometimes useful to describe a variable expressed as a function of angle in terms of Legendre polynomials

$$y(x) = \sum_{n=0}^{\infty} a_n P_n(x)$$

where $P_n(x)$ is a Legendre polynomial of degree n, x is $\cos(\theta_\alpha)$, and a_n are the coefficients of the fit. Refer to the `legendre` function for information about generating Legendre polynomials.

For the alpha-emission data, you can directly associate the coefficients with the nuclear dynamics by invoking a theoretical model, which is described in [8]. Additionally, the theoretical model introduces constraints for the infinite sum shown above. In particular, by considering the angular momentum of the reaction, a fourth-degree Legendre polynomial using only even terms should describe the data effectively.

You can generate Legendre polynomials with Rodrigues' formula:

$$P_n(x) = \frac{1}{2^n n!}\left(\frac{d}{dx}\right)^n (x^2 - 1)^n$$

The Legendre polynomials up to fourth degree are given below.

Table 3-4: Legendre Polynomials up to Fourth Degree

n	$P_n(x)$
0	1
1	x
2	$(1/2)(3x^2 - 1)$
3	$(1/2)(5x^3 - 3x)$
4	$(1/8)(35x^4 - 30x^2 + 3)$

The first step is to load the ^{12}C alpha-emission data from the file carbon12alpha.mat, which is provided with the toolbox.

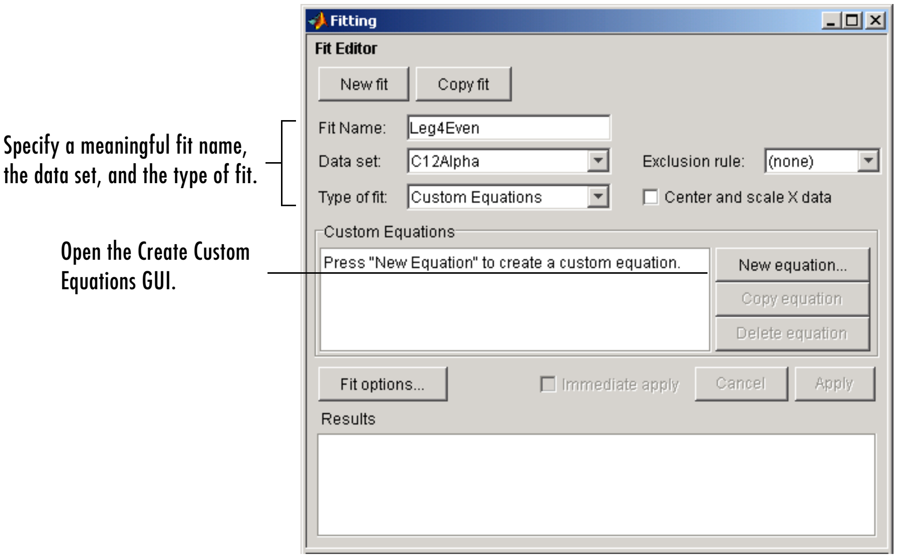
```
load carbon12alpha
```

The workspace now contains two new variables, angle and counts:

- angle is a vector of angles (in radians) ranging from 10° to 240° in 10° increments.
- counts is a vector of raw alpha particle counts that correspond to the emission angles in angle.

Import these two variables into the Curve Fitting Toolbox and name the data set C12Alpha.

The **Fit Editor** for a custom equation fit type is shown below.



Specify a meaningful fit name, the data set, and the type of fit.

Open the Create Custom Equations GUI.

Fit Name: Leg4Even

Data set: C12Alpha

Exclusion rule: (none)

Type of fit: Custom Equations

Center and scale X data

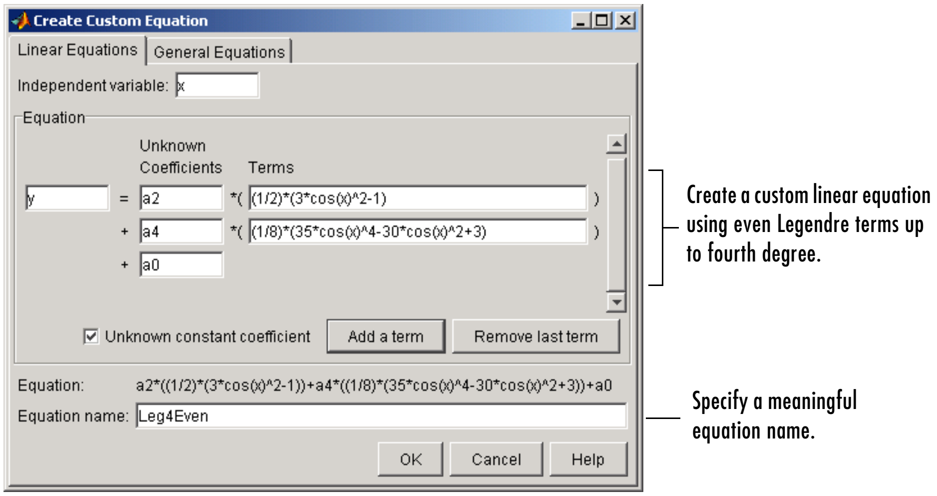
Custom Equations

Press "New Equation" to create a custom equation.

Fit the data using a fourth-degree Legendre polynomial with only even terms:

$$y_1(x) = a_0 + a_2\left(\frac{1}{2}\right)(3x^2 - 1) + a_4\left(\frac{1}{8}\right)(35x^4 - 30x^2 + 3)$$

Because the Legendre polynomials depend only on the predictor variable and constants, you use the Linear Equations pane on the Create Custom Equation GUI. This pane is shown below for the model given by $y_1(x)$. Note that because `angle` is given in radians, the argument of the Legendre terms is given by $\cos(\theta_\alpha)$.


Create Custom Equation
Linear Equations
General Equations
Unknown Coefficients
Terms
Unknown constant coefficient
Add a term
Remove last term
OK
Cancel
Help
Create a custom linear equation using even Legendre terms up to fourth degree.
Specify a meaningful equation name.

Independent variable: x

Equation:

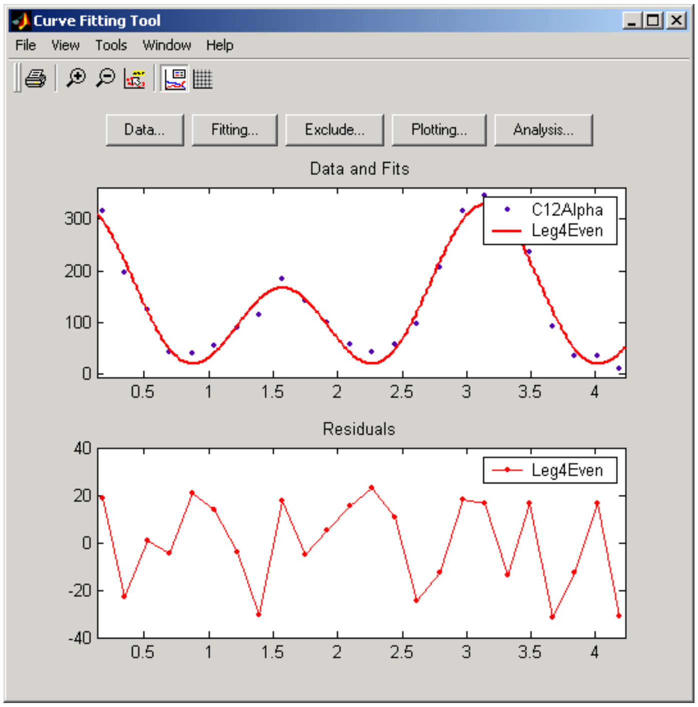
y = a2 *((1/2)*(3*cos(x)^2-1))
+ a4 *((1/8)*(35*cos(x)^4-30*cos(x)^2+3))
+ a0

☑ Unknown constant coefficient

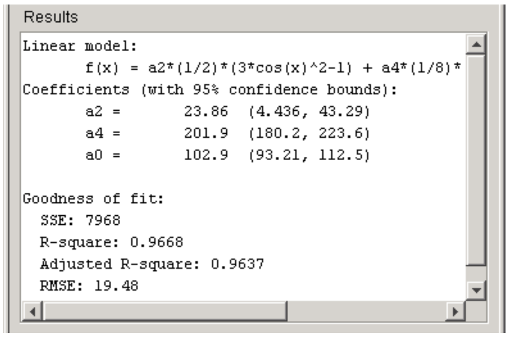
Equation: a2*((1/2)*(3*cos(x)^2-1))+a4*((1/8)*(35*cos(x)^4-30*cos(x)^2+3))+a0

Equation name: Leg4Even

The fit and residuals are shown below. The fit appears to follow the trend of the data well, while the residuals appear to be randomly distributed and do not exhibit any systematic behavior.


Curve Fitting Tool
File View Tools Window Help
Data... Fitting... Exclude... Plotting... Analysis...
Data and Fits
C12Alpha
Leg4Even
Residuals
Leg4Even

The numerical fit results are shown below. The 95% confidence bounds indicate that the coefficients associated with $P_0(x)$ and $P_4(x)$ are known fairly accurately, but that the $P_2(x)$ coefficient has a relatively large uncertainty.



Results

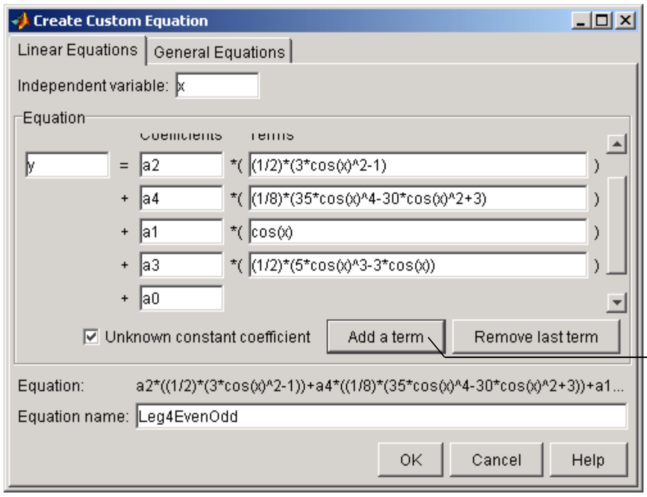
```
Linear model:
       f(x) = a2*(1/2)*(3*cos(x)^2-1) + a4*(1/8)*
Coefficients (with 95% confidence bounds):
       a2 =       23.86  (4.436, 43.29)
       a4 =       201.9  (180.2, 223.6)
       a0 =       102.9  (93.21, 112.5)

Goodness of fit:
  SSE: 7968
  R-square: 0.9668
  Adjusted R-square: 0.9637
  RMSE: 19.48
```

The coefficients associated with $P_0(x)$ and $P_4(x)$ are known accurately, but the $P_2(x)$ coefficient has a larger uncertainty.

To confirm the theoretical argument that the alpha-emission data is best described by a fourth-degree Legendre polynomial with only even terms, fit the data using both even and odd terms:

$$y_2(x) = y_1(x) + a_1 x + a_3\left(\frac{1}{2}\right)(5x^3 - 3x)$$

The Linear Equations pane of the Create Custom Equation GUI is shown below for the model given by $y_2(x)$.



Create Custom Equation

Linear Equations | General Equations

Independent variable: x

Equation

		Coefficients		Terms	
y	=	a2	*(	(1/2)*(3*cos(x)^2-1)	)
	+	a4	*(	(1/8)*(35*cos(x)^4-30*cos(x)^2+3)	)
	+	a1	*(	cos(x)	)
	+	a3	*(	(1/2)*(5*cos(x)^3-3*cos(x))	)
	+	a0			

☑ Unknown constant coefficient

Add a term | Remove last term

Equation: a2*((1/2)*(3*cos(x)^2-1))+a4*((1/8)*(35*cos(x)^4-30*cos(x)^2+3))+a1...

Equation name: Leg4EvenOdd

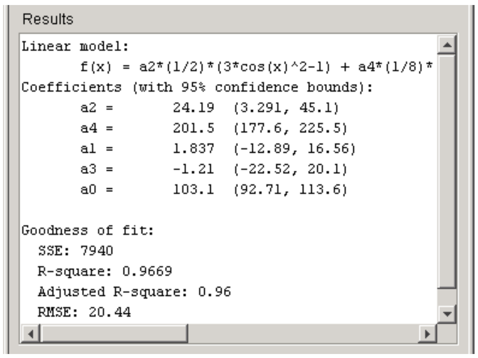
OK | Cancel | Help

Create a custom linear equation using even and odd Legendre terms up to fourth degree.

Click **Add a term** to add the odd Legendre terms.

Specify a meaningful equation name.

The numerical results indicate that the odd Legendre terms do not contribute significantly to the fit, and the even Legendre terms are essentially unchanged from the previous fit. This confirms that the initial model choice is the best one.



Results

```
Linear model:
       f(x) = a2*(1/2)*(3*cos(x)^2-1) + a4*(1/8)*
Coefficients (with 95% confidence bounds):
       a2 =       24.19  (3.291, 45.1)
       a4 =       201.5  (177.6, 225.5)
       a1 =       1.837  (-12.89, 16.56)
       a3 =       -1.21  (-22.52, 20.1)
       a0 =       103.1  (92.71, 113.6)

Goodness of fit:
  SSE: 7940
  R-square: 0.9669
  Adjusted R-square: 0.96
  RMSE: 20.44
```

The odd Legendre coefficients should not be included in the fit because their values are small and their confidence bounds are large.

General Equation: Fourier Series Fit

This example fits the ENSO data using several custom nonlinear equations. The ENSO data consists of monthly averaged atmospheric pressure differences between Easter Island and Darwin, Australia. This difference drives the trade winds in the southern hemisphere.

As shown in “Example: Smoothing Data” on page 2-21, the ENSO data is clearly periodic, which suggests it can be described by a Fourier series

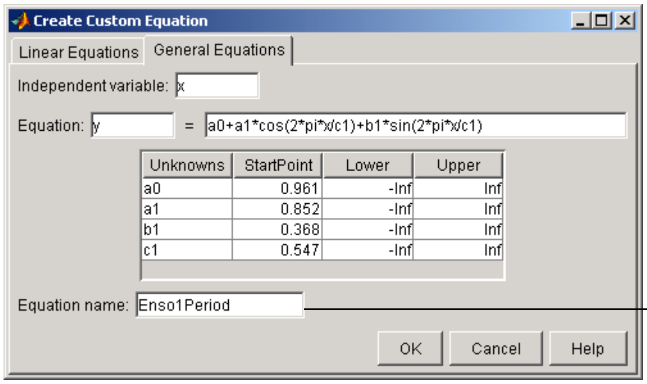
$$y(x) = a_0 + \sum_{i=1}^{\infty} a_i \cos\left(2\pi \frac{x}{c_i}\right) + b_i \sin\left(2\pi \frac{x}{c_i}\right)$$

where a_i and b_i are the amplitudes, and c_i are the periods (cycles) of the data. The question to be answered in this example is how many cycles exist? As a first attempt, assume a 12 month cycle and fit the data using one sine term and one cosine term.

$$y_1(x) = a_0 + a_1 \cos\left(2\pi \frac{x}{c_1}\right) + b_1 \sin\left(2\pi \frac{x}{c_1}\right)$$

If the fit does not describe the data well, add additional sine and cosine terms with unique period coefficients until a good fit is obtained.

Because there is an unknown coefficient c_1 included as part of the trigonometric function arguments, the equation is nonlinear. Therefore, you must specify the equation using the General Equations pane of the Create Custom Equation GUI. This pane is shown below for the equation given by $y_1(x)$.



Independent variable: x

Equation: y = a0+a1*cos(2*pi*x/c1)+b1*sin(2*pi*x/c1)

Unknowns	StartPoint	Lower	Upper
a0	0.961	-Inf	Inf
a1	0.852	-Inf	Inf
b1	0.368	-Inf	Inf
c1	0.547	-Inf	Inf

Equation name: Enso1Period

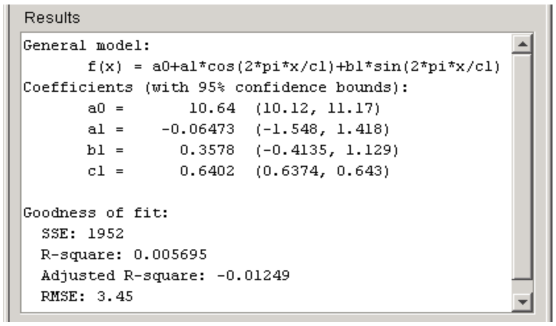
Assume one 12 month cycle.

By default, the coefficients are unbounded and have random starting values between 0 and 1.

Specify a meaningful equation name.

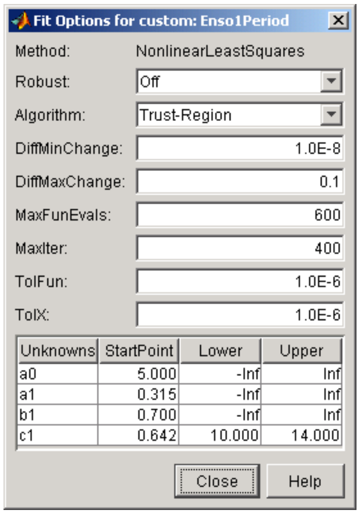
Note that the toolbox includes the Fourier series as a nonlinear library equation. However, the library equation does not meet the needs of this example because its terms are defined as fixed multiples of the fundamental frequency w. Refer to “Fourier Series” on page 3-16 for more information.

The numerical results shown below indicate that the fit does not describe the data well. In particular, the fitted value for c1 is unreasonably small. Because the starting points are randomly selected, your initial fit results might differ from the results shown here.



```
General model:
       f(x) = a0+a1*cos(2*pi*x/c1)+b1*sin(2*pi*x/c1)
Coefficients (with 95% confidence bounds):
       a0 =       10.64  (10.12, 11.17)
       a1 =    -0.06473  (-1.548, 1.418)
       b1 =      0.3578  (-0.4135, 1.129)
       c1 =      0.6402  (0.6374, 0.643)

Goodness of fit:
  SSE: 1952
  R-square: 0.005695
  Adjusted R-square: -0.01249
  RMSE: 3.45
```

To assist the fitting procedure, constrain c1 to a value between 10 and 14. To define constraints for unknown coefficients, use the Fit Options GUI, which you open by clicking the **Fit options** button in the Fitting GUI.

