Version 10

FitAll

nonlinear regression analysis

Reference Guide

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Contents

Introduction

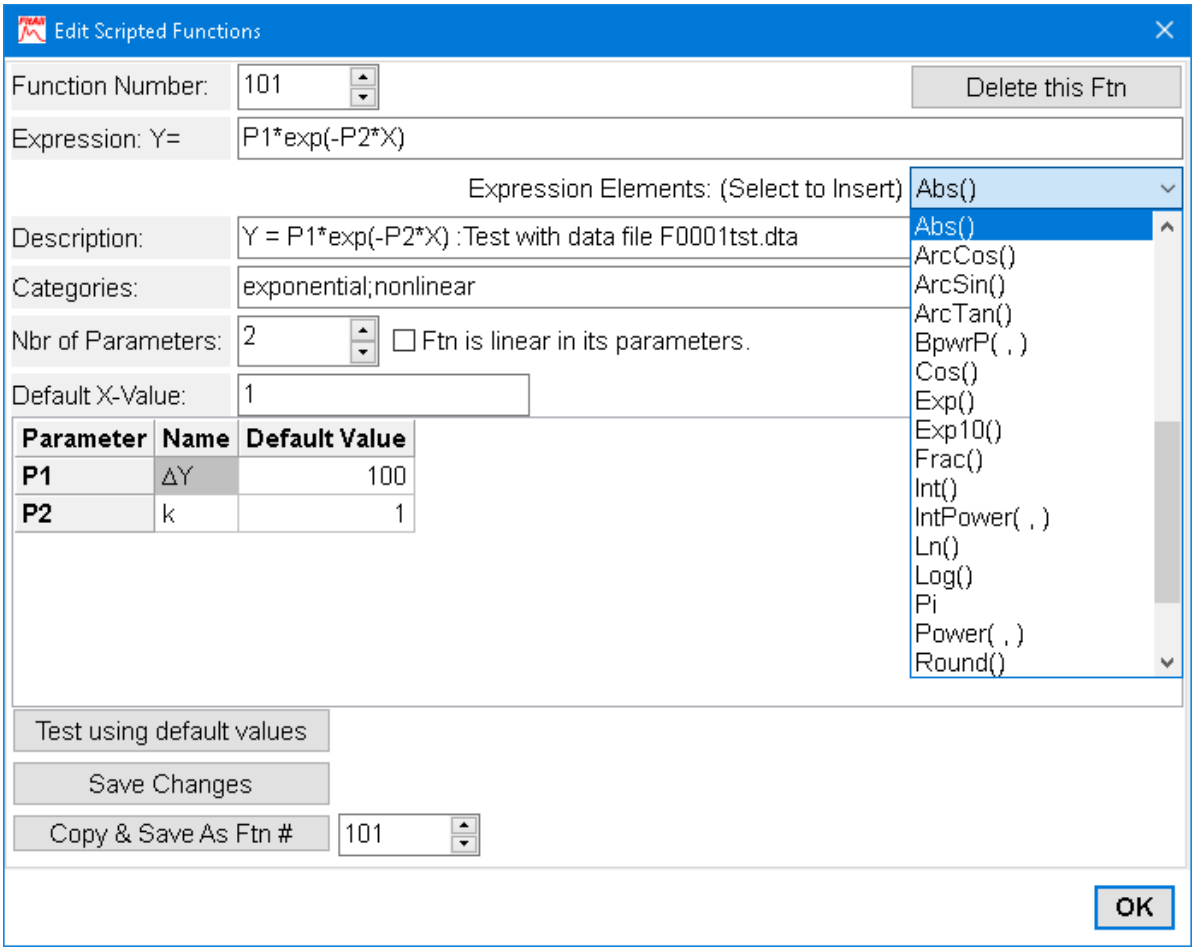
This ***FitAll***™ Reference Guide describes the function of each of the menu selections, provides a 'How to' section that will help you to make better use of ***FitAll*** and has an appendix that provides contact and additional technical information about ***FitAll***.

What's New

New In FitAll version 10

FitAll version 10 has been enhanced to include the following new features:

? **NEW:** A **Scripted Functions** feature has been added.
This makes is possible for you to add up to 100 functions to ***FitAll*** by filling out a simple form.



The advantages are:
(i) You can quickly add single-line custom function expressions to ***FitAll*** without the need for a compiler.
(ii) Each function can contain one independent variable, X, and up to ten (10) parameters, P,

The disadvantages are:
(i) ***FitAll*** will not be able to automatically determine the initial parameter estimates that are required when analyzing nonlinear functions.
(ii) The regression analysis will be slower than if the function had been compiled into a ***FitAll*** function library

? **NEW:** Almost all forms and dialogs now use the font that is set via the new Options > Change Font menu selection.
This makes it easier to read the text on small, high resolution monitors.

? **IMPROVED:** Most dialogs and forms have been modified to make them easier to read.

? **CHANGED: *FitAll*** Function Libraries can only be modified and compiled using the Lazarus / Free Pascal Compiler, which is a free, open source Object Pascal compiler.
Support for the Delphi compiler was discontinued because most users found it to be too costly.

? **DISCONTINUED:** Support for MS Windows Vista and earlier has been discontinued because they are no longer supported by Microsoft.

? **DISCONTINUED:** Support for ActiveX / COM Automation.
That is, ***FitAll*** can no longer act as an automation server and be controlled by other programs using ActiveX / COM automation.
(This was done because no current ***FitAll*** users are using or even contemplating using this feature.)

New In FitAll version 9

FitAll version 9 has been enhanced to include the following new features:

- ***FitAll*** now takes advantage of some of the features that were introduced in MS Windows 8.1 and 10.

  The most noticeable change is that ***FitAll*** now will automatically adjust the font and images sizes when it is run on a computer with a high resolution monitor or its main window is moved to a monitor that has a different resolution.

- The ***FitAll*** API now has functions to determine the roots of 2^{nd} to 10^{th} -order polynomials.

- The ***FitAll*** Chemistry Functions Library now has many new functions that can be used to determine the concentration, and acid dissociation constants, pKa's, of weak monoprotic, diprotic and triprotic acids as well as mixtures of monoprotic acids when titrated with a strong base. All of the solutions may or may not contain a strong acid, the concentration of which also can determined.

- ***FitAll*** can now **display help documents for the User Defined Functions**, UDFs, that you have created.

  This makes it possible for you, your colleagues and your students to get some help for the functions that you developed.

  The help files can be MS Word (*doc, *.docx), Rich Text (*.rtf), Open Document Text (*.odt), Text (*.txt) or Portable Document Format (*.pdf) files

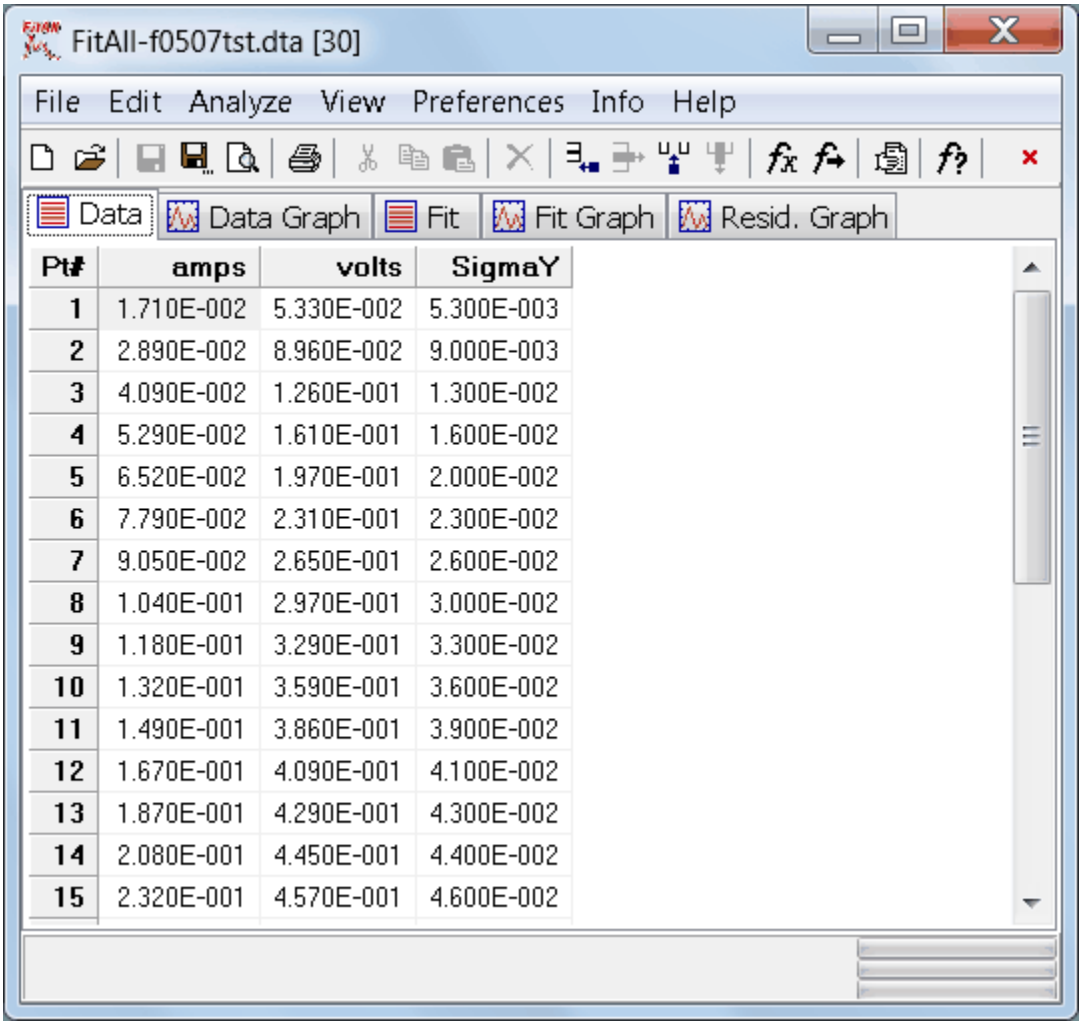
- Support for MS Windows XP has been discontinued.

New In FitAll version 8

FitAll version 8 has been enhanced to include the following new features:

- The most noticeable change is to the main user interface, which is of the "tabbed notebook" type rather than the previous "multi-document" type.

  This makes it easier to see which windows are open and to switch between them. The tabs may, optionally, include a small icon (graphic) that indicates whether the tab contains text or a graph.



Pt#	amps	volts	SigmaY
1	1.710E-002	5.330E-002	5.300E-003
2	2.890E-002	8.960E-002	9.000E-003
3	4.090E-002	1.260E-001	1.300E-002
4	5.290E-002	1.610E-001	1.600E-002
5	6.520E-002	1.970E-001	2.000E-002
6	7.790E-002	2.310E-001	2.300E-002
7	9.050E-002	2.650E-001	2.600E-002
8	1.040E-001	2.970E-001	3.000E-002
9	1.180E-001	3.290E-001	3.300E-002
10	1.320E-001	3.590E-001	3.600E-002
11	1.490E-001	3.860E-001	3.900E-002
12	1.670E-001	4.090E-001	4.100E-002
13	1.870E-001	4.290E-001	4.300E-002
14	2.080E-001	4.450E-001	4.400E-002
15	2.320E-001	4.570E-001	4.600E-002

- Switching the X- (bottom) and Y- (left) axes has been improved to ensure that the axis captions are properly switched.

- .All of the Solar Cell functions have been extended so that they can be used to analyze IV data obtained from "modules" as well as from "single cells".

  Previously, for a module with the solar cells connected in series, it was necessary to divide the measured voltage values by the number of cells. Now, an adjustable constant, Ns, can be set to the number of cells that are connected in series and the unmodified data can be directly analyzed.

A similar situation also applies to modules in which the solar cells are connected in parallel.

- Several new functions, including but not limited to GammaP, GammaQ, IsInfinite, IsNAN, IsZero, Sinh, Cosh, Tanh, have been added to the ***FitAll*** API. This makes it easier for programmers, who are adding their own functions to ***FitAll*** **Research Edition**, to more easily add more complicated functions of their own.

- ***FitAll*** now makes more efficient use of the computer's memory.

- ***FitAll*** now makes more efficient use of the computer's memory.

- MS Windows 8 is now supported.

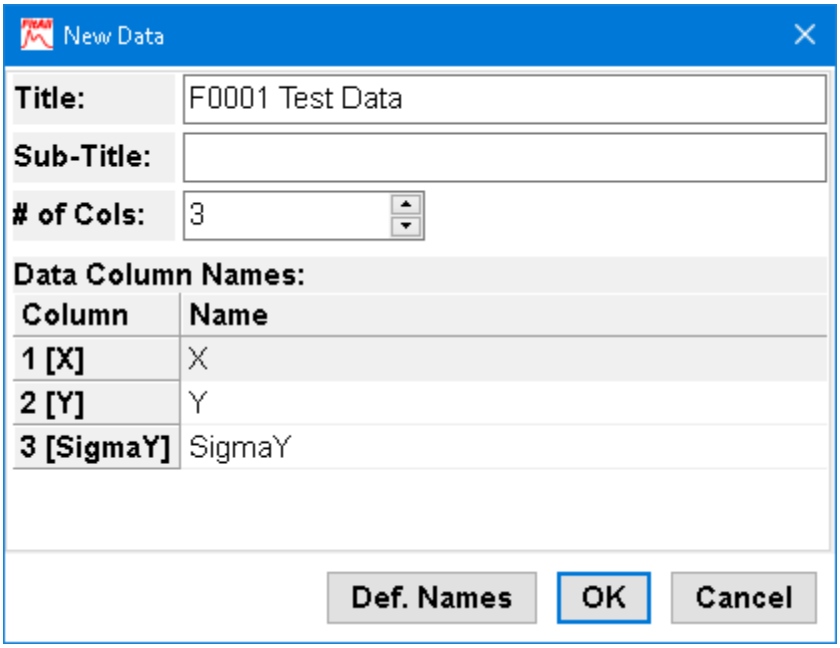
- MS Windows 2000 support has been discontinued.

File

New

Choose File > New, press **Ctrl+N** or click the button to create a new set of data.

When you select File > New, the 'New Data' dialog box appears. It looks like this:



Click the **Ok** button to accept your choices or click the **Cancel** button if you decide not to create a new data set.

FitAll will then switch to the Data window, which will contain one data point.

An initial value of zero is assigned to the number in each column, with the exception of the last column, the SigmaY column, which may be assigned a value of one (See: Options > Preferences > Set new SigmaY's to 1.0 128).

To add another data point at the end of the list, press the Insert key or choose Edit > Add point 35.

After entering your data, save it to disk before doing anything else. This will minimize the possibility of accidental data loss.

> **NOTE:**
> You can quickly and easily spot data entry errors by plotting the data graph 108.

Title

Enter a title for your data set in the Title edit field.

FitAll will use this as the default title for graphs.

Sub-Title

Enter a sub-title for your data set in the Sub-Title edit field.

Number of columns

Use this spin-edit box to set the number of data columns.

Each data set must have at least three data columns, which hold the X, Y and SigmaY data.

If you only have data for the X and Y columns, choose three columns, anyway.

Initially, the maximum number of data columns is limited to eight. If you need more, use the Options > Preferences > Max data columns 127 setting to set a higher value.

> **NOTE:**
> The amount of memory that your computer has may limit the size of data sets that you can use.

Data Column names

Enter a name for each data column.

To enter a new column name:

- Click on the column name that you want to change.
- Type in that name you want.
- Press the Enter key to accept your change, or press the Esc key to cancel it.

To edit a column name:

- Double click the column name you want to edit, or highlight it and press the F2 key.
- Make the changes the you want.
- Press the Enter key to accept your change, or press the Escape key to cancel your change.

Def. names

Click this button to have ***FitAll*** assign default names to the data columns. The assigned column names will be "X1", "X2", ..., "Y", and "SigmaY".

Open

Choose File > Open, press **Ctrl+O** or click the  button to retrieve data from a disk file (See: Opening a Data File in the Getting Started Guide).

Opening a data file replaces the data currently in memory with that from the disk file.

If the data currently in the computer's memory has not been saved or if it has changed since it was last saved, you will be asked whether to save it before it is replaced by the new data.

> **NOTE:**
> ***FitAll*** normally expects data files to have the file name extension ".DTA". If you choose to open a file with a different file name extension, ***FitAll*** will still read it as long as it has the correct structure (See: DTA Files 192 in the Appendix).

Also See

File > Import Text Data... 12

File > Join... 17

File > Reopen... 16

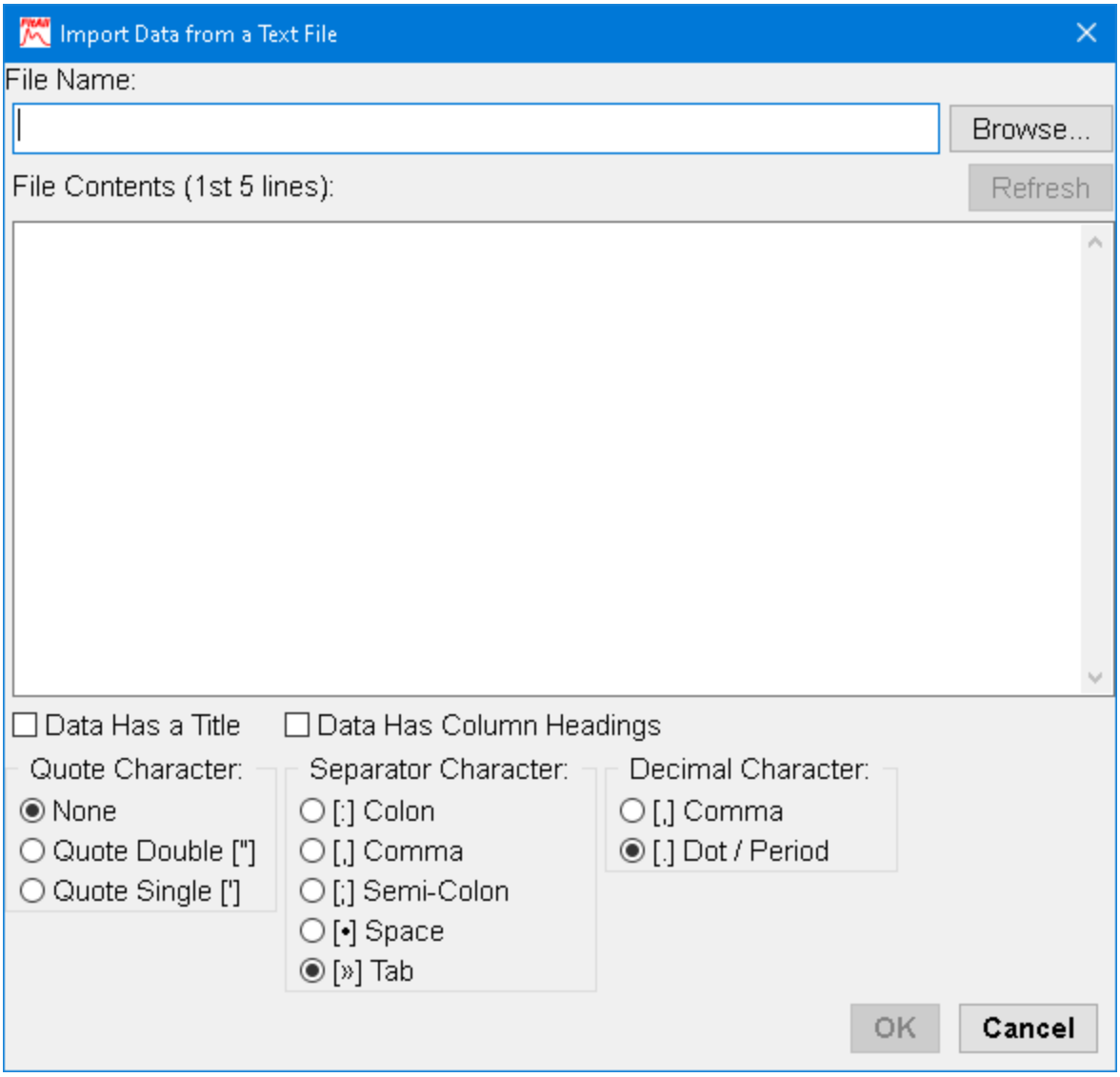
Import text data ...

Choose File > Import Text Data... to retrieve data from a disk text file that has a structure that does not correspond to the standard ".dta" format.

> **NOTE:**
> The structure of "Comma Separated Values", CSV, data files is best regarded as a "pseudo standard".
>
> Depending on which program generated the ".CSV" data file, the characters used to enclose, quote, text values, to separate data values and to indicate the decimal position in numeric values may differ.
>
> The "Import Text Data" makes it possible to import the data from such files into ***FitAll***.

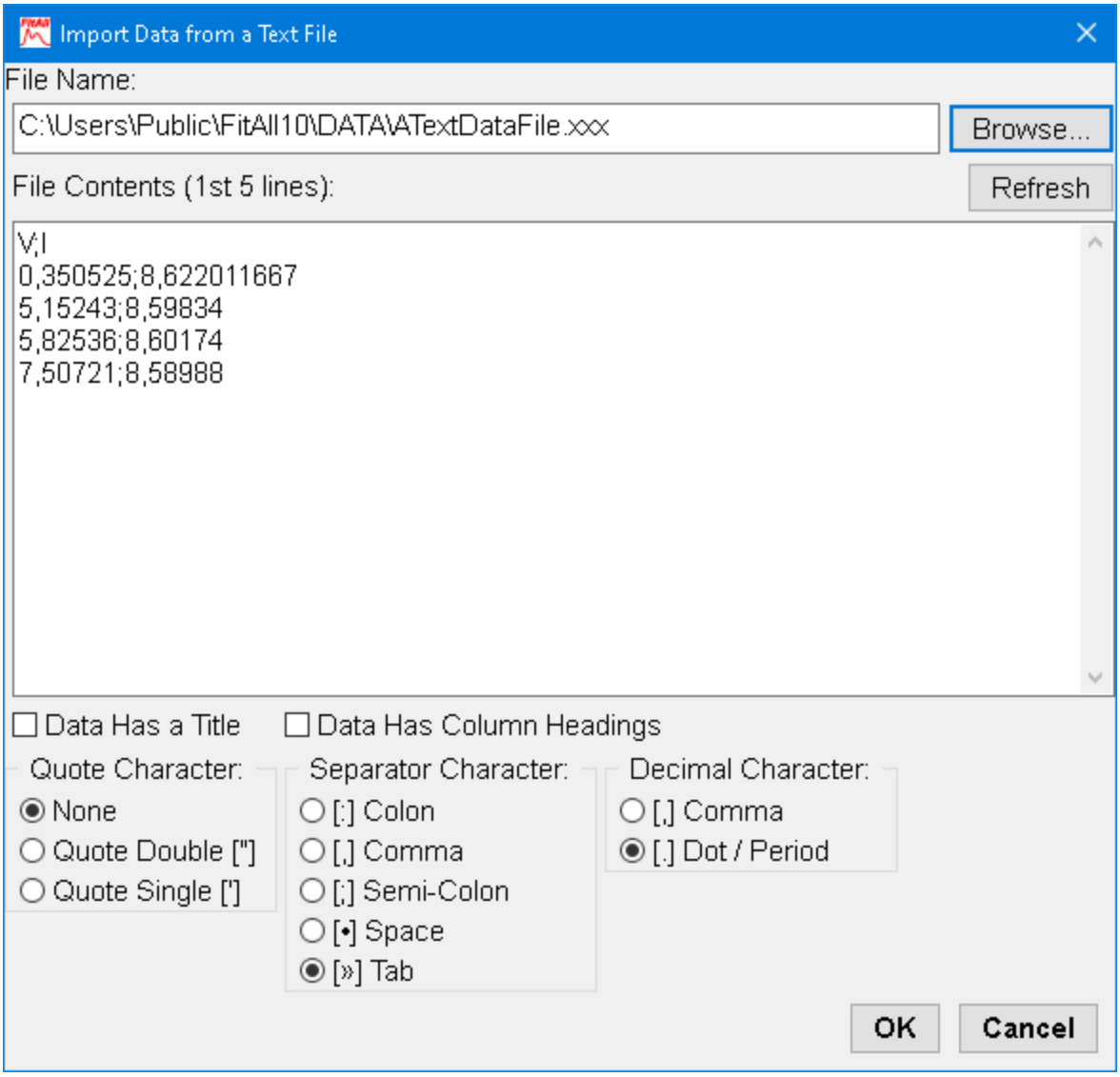
The general file structure that can be imported is described in the Appendix as XXX Data Files 200.

When you click the menu selections File > Import Text Data... a dialog like the following will appear.



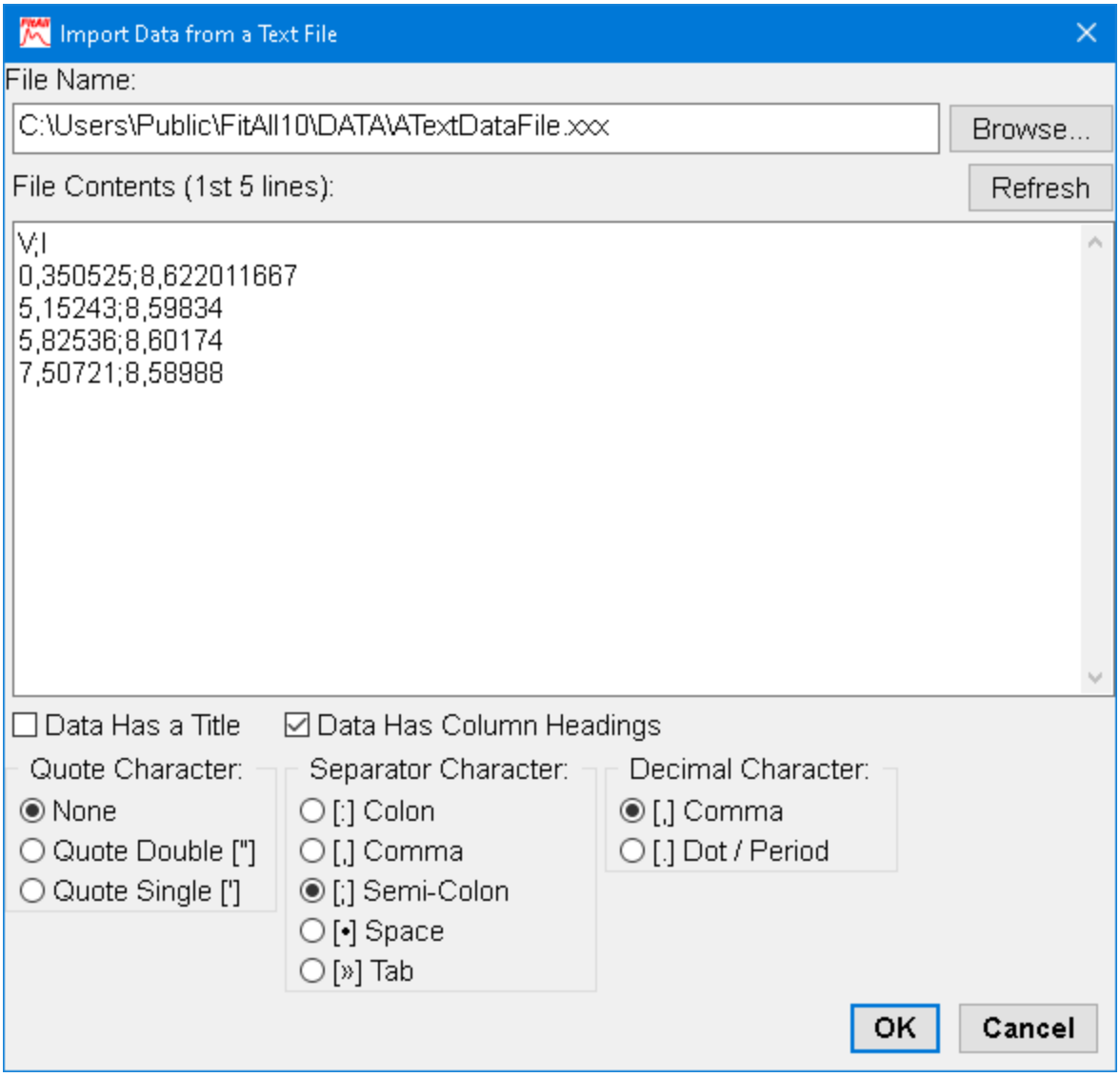
Click the "Browse" button and open the data file that you want to import into ***FitAll***.

The result could look like this:



After viewing the first five lines of the file contents, change the "Quote Character", "Separator Character" and "Decimal Character" to appropriate values.

In the above example, the result should look like this:



Click the **OK** button to import the data.

Opening a data file replaces the data currently in memory with that from the disk file.

If the data currently in the computer's memory has not been saved or if it has changed since it was last saved, you will be asked whether to save it before it is replaced by the new data.

> **NOTE:**
> After the data is imported, ***FitAll*** will change the file name extension to ".DTA". This is done so that when the data is next saved it will be saved in the standard ***FitAll*** data format.

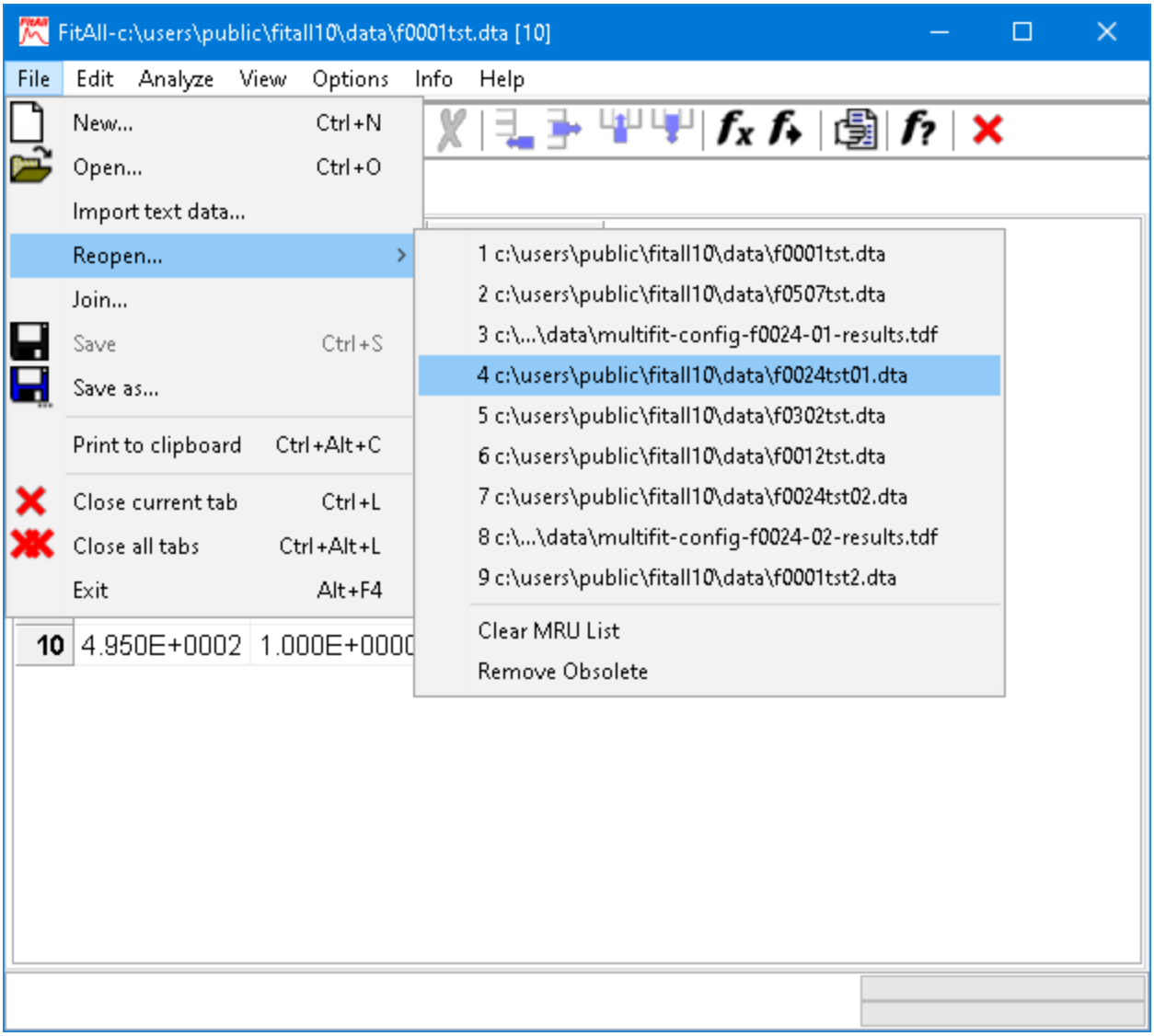
Also See

XXX Data Files 200

DTA Data Files 192

Reopen...

Choose File > Reopen recent to retrieve a data set that you have recently used.



NOTE:
Depending on which Preferences 129 are set, the File > Reopen recent... menu selection may or may not be available.

Also See

File > Open... 11

Join...

Choose File > Join to append data from an existing file to the data in memory.

The number of data columns in the file must be the same as the number of columns in the data set that is in your computer's memory.

After joining a set of data, you will probably want to sort it using the Edit > data Sort 48 menu selection or right click in the data window and choosing data Sort... from the context menu.

Save

Choose File > Save, press **Ctrl+S** or click the  button when the Data window has the focus to save the data, that is in your computer's memory, to a disk file.

> **NOTE:**
> This menu selection is only available when the Data window is active and the data has changed since it was last saved.

The data will be saved with its current file name.

To save the data with a different file name, select the File > Save as... 19 menu choice or click the  button on the toolbar.

> **NOTE:**
> The contents of other windows, for example, the data graph or the results window also can be saved to disk using the File > Save as... 19 menu selection.

Also See

File > Save as... 19

Save as...

Data window

When the Data window is active, ***FitAll*** will automatically add the ".DTA" extension, if you do not specify a file name extension.

If you specify an extension other than ".dta", ***FitAll*** will save it in the same format as a DTA 192 file unless you specify a ".CSV" 194 , ".SDF 198" or ".TDF" 196 extension (See: File Structures 192 in the Appendix).

Windows Containing Text

When the active window contains text, such as the Results window, ***FitAll*** will suggest a file name based on the data file name and the window's name. The contents of the window will then be saved as a standard ASCII text file.

If you change the file name extension to something other than ".txt", ***FitAll*** will still save the contents of the window as a standard ASCII text file.

Windows Containing A Graph

When the active window contains a graph, such as the data graph window, ***FitAll*** will suggest a file name based on the data file name and the window's name.

By default, the file name extension will be ".emf". The ".emf" extension indicates that the graph will be saved as a Windows Enhanced Meta file. Many Windows programs can import graphics files that use this format.

FitAll can save graphs as a:

- Bitmap (.bmp) file.
- Graphics Interchange Format (.gif) file.
- JPEG (.jpg) file, which easily can be incorporated into web pages.
- Portable Network Graphics (.png) file.

Print to clipboard

Choose File > Print to clipboard or press **Ctrl+Alt+C** to copy the contents of the active window to MS Windows' Clipboard.

If the active window is a text window, such as the 'Data' or 'Fit' windows, its contents will be copied to the clipboard.

If the active window is a graph window, such as the 'data graph' or 'fit graph' windows, its contents will be copied to the clipboard as a 'Picture' (a bitmap). Pictures can be 'pasted' into many Windows applications, including word processors such as MS Word for Windows and LibreOffice Writer.

> **NOTE:**
> For graph windows in ***FitAll***, this command does the same thing as the Edit, Copy 28 command.
>
> For windows that contain text, printing to the clipboard copies the window's column and row headings as well as the column values.

Also See

Edit > Generate Report 73

Close current tab

Choose File > Close current tab, press **Ctrl+L** or click the  button at the right end of the toolbar to close the currently active tab/window.

Also See

File > Close all tabs 22

Close all tabs

Choose File > Close all tabs or press **Ctrl+Alt+L** to close all currently open tabs/windows.

Also See

File > Close current tab 21

Exit

Choose File > Exit or press **Alt+F4** to quit ***FitAll*** and return to Windows.

If the data in memory has not been saved since it was last modified, you will asked whether you want to save it before quitting.

Edit

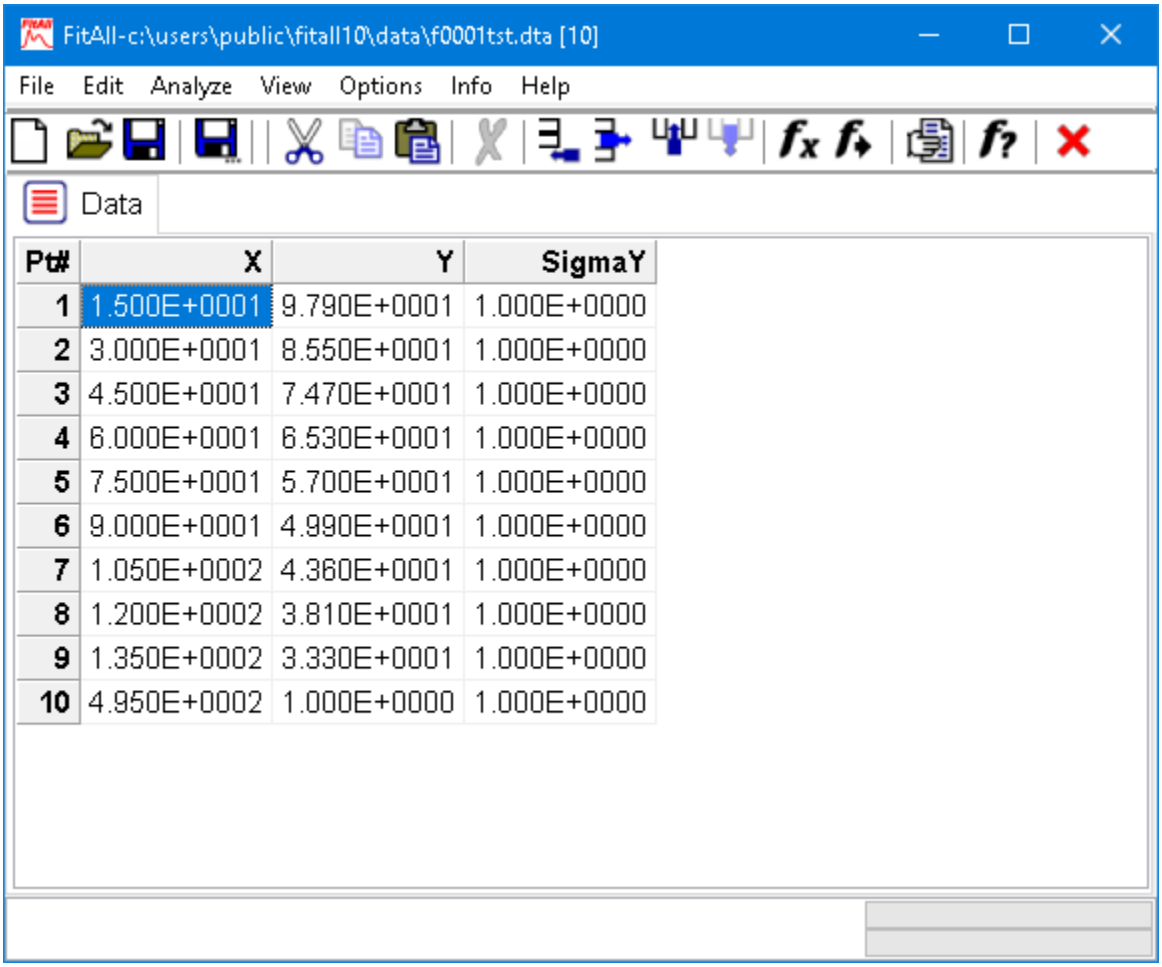
Cut

Choose Edit > Cut, press **Ctrl+X** or click the button to delete the selected data points in the Data window and copy them to the Windows Clipboard.

The Edit > Cut and Edit > Paste selections can be used together to change the order of the data points in the data set. You might, for example, want to move one or more 'bad' data points out of the analysis range without actually deleting them from the data set.

> **NOTE:**
> This command is available only when the 'Data' window is active and one or more data points are selected.

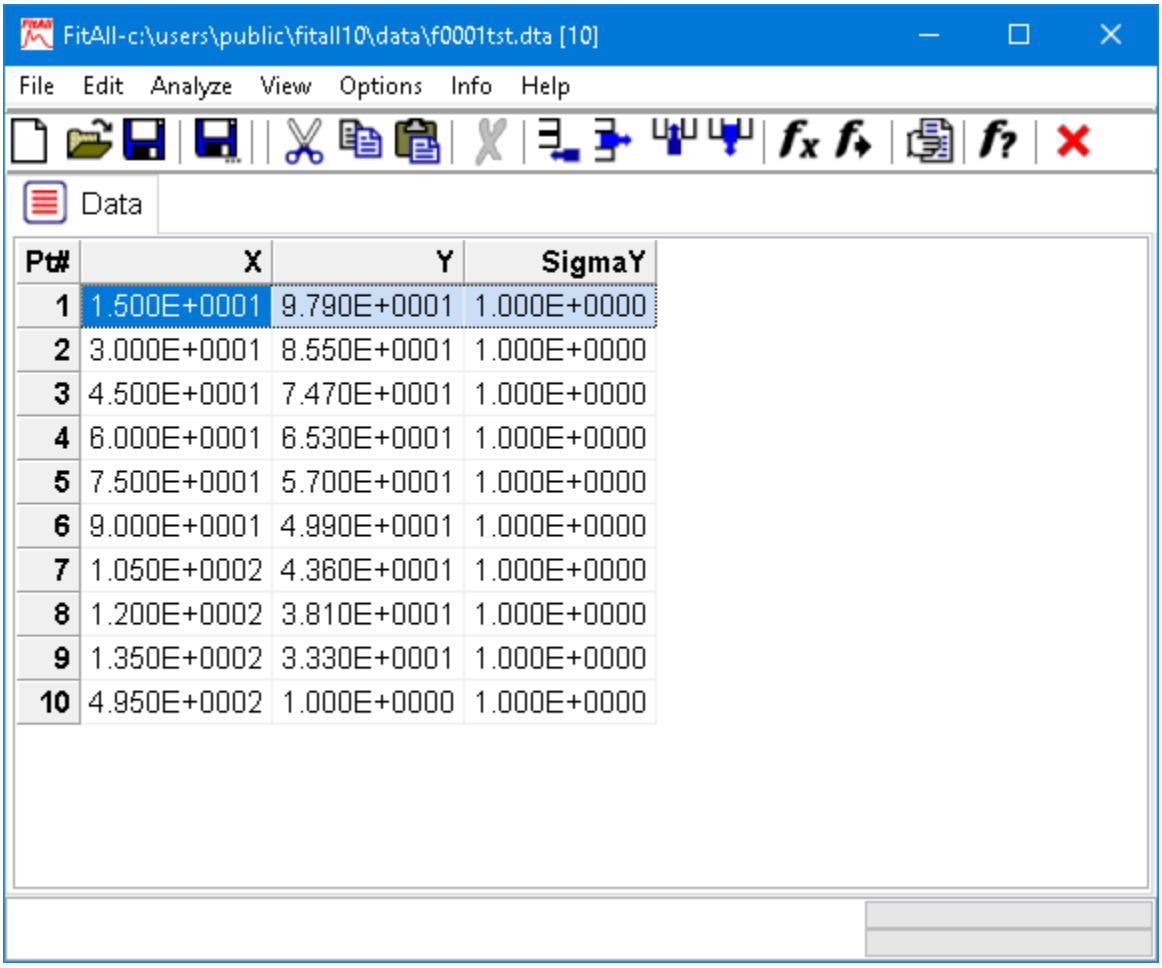
To select a row of data click on the 'Row row number'. You can use the Shift key to select more than one row.



Pt#	X	Y	SigmaY
1	1.500E+0001	9.790E+0001	1.000E+0000
2	3.000E+0001	8.550E+0001	1.000E+0000
3	4.500E+0001	7.470E+0001	1.000E+0000
4	6.000E+0001	6.530E+0001	1.000E+0000
5	7.500E+0001	5.700E+0001	1.000E+0000
6	9.000E+0001	4.990E+0001	1.000E+0000
7	1.050E+0002	4.360E+0001	1.000E+0000
8	1.200E+0002	3.810E+0001	1.000E+0000
9	1.350E+0002	3.330E+0001	1.000E+0000
10	4.950E+0002	1.000E+0000	1.000E+0000

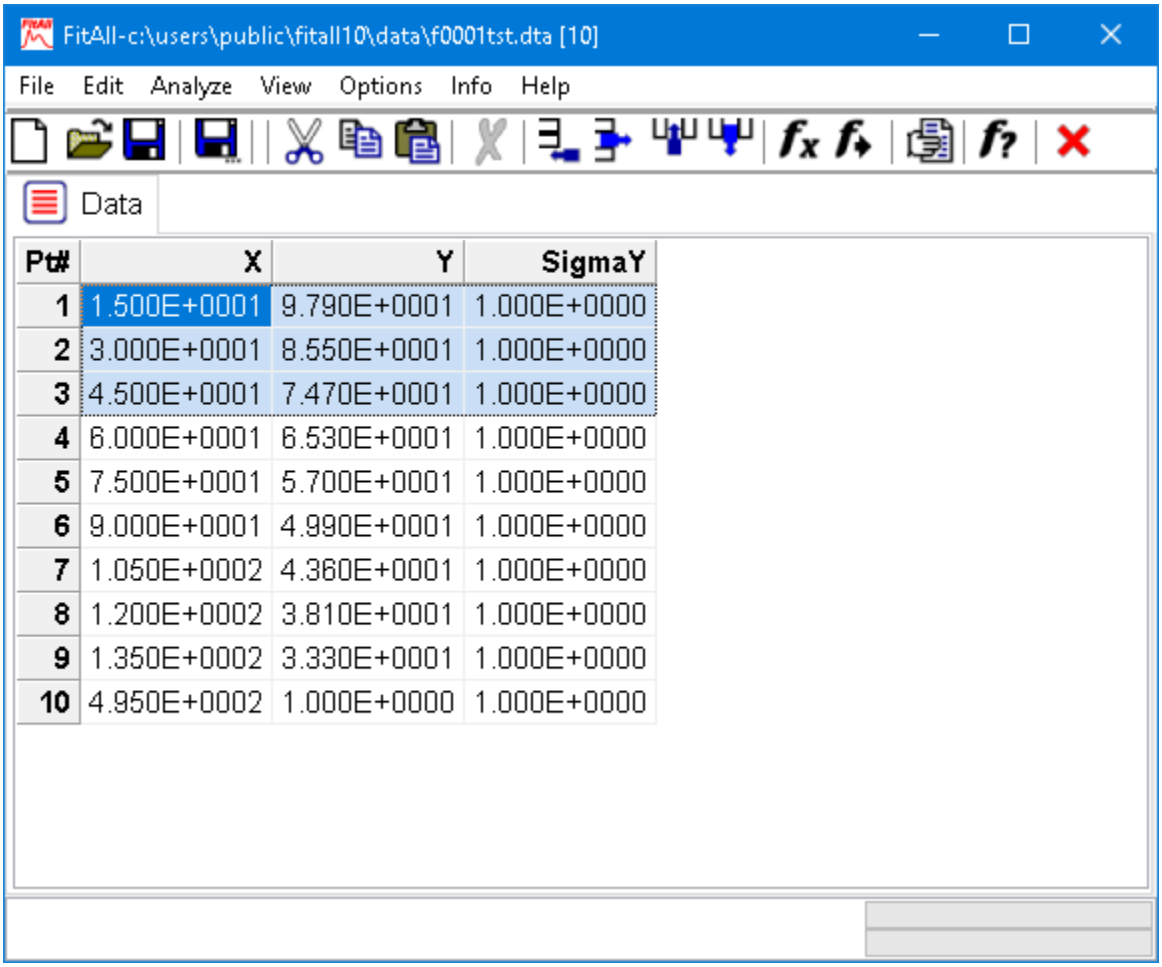
For example:

- Click on the row number 1.



Pt#	X	Y	SigmaY
1	1.500E+0001	9.790E+0001	1.000E+0000
2	3.000E+0001	8.550E+0001	1.000E+0000
3	4.500E+0001	7.470E+0001	1.000E+0000
4	6.000E+0001	6.530E+0001	1.000E+0000
5	7.500E+0001	5.700E+0001	1.000E+0000
6	9.000E+0001	4.990E+0001	1.000E+0000
7	1.050E+0002	4.360E+0001	1.000E+0000
8	1.200E+0002	3.810E+0001	1.000E+0000
9	1.350E+0002	3.330E+0001	1.000E+0000
10	4.950E+0002	1.000E+0000	1.000E+0000

- Hold down the Shift key and click on the Pt# number three (3). The result should look like this:



Pt#	X	Y	SigmaY
1	1.500E+0001	9.790E+0001	1.000E+0000
2	3.000E+0001	8.550E+0001	1.000E+0000
3	4.500E+0001	7.470E+0001	1.000E+0000
4	6.000E+0001	6.530E+0001	1.000E+0000
5	7.500E+0001	5.700E+0001	1.000E+0000
6	9.000E+0001	4.990E+0001	1.000E+0000
7	1.050E+0002	4.360E+0001	1.000E+0000
8	1.200E+0002	3.810E+0001	1.000E+0000
9	1.350E+0002	3.330E+0001	1.000E+0000
10	4.950E+0002	1.000E+0000	1.000E+0000

NOTE:
You also can select rows of data using the shift and arrow keys.

Copy

Choose Edit > Copy, press **Ctrl+C** or click the  button to copy the selected text in the Data Window or the graph in a graph-containing window to the Windows Clipboard.

Also See

Edit > Generate Report 73

File > Print to clipboard 20

Paste

Choose Edit > Paste, press **Ctrl+V** or click the  button to copy data points from MS Windows' Clipboard to ***FitAll***'s Data window.

NOTES:

1. The Data window is the only window in ***FitAll*** into which data can be pasted.
2. If there are fewer columns of data in the text that is to be pasted than are present in the current data set, the additional columns will be assigned a value of 1.0 or 0.0 depending on the Set new SigmaY's to 1.0 128 setting on the Options > Preferences 126 menu.
3. If one or more rows of data are selected, the pasted data will replace selected rows of data.
4. If all the data rows are selected

   (a) And the first column of the first row of the text to be pasted contains a column heading, rather than a number, the headings also will be pasted into ***FitAll***.

   (b) And the text to be pasted only contains numbers, the column headings in ***FitAll*** will not be changed.

   (c) And the pasted data contains a different number of columns, the number of data columns in ***FitAll*** will be adjusted to match the number of columns in the pasted data.

Also See

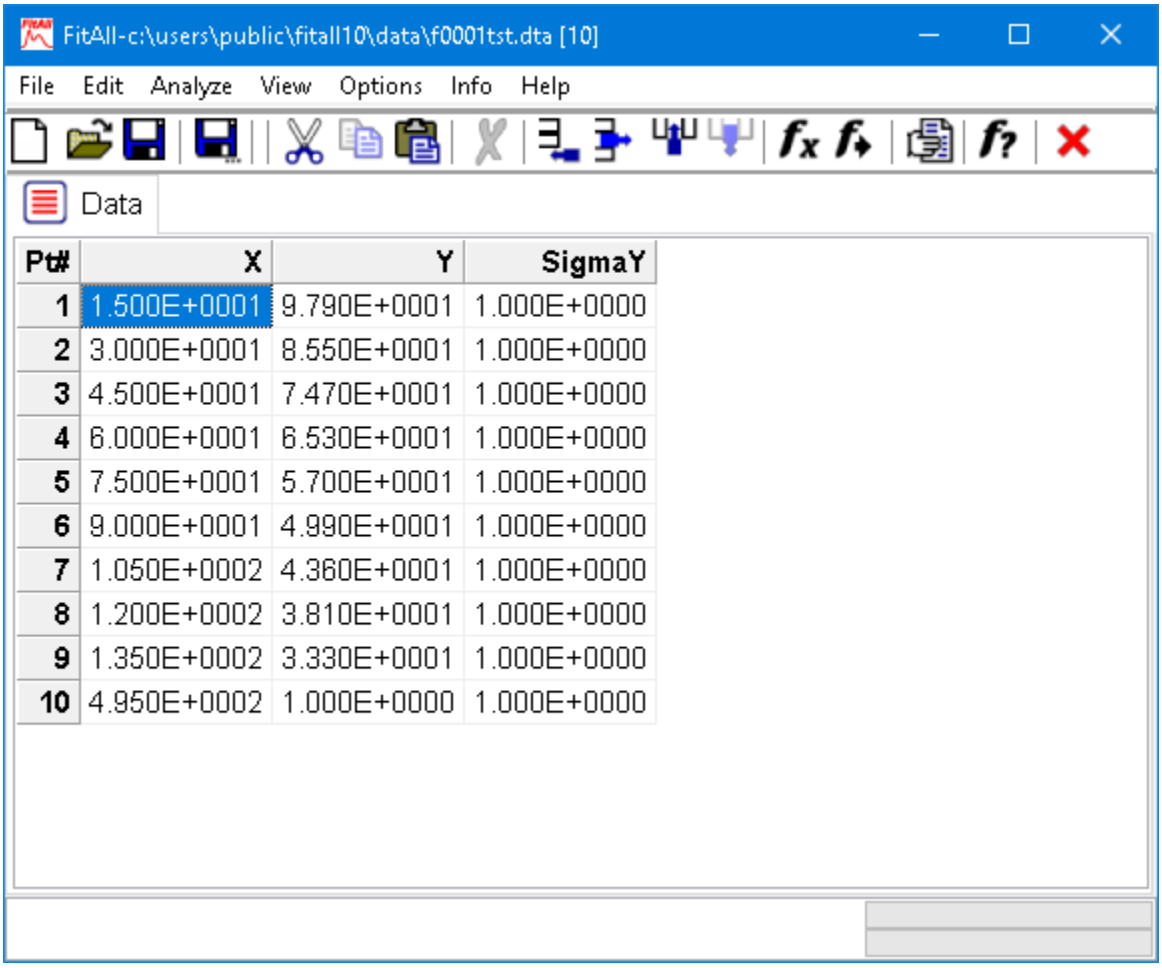
Edit > Copy 28

Edit > Cut 25

Delete

Choose Edit > Delete, press **Delete** or click the ✕ or ⇥ buttons to delete the selected data points in the Data window.

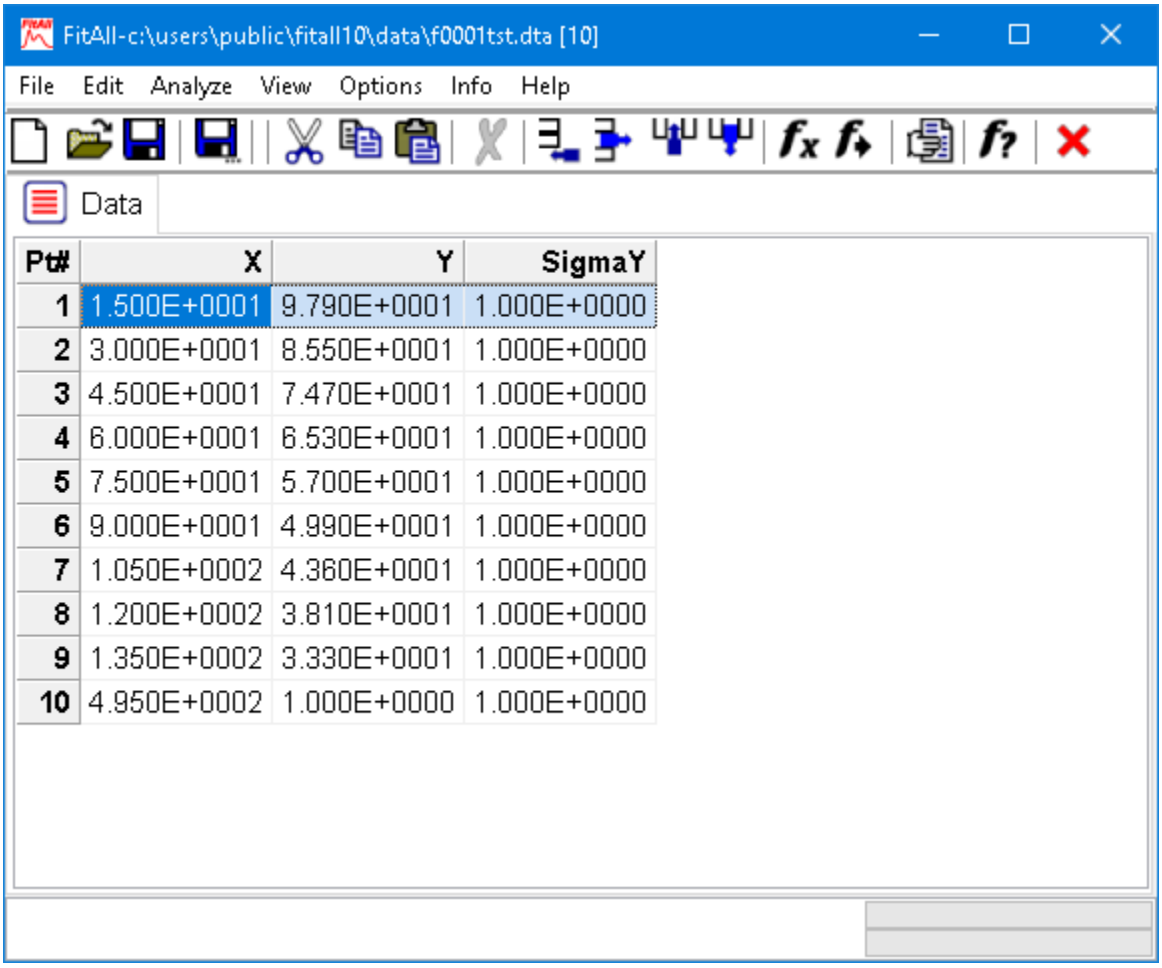
To select a row of data click on the 'Row row number'. You can use the Shift key to select more than one row.



Pt#	X	Y	SigmaY
1	1.500E+0001	9.790E+0001	1.000E+0000
2	3.000E+0001	8.550E+0001	1.000E+0000
3	4.500E+0001	7.470E+0001	1.000E+0000
4	6.000E+0001	6.530E+0001	1.000E+0000
5	7.500E+0001	5.700E+0001	1.000E+0000
6	9.000E+0001	4.990E+0001	1.000E+0000
7	1.050E+0002	4.360E+0001	1.000E+0000
8	1.200E+0002	3.810E+0001	1.000E+0000
9	1.350E+0002	3.330E+0001	1.000E+0000
10	4.950E+0002	1.000E+0000	1.000E+0000

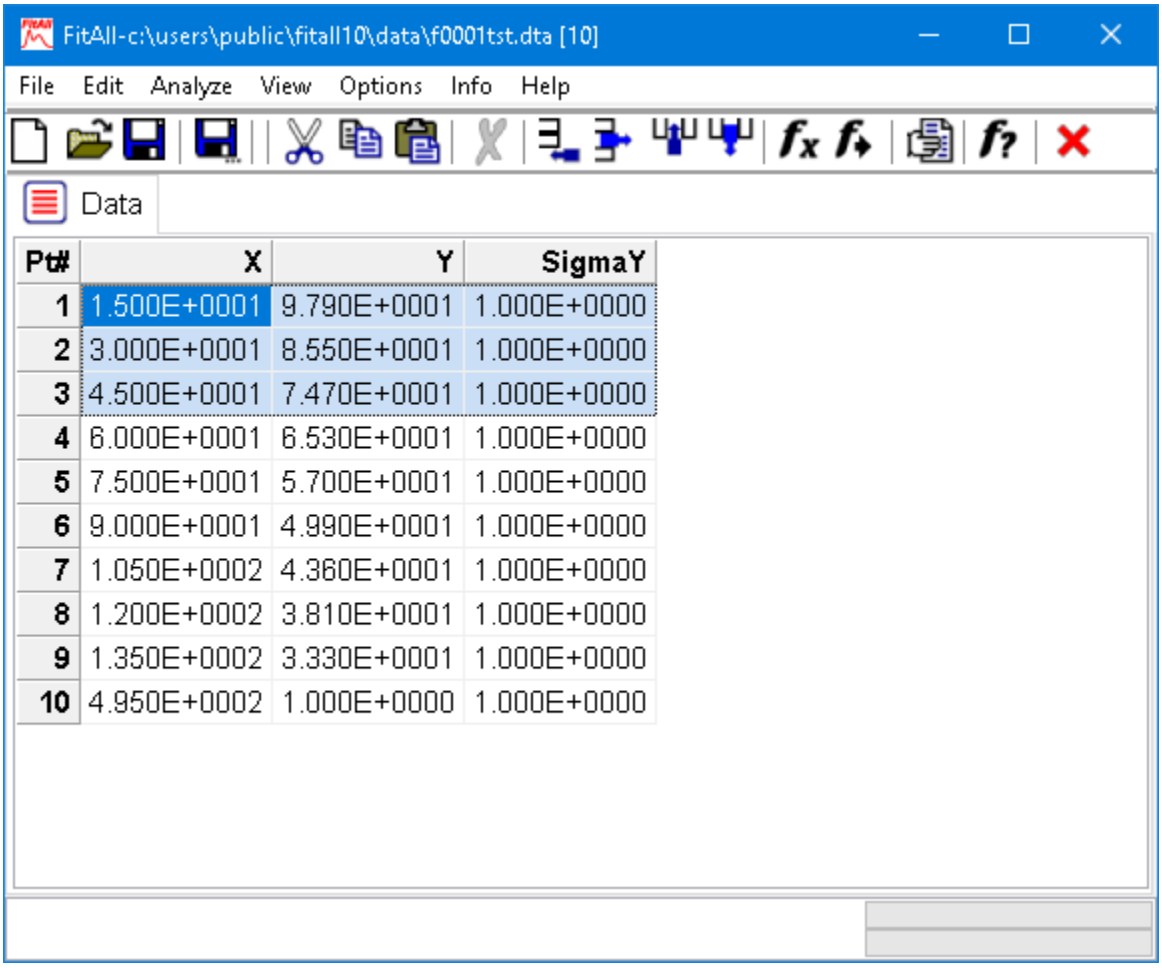
For example:

- Click on the row number 1.



Pt#	X	Y	SigmaY
1	1.500E+0001	9.790E+0001	1.000E+0000
2	3.000E+0001	8.550E+0001	1.000E+0000
3	4.500E+0001	7.470E+0001	1.000E+0000
4	6.000E+0001	6.530E+0001	1.000E+0000
5	7.500E+0001	5.700E+0001	1.000E+0000
6	9.000E+0001	4.990E+0001	1.000E+0000
7	1.050E+0002	4.360E+0001	1.000E+0000
8	1.200E+0002	3.810E+0001	1.000E+0000
9	1.350E+0002	3.330E+0001	1.000E+0000
10	4.950E+0002	1.000E+0000	1.000E+0000

- Hold down the Shift key and click on the Pt# number three (3). The result should look like this:



Pt#	X	Y	SigmaY
1	1.500E+0001	9.790E+0001	1.000E+0000
2	3.000E+0001	8.550E+0001	1.000E+0000
3	4.500E+0001	7.470E+0001	1.000E+0000
4	6.000E+0001	6.530E+0001	1.000E+0000
5	7.500E+0001	5.700E+0001	1.000E+0000
6	9.000E+0001	4.990E+0001	1.000E+0000
7	1.050E+0002	4.360E+0001	1.000E+0000
8	1.200E+0002	3.810E+0001	1.000E+0000
9	1.350E+0002	3.330E+0001	1.000E+0000
10	4.950E+0002	1.000E+0000	1.000E+0000

NOTE:
You also can select rows of data using the shift and arrow keys.

Select all

Choose Edit > Select all or press **Ctrl+A** to select all of the data points in ***FitAll***'s Data window.

Also See

Edit > Unselect all 34.

Unselect all

Choose Edit > Unselect all or press **Ctrl+U** to de-select all of the text in a text containing window, such as the Data window.

Also See

Edit > Select all 33.

Row(s) Add

Click Edit > Add point (row), press the **Insert** key or click the  button to add (append) a data point to the end of the data set.

The initial values in all the columns will be zero, with the possible exception of the last column.

The value in the last data column, the SigmaY column, may be one or zero, depending on the Options > Preferences > Set new SigmaY's to 1.0  setting.

To enter the values you actually want:

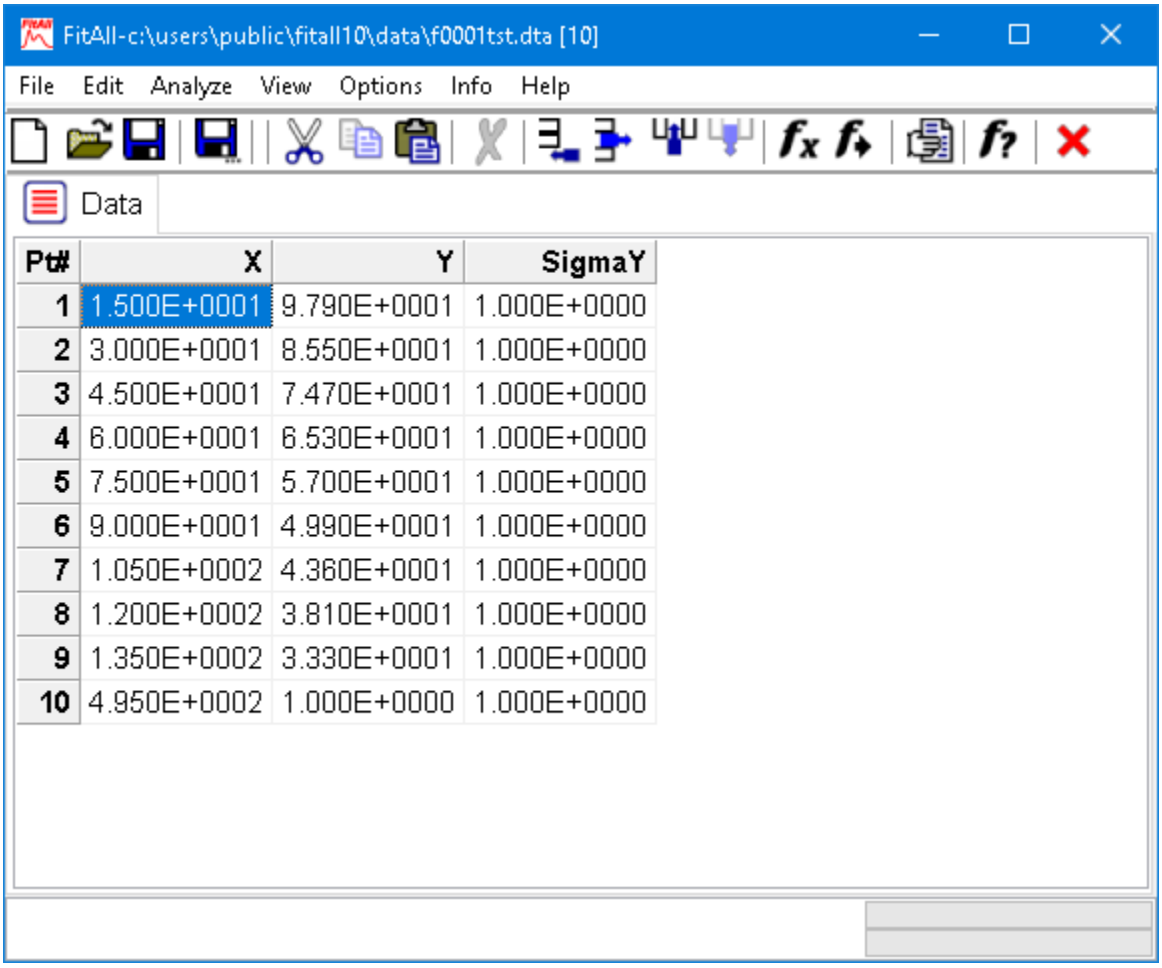
- Click on the value you want to change or use the arrow keys to highlight it.
- Type in the new value or press the **F2** key to edit the value.
- Press the **Enter** key.

For a more detailed example, see Entering and Editing Data in the Getting Started Guide.

Row(s) Delete

After selecting one or more rows of data, choose Edit > Delete, press the **Delete** key or click the button to delete the 'selected' data point(s) in the Data window.

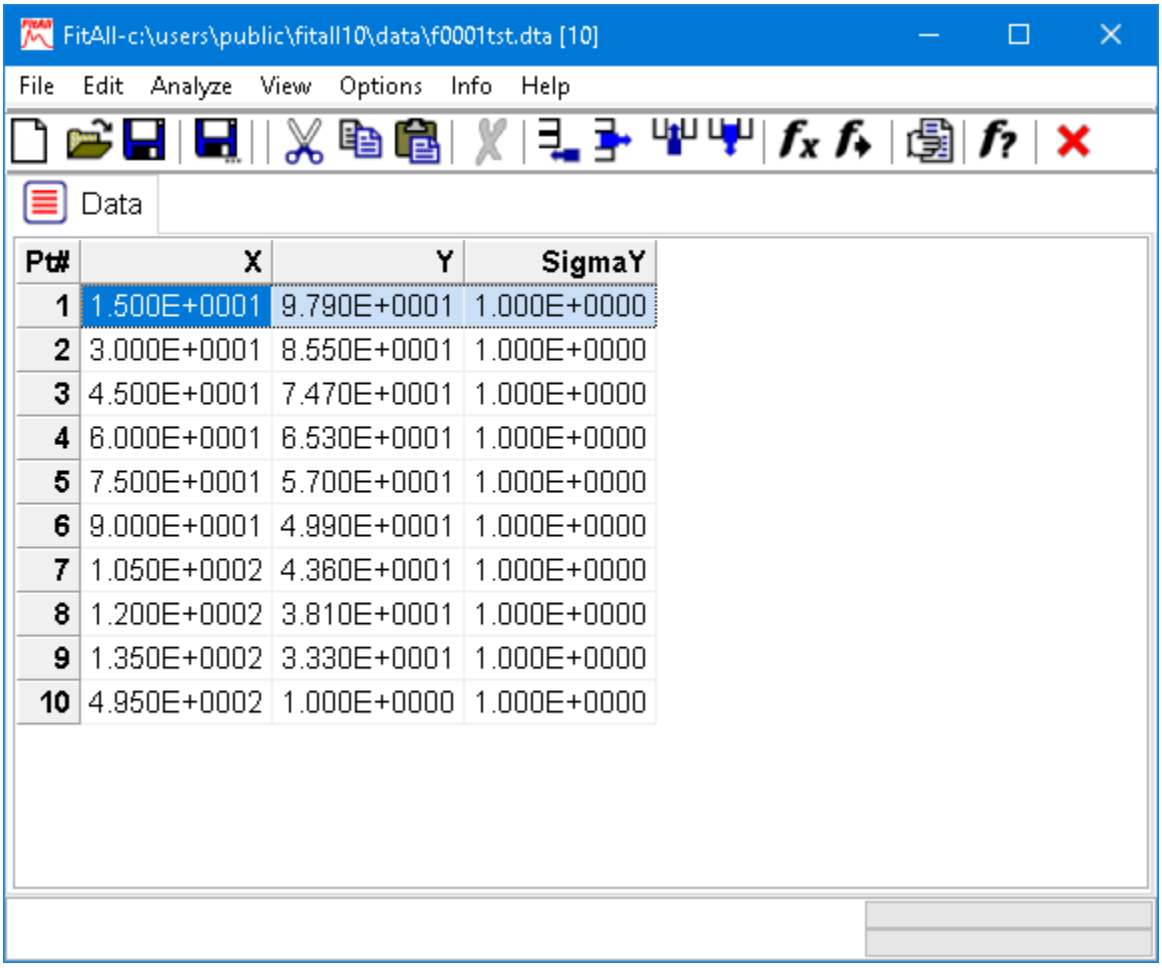
To select a row of data click on the 'Row row number'. You can use the Shift key to select more than one row.



Pt#	X	Y	SigmaY
1	1.500E+0001	9.790E+0001	1.000E+0000
2	3.000E+0001	8.550E+0001	1.000E+0000
3	4.500E+0001	7.470E+0001	1.000E+0000
4	6.000E+0001	6.530E+0001	1.000E+0000
5	7.500E+0001	5.700E+0001	1.000E+0000
6	9.000E+0001	4.990E+0001	1.000E+0000
7	1.050E+0002	4.360E+0001	1.000E+0000
8	1.200E+0002	3.810E+0001	1.000E+0000
9	1.350E+0002	3.330E+0001	1.000E+0000
10	4.950E+0002	1.000E+0000	1.000E+0000

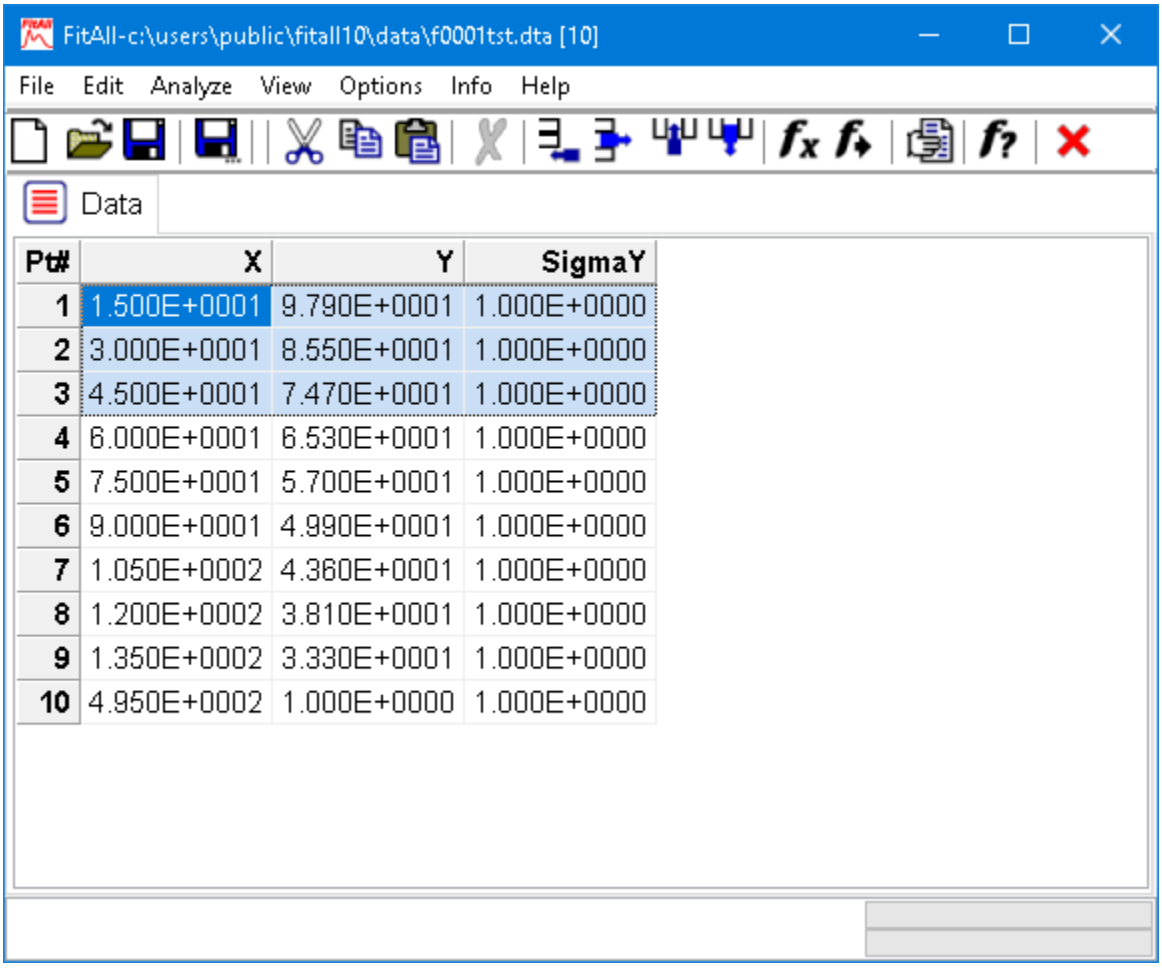
For example:

- Click on the row number 1.



Pt#	X	Y	SigmaY
1	1.500E+0001	9.790E+0001	1.000E+0000
2	3.000E+0001	8.550E+0001	1.000E+0000
3	4.500E+0001	7.470E+0001	1.000E+0000
4	6.000E+0001	6.530E+0001	1.000E+0000
5	7.500E+0001	5.700E+0001	1.000E+0000
6	9.000E+0001	4.990E+0001	1.000E+0000
7	1.050E+0002	4.360E+0001	1.000E+0000
8	1.200E+0002	3.810E+0001	1.000E+0000
9	1.350E+0002	3.330E+0001	1.000E+0000
10	4.950E+0002	1.000E+0000	1.000E+0000

- Hold down the Shift key and click on the Pt# number three (3). The result should look like this:



Pt#	X	Y	SigmaY
1	1.500E+0001	9.790E+0001	1.000E+0000
2	3.000E+0001	8.550E+0001	1.000E+0000
3	4.500E+0001	7.470E+0001	1.000E+0000
4	6.000E+0001	6.530E+0001	1.000E+0000
5	7.500E+0001	5.700E+0001	1.000E+0000
6	9.000E+0001	4.990E+0001	1.000E+0000
7	1.050E+0002	4.360E+0001	1.000E+0000
8	1.200E+0002	3.810E+0001	1.000E+0000
9	1.350E+0002	3.330E+0001	1.000E+0000
10	4.950E+0002	1.000E+0000	1.000E+0000

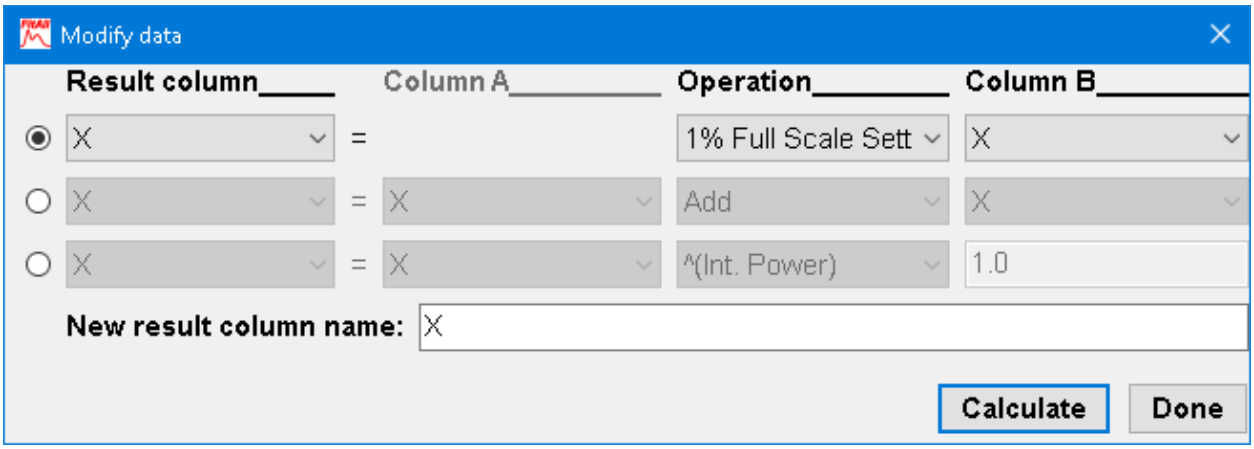
NOTE:
You also can select rows of data using the shift and arrow keys.

data Modify...

Choose Edit > data Modify... or press **Alt+M** to modify your data one column at a time.

> **NOTE:**
> This menu selection is available only when there is data available and the 'Data window' is the active window.

When you choose Edit > data Modify... the 'Modify data' dialog box appears. It looks like this:



To modify a column of data:

- Choose one of the three equations shown in the Modify data dialog box by clicking the top, middle or bottom radio button at the left side of the dialog box.
- Use the Result Column drop-down list to choose the data column into which the results of the calculations will be placed.
- Use the Column A and Column B drop-down lists to choose the data columns that will be used in the calculation.
- Use the Operation drop-down list to choose the arithmetic operation that will be performed. The available operations include such arithmetic operations as: absolute value, multiply, divide, Log, Ln and exponential to the base 10 or base e.
- Use the 'New result column name' edit box to assign a new name (title) to the result column.
- Click the Calculate button to do the calculation.
- Repeat the steps above to make additional data modifications.
- Click the Done button.

One column operations

- **1% Full Scale Setting**: Each element of the Result column is replaced by one percent of the *full-scale setting* of the value in Column B; that is, R = 0.01*FSS(B).

  The full-scale setting is determined by rounding the absolute value of B to the next highest power of ten.

  For example:
  for B-values from 0.0100 to 0.0999 the FSS is 0.1,
  for B-values from 0.100 to 0.999 the FSS is 1.0 and
  for B-values from 1.00 to 9.99 the FSS is 10.

  This *may* be useful in estimating the error (precision) of measured Y-values when the Y-values in one experiment span several orders of magnitude.

  NOTE 1:
  Typical measurement instruments, such as (auto-ranging) voltmeters, often have a precision that is directly proportional to their full-scale setting.

  NOTE 2:
  FitAll has a weighting factor called 1/(0.01*FSS) that will automatically calculate and use the FSS when weighting the regression analysis.

- **1/**: Each element of the Result column is replaced by the reciprocal of the value in Column B; that is, R = (1/B).

- **10^**: Each element of the Result column is replaced by 10 raised to the power of the value in Column B; that is, $R = 10^B$.

- **Abs**: Each element of the Result column is replaced by the positive value of the value in Column B; that is, R = |B|.

- **ArcCos**: Each element of the Result column is replaced by the ARCCOSINE of the value in Column B; that is, R = ArcCos(B).

- **ArcSin**: Each element of the Result column is replaced by the ARCSIN of the value in Column B; that is, R = Arcsin(B).

- **ArcTan**: Each element of the Result column is replaced by the ARCTANGENT of the value in Column B; that is, R = ArcTan(B).

- **Cos**: Each element of the Result column is replaced by the COSINE of the value in Column B; that is, R = Cos(B). The Column B values are assumed to be in radians.

- **Cube**: Each element of the Result column is replaced by the cube of the value in Column B; that is, $R=B^3$.

- **Cube root(**: Each element of the Result column is replaced by the cube root of the value in Column B; that is, $R = B^{(1/3)}$.

- **Degrees to Radians**: Each element of the Result column is replaced by 2π times the value in Column B; that is, $R = B * 2\pi$.

- **Exp**: Each element of the Result column is replaced by e raised to the power of the value in Column B; that is, $R = e^B$.

- **FFT**: Each element of the Result column is replaced by the **Fast Fourier Transform** (FFT) of the value in Column B; that is, R = FFT(B).

  The FFT procedure assumes that:

  1. The data to be analyzed contains an integer power of two (that is, 2i) data points to a maximum of 65,536 (which is equal to 216) points. If it does not, FitAll will, during the calculations, append a sufficient number of data points with a value of zero so that there are 2i data point to analyze. For example, if the actual data set contains 200 data points, FitAll will append 56 data points with a value of zero so that there are a total of 256 (= 28) data points to analyze.

  2. All the data are "real"-valued.

  3. The data were collected at a constant interval, D. For example if the time between each measurement was ten seconds then D = 10 s.

  The simplest way to display the results of the FFT transform is to plot the FFT values versus the Point Number in a data graph.

  The frequency at each data point can be calculated using the formula:

  f(i) = (i-1) / (2 * N * D), in which

  i is the point number, which has values from 1 to Npts,

  N is the number of data points that ***FitAll*** used in its calculations. For example, if the data set contains 200 data points, the value of N is 256, which is the smallest integer power of two that is greater than or equal to the number of data points in the data set, and

  D is the time difference between two adjacent data points.

- **FFT***: Each element of the Result column is replaced by the **Inverse Fast Fourier Transform** (FFT^*) of the value in Column B; that is, $R = FFT^*(B)$.

  The FFT* procedure makes the same assumptions as the FFT procedure.

NOTE:
If an inverse FFT, FFT^*, is applied to the result of the FFT of a column of data the final result will *not* be identical to the original data.

This is because the FFT calculates the amplitude at a *finite* number of frequencies.

- **Hours to Minutes**: Each element of the Result column is replaced by 60 times the value in Column B; that is, R = B*60.

- **Hours to mS**: Each element of the Result column is replaced by 3,600,000 times the value in Column B; that is, R = B*3600000.

- **Hours to Secs**: Each element of the Result column is replaced by 3,600 times the value in Column B; that is, R = B*3600.

- **Ln(Abs(**: Each element of the Result column is replaced by the natural logarithm of the value in Column B; that is, R = Ln|B|.

- **Log(Abs(**: Each element of the Result column is replaced by the base ten logarithm of the absolute value in Column B; that is, R=Log|B|.

- **Minutes to Hours**: Each element of the Result column is replaced by 1/60 times the value in Column B; that is, R = B/60.

- **Minutes to mS**: Each element of the Result column is replaced by 60,000 times the value in Column B; that is, R = B*60000.

- **Minutes to Secs**: Each element of the Result column is replaced by 60 times the value in Column B; that is, R = B*60.

- **mS to Hours**: Each element of the Result column is replaced by 1/3,600,000 times the value in Column B; that is, R = B/3600000.

- **mS to Minutes**: Each element of the Result column is replaced by 1/60,000 times the value in Column B; that is, R = B/60000.

- **mS to Seconds**: Each element of the Result column is replaced by 1/1,000 times the value in Column B; that is, R = B/1000.

- **Radians to Degrees**: Each element of the Result column is replaced by 1/(2π) times the value in Column B; that is, R = B / 2π.

- **Random Number**: Each element of the Result column is replaced by a (pseudo) random number such that the average of the values is zero, 0, and the standard deviation is 1.0.

- **Sin**: Each element of the Result column is replaced by the SINE of the value in Column B; that is, R = Sin(B). The Column B values are assumed to be in radians.

- **Secs to Hours**: Each element of the Result column is replaced by 1/3,600 times the value in Column B; that is, R = B/3600.

- **Secs to Minutes**: Each element of the Result column is replaced by 1/60 times the value in Column B; that is, R = B/60.

- **Secs to mS**: Each element of the Result column is replaced by 1,000 times the value in Column B; that is, R = B*1000.

- **Square**: Each element of the Result column is replaced by the square of the value in Column B; that is, R = B^2.

- **Square root(Abs(**: Each element of the Result column is replaced by the square root of the value in Column B; that is, R = $\sqrt{|B|}$.

- **Tan**: Each element of the Result column is replaced by the TANGENT of the value in Column B; that is, R = Tan(B). The Column B values are assumed to be in radians.

Two column operations

- **Add**: Each element of the Result column is replaced by the sum of the values in Column A and B, that is R = A + B.

- **Differentiate wrt**: Each element of the Result column is replaced by the derivative of the value in Column A taken with respect to the value in Column B; that is, R = $\partial A/\partial B$.

  The derivative is calculated using a 'natural' cubic spline. This is equivalent to using a sliding second-order polynomial.

  The derivatives at the first and last points are calculated using linear interpolation. The data are assumed to be sorted on Column B.

- **Divide by**: Each element of the Result column is replaced the values in Column A divided by the value in Column B; that is, R = A / B.

- **Integrate wrt**: Each element of the Result column is replaced by the area under the curve of a plot of the values in Column A vs. the values in Column B; that is, R = $\int AdB$.

  The area (integral) is calculated using linear interpolation (the trapezoid rule). The incremental change in the area for the i^{th} data point is given by: $(A_i + A_{i-1}) * (B_i - B_{i-1}) /2$.

  The data are assumed be sorted on Column B.

- **Multiply by**: Each element of the Result column is replaced product of the values in Column A and B; that is, R = A * B.

- **Polar ΘR to X**: Each element of the Result column is replaced by the Cartesian Coordinate value X from the Polar coordinates Theta, Θ, and R; that is, Result = B*Cos(A).

  It is assumed that Column A contains the Θ values and Column B contains the R values.

  It is essential that the Result Column is **not** either column A or B.

- **Polar ΘR to Y**: Each element of the Result column is replaced by the Cartesian Coordinate value X from the Polar coordinates Theta, Θ, and R; that is, Result = B*Sin(A).

  It is assumed that Column A contains the Θ values and Column B contains the R values.

  It is essential that the Result Column is **not** either column A or B.

- **Subtract**: Each element of the Result column is replaced by the difference between the values in Column A and B; that is, R = A - B.

- **XY to Polar R**: Each element of the Result column is replaced by the Polar coordinate Radius value, R, from the Cartesian coordinate values X and Y; that is, Result = $\sqrt{(A^2 + B^2)}$.

  It is assumed that Column A contains the X values and Column B contains the Y values.

  It is essential that the Result Column is **not** either column A or B.

- **XY to Polar Θ**: Each element of the Result column is replaced by the Polar coordinate Theta value, Θ, from the Cartesian coordinate values X and Y; that is, Result = Arctan2(B, A).

  It is assumed that Column A contains the X values and Column B contains the Y values.

  It is essential that the Result Column is **not** either column A or B.

One column and a constant operations

- **^(Integer power)**: Each element of the Result column is obtained by raising the value in Column A to the power of the constant; that is, $R = A^{const}$.

  The constant value must be an integer (whole) number. If it is not, ***FitAll*** will round it to the nearest whole number.

- **Abs()^**: Each element of the Result column is obtained by raising the absolute value of the corresponding value in Column A to the power of the constant; that is, $R = |A|^{const}$.

  The constant value can be a fraction; that is, it does not have to be a whole (integer) number.

- **Add**: Each element of the Result column is the sum of the corresponding element in Column A and the constant; that is, R = A + Const.

- **Divide by**: Each element of the Result column is the dividend of the corresponding element in Column A and the constant; that is, R = A / Const.

- **Limit <=**: Each element of the Result column is set to the corresponding value in column A if it is less than or equal to 'The Constant'; otherwise it is set to 'The Constant' value; that is, R = A if A <= Const otherwise R = Const.

- **Limit >=**: Each element of the Result column is set to the corresponding value in column A if it is greater than or equal to 'The Constant'; otherwise, it is set to 'The Constant' value; that is, R = A if A is >= Const otherwise R = Const.

- **Rnd to N sig. figs.**: Each element of the Result column is obtained by rounding the value in Column A to N significant figures.

  The constant value must be an integer (whole) number between 1 and 20. If it is not, ***FitAll*** will round it to the nearest whole number.

- **Subtract**: Each element of the Result column is the difference of the corresponding element in Column A and the constant; that is, R = A - Const.

- **Multiply by**: Each element of the Result column is the product of the corresponding element in Column A and the constant; that is, R = A * Const.

- **Smooth Boxcar**: Smooths one column of data by averaging the "Constant" number of adjacent data points.

  The constant you specify will be rounded to the nearest whole (integer) number.

  If you enter a value of one, 1, for the constant no smoothing will be done.

- **Smooth FFT**: Smooths one column of data using a Fast Fourier transform (FFT) as a 'low pass filter'. When you choose this type of smoothing, the 'Constant' value determines the 'amount of smoothing'. This number is approximately equivalent to the number of data points that are 'averaged'.

  The number that you enter does not have to be an integer. For example, 3, 3.5 and 6.27 are acceptable values for the constant.