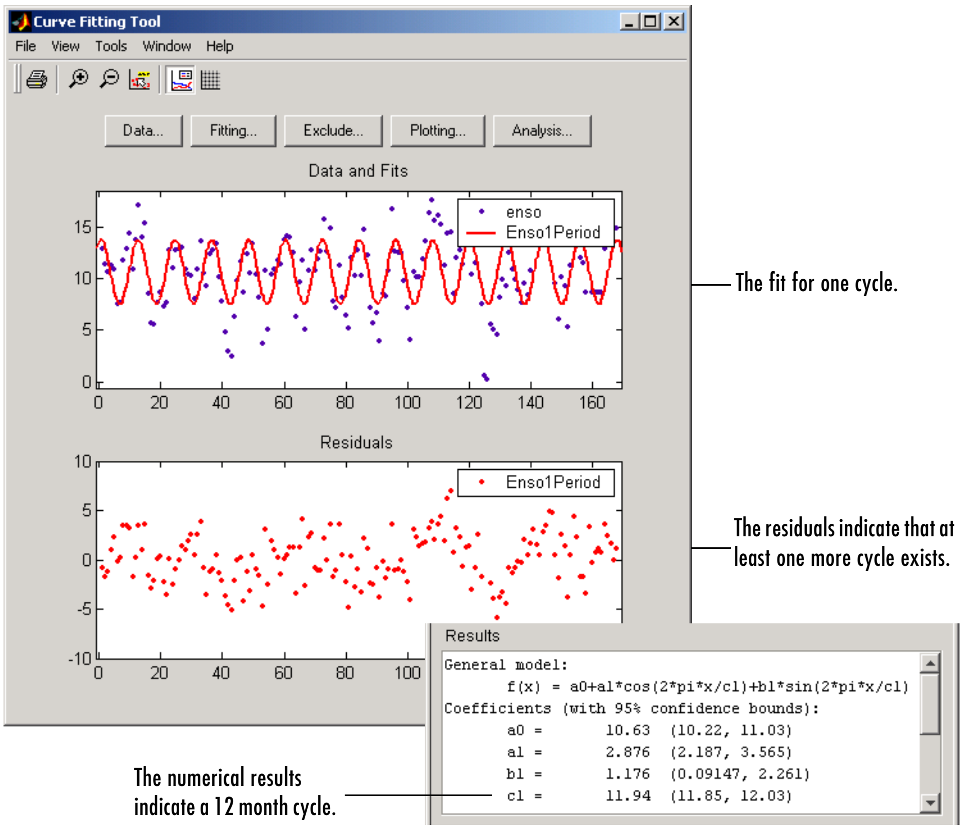


Method:	NonlinearLeastSquares
Robust:	Off
Algorithm:	Trust-Region
DiffMinChange:	1.0E-8
DiffMaxChange:	0.1
MaxFunEvals:	600
MaxIter:	400
TolFun:	1.0E-6
TolX:	1.0E-6

Unknowns	StartPoint	Lower	Upper
a0	5.000	-Inf	Inf
a1	0.315	-Inf	Inf
b1	0.700	-Inf	Inf
c1	0.642	10.000	14.000

Constrain the cycle to be between 10 and 14 months.

The fit, residuals, and numerical results are shown below.


Curve Fitting Tool
File View Tools Window Help
Data... Fitting... Exclude... Plotting... Analysis...
Data and Fits
enso
Enso1Period
Residuals
Enso1Period
Results
The fit for one cycle.
The residuals indicate that at least one more cycle exists.
The numerical results indicate a 12 month cycle.

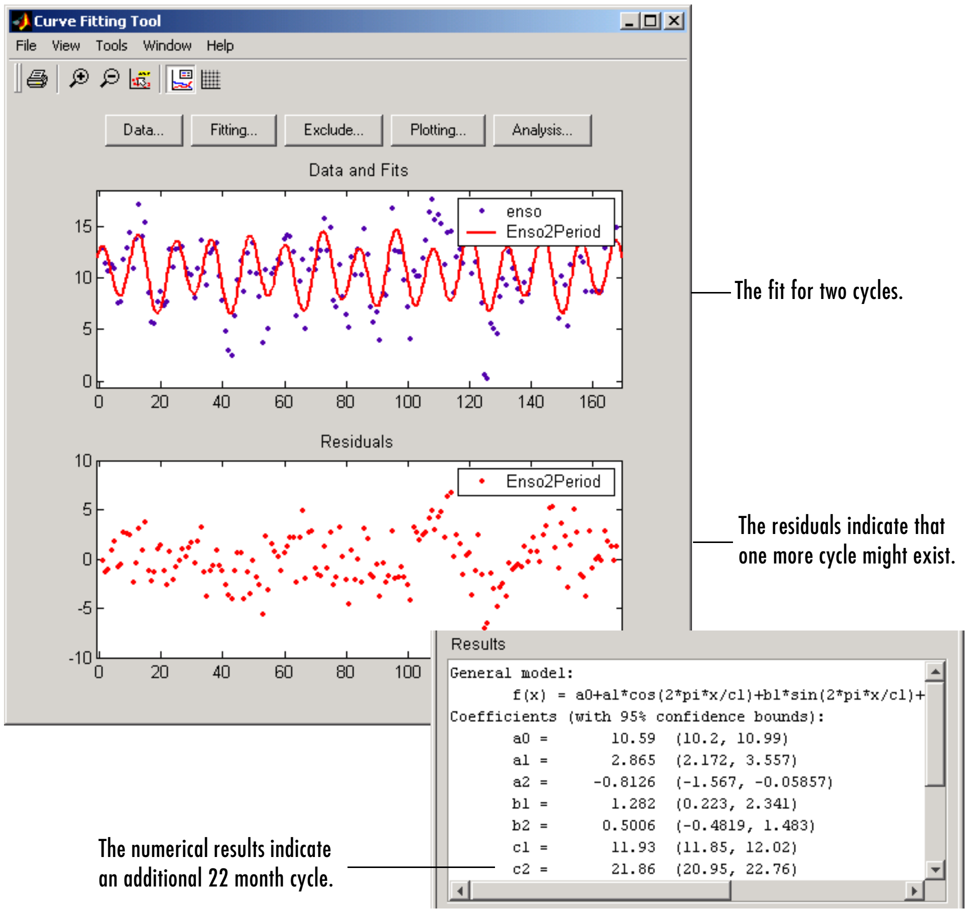
```
General model:
       f(x) = a0+a1*cos(2*pi*x/c1)+b1*sin(2*pi*x/c1)
Coefficients (with 95% confidence bounds):
       a0 =       10.63  (10.22, 11.03)
       a1 =       2.876  (2.187, 3.565)
       b1 =       1.176  (0.09147, 2.261)
       c1 =       11.94  (11.85, 12.03)
```

The fit appears to be reasonable for some of the data points but clearly does not describe the entire data set very well. As predicted, the numerical results indicate a cycle of approximately 12 months. However, the residuals show a systematic periodic distribution indicating that there are additional cycles that you should include in the fit equation. Therefore, as a second attempt, add an additional sine and cosine term to $y_1(x)$

$$y_2(x) = y_1(x) + a_2\cos\left(2\pi\frac{x}{c_2}\right) + b_2\sin\left(2\pi\frac{x}{c_2}\right)$$

and constrain the upper and lower bounds of c_2 to be roughly twice the bounds used for c_1.

The fit, residuals, and numerical results are shown below.


Curve Fitting Tool
File View Tools Window Help
Data... Fitting... Exclude... Plotting... Analysis...
Data and Fits
enso
Enso2Period
Residuals
Enso2Period
Results
The fit for two cycles.
The residuals indicate that one more cycle might exist.
The numerical results indicate an additional 22 month cycle.

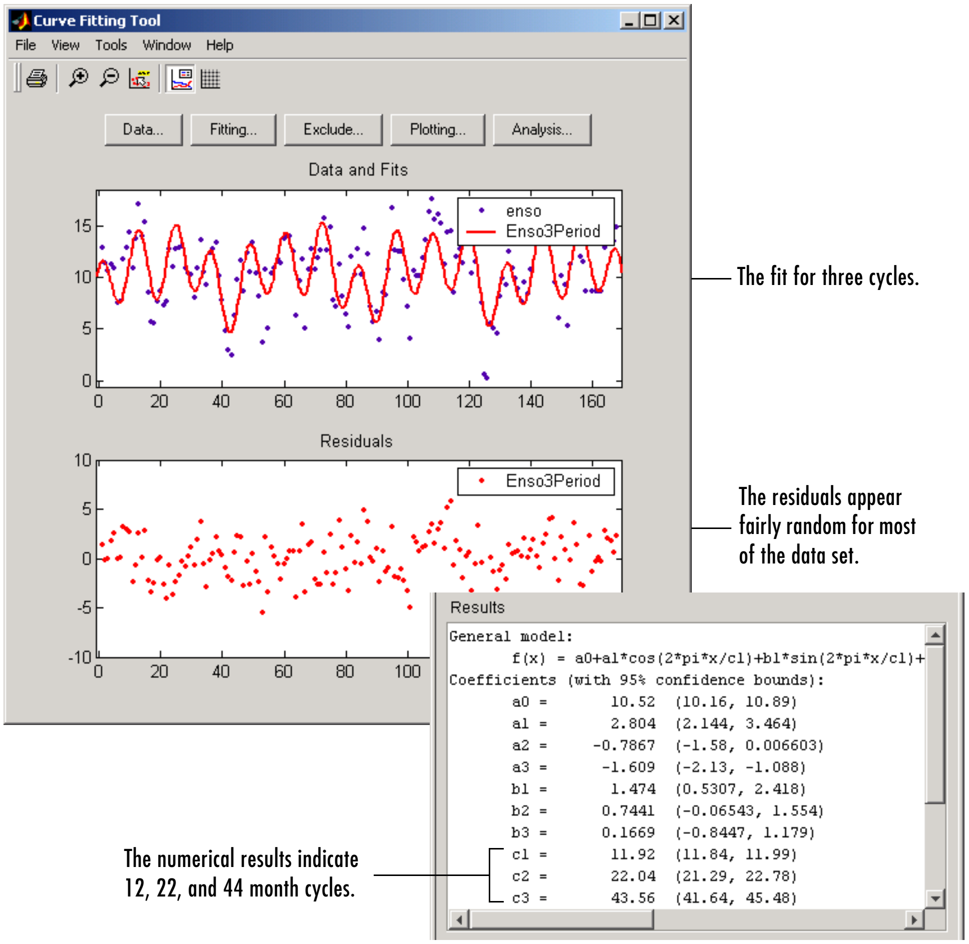
```
General model:
     f(x) = a0+a1*cos(2*pi*x/c1)+b1*sin(2*pi*x/c1)+
Coefficients (with 95% confidence bounds):
       a0 =       10.59  (10.2, 10.99)
       a1 =       2.865  (2.172, 3.557)
       a2 =     -0.8126  (-1.567, -0.05857)
       b1 =       1.282  (0.223, 2.341)
       b2 =      0.5006  (-0.4819, 1.483)
       c1 =       11.93  (11.85, 12.02)
       c2 =       21.86  (20.95, 22.76)
```

The fit appears to be reasonable for most of the data points. However, the residuals indicate that you should include another cycle to the fit equation. Therefore, as a third attempt, add an additional sine and cosine term to $y_2(x)$

$$y_3(x) = y_2(x) + a_3\cos\left(2\pi\frac{x}{c_3}\right) + b_3\sin\left(2\pi\frac{x}{c_3}\right)$$

and constrain the lower bound of c_3 to be roughly three times the value of c_1.

The fit, residuals, and numerical results are shown below.


Curve Fitting Tool
File View Tools Window Help
Data... Fitting... Exclude... Plotting... Analysis...
Data and Fits
enso
Enso3Period
Residuals
Enso3Period
Results
The fit for three cycles.
The residuals appear fairly random for most of the data set.
The numerical results indicate 12, 22, and 44 month cycles.

```
General model:
      f(x) = a0+a1*cos(2*pi*x/c1)+b1*sin(2*pi*x/c1)+
Coefficients (with 95% confidence bounds):
      a0 =       10.52  (10.16, 10.89)
      a1 =       2.804  (2.144, 3.464)
      a2 =     -0.7867  (-1.58, 0.006603)
      a3 =      -1.609  (-2.13, -1.088)
      b1 =       1.474  (0.5307, 2.418)
      b2 =      0.7441  (-0.06543, 1.554)
      b3 =      0.1669  (-0.8447, 1.179)
      c1 =       11.92  (11.84, 11.99)
      c2 =       22.04  (21.29, 22.78)
      c3 =       43.56  (41.64, 45.48)
```

The fit is an improvement over the previous two fits, and appears to account for most of the cycles present in the ENSO data set. The residuals appear random for most of the data, although a pattern is still visible indicating that additional cycles may be present, or you can improve the fitted amplitudes.

In conclusion, Fourier analysis of the data reveals three significant cycles. The annual cycle is the strongest, but cycles with periods of approximately 44 and 22 months are also present. These cycles correspond to El Nino and the Southern Oscillation (ENSO).

General Equation: Gaussian Fit with Exponential Background

This example fits two poorly resolved Gaussian peaks on a decaying exponential background using a general (nonlinear) custom model. To get started, load the data from the file `gauss3.mat`, which is provided with the toolbox.

```
load gauss3
```

The workspace now contains two new variables, `xpeak` and `ypeak`:

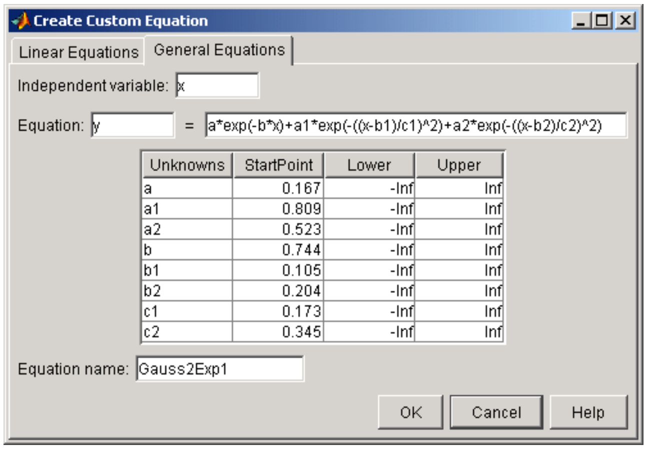
- `xpeak` is a vector of predictor values.
- `ypeak` is a vector of response values.

Import these two variables into the Curve Fitting Toolbox and accept the default data set name `ypeak vs. xpeak`.

You will fit the data with the following equation

$$y(x) = ae^{-bx} + a_1 e^{-\left(\frac{x-b_1}{c_1}\right)^2} + a_2 e^{-\left(\frac{x-b_2}{c_2}\right)^2}$$

where a_i are the peak amplitudes, b_i are the peak centroids, and c_i are related to the peak widths. Because there are unknown coefficients included as part of the exponential function arguments, the equation is nonlinear. Therefore, you must specify the equation using the General Equations pane of the Create Custom Equation GUI. This pane is shown below for $y(x)$.



Independent variable: x

Equation: y = a*exp(-b*x)+a1*exp(-((x-b1)/c1)^2)+a2*exp(-((x-b2)/c2)^2)

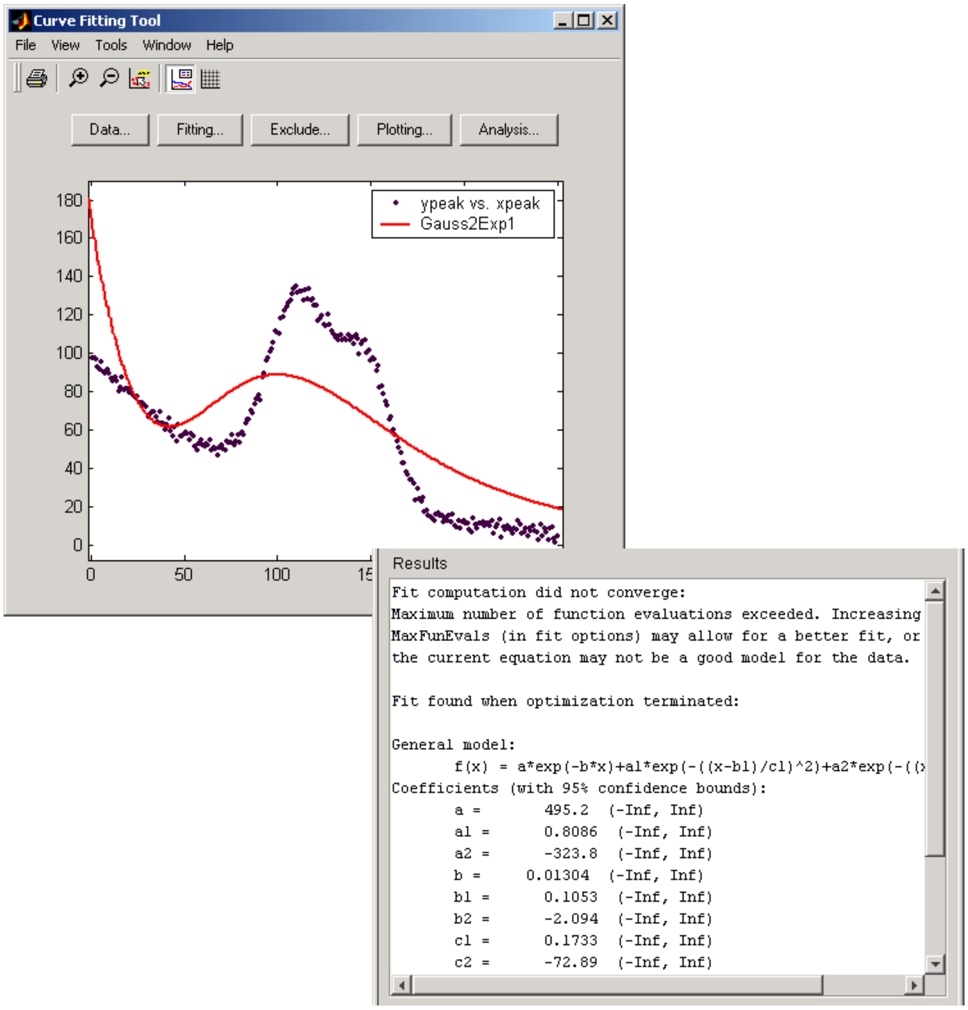
Unknowns	StartPoint	Lower	Upper
a	0.167	-Inf	Inf
a1	0.809	-Inf	Inf
a2	0.523	-Inf	Inf
b	0.744	-Inf	Inf
b1	0.105	-Inf	Inf
b2	0.204	-Inf	Inf
c1	0.173	-Inf	Inf
c2	0.345	-Inf	Inf

Equation name: Gauss2Exp1

Two Gaussian peaks on an exponential background.

By default, the coefficients are unbounded and have random starting values between 0 and 1.

The data, fit, and numerical fit results are shown below. Clearly, the fit is poor.