  If you enter zero, 0, no smoothing will be done.

  FitAll assumes that the data are sorted on the independent variable. That is, when smoothing the Y-data, it is assumed that the data has been sorted on X.

  FFT smoothing is restricted to data sets with 2,097,152 or fewer data points.

- **Rotate X CC Degrees**: Modifies the values of the specified column assuming that it contains X-values and the corresponding Y-values are specified by the data set's Y-values; that is, the second last data column.

  The resulting values will correspond to the values obtained if the X and Y axes are rotated in a counter-clockwise direction by the specified number of degrees.

  It is very important that the Result column is NOT the current X, or a specified, column.

  Prior to applying this data modification create a new data column and specify the new column as the Result column.

  The reason for doing the above is that it is more than likely that you also will want to rotate the Y-values and the Y-value rotation requires the original X-values.

- **Rotate Y CC Degrees**: Modifies the values of the specified column assuming that it contains Y-values and the corresponding X-values are specified by the data set's X-values; that is, the first data column.

  The resulting values will correspond to the values obtained if the X and Y axes are rotated in a counter-clockwise direction by the specified number of degrees.

  It is very important that the Result column is NOT the current Y, or a specified, column.

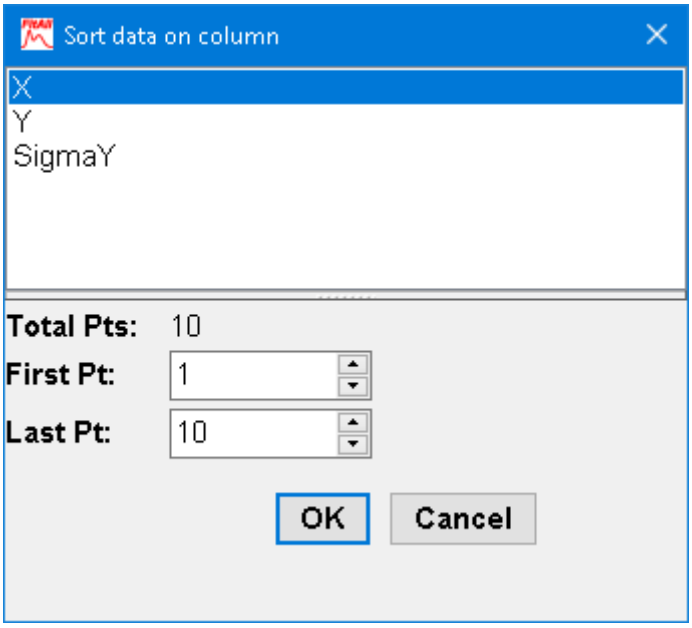
  Prior to applying this data modification create a new data column and specify the new column as the Result column.

  The reason for doing the above is that it is more than likely that you also will want to rotate the X-values and the X-value rotation requires the original Y-values.

data Sort...

Choose Edit > data Sort... to sort your data.

When you choose Edit > data Sort the 'Sort data on column' dialog box appears. It looks like this:



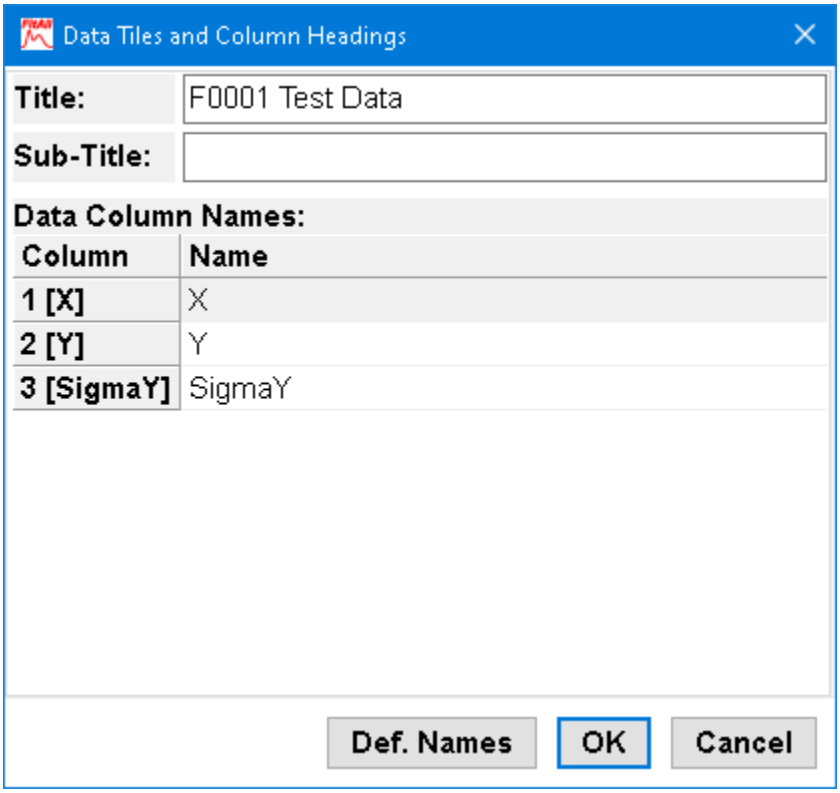
- Click the name of the column on which you want to sort the data.
- If you want to sort only some of the data, change the "First Pt." and "Last Pt." values to reduce the range of data points that will be sorted. By default all of the data points will be included in the sort operation.
- Click the **OK** button.

> **NOTE:**
> When ***FitAll*** does automatic initial estimates of the parameter values it normally expects the data to be sorted on the first, X, data column.

data Titles...

Click the Edit > data Titles... menu selections or press **Ctrl+T** to edit the data set's titles.

The 'Data Titles and Column Headings' dialog box will appear. It should look like this:



Title

Use the 'Title' edit box to enter a title for the data set.

Sub-Title

Use the 'sub-Title' edit box to enter a sub-title for the data set.

Data Column Names

Use the 'Data Column Names' table to change the data column names.

Use the up and down arrow keys to highlight the name you want to change. Type in the new column name.

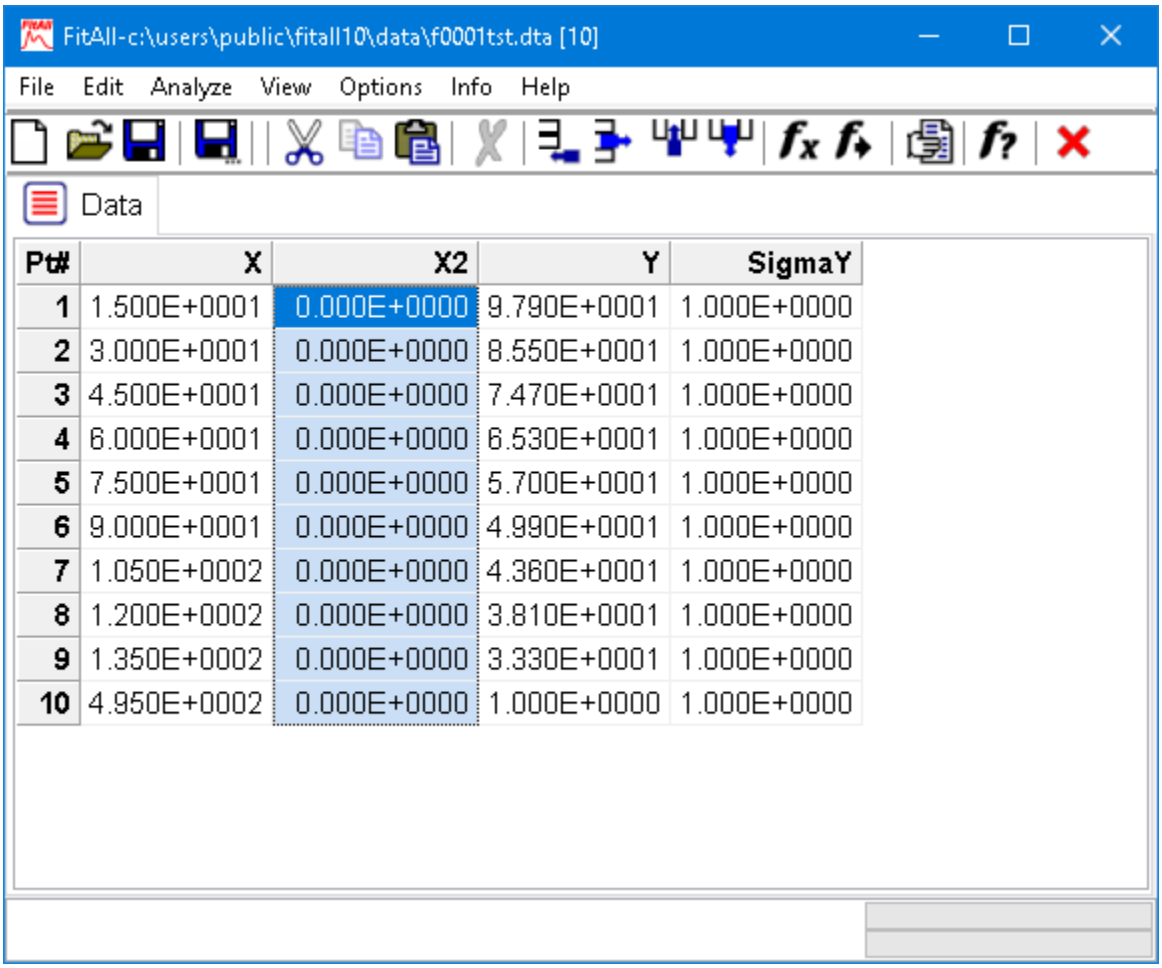
Def. Names

Click the "Def. Names" button to set the data column names to "X1, X2, ..., Y, SigmaY".

column Delete

After selection on or more data columns, choose Edit > column Delete or click the button to delete selected columns of data.

To select a data column click on the column title. The column will be highlighted. The data window may look like this:



Pt#	X	X2	Y	SigmaY
1	1.500E+0001	0.000E+0000	9.790E+0001	1.000E+0000
2	3.000E+0001	0.000E+0000	8.550E+0001	1.000E+0000
3	4.500E+0001	0.000E+0000	7.470E+0001	1.000E+0000
4	6.000E+0001	0.000E+0000	6.530E+0001	1.000E+0000
5	7.500E+0001	0.000E+0000	5.700E+0001	1.000E+0000
6	9.000E+0001	0.000E+0000	4.990E+0001	1.000E+0000
7	1.050E+0002	0.000E+0000	4.360E+0001	1.000E+0000
8	1.200E+0002	0.000E+0000	3.810E+0001	1.000E+0000
9	1.350E+0002	0.000E+0000	3.330E+0001	1.000E+0000
10	4.950E+0002	0.000E+0000	1.000E+0000	1.000E+0000

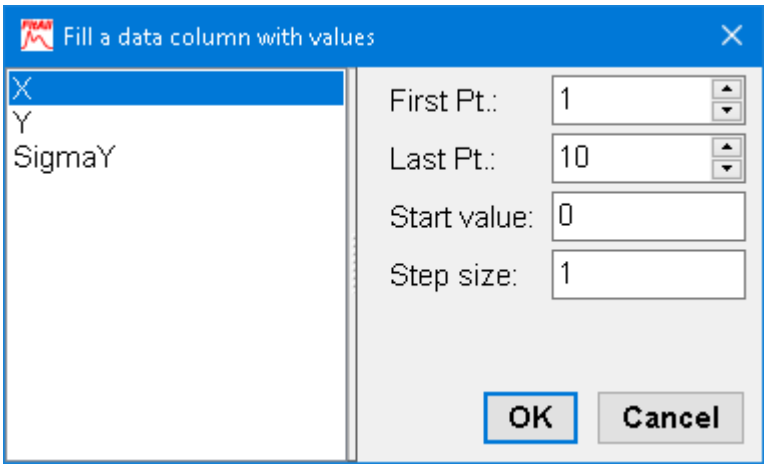
NOTE:
You also can select columns of data using the shift and arrow keys.

NOTE:
Since a ***FitAll*** data set must have at least three data columns, ***FitAll*** will only delete a column of data if there are at least four columns in the current data set

column Fill...

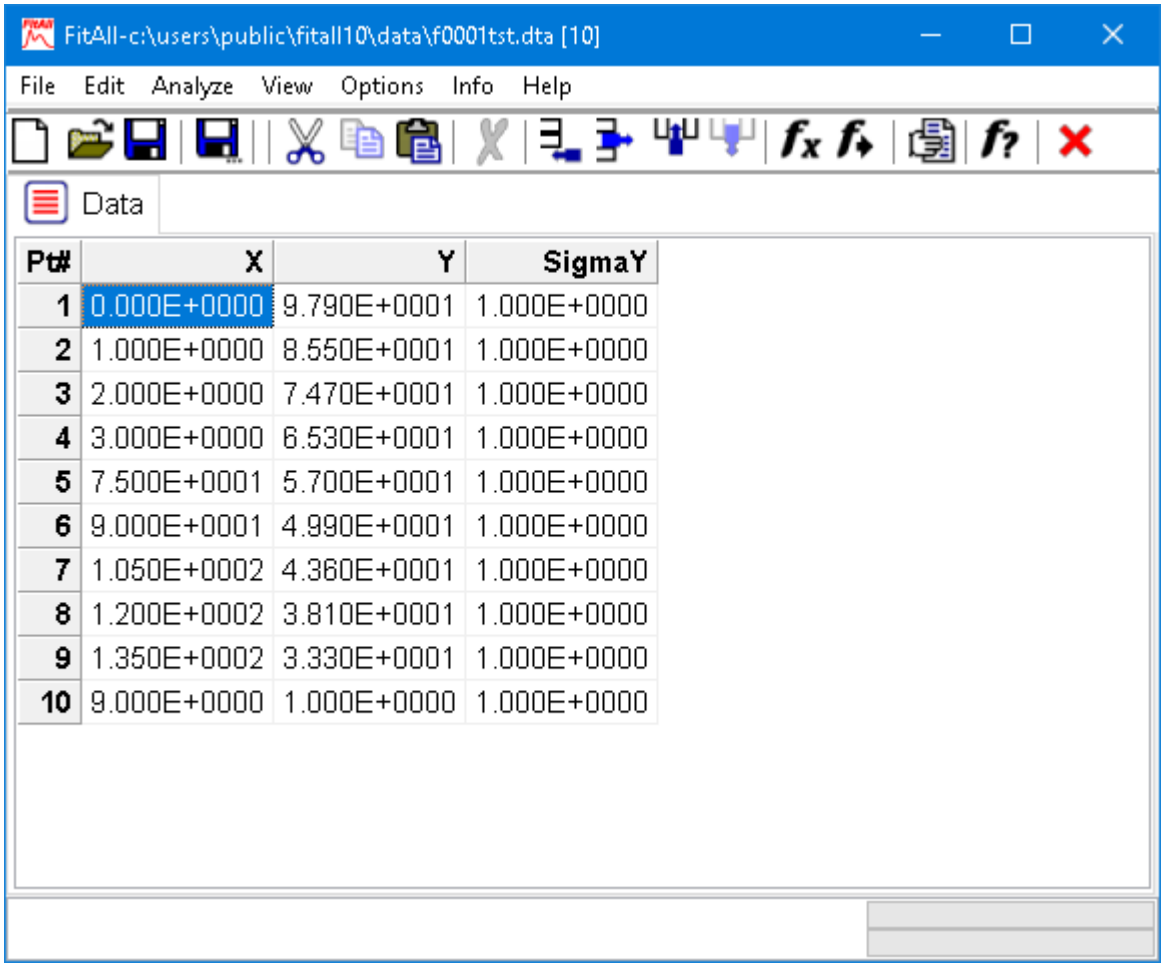
Choose Edit > column Fill... to set all of the data values in one column at once.

When you choose Edit > column Fill... the 'Fill a data column with values' dialog box appears. It looks like this:



- Select (highlight) the name of the column, that is to be filled with values, in the list box at the left side of the dialog.
- Change the value in the "First Pt." spin edit control as appropriate.
- Change the value in the "Last Pt." spin edit control as appropriate.
- Enter a starting value in the 'Start value' edit box.
- Enter a step size in the 'Step size' edit box.
- Click the **OK** button.

The result could look like this:



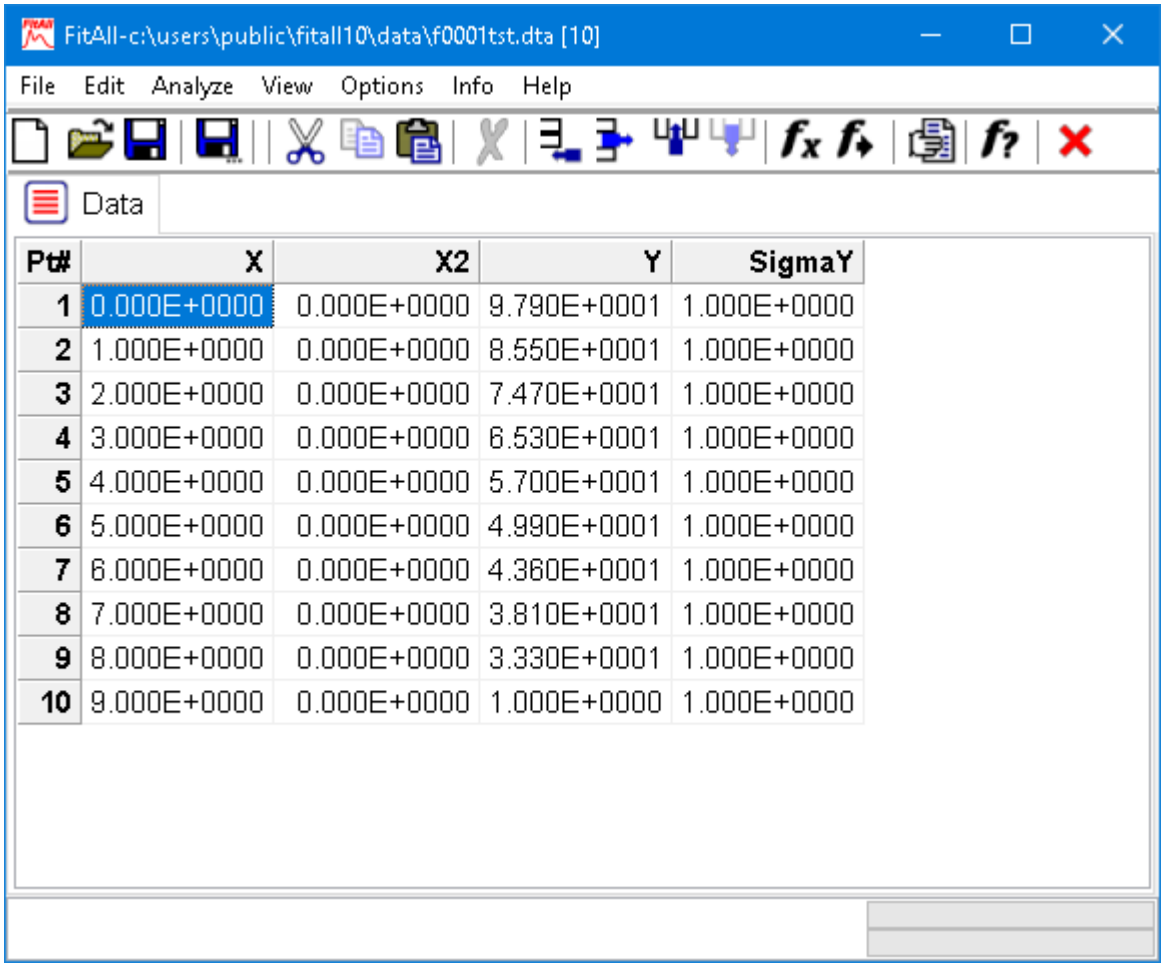
Pt#	X	Y	SigmaY
1	0.000E+0000	9.790E+0001	1.000E+0000
2	1.000E+0000	8.550E+0001	1.000E+0000
3	2.000E+0000	7.470E+0001	1.000E+0000
4	3.000E+0000	6.530E+0001	1.000E+0000
5	7.500E+0001	5.700E+0001	1.000E+0000
6	9.000E+0001	4.990E+0001	1.000E+0000
7	1.050E+0002	4.360E+0001	1.000E+0000
8	1.200E+0002	3.810E+0001	1.000E+0000
9	1.350E+0002	3.330E+0001	1.000E+0000
10	9.000E+0000	1.000E+0000	1.000E+0000

column Insert

Choose Edit > column Insert or click the button to insert a new data column into the data set that is currently in memory.

> **NOTE:**
> This option is only available when the 'Data window' is the active window.

After choosing this menu selection the data window may look like this:



Pt#	X	X2	Y	SigmaY
1	0.000E+0000	0.000E+0000	9.790E+0001	1.000E+0000
2	1.000E+0000	0.000E+0000	8.550E+0001	1.000E+0000
3	2.000E+0000	0.000E+0000	7.470E+0001	1.000E+0000
4	3.000E+0000	0.000E+0000	6.530E+0001	1.000E+0000
5	4.000E+0000	0.000E+0000	5.700E+0001	1.000E+0000
6	5.000E+0000	0.000E+0000	4.990E+0001	1.000E+0000
7	6.000E+0000	0.000E+0000	4.360E+0001	1.000E+0000
8	7.000E+0000	0.000E+0000	3.810E+0001	1.000E+0000
9	8.000E+0000	0.000E+0000	3.330E+0001	1.000E+0000
10	9.000E+0000	0.000E+0000	1.000E+0000	1.000E+0000

> **NOTE:**
> The new column is automatically inserted as the third last column in the data set and all of its values are zero. This corresponds to the last of the independent variable columns.

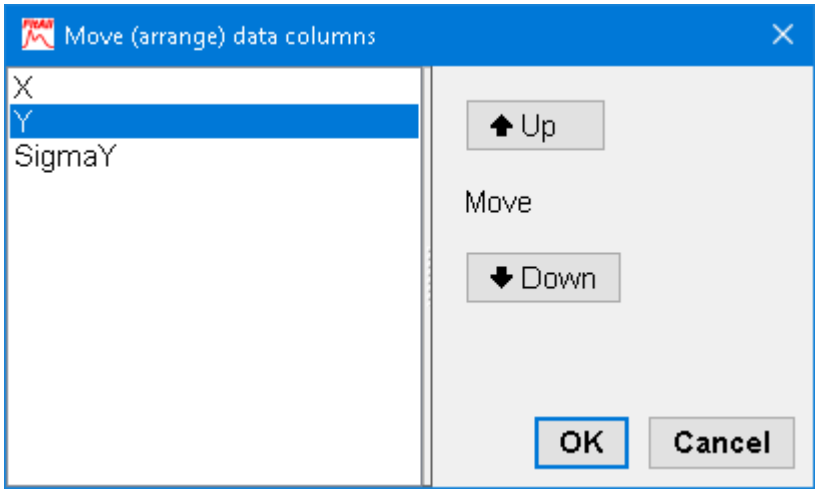
If you want the new column at a different location, you can change its position using the Edit > column Move... 54 menu selection or by selecting the column heading and dragging it to its new position.

column Move...

Choose Edit > column Move... to change the order of the data columns in the data set that is currently in memory.

> **NOTE:**
> This option is only available when the 'Data window' is the active window.

When you choose Edit > column Move... the 'Move data columns' dialog box appears. It looks like this:



- Select one of the columns in the listbox at the left of the dialog by clicking on it.
- Click either the Up or Down button to change the position of the currently selected column.
- Click the OK button when the columns are in the order that you want them.

It also is possible to "drag" a column from one position to another. Here's how to do it:

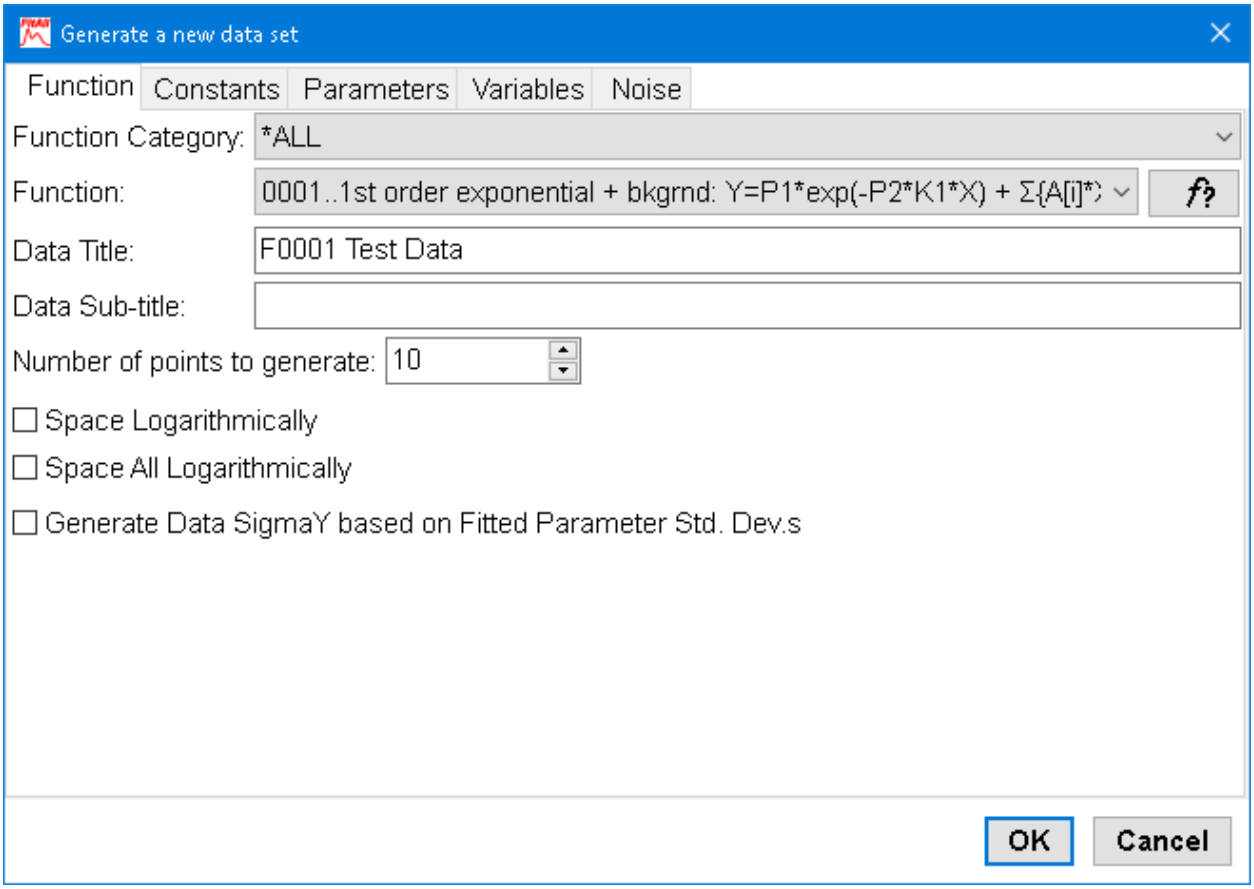
- Click on the title of the column that you want to move. (This will select/highlight it).
- "Click and drag" the column title to its new position.
- Release the mouse button.

Generate data set...

Choose Edit > Generate data set... to create a set of data that is calculated using one of ***FitAll***'s defined functions with the constants and parameters of your choice.

Use this menu selection to create sample data sets or data sets that can be used as calibration curves.

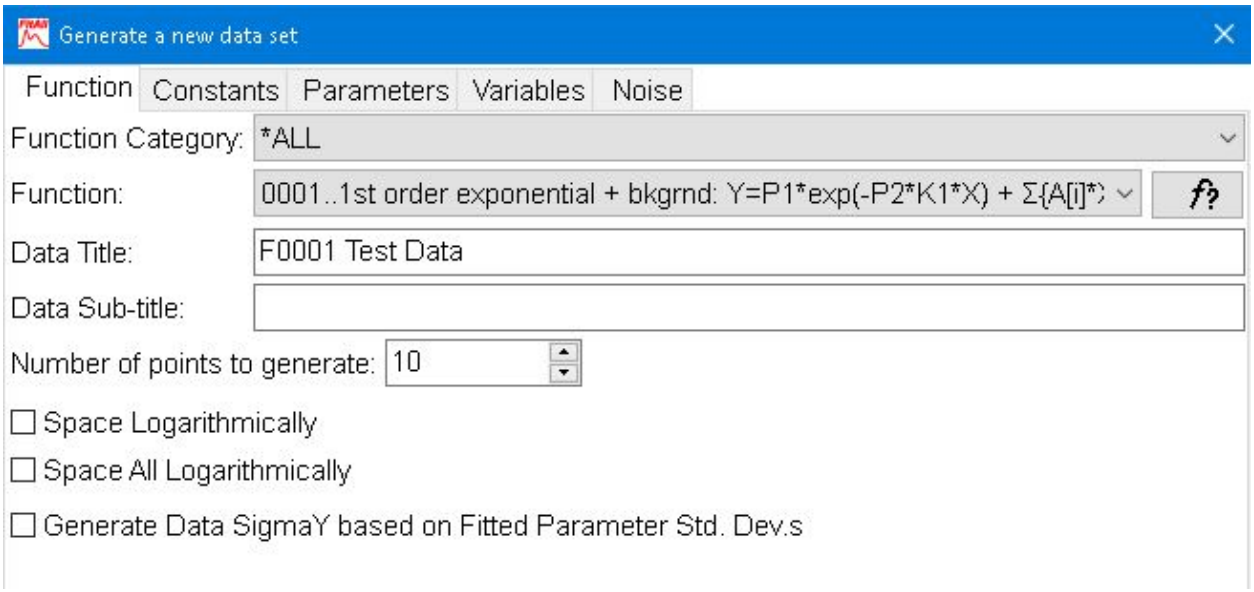
When you choose Edit > Generate data set... the 'Generate new data set' dialog box appears. It looks like this:



and has five tabs -- Function 56, Constants 57, Parameters 57, Variables 58 and Noise 58.

- Click on each of the tabs in turn and change the settings to what you want them to be.
- Click the **OK** button.

Function



Ftn Category

Use the Ftn Category drop down list to restrict (limit) the list of selectable functions.

> **NOTE:**
> Only the functions in the category that you select will be displayed in the Function drop down list.

Function

Use the Function drop down list to select the function that you want to use to generate a new set of data.

If more than one variation of the function is available, one or more dialog boxes requesting additional information will appear. In each dialog, enter an appropriate value and click the **OK** button.

Help for Current Function, f?

Click the f? button to display Help for the currently selected function.

Data Title

Use the Data Title edit box to enter a title for the data set.

Data Sub-Title

Use the Data Sub-Title edit box to enter a sub-title for the data set.

Number of points to generate

Use the 'Number of points to generate' spin-edit box to enter the number of data points that should be calculated.

The minimum value is two (2) and the maximum value depends on the Preferences, Max. data points 126 setting.

NOTE:
The Variables tab is used to set the minimum and maximum values of the X-variables (that is, the independent variables) that will be used in the calculation.

If you are going to have the X-values range from 0 to 10 then set the number of data points to 11 so that the actual X-values are 0, 1, 2, .., 10.

Space Logarithmically

Check this item if you want the first X-variable's spacing between the calculated data points to be logarithmic.

This is useful if graphs of the data usually use a logarithmic scale.

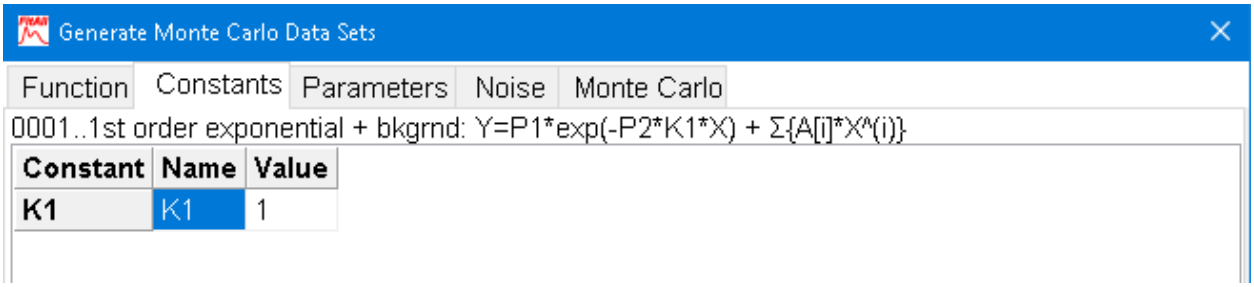
Space All Logarithmically

Check this item if you want all of the X-variables' spacings between the calculated data points to be logarithmic. (This assumes that there is more than one X-variable.)

Generate Data SigmaY

Check this item if you want ***FitAll*** to use the parameter standard deviations from the last analysis to calculate the estimated error (standard deviation) of the calculated Y-values.

Constants



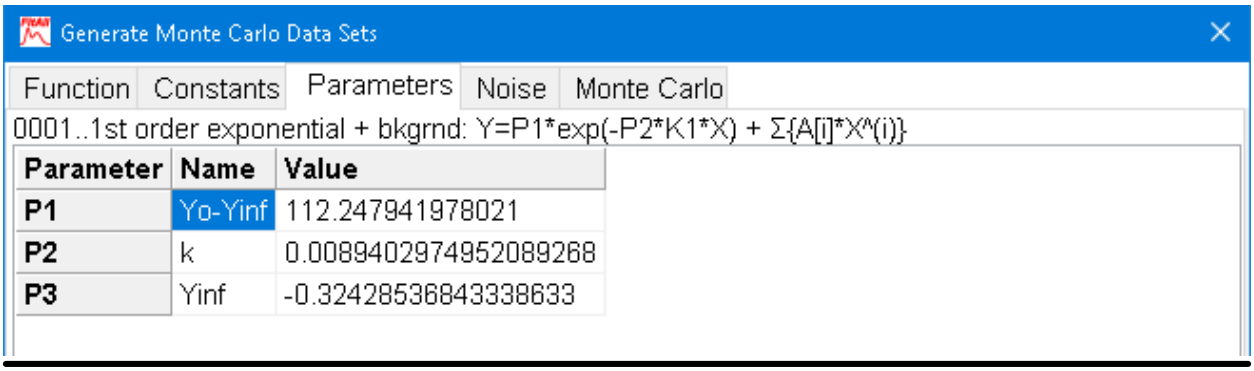
Name

Initially, the names displayed in the 'Name' column are the current default constant names for the selected function. You can change the names to whatever you want.

Value

Initially, the values displayed in the 'Value' column are the current constant values for the selected function. You can change the values to whatever you want.

Parameters



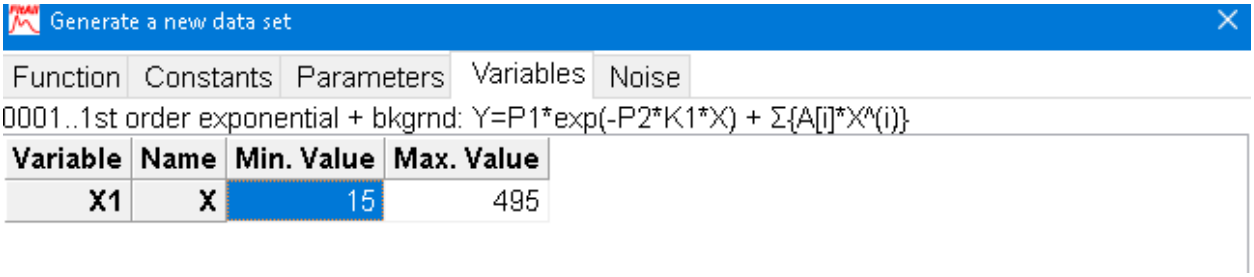
Name

Initially, the names displayed in the 'Name' column are the current default parameter names for the selected function. You can change the names to whatever you want.

Value

Initially, the values displayed in the 'Value' column are the current parameter values for the selected function. You can change the values to whatever you want.

Variables



Name

Initially, the names displayed in the 'Name' column are the current independent variable names for the selected function. You can change the names to whatever you want.

Min. Value

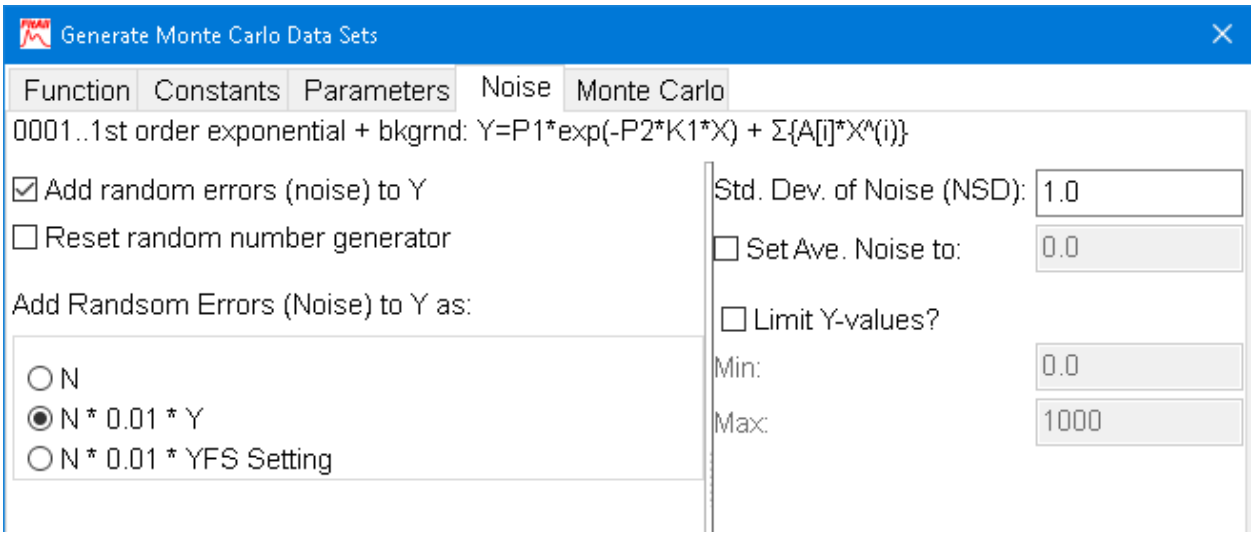
When ***FitAll*** generates a data set, it uses the 'Number of points to generate' value, the 'Min. Value' and the 'Max. Value' of each of the independent, X, variables to calculate a set of equally space independent variable values at which the function will be evaluated.

Use the 'Min. Value' edit box to set the smallest value of the independent variable.

Max. Value

Use the 'Max. Value' edit box to set the largest value of the independent variable.

Noise



Add random errors (noise) to Y

Select this check box to have ***FitAll*** generate a set of errors that will be added to the calculated values of Y. The absolute value of the errors will be placed in the 'SigmaY' data column.

Do not check this box if you are generating a set of data to be used for a calibration plot.

Reset random number generator

Select this check box if you want ***FitAll*** to initialize the random number generator just before the data set is calculated.

In most circumstances this item should not be checked.

Add noise (random errors) to Y as

Use these radio button to choose how you want the noise values calculated before they are added to the Y-value. The noise values also are stored in the last data column, the SigmaY column.

There are three choices:

- **N**: For each data set, a set of random numbers is generated with the desired standard deviation and an average of approximately zero. The specified average is then added to each of the noise values. The result is then added to the Y-value.

- **N*0.01*Y:** For each data set, a set of random numbers is generated with the desired standard deviation and an average of approximately zero. The specified average is then added to each of the noise values. These values are then multiplied by 0.01 (i.e., 1%) and the Y-value. The result is then added to the Y-value.

  Noise values of this type can be used to approximate measurement errors that are proportional to the value of the (measured) independent variable, Y.

- **N*0.01*YFS Setting**: For each data set, a set of random numbers is generated with the desired standard deviation and an average of approximately zero. The specified average is then added to each of the noise values. These values are then multiplied by 0.01 (i.e., 1%) and the 'Full Scale Yrange' value. The result is then added to the Y-value.

  Noise values of this type can be used to approximate instrumental measurement errors that are proportional to the full-scale range setting typical of most measurement equipment.

  The full-scale range setting is determined by rounding the absolute value of Y to the next highest power of ten.

  For example:

  for Y-values from 0.0100 to 0.0999 the YFSRange is 0.1,

  for Y-values from 0.100 to 0.999 the YFSRange is 1.0 and

  for Y-values from 1.00 to 9.99 the YFSRange is 10.

  > **NOTE:**
  > If the Y-values in the data span more than an order of magnitude, this type of noise is probably the most representative of the actual experimental noise.

Also, when fitting the data it is likely most appropriate to use a weighting factor of $1/Y^2$.

Std. Dev. of Noise (NSD)

Use the 'Std. Dev. of Noise (NSD)' edit box to set the standard deviation of the random numbers (noise) that will be added to the dependent, Y, variable values. These values also will be placed in the 'SigmaY' data column, that is, the last data column.

Average Noise Value

Use the 'Average noise value' check and edit boxes if you want the average of the added noise values to differ from (approximately) zero.

Limit Y-Values

Use the "Use Limits" check box to determine whether ***FitAll*** will place limits on the Y-value.

Use the Min and Max edit boxes to set the values of these limits.

Depending on the size of the random errors (noise) being added to the Y-value, the final Y-value could end up having an unrealistic or physically meaningless value or a value that would exceed the range of the 'hypothetical' instrument that is making the measurements.

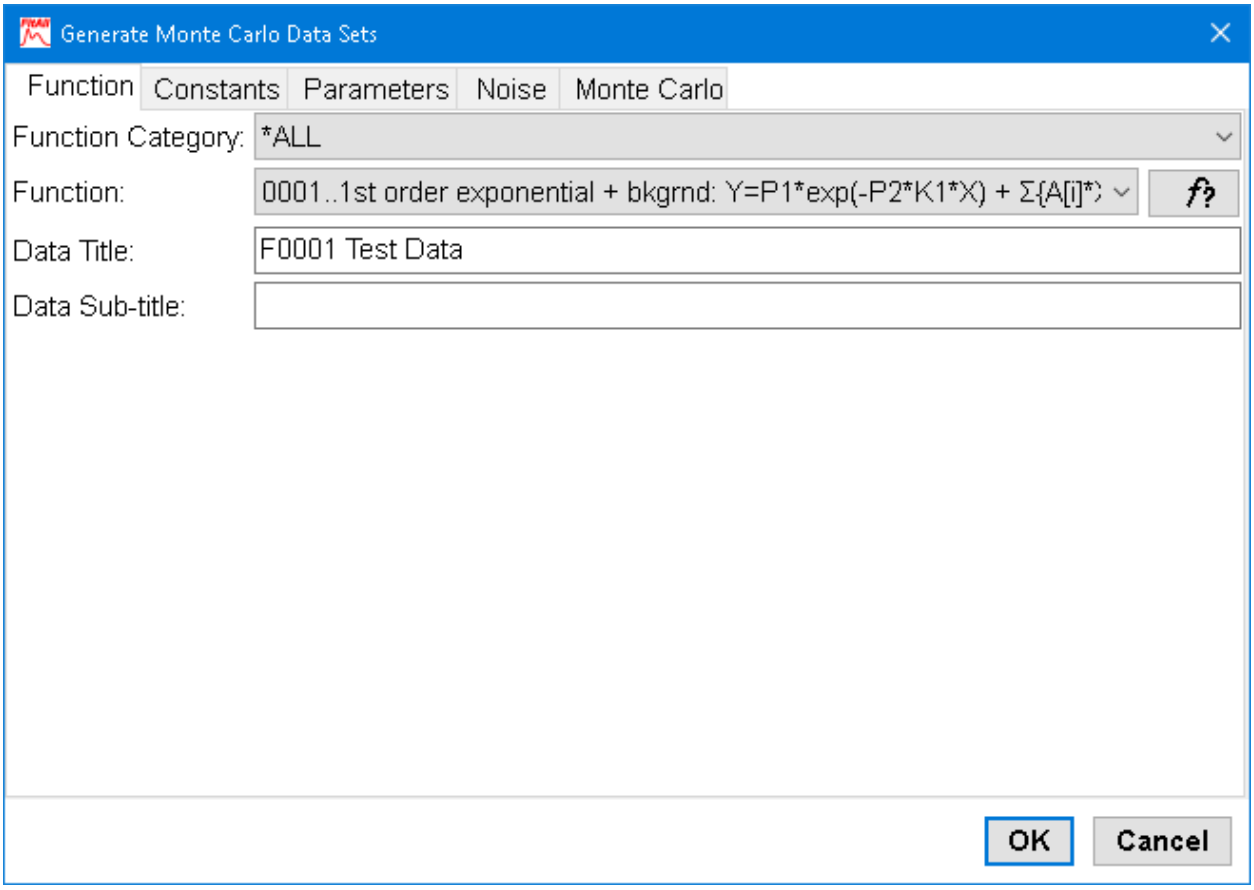
For example, adding a negative value of the noise to a very small Y-value might produce a negative result which may be physically impossible. In such a case, it would be useful to set the minimum value to zero.

Generate Monte Carlo data sets...

Choose Edit > Generate Monte Carlo data sets to create one or more sets of data using one of the functions and the values of your choice for the parameters, constants and noise.

The values of the independent variable(s), X, used when generating the data are obtained from the data currently in memory.

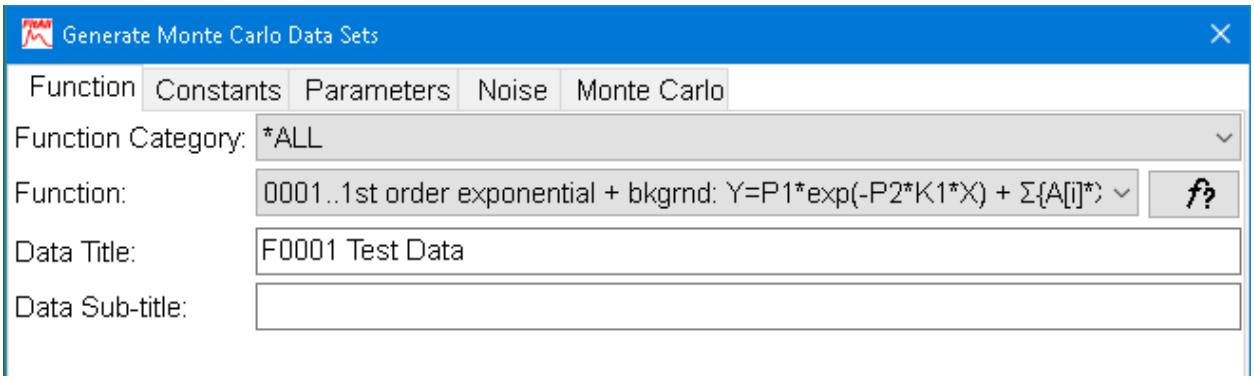
When you select Edit > Generate Monte Carlo data sets, the 'Generate Monte Carlo data sets' dialog box appears. It looks like this:



and has five tabs -- Function 62, Constants 63, Parameters 64, Noise 65 and Monte Carlo 67.

Click on each of the tabs in turn and change the settings to what you want, then click the **OK** button.

Function



Ftn Category

Use the Ftn Category drop down list to restrict (limit) the list of selectable functions.

> **NOTE:**
> Only the functions in the category that you select will be displayed in the Function drop down list.

Function

Use the Function drop down list to select the function that you want to use to generate the new data sets.

If more than one variation of the function is available, one or more dialog boxes requesting additional information will appear. In each dialog, enter an appropriate value and click the **OK** button.

Help for Current Function, f?

Click the f? button to display Help for the currently selected function.

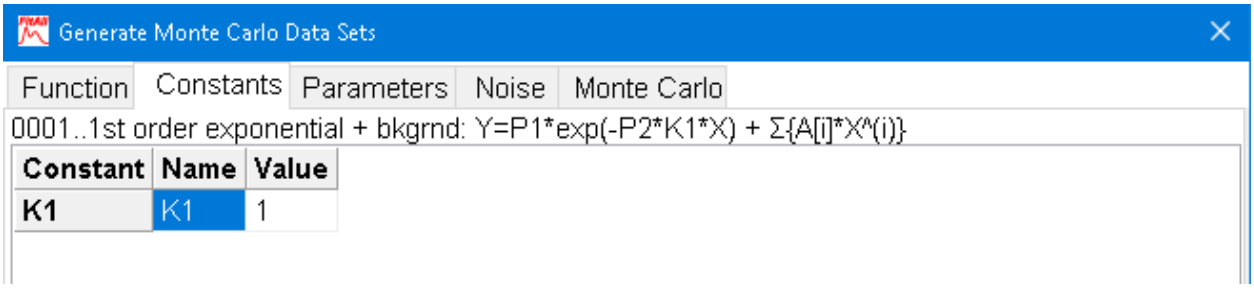
Data Title

Use the Data Title edit box to enter a title for the data sets.

Data Sub-Title

Use the Data Sub-Title edit box to enter a sub-title for the data sets.

Constants



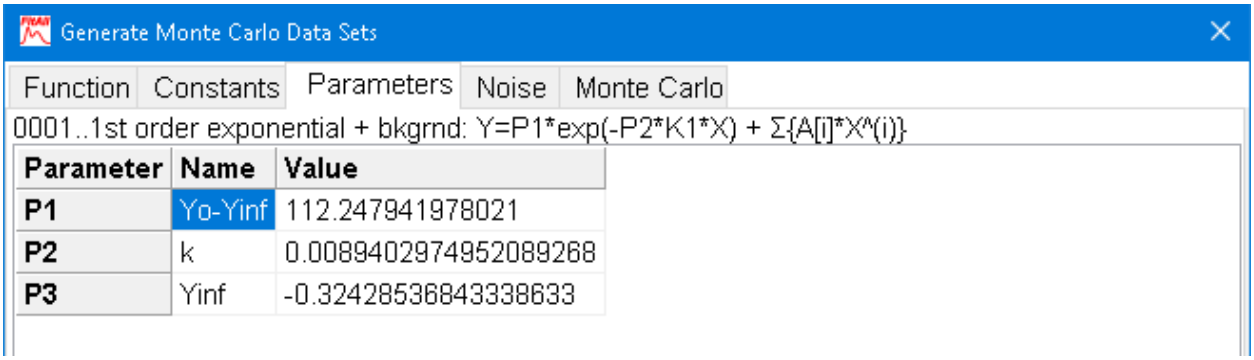
Name

Initially, the names displayed in the 'Name' column are the current default constant names for the selected function. You can change the names to whatever you want.

Value

Initially, the values displayed in the 'Value' column are the current constant values for the selected function. You can change the values to whatever you want.

Parameters



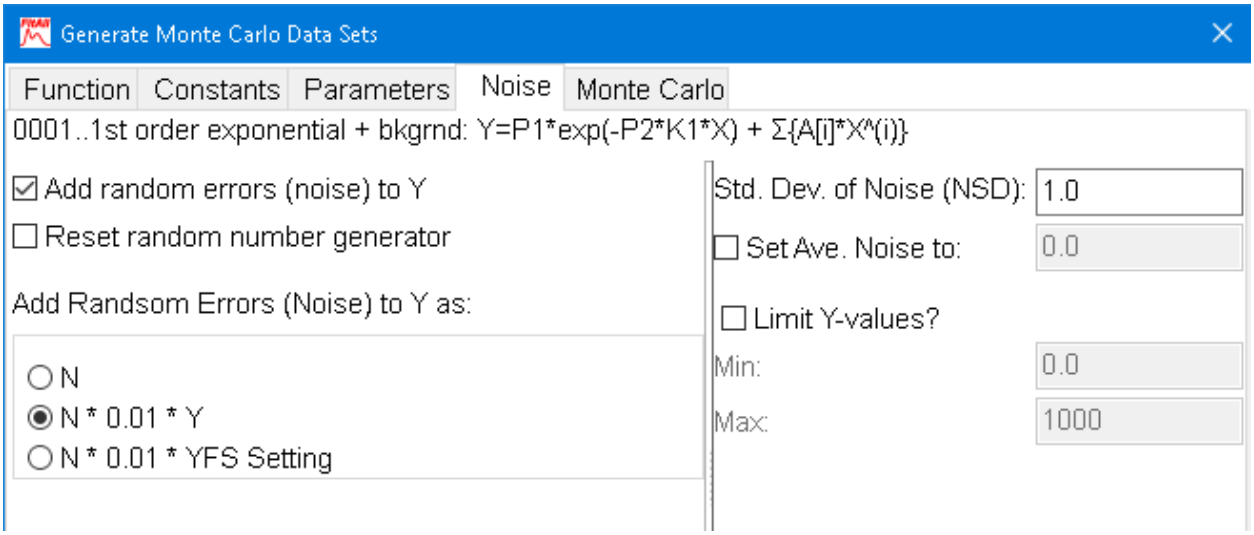
Name

Initially, the names displayed in the 'Name' column are the current default parameter names for the selected function. You can change the names to whatever you want.

Value

Initially, the values displayed in the 'Value' column are the current parameter values for the selected function. You can change the values to whatever you want.

Noise



Add random errors (noise) to Y

Select this check box to have ***FitAll*** generate a set of errors that will be added to the calculated values of Y. The absolute value of the errors will be placed in the 'SigmaY' data column.

Do not check this box if you are generating a set of data to be used for a calibration plot.

Reset random number generator

Select this check box if you want ***FitAll*** to initialize the random number generator just before the data set is calculated.

In most circumstances this item should not be checked.

Add noise (random errors) to Y as

Use these radio button to choose how you want the noise values calculated before they are added to the Y-value. The noise values also are stored in the last data column, the SigmaY column.

There are three choices:

- **N**: For each data set, a set of random numbers is generated with the desired standard deviation and an average of approximately zero. The specified average is then added to each of the noise values. The result is then added to the Y-value.

- **N*0.01*Y**: For each data set, a set of random numbers is generated with the desired standard deviation and an average of approximately zero. The specified average is then added to each of the noise values. These values are then multiplied by 0.01 (i.e., 1%) and the Y-value. The result is then added to the Y-value.

  Noise values of this type can be used to approximate measurement errors that are proportional to the value of the (measured) independent variable, Y.

- **N*0.01*YFS**: For each data set, a set of random numbers is generated with the desired standard deviation and an average of approximately zero. The specified average is then added to each of the noise values. These values are then multiplied by 0.01 (i.e., 1%) and the 'Full Scale Yrange' value. The result is then added to the Y-value.

Noise values of this type can be used to approximate instrumental measurement errors that are proportional to the full-scale range setting typical of most measurement equipment.

The full-scale range setting is determined by rounding the absolute value of Y to the next highest power of ten.

For example:

for Y-values from 0.0100 to 0.0999 the YFSRange is 0.1,

for Y-values from 0.100 to 0.999 the YFSRange is 1.0 and

for Y-values from 1.00 to 9.99 the YFSRange is 10.

> **NOTE:**
> If the Y-values in the data span more than an order of magnitude, this type of noise is probably the most representative of the actual experimental noise.
>
> Also, when fitting the data it is likely most appropriate to use a weighting factor of $1/Y^2$.

Std. Dev. of Noise (NSD)

Use the 'Std. Dev. of Noise (NSD)' edit box to set the standard deviation of the random numbers (noise) that will be added to the dependent, Y, variable values. These values also will be placed in the 'SigmaY' data column, that is, the last data column.

Average Noise Value

Use the 'Average noise value' check and edit boxes if you want the average of the added noise values to differ from (approximately) zero.

Limit Y-Values

Select (check) the 'Limit Y-Values' check box if you want ***FitAll*** to limit (constrain) the generated Y-values to the range Min <= Y <= Max.

- **Min**: Use the 'Min' edit box to enter the minimum Y-value that will be generated. If a generated Y-value is less than the specified Min. value, ***FitAll*** will adjust the added noise value so that the resulting Y-value is equal to the specified Min value.

- **Max**: Use the 'Max' edit box to enter the maximum Y-value that will be generated. If a generated Y-value is greater than the specified Max. value, ***FitAll*** will adjust the added noise value so that the resulting Y-value is equal to the specified Max. value.

CAUTION:

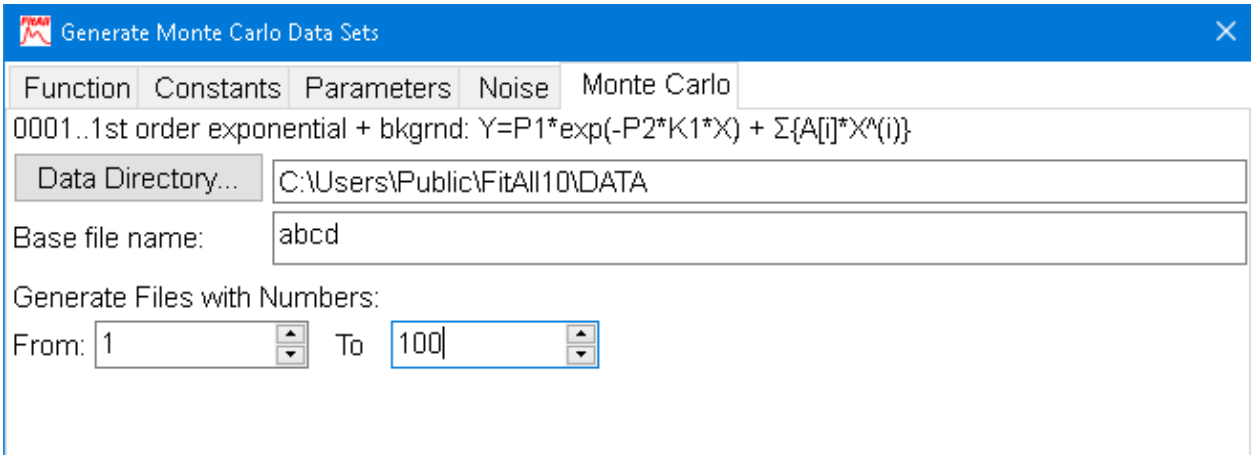
If any of the Y-values are adjusted, the statistics and validity of any subsequent Monte Carlo analysis will be very questionable!

This option has been provided to allow you to simulate how an instrument's response may affect the results. -- If the monitoring instrument's range is exceeded, it may report a limiting value.

This option may be useful in investigating how instrumental (or measurement) range limitations affect (and potentially distort) the analysis results.

Exercise extreme caution when using this option.

Monte Carlo



Data Directory

Click the 'Data Directory' button to select the directory (folder) in which the data files are to be saved. The Browse For Folder dialog that appears looks like this:

Base file name

Use the 'Base file name for data sets' edit box to enter a base file name for the generated data files. ***FitAll*** will create file names based on this name by adding an additional five characters to the name.

For example, if the entered name is 'ABCD', ***FitAll*** will created a series of files named ABCD0000001.DTA, ABCD0000002.DTA, etc. each containing one set of generated data.

NOTE:
A special file named ABCD00000.DTA also will be created. This data file contains the parameter values that were used to generate the data and has the same format as the results data file that is created when Monte Carlo analyses are done.

Generate Files with Numbers

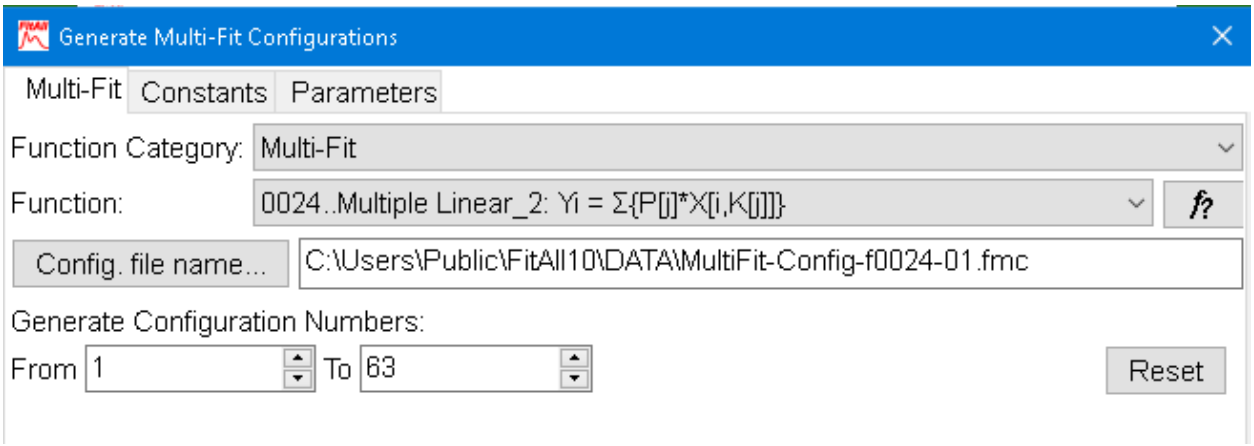
Use the **From** spin-edit box to enter the number of the first data set that ***FitAll*** should generate. The maximum value is 2,000,000.

Use the **To** spin-edit box to enter the number of the last data set that ***FitAll*** should generate. The maximum value is 2,000,000 and must be greater than or equal to the first file number.

Generate Multi-Fit Configs...

Choose Edit > Generate Multi-Fit Configs to create a file containing a set of function configurations (variations) that can be used to analyze one set of data with many different forms (variations) of the basic function.

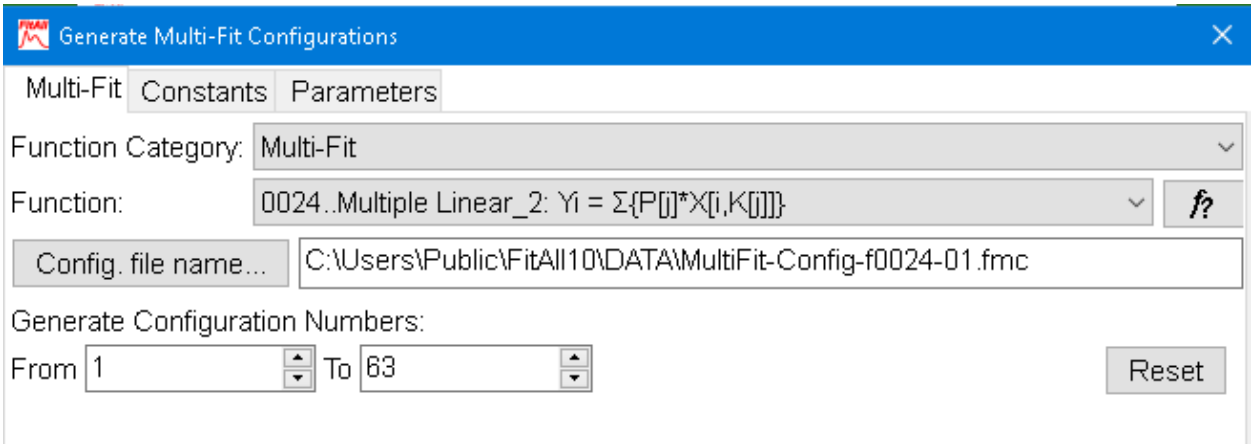
When you select Edit > Generate Multi-Fit Configs, the 'Generate Multi-Fit Configurations' dialog box appears. It looks like this:



and has three tabs -- Function 70, Constants 71 and Parameters 72.

Click on each of the tabs in turn and change the settings to what you want, then click the **OK** button.

Function



Ftn Category

Use the Ftn Category drop down list to restrict (limit) the list of selectable functions.

> **NOTE:**
> Only the functions in the category that you select will be displayed in the Function drop down list.

Function

Use the Function drop down list to select the function that you want to use to generate the multi-fit configurations.

If more than one variation of the function is available, one or more dialog boxes requesting additional information will appear. In each dialog, enter a value that corresponds to the function variation that has the largest number of parameters and click the **OK** button.

Help for Current Function, *f?*

Click the *f?* button to display Help for the currently selected function.

Config. file name

Click the 'Config. file name' button to select / create a file that will contain the generated configuration information. The file name extension 'fmc' stands for ***FitAll*** Multi-fit Configuration file.

Generate Configuration Numbers

Enter the number of the first configuration that you want saved to (or appended to) the configuration file in the **From** spin-edit.

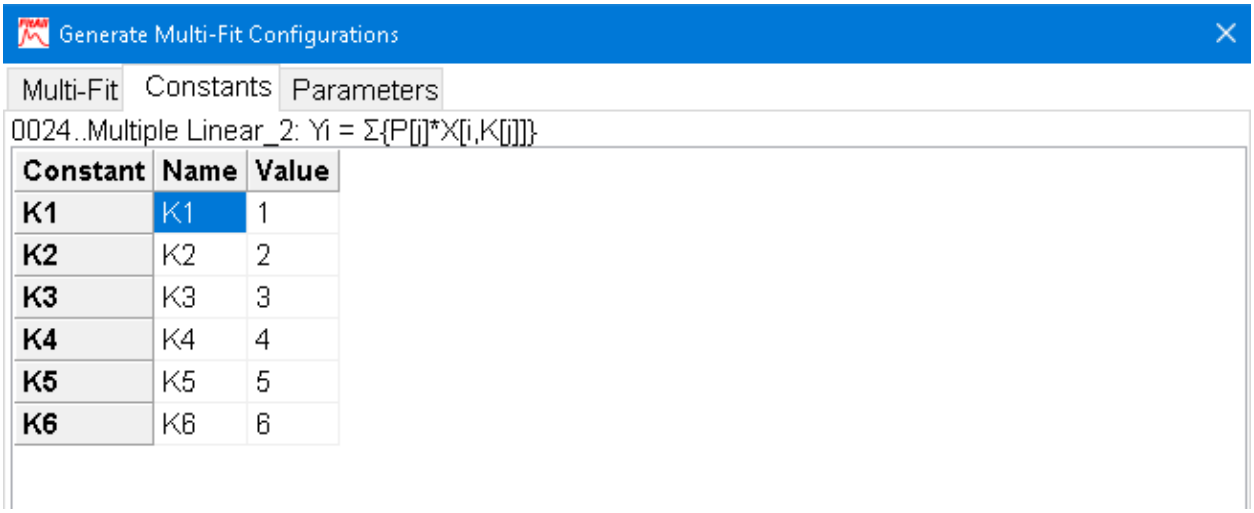
In most cases, the value should be 1 (one).

However, if the function being used has a very large number of variations, it is possible that you may have stopped the configuration generation process before it had generated all possible configurations. In such a case, you may want to start generating additional configurations at the point following those that have already been generated and append the these configurations to the existing configuration file.

Enter the number of the last configuration that you want saved to (or appended to) the configuration file in the **To** spin-edit.

Click the **Reset** button to reset the first and last configuration numbers to 1 and the maximum number of configurations can be generated for the current settings.

Constants



Name

Initially, the names displayed in the 'Name' column are the current default constant names for the selected function. You can change the names to whatever you want.

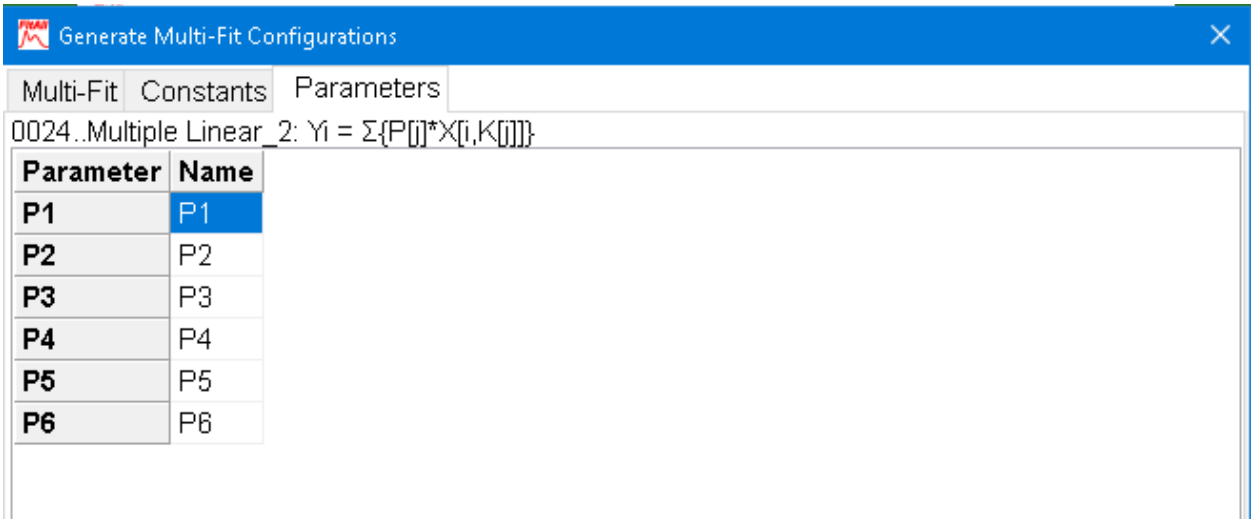
Value

Initially, the values displayed in the 'Value' column are the current constant values for the selected function. You can change the values to whatever you want.

FitAll, in its current implementation, changes the values of the constants when it generates the different 'Multi-Fit Configurations'.

> **NOTE:**
> Only a very small number of ***FitAll***'s functions are 'Multi-Fit enabled'.

Parameters



Name

Initially, the names displayed in the 'Name' column are the current default parameter names for the selected function. You can change the names to whatever you want.

Value

Initially, the values displayed in the 'Value' column are the current parameter values for the selected function. You can change the values to whatever you want. For non-linear functions the parameter values that you enter will be used as the initial estimates when the fit is done.

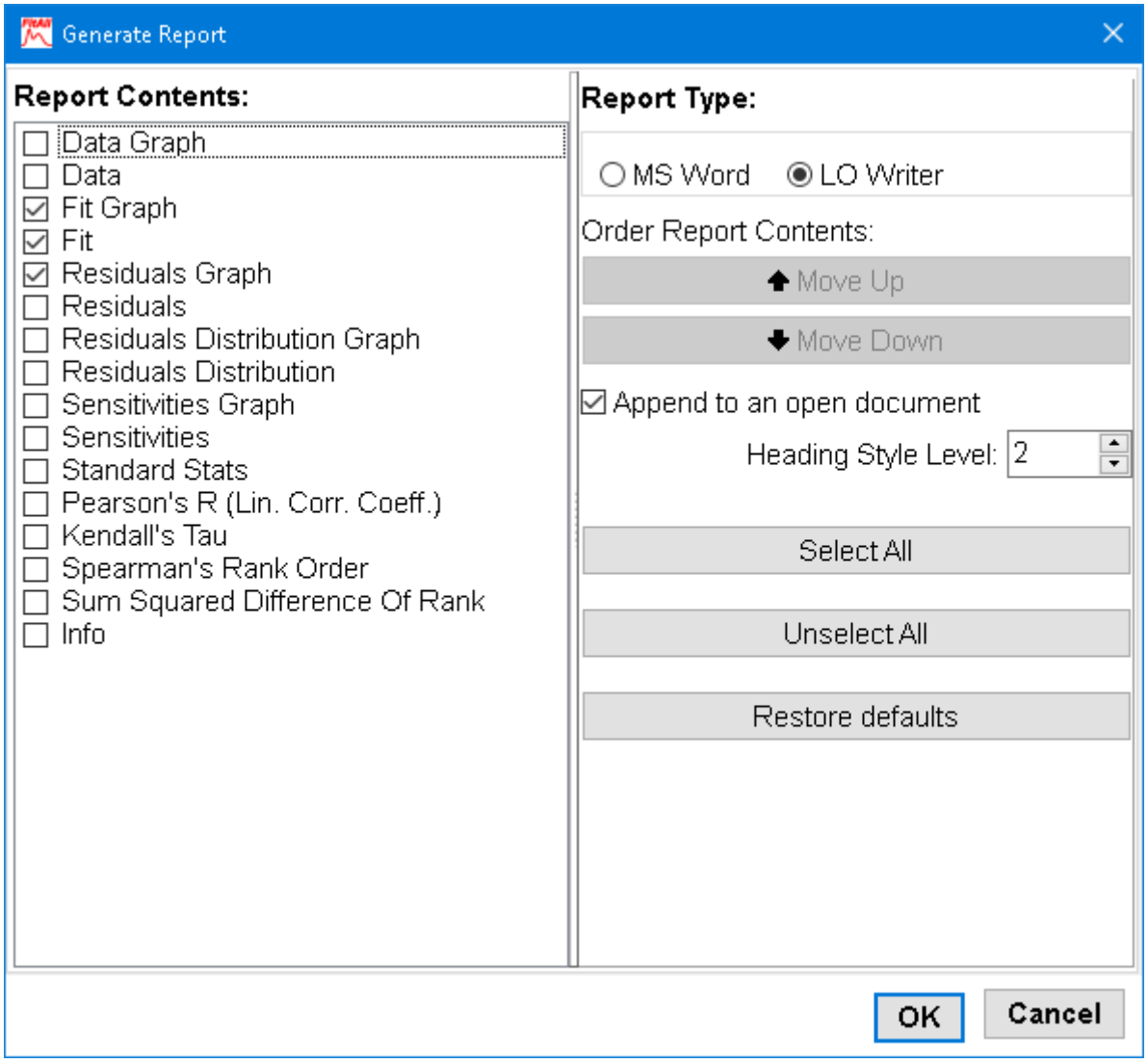
> **NOTE:**
> The 'Value' column is not displayed when the selected function is linear in its parameter as initial parameter estimates are not required for a lls analysis.

Generate Report

Click the Edit > Generate Report... menu selections or click the button to create a MS Word or Excel report (document) that contains the results of your analysis.

Each report can contain the contents of any or all of ***FitAll***'s windows.

When you choose Edit > Generate Report... the 'Generate Report' dialog box appears. It looks like this:



Report Contents

Select (check) the report elements that you want to include in the report.

Report Type

Select (click) on of the **MS Word** or **LO Writer** radio buttons to choose the type of report that you want ***FitAll*** to create.

Order Report Contents

Select (click to highlight) one of the items in the 'Report Contents' check list and click the 'Move Up' and 'Move Down' buttons to change the order of the report's contents.

> **NOTE:**
> Only those items in the 'Report Contents' check list that are checked will appear in the report.

Append to Existing Report

Select (check) the 'Append to Existing Report' check box if you want the generated report appended (added) to an existing open document.

> **NOTE:**
> The report will be added to the end of the open and active document. It will NOT be inserted at the cursor position.
>
> This can be very useful when you are writing a report at the same time that you are analyzing your data or are otherwise documenting the fits as you do them.

Heading Style Level

Each element in the report has a heading, such as 'Data', Data Graph', 'Fit' or 'Fit Graph'.

In MS Word and LO Writer the headings are formatted with a 'heading style', such as 'Heading 1' or 'Heading 2'.

The 'Heading Style Level', which can have values from 0 to 9, applies the standard Heading Style (1 to 9) to the heading text. A value of 0 means that the 'Normal' style will be applied to the heading text.

Select All

Click the 'Select All' button to include all possible results and information in the report.

Unselect All

Click the 'Unselect All' button to remove all possible results and information in the report so that you can more easily select the one or two items that you actually want in the report.

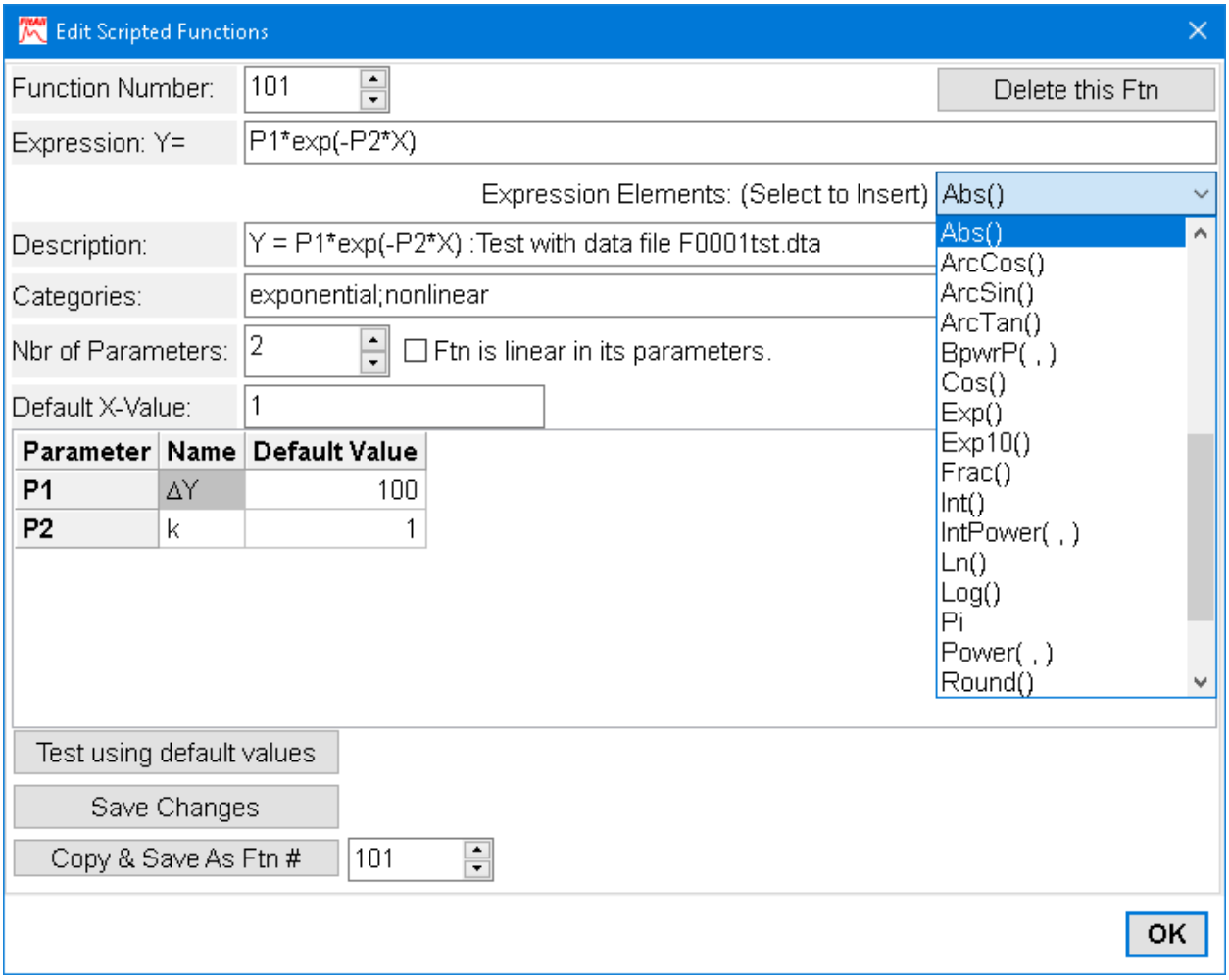
Restore defaults

Click the 'Restore defaults' button to change the report settings to ***FitAll***'s standard (default) settings.Enter topic text here.

Scripted Ftns...

Scripted functions are functions that can be defined by a one line expression

When you select Edit > Scripted Ftns..., the 'Edit Scripted Functions' dialog box appears. It looks like this:



Function Number:

Use this spin-edit to select the function number, from 101 to 200, that is to be created or edited.
(Note: The Evaluation Edition is limited to function numbers 101 to 103.)

> **NOTE:**
> Changing the function number after making changes to a function definition does NOT save the changes.
> You MUST click the "Save Changes" button to save the changes that you have made.

Delete this Ftn:

Click this button to delete / remove the current function definition.

Expression: Y=

Enter the expression for the right hand side of the equation, Y = f(X, Pn), in which X is the independent variable and the Pn's are the parameters to be resolved
For example: P1 + P2*X is the expression for a straight line that has an intercept of P1 and a slope of P2.

Expression Elements (Select to insert):

Use this drop down combobox to choose an expression element to insert into the Expression edit at the cursor or simply to view the list of elements that can be entered into the Expression edit.

Valid Expression Definition Elements and Operations

Element	**Description**
X	The independent variable.
P1, .., P10	The parameters to be resolved, starting with P1.
+	Addition operator.
-	Subtraction operator.
*	Multiplication operator.
/	Division operator.
( )	Parentheses to group operations.
Abs(V)	The result is the absolute value of V.
ArcCos(V)	The result is the ArcCosine in radians of the value, V.
ArcSin(V)	The result is the ArcSine in radians of the value, V.
ArcTan(V)	The result is the ArcTangent in radians of the value, V.
BpwrP(V1, V2)	The result is the absolute value of V1 raised to the power V2; that is, $\|V1\|^{V2}$. Note: This is the same as Power(V1,V2).
Cos(V)	The result is the Cosine of the value V radians.
Exp(V)	The result is e raised to the power V; that is, e^V
Exp10(V)	The result is 10 raised to the power V; that is, 10^V

Element	Description
Frac(V)	The result is the fractional part of V. For example Frac(1.234) is 0.234.
Int(V)	The result is the integer part of V. For example Int(1.234) is 1.
IntPower(V1, V2)	The result is the value of V1 raised to the integer power V2; that is, $V1^{V2}$.
Ln(V)	The result is the natural logarithm of the absolute value of V; that is, Ln|V| .
Log(V)	The result is the base 10 logarithm of the absolute value of V; that is, Log|V|.
Pi	The constant π, which is equal to 3.14159265358979.
Power(V1, V2)	The result is the absolute value of V1 raised to the power V2; that is, $\|V1\|^{V2}$.
Round(V)	The result is the integer result of rounding V. For example, Round(10.4) is 10 and Round(10.6) is 11.
Sin(V)	The result is the sine of V radians.
Sqr(V)	The result is the square of V; that is V^2
Sqrt(V)	The result is the square root of V; that is, $\sqrt{V}$
Trunc(V)	The result is the integer result of truncating V. For example, Trunc(10.4) is 10 and Trunc(10.6) is 10.

Description:

This description added here appears in the function drop down list used in the setup the analysis 92 dialog.

Categories:

This semi-colon, ";", delimited list of categories used to filter the list of functions that appear in the drop down list used in the setup the analysis 92 dialog.

Nbr of Parameters:

Number of parameters contained in the function's expression and will be resolved by the regression analysis.

Ftn is linear in its parameters:

Select, check, this checkbox if the function expression is linear in its parameters, P; that is, it is of the general form $Y = \sum_j Pj*f(x)$

Default X-Value:

The value of the independent variable, X, that is used when testing the function.

Parameter

The parameters that are to be used in the expression. Which parameters are available is set using the "Nbr of Parameters" spin-edit.

Name:

Descriptive names of the parameters.

Default Value:

The default values of the parameters that are used when testing the correctness of the function.

Test using default values:

Click this button to evaluate the function using the default values the parameters, P, and the independent variable, X.

Save Changes Button:

Click this button to save the changes.

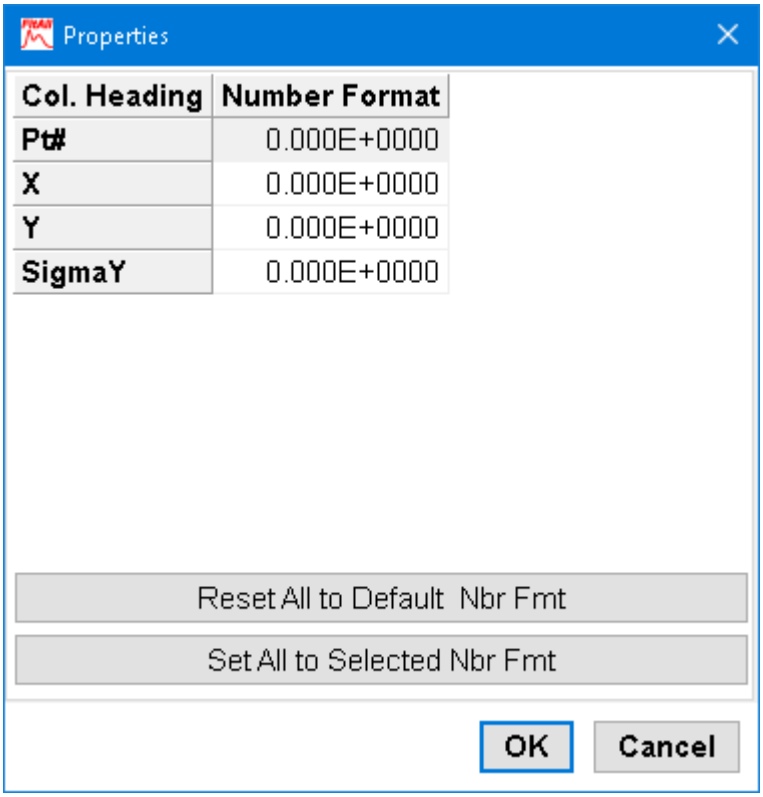
Copy and Save As Ftn#:

Use this button and the accompanying spin-edit to copy and save the current function definition with a different function number.
This is a convenient way to create a new function definition that is similar to the current definition.

Properties...

Text Window

Most text windows contain a grid in which columns of numbers are displayed. The Properties dialog for text windows looks like this:



Column Number

Use this spin edit to select a column.

Col. Number Format

Use this drop down edit to view and change the number format of the selected column.

Reset All to Default Num Fmt

Click this button to set the numeric format for all columns in the active window to the default numeric format.

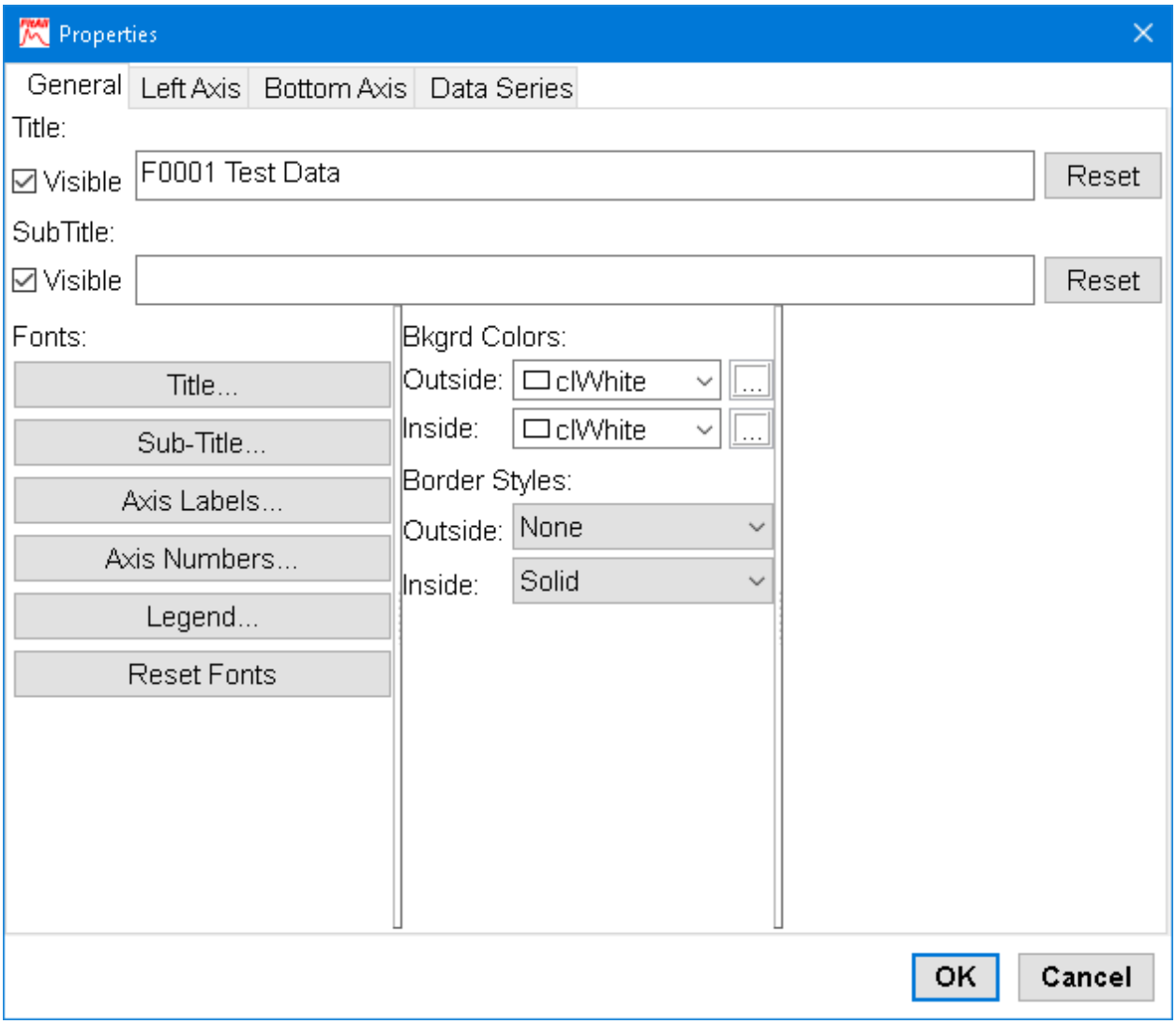
> **NOTE:**
> The default numeric format can be changed by choosing the Options > Preferences 126 menu selection and changing the value of 'Default Number Format' on the 'General' tab.

Set All to Selected Nbr Fmt

Click this button to set the number format for all columns in the active window to the current column's numeric format.

Graph Window

The Properties dialog for windows that contain a graph looks like this:

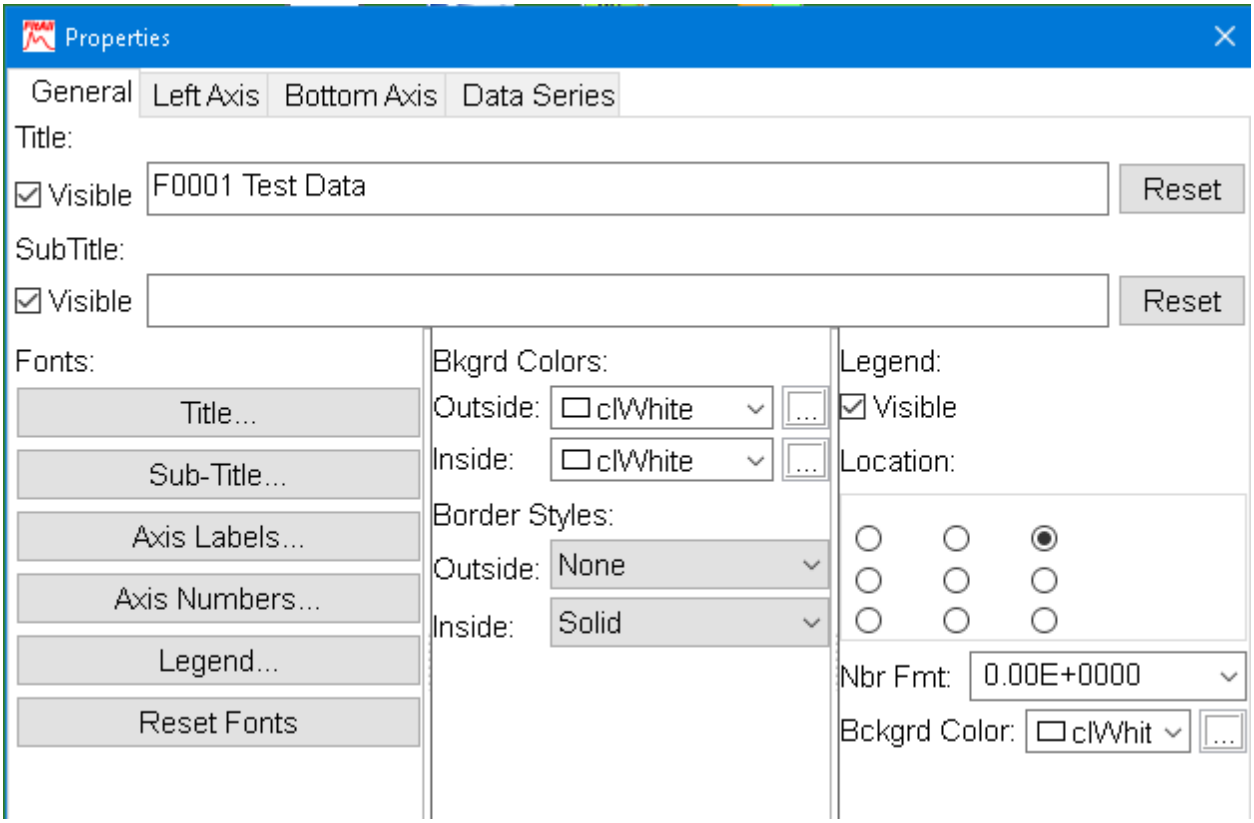


The dialog contains a least four tabs on which are general settings, bottom and left axis settings and one tab with settings for each data series. Only the 'sensitivities graph' displays more than one data series.