Curve Fitting Tool
File View Tools Window Help
Data... Fitting... Exclude... Plotting... Analysis...
ypeak vs. xpeak
Gauss2Exp1
Results

```
Fit computation did not converge:
Maximum number of function evaluations exceeded. Increasing
MaxFunEvals (in fit options) may allow for a better fit, or
the current equation may not be a good model for the data.

Fit found when optimization terminated:

General model:
       f(x) = a*exp(-b*x)+a1*exp(-((x-b1)/c1)^2)+a2*exp(-((x
Coefficients (with 95% confidence bounds):
       a =       495.2  (-Inf, Inf)
       a1 =      0.8086  (-Inf, Inf)
       a2 =      -323.8  (-Inf, Inf)
       b =     0.01304  (-Inf, Inf)
       b1 =      0.1053  (-Inf, Inf)
       b2 =      -2.094  (-Inf, Inf)
       c1 =      0.1733  (-Inf, Inf)
       c2 =      -72.89  (-Inf, Inf)
```

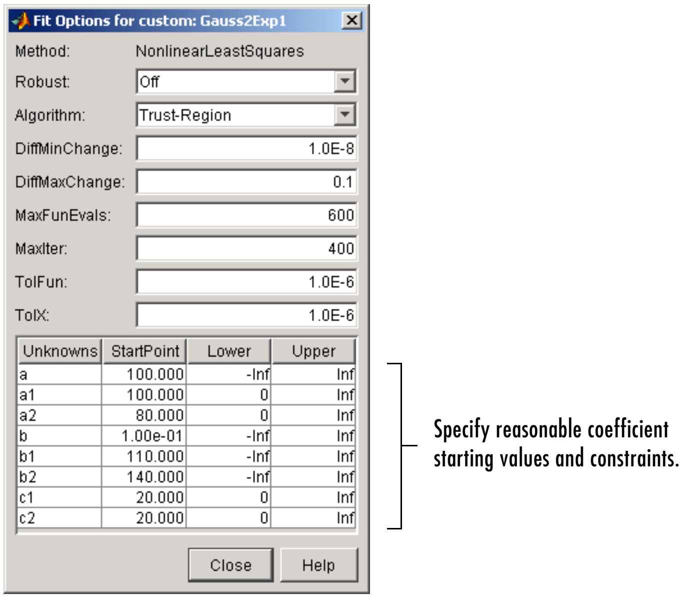
Because the starting points are randomly selected, your initial fit results might differ from the results shown here.

The results include this warning message.

```
Fit computation did not converge:
Maximum number of function evaluations exceeded. Increasing
MaxFunEvals (in fit options) may allow for a better fit, or
the current equation may not be a good model for the data.
```

To improve the fit for this example, specify reasonable starting points for the coefficients. Deducing the starting points is particularly easy for the current model because the Gaussian coefficients have a straightforward interpretation and the exponential background is well defined. Additionally, as the peak amplitudes and widths cannot be negative, constrain a_1, a_2, c_1, and c_2 to be greater then zero.

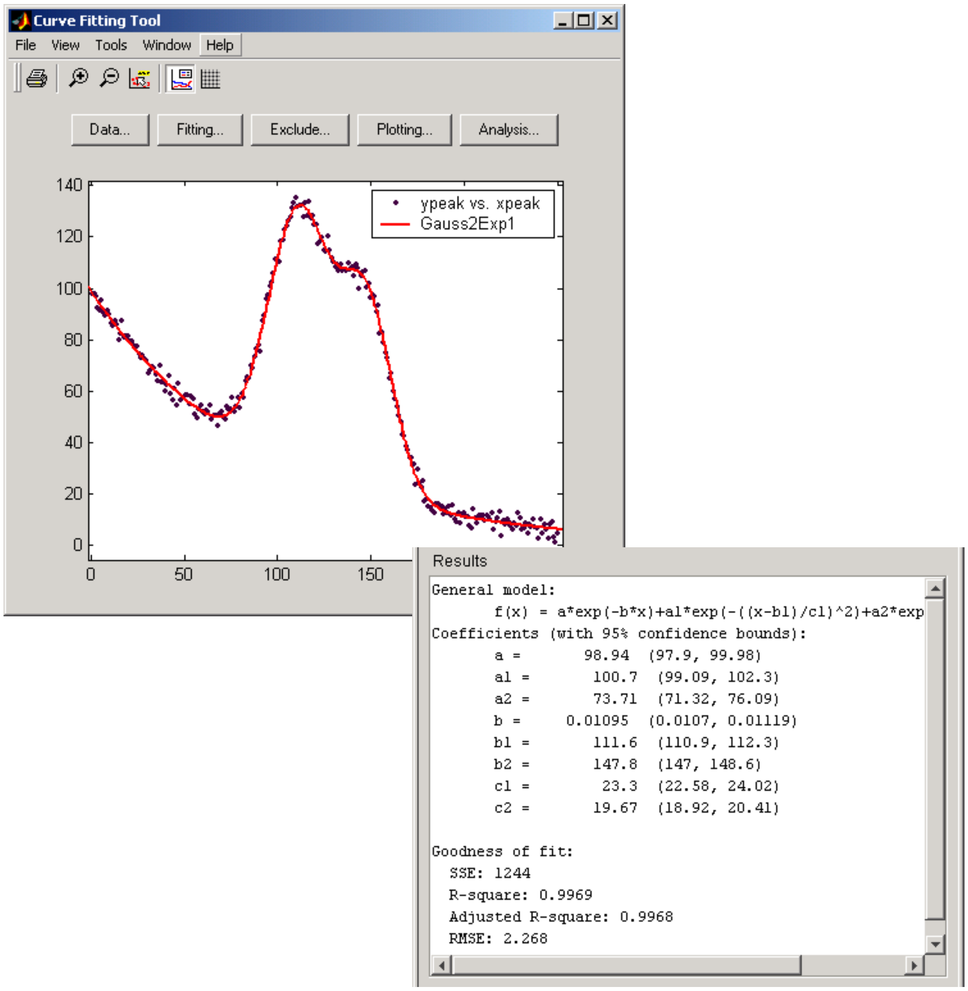
To define starting values and constraints for unknown coefficients, use the Fit Options GUI, which you open by clicking the **Fit options** button. The starting values and constraints are shown below.


Fit Options for custom: Gauss2Exp1
Close
Help
Specify reasonable coefficient starting values and constraints.

Method:	NonlinearLeastSquares
Robust:	Off
Algorithm:	Trust-Region
DiffMinChange:	1.0E-8
DiffMaxChange:	0.1
MaxFunEvals:	600
MaxIter:	400
TolFun:	1.0E-6
TolX:	1.0E-6

Unknowns	StartPoint	Lower	Upper
a	100.000	-Inf	Inf
a1	100.000	0	Inf
a2	80.000	0	Inf
b	1.00e-01	-Inf	Inf
b1	110.000	-Inf	Inf
b2	140.000	-Inf	Inf
c1	20.000	0	Inf
c2	20.000	0	Inf

The data, fit, residuals, and numerical results are shown below.


Curve Fitting Tool
File View Tools Window Help
Data... Fitting... Exclude... Plotting... Analysis...
ypeak vs. xpeak
Gauss2Exp1
Results

```
General model:
       f(x) = a*exp(-b*x)+a1*exp(-((x-b1)/c1)^2)+a2*exp
Coefficients (with 95% confidence bounds):
       a =       98.94  (97.9, 99.98)
       a1 =       100.7  (99.09, 102.3)
       a2 =       73.71  (71.32, 76.09)
       b =     0.01095  (0.0107, 0.01119)
       b1 =       111.6  (110.9, 112.3)
       b2 =       147.8  (147, 148.6)
       c1 =        23.3  (22.58, 24.02)
       c2 =       19.67  (18.92, 20.41)

Goodness of fit:
  SSE: 1244
  R-square: 0.9969
  Adjusted R-square: 0.9968
  RMSE: 2.268
```

Example: Robust Fit

This example fits data that is assumed to contain one outlier. The data consists of the 2000 United States presidential election results for the state of Florida. The fit model is a first degree polynomial and the fit method is robust linear least squares with bisquare weights.

In the 2000 presidential election, many residents of Palm Beach County, Florida, complained that the design of the election ballot was confusing, which they claim led them to vote for the Reform candidate Pat Buchanan instead of the Democratic candidate Al Gore. The so-called "butterfly ballot" was used only in Palm Beach County and only for the election-day ballots for the presidential race. As you will see, the number of Buchanan votes for Palm Beach is far removed from the bulk of data, which suggests that the data point should be treated as an outlier.

To get started, load the Florida election result data from the file `flvote2k.mat`, which is provided with the toolbox.

```
load flvote2k
```

The workspace now contains these three new variables:

- `buchanan` is a vector of votes for the Reform Party candidate Pat Buchanan.
- `bush` is a vector of votes for the Republican Party candidate George Bush.
- `gore` is a vector of votes for the Democratic Party candidate Al Gore.

Each variable contains 68 elements, which correspond to the 67 Florida counties plus the absentee ballots. The names of the counties are given in the variable `counties`. From these variables, create two data sets with the Buchanan votes as the response data: `buchanan vs. bush` and `buchanan vs. gore`.

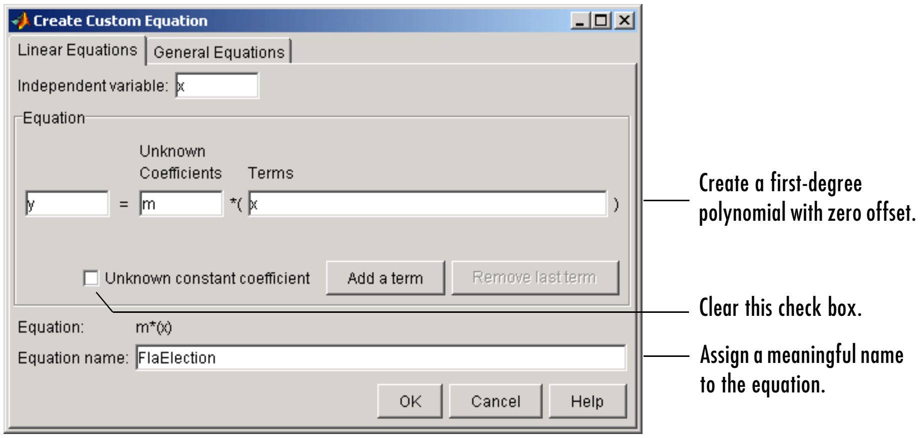
For this example, assume that the relationship between the response and predictor data is linear with an offset of zero.

buchanan votes = (bush votes)(m1)
buchanan votes = (gore votes)(m2)

m1 is the number of Bush votes expected for each Buchanan vote, and m2 is the number of Gore votes expected for each Buchanan vote.

To create a first-degree polynomial equation with zero offset, you must create a custom linear equation. As described in "Example: Fitting with Custom Equations" on page 3-46, you can create a custom equation using the Fitting GUI by selecting **Custom Equations** from the **Type of fit** list, and then clicking the **New Equation** button.

The Linear Equations pane of the Create Custom Equation GUI is shown below.



Independent variable: x

y = m *(x)

☐ Unknown constant coefficient

Equation: m*(x)

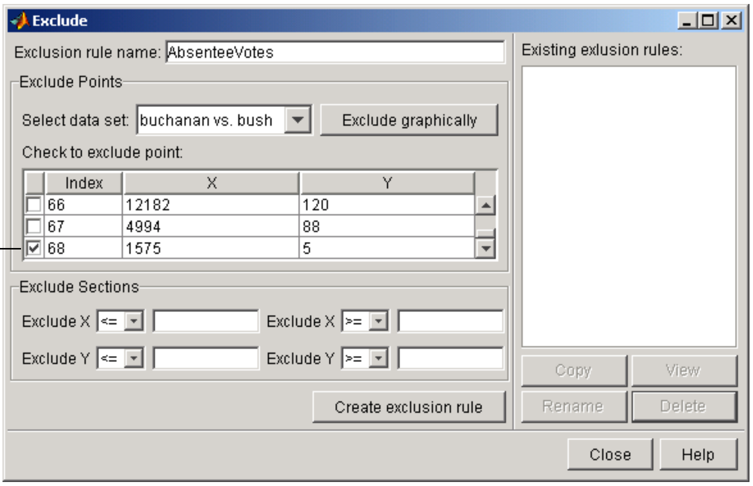
Equation name: FlaElection

Before fitting, you should exclude the data point associated with the absentee ballots from each data set because these voters did not use the butterfly ballot. As described in "Marking Outliers" on page 2-27, you can exclude individual data points from a fit either graphically or numerically using the Exclude GUI. For this example, you should exclude the data numerically. The index of the absentee ballot data is given by

```
ind = find(strcmp(counties,'Absentee Ballots'))
ind =
    68
```

The Exclude GUI is shown below.

Mark the absentee votes to be excluded.



	Index	X	Y
☐	66	12182	120
☐	67	4994	88
☑	68	1575	5

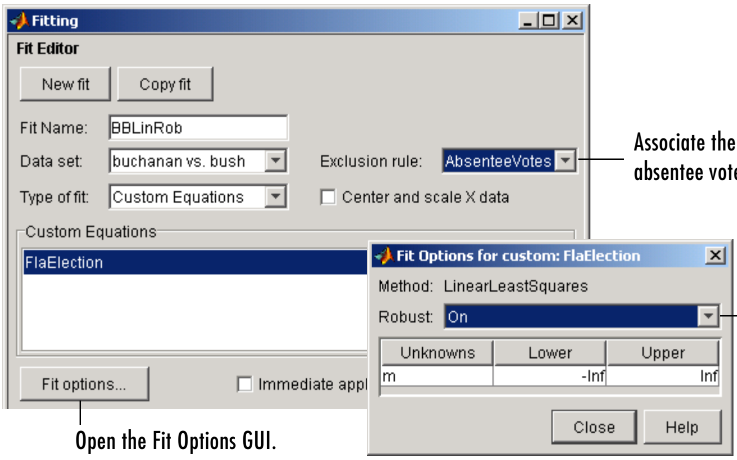
The exclusion rule is named `AbsenteeVotes`. You use the Fitting GUI to associate an exclusion rule with the data set to be fit.

For each data set, perform a robust fit with bisquare weights using the `FlaElection` equation defined above. For comparison purposes, also perform a regular linear least squares fit. Refer to "Robust Least Squares" on page 3-11 for a description of the robust fitting methods provided by the toolbox.

You can identify the Palm Beach County data in the scatter plot by using the data tips feature, and knowing the index number of the data point.

```
ind = find(strcmp(counties,'Palm Beach'))
ind =
    50
```

The **Fit Editor** and the Fit Options GUI are shown below for a robust fit.



Fit Name: BBLinRob
Data set: buchanan vs. bush
Exclusion rule: AbsenteeVotes
Type of fit: Custom Equations
☐ Center and scale X data
Custom Equations: FlaElection

Fit Options for custom: FlaElection
Method: LinearLeastSquares
Robust: On

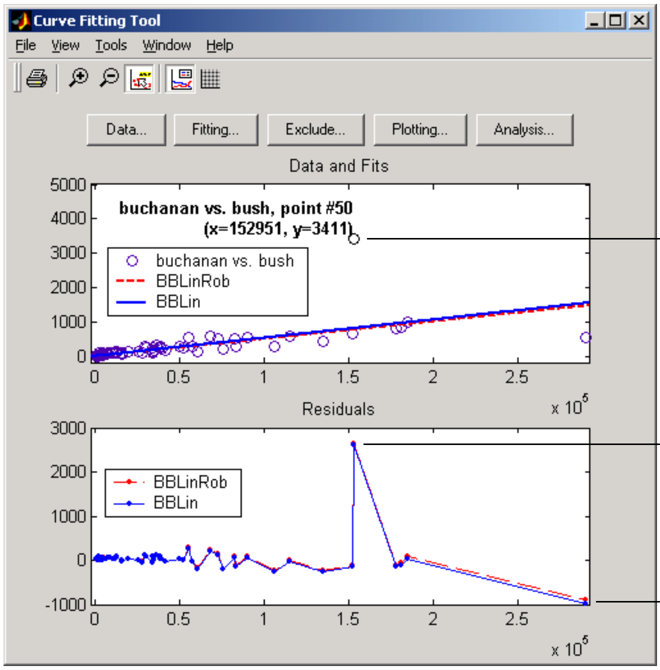
Unknowns	Lower	Upper
m	-Inf	Inf

Associate the excluded absentee votes with the fit.

Choose robust fitting with bisquare weights.

Open the Fit Options GUI.

The data, robust and regular least squares fits, and residuals for the buchanan vs. bush data set are shown below.



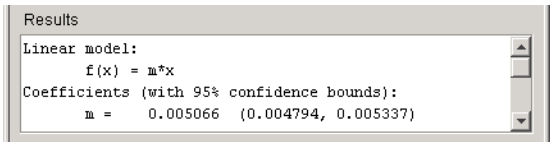
The data tip shows that Buchanan received 3411 votes in Palm Beach County.

The Palm Beach County residual is very large.

The Miami/Dade County residual is also very large.

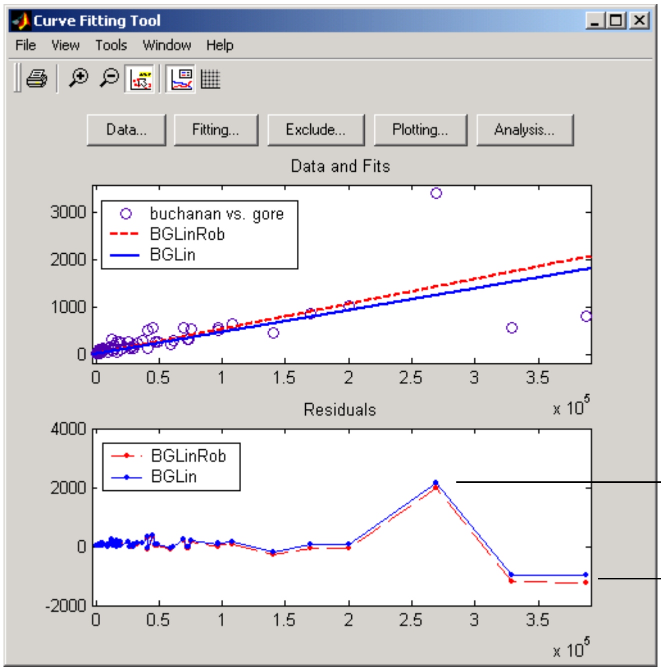
The graphical results show that the linear model is reasonable for the majority of data points, and the residuals appear to be randomly scattered around zero. However, two residuals stand out. The largest residual corresponds to Palm Beach County. The other residual is at the largest predictor value, and corresponds to Miami/Dade County.

The numerical results are shown below. The inverse slope of the robust fit indicates that Buchanan should receive one vote for every 197.4 Bush votes.



```
Linear model:
       f(x) = m*x
Coefficients (with 95% confidence bounds):
       m =    0.005066  (0.004794, 0.005337)
```

The data, robust and regular least squares fits, and residuals for the `buchanan vs. gore` data set are shown below.

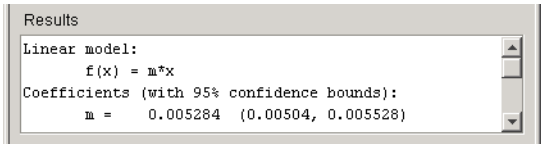


The Palm Beach County residual is very large.

The Miami/Dade and Broward County residuals are also very large.

Again, the graphical results show that the linear model is reasonable for the majority of data points, and the residuals appear to be randomly scattered around zero. However, three residuals stand out. The largest residual corresponds to Palm Beach County. The other residuals are at the two largest predictor values, and correspond to Miami/Dade County and Broward County.