Only those properties that apply to the current graph are visible and changeable. For example, the 'fit graph' can have a legend, but the 'data graph' can not.

In most cases, changing a property will be immediately reflected in the graph. That is, you do not have to close the Properties dialog box to see the changes.

General



Title

Use the edit box to change the title text.

Visible

Use this check box to determine whether the title is displayed on the graph.

Reset

By default, the title is the same as the data set's title. If you wish to change it, un-check this setting and then edit the title text.

Sub-Title

Use the edit box to change the sub-title text.

Visible

Use this check box to determine whether the sub-title is displayed on the graph.

Reset to Default

By default, the sub-title is the same as the data set's sub-title. If you wish to change it, un-check this setting and then edit the sub-title text.

Fonts

Click one of the buttons in the Fonts group to view and change the font that is used for the **Title**, **Sub-Title**, **Axis labels**, **Axis numbers** and **Legend** text.

Bckgrd Colors

Click the small button to the left of the '**Outside**' label to change the background color around the outside of the graph; that is, the part of the graph on which the title, sub-title and Axis labels are displayed.

Click the small button to the left of the '**Inside**' label to change the background color on the inside of the graph; that is, the part of the graph on which the data points and legend are displayed.

Border Styles

Use the '**Outside**' and '**Inside**' drop down lists to choose a border style.

For example, choosing an outside border style of 'Solid3' will draw a thick line around the entire graph.

Legend

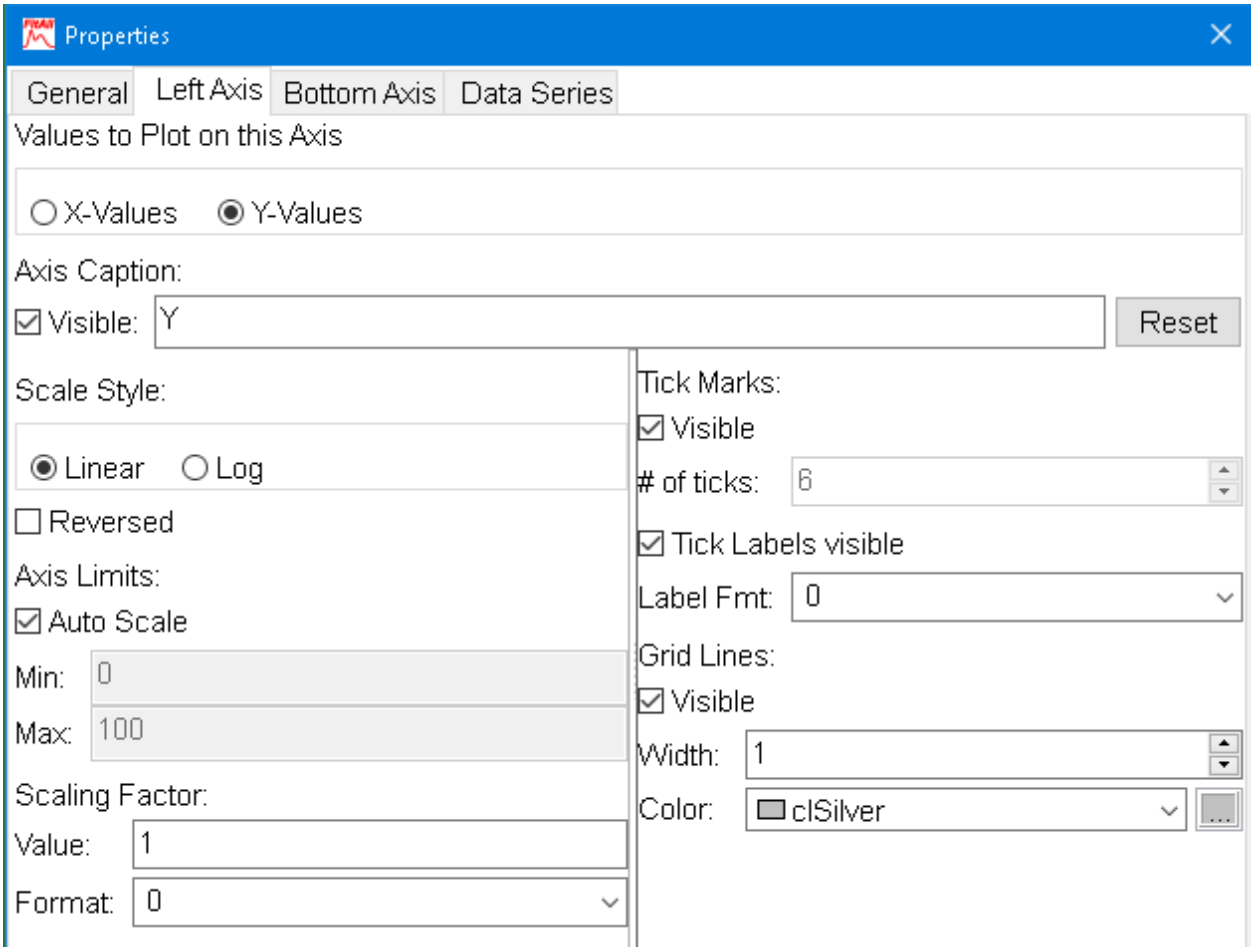
Check the **Visible** check box to make the legend visible.

Select the **Location** radio button that corresponds to relative position where you want the legend to appear.

Use the **Number Fmt** drop down list to select the format to be used when displaying numbers in the legend. At present, only the 'fit graph' has numbers in its legend.

Select the small button to the left of the **Bckgrd Color** label to change the legend's background color.

Axis



Values to Plot on this axis

By default, ***FitAll*** plots the X-values, the independent variable, on the bottom axis and the Y-values, the dependent variable, on the left axis.

You can change this by selecting either the X or Y radio button.

> **NOTE:**
> If you select the Y radio button in the Bottom Axis tab, ***FitAll*** will automatically select the X radio button in the Left Axis tab.
>
> That is, ***FitAll*** always will plot the X vs. Y values -- this option simply determines whether the X-values are plotted on the bottom or left axis.

In most cases, it is appropriate to plot the X-values along the bottom axis. However, there can be situations in which it is desirable to change this.

For example, in the solar cell functions, function numbers 0504 to 0507, the dependent variable, Y, is the voltage and the independent variable, X, is the current. However, in solar cell, electrochemistry and other related fields it is traditional to plot the current, X in these cases, on the left axis and the voltage, Y, on the bottom axis.

Axis Caption

Use the edit box to change the axis caption's text.

Visible

Use this check box to determine whether the axis caption is displayed on the graph.

Reset to Default

By default, the axis caption is the same as the data set's axis title. If you wish to change it, un-check this setting and then edit the axis caption text.

Scale Style

Use the **Reversed** check box to change how the values are plotted. Normally ***FitAll*** makes plots the smallest values at the lower left corner of the graph. If the **Reversed** check box is checked, the largest value for the axis in question will be plotted at the lower left corner of the graph.

Select the **Linear** radio button to have axis use a linear scale.

Select the **Log** radio button to have the axis use a logarithmic scale.

Scale Factor

Use the **Value** edit box to enter the number by which the axis values will be divided. The result will be that the numeric axis labels will be scaled by the value amount.

For example, if the original numeric labels on the axis were 0.00, 500.00 and 1000.00 and a scaling factor value of **100** was entered, the new numeric axis labels would be 0.00, 5.00 and 10.00. Also, the axis label will be "original axis label **/ 100**"

Use the **Format** drop down list to set the format of the divisor displayed in the axis label.

Limits

Check the **AutoScale** checkbox if you want ***FitAll*** to automatically determine the axis limits and the number of "tic marks".

If you want to set the axis limits yourself, uncheck the **AutoScale** check box and enter the minimum and maximum axis values in the **Min** and **Max** edit boxes.

Ticks

When the **Visible** checkbox is checked, the tic marks are displayed on the graph.

The **# of tick marks** spin edit determines the number of tic marks that will appear. The minimum value is two.

Check the **Labels visible** checkbox if you want the numeric values displayed next to the tic marks.

Use the **Label Fmt** drop down list to set the format of the numbers that are displayed next to each tic mark.

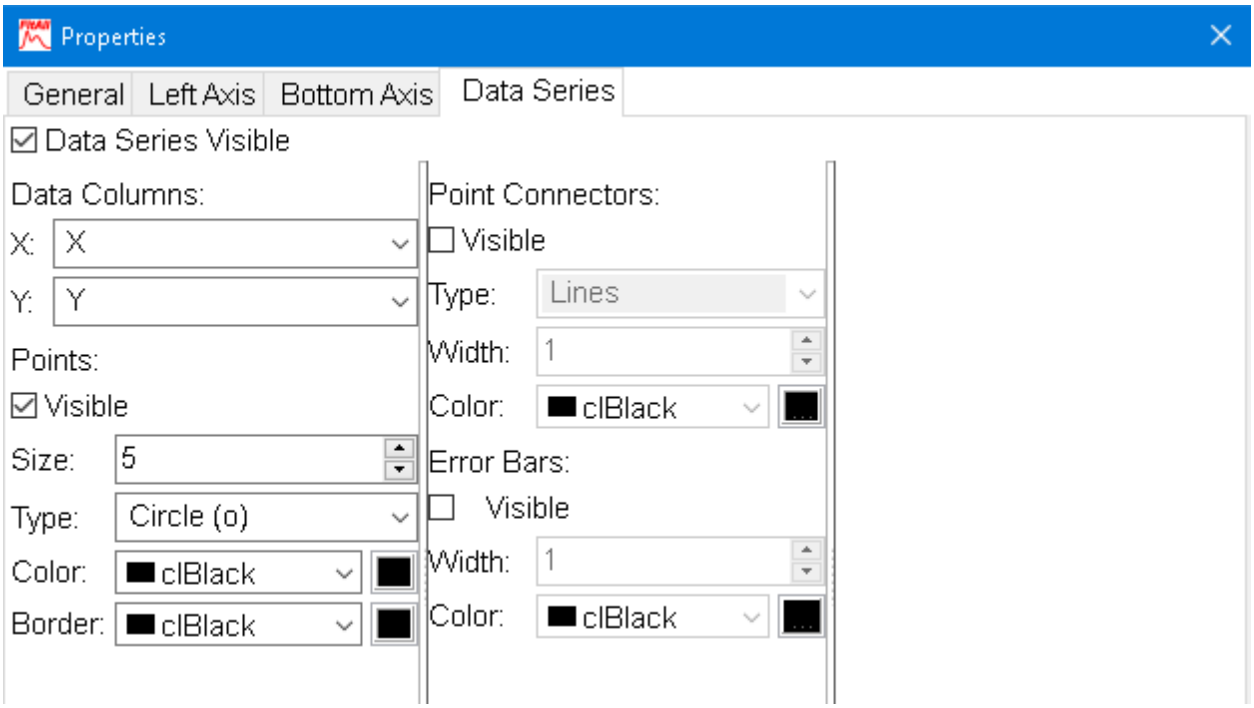
Grid Lines

When the **Visible** checkbox is checked, the grid lines are displayed on the graph.

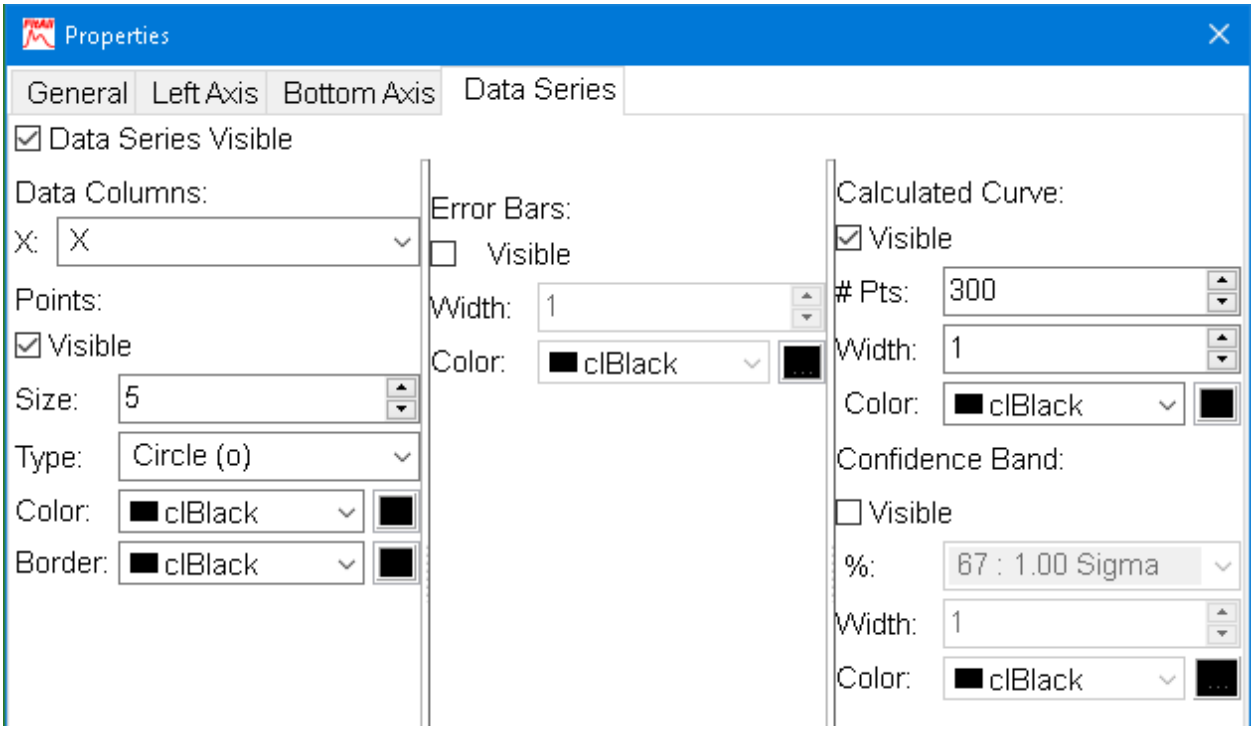
Use the **Width** spin edit to set the thickness of the grid lines.

Click the small button to the left of the **Color** label to choose the grid line color.

Data Series



OR



The properties available on the Data Series tab depend on the type of graph that is being displayed. For example, the 'Fit Curve' and 'Confidence Band' groups of properties are only available for the 'fit graph' window.

Visible

When the **Visible** checkbox is checked, the data series is displayed on the graph.

Data Columns

Use the **Data Columns** drop down list to select the data column that will be plotted on the X- or Y-axis. For example, you may want to plot the "point number" rather than the actual value along one of the axes.

Points

When the **Visible** checkbox is checked, the data points are displayed on the graph.

Use the **Size** spin edit to set the size of the data points.

Click the small button to the left of the **Color** label to choose the data point's color.

Click the small button to the left of the **Border Color** label to choose the color of the data point's border (outline).

Error Bars

When the **Visible** checkbox is checked, the error bars are displayed on the graph.

Click the small button to the left of the **Color** label to choose the error bar's color.

Point Connectors

When the **Visible** checkbox is checked, the connector lines between data points are displayed on the graph.

Use the drop down list to select the type of **connector lines** that you want to be drawn between the data points.

Use the **Width** spin edit to set the thickness of the connector lines.

Click the small button to the left of the **Color** label to choose the color of the point connectors.

Fit Curve

> **NOTE:**
> The fit curve is only displayed in the fit graph window.

When the **Visible** checkbox is checked, the calculated fit curve through data points is displayed on the graph.

Use the **# Pts** spin edit to set the number of calculated points that will be used to draw the "smooth" curve through the actual data points. The higher the number, the "smoother" the calculated curve; however, the higher the number, the longer it will take to draw the graph.

Use the **Width** spin edit to set the thickness of the fit curve.

Click the small button to the left of the **Color** label to choose the color of the point connectors.

Confidence Band

> **NOTE:**
> The confidence lines are only displayed in the fit graph window.

When the **Visible** checkbox is checked, the confidence band lines are displayed on the graph.

Use the **%** drop down list to select the percent confidence that you want the confidence lines to illustrate.

You can choose confidence curves that corresponds to the 50% (CM=0.67), 67% (CM=1), 95% (CM=1.96) or 99% (CM=2.58) confidence interval. Two additional lines are drawn using the formulas:

$$Y_i = f(x_i, P_j) + CM * \sum_j \left(\left| \frac{\partial f}{\partial P_j} \right| \delta P_j \right)$$

and

$$Y_i = f(x_i, P_j) - CM * \sum_j \left(\left| \frac{\partial f}{\partial P_j} \right| \delta P_j \right)$$

When evaluating the goodness of fit:

- The standard deviation of the parameters indicates how well determined or significant each of the resolved parameters is.
- Tends in the residuals graph can help you determine the appropriateness of a particular function or identify data collection biases (determinant errors).
- Plotting the confidence band can assist you in visualizing the fit quality. The 50% confidence band (that is, when the 'confidence multiplier', CM, is equal to 0.67) is often called the 'Probable Error'.
- A confidence band of 67% indicates that there is a 67% probability that the 'true' value of the function is within that band.
- A 'sensitivities graph' can help you visually determine the data range over which the calculated function's value is most influenced by each parameter.

Use the **Width** spin edit to set the thickness of the confidence band lines.

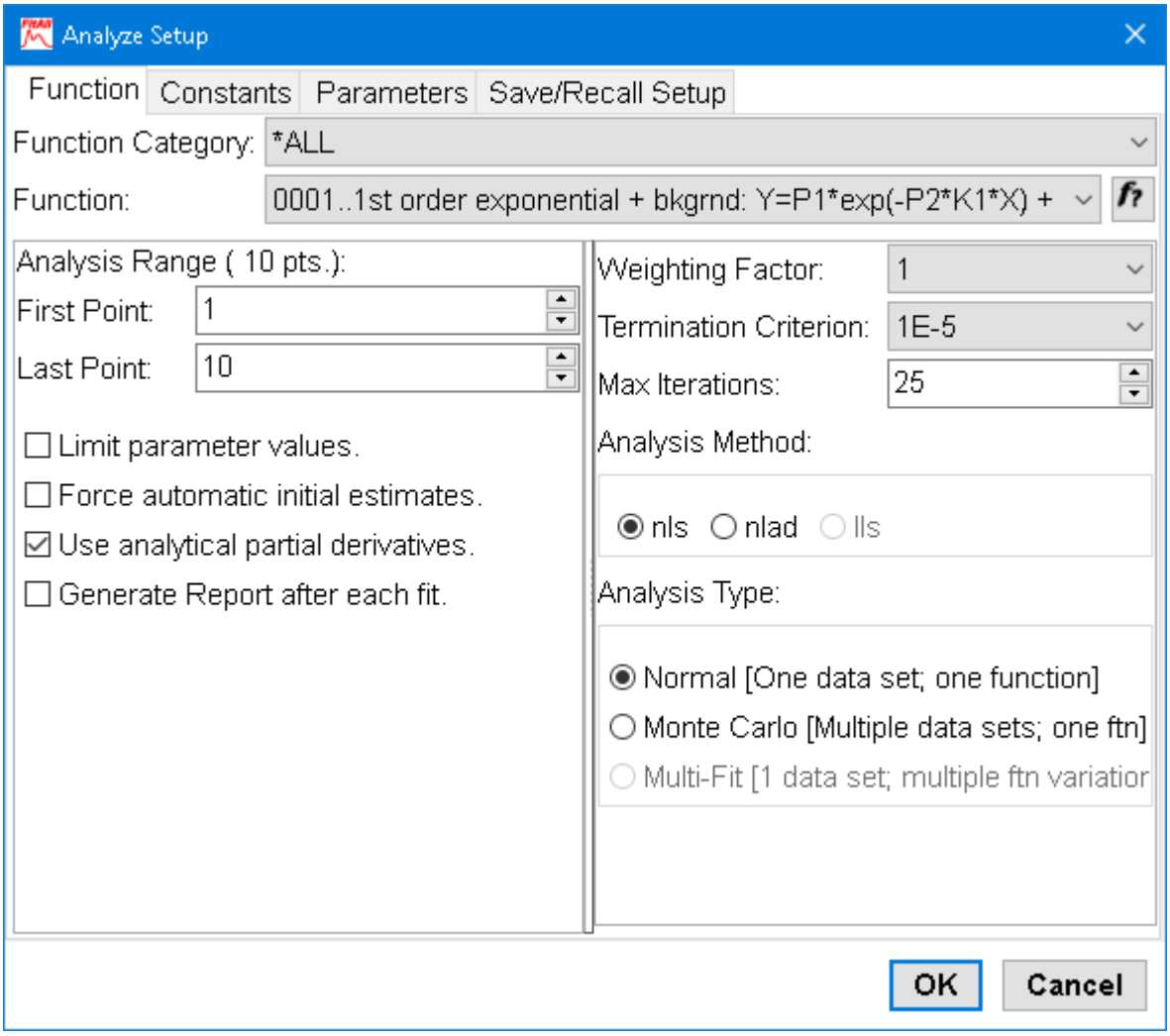
Click the small button to the left of the **Color** label to choose the color of the confidence band lines.

Analyze

Setup...

Choose Analyze > Setup, press **Alt+S** or click the f_x button to setup the data analysis.

When you select Analyze > Setup the 'Analyze Set Up' dialog appears. It looks like this:

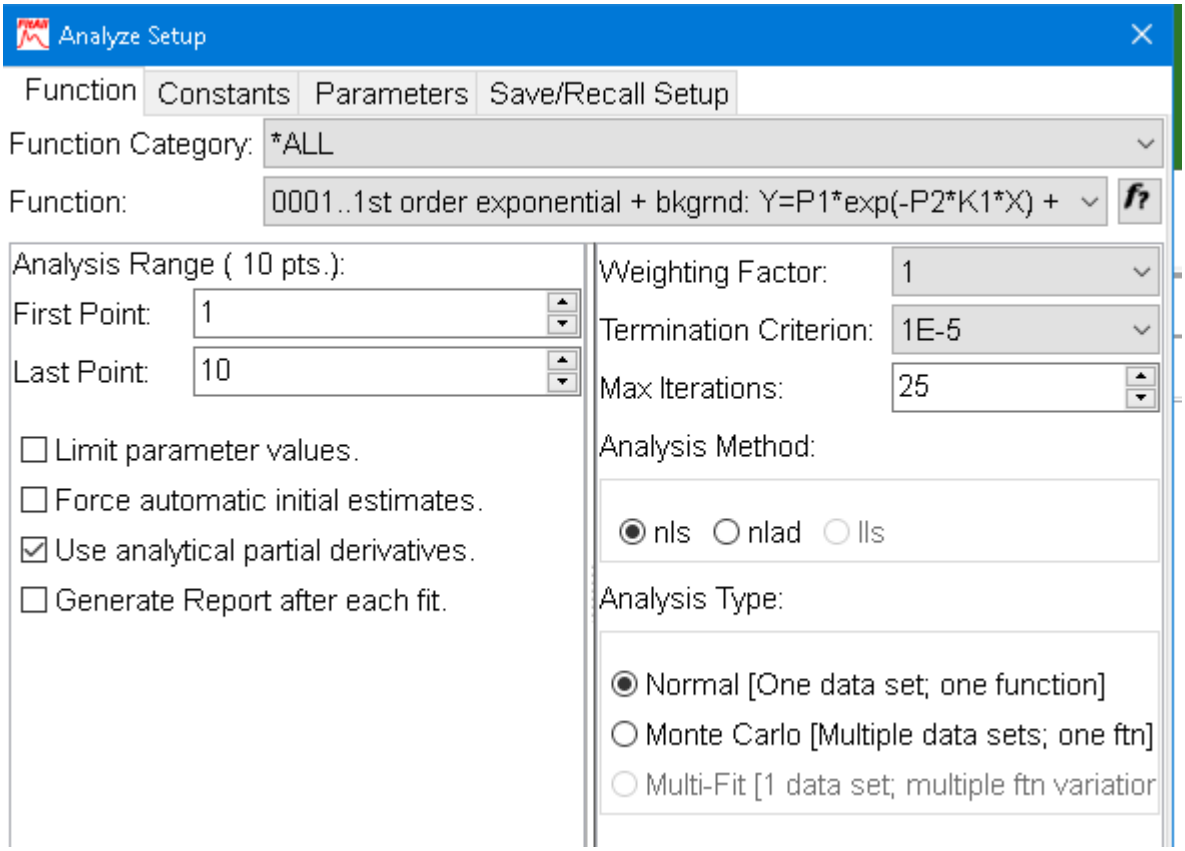


NOTE:
Not all of the tabs will be visible.

Which tabs are visible is determined by the current function and the analysis settings.

For example, if the current function does not have any constants, the 'Constants' tab will not be visible.

Function



Function Category

Use the Ftn Category drop down list to restrict (limit) the list of selectable functions.

> **NOTE:**
> Only the functions in the category that you select will be displayed in the Function drop down list.
>
> **HINT:**
> If you typically use a small number of the available functions you can add categories of your own so that only those functions are displayed in the Function drop down list.
>
> See Options > Preferences > Ftn categories 134 to see how to add categories of your own.

Function

Use the Function drop down list to select the function that you want to use to analyze the current data set.

If more than one variation of the function is available, one or more dialog boxes requesting additional information may appear. In each dialog, enter an appropriate value and click the **OK** button.

> **NOTE:**
> The dialog boxes requesting additional information are only displayed when the function is initially selected. If you want to see or change the settings you've made, expand the Function drop-down list and click on the same function.

Help for Current Function, f?

Click the f? button to display Help for the currently selected function.

Analysis Range

Use the **First Point** and **Last Point** spin edits to set the range of data points that you want to be used in the regression analysis,

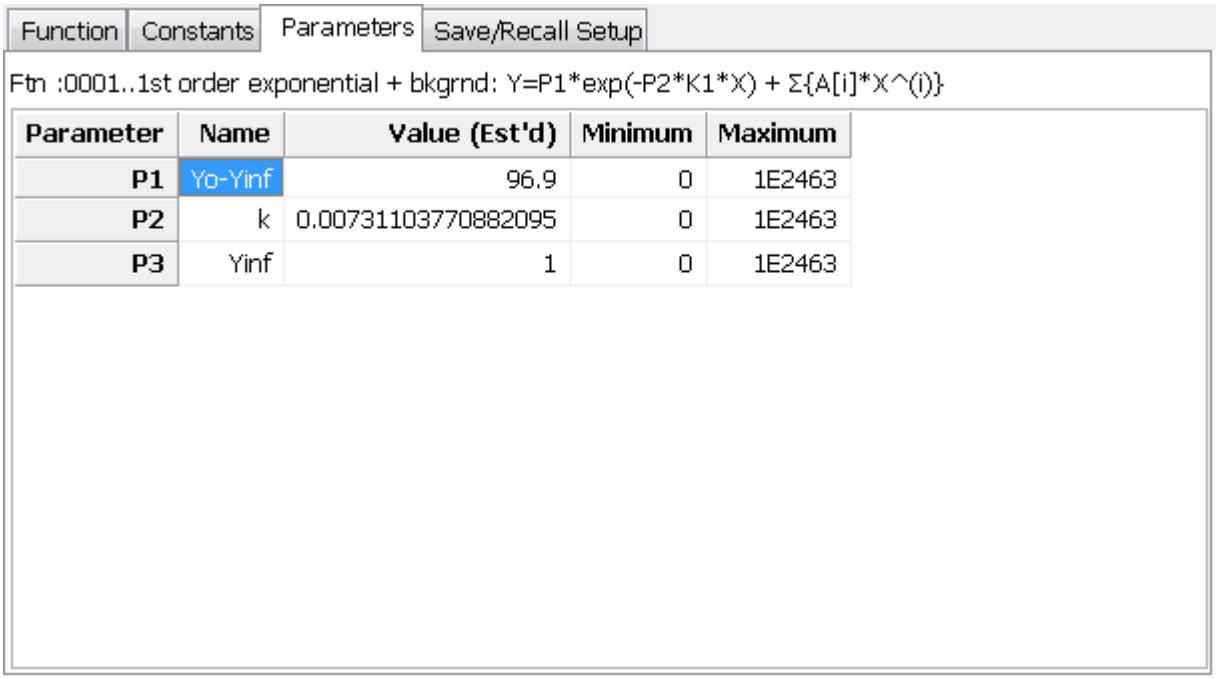
Limit parameter values

Check this item if you want to limit the value of one or more of the parameters' values to a specific range of values.

When ***FitAll*** analyzes a set of data, it adjusts the value of each parameter after each iteration. For some functions, more than one solution may be possible and ***FitAll*** *may* assign an unrealistic value to one or more of the parameters. To prevent this from happening, you can assign upper and lower limits to a parameter's value. When you do this, ***FitAll*** will ensure that the parameter's value is limited to the range you specify.

> **NOTE:**
> When you select a function from the Function drop down list most functions that are likely to require parameter limits will automatically check this item.

When checked, the Analyze > Setup > Parameters 99 tab will include columns in which you can enter the maximum and minimum parameter values and will look like this:



Force automatic initial estimates

This check box tells ***FitAll*** to re-evaluate its estimates of the parameter values before every analysis.

Check this option if you are analyzing several sets of data with the same function and you know that:

- The parameter values resulting from the regression analysis will have widely different values.
- ***FitAll*** makes sufficiently good initial estimates.
- Do not check this option if you want to use the results of the previous analysis as the starting point for the analysis you are about to do.

> **NOTE:**
> To manually instruct ***FitAll*** to generate initial parameter estimates:
>
> - Select (Click) the 'Parameters' tab.
> - Click the 'Initial Estimates' button.

Use analytical partial derivatives

This check box should be checked.

When ***FitAll*** is fitting a set of data, it adjusts the value of each parameter after each iteration. To determine how large the adjustment should be, it must calculate the partial derivatives of the function with respect to each of the parameters. ***FitAll*** always does this calculation numerically and then updates these values using an analytical expression for the required partial derivative when the required analytical expression is available.

If this item is not checked, ***FitAll*** will not update the numerically calculated values.

In most cases, the solution arrived at will be the same, whether or not this item is checked.

This option is primarily for the use of those who have the Research Edition and are creating user defined ***FitAll*** **Function Libraries** (ffl's) of their own.

Generate Report after each fit

When checked ***FitAll*** will generate an Excel or Word report whenever it successfully fits a set of data.

The type of report and its contents can be set by selecting Preferences, Report 135.

> **NOTE:**
> When doing Batch Mode, Monte Carlo or Multi-Fit Analyses a large number of reports may be created -- This can be very time consuming.

Weighting Factor

Use this drop down list to select one of the five available weighting schemes.

The weighting factors that can be selected are: $1/(SigmaY)^2$, 1, 1/Y, $1/(0.1*Y)^2$ and $1/(0.01*Y)^2$.

Weighting Factor	**Comment**
$1/(SigmaY)^2$	The weighting factor used is proportional to the reciprocal of the square of the Y-values' standard deviation.
1	All data points are equally weighted. That is, all measured values of the function are assumed to be of equal precision. Use this weighting scheme unless you know that the errors associated with the data are different.
1/Y	The weighting factor used is proportional to the inverse of the value of the function. Use this weighting scheme when the data is distributed around each point according to a Poisson distribution rather than a Gaussian distribution as is assumed to be the case in the least-squares method. A Poisson distribution assumes that $(SigmaY)^2$ is directly proportional to the value of Y. Poisson distributions are normally encountered in counting experiments; that is, in situations in which the magnitude of the measured value of the function is determined by summing (counting) the number of times that a particular event occurs.
$1/(0.01*Y)^2$	This weighting factor assumes that the standard deviation, SigmaY[i], of the function is equal to 1% of the function's measured value.

Weighting Factor	Comment
$1/(0.01*FSS)^2$	This weighting factor assumes that the standard deviation, SigmaY[i], of the function is equal to 1% of the measurement instrument's Full-Scale Setting, FSS, that was required to measure the function's value. This weighting scheme is intended to reflect the measurement errors that are usual with most common measurement instruments, such as (auto-ranging) voltmeters. For example: for Y-values from 0.0100 to 0.0999 the FSS is 0.1, and for Y-values from 1.00 to 9.99 the FSS is 10.

Termination Criterion

FitAll alters its estimate of the parameter values at each iteration so that successive values of the reduced chi-square statistic becomes smaller.

The termination criterion is used to determine when the difference between the calculated curve and the actual data points is small enough to assume that the final (correct) values of the parameters have been determined.

The actual convergence test used is: $\Delta\chi/\chi^2$ <= Termination criterion.

If the termination criterion's value is large, for example 0.1, relatively few iterations will be required in order to get a fit. However, the accuracy and precision of the calculated parameters *may* be low.

If the termination criterion's value is small, for example 10^{-15}, a relatively large number of iterations may be required before ***FitAll*** converges to the final parameter values. The final values, however, generally will be more precise than if a large value of the termination criterion had been used.

If the termination criterion's value is too small, numeric truncation errors may prevent convergence from ever occurring.

The termination criterion's default value of 0.001 is appropriate for a wide range of fitting functions and data sets.

Max. Iterations

FitAll uses an iterative process to locate the best-fit parameter values. That is, it starts with initial guesses and, by repeating the calculations (iterating), it refines these values until the difference between the calculated values and the actual values is at a minimum.

If the initial guesses are too far from the final values or if the data are not well dispersed over an appropriate range, the number of iterations required can be very large. In such circumstances, it may take a long time to obtain the final results.

The 'Max. iterations' value tells ***FitAll*** to stop after that number of iterations, even if a best-fit has not been obtained. You will then be given the option of terminating or continuing with the analysis.

CAUTION:
The final results reported by ***FitAll*** do not indicate whether the analysis was stopped before the termination criterion was met!

Analysis Method

FitAll can analyze your data using one of three methods.

Select (click) the radio button corresponding to the analysis method that you want to use when fitting your data (See: Theory Behind FitAll 205).

For functions that are non-linear in their parameters, either the non-linear least-squares, **nlls** 207, or non-linear absolute deviations, **nllad** 208, methods can be used.

For functions that are linear in their parameters the linear least-squares, **lls** 206, method will be used.

Analysis Type

Select (click) the radio button that corresponds to the analysis type that you want to use.

- **Normal**: Choose this analysis type to do one analysis using the current function and settings. This is the most commonly used analysis type.

- **Monte Carlo**: Choose this analysis type to analyze multiple data sets with the same function and initial settings (See: Edit > Generate Monte Carlo data sets 67 and Analyze > Setup Monte Carlo 100).

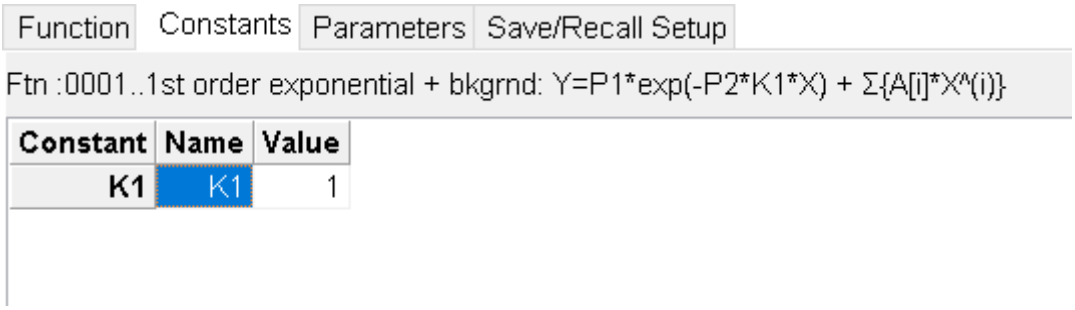
  When checked, the Monte Carlo 100 tab is enabled (visible) and allows you to enter the additional information required by ***FitAll*** to analyze multiple data sets.

- **Multi-Fit**: Choose this analysis type to analyze one set of data with many different initial settings; that is, with different variations of the same function (See: Edit > Generate Multi-Fit Configs... 69).

  Only some of the functions in ***FitAll*** are "Multi-Fit enabled" (See: Analyze > Multi-Fit 105).

  When checked, the Multi-Fit tab is visible and allows you to enter the additional information required by ***FitAll*** to do multiple analyses of the same data set.

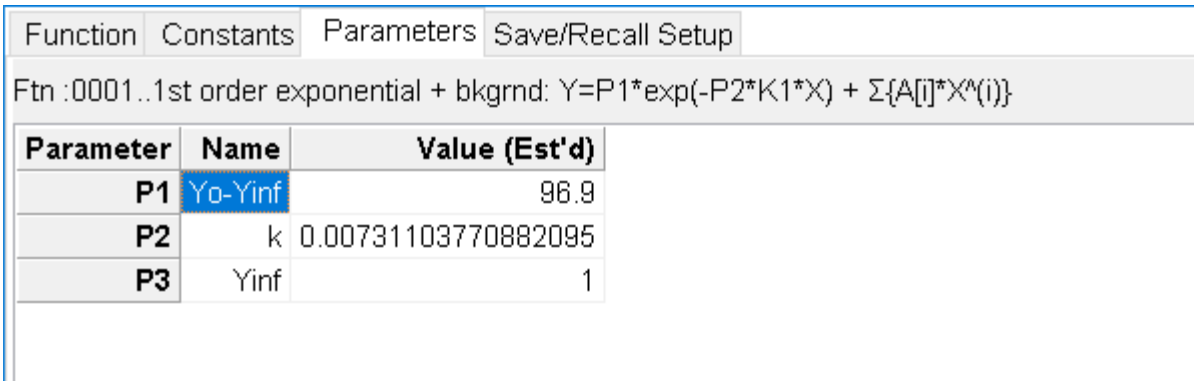
Constants



The 'Constants' tab in the 'Analyze Set Up' dialog allows you to change the names and values of the current function's constants.

To edit or change a name or value, select the value you want to change by clicking on the cell and (a) entering the new value or (b) press the **F2** key and edit the existing value.

Parameters



The 'Parameters' tab in the 'Analyze Set Up' dialog allows you to change the names and values of the current function's parameters.

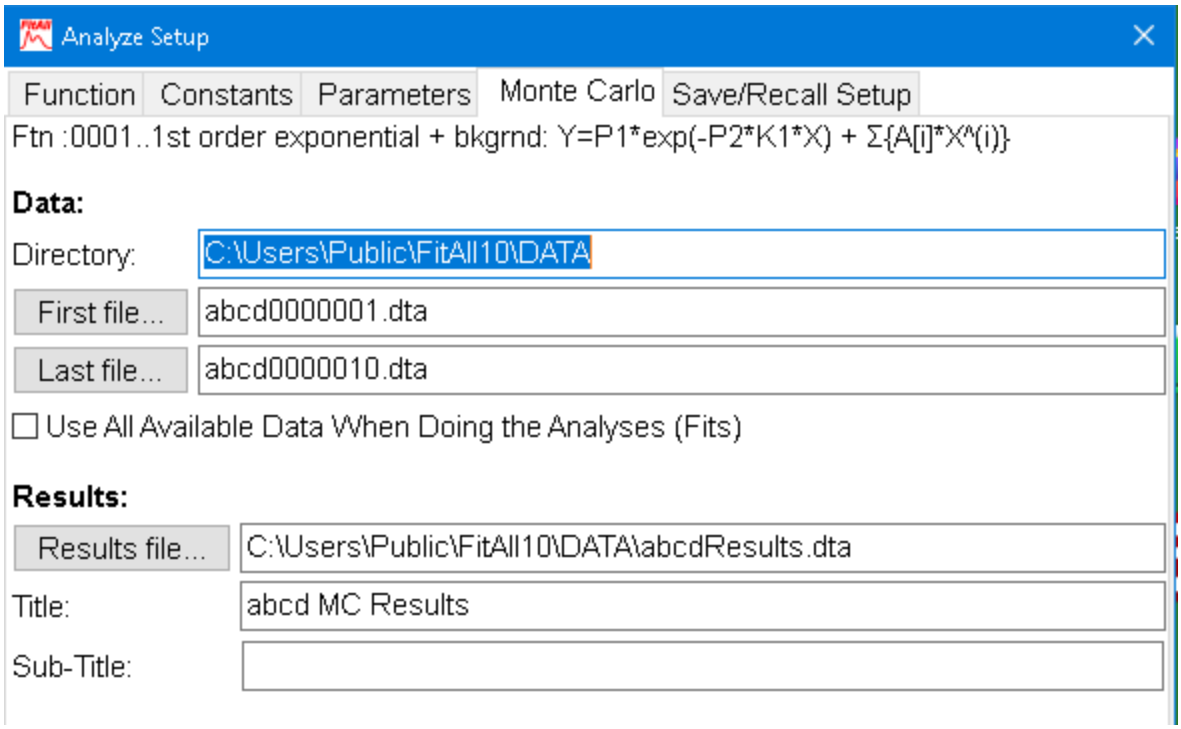
To edit or change a name or value, select the value you want to change by clicking on the cell and (a) entering the new value or (b) press the **F2** key and edit the existing value.

Initial Estimates

To have ***FitAll*** automatically calculate the initial estimated values of the parameters, click the 'Initial Estimates' button.

> **NOTE:**
> ***FitAll*** can not calculate initial estimates for every function.
>
> If ***FitAll*** is unable to calculate the initial estimate, the parameter values will not change and a message dialog will appear indicating that it was not able to calculate the initial estimates.
>
> FitAll can not automatically calculated the required initial estimates for any of the Scripted Functions that you may ceate. (Edit > Scripted Ftns 75

Monte Carlo



To do a Monte Carlo analysis it is necessary to tell ***FitAll*** which data files should be analyzed as well as the data file in which the results of the analyses should be saved.

Data

FitAll assumes that:

- All of the files to be analyzed have file names that include a five digit number at the end, for example, 'abcd00001.dta'.
- All of the files to be analyzed have the same 'base file name'; for example, abcd.
- All of the files to be analyzed are located in the same directory (folder).

Click the '**First File...**' button to select the first file that should be analyzed. The name of this file should contain the smallest number.

Click the '**Last File...**' button to select the last file that should be analyzed. The name of this file should contain the largest number.

> **NOTE:**
> If there are 'gaps' in the numbers, ***FitAll*** will automatically go on to the next file.

Check the '**Use All Available Data When Doing the Analyses (Fits)**' check box if you are using the Monte Carlo analysis feature to do batch mode processing 154 of a number of data files that may not have the same number of data points. When this selection is checked ***FitAll*** will automatically adjust the data range to include all of the data in each of the data files that it analyzes.

Results

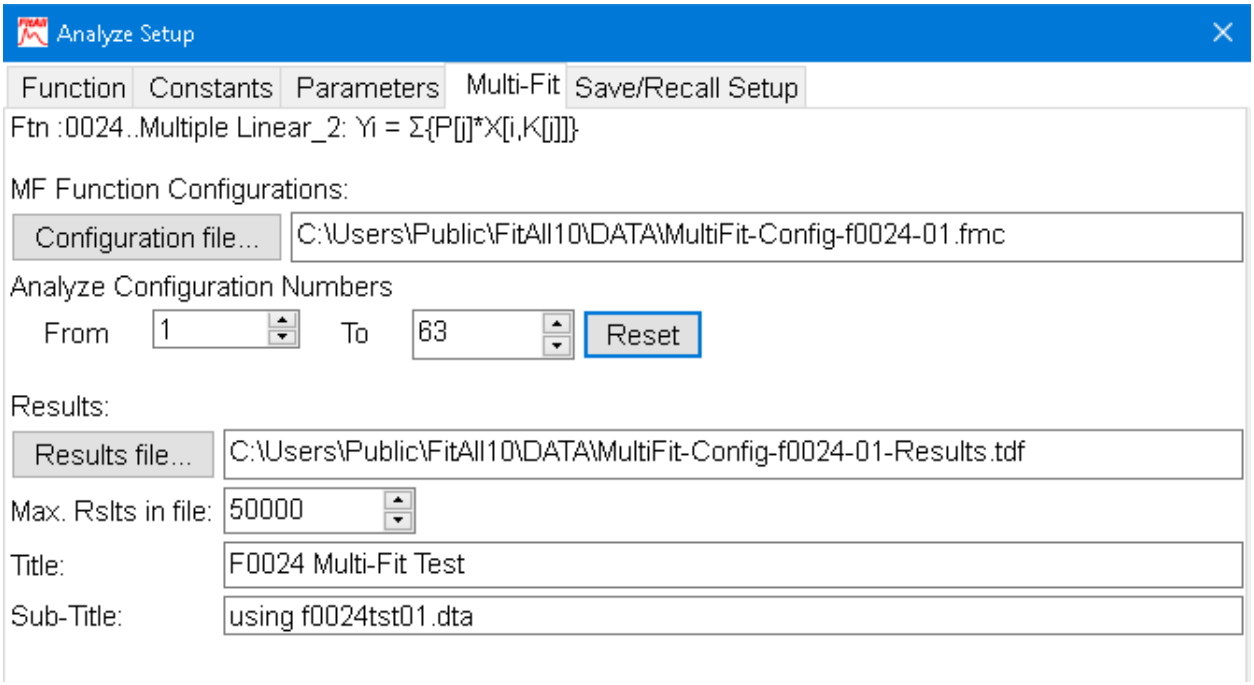
Click the '**Results file...'** button to select or create the data file in to which the results of the analyses will be saved.

> **NOTE:**
> If the file already exists, the results from the current analyses will be appended (added) to it.

Use the **Title** edit box to enter the 'title' that will be entered into the results data set.

Use the **Sub-Title** edit box to enter the 'sub-title' that will be entered into the results data set.

Multi-Fit



Before doing a Multi-Fit analysis it is necessary to tell ***FitAll*** which configuration file should be used as well as the file into which the results of the analyses should be saved.

MF Function Configurations:

Configuration file:

Click the 'Configuration file...' button to locate the file that contains the multi-fit function configurations that are to be evaluated.

> **NOTE:**
> The configuration file will normally have been created using the menu selections Edit > Generate Multi-Fit Configs 69.

Analyze Configuration Numbers:

Use the **First** and **Last** spin-edits to identify the function configurations that should be evaluated during the multi-fit analyses.

Initially, **First** should be set to 1, one, and **Last** to a large number so that all of the configurations are analyzed.

If there are many configurations to evaluate, it may be that not all were initially analyzed; for example, because of the time required, the analyses may have been stopped before all were completed. Under such circumstances you can re-start the analyses with a value of **First** that is one larger than the last one analyzed and append the results to the same results file.

NOTE:
If the **First** and **Last** configuration numbers are equal ***FitAll*** will retrieve the configuration and do the analysis, *but it will not append the results to the results file*.

This makes it possible selectively analyze one configuration and view the results of that particular configuration of the function.

Reset

Click this button to reset the **First** and **Last** numbers to the lowest and highest configuration numbers that are available in the configuration file.

Results:

Results file...:

Click the 'Results file...' button to create the file in which the results of the analyses will be saved.

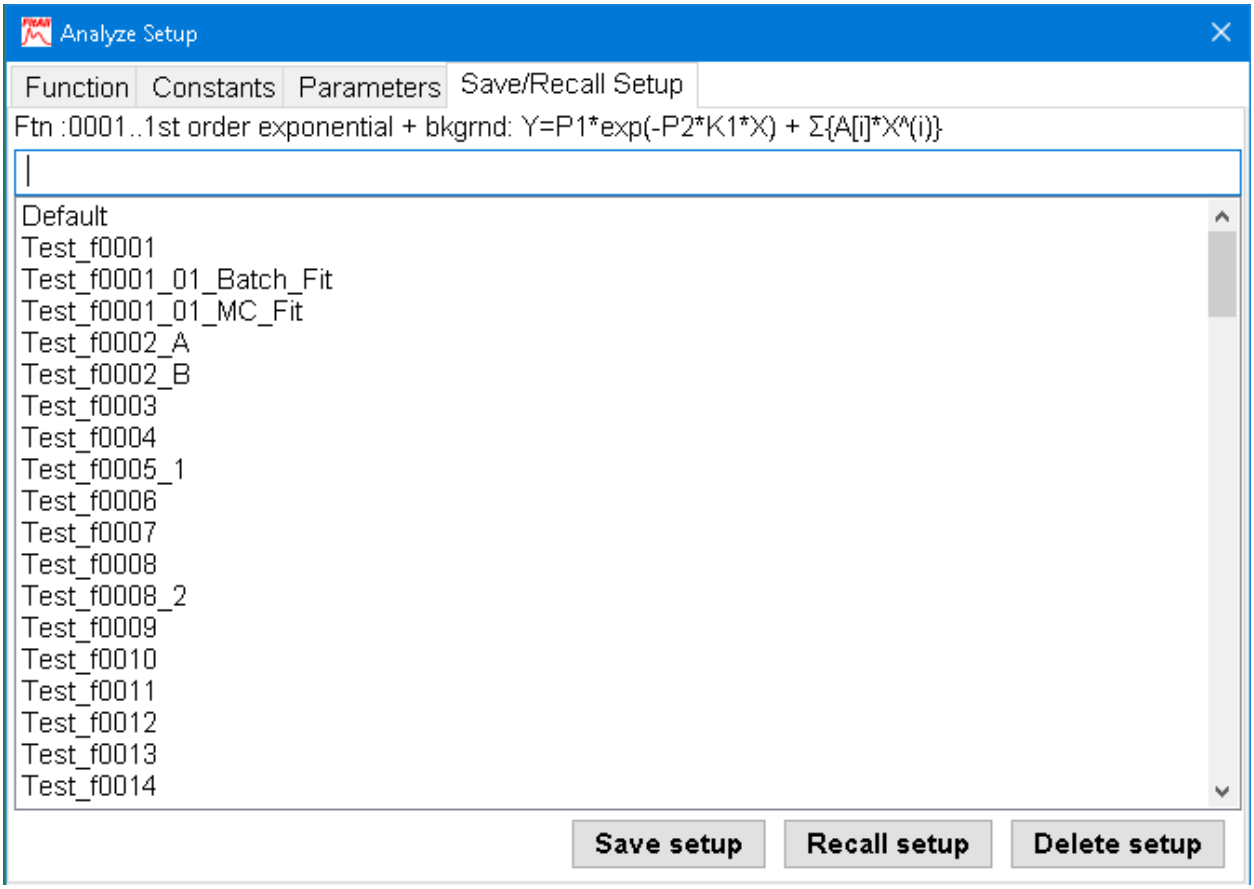
Title:

Use the 'Title' edit box to enter the title of the results data set.

Sub-Title:

Use the 'Sub-Title' edit box to enter the sub-title of the results data set.

Save / Recall Setup



Save setup

Click the 'Save setup' button to save the current analysis setup with the name in the edit box at the top of the combo box.

If that particular setup already exists, you will be given a chance to cancel the operation.

Recall setup

Click on one of the existing setup names to select it, then click the 'Recall setup' button to retrieve all of the analysis settings that you previously saved using this name.

Delete setup

If an analysis setup that you previously saved is no longer relevant to your needs, you can delete it by clicking on its name to select it and then clicking the 'Delete setup' button.

Analyze

Choose Analyze > Analyze, press **Alt+N** or click the  button to fit the data; that is, to do the regression analysis.

This menu item changes depending on the 'Analysis Type' that is selected in the Analyze > Setup, Function 92 dialog box.

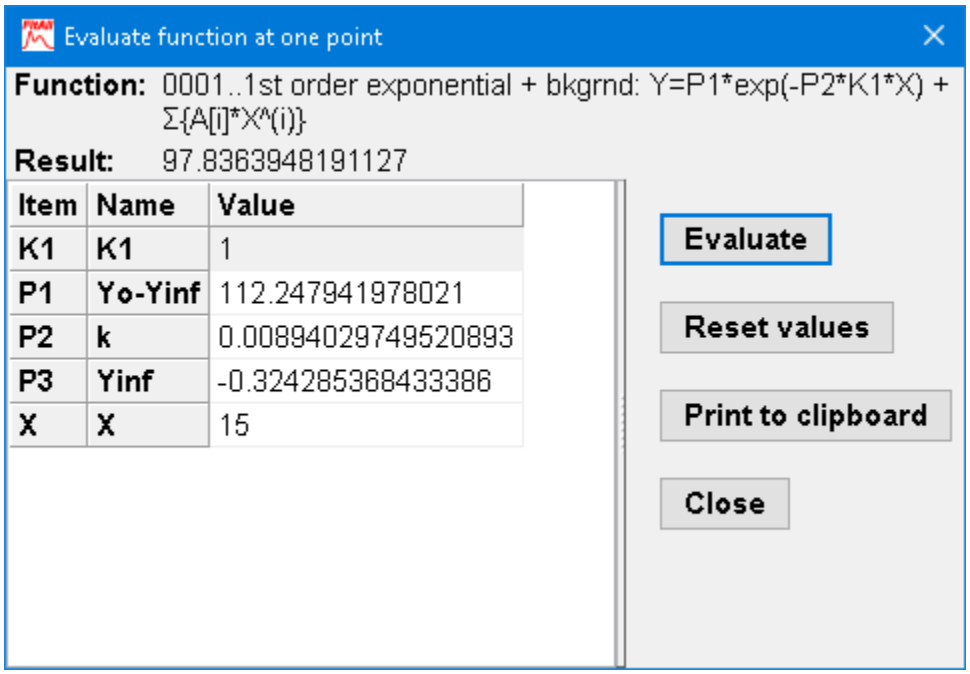
The following table shows the correspondence between the Analysis Type and the Analyze Menu's text.

Analysis Type	**Analyze Menu's Text**
Normal	Analyze
Monte Carlo	Analyze Monte Carlo
Multi-Fit	Analyze Multi-Fit.

One point...

Choose Analyze > One point... to evaluate the current function with a particular set of parameters, constants and independent variables.

When you select Analyze, One point the 'Evaluate function at one point' dialog appears. It looks like this:



If you want to generate a set of data with equally spaced (either linearly or logarithmically) values of the independent variable(s), X, use the Edit > Generate data set 55 menu selections.

Value

Enter the values that you want into the appropriate rows of the value's column.

Evaluate

Click the 'Evaluate' button to have ***FitAll*** do the calculation and display the result in the 'Result' field.

Reset values

Click the 'Reset values' button to have ***FitAll*** reset all values of the parameters, constants and independent variables.

Print to clipboard

Click the 'Print to clipboard' button to copy all of the text in the 'Evaluate One Point' dialog to the Windows clipboard. You can then paste the result into another document, such as a MS Word or Excel document, for future reference.

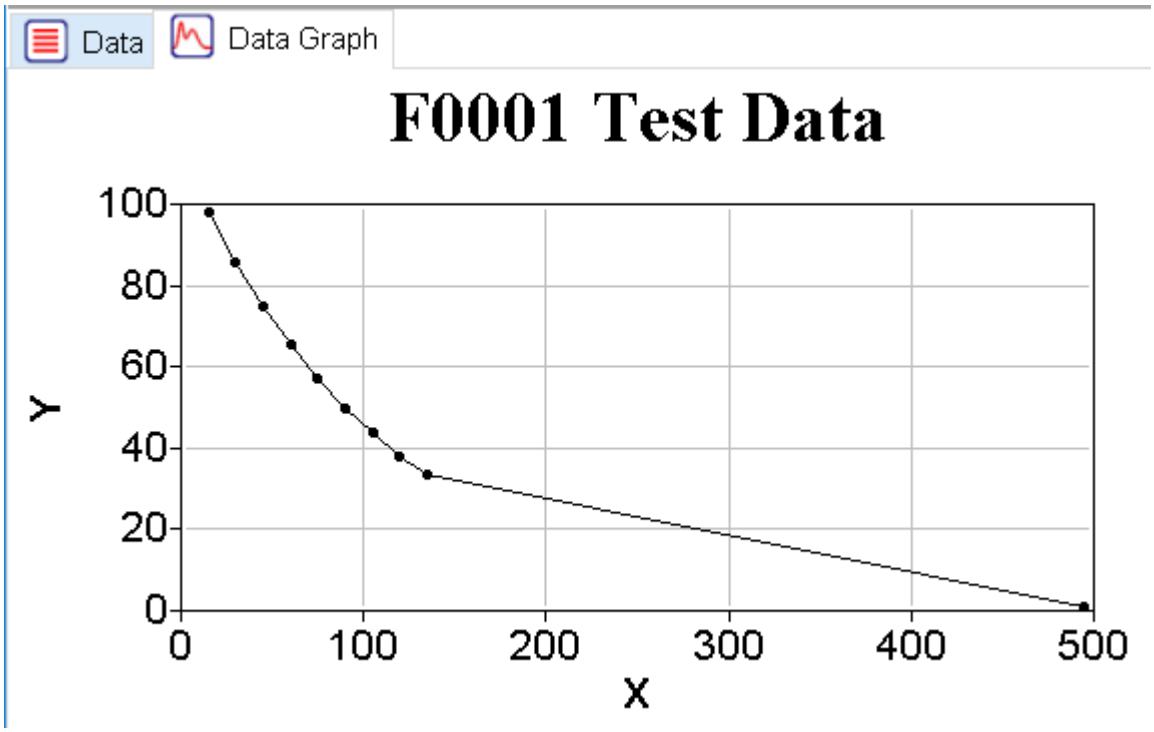
Close

Click the 'Close' button to return to ***FitAll***.

View

data graph

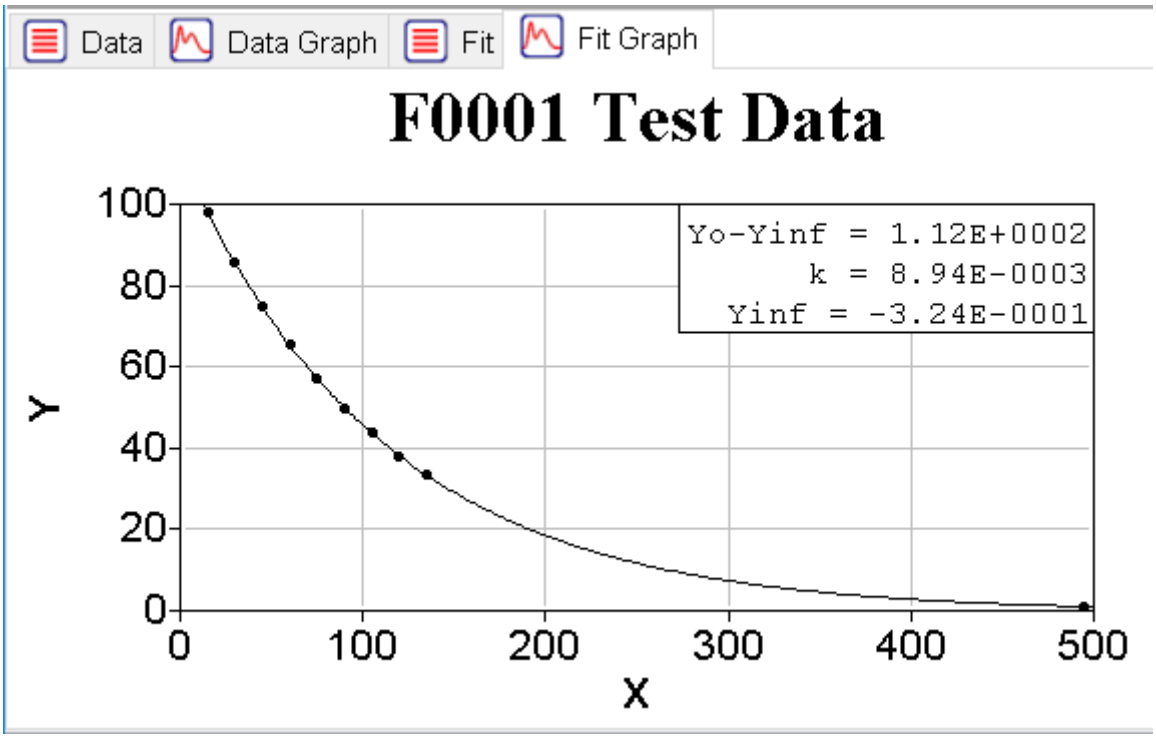
Choose View > data graph to see a graph of the data. The graph could look like this:



To change the appearance of the graph, select the menu options Edit > Properties... or right click in the graph window and click Properties on the context menu that appears.

fit graph

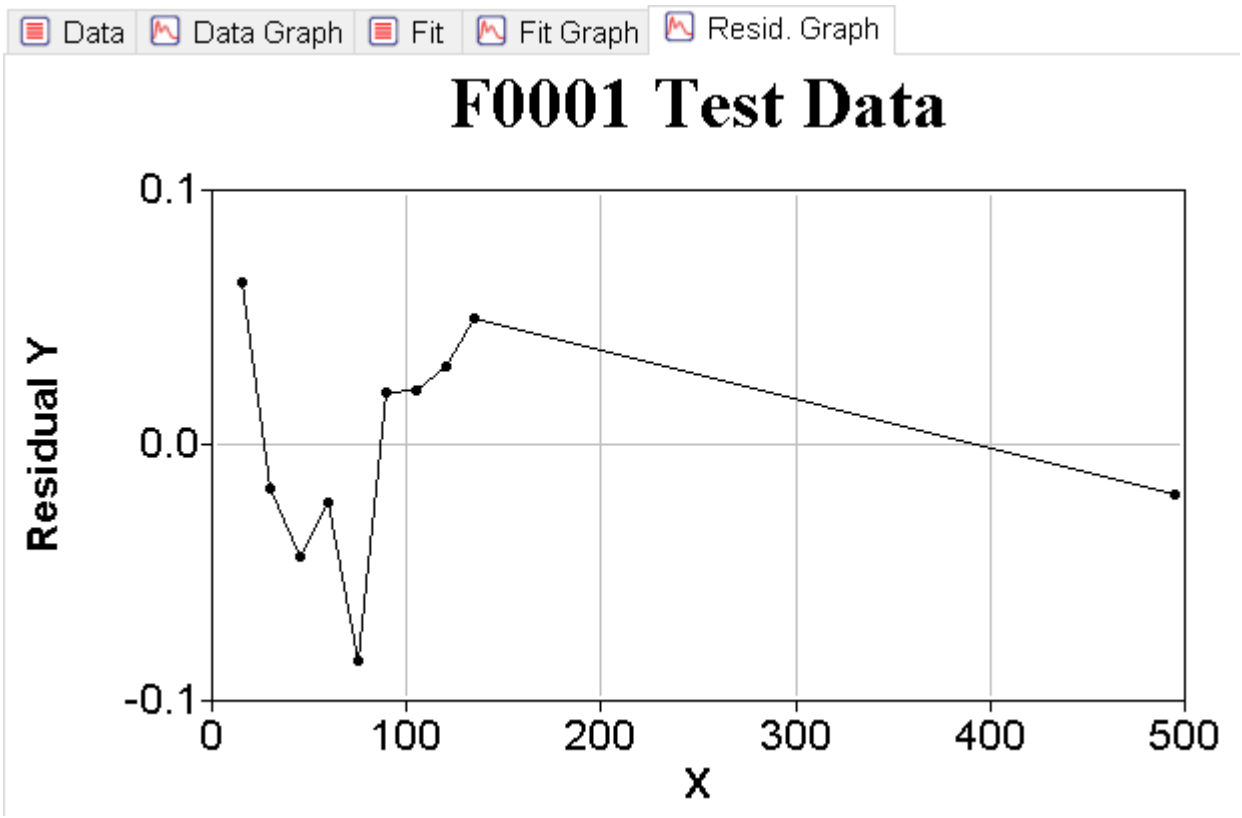
Choose View > fit graph to see a graph of the data. The graph could look like this:



To change the appearance of the graph, select the menu options Edit > Properties... 81 or right click in the graph window and click Properties on the context menu that appears.

residuals graph

Choose View > residuals graph to see a residuals graph; that is, a graph that displays the difference between the observed and calculated values of Y vs. X. The graph could look like this:



To change the appearance of the graph, select the menu options Edit > Properties... 81 or right click in the graph window and click Properties on the context menu that appears.

The residuals graph plots the difference between the calculated and observed values of the function.

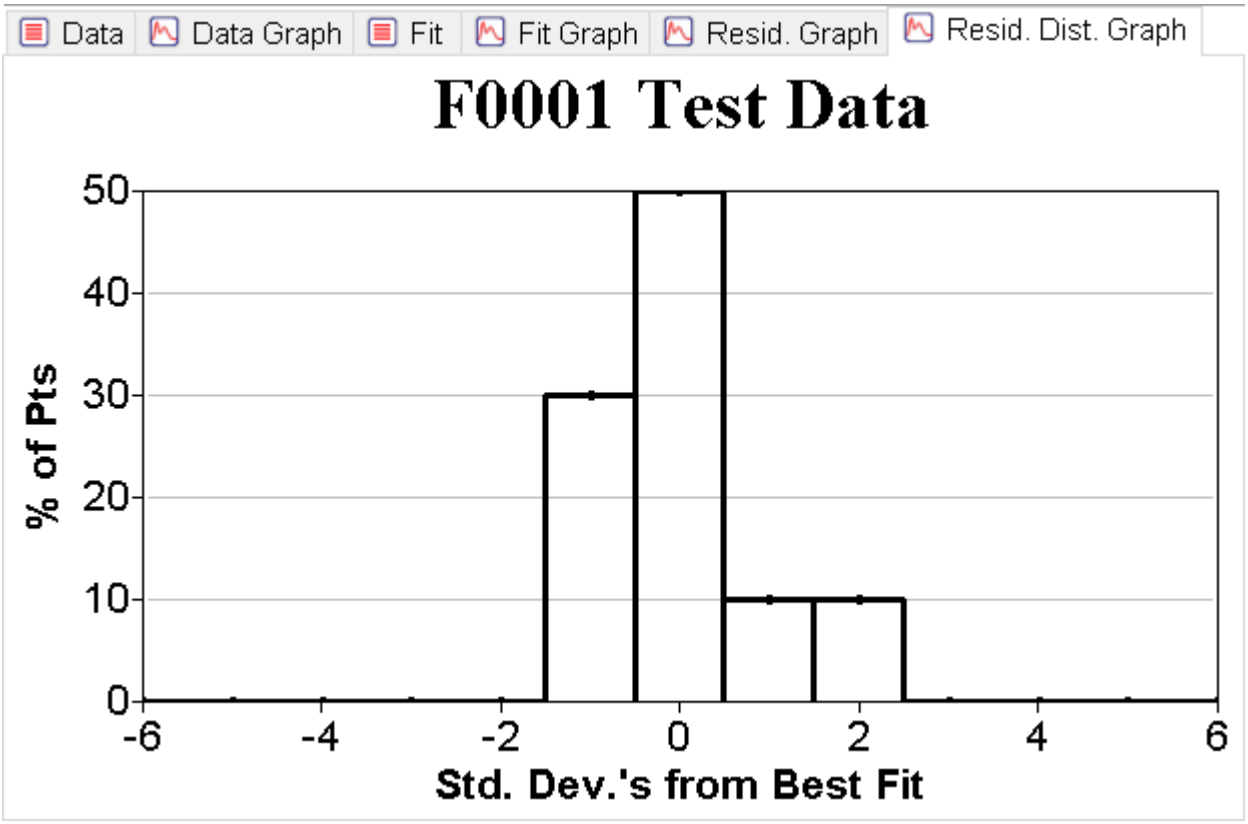
It provides a quick, visual way of determining whether the function used to fit the data is a good or bad model for the data.

If the function used in the analysis is a good model, the residuals graph will show the points randomly distributed about the zero line. On the other hand, if the residuals graph shows a trend, the function used is probably not a good model.

Even when the standard deviations of the fit and of the parameters are quite small, you should investigate the reasons for trends in the residuals plot. It may be that the function selected is almost a good model, but needs one or more parameters in it or it may be that some determinant error was introduced during data collection.

residuals distribution graph

Choose View > residuals distribution graph to see a residual distribution graph; that is, a graph that displays the percentage of data points that are within one or more standard deviations of the best fit. The graph could look like this:



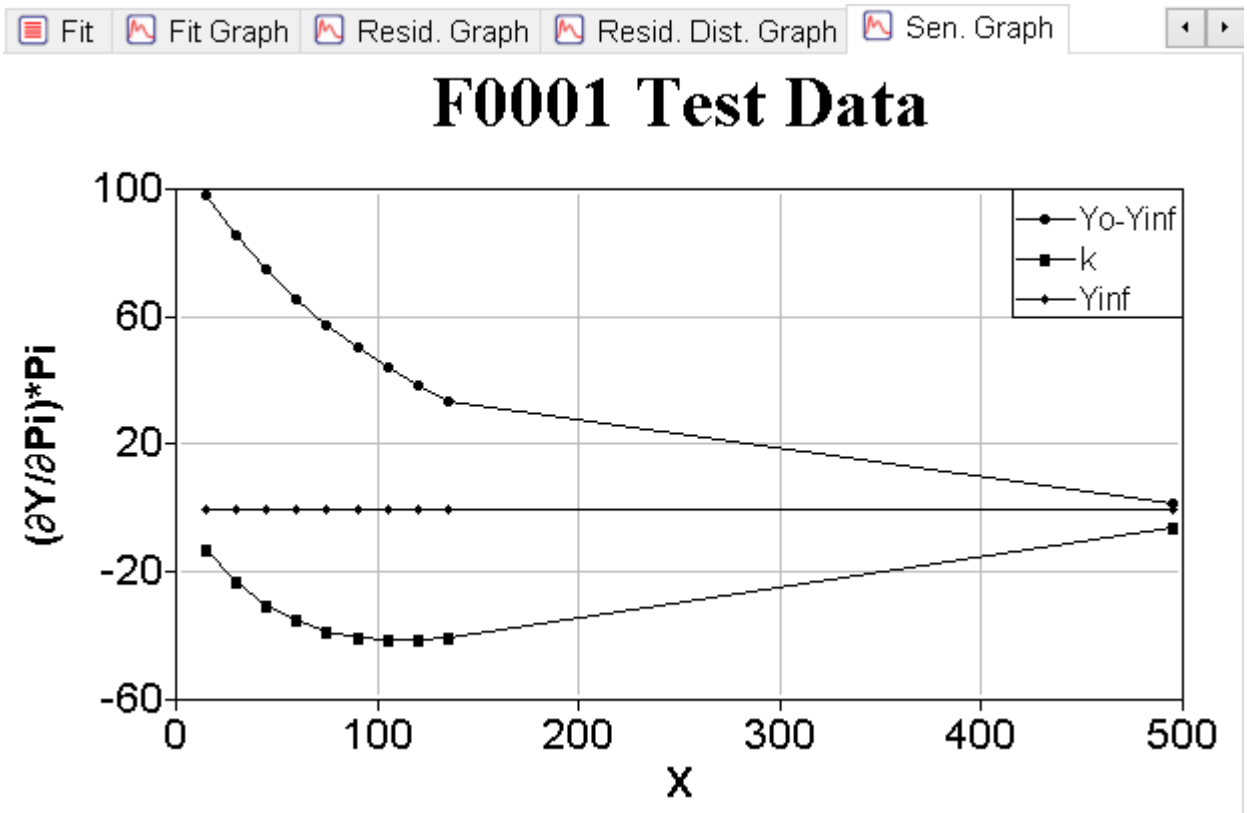
To change the appearance of the graph, select the menu options Edit > Properties... or right click in the graph window and click Properties on the context menu that appears.

The residuals distribution graph plots a histogram of the fraction of data points (as a percentage) versus their deviations from the best fit line. Each bar in the graph is 1.0 standard deviations wide.

It provides a quick, visual, way of determining whether the residuals (and, therefore, the measurement errors) are 'normally' distributed. The non-linear least squares (nlls) and linear least squares (lls) methods assume a 'normal' or Gaussian error distribution, while the non-linear least absolute deviations (nllad) method does not.

sensitivities graph

Choose View > sensitivities graph to see a sensitivities graph; that is, a graph that displays of the parameter sensitivity of the dependent variable, Y, on each of the parameters vs. X. The graph could look like this:



To change the appearance of the graph, select the menu options Edit > Properties... 81 or right click in the graph window and click Properties on the context menu that appears.

The sensitivities graph plots the 'parameter sensitivity' for each of the function's resolved parameters.

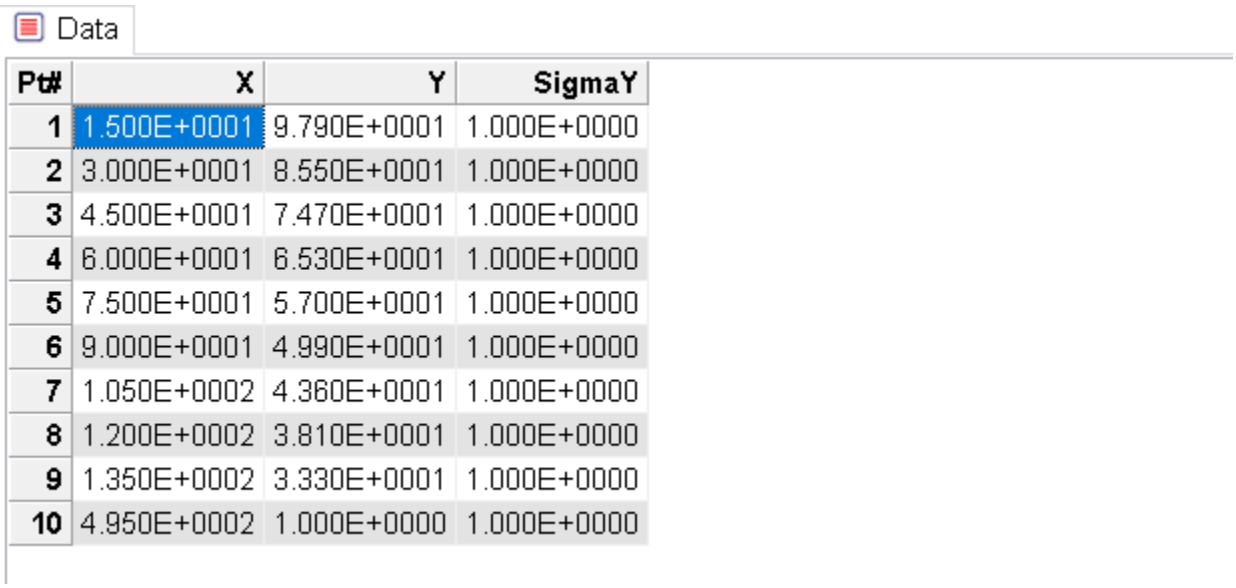
A parameter's sensitivity is given by the relationship:

$$\text{Parameter j Sensitivity} = \left(\frac{\partial f}{\partial Pj}\right) * Pj$$

The 'sensitivities graph' can help you visually determine the data range over which the calculated function's value is most influenced by each of its parameters.

Data

Choose View > Data to view and edit the data.


Data

Pt#	X	Y	SigmaY
1	1.500E+0001	9.790E+0001	1.000E+0000
2	3.000E+0001	8.550E+0001	1.000E+0000
3	4.500E+0001	7.470E+0001	1.000E+0000
4	6.000E+0001	6.530E+0001	1.000E+0000
5	7.500E+0001	5.700E+0001	1.000E+0000
6	9.000E+0001	4.990E+0001	1.000E+0000
7	1.050E+0002	4.360E+0001	1.000E+0000
8	1.200E+0002	3.810E+0001	1.000E+0000
9	1.350E+0002	3.330E+0001	1.000E+0000
10	4.950E+0002	1.000E+0000	1.000E+0000

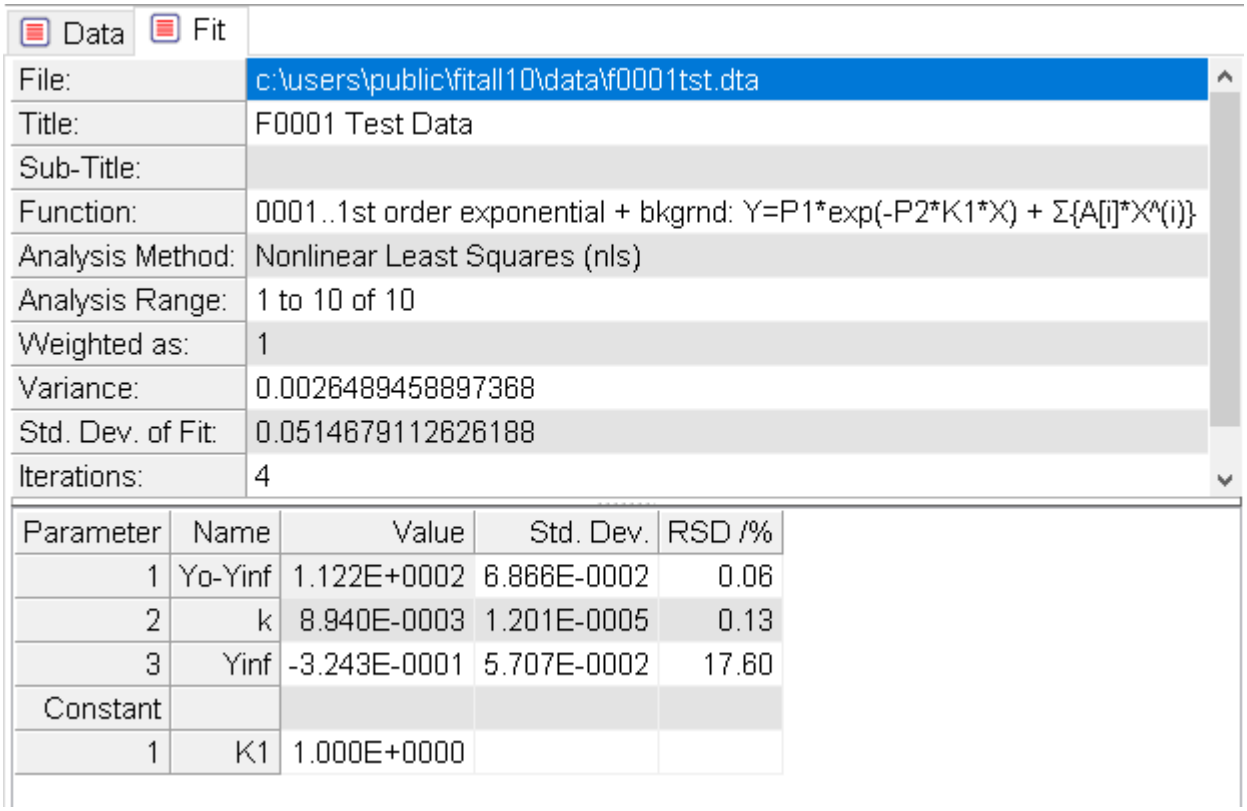
You can only edit and modify your data when the Data window is the active window; that is, when the cursor is in the Data window. (See: Entering and Editing Data in the Getting Started Guide).

To change the format of the numbers, select the menu options Edit > Properties... or right-click in the window and click Properties on the context menu that appears.

Fit

Choose View > Fit to see the results of the analysis in the Fit window.

The Fit window should look like this:



Data | Fit

File:	c:\users\public\fitall10\data\f0001tst.dta
Title:	F0001 Test Data
Sub-Title:	
Function:	0001..1st order exponential + bkgrnd: Y=P1*exp(-P2*K1*X) + Σ{A[i]*X^(i)}
Analysis Method:	Nonlinear Least Squares (nls)
Analysis Range:	1 to 10 of 10
Weighted as:	1
Variance:	0.0026489458897368
Std. Dev. of Fit:	0.0514679112626188
Iterations:	4

Parameter	Name	Value	Std. Dev.	RSD /%
1	Yo-Yinf	1.122E+0002	6.866E-0002	0.06
2	k	8.940E-0003	1.201E-0005	0.13
3	Yinf	-3.243E-0001	5.707E-0002	17.60
Constant				
1	K1	1.000E+0000		

It shows:

- The file name of the data that was analyzed.
- The title of the data set.
- The name of the function that was used in the analysis.
- The analysis method used to do the fit. This can be Non-linear least-squares (nlls), non-linear absolute deviations (nllad) or linear least squares (lls).
- The range of data points used in the analysis.
- The weighting scheme used.
- The variance or the reduced chi square, χ^2/ν, statistic when non-linear least squares (nlls) and linear least squares (lls) fitting are used and the average absolute deviation when non-linear least absolute deviations (nllad) fitting is used.
- The standard deviation of the fit.
- The number of iterations required to obtain the fit.

- For each of the parameters, its name, its resolved value and its estimated error, which is given as the standard deviation when the nlls or lls analysis methods are used or as the absolute deviation when the nllad method is used.

The standard deviation of the fit is calculated as the square root of the variance using the formula:

$$\text{Std. Dev. of Fit} = \sqrt{\frac{\Sigma\left(Y - Y_{calc}\right)^2}{\left(\text{LastPt} - \text{FirstPt} + 1 - \text{NTerms}\right)}}$$

in which NTerms is the number of parameters resolved and FirstPt to LastPt is the range of data points used in the analysis.

The standard deviation of each of the resolved parameters is calculated in a similar manner.

The relative standard deviation, RSD /%, or the relative absolute deviation, RAD /%, of the resolved parameters also will be displayed if the 'Display Rel. Std. Dev. in Fit Window 128' option in the Preferences dialog is checked.

If limiting parameter values were used during the regression analysis, the table also will contain a list of the parameter limits.

CAUTION:
If one or more of the parameter values is equal to one of its limits, the analysis is NOT statistically valid.

NOTE:
The values of the lower and upper limits are only displayed if one or more of the parameter values are outside the ranges defined by the limits.

To change the format of the numbers, select the menu options Edit > Properties... 80 or right click in the window and click Properties on the context menu that appears.

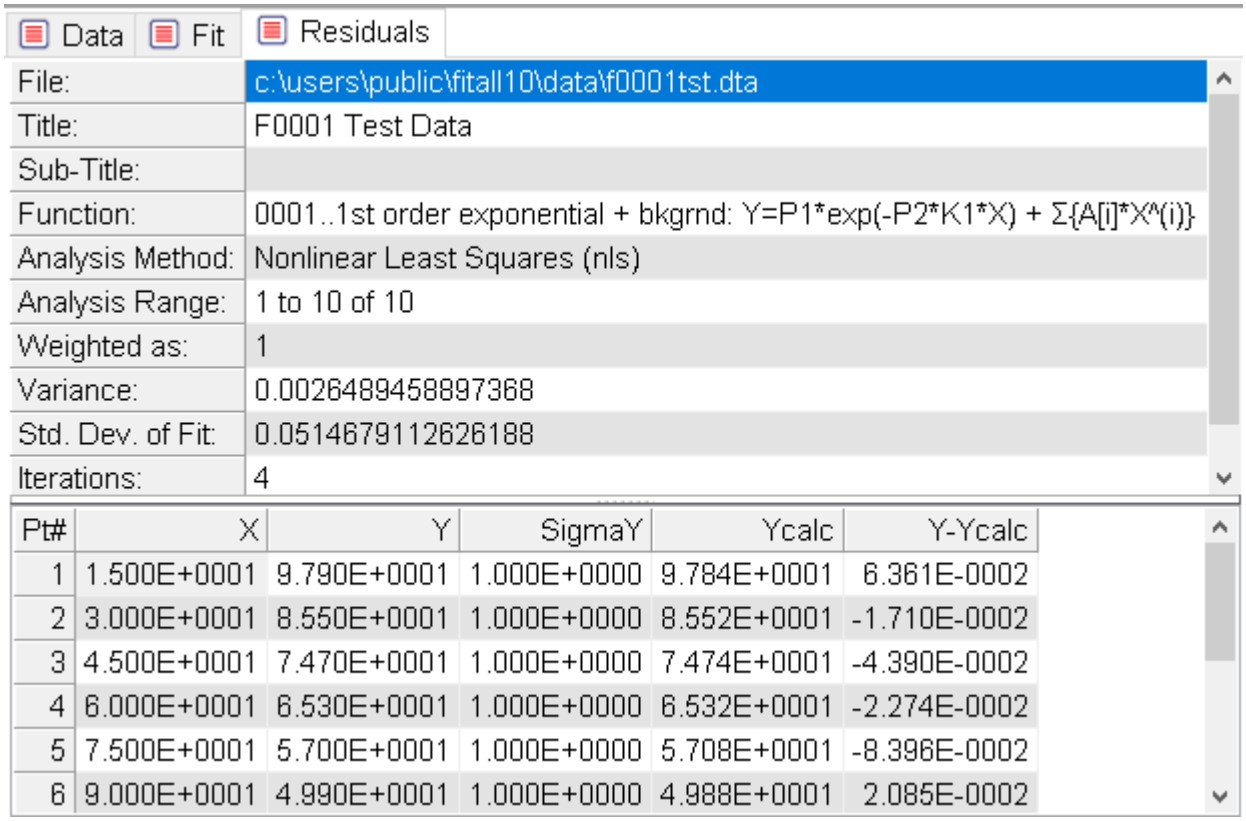
Residuals

Choose View > Residuals to view a table containing the:

- Data.
- Residuals; that is, the difference between the observed and calculated values of the function.

> **NOTE:**
> The residuals only are meaningful after an analysis has been completed.

The Residuals window looks like this:



Pt#	X	Y	SigmaY	Ycalc	Y-Ycalc
1	1.500E+0001	9.790E+0001	1.000E+0000	9.784E+0001	6.361E-0002
2	3.000E+0001	8.550E+0001	1.000E+0000	8.552E+0001	-1.710E-0002
3	4.500E+0001	7.470E+0001	1.000E+0000	7.474E+0001	-4.390E-0002
4	6.000E+0001	6.530E+0001	1.000E+0000	6.532E+0001	-2.274E-0002
5	7.500E+0001	5.700E+0001	1.000E+0000	5.708E+0001	-8.396E-0002
6	9.000E+0001	4.990E+0001	1.000E+0000	4.988E+0001	2.085E-0002

To change the format of the numbers, select the menu options Edit > Properties... or right click in the window and click Properties on the context menu that appears.

Residuals distribution

Choose View > Residuals distribution to view a table containing the data that is used to construct the residuals distribution graph.

> **NOTE:**
> The residuals distribution data are meaningful only after an analysis has been completed.

The 'Residuals distribution' window looks like this:

Data | Fit | Residuals | Residuals Dist.

File:	c:\users\public\fitall10\data\f0001tst.dta
Title:	F0001 Test Data
Sub-Title:	
Function:	0001..1st order exponential + bkgrnd: Y=P1*exp(-P2*K1*X) + Σ{A[i]*X^(i)}
Analysis Method:	Nonlinear Least Squares (nls)
Analysis Range:	1 to 10 of 10
Weighted as:	1
Variance:	0.0026489458897368
Std. Dev. of Fit:	0.0514679112626188
Iterations:	4

Std. Dev.'s from Best Fit	# of Pts	% of Pts
-6.5 to -5.5	0	0.00
-5.5 to -4.5	0	0.00
-4.5 to -3.5	0	0.00
-3.5 to -2.5	0	0.00
-2.5 to -1.5	0	0.00
-1.5 to -0.5	3	30.00

To change the format of the numbers, select the menu options Edit > Properties... or right click in the window and click Properties on the context menu that appears.

Sensitivities

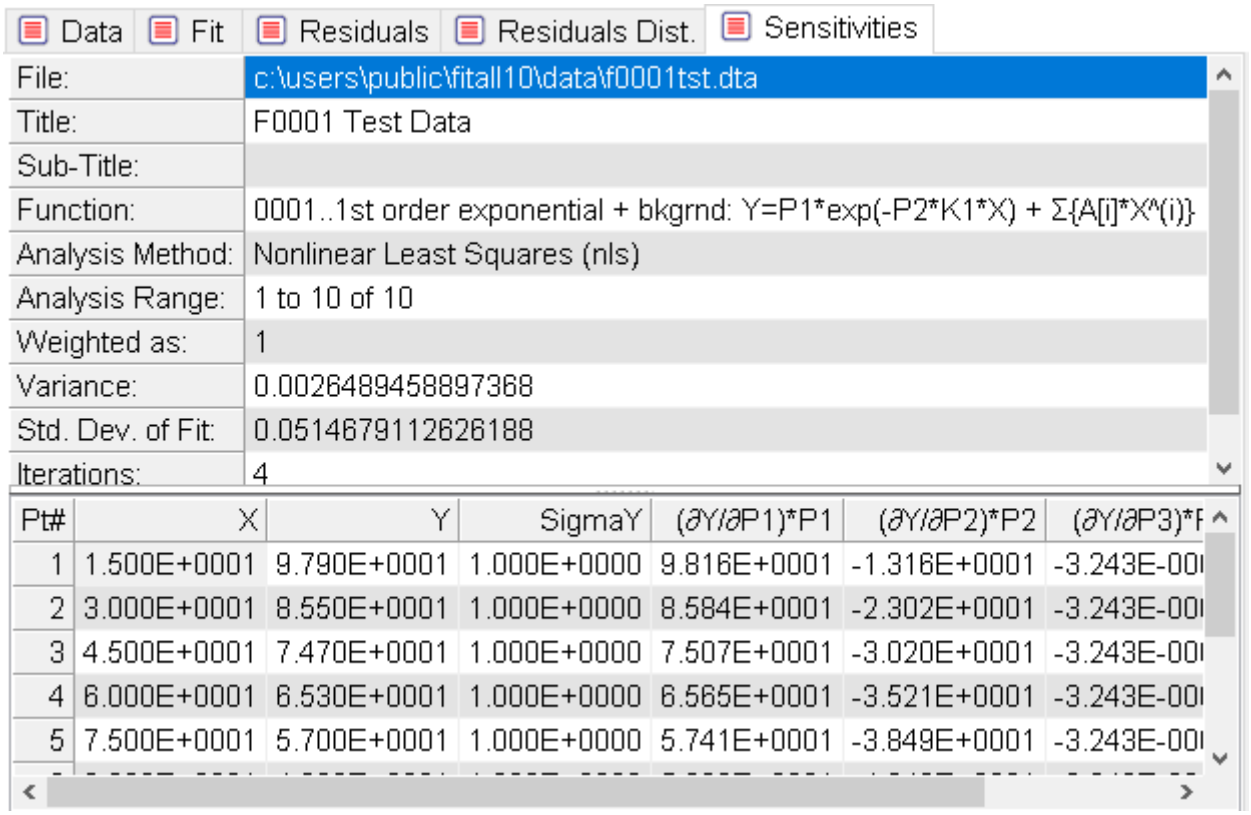
Choose View > Sensitivities to view a table containing the:

- Data.
- Parameter sensitivities, that is, the partial derivative of the function with respect to the parameter multiplied by the parameter's value.

To see a graph of the parameter sensitivities, choose the View > sensitivities graph 112 menu selections.

> **NOTE:**
> The parameter sensitivities are meaningful only after an analysis has been completed.