The numerical results are shown below. The inverse slope of the robust fit indicates that Buchanan should receive one vote for every 189.3 Gore votes.



```
Linear model:
      f(x) = m*x
Coefficients (with 95% confidence bounds):
      m =    0.005284  (0.00504, 0.005528)
```

Using the fitted slope value, you can determine the expected number of votes that Buchanan should have received for each fit. For the Buchanan versus Bush data, you evaluate the fit at a predictor value of 152,951. For the Buchanan versus Gore data, you evaluate the fit at a predictor value of 269,732. These results are shown below for both data sets and both fits.

Table 3-5: Expected Buchanan Votes in Palm Beach County

Data Set	Fit	Expected Buchanan Votes
Buchanan vs. Bush	Regular least squares	814
	Robust least squares	775
Buchanan vs. Gore	Regular least squares	1246
	Robust least squares	1425

The robust results for the Buchanan versus Bush data suggest that Buchanan received 3411 – 775 = 2636 excess votes, while robust results for the Buchanan versus Gore data suggest that Buchanan received 3411 – 1425 = 1986 excess votes.

The margin of victory for George Bush is given by

```
margin = sum(bush) sum(gore)
margin =

   537
```

Therefore, the voter intention comes into play because in both cases, the margin of victory is less than the excess Buchanan votes.

In conclusion, the analysis of the 2000 United States presidential election results for the state of Florida suggests that the Reform Party candidate received an excess number of votes in Palm Beach County, and that this excess number was a crucial factor in determining the election outcome. However, additional analysis is required before a final conclusion can be made.

Nonparametric Fitting

In some cases, you are not concerned about extracting or interpreting fitted parameters. Instead, you might simply want to draw a smooth curve through your data. Fitting of this type is called *nonparametric fitting*. The Curve Fitting Toolbox supports these nonparametric fitting methods:

- Interpolants — Estimate values that lie between known data points.
- Smoothing spline — Create a smooth curve through the data. You adjust the level of smoothness by varying a parameter that changes the curve from a least squares straight-line approximation to a cubic spline interpolant.

For more information about interpolation, refer to "Polynomials and Interpolation" and the `interp1` function in the MATLAB documentation. For more information about smoothing splines, refer to "Tutorial" and the `csaps` function in the Spline Toolbox documentation.

Interpolants

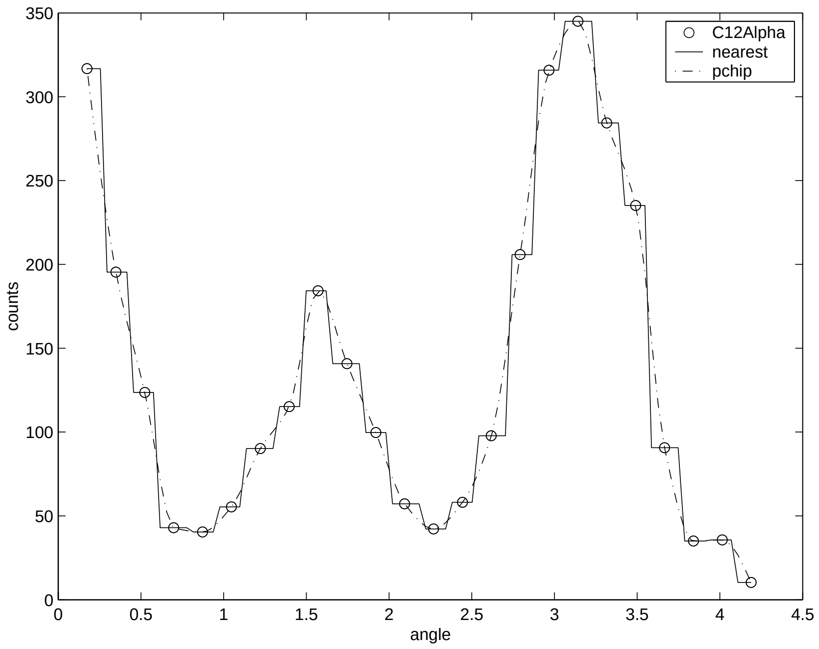
Interpolation is a process for estimating values that lie between known data points. The supported interpolant methods are shown below.

Table 3-6: Interpolant Methods

Method	Description
Linear	Linear interpolation. This method fits a different linear polynomial between each pair of data points.
Nearest neighbor	Nearest neighbor interpolation. This method sets the value of an interpolated point to the value of the nearest data point. Therefore, this method does not generate any new data points.
Cubic spline	Cubic spline interpolation. This method fits a different cubic polynomial between each pair of data points.
Shape-preserving	Piecewise cubic Hermite interpolation (PCHIP). This method preserves monotonicity and the shape of the data.

The type of interpolant you should use depends on the characteristics of the data being fit, the required smoothness of the curve, speed considerations, postfit analysis requirements, and so on. The linear and nearest neighbor methods are fast, but the resulting curves are not very smooth. The cubic spline and shape-preserving methods are slower, but the resulting curves are often very smooth.

For example, the nuclear reaction data from the file `carbon12alpha.mat` is shown below with a nearest neighbor interpolant fit and a shape-preserving (PCHIP) interpolant fit. Clearly, the nearest neighbor interpolant does not follow the data as well as the shape-preserving interpolant. The difference between these two fits can be important if you are interpolating. However, if you want to integrate the data to get a sense of the total unormalized strength of the reaction, then both fits provide nearly identical answers for reasonable integration bin widths.



Note Goodness of fit statistics, prediction bounds, and weights are not defined for interpolants. Additionally, the fit residuals are always zero (within computer precision) because interpolants pass through the data points.

Interpolants are defined as *piecewise polynomials* because the fitted curve is constructed from many "pieces." For cubic spline and PCHIP interpolation, each piece is described by four coefficients, which are calculated using a cubic (third-degree) polynomial. Refer to the `spline` function for more information about cubic spline interpolation. Refer to the `pchip` function for more information about shape-preserving interpolation, and for a comparison of the two methods.

Parametric polynomial fits result in a global fit where one set of fitted coefficients describes the entire data set. As a result, the fit can be erratic. Because piecewise polynomials always produce a smooth fit, they are more flexible than parametric polynomials and can be effectively used for a wider range of data sets.

Smoothing Spline

If your data is noisy, you might want to fit it using a smoothing spline. Alternatively, you can use one of the smoothing methods described in "Smoothing Data" on page 2-9.

The smoothing spline s is constructed for the specified *smoothing parameter p* and the specified weights w_i. The smoothing spline minimizes

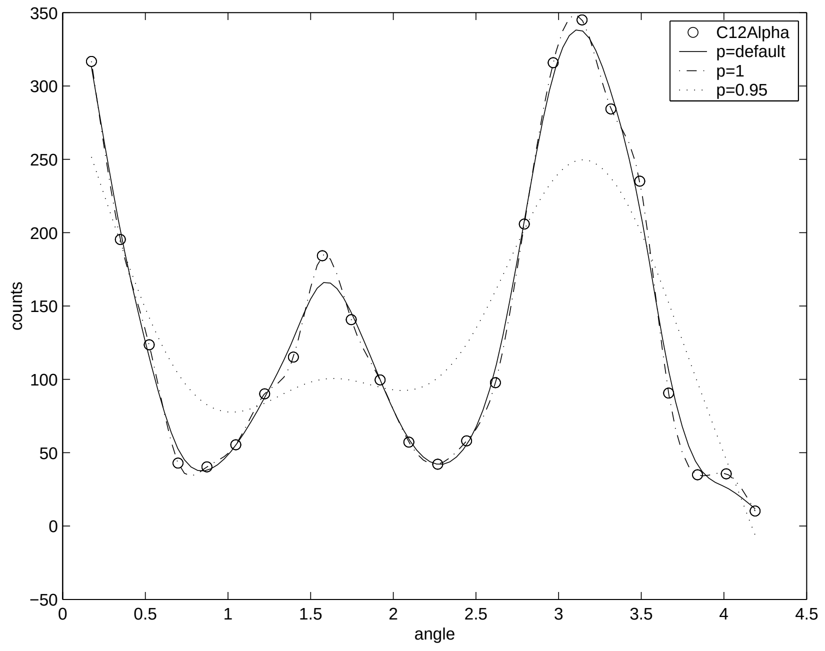
$$p\sum_{i} w_i(y_i - s(x_i))^2 + (1-p)\int\left(\frac{d^2 s}{dx^2}\right)^2 dx$$

If the weights are not specified, they are assumed to be 1 for all data points.

p is defined between 0 and 1. $p = 0$ produces a least squares straight line fit to the data, while $p = 1$ produces a cubic spline interpolant. If you do not specify the smoothing parameter, it is automatically selected in the "interesting range." The interesting range of p is often near $1/(1+h^3/6)$ where h is the average spacing of the data points, and it is typically much smaller than the allowed range of the parameter. Because smoothing splines have an associated parameter, you can consider these fits to be parametric. However, smoothing splines are also piecewise polynomials like cubic spline or shape-preserving interpolants and are considered a nonparametric fit type in this guide.

Note The smoothing spline algorithm used by the Curve Fitting Toolbox is based on the `csaps` function included with the Spline Toolbox. Refer to the `csaps` reference pages for detailed information about smoothing splines.

The nuclear reaction data from the file `carbon12alpha.mat` is shown below with three smoothing spline fits. The default smoothing parameter (p = 0.99) produces the smoothest curve. The cubic spline curve (p = 1) goes through all the data points, but is not quite as smooth. The third curve (p = 0.95) misses the data by wide margin and illustrates how small the “interesting range” of p can be.

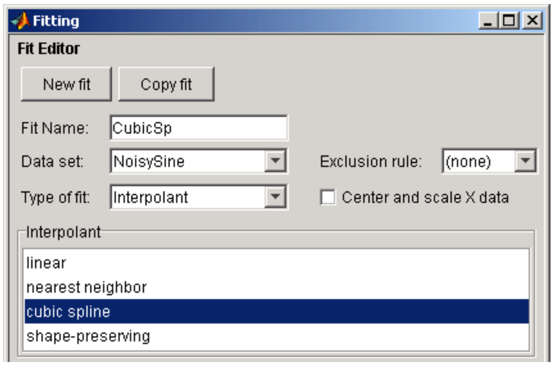


Example: Nonparametric Fit

This example fits the following data using a cubic spline interpolant and several smoothing splines.

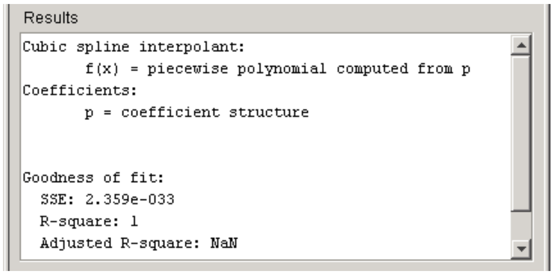
```
rand('state',0);
x = (4*pi)*[0 1 rand(1,25)];
y = sin(x) + .2*(rand(size(x))-.5);
```

As shown below, you can fit the data with a cubic spline by selecting **Interpolant** from the **Type of fit** list.



Fit Name: CubicSp
Data set: NoisySine
Exclusion rule: (none)
Type of fit: Interpolant
☐ Center and scale X data
Interpolant: cubic spline

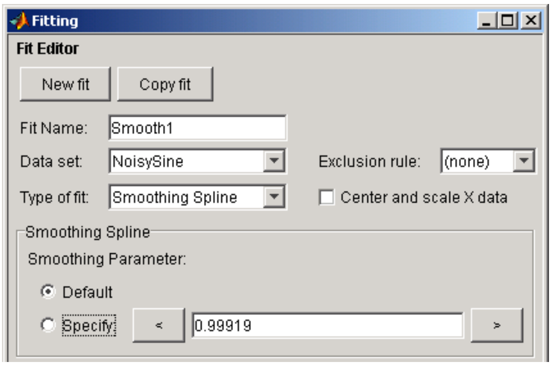
The results shown below indicate that goodness of fit statistics are not defined for interpolants.



```
Results
Cubic spline interpolant:
       f(x) = piecewise polynomial computed from p
Coefficients:
       p = coefficient structure


Goodness of fit:
  SSE: 2.359e-033
  R-square: 1
  Adjusted R-square: NaN
```

As described in “Interpolants” on page 3-68, cubic spline interpolation is defined as a piecewise polynomial that results in a structure of coefficients. The number of “pieces” in the structure is one less than the number of fitted data points, and the number of coefficients for each piece is four because the polynomial degree is three. The toolbox does not allow you to access the structure of coefficients.

As shown below, you can fit the data with a smoothing spline by selecting **Smoothing Spline** in the **Type of fit** list.



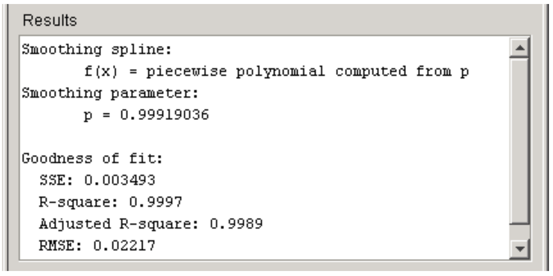
Fit Name: Smooth1
Data set: NoisySine
Exclusion rule: (none)
Type of fit: Smoothing Spline
☐ Center and scale X data
(● Default) ○ Specify: 0.99919

The default smoothing parameter is based on the data set you fit.

The level of smoothness is given by the **Smoothing Parameter**. The default smoothing parameter value depends on the data set, and is automatically calculated by the toolbox after you click the **Apply** button.

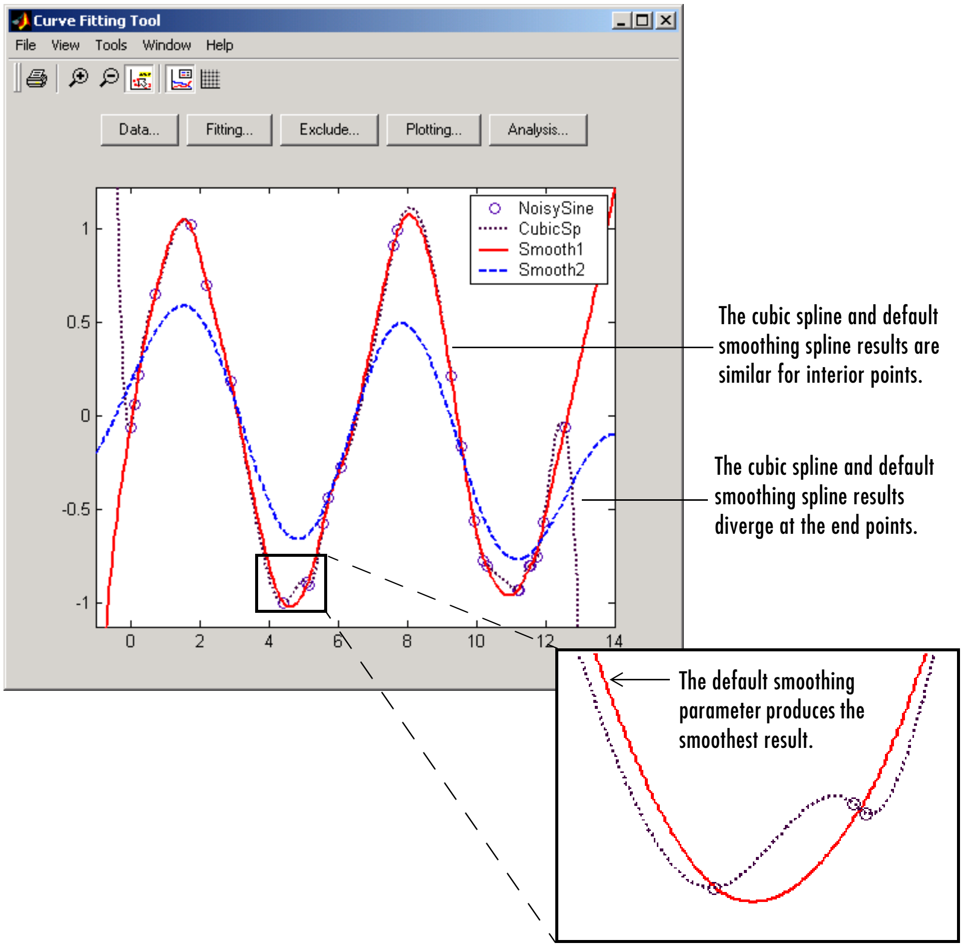
For this data set, the default smoothing parameter is close to 1, indicating that the smoothing spline is nearly cubic and comes very close to passing through each data point. Create a fit for the default smoothing parameter and name it `Smooth1`. If you do not like the level of smoothing produced by the default smoothing parameter, you can specify any value between 0 and 1. A value of 0 produces a piecewise linear polynomial fit, while a value of 1 produces a piecewise cubic polynomial fit, which passes through all the data points. For comparison purposes, create another smoothing spline fit using a smoothing parameter of 0.5 and name the fit `Smooth2`.

The numerical results for the smoothing spline fit `Smooth1` are shown below.



```
Smoothing spline:
       f(x) = piecewise polynomial computed from p
Smoothing parameter:
       p = 0.99919036

Goodness of fit:
  SSE: 0.003493
  R-square: 0.9997
  Adjusted R-square: 0.9989
  RMSE: 0.02217
```

The data and fits are shown below. The default abscissa scale was increased to show the fit behavior beyond the data limits. You change the axes limits with **Tools->Axes Limit Control** menu item.


Curve Fitting Tool
File View Tools Window Help
Data... Fitting... Exclude... Plotting... Analysis...
NoisySine
CubicSp
Smooth1
Smooth2
1
0.5
0
-0.5
-1
0
2
4
6
8
10
12
14
The cubic spline and default smoothing spline results are similar for interior points.
The cubic spline and default smoothing spline results diverge at the end points.
The default smoothing parameter produces the smoothest result.

Note that the default smoothing parameter produces the smoothest curve. As the smoothing parameter increases beyond the default value, the associated curve approaches the cubic spline curve.

Selected Bibliography

[1] Draper, N.R and H. Smith, *Applied Regression Analysis*, 3rd Ed., John Wiley & Sons, New York, 1998.

[2] Bevington, P.R. and D.K. Robinson, *Data Reduction and Error Analysis for the Physical Sciences*, 2nd Ed., WCB/McGraw-Hill, Boston, 1992.

[3] Daniel, C. and F.S. Wood, *Fitting Equations to Data*, John Wiley & Sons, New York, 1980.

[4] Branch, M.A., T.F. Coleman, and Y. Li, "A Subspace, Interior, and Conjugate Gradient Method for Large-Scale Bound-Constrained Minimization Problems," *SIAM Journal on Scientific Computing*, Vol. 21, Number 1, pp. 1-23, 1999.

[5] Levenberg, K., "A Method for the Solution of Certain Problems in Least Squares," *Quart. Appl. Math*, Vol. 2, pp. 164-168, 1944.

[6] Marquardt, D., "An Algorithm for Least Squares Estimation of Nonlinear Parameters," *SIAM J. Appl. Math*, Vol. 11, pp. 431-441, 1963.

[7] DuMouchel, W. and F. O'Brien, "Integrating a Robust Option into a Multiple Regression Computing Environment," in *Computing Science and Statistics: Proceedings of the 21st Symposium on the Interface*, (K. Berk and L. Malone, eds.), American Statistical Association, Alexandria, VA, pp. 297-301, 1989.