The Sensitivities table looks like this:

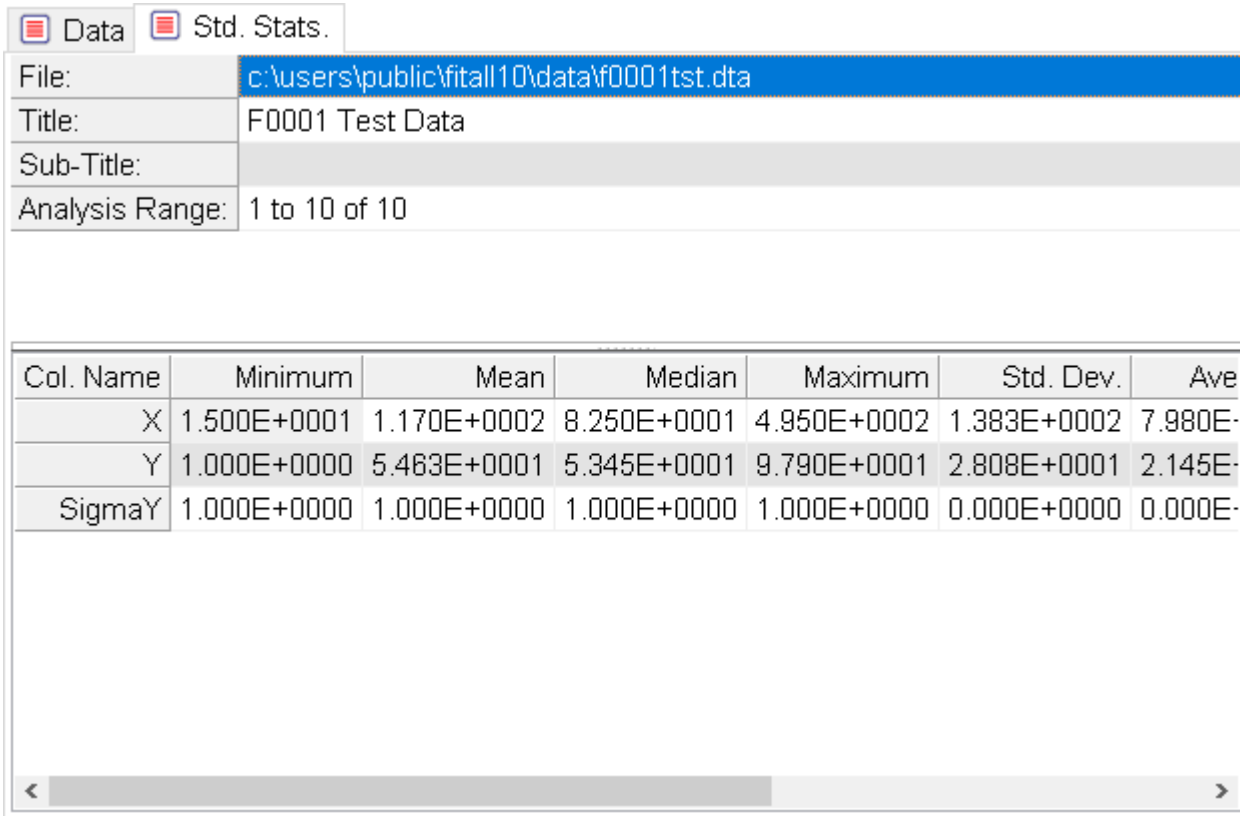


To change the format of the numbers, select the menu options Edit, Properties... 80 or right click in the window and click Properties on the context menu that appears.

Standard stats

Choose View > Standard stats to view a table containing some standard statistical values for each of the current data set's columns, including the:

- Minimum.
- Mean (average).
- Median.
- Maximum.
- Standard deviation.
- Average deviation.
- Skew.
- Kurtosis.



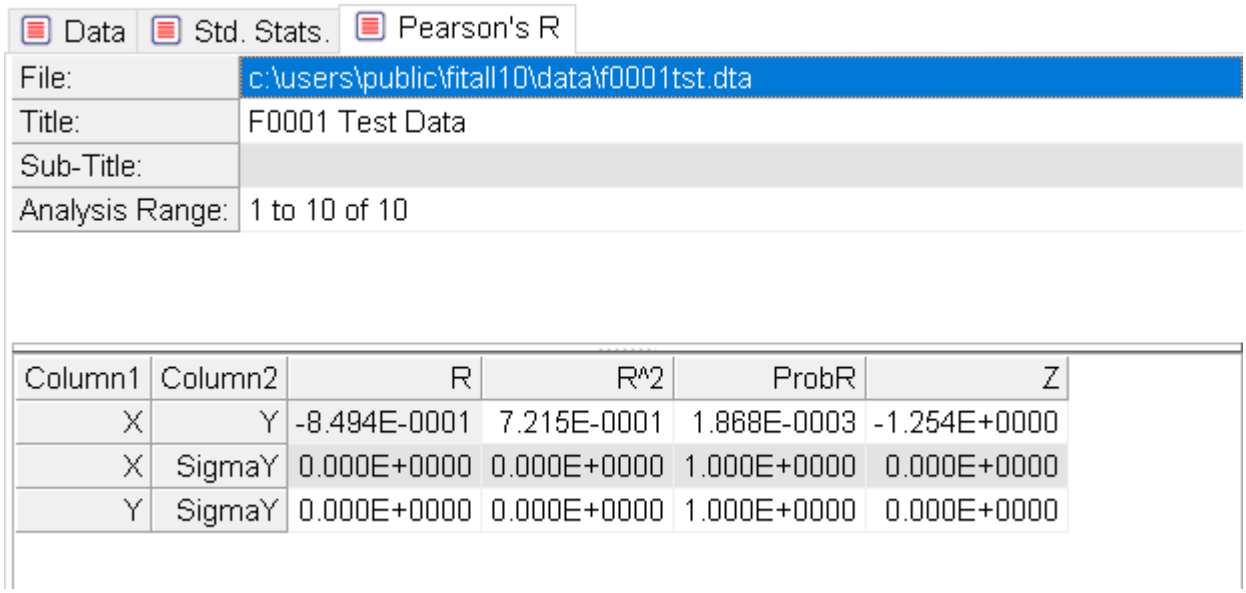
The values are calculated using the data analysis range specified in the Analyze > Setup 93 dialog.

To change the format of the numbers, select the menu options Edit > Properties... 80 or right click in the window and click Properties on the context menu that appears.

Pearson's R (Linear Corr. Coeff.)

Choose View > Pearson's R to view a table containing Pearson's R.

Pearson's is also known as the Linear Correlation Coefficient and provides a measure of the correlation between two columns of numbers.



Column1	Column2	R	R^2	ProbR	Z
X	Y	-8.494E-0001	7.215E-0001	1.868E-0003	-1.254E+0000
X	SigmaY	0.000E+0000	0.000E+0000	1.000E+0000	0.000E+0000
Y	SigmaY	0.000E+0000	0.000E+0000	1.000E+0000	0.000E+0000

The values are calculated using the data analysis range specified in the Analyze > Setup 93 dialog.

- **R** is Pearson's R; that is, the linear correlation coefficient. The values of R range from -1 to +1.

  If R = 1, there is a complete positive correlation; that is, the points fall on a perfect straight line with a positive slope.

  If R = -1, there is a complete negative correlation; that is, the points fall on a perfect straight line with a negative slope.

  A value of R near zero indicates that the data are uncorrelated.

- **R^2** is the square of R; that is, R * R. Often, R^2, rather than R, is reported as the linear correlation coefficient.

- **ProbR** is the probability that the absolute value of R should be greater than its calculated value.

  Small values of ProbR indicate that the value of R and R^2 are likely to be significant.

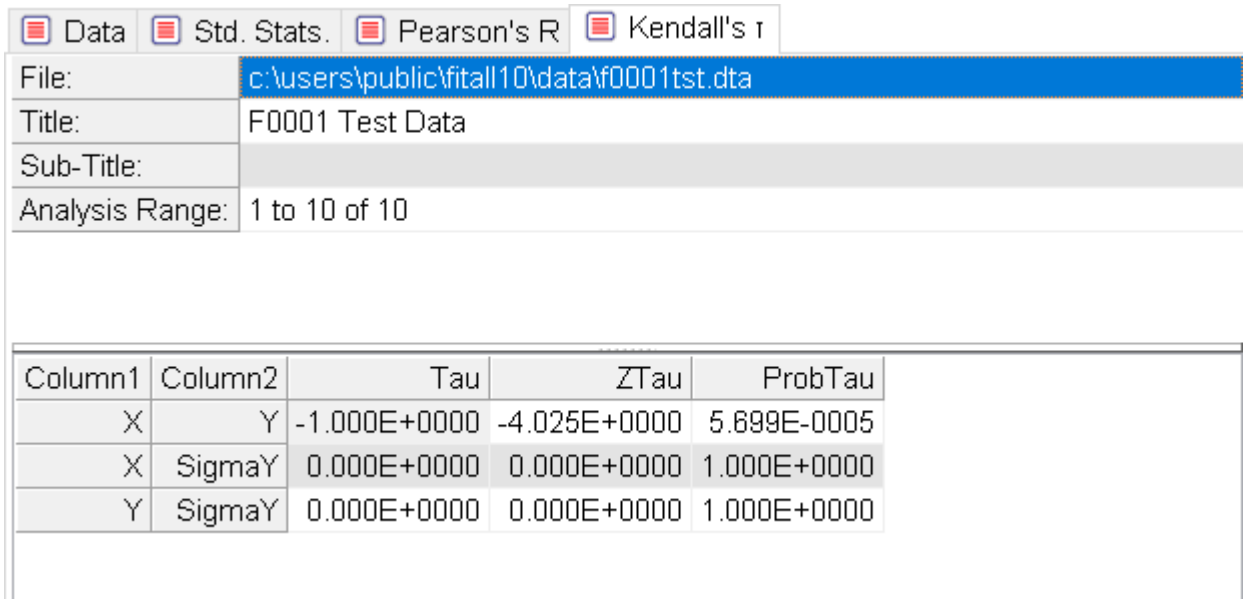
- **Z** is obtained using Fisher's z-transformation.

  This value can be used to compare the significance of the difference between two measured R-values.

To change the format of the numbers, select the menu options Edit > Properties... 80 or right click in the window and click Properties on the context menu that appears.

Kendall's tau

Choose View > Kendall's tau to view a table containing Kendall's Tau, which is a non-parametric statistic that measures the correlation between two columns of numbers.



Column1	Column2	Tau	ZTau	ProbTau
X	Y	-1.000E+0000	-4.025E+0000	5.699E-0005
X	SigmaY	0.000E+0000	0.000E+0000	1.000E+0000
Y	SigmaY	0.000E+0000	0.000E+0000	1.000E+0000

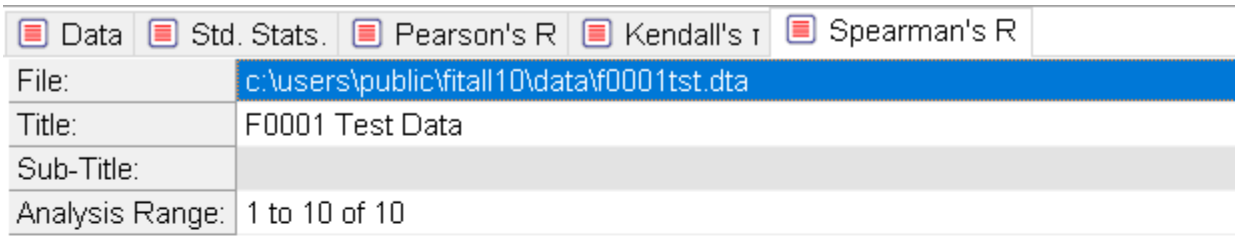
The values are calculated using the data analysis range specified in the Analyze > Setup 93 dialog.

- **Tau** is Kendall's Tau.
- **Ztau** is the number of standard deviations from zero.
  Small values of Ztau indicate a significant correlation or anti-correlation.

To change the format of the numbers, select the menu options Edit > Properties... 80 or right click in the window and click Properties on the context menu that appears.

Spearman's rank-order

Choose View > Spearman's rank-order to view a table containing Spearman's rank-order, which is a non-parametric statistic that measures the correlation between two columns of numbers.



Data | Std. Stats. | Pearson's R | Kendall's τ | Spearman's R

File:	c:\users\public\fitall10\data\f0001tst.dta
Title:	F0001 Test Data
Sub-Title:	
Analysis Range:	1 to 10 of 10

Column1	Column2	Rs	ProbRs
X	Y	-1.000E+0000	6.045E-0076
X	SigmaY	0.000E+0000	1.000E+0000
Y	SigmaY	0.000E+0000	1.000E+0000

The values are calculated using the data analysis range specified in the Analyze > Setup 93 dialog.

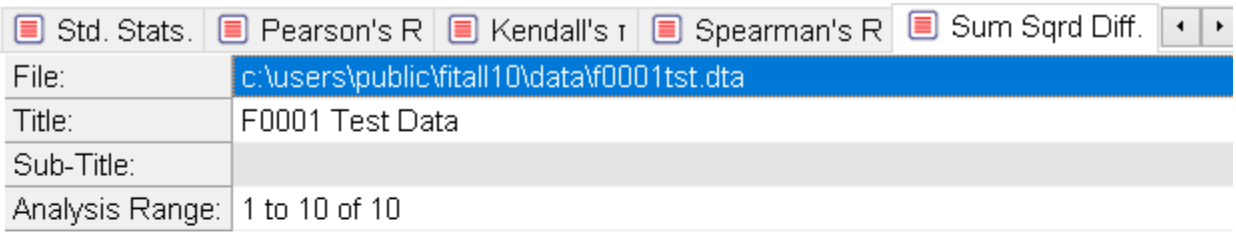
- **Rs** is the Spearman Rank-Order Correlation Coefficient.
- **ProbRs** is the two-sided significance of Rs' deviation from zero.

Small values of ProbRs indicate a significant correlation or anti-correlation.

To change the format of the numbers, select the menu options Edit > Properties... 80 or right click in the window and click Properties on the context menu that appears.

Sum squared diff. of rank

Choose View > Sum squared diff. of rank to view a table containing Sum squared differences of rank, which is a non-parametric statistic that measures the correlation between two columns of numbers.



Column1	Column2	D	ZD	ProbD
X	Y	3.300E+0002	3.000E+0000	2.700E-0003
X	SigmaY	8.250E+0001	0.000E+0000	0.000E+0000
Y	SigmaY	8.250E+0001	0.000E+0000	0.000E+0000

The values are calculated using the data analysis range specified in the Analyze > Setup 93 dialog.

- **D** is the sum-squared difference of ranks.
- **ZD** is the number of standard deviations by which D deviates from its null-hypothesis expected value.
- **ProbD** is the two-sided significance level of the deviation of D from its null-hypothesis value.

Small values of ProbD indicate a significant correlation or anti-correlation.

To change the format of the numbers, select the menu options Edit > Properties... 80 or right click in the window and click Properties on the context menu that appears.

Options

Change Font

FitAll Default

Click the menu items Options > Change Font > FitAll Default to set the font that ***FitAll*** will use to Arial, Regular, 8 pt.

Font...

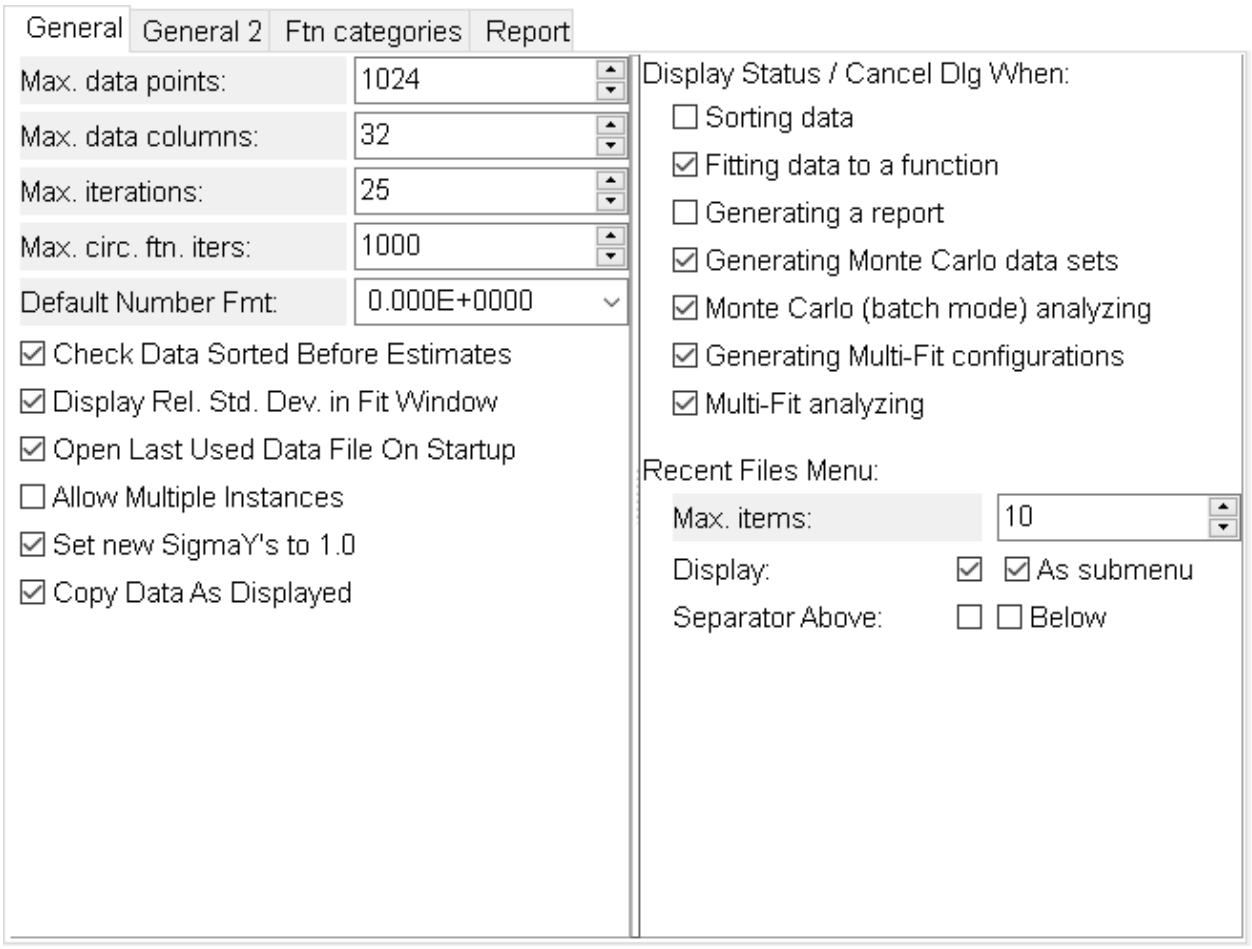
Click the menu items Options > Change Font > Font... to set the font that ***FitAll*** will use to whatever you like.

System Default

Click the menu items Options > Change Font > System Default to set the font that ***FitAll*** will use to Segoe UI, Regular, 7 pt.

Preferences

General



Max. data points

Use this spin-edit box to enter the maximum number of data points in a data set.

The amount of memory installed in your computer may restrict the maximum value to a number less than ***FitAll***'s upper limit of 65,536.

> **NOTE:**
> If the Max. data points or Max. data columns is changed the current data set will be removed from the computer's memory and all windows will be closed.

Max. data columns

Use this spin-edit box to set the maximum number of data columns in a data set.

The amount of memory installed in your computer may restrict the maximum value to a number less than ***FitAll***'s upper limit of 64.

> **NOTE:**
> If the Max. data points or Max. data columns is changed the current data set will be removed from the computer's memory and all windows will be closed.

Max. iterations

Use this spin-edit box to set the maximum number of iterations that will be used to analyze a function.

> **NOTE:**
> The Max. iterations setting also can be changed in the Analyze,Setup 96 dialog.

FitAll uses an iterative process to locate the best-fit parameter values. That is, it starts with initial guesses and, by repeating the calculations (iterating), it refines these values until the difference between the calculated values and the actual values is at a minimum.

If the initial guesses are too far from the final values or if the data are not well dispersed over an appropriate range, the number of iterations required can be very large. In such circumstances, it may take a long time to obtain the final results.

The 'Maximum iterations' value tells ***FitAll*** to stop after that number of iterations, even if a best-fit has not been obtained. You will then be given the option of terminating or continuing with the analysis.

> **CAUTION:**
> The final results reported by ***FitAll*** do not indicate whether the analysis was stopped before the termination criterion was met.

Max. circ. ftn. iterations

Use this spin-edit box to set the maximum number of iterations that will be used to evaluate a 'circularly defined' (implicit) function.

Implicit (circularly defined) functions are functions in which the function's value depends on its own magnitude; that is, the function, Y, is defined as Y = f(X, Y) rather than the more common Y = f(x).

Functions 0416, 0501 to 0503 and 0505 to 0507 are examples of implicit functions. ***FitAll*** uses an iterative (successive approximation) method to evaluate functions of this type. The value of 'Circ. ftn. max. iterations' constant is the maximum number of iterations that ***FitAll*** will use in evaluating the function.

The default value of 50 is adequate in the vast majority of cases. Increase this value if it seems that the function evaluations are not correct.

Default Number Fmt

Use this drop-down list to select the default format that ***FitAll*** should use when displaying numeric values.

Set New SigmaY's to 1.0

Select this check box if you want ***FitAll*** to assign a value of 1.0 rather than zero to SigmaY when you add a new data point (see: Edit, Add point 35).

> **NOTE:**
> This setting also affects how data is entered when pasted from the Windows Clipboard into the data window.
>
> If the number of columns of data in the text that is being pasted into the data window is less than the number of data columns in the current data set the extra data columns will be assigned a value of one if the 'Set New SigmaY's to 1.0' is checked, otherwise a value of zero will be assigned to the extra data columns.

Display All Data in Graphs

By default, ***FitAll*** displays the data points that were used in the regression analysis in the Fit, Residuals, Residuals Distribution and Sensitivity graphs.

Check this option to have all of the data points displayed, even if some of them were not used in the regression analysis.

This can be useful for getting a visual feeling of how important the "missing" data points are to the analysis or if they deviate significantly from the fitted curve when they are not included when doing the fit.

> **NOTE:**
> The Data graph always displays all of the data points.

Display Rel. Std. Dev. in Fit Window

Check this option to have the Fit Window display an extra column that contains the relative standard deviation, RSD /%, or the relative absolute deviation, RAD /%.

Open Last Used Data File On Startup

Select this check box if you want ***FitAll*** to open the last used data file when it starts-up.

Allow Multiple Instances

Select this check box if you want to run more than one copy (instance) of ***FitAll*** at a time.

- When this option *is* checked, double clicking on the ***FitAll*** icon will start up a new copy of ***FitAll***, even if one is already running.
- When this option is *not* checked, double clicking on the ***FitAll*** icon will start the first copy of ***FitAll*** or switch to a currently running copy of ***FitAll***, if one is active.

> **NOTE:**
> To do a 'side-by-side' comparison of the fit of two different functions to the same data, run two instances of ***FitAll*** and analyze the same data with a different function in each instance.

Check Data Sorted Before Estimates

Select this check box if you want ***FitAll*** to check whether the data has been sorted before it makes its initial estimates.

When ***FitAll*** makes its Initial Parameter Estimates it normally expects the data to be sorted on the first data column. If the data is not sorted, the initial estimates may not be appropriate.

Copy Data As Displayed

Select this check box if you want ***FitAll*** to copy its data to the Clipboard as it is displayed in the data window/tab. If not checked, the data will be copied using as many significant digits as are required and in a format that minimizes the number of characters in the number.

Font

Click this button to choose the font that ***FitAll*** will use to display information in its text windows, such as the data, fit, residuals and info windows.

Display Status / Cancel Dialog

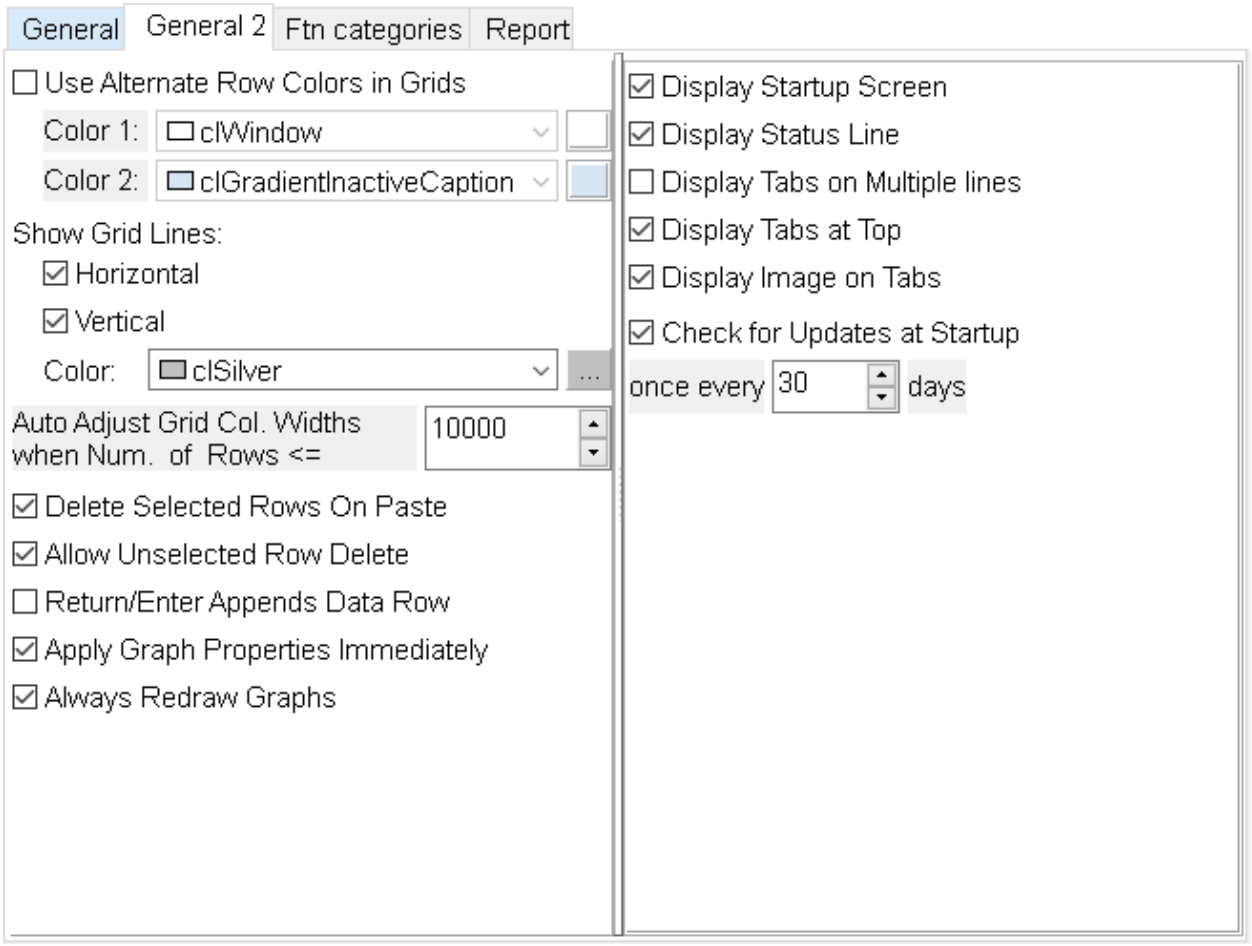
- **Sorting data**: Check this item if you want to be able to cancel a data sort operation before it is completed.
- **Fitting data to a function**: Check this item if you want to be able to cancel the fitting operation before it is completed.
- **Generating a report**: Check this item if you want to be able to cancel the report generation operation before it is completed.
- **Generating Monte Carlo data sets**: Check this item if you want to be able to cancel the generate Monte Carlo data sets operation before it is completed.
- **Monte Carlo (batch mode) analyzing**: Check this item if you want to be able to cancel the Monte Carlo analysis operation before it is completed.
- **Generating Multi-Fit configurations**: Check this item if you want to be able to cancel the Multi-Fit configuration generation before it is completed.
- **Multi-Fit analyzing**: Check this item if you want to be able to cancel the Multi-Fit analyzing operation before it is completed.

Recent files menu items

- **Display**: Check this item if you want the names of recently used data files listed in the File menu.
- **As submenu**: Check this item if you want the list of recently used data files to appear as a sub-menu item under the main File menu. When this is not checked, the names of the recently used data files are displayed directly on the File menu.
- **Separator Above**: Check this item if you want a separator bar above the first listed file or the sub-menu.
- **Separator Below**: Check this item if you want a separator bar below the last listed file or the sub-menu.

- **Max. items**: Use this spin-edit box to set the number of recently used files you want to appear in the recently used file list under the File menu item.

General 2



Use Alternate Row Colors in Grids

Check this item if you want alternate rows in most grids to have a different color.

Click on the Alternate Row Color 1 and 2 color boxes to change the colors that will be used.

Auto. Adjust Col. Widths

FitAll normally adjusts the widths of columns whenever a window that contains a table is displayed.

With large data sets, for example of 10,000 data points or more, the display of the window can be rather slow.

Use this setting to indicate when ***FitAll*** should or should not automatically adjust the column widths in a table.

Delete Selected Rows On Paste

When checked and pasting rows of data into the Data window any selected rows will be deleted before the new data is pasted into the window.

Allow Unselected Row Delete

When editing the data allow the **Ctrl + De**l key or the to delete the row even when the entire row is not selected.

Return / Enter Appends Data Row

Select this check box if you want ***FitAll*** to automatically append a row in the data window when the cursor is in the last row and column. This can speed up entering data into the data window.

Apply Graph Properties Immediately

When changing the properties 81 of a graph ***FitAll*** normally applies each change to the current graph as the property is changed.

With large data sets, for example of 100,000 data points or more, some of the property changes may be somewhat time consuming.

Uncheck this check box to have ***FitAll*** delay applying the changes until the Properties dialog box is closed.

Always Redraw Graphs

When ***FitAll*** displays a graph window it normally recalculates and redraws the graph.

With large data sets, for example of 100,000 data points or more, this may be somewhat time consuming.

Uncheck this check box to have ***FitAll*** automatically save the graph as a bitmap and then redisplay the bitmap rather than recalculating and re-plotting the graph. This will speed up the display of graph windows, but occasionally the redisplayed graph window may be partially obscured by portions of another window that was overlapping the graph window.

Display Startup Screen

By default, ***FitAll*** displays a startup dialog screen when it starts up.

When ***FitAll*** starts it often loads the most recently used data file. If there is a large number of data points in the file, for example 100,000 or more, this may be time consuming and the startup screen will show that ***FitAll*** is actually starting up and loading data.

If you do not want the startup screen to appear, uncheck this checkbox.

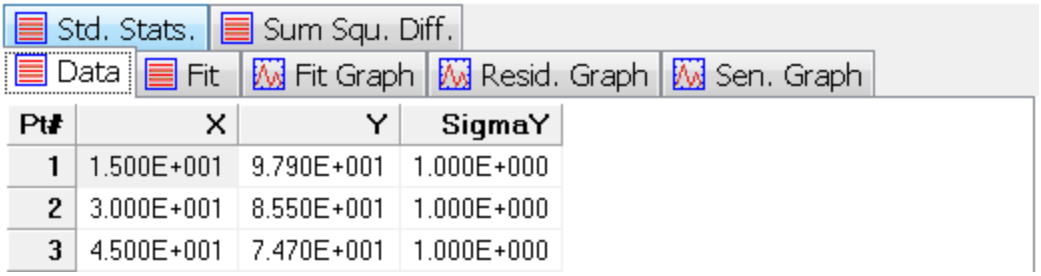
Display status line

Select this check box if you want ***FitAll*** to display a status line at the bottom of its 'desktop'.

Display Tabs on Multiple Lines

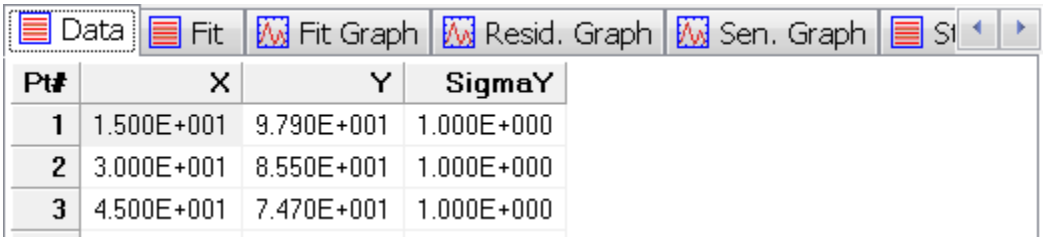
Select this check box if you want ***FitAll*** to display the window tabs on multiple lines when there are more tabs than can be displayed in a single row and still have all of the tabs visible. If this is not checked scroll buttons will appear so that the tabs can be scrolled in and out of view.

For example, the row of tabs could look like this:



Pt#	X	Y	SigmaY
1	1.500E+001	9.790E+001	1.000E+000
2	3.000E+001	8.550E+001	1.000E+000
3	4.500E+001	7.470E+001	1.000E+000

or this:



Pt#	X	Y	SigmaY
1	1.500E+001	9.790E+001	1.000E+000
2	3.000E+001	8.550E+001	1.000E+000
3	4.500E+001	7.470E+001	1.000E+000

Display Tabs at Top

Select this check box if you want ***FitAll*** to display the tabs with the Window names at the top. If not checked, the tabs will be displayed at the bottom of the main window.

Display Image on Tabs

Select this check box if you want ***FitAll*** to display a small image on the tabs to indicate whether the tab contains a window that contains a graph or text.

Check for Updates at Startup

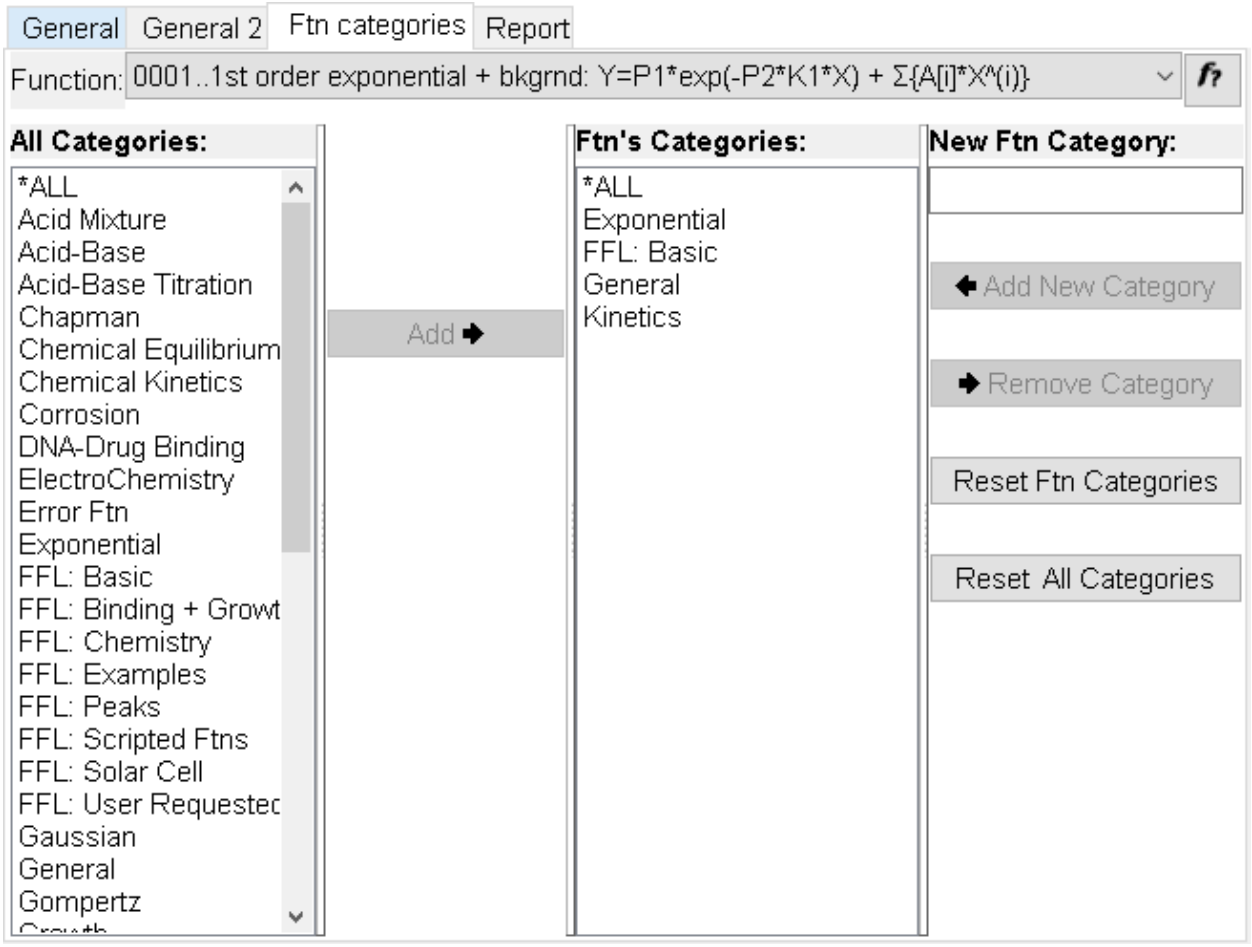
FitAll automatically checks ***MTR* Software**'s website for updates once every 30 days.

To change how often ***FitAll*** automatically checks for updates, use the "Days" spin-edit.

If you do not want ***FitAll*** to automatically check for updates uncheck this checkbox.

> **NOTE:**
> At any time, you can check for updates by making the menu selections Help > Check for Updates.. 139 or by using the Windows menu selections Start > Programs > FitAll80 > Check for Updates.

Ftn categories



Function

Use this drop down list box to select the function whose categories you want to view or change.

Help for Current Function, f?

Click the f? button to display Help for the currently selected function.

All Categories

The 'All Categories List Box' lists all of the function categories that have been defined and have been assigned to at least one of the available functions.

Add

Click this button to add the category highlighted in the 'All Categories' list to the 'Function Categories' list for the current function.

Function Categories

The 'Function Categories List Box' list the categories associated with the currently selected function.

New Ftn Category

Enter a new category into this edit box.

When you are sure that you actually want to add the new category, click the 'Add New Category' button. It will be added to the current Function Categories list and to the All Categories lists.

> **NOTE:**
> The list of function categories is sorted alphabetically.
> If you name your new category something like "* My Favourite Ftns" it will appear at the top of the list.

Add New Category

Click the 'Add New Category' button to add the category in the 'New Ftn category' edit box to the current function.

Remove Category

Click this button to remove the category that is highlighted in the 'function's categories' list.

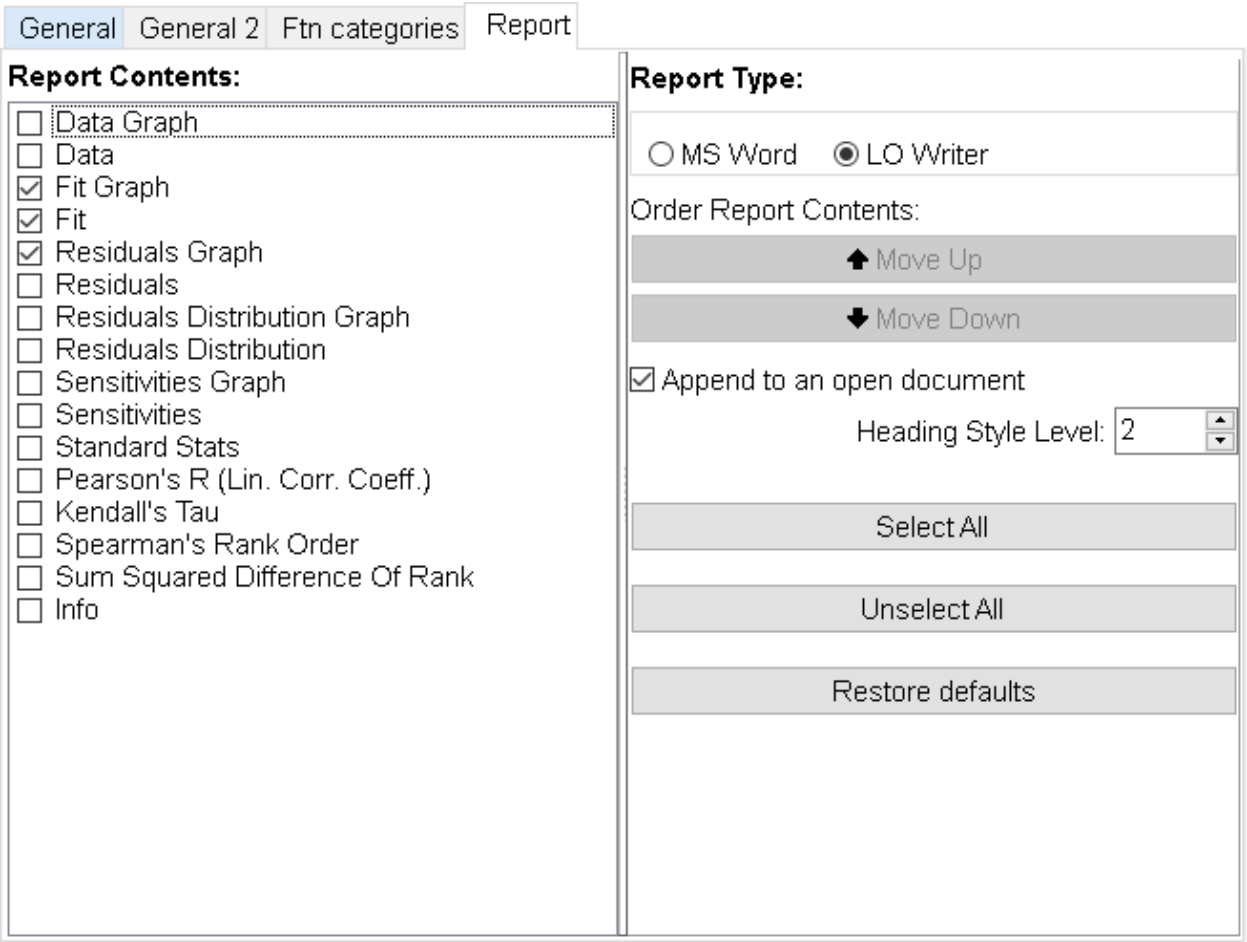
Reset Ftn Categories

Click this button to reset the current function's categories to its default values.

Reset All Categories

Click this button to reset all of the functions' categories to the default values.

Report



Report Contents

Select (check) the report elements that you want to include in the report.

Report Type

Select (click) on of the **MS Word** or **LO Writer** radio buttons to choose the type of report that you want ***FitAll*** to create.

Order Report Contents

Select (click to highlight) one of the items in the 'Report Contents' check list and click the 'Move Up' and 'Move Down' buttons to change the order of the report's contents.

> **NOTE:**
> Only those items in the 'Report Contents' check list that are checked will appear in the report.

Append to Existing Report

Select (check) the 'Append to Existing Report' check box if you want the generated report appended (added) to an existing open document.

> **NOTE:**
> The report will be added to the end of the open and active document. It will NOT be inserted at the cursor position.
>
> This can be very useful when you are writing a report at the same time that you are analyzing your data or are otherwise documenting the fits as you do them.

Heading Style Level

Each element in the report has a heading, such as 'Data', Data Graph', 'Fit' or 'Fit Graph'.

In MS Word and LO Writer the headings are formatted with a 'heading style', such as 'Heading 1' or 'Heading 2'.

The 'Heading Style Level', which can have values from 0 to 9, applies the standard Heading Style (1 to 9) to the heading text. A value of 0 means that the 'Normal' style will be applied to the heading text.

Select All

Click the 'Select All' button to include all possible results and information in the report.

Unselect All

Click the 'Unselect All' button to remove all possible results and information in the report so that you can more easily select the one or two items that you actually want in the report.

Restore defaults

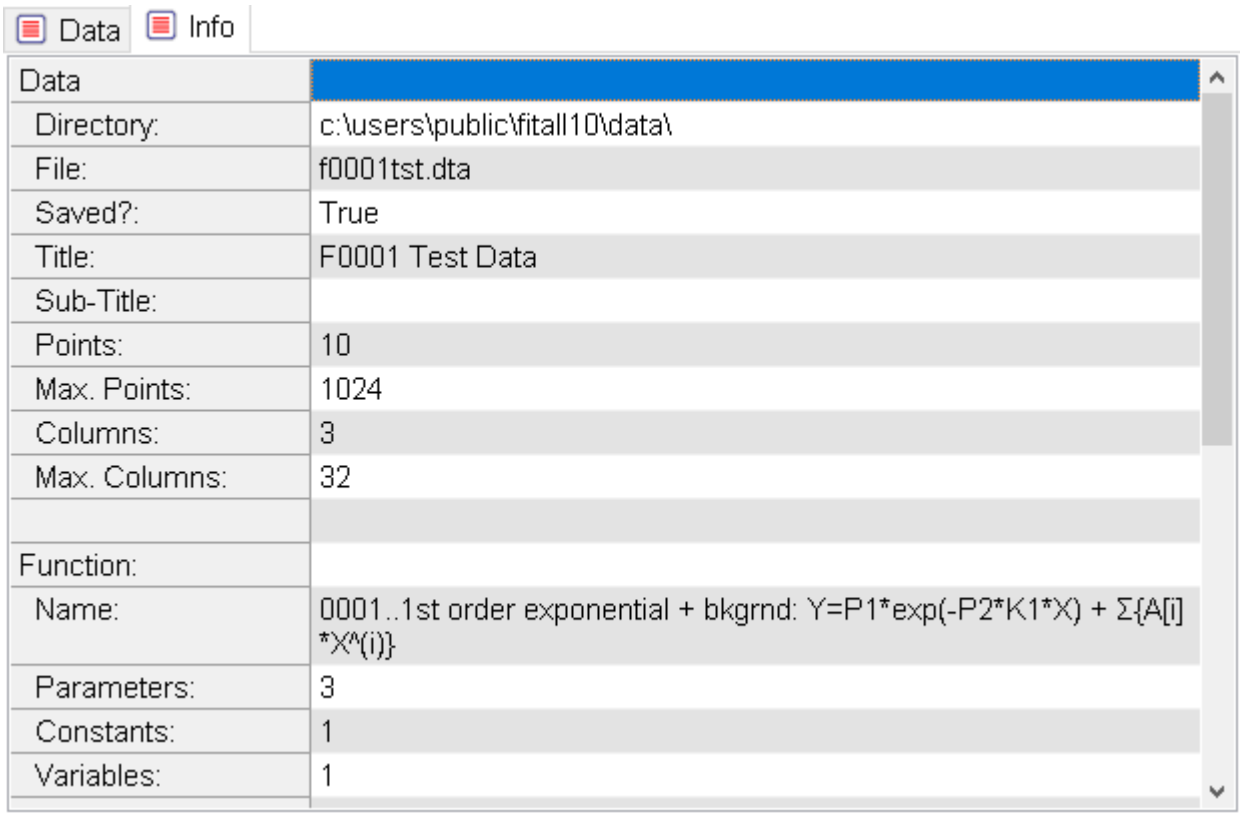
Click the 'Restore defaults' button to change the report settings to ***FitAll***'s standard (default) settings.Enter topic text here.