[8] DeAngelis, D.J., J.R. Calarco, J.E. Wise, H.J. Emrich, R. Neuhausen, and H. Weyand, "Multipole Strength in ^{12}C from the $(e,e'\alpha)$ Reaction for Momentum Transfers up to 0.61 fm^{-1}," *Phys. Rev. C*, Vol. 52, Number 1, pp. 61-75 (1995).

Function Reference

This chapter describes the toolbox M-file functions that you use directly. A number of other M-file helper functions are provided with this toolbox to support the functions listed below. These helper functions are not documented because they are not intended for direct use.

Functions — Categorical List

Fitting Data

`cfit`	Create a cfit object
`fit`	Fit data using a library or custom model, a smoothing spline, or an interpolant
`fitoptions`	Create or modify a fit options object
`fittype`	Create a fit type object

Getting Information and Help

`cflibhelp`	Display information about library models, splines, and interpolants
`disp`	Display descriptive information for Curve Fitting Toolbox objects

Getting and Setting Properties

`get`	Return properties for a fit options object
`set`	Configure or display property values for a fit options object

Preprocessing Data

`excludedata`	Specify data to be excluded from a fit
`smooth`	Smooth the response data

Postprocessing Data

`confint`	Compute confidence bounds for fitted coefficients
`differentiate`	Differentiate a fit result object
`integrate`	Integrate a fit result object
`predint`	Compute prediction bounds for new observations or for the function

General Purpose

`cftool`	Open the Curve Fitting Tool
`datastats`	Return descriptive statistics about the data
`feval`	Evaluate a fit result object or a fit type object
`plot`	Plot data, fit, prediction bounds, outliers, and residuals

Functions — Alphabetical List

This section contains function reference pages listed alphabetically.

Purpose

Create a cfit object

Syntax

```
fmodel = cfit(ftype,coef1,coef2,...)
```

Arguments

`ftype`	A fit type object representing a custom or library model.
`coef1,coef2,...`	The model coefficients.
`fmodel`	The cfit object.

Description

`fmodel = cfit(ftype,coef1,coef2,...)` creates the cfit object `fmodel` based on the custom or library model specified by `ftype`, and with the coefficients specified by `coef1`, `coef2`, and so on. You create `ftype` with the `fittype` function.

Remarks

`cfit` is called by the `fit` function. You should call `cfit` directly if you want to assign coefficients and problem parameters to a model without performing a fit.

Example

Create a fit type object and assign values to the coefficients and to the problem parameter.

```
m = fittype('a*x^2+b*exp(n*x)','prob','n');
f = cfit(m,pi,10.3,3);
```

See Also

`fit`, `fittype`

cflibhelp

Purpose Display information about library models, splines, and interpolants

Syntax

```
cflibhelp
cflibhelp group
```

Arguments

group	The name of the fit type group.

Description `cflibhelp` displays the names, equations, and descriptions for all the fit types in the curve fitting library. You can use the fit type name as an input parameter to the `fit`, `cfit`, and `fittype` functions.

`cflibhelp` *group* displays the names, equations, and descriptions for the fit type group specified by *group*. The supported fit type groups are given below.

Group	Description
`distribution`	Distribution models such as Weibull
`exponential`	One-term and two-term exponential equations
`fourier`	Sums of sine and cosine equations up to eight terms
`gaussian`	Sums of Gaussian equations up to eight terms
`interpolant`	Interpolant fit types including linear, nearest neighbor, cubic spline, and shape-preserving interpolation
`polynomial`	Polynomial equations up to ninth degree
`power`	One-term and two-term power equations
`rational`	Ratios of polynomial equations up to degree 5 in both numerator and denominator
`sin`	Sums of sine equations up to eight terms
`spline`	Cubic spline and smoothing spline fit types

For more information about the toolbox library models, refer to “Library Models” on page 3-16. For more information about the toolbox library interpolants and splines, refer to “Nonparametric Fitting” on page 3-68.

Example

Display the names and descriptions for the spline fit type group.

```
cflibhelp spline

SPLINES

        SPLINETYPE              DESCRIPTION

        cubicspline             cubic interpolating spline
        smoothingspline         smoothing spline
```

Display the model names and equations for the polynomial fit type group.

```
cflibhelp polynomial

  POLYNOMIAL MODELS

        MODELNAME              EQUATION

          poly1                 Y = p1*x+p2
          poly2                 Y = p1*x^2+p2*x+p3
          poly3                 Y = p1*x^3+p2*x^2+...+p4
          ...
          poly9                 Y = p1*x^9+p2*x^8+...+p10
```

See Also

`cfit`, `fit`, `fittype`

cftool

Purpose Open the Curve Fitting Tool

Syntax

```
cftool
cftool(xdata,ydata)
```

Arguments

`xdata`	A vector of predictor data.
`ydata`	A vector of response data.

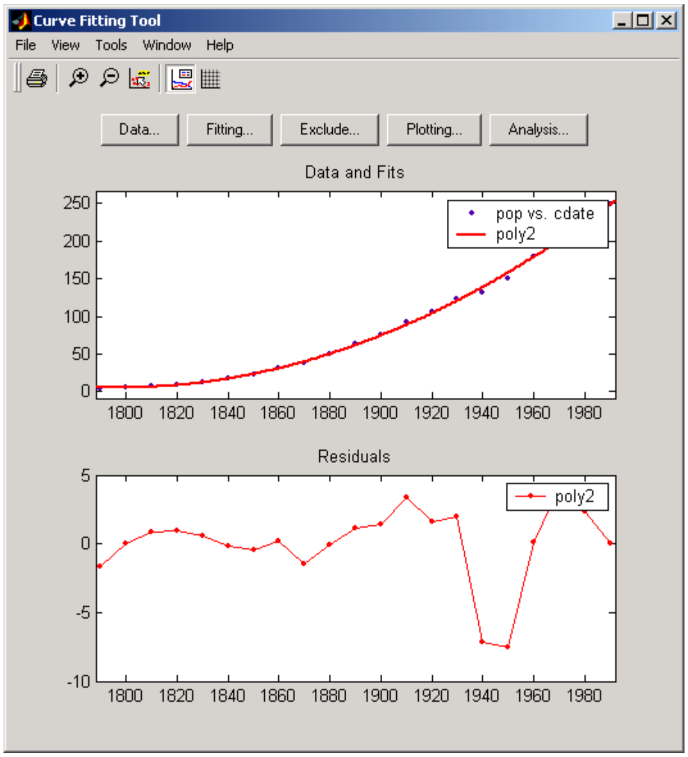
Description `cftool` opens the Curve Fitting Tool.

`cftool(xdata,ydata)` opens the Curve Fitting Tool with predictor data specified by `xdata` and response data specified by `ydata`. `xdata` and `ydata` must be vectors of the same size. `Infs` and `NaNs` are ignored because you cannot fit data containing these values. Additionally, only the real component of a complex value is used.

Remarks The Curve Fitting Tool is a graphical user interface (GUI) that allows you to

- Visually explore data and fits as scatter plots
- Graphically evaluate the goodness of fit using residuals and prediction bounds
- Access GUIs for importing, preprocessing, and fitting data, and for plotting and analyzing fits to the data

The Curve Fitting Tool is shown below. The data is from the census MAT-file, and the fit is a quadratic polynomial. The residuals are shown as a line plot below the data and fit.



The Curve Fitting Tool provides several features that facilitate data and fit exploration. Refer to “Viewing Data” on page 2-6 for a description of these features.

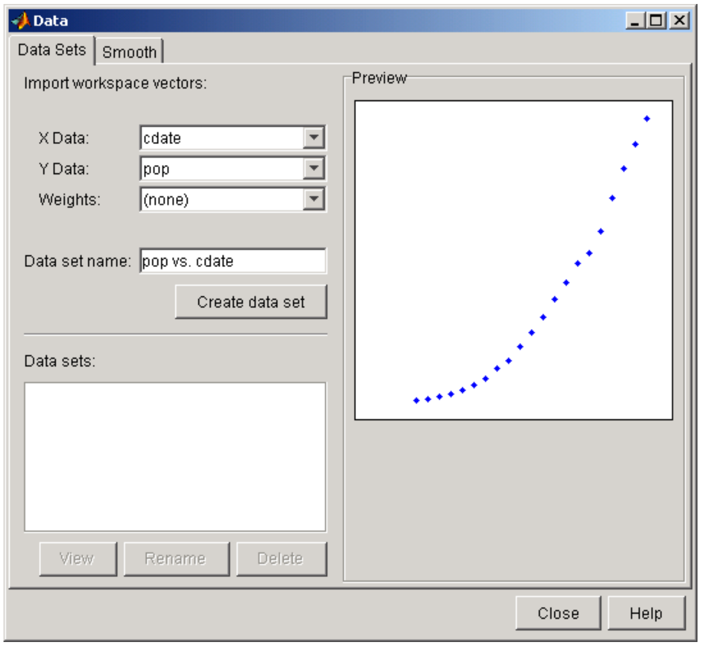
By clicking the **Data**, **Fitting**, **Exclude**, **Plotting**, or **Analysis** buttons, you can open the associated GUIs, which are described below. For a complete example that uses many of these GUIs, refer to Chapter 1, “Getting Started with the Curve Fitting Toolbox.”

The Data GUI

The Data GUI allows you to

- Import, preview, name, and delete data sets
- Smooth noisy data

The Data GUI is shown below with the census data loaded.



Import workspace vectors:

X Data: cdate

Y Data: pop

Weights: (none)

Data set name: pop vs. cdate

Data sets:

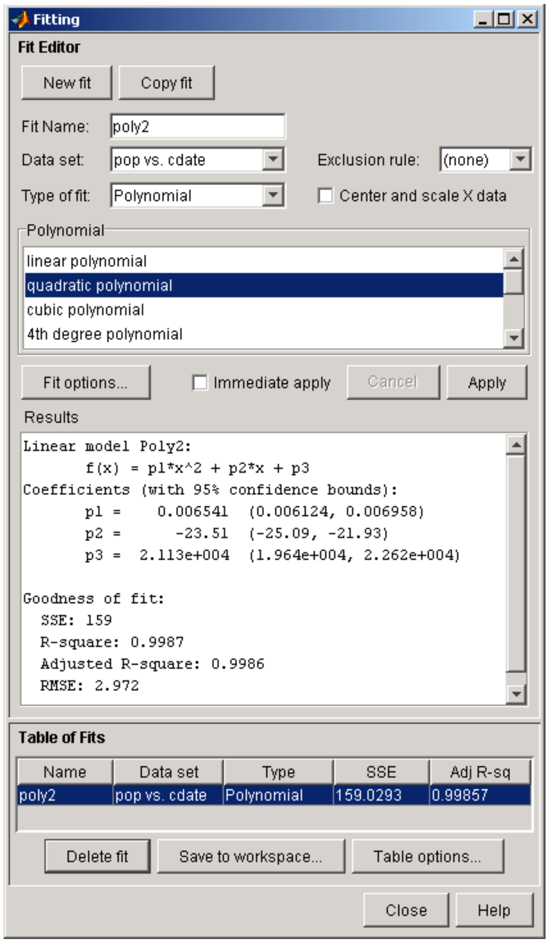
Refer to Chapter 2, “Importing, Viewing, and Preprocessing Data” for more information about the Data GUI.

The Fitting GUI

The Fitting GUI allows you to

- Fit data using a parametric or nonparametric equation
- Examine and compare fit results including fitted coefficient values and goodness of fit statistics
- Keep track of all the data sets and fits for the current session

The Fitting GUI shown below displays the results of fitting the census data to a quadratic polynomial.



Fit Name: poly2
Data set: pop vs. cdate
Exclusion rule: (none)
Type of fit: Polynomial
Center and scale X data

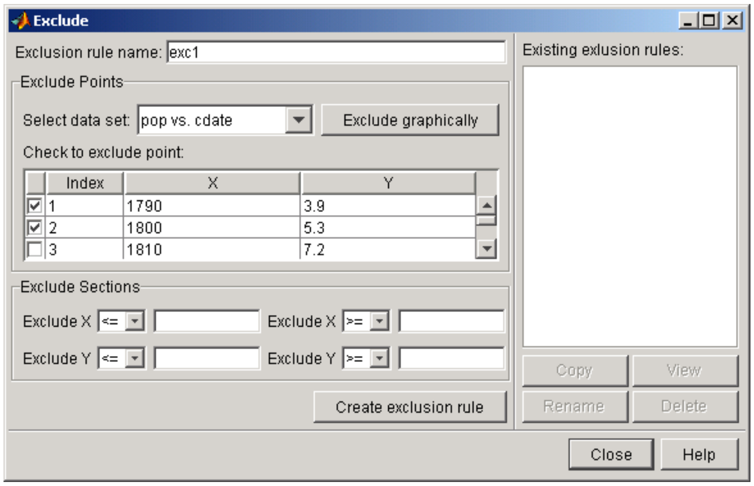
Polynomial
- linear polynomial
- quadratic polynomial
- cubic polynomial
- 4th degree polynomial

```
Linear model Poly2:
       f(x) = p1*x^2 + p2*x + p3
Coefficients (with 95% confidence bounds):
       p1 =    0.006541  (0.006124, 0.006958)
       p2 =      -23.51  (-25.09, -21.93)
       p3 =  2.113e+004  (1.964e+004, 2.262e+004)

Goodness of fit:
  SSE: 159
  R-square: 0.9987
  Adjusted R-square: 0.9986
  RMSE: 2.972
```

Name	Data set	Type	SSE	Adj R-sq
poly2	pop vs. cdate	Polynomial	159.0293	0.99857

The Exclude GUI

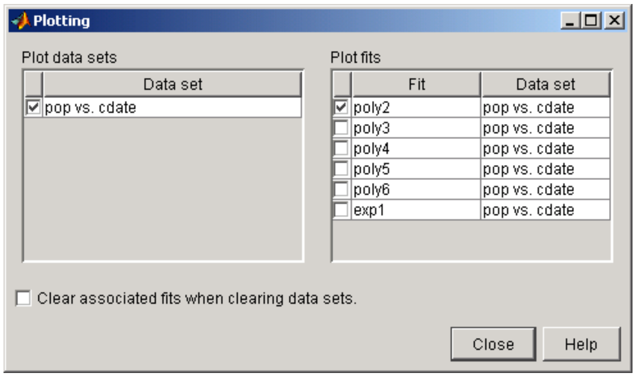
The Exclude GUI allows you to create exclusion rules for a data set. An exclusion rule identifies data to be excluded while fitting. The excluded data can be individual data points, or a section of predictor or response data. The Exclude GUI shown below indicates that the first two data points of the census data are marked for exclusion, and that this exclusion rule is named `exc1`.



	Index	X	Y
✓	1	1790	3.9
✓	2	1800	5.3
☐	3	1810	7.2

The Plotting GUI

The Plotting GUI allows you to control the data sets and fits displayed by the Curve Fitting Tool. The Plotting GUI shown below indicates that the census data and the fit `poly2` are displayed by the Curve Fitting Tool.



	Data set
✓	pop vs. cdate

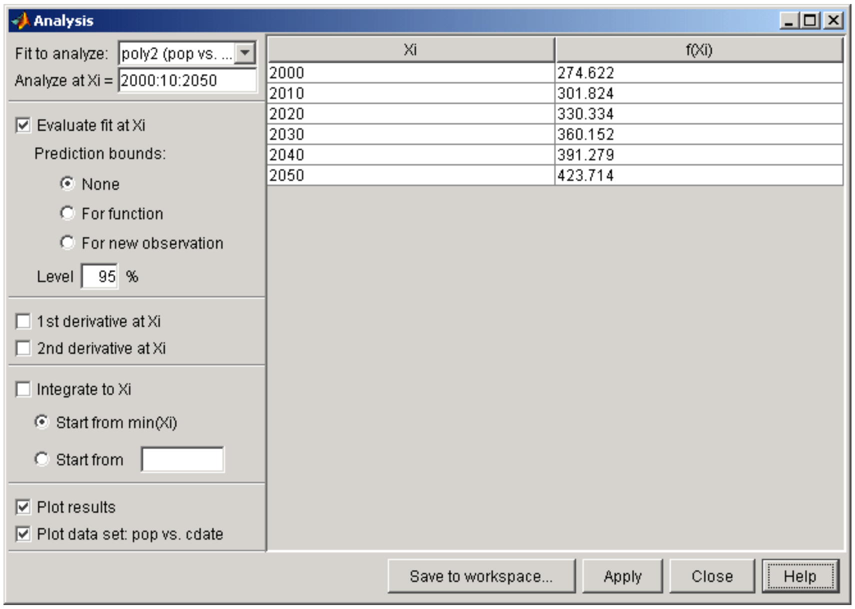
	Fit	Data set
✓	poly2	pop vs. cdate
☐	poly3	pop vs. cdate
☐	poly4	pop vs. cdate
☐	poly5	pop vs. cdate
☐	poly6	pop vs. cdate
☐	exp1	pop vs. cdate

The Analysis GUI

The Analysis GUI allows you to

- Evaluate (interpolate or extrapolate), differentiate, or integrate a fit
- Plot the analysis results and the data set

The Analysis GUI shown below displays the numerical results of extrapolating the census data from the year 2000 to the year 2050 in 10-year increments.



Fit to analyze: poly2 (pop vs. ...
Analyze at Xi = 2000:10:2050

☑ Evaluate fit at Xi
Prediction bounds: [✓ None] For function / For new observation
Level 95 %

☐ 1st derivative at Xi
☐ 2nd derivative at Xi

☐ Integrate to Xi
[✓ Start from min(Xi)] Start from

☑ Plot results
☑ Plot data set: pop vs. cdate

Xi	f(Xi)
2000	274.622
2010	301.824
2020	330.334
2030	360.152
2040	391.279
2050	423.714

Refer to "Analyzing the Fit" on page 1-17 for an example that uses the Analysis GUI.

confint

Purpose

Compute confidence bounds for fitted coefficients

Syntax

```
ci = confint(fresult)
ci = confint(fresult,level)
```

Arguments

`fresult`	A fit result object.
`level`	The confidence level.
`ci`	An array of confidence bounds.

Description

`ci = confint(fresult)` returns 95% confidence bounds to `ci` for the fit coefficients associated with `fresult`. `fresult` is the fit result object returned by the `fit` function. `ci` is a 2-by-n array where n is the number of coefficients associated with `fresult`. The top row of the array contains the lower bound, while the bottom row of the array contains the upper bound for each coefficient

`ci = confint(fresult,level)` returns confidence bounds for the confidence level specified by `level`. You specify `level` on the interval (0,1). For example, if `level` is 0.99, then 99% confidence bounds are calculated.

Remarks

To calculate confidence bounds, `confint` uses R^{-1} (the inverse R factor from QR decomposition of the Jacobian), the degrees of freedom for error, and the root mean squared error. This information is automatically returned by the `fit` function and contained within the fit result object.

If coefficients are bounded and one or more of the estimates are at their bounds, those estimates are regarded as fixed and do not have confidence bounds. Note that you cannot calculate confidence bounds for the smoothing spline and interpolant fit types.

Example

Fit the census data to a second-degree polynomial. The display for `fresult` includes the 95% confidence bounds for the fitted coefficients.

```
load census
fresult = fit(cdate,pop,'poly2')

fresult =
     Linear model Poly2:
       fresult(x) = p1*x^2 + p2*x + p3
     Coefficients (with 95% confidence bounds):
       p1 =    0.006541  (0.006124, 0.006958)
       p2 =      -23.51  (-25.09, -21.93)
       p3 =  2.113e+004  (1.964e+004, 2.262e+004)
```

Calculate 95% confidence bounds for the fitted coefficients using `confint`.

```
ci = confint(fresult,0.95)
ci =

    0.0061242      -25.086        19641
    0.0069581      -21.934        22618
```

Note that the `fit` display and the array returned by `confint` present the confidence bounds using slightly different formats. The `fit` display mimics an n-by-3 array where n is the number of coefficients, the first column is the coefficient variable, the second column is the fitted coefficient value, and the third column is the lower and upper bound. `confint` returns a 2-by-n array where the top row contains the lower bound and the bottom row contains the upper bound for each coefficient.

See Also

`fit`

datastats

Purpose

Return descriptive statistics about the data

Syntax

```
xds = datastats(xdata)
[xds,yds] = datastats(xdata,ydata)
```

Arguments

`xdata`	A column vector of predictor data.
`ydata`	A column vector of response data.
`xds`	A structure containing descriptive statistics for `xdata`.
`yds`	A structure containing descriptive statistics for `ydata`.

Description

`xds = datastats(xdata)` returns statistics for `xdata` to the structure `xds`. The structure contains the fields shown below.

Field	**Description**
`num`	The number of data values
`max`	The maximum data value
`min`	The minimum data value
`mean`	The mean value of the data
`median`	The median value of the data
`range`	The range of the data
`std`	The standard deviation of the data

`[xds,yds] = datastats(xdata,ydata)` returns statistics for `xdata` and `ydata` to the structures `xds` and `yds`, respectively. `xds` and `yds` contain the fields shown above. `xdata` and `ydata` are column vectors of the same size.

Remarks

If `xdata` or `ydata` contains complex values, only the real part of the value is used in the statistics computations. If the data contains `Inf`s or `NaN`s, they are processed using the usual MATLAB rules.

Example

Return data statistics for the census data.

```
load census
[xds,yds] = datastats(cdate,pop)

xds = 

       num: 21
       max: 1990
       min: 1790
      mean: 1890
    median: 1890
     range: 200
       std: 62.048

yds = 

       num: 21
       max: 248.7
       min: 3.9
      mean: 85.729
    median: 62.9
     range: 244.8
       std: 78.601
```

differentiate

Purpose

Differentiate a fit result object

Syntax

```
deriv1 = differentiate(fitresult,x)
[deriv1,deriv2] = differentiate(...)
```

Arguments

`fresult`	A fit result object.
`x`	A column vector of values at which `fresult` is differentiated.
`deriv1`	A column vector of first derivatives.
`deriv2`	A column vector of second derivatives.

Description

`deriv1 = differentiate(fitresult,x)` differentiates the fit result object `fresult` at the points specified by `x` and returns the result to `deriv1`. You can generate `fresult` with the `fit` function or the `cfit` function.

`[deriv1,deriv2] = differentiate(...)` computes the first derivative `deriv1`, and the second derivative `deriv2` for the specified fit result object.

Remarks

For library equations with closed forms, analytic derivatives are calculated. For all other equations, the first derivative is calculated using the central difference quotient

$$y' = \frac{y_{x+h} - y_{x-h}}{2h}$$

where x is the predictor value at which the derivative is calculated, h is a small number, y_{x+h} is `fresult` evaluated at $x+h$, and y_{x-h} is `fresult` evaluated at $x-h$. The second derivative is calculated using the expression

$$y'' = \frac{y_{x+h} + y_{x-h} - 2y_x}{h^2}$$

Example

Create a noisy sine wave on the interval [0, 4π].

```
rand('state',0);
x = linspace(0,4*pi,200)';
y = sin(x) + (rand(size(x))-0.5)*0.2;
```

Create a custom fit type, and fit the data using reasonable starting values.

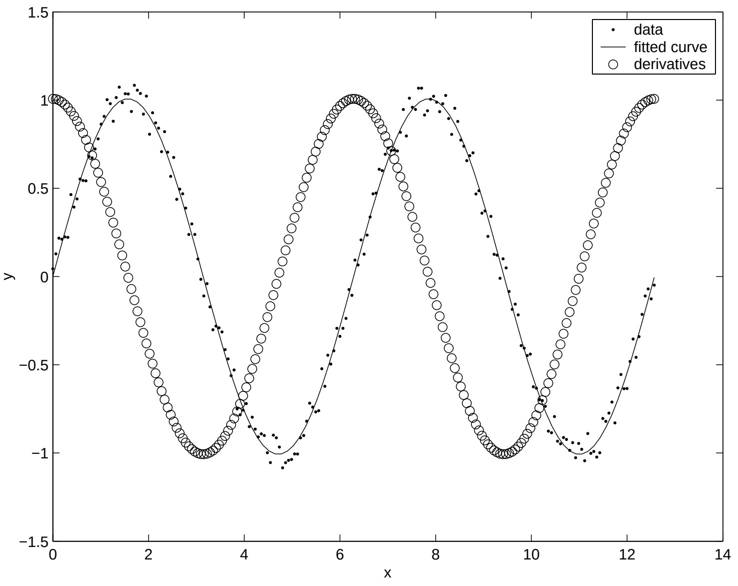
```
ftype = fittype('a*sin(b*x)');
fopts = fitoptions('Method','Nonlinear','start',[1 1]);
fit1 = fit(x,y,ftype,fopts);
```

Calculate the first derivative for each value of `x`.

```
deriv1 = differentiate(fit1,x);
```

Plot the data, the fit to the data, and the first derivatives.

```
plot(fit1,'k-',x,y,'b.');hold on
plot(x,deriv1,'ro')
legend('data','fitted curve','derivatives')
```



See Also

`cfit`, `fit`, `integrate`

disp

Purpose Display descriptive information for Curve Fitting Toolbox objects

Syntax

```
obj
disp(obj)
```

Arguments

`obj`	A Curve Fitting Toolbox object.

Description `obj` or `disp(obj)` displays descriptive information for `obj`. You can create `obj` with the `fit` or `cfit` function, the `fitoptions` function, or the `fittype` function.

Example The display for a custom fit type object is shown below.

```
ftype = fittype('a*x^2+b*x+c+d*exp(-e*x)')

ftype =
     General model:
       ftype(a,b,c,d,e,x) = a*x^2+b*x+c+d*exp(-e*x)
```

The display for a fit options object is shown below.

```
fopts = fitoptions('Method','Nonlinear','Normalize','on')

fopts =
        Normalize: 'on'
          Exclude: []
          Weights: []
           Method: 'NonlinearLeastSquares'
           Robust: 'Off'
       StartPoint: []
            Lower: []
            Upper: []
        Algorithm: 'Trust-Region'
    DiffMinChange: 1e-008
    DiffMaxChange: 0.1
          Display: 'Notify'
      MaxFunEvals: 600
          MaxIter: 400
           TolFun: 1e-006
             TolX: 1e-006
```

Note that all fit types have the Normalize, Exclude, Weights, and Method fit options. Additional fit options are available depending on the Method value. For example, if Method is SmoothingSpline, the SmoothingParam fit option is available.

The display for a fit result object is shown below.

```
fresult = fit(cdate,pop,ftype,fopts)

Warning: Start point not provided, choosing random start point.
Maximum number of function evaluations exceeded. Increasing
MaxFunEvals (in fit options) may allow for a better fit, or
the current equation may not be a good model for the data.

fresult =

     General model:
       fresult(x) = a*x^2+b*x+c+d*exp(-e*x)
       where x is normalized by mean 1890 and std 62.05
     Coefficients (with 95% confidence bounds):
       a =       21.14  (-27.61, 69.89)
       b =       64.49  (-188.5, 317.4)
       c =       49.92  (-421.5, 521.4)
       d =       11.96  (-458, 481.9)
       e =     -0.7745  (-10.25, 8.701)
```

See Also cfit, fit, fitoptions, fittype

excludedata

Purpose

Specify data to be excluded from a fit

Syntax

```
outliers = excludedata(xdata,ydata,'MethodName',MethodValue)
```

Arguments

`xdata`	A column vector of predictor data.
`ydata`	A column vector of response data.
`'MethodName'`	The data exclusion method.
`MethodValue`	The value associated with *`MethodName`*.
`outliers`	A logical vector that defines data to be excluded from a fit.

Description

`outliers = excludedata(xdata,ydata,'MethodName',MethodValue)` identifies data to be excluded from a fit using the specified *`MethodName`* and `MethodValue`. `outliers` is a logical vector containing 1's marking data points to exclude while fitting, and 0's marking data points to include while fitting. The data exclusion methods are given below.

Method	Description
`box`	A four-element vector that specifies a box of data to include in a fit. Data outside the box is excluded. You specify the box as [x_{min} x_{max} y_{min} y_{max}].
`domain`	A two-element vector that specifies the domain of data to include in a fit. Data outside this domain is excluded. You specify the domain as [x_{min} x_{max}].
`indices`	A vector specifying the indices of the data points to be excluded.
`range`	A two-element vector that specifies the range of data to include in a fit. Data outside this range is excluded. You specify the range as [y_{min} y_{max}].

Remarks

You can combine data exclusion methods using logical operators. For example, to combine methods using the | (OR) operator

```
outliers = excludedata(xdata,ydata,'indices',[3 5]);
outliers = outliers|excludedata(xdata,ydata,'box',[1 10 0 90]);
```

In some cases, you might want to use the ~ (NOT) operator to specify a box that contains all the data to exclude.

```
outliers = ~excludedata(xdata,ydata,'box',[1 10 0 90]);
```

Example

Generate random data in the interval [0, 15], create a sine wave with noise, and add two outliers with the value 2.

```
rand('state',0);
x = 15*rand(150,1);
y = sin(x) + (rand(size(x))-0.5)*0.5;
y(ceil(length(x)*rand(2,1))) = 2;
```

Identify outliers that are outside the interval [-1.5, 1.5] using the `range` method.

```
outliers = excludedata(x,y,'range',[-1.5 1.5]);
```

Identify the same outliers using the `indices` method.

```
ind = find((y>1.5)|(y<-1.5));
outliers = excludedata(x,y,'indices',ind);
```

You can pass `outliers` to the `fit` function to exclude the specified data points from a fit.

```
ftype = fittype('a*sin(b*x)');
fresult = fit(x,y,ftype,'startpoint',[1 1],'exclude',outliers);
```

See Also

`fit`

feval

Purpose

Evaluate a fit result object or a fit type object

Syntax

```
f = feval(fresult,x)
f = feval(ftype,coef1,coef2,...,x)
```

Arguments

`fresult`	A fit result object.
`x`	A column vector of values at which `fresult` or `ftype` is evaluated.
`ftype`	A fit type object.
`coef1,coef2,...`	The model coefficients assigned to `ftype`.
`f`	A column vector containing the result of evaluating `fresult` or `ftype` at `x`.

Description

`f = feval(fresult,x)` evaluates the fit result object `fresult` at the values specified by `x`, and returns the result to `f`. You create a fit result object with the `fit` function.

`f = feval(ftype,coef1,coef2,...,x)` evaluates the fit type object `ftype` using the coefficients specified by `coef1`, `coef2`, and so on. You create a fit type object with the `fittype` function.

Remarks

You can also evaluate a fit result or a fit type object using the following syntax.

```
f = fresult(x);
f = ftype(coef1,coef2,...,x);
```

Example

Create a fit type object and evaluate the object at `x` using the specified model coefficients.

```
x = (0:0.1:10)';
ftype = fittype('a*x^2+b*x');
f = feval(ftype,1,2,x);
```

Create a fit result object and evaluate the object over a finer range in x.

```
y = x.^2+(rand(size(x))-0.5);
xx = (0:0.05:10)';
fresult = fit(x,y,ftype);
f = feval(fresult,xx);
```

See Also

fit, fittype

Purpose

Fit data using a library or custom model, a smoothing spline, or an interpolant

Syntax

```
fresult = fit(xdata,ydata,'ltype')
fresult = fit(xdata,ydata,'ltype','PropertyName',PropertyValue, )
fresult = fit(xdata,ydata,'ltype',opts)
fresult = fit(xdata,ydata,'ltype',...,'problem',values)
fresult = fit(xdata,ydata,ftype,...)
[fresult,gof] = fit( )
[fresult,gof,output] = fit( )
```

Arguments

`xdata`	A column vector of predictor data.
`ydata`	A column vector of response data.
`'ltype'`	The name of a library model, spline, or interpolant.
`'PropertyName'`	The name of a fit options property.
`PropertyValue`	A valid value for *`PropertyName`*.
`opts`	A fit options object.
`'problem'`	Specify problem parameters.
`values`	A cell array of problem parameter values.
`ftype`	A fit type object.
`fresult`	The fit result object.
`gof`	Goodness of fit statistics.
`output`	A structure containing information that is associated with the fitting procedure.

Description

`fresult = fit(xdata,ydata,'ltype')` fits the data specified by `xdata` and `ydata` to the library model, interpolant, or smoothing spline specified by *`ltype`*. The fit result is returned to `fresult`. You can display the library fit type names with the `cflibhelp` function. `xdata` and `ydata` cannot contain `Inf`s or `NaN`s. Additionally, only the real part of a complex value is used.

`fresult = fit(xdata,ydata,'`*`ltype`*`','`*`PropertyName`*`', PropertyValue,...)` fits the data using the options specified by *`PropertyName`* and `PropertyValue`. You can display the fit options available for the specified library fit type with the `fitoptions` function.

`fresult = fit(xdata,ydata,'`*`ltype`*`',opts)` fits the data using options specified by the fit options object `opts`. You create a fit options object with the `fitoptions` function. This is an alternative syntax to specifying property name/property value pairs.

`fresult = fit(xdata,ydata,'`*`ltype`*`',...,'`**`problem`**`',values)` assigns `values` to problem parameters. `values` is a cell array with one element per parameter. Problem parameters are problem-dependent constants that you define as part of your model. See `fittype` for more information on problem parameters.

`fresult = fit(xdata,ydata,ftype,...)` fits the data to the fit type object specified by `ftype`. You create a fit type object with the `fittype` function.

`[fresult,gof] = fit(...)` returns goodness of fit statistics to the structure `gof`. The `gof` structure includes the fields shown below.

Field	**Description**
`sse`	Sum of squares due to error
`rsquare`	Coefficient of determination
`dfe`	Degrees of freedom
`adjrsquare`	Degree-of-freedom adjusted coefficient of determination
`rmse`	Root mean squared error (standard error)

`[fresult,gof,output] = fit(...)` returns the structure `output`, which contains information that is associated with the fitting procedure used. Supported fitting procedures include linear least squares, robust nonlinear least squares, and so on. Some information applies to all fitting procedures, while other information is relevant only for particular fitting procedures. For example, the information returned for nonlinear least squares fits is given below.

Field	Description
`numobs`	Number of observations (response values).
`numparam`	Number of unknown parameters to fit.
`residuals`	Vector of residuals.
`Jacobian`	Jacobian matrix.
`exitflag`	Describes the exit condition. If `exitflag` > 0, the function converged to a solution. If `exitflag` = 0, the maximum number of function evaluations or iterations was exceeded. If `exitflag` < 0, the function did not converge to a solution.
`iterations`	Number of iterations used to complete the fit.
`funcCount`	Number of function evaluations used to complete the fit.
`firstorderopt`	Measure of first-order optimality.
`algorithm`	Fitting algorithm used.

Remarks

For rationals and Weibull library models, the coefficient starting values are randomly selected in the range [0,1]. Therefore, if you perform multiple fits to a data set using the same equation, you might get different coefficient results due to different starting values. To avoid this situation, you should pass in a vector of starting values each time you fit, or define a specific state for the random number generator, `rand` or `randn`, before fitting.

For all other library models, optimal starting points are automatically calculated. These values depend on the data, and are based on model-specific heuristics.

Example

Fit the census data with a second-degree polynomial library model and return the goodness of fit statistics and the output structure.

```
load census
[fit1,gof1,out1] = fit(cdate,pop,'poly2');
```

Normalize the data and fit with a third-degree polynomial.

```
[fit1,gof1,out1] = fit(cdate,pop,'poly3','Normalize','on');
```

Fit the data with a single-term exponential library model.

```
[fit2,gof2,out2] = fit(cdate,pop,'exp1','Normalize','on');
```

Create a fit options object, and try to find a better fit by overriding the default starting points for the fit coefficients.

```
opts = fitoptions('exp1','Norm','on','start',[100 0.1]);
[fit3,gof3,out3] = fit(cdate,pop,'exp1',opts);
```

Fit the data to a custom model that contains the problem parameter `n`.

```
mymodel = fittype('a*exp(b*n*x)+c','problem','n');
opts = fitoptions(mymodel);
set(opts,'normalize','on')
[fit4,gof4,out4] = fit(cdate,pop,mymodel,opts,'problem',{2});

Warning: Start point not provided, choosing random start point.
```

The warning occurs whenever you fit data with a custom nonlinear model and do not provide starting points.

See Also

`cflibhelp`, `fitoptions`, `fittype`

fitoptions

Purpose

Create or modify a fit options object

Syntax

```
opts = fitoptions
opts = fitoptions('ltype')
opts = fitoptions('ltype','PropertyName',PropertyValue,...)
opts = fitoptions('method',value)
opts = fitoptions('method',value,'PropertyName',PropertyValue,...)
opts = fitoptions(opts,'PropertyName',PropertyValue,...)
opts = fitoptions(opts,newopts)
```

Arguments

`'ltype'`	The name of a library model, spline, or interpolant.
`'PropertyName'`	The name of a fit options property.
`PropertyValue`	A valid value for *`PropertyName`*.
`'method'`	Specify a toolbox fitting method.
`value`	A supported fitting method.
`opts,newopts`	A fit options object.

Description

`opts = fitoptions` creates the empty fit options object `opts`. The returned options are supported by all fitting methods, and are given by the following properties. Note that curly braces denote default property values.

Property	**Description**
`Normalize`	Specifies whether the data is centered and scaled. The value can be `{'off'}` or `'on'`.
`Exclude`	A vector of one or more data points to exclude from the fit. You can use the `excludedata` function to create this vector.
`Weights`	A vector of weights associated with the response data.
`Method`	The fitting method. The value is `None` for an empty object. A complete list of supported fitting methods is given below.

`opts = fitoptions('`*`ltype`*`')` creates a default fit options object for the library or custom fit type specified by *`ltype`*. You can display the library model, interpolant, and smoothing spline names with the `cflibhelp` function.

`opts = fitoptions('`*`ltype`*`','`*`PropertyName`*`',PropertyValue,...)` creates a fit options object for the specified library fit type, and with the specified property names and property values. Note that you can specify *`PropertyName`* or `PropertyValue` without regard to case, and you can make use of name completion by supplying the minimum number of characters that uniquely identify the string.

`opts = fitoptions('`**`method`**`',value)` creates a default fit options object for the fitting method specified by `value`. A complete list of supported fitting methods is given below.

`opts = fitoptions('`**`method`**`',value,'PropertyName',PropertyValue,...)` creates a default fit options object for the specified fitting method, and with the specified property names and property values.

`opts = fitoptions(opts,'`*`PropertyName`*`',PropertyValue,...)` modifies the existing fit options object with the specified property names and property values.

`opts = fitoptions(opts,newopts)` combines the existing fit options object `opts` with a new fit options object `newopts`. If both objects have the same `Method` value, the nonempty properties in `newopts` override the corresponding properties in `opts`. If the objects have different `Method` values, the output object will have the same `Method` as `opts`, and only the `Normalize`, `Exclude`, and `Weights` properties of `newopts` will override the corresponding properties in `opts`.

Remarks

To display the possible fit options property values, use the `set` function.

```
set(opts)
```

To display the current fit options property values, use the `get` function.

```
get(opts)
```

Note that you can configure or display a single property value using the dot notation. See below for an example.

Additional Fit Options

If `Method` is `NearestInterpolant`, `LinearInterpolant`, `PchipInterpolant`, or `CubicSplineInterpolant`, there are no additional fit options.

If `Method` is `SmoothingSpline`, the `SmoothingParam` property is available to configure the smoothing parameter. You can specify any value between 0 and 1. The default value depends on the data set.

If `Method` is `LinearLeastSquares`, the additional fit option properties shown below are available.

Property	Description
`Robust`	Specifies whether to use the robust linear least squares fitting method. The value can be `{'off'}` or `'on'`.
`Lower`	A vector of lower bounds on the coefficients to be fitted. The coefficients are specified by the input argument `ftype` for `fit`. The default value of `Lower` is an empty vector indicating that the fit is not constrained by lower bounds. If bounds are specified, the vector length must equal the number of coefficients. An unconstrained lower bound is specified by `-Inf`.
`Upper`	A vector of upper bounds on the coefficients to be fitted. The coefficients are specified by the input argument `ftype` for `fit`. The default value of `Upper` is an empty vector indicating that the fit is not constrained by upper bounds. If bounds are specified, the vector length must equal the number of coefficients. An unconstrained upper bound is specified by `Inf`.

If `Method` is `NonlinearLeastSquares`, the additional fit option properties shown below are available.

Property	Description
`Robust`	Specifies whether to use the robust nonlinear least squares fitting method. The value can be `{'off'}` or `'on'`.
`Lower`	A vector of lower bounds on the coefficients to be fitted. The coefficients are specified by the input argument `ftype` for `fit`. The default value of `Lower` is an empty vector indicating that the fit is not constrained by lower bounds. If bounds are specified, the vector length must equal the number of coefficients. An unconstrained lower bound is specified by `-Inf`.
`Upper`	A vector of upper bounds on the coefficients to be fitted. The coefficients are specified by the input argument `ftype` for `fit`. The default value of `Upper` is an empty vector indicating that the fit is not constrained by upper bounds. If bounds are specified, the vector length must equal the number of coefficients. An unconstrained upper bound is specified by `Inf`.
`StartPoint`	Vector of coefficient starting values. The coefficients are specified by the input argument `ftype` for `fit`. The default value of `StartPoint` is an empty vector. If the default value is passed to the `fit` function, then starting points for some library models are determined heuristically. For other models, the values are selected randomly on the interval (0,1).
`Algorithm`	Algorithm used for the fitting procedure. The value can be `'Levenberg-Marquardt'`,`'Gauss-Newton'`, or `{'Trust-Region'}`.
`DiffMax Change`	Maximum change in coefficients for finite difference gradients. The default value is 0.1.

Property	Description (Continued)
DiffMin Change	Minimum change in coefficients for finite difference gradients. The default value is 10^{-8}.
Display	Level of display. {'notify'} displays output only if the fit does not converge. 'final' displays only the final output. 'iter' displays output at each iteration. 'off' displays no output.
MaxFunEvals	Maximum number of function (model) evaluations allowed. The default value is 600.
MaxIter	Maximum number of fit iterations allowed. The default value is 400.
TolFun	Termination tolerance on the function (model) value. The default value is 10^{-6}.
TolX	Termination tolerance on coefficients. The default value is 10^{-6}.

Note For the properties Upper, Lower, and StartPoint, the order of the entries in the vector corresponds to the alphabetical order of the coefficients, not the order in which they appear in the expression ftype. For example, if you create ftype by the command ftype = fittype('b*x^2+c*x+a'), setting StartPoint to [1 3 5] assigns a = 1, b = 3, and c = 5.

Example

Create an empty fit options object and configure the object so that data is normalized before fitting.

```
opts = fitoptions;
opts.Normal = 'on'

opts =

    Normalize: 'on'
      Exclude: []
```

```
          Weights: []
           Method: 'None'
```

Creating an empty fit options object is particularly useful when you want to configure only the `Normalize`, `Exclude`, or `Weights` properties for a data set, and then fit the data using the same fit options object, but with different fitting methods. For example, fit the census data using a third-degree polynomial, a one-term exponential, and a cubic spline.

```
load census
f1 = fit(cdate,pop,'poly3',opts);
f2 = fit(cdate,pop,'exp1',opts);
f3 = fit(cdate,pop,'cubicsp',opts);
```

You can return values for some fit options with the `fit` function. For example, fit the census data using a smoothing spline and return the default smoothing parameter. Note that this value is based on the data passed to `fit`.

```
[f,gof,out] = fit(cdate,pop,'smooth');
smoothparam = out.p
smoothparam =

    0.0089
```

Increase the default smoothing parameter by about 10% and fit again.

```
opts = fitoptions('Method','Smooth','SmoothingParam',0.0098);
[f,gof,out] = fit(cdate,pop,'smooth',opts);
```

Create two noisy Gaussian peaks — one with a small width, and one with a large width.

```
a1 = 15; b1 = 3; c1 = 0.02;
a2 = 35; b2 = 7.5; c2 = 4;
x = (1:0.01:10)';
rand('state',0)
gdata = a1*exp(-((x-b1)/c1).^2) + a2*exp(-((x-b2)/c2).^2) ...
    + 5*(rand(size(x))-.5);
```

Fit the data using the two-term Gaussian library model.

```
ftype = fittype('gauss2');
gfit = fit(x,gdata,ftype);

Maximum number of function evaluations exceeded. Increasing
MaxFunEvals (in fit options) may allow for a better fit, or
the current equation may not be a good model for the data.
```

Because the `Display` property is set to its default value `Notify`, a message is included as part of the display due to the fit not converging. The message indicates that you should try increasing the number of function evaluations.

The fit results are shown below.

```
gfit
gfit =
     General model Gauss2:
      gfit(x) =  a1*exp(-((x-b1)/c1)^2) + a2*exp(-((x-b2)/c2)^2)
     Coefficients (with 95% confidence bounds):
       a1 =       43.59  (-411.9, 499.1)
       b1 =       7.803  (0.7442, 14.86)
       c1 =       4.371  (-3.065, 11.81)
       a2 =      -10.86  (-373.4, 351.7)
       b2 =       11.05  (-190.4, 212.5)
       c2 =       6.985  (-124.6, 138.5)
```

As you can see by examining the fitted coefficients, it is clear that the algorithm has difficulty fitting the narrow peak, and does a good job fitting the broad peak. In particular, note that the fitted value of the `a2` coefficient is negative. To help the fitting procedure converge, specify that the lower bounds of the amplitude and width parameters for both peaks must be greater than zero. To do this, create a fit options object for the `gauss2` model and configure the `Lower` property to zero for `a1`, `c1`, `a2`, and `c2`, but leave `b1` and `b2` unconstrained.

```
opts = fitoptions('gauss2');
opts.Lower = [0 -Inf 0 0 -Inf 0];
```

Fit the data using the new constraints.

```
gfit = fit(x,gdata,ftype,opts)
gfit =
     General model Gauss2:
      gfit(x) =  a1*exp(-((x-b1)/c1)^2) + a2*exp(-((x-b2)/c2)^2)
     Coefficients (with 95% confidence bounds):
       a1 =          35  (34.82, 35.17)
       b1 =        7.48  (7.455, 7.504)
       c1 =       3.993  (3.955, 4.03)
       a2 =       4.824  (2.964, 6.684)
       b2 =           3  (2.99, 3.01)
       c2 =     0.03209  (0.01774, 0.04643)
```

This is a much better fit, although you can still improve the `a2` value.

See Also

`cflibhelp`, `fit`, `get`, `set`

fittype

Purpose Create a fit type object

Syntax

```
ftype = fittype('ltype')
ftype = fittype('expr')
ftype = fittype('expr','PropertyName',PropertyValue,...)
```

Arguments

`'ltype'`	The name of a library model, spline, or interpolant.
`'expr'`	An expression representing a custom model.
`'PropertyName'`	The name of a fit type object property.
`PropertyValue`	A valid value for *PropertyName*.
`ftype`	A fit type object.

Description

`ftype = fittype('ltype')` creates the fit type object `ftype` from the library model, spline, or interpolant specified by *ltype*. You can display the library fit type names with the `cflibhelp` function.

`ftype = fittype('expr')` creates the fit type object from the expression specified by `expr`. The expression `expr` represents the custom model you will use to fit your data. To create a general (nonlinear) custom model, specify the entire equation as one expression. To create a linear custom model, pass in a cell array of expressions to `expr` but do not include the coefficients. Each element of the cell array corresponds to one term of the model. If there is a constant term, use "1" as the corresponding element in the cell array.

By default, the independent variable is assumed to be `x`, the dependent variable is assumed to be `y`, there are no problem-dependent variables, and all other variables are assumed to be coefficients of the model. All coefficients must be scalars.

`ftype = fittype('expr','PropertyName',PropertyValue,...)` creates a fit type object using the specified property name/property value pairs. The supported property names are given below.

Property Name	Description
`coefficients`	Specify the coefficient names. Use a cell array if there are multiple names.
`dependent`	Specify the dependent (response) variable name.
`independent`	Specify the independent (predictor) variable name.
`options`	Specify the default fit options for the current expression.
`problem`	Specify the problem-dependent (constant) names. Use a cell array if there are multiple names.

Example

Create a fit type object for a custom general equation and define the problem-dependent name to be `n`.

```
ftype = fittype('a*x+b*exp(n*x)','problem','n');
```

Define the independent variable to be `chan`.

```
ftype = fittype('a*chan+b*exp(n*chan)','ind','chan','prob','n')

ftype =
     General model:
       ftype(a,b,n,chan) = a*chan+b*exp(n*chan)
```

Create a fit type object for a custom linear equation and specify names for the coefficients.

```
ftype = fittype({'cos(x)','1'},'coeff',{'a1','a2'})

ftype =
     Linear model:
       ftype(a1,a2,x) = a1*cos(x) + a2
```

Create a fit type object for the `rat33` library model. Note that the display includes the full equation.

```
ftype = fittype('rat33')

ftype =
   General model Rat33:
   ftype(p1,p2,p3,p4,q1,q2,q3,x) = (p1*x^3 + p2*x^2 + p3*x + p4)/
                (x^3 + q1*x^2 + q2*x + q3)
```

Create a fit type object and include the existing fit options object `opts`, and fit to the census data.

```
load census
opts = fitoptions('Method','Nonlinear','Normalize','On');
ftype = fittype('a*exp(b*x)+c','options',opts);
f1 = fit(cdate,pop,ftype);
```

Purpose

Return properties for a fit options object

Syntax

```
get(opts)
a = get(opts)
a = get(opts,'PropertyName')
```

Arguments

`opts`	A fit options object.
'*`PropertyName`*'	The name of a fit options property, or a cell array of property names.
`a`	A structure or cell array of fit options property values.

Description

`get(opts)` returns all property names and their current values to the command line for the fit options object `opts`.

`a = get(opts)` returns the structure a where each field name is the name of a property of `opts`, and each field contains the value of that property.

`a = get(opts,'`*`PropertyName`*`')` returns the value of the property specified by *`PropertyName`* for `opts`. If *`PropertyName`* is replaced by a cell array of strings containing property names, `get` returns a cell array of values to `a`.

Example

Create a fit options object for a second-degree polynomial, and return the current property values to the command line.

```
opts = fitoptions('poly2');
get(opts)

ans =
    Normalize: 'off'
      Exclude: []
      Weights: []
       Method: 'LinearLeastSquares'
       Robust: 'Off'
        Lower: []
        Upper: []
```

See Also

`set`

integrate

Purpose

Integrate a fit result object

Syntax

```
inty = integrate(fresult,x,x0)
```

Arguments

`fresult`	A fit result object.
`x`	The values at which `fresult` is integrated.
`x0`	The integration starting point.
`inty`	A vector of integration values.

Description

`inty = integrate(fresult,x,x0)` integrates the fit result object `fresult` at the values specified by `x` starting from `x0`, and returns the result to `inty`. The `fresult` object is a fit result object generated by the `fit` function. `x` is a scalar or column vector and `inty` is the same size as `x`. `x0` is a scalar.

Example

Create a noisy sine wave on the interval [-2π, 2π].

```
rand('state',0);
x = (-2*pi:0.1:2*pi)';
y = sin(x) + (rand(size(x))-0.5)*0.2;
```

Create a custom fit type, and fit the data using reasonable starting values.

```
ftype = fittype('a*sin(b*x)');
fit1 = fit(x,y,ftype,'startpoint',[1 1]);
```

Calculate the integral for each value of `x` starting at `-2*pi`

```
inty = integrate(fit1,x,x(1));
```

See Also

`differentiate`, `cfit`, `fit`, `quad`

Purpose

Plot data, fit, prediction bounds, outliers, and residuals

Syntax

```
plot(fresult)
plot(fresult,xdata,ydata)
plot(fresult,xdata,ydata,'s')
plot(fresult,'s1',xdata,ydata,'s2')
plot(fresult,xdata,ydata,outliers)
plot(fresult,xdata,ydata,outliers,'s')
plot(...,'ptype1','ptype2',...)
plot(...,'ptype1','ptype2',...,conflev)
h = plot( )
```

Arguments

`fresult`	A fit result object.
`xdata`	A column vector of predictor data.
`ydata`	A column vector of response data.
`s,s1,s2`	The plot symbols, plot colors, and line type.
`outliers`	A vector of outliers.
`'`*`ptype`*`'`	The plot type. You can specify multiple plot types as a cell array of strings.
`conflev`	The confidence level.
`h`	A vector of plot handles.

Description

`plot(fresult)` plots the fit result object `fresult`. `fresult` is a fit result object generated by the `fit` function.

`plot(fresult,xdata,ydata)` plots the fit result object, the predictor data specified by `xdata`, and the response data specified by `ydata`.

`plot(fresult,xdata,ydata,'s')` plots the predictor and response data using the color, symbol, and line type specified by the string `s`. Refer to the built-in `plot` function for color, symbol, and line type options.

`plot(fresult,'s1',xdata,ydata,'s2')` plots the fit result object using the color, symbol, and line type specified by the string `s1`, and plots the predictor and response data using the color, symbol, and line type specified by the string `s2`.

`plot(fresult,xdata,ydata,outliers)` plots the outliers specified by `outliers` in a different color. `outliers` must be the same size as `xdata` and `ydata`. You identify data points as outliers with the `excludedata` function.

`plot(fresult,xdata,ydata,outliers,'s')` plots the outliers using the color, symbol, and line type specified by the string `s`.

`plot(...,'`*`ptype1`*`','`*`ptype2`*`',...)` plots the plot types specified by *`ptype1`*, *`ptype2`*, and so on. *`ptype`* can be a single plot type or multiple plot types, which you can specify as a cell array of strings. For one plot type or none (the default), `plot` behaves like the built-in `plot` command and draws into the current figure and axes. This way, you can use commands like `subplot` and `hold` to arrange plots in a figure window and to superimpose multiple fits into the same graph. For multiple plot types, `plot` uses `subplot` to create one set of axes per plot type. The supported plot types are given below.

Plot Type	**Description**
`fit`	Plot the data and the fit (default).
`predfunc`	Same as `fit` but with prediction bounds for the function.
`predobs`	Same as `fit` but with prediction bounds for a new observation.
`residuals`	Plot the residuals. The fit corresponds to the zero line.
`stresiduals`	Plot the standardized residuals. The fit corresponds to the zero line. Standardized residuals are the ordinary residuals divided by their standard deviation. Standardizing puts all residuals on a common scale (units of standard deviations) and makes it easier to quantify how far a point is from the fitted curve.

`plot(...,'ptype1','ptype2',...,conflev)` plots prediction bounds with the confidence level specified by `conflev`. `conflev` must be between 0 and 1. The default value is 0.95 for 95% confidence levels.

`h = plot( )` returns a vector of handles to `h`.

Remarks

To plot error bars, use the `errorbar` function. For example, if you have a vector of weights `w` (reciprocal variances) associated with the response data `ydata`, you can plot symmetric error bars with the following command.

```
errorbar(xdata,ydata,1./sqrt(w))
```

Example

Create a noisy sine wave on the interval [-2π, 2π] and add two outliers with the value 2.

```
rand('state',2);
x = (-2*pi:0.1:2*pi)';
y = sin(x) + (rand(size(x))-0.5)*0.2;
y(ceil(length(x)*rand(2,1))) = 2;
```

Identify outliers that are outside the interval [-1.5, 1.5] using the `range` method.

```
outliers = excludedata(x,y,'range',[-1.5 1.5]);
```

Create a custom fit type, define fit options that exclude the outliers from the fit and define reasonable starting values, and fit the data.

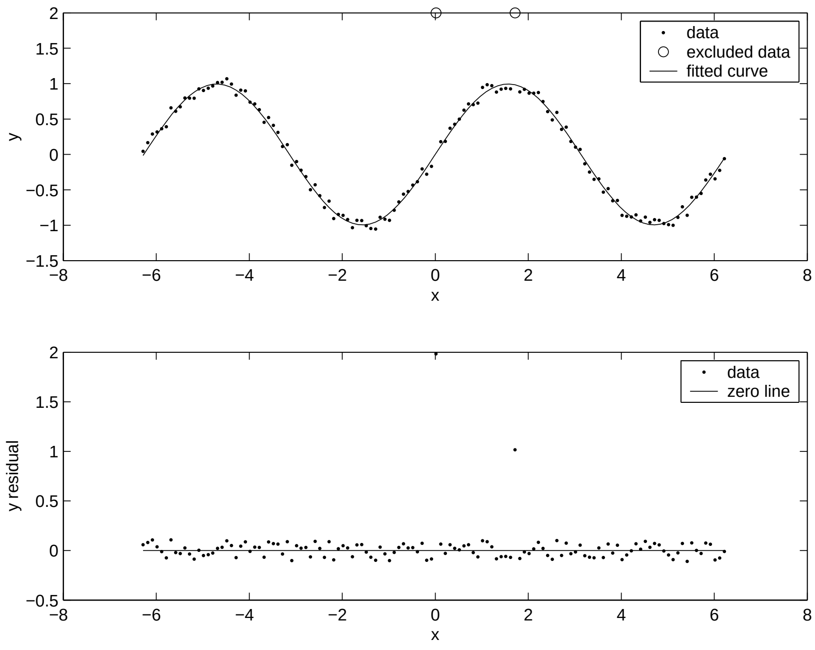
```
ftype = fittype('a*sin(b*x)');
opts = fitoptions('Method','NonLinear','excl',outliers,...
'Start',[1 1]);
fit1 = fit(x,y,ftype,opts);
```

Plot the data, the fit to the data, and mark the outliers.

```
subplot(2,1,1)
plot(fit1,'k-',x,y,'b.',outliers,'ro');
```

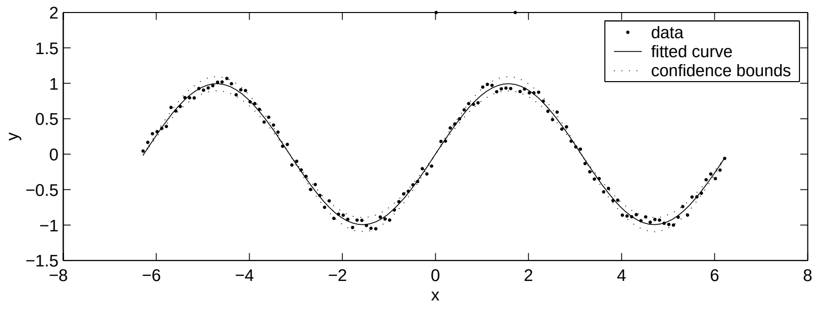
Plot the residuals.

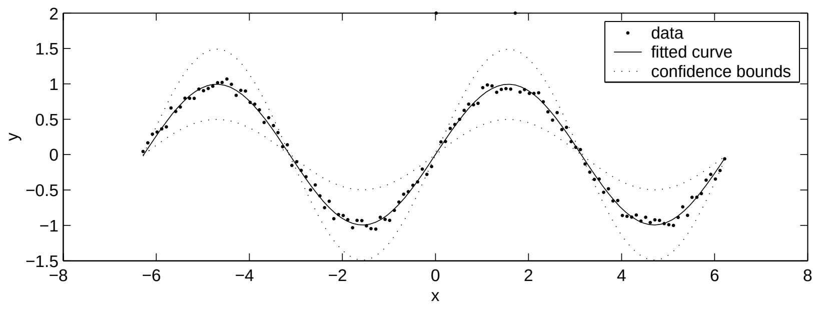
```
subplot(2,1,2)
plot(fit1,'k-',x,y,'b.','residuals');
```



Plot 99% confidence and prediction bounds for the function and for a new observation.

```
plot(fit1,'k-',x,y,'b.','predfunc','predobs',0.99);
```





See Also

`errorbar`, `plot` (built-in), `subplot`

predint

Purpose

Compute prediction bounds for new observations or for the function

Syntax

```
ci = predint(fresult,x)
ci = predint(fresult,x,level)
ci = predint(fresult,x,level,'intopt','simopt')
[ci,ypred] = predint(...)
```

Arguments

`fresult`	A fit result object.
`x`	The values at which predictions are calculated.
`level`	Confidence level. The value must be between 0 and 1. The default value is 0.95.
`'intopt'`	Can be `observation` (the default) to compute bounds for new response values, or `functional` to compute bounds for the fit evaluated at `x`.
`'simopt'`	Can be `off` (the default) to compute nonsimultaneous bounds, or `on` to compute simultaneous bounds.
`ci`	An array of upper and lower prediction bounds.
`ypred`	The predicted (fitted) value of `fresult` evaluated at `x`.

Description

`ci = predint(fresult,x)` returns prediction bounds for new response (observation) values at the predictor values specified by `x`. The confidence level of the predictions is 95%. `ci` contains the upper and lower prediction bounds. `fresult` is the fit result object returned by the `fit` function. You can compute prediction bounds only for parametric fits. To compute confidence bounds for the fitted parameters, use the `confint` function.

`ci = predint(fresult,x,level)` returns prediction bounds with a confidence level specified by `level`.

`ci = predint(fitresult,x,level,'intopt','simopt')` specifies the type of bounds to compute. If *`intopt`* is `functional`, the bounds measure the uncertainty in estimating the function (the fitted curve). If *`intopt`* is `observation`, the bounds are wider to represent the additional uncertainty in predicting a new response value (the fitted curve plus random noise).

If *`simopt`* is `off`, nonsimultaneous bounds are calculated. If *`simopt`* is `on`, simultaneous bounds are calculated. Nonsimultaneous bounds take into account only individual `x` values. Simultaneous bounds take into account all `x` values.

`[ci,ypred] = predint(...)` returns the predicted (fitted) value of `fresult` evaluated at `x`.

Example

Generate some data and add noise.

```
x = (0:0.2:10)';
coef = [2 -0.2];
rand('state',0)
y = coef(1)*exp(coef(2)*x) + (rand(size(x))-0.5)*0.5;
```

Fit the data using a single-term exponential and define the range over which prediction bounds are calculated.

```
fresult = fit(x,y,'exp1');
```

Return the prediction bounds for the function as well as the predicted values of the fit using nonsimultaneous and simultaneous bounds with a 95% confidence level. For nonsimultaneous bounds, given a single predetermined predictor value, you have 95% confidence that the true function lies between the confidence bounds. For simultaneous bounds, you have 95% confidence that the function at all predictor values lies between the bounds.

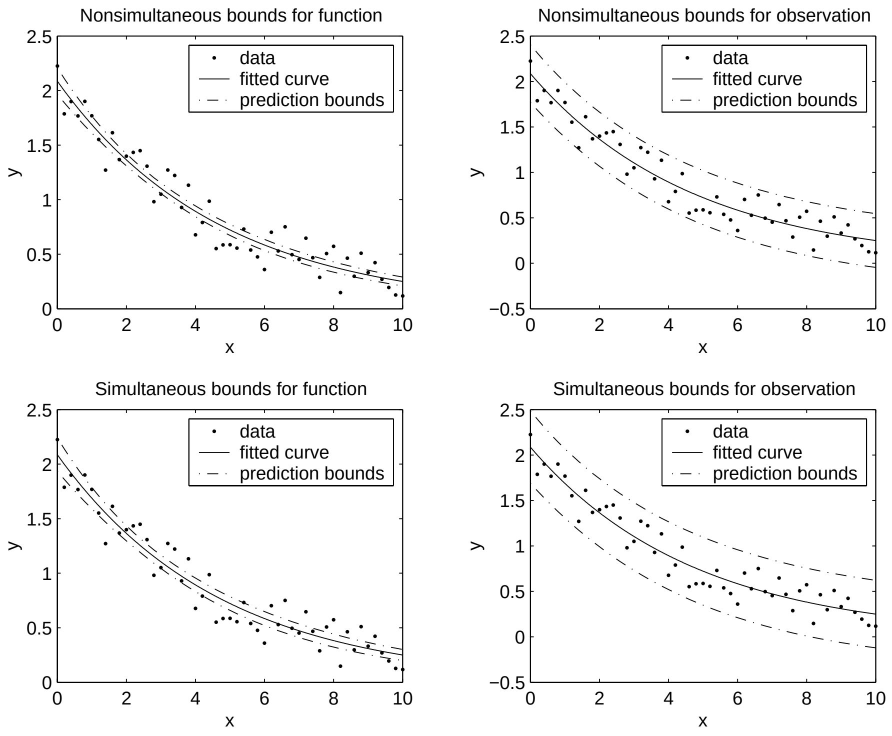
```
[c1,ypred1] = predint(fresult,x,0.95,'fun','off');
[c2,ypred2] = predint(fresult,x,0.95,'fun','on');
```

Return the prediction bounds for new observations as well as the predicted values of the fit using nonsimultaneous and simultaneous bounds with a 95% confidence level. For nonsimultaneous bounds, given a single predictor value, you have 95% confidence that a new observation lies between the confidence bounds. For simultaneous bounds, regardless of the predictor value, you have 95% confidence that a new observation lies between the bounds.

```
[c3,ypred3] = predint(fresult,x,0.95,'obs','off');
[c4,ypred4] = predint(fresult,x,0.95,'obs','on');
```

Plot the data, fit, and confidence bounds.

```
subplot(2,2,1), plot(fresult,x,y), hold on, plot(x,c1,'k-.')
legend('data','fitted curve','prediction bounds')
title('Nonsimultaneous bounds for function')
subplot(2,2,3), plot(fresult,x,y), hold on, plot(x,c2,'k-.')
legend('data','fitted curve','prediction bounds')
title('Simultaneous bounds for function')
subplot(2,2,2), plot(fresult,x,y), hold on; plot(x,c3,'k-.')
legend('data','fitted curve','prediction bounds')
title('Nonsimultaneous bounds for observation')
subplot(2,2,4), plot(fresult,x,y), hold on, plot(x,c4,'k-.')
legend('data','fitted curve','prediction bounds')
title('Simultaneous bounds for observation')
```



See Also

`confint`, `fit`

Purpose

Configure or display property values for a fit options object

Syntax

```
set(opts)
a = set(opts)
set(opts,'PropertyName',PropertyValue,...)
set(opts,PN,PV)
set(opts,S)
```

Arguments

`opts`	A fit options object.
'*`PropertyName`*'	A property name for `opts`.
`PropertyValue`	A property value supported by *`PropertyName`*.
`PN`	A cell array of property names.
`PV`	A cell array of property values.
S	A structure with property names and property values.
`a`	A structure array whose field names are the property names for `opts`, or cell array of possible values.

Description

`set(opts)` displays all configurable property values for the fit options object `opts`. If a property has a finite list of possible string values, these values are also displayed.

`a = set(opts)` returns all configurable properties and their possible values for `opts` to the structure `a`. The field names of `a` are the property names of `opts`, and the field values are cell arrays of possible property values. If the property does not have a finite set of possible values, the cell array is empty.

`set(opts,'`*`PropertyName`*`',PropertyValue,...)` configures multiple property values with a single command.

`set(opts,PN,PV)` configures the properties specified in the cell array of strings `PN` to the corresponding values in the cell array `PV`.

`set(opts,S)` configures the named properties to the specified values for `opts`. The structure `S` has field names given by the fit options object properties, and the field values are the values of the corresponding properties.

Example

Create a custom nonlinear model, and create a default fit options object for the model.

```
mymodel = fittype('a*x^2+b*exp(n*c*x)','prob','n');
opts = fitoptions(mymodel);
```

Configure the `Robust` and `Normalize` properties using property name/property value pairs.

```
set(opts,'Robust','LAR','Normalize','On')
```

Configure the `Display`, `Lower`, and `Algorithm` properties using cell arrays of property names and property values.

```
set(opts,{'Disp','Low','Alg'},{'Final',[0 0 0],'Levenberg'})
```

See Also

`fitoptions`, `get`

Purpose

Smooth the response data

Syntax

```
yy = smooth(ydata)
yy = smooth(ydata,span)
yy = smooth(ydata,'method')
yy = smooth(ydata,span,'method')
yy = smooth(ydata,'sgolay',degree)
yy = smooth(ydata,span,'sgolay',degree)
yy = smooth(xdata,ydata,...)
```

Arguments

`ydata`	A column vector of response data.
`span`	The number of data points to include for each smooth calculation.
`'method'`	The smoothing method.
`'sgolay'`	Use Savitzky-Golay smoothing.
`degree`	The polynomial degree for the Savitzky-Golay method.
`xdata`	A column vector of predictor data.
`yy`	A vector of smoothed response data.

Description

`yy = smooth(ydata)` smooths the response data specified by `ydata` using the moving average method. The default number of data points in the average (the span) is five. `yy` is the smoothed response data. Note that you need not specify the predictor data if it is sorted and uniform.

`yy = smooth(ydata,span)` uses the number of data points specified by `span` in the moving average calculation. `span` must be odd.

`yy = smooth(ydata,'method')` smooths the response data using the method specified by *`method`* and the default span. The supported smoothing methods are given below. For the Savitzky-Golay method, the default polynomial degree is 2.

Method	Description
`moving`	Moving average filter.
`lowess`	Locally weighted scatter plot smooth using least squares linear polynomial fitting.
`loess`	Locally weighted scatter plot smooth using least squares quadratic polynomial fitting.
`sgolay`	Savitzky-Golay filter. Note that the algorithm used by the toolbox can accept nonuniform predictor data.
`rlowess`	Lowess smoothing that is resistant to outliers.
`rloess`	Loess smoothing that is resistant to outliers.

`yy = smooth(ydata,span,'`*`method`*`')` smooths data using the specified `span` and *`method`*. For the `loess` and `lowess` methods, you can specify `span` as a percentage of the total number of data points. In this case, `span` must be less than or equal to 1. For the moving average and Savitzky-Golay methods, `span` must be odd. If an even `span` is specified, it is reduced by 1.

`yy = smooth(ydata,'`**`sgolay`**`',degree)` uses the Savitzky-Golay method with polynomial degree specified by `degree`.

`yy = smooth(ydata,span,'`**`sgolay`**`',degree)` uses the number of data points specified by `span` in the Savitzky-Golay calculation. `span` must be odd and `degree` must be less than `span`.

`yy = smooth(xdata,ydata,...)` smooths the data specified by `ydata` and the associated predictor data, `xdata`. You should specify the predictor data when it is not uniformly spaced or it is not sorted. If `xdata` is not uniform and you do not specify `method`, `lowess` is used. If the smoothing method requires `xdata` to be sorted, the sorting occurs automatically.

Remarks

For the moving average and Savitzky-Golay methods, `span` must be odd. If an even `span` is specified, it is reduced by 1. If `span` is greater than the length of `ydata`, it is reduced to the length of `ydata`.

Use robust smoothing when you want to assign lower weight to outliers. The robust smoothing algorithm uses the 6*MAD* method, which assigns zero weight to data outside six mean absolute deviations.

Another way to generate a vector of smoothed response values is to fit your data using a smoothing spline. Refer to the `fit` function for more information.

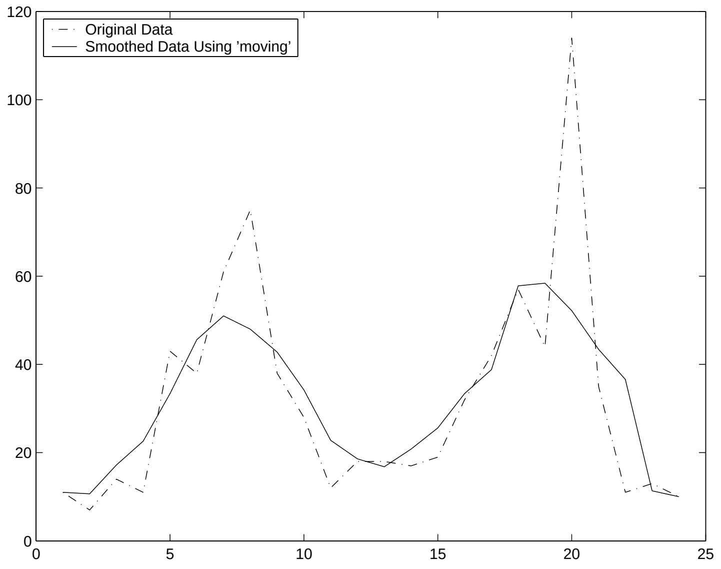
Example

Suppose you want to smooth traffic count data with a moving average filter to see the average traffic flow over a 5-hour window (`span` is 5).

```
load count.dat
y = count(:,1);
yy = smooth(y);
```

Plot the original data and the smoothed data.

```
t = 1:length(y);
plot(t,y,'r-.',t,yy,'b-')
legend('Original Data','Smoothed Data Using ''moving''',2)
```



The first four elements of yy are given by

```
yy(1) = y(1)
yy(2) = (y(1)+y(2)+y(3))/3
yy(3) = (y(1)+y(2)+y(3)+y(4)+y(5))/5
yy(4) = (y(2)+y(3)+y(4)+y(5)+y(6))/5
```

Because of the way that the end points are treated, the result shown above differs from the result returned by the `filter` function described in “Difference Equations and Filtering” in the MATLAB documentation.

In this example, generate random data between 0 and 15, create a sine wave with noise, and add two outliers with the value 3.

```
rand('state',2);
x = 15*rand(150,1);
y = sin(x) + (rand(size(x))-0.5)*0.5;
y(ceil(length(x)*rand(2,1))) = 3;
```

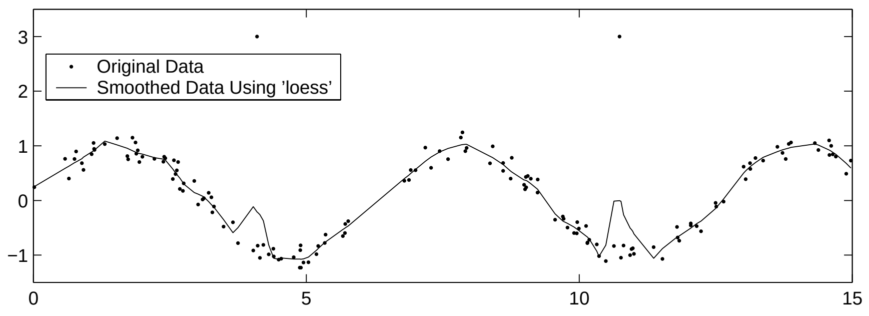
Smooth the data using the `loess` and `rloess` methods with the span specified as 10% of the data.

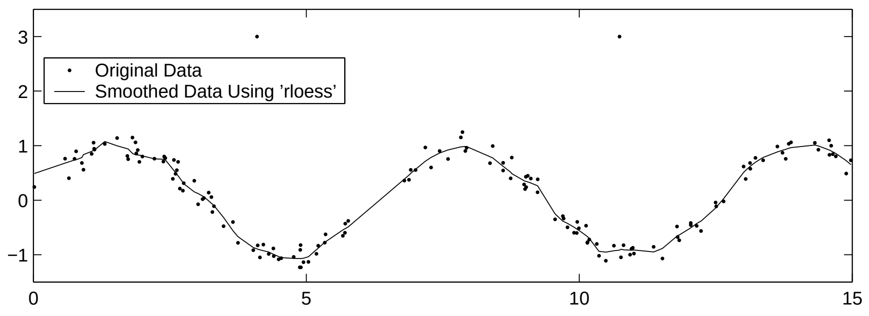
```
yy1 = smooth(x,y,0.1,'loess');
yy2 = smooth(x,y,0.1,'rloess');
```

Plot original data and the smoothed data.

```
[xx,ind] = sort(x);
subplot(2,1,1)
plot(xx,y(ind),'r.',xx,yy1(ind),'k-')
set(gca,'YLim',[-1.5 3.5])
legend('Original Data','Smoothed Data Using ''loess''',2)
subplot(2,1,2)
plot(xx,y(ind),'r.',xx,yy2(ind),'k-')
set(gca,'YLim',[-1.5 3.5])
legend('Original Data','Smoothed Data Using ''rloess''',2)
```

Note how the outliers have less effect with the robust method.





See Also

`fit`, `sort`

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