Also See

File, Print to clipboard 20

Info

Choose Info to open the 'Info' window which looks like this:



This window provides some basic information about the current state of ***FitAll*** and your computer, including:

- The name and location of the current data file.
- Whether the data has been saved since it was last modified.
- The current analysis function.
- The version of ***FitAll***.
- The first six characters of ***FitAll***'s serial number.
- The ***FitAll*** Function Libraries (FFL's) that are loaded.
- The MS Windows version
- The MS Excel version
- The MS Word version
- The Open Office version

- The total amount of memory in the computer.
- The computer's CPU speed.

Help

Contents

Choose Help > Contents to open the ***FitAll*** Reference Guide.

The on-line table of contents list other ***FitAll*** Guides, such as the ***FitAll*** Getting Started Guide and one or more of ***FitAll***'s Function Library guides.

Pressing the **F1** key will, in many cases, display a context sensitive help item in the on-line ***FitAll*** Reference Guide.

You also can view the on-line ***FitAll*** Reference Guide by selecting the Windows menu items Start > Programs > FitAll10 > Reference Guide.

Current Function...

Choose Help > Current Function or click the toolbar button,  , to open the ***FitAll*** Function Guide that describes the currently selected function.

User Defined Functions...

Choose Help > User Defined Functions... to open a dialog box that provides a list of all the available help documents that are available for the user defined functions.

This menu item will not be displayed if there are no UDF help documents.

Check for Updates...

Click the menu items Help > Check for Updates to connect to ***MTR* Software**'s web site to see if an update is available.

If an update is available you will be given the opportunity to download and install it.

> **NOTE:**
>
> - You also can check for updates by using the Windows menu selections Start, Programs > FitAll10, Check for Updates.
> - You can change when and if ***FitAll*** automatically checks for updates by selecting the menu items Options > Preferences > General 2 > Check for Updates at startup 132.

FitAll on the Web...

Click the menu items Help > FitAll on the Web... to automatically start your default web browser and link to ***MTR* Software**'s home page. Of course, your computer must have an active connection to the Internet for this to work.

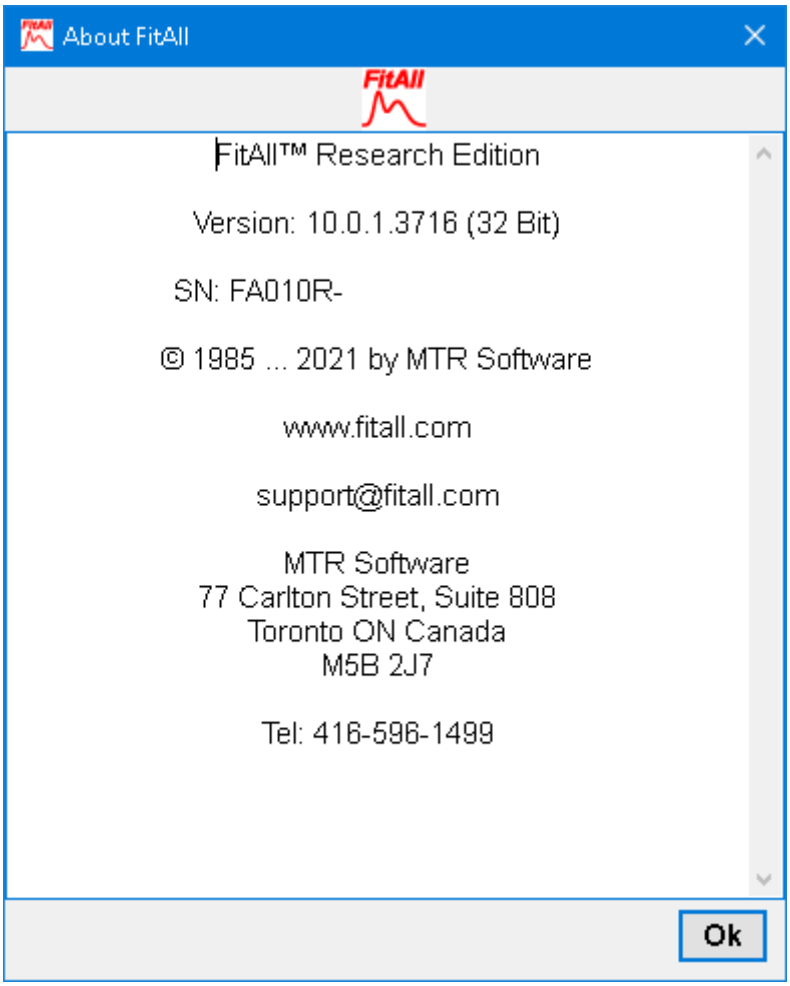
email FitAll Support...

Click the menu items Help > email FitAll Support to automatically start your email program with a new message addressed to support@fitall.com having a subject of ***FitAll*** Support and ***FitAll***'s version and serial numbers in the body of the message.

Complete the message with your question or request and send it.

About FitAll

Choose Help > About FitAll to display the 'About ***FitAll***' dialog box. It looks like this:



How To

Add Scripted Functions

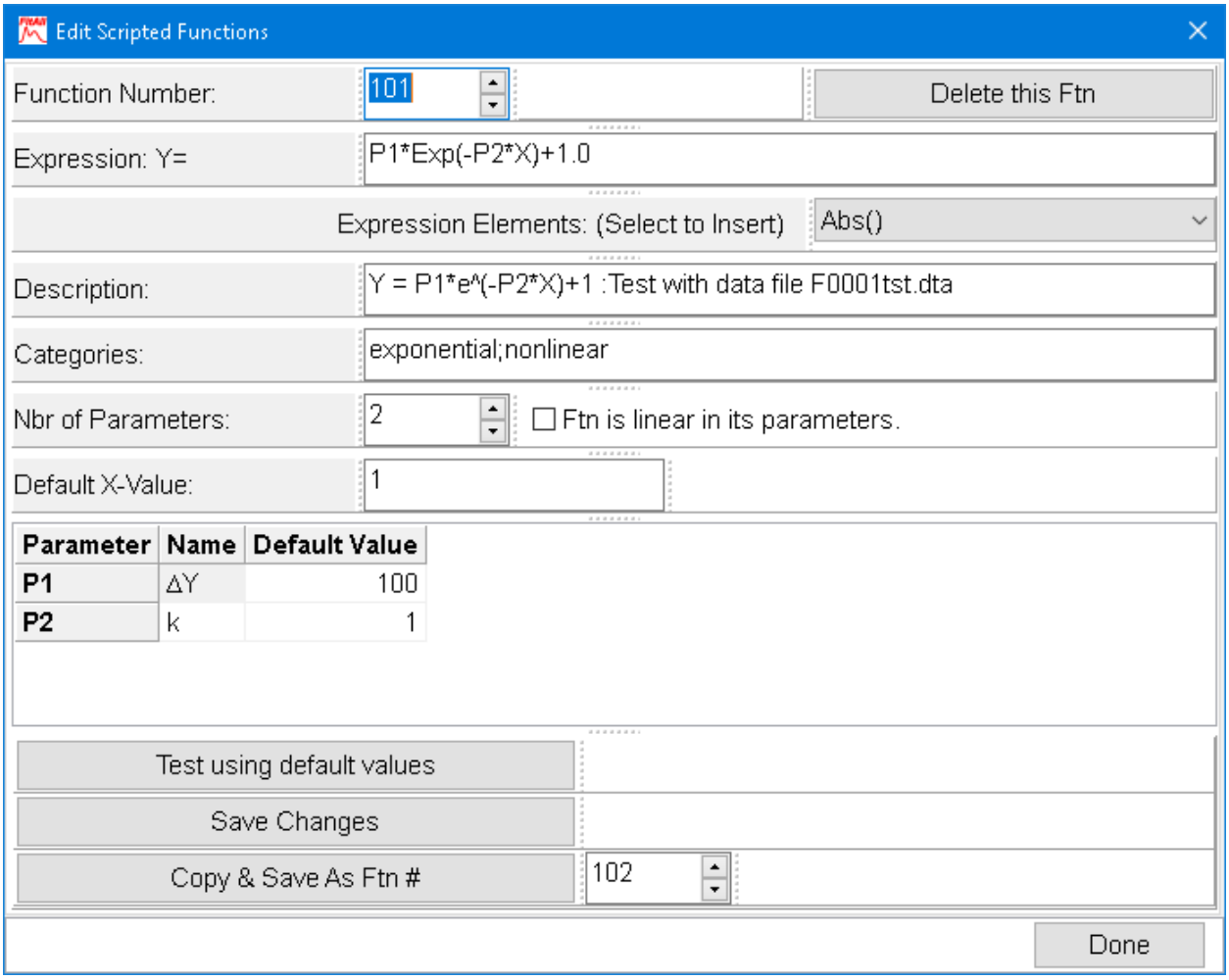
To add your own scripted function to ***FitAll*** do the following:

1. Decide on the function that you would like to add and write down an expression for it using "X" as the independent variable and "P1", "P2", etc. as the parameters that are to be resolved.

   For example, if you want to fit your data to a straight line the function would be
   Y = P1 + P2 * X
   in which P1 is the intercept and P2 is the slope of the line.

   Note that the function (a) has two (2) parameters and (b) is "linear" in its parameters.

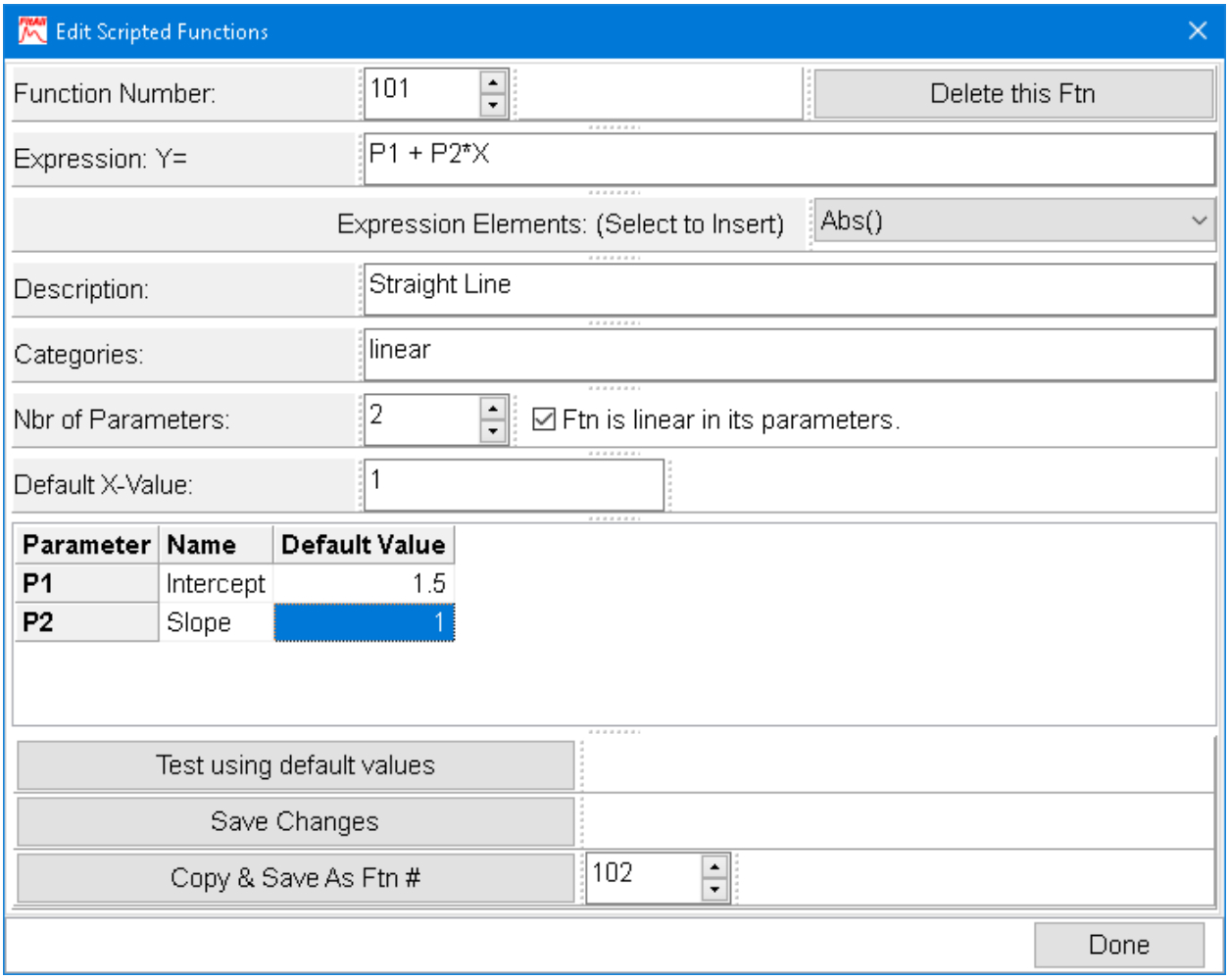
2. Make the menu selection Edit > Scripted Ftns.... The "Edit Scripted Functions" dialog that appears will look like this:



3. Use the Function Number spin edit to choose a function that has not yet been defined; that is, one in which most of the entries in the dialog are blank.
   Or simply edit the entries for an existing function to change its definition.

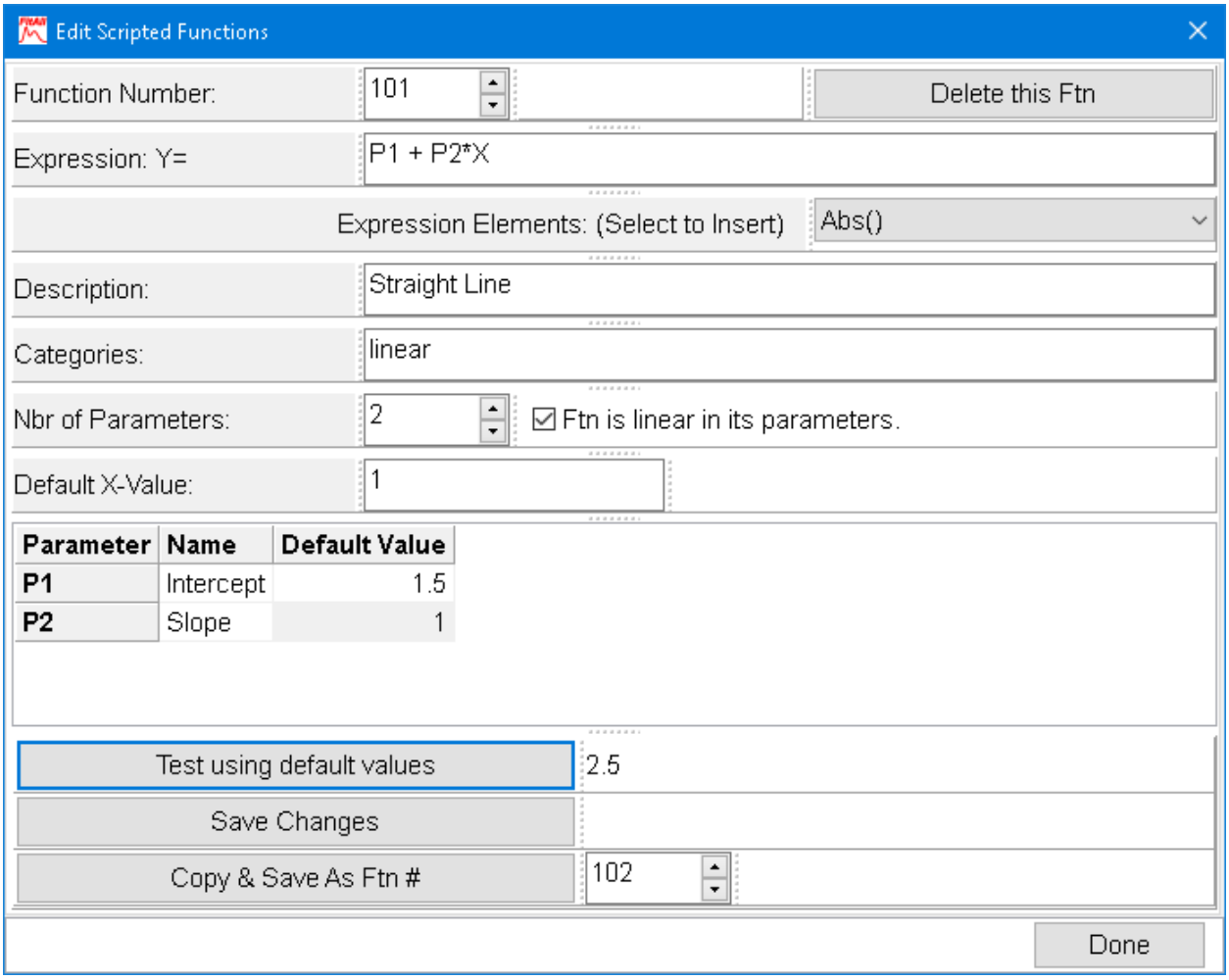
   In this example, edit the definition of function 101.

4. After making your changes the dialog should look like this:



Note that:
(a) The Description must not be blank. If it is blank the function will not appear in the list of available analysis functions.
(b) The "Ftn is linear in its parameters" checkbox has been checked because the function is linear in its parameters.
(c) The names "Intercept" and "Slope" have been assigned to the parameters P1 and P2.

5. Click the "Test using default values" button to make sure that the expression is valid and will give the expected result when evaluated.
The dialog should look like this



Note that you can change the default X-value and parameter values and test the function evaluation again.

6. Click the "Save Changes" button to save the scripted function definition.

7. Click the "Done" button. When next setting up an analysis this function will appear in the list of available functions.

Change Data Column Order

This "How To" illustrates how to change the order of the data columns in the current data set.

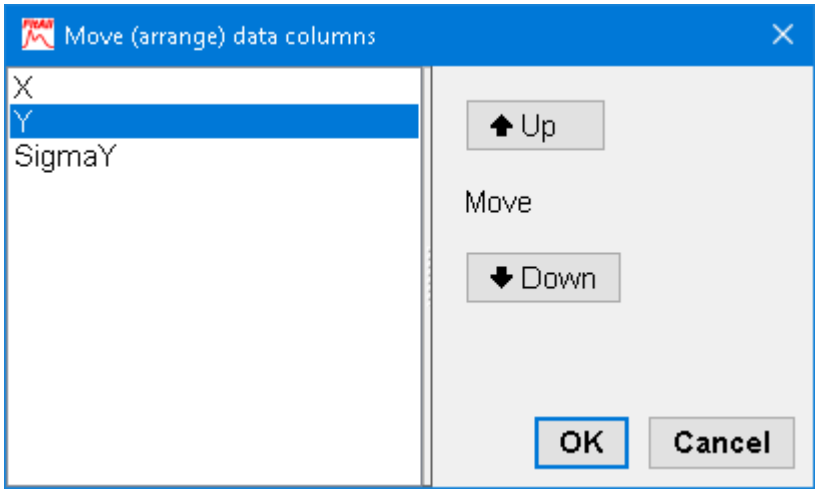
Changing the data column order may be useful in a number of situations. For example:

1. Data that is copied and pasted from another program into ***FitAll*** may not have the data columns organized in the way that the analysis function expects, or

2. You want to analyze the same set of data with two different functions, such as function numbers 0502 and 0512, but the two functions expect the order of the data columns to be different.

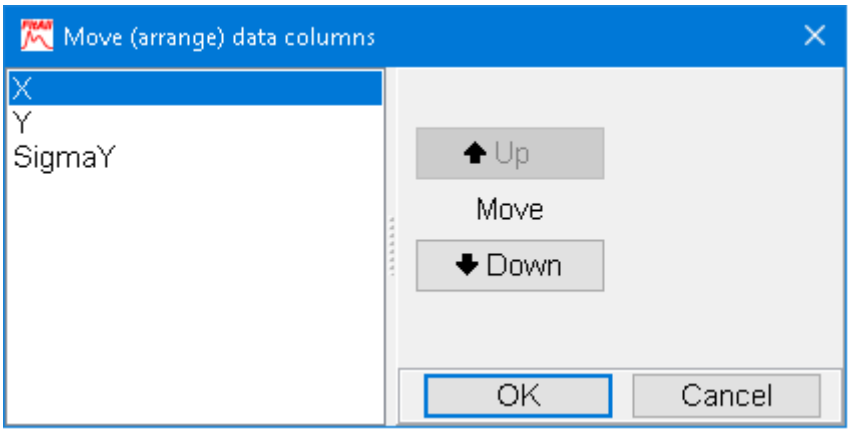
Here's how to do it:

1. Open a data file. The result may look like this:

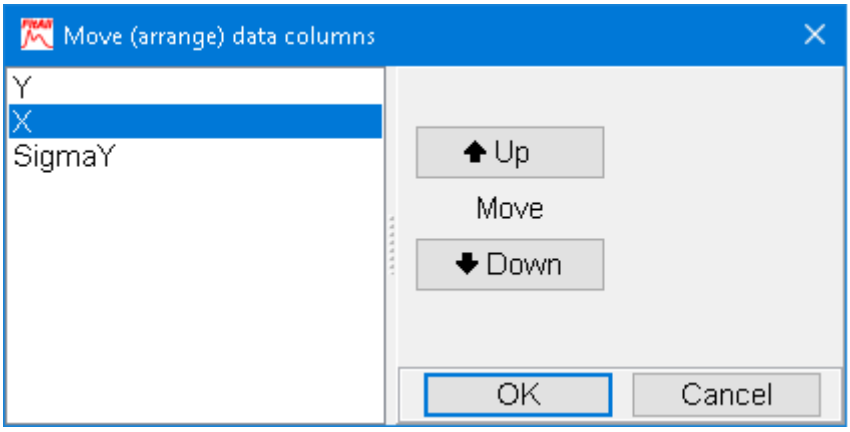


2. Click the menu selections Edit > column Move... (or right-click in the Data window and then click on the column Move... item in the context menu that appears).

   The "Move data columns" dialog will appear and looks like this:



3. Click the "Down" (or "Up") button to change the data column order. The result may look like this:



4. Click the **OK** button. The result may look like this:

Data

Pt#	Y	X	SigmaY
1	9.790E+0001	1.500E+0001	1.000E+0000
2	8.550E+0001	3.000E+0001	1.000E+0000
3	7.470E+0001	4.500E+0001	1.000E+0000
4	6.530E+0001	6.000E+0001	1.000E+0000
5	5.700E+0001	7.500E+0001	1.000E+0000
6	4.990E+0001	9.000E+0001	1.000E+0000
7	4.360E+0001	1.050E+0002	1.000E+0000
8	3.810E+0001	1.200E+0002	1.000E+0000
9	3.330E+0001	1.350E+0002	1.000E+0000
10	1.000E+0000	4.950E+0002	1.000E+0000

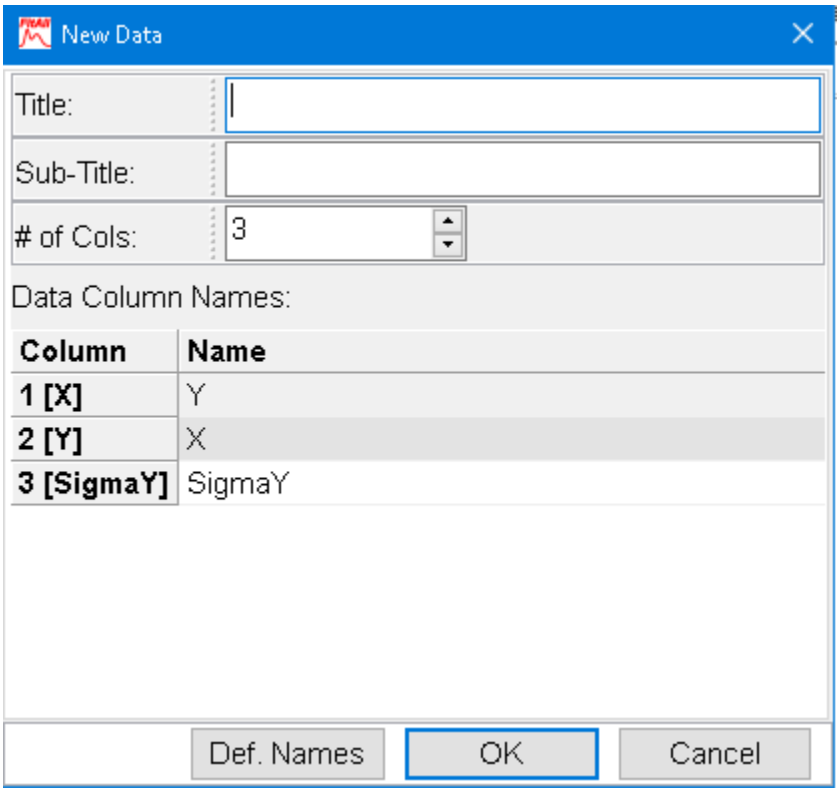
Copy Data From a SpreadSheet Program to FitAll

This "How To" illustrates how to copy data from a spreadsheet program, such as MS Excel, to ***FitAll***.

It is equally applicable to other spreadsheet programs and even text editors and word processors that can organize and copy columns of data to the MS Windows' clipboard.

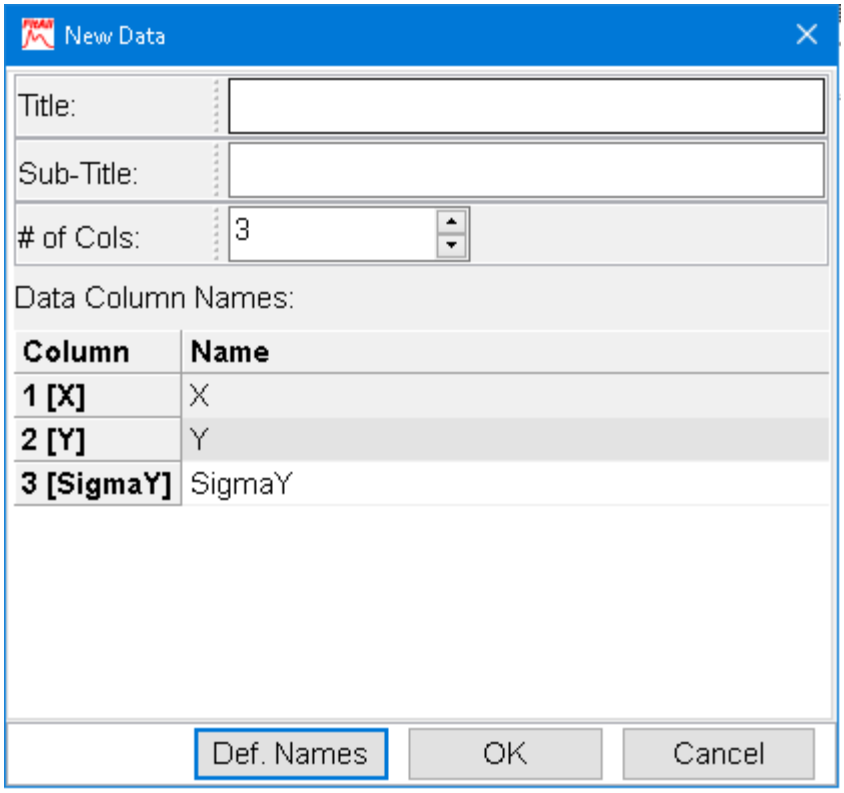
The first thing to do is to start ***FitAll*** and then create a new data set by clicking the menu selections File > New.

The "New Data" dialog will appear and looks like this:



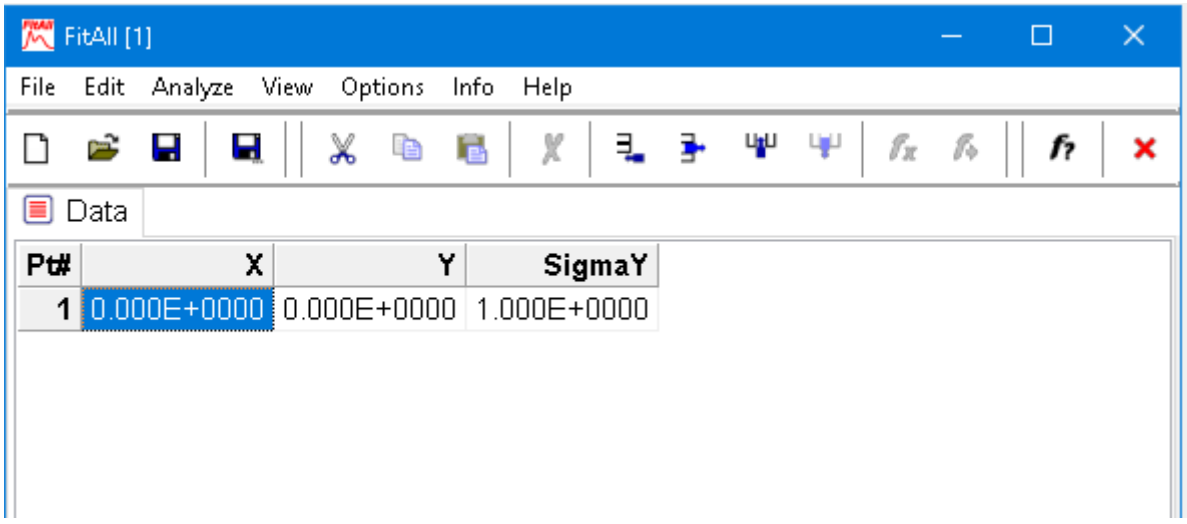
Click **Def. Names** button to assign the standard names to the data columns.

Note: Each ***FitAll*** data set must contain at least three columns of data.



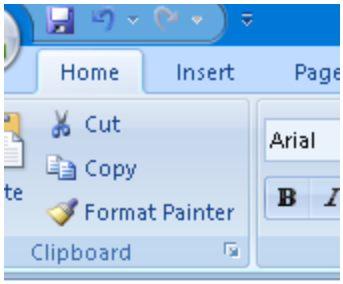
Click the **OK** button.

FitAll will display its Data window and automatically insert one data point into the data set.



Open Excel or another spreadsheet with a set of data and select (highlight) the columns of data that are to be copied to ***FitAll***.

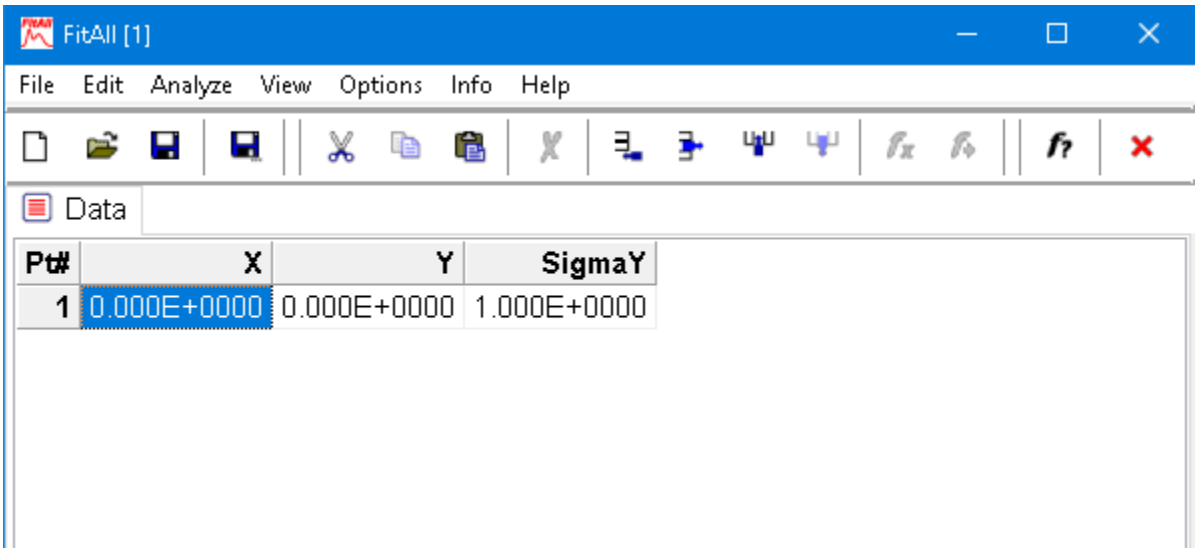
Note: If the column headings (column names) are included in selection they will be pasted into ***FitAll*** if all of the data is in ***FitAll***'s data window is to be replaced.



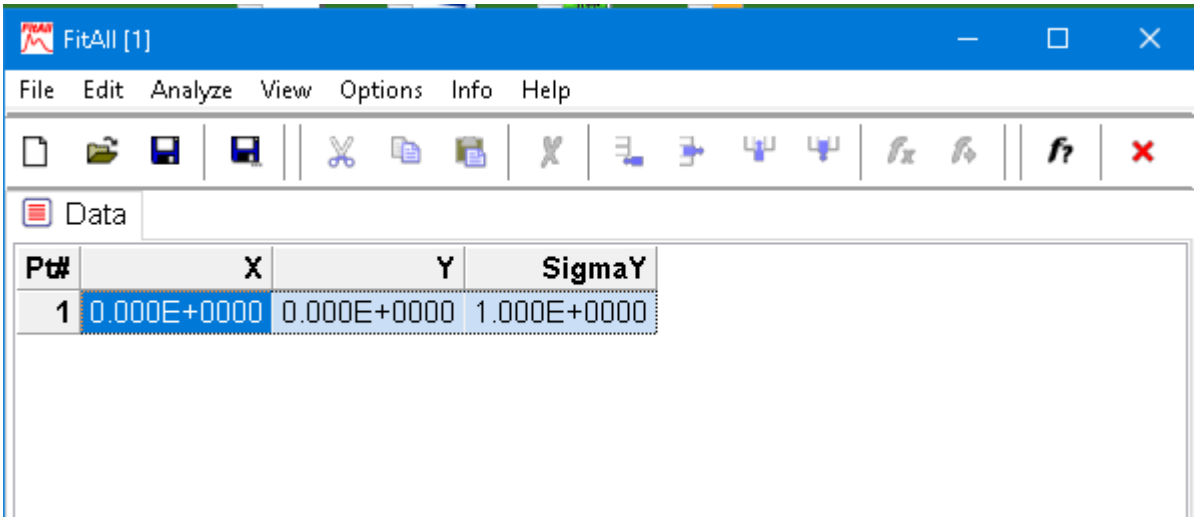
A	B
amps	volts
1.71E-02	5.33E-02
2.89E-02	8.96E-02
4.09E-02	1.26E-01
5.29E-02	1.61E-01
6.52E-02	1.97E-01
7.79E-02	2.31E-01
9.05E-02	2.65E-01
1.04E-01	2.97E-01
1.18E-01	3.29E-01
1.32E-01	3.59E-01
1.49E-01	3.86E-01
1.67E-01	4.09E-01
1.87E-01	4.29E-01
2.08E-01	4.45E-01
2.32E-01	4.57E-01
2.56E-01	4.68E-01
2.81E-01	4.76E-01
3.07E-01	4.83E-01
3.33E-01	4.89E-01
3.60E-01	4.94E-01
3.87E-01	4.99E-01
4.15E-01	5.03E-01
4.16E-01	5.03E-01
1.02E+00	5.48E-01
1.63E+00	5.68E-01
2.25E+00	5.81E-01
2.87E+00	5.92E-01
3.48E+00	6.01E-01
4.10E+00	6.08E-01
4.70E+00	6.15E-01

Press **Ctrl+C** (or the menu selections Edit > Copy) to copy the selected data to Windows' clipboard.

Return to ***FitAll***

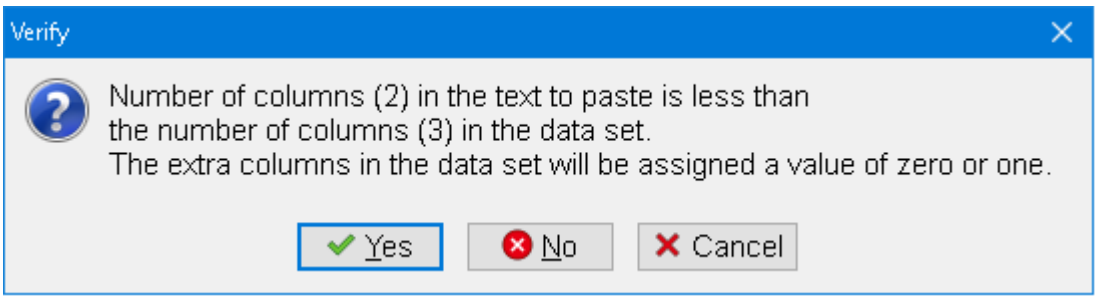


Press **Ctrl+A** (or click the menu selections Edit > Select All) to select all of the data in ***FitAll***'s data window.



Press **Ctrl+V** (or click the menu selections Edit > Paste) to paste the copied data into ***FitAll***.

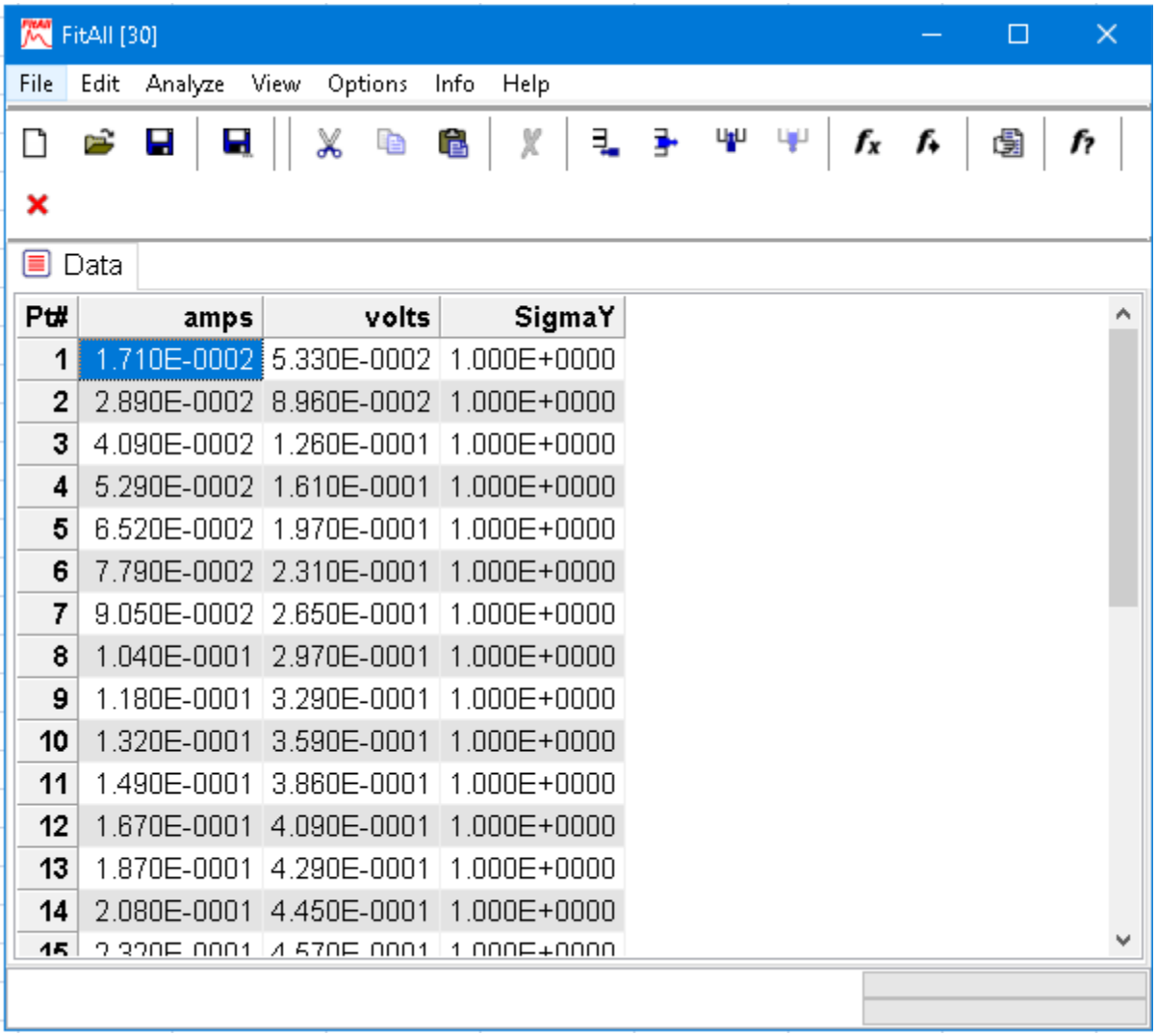
A warning message, like the one below, may appear.



Note: Whether a value of zero or one is assigned to the extra data columns is determine by the setting of the "Set New SigmaY's to 1.0 128" checkbox on the "Options > Preferences > Genera 126" page.

Click the **OK** button.

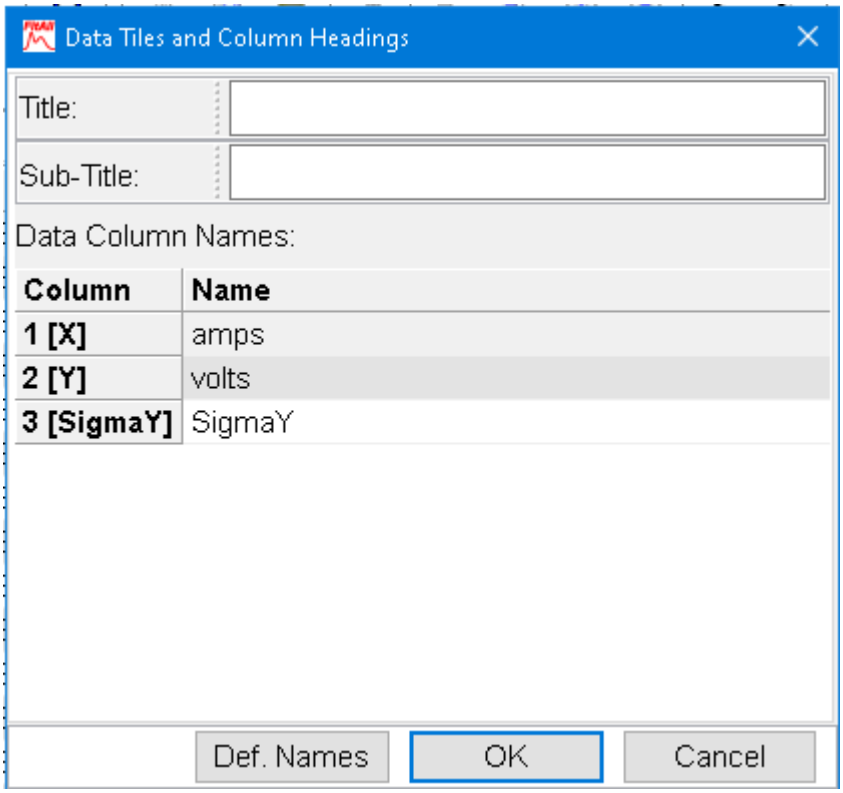
The result should look like this:



Pt#	amps	volts	SigmaY
1	1.710E-0002	5.330E-0002	1.000E+0000
2	2.890E-0002	8.960E-0002	1.000E+0000
3	4.090E-0002	1.260E-0001	1.000E+0000
4	5.290E-0002	1.610E-0001	1.000E+0000
5	6.520E-0002	1.970E-0001	1.000E+0000
6	7.790E-0002	2.310E-0001	1.000E+0000
7	9.050E-0002	2.650E-0001	1.000E+0000
8	1.040E-0001	2.970E-0001	1.000E+0000
9	1.180E-0001	3.290E-0001	1.000E+0000
10	1.320E-0001	3.590E-0001	1.000E+0000
11	1.490E-0001	3.860E-0001	1.000E+0000
12	1.670E-0001	4.090E-0001	1.000E+0000
13	1.870E-0001	4.290E-0001	1.000E+0000
14	2.080E-0001	4.450E-0001	1.000E+0000
15	2.320E-0001	4.570E-0001	1.000E+0000

Note: Since the data to be pasted consisted of only two columns and the column headings were included the first two column heading were changed and the third column's values were assigned a value of one.

To change the data set title and column headings click the menu selections Edit > data Titles.



Click the **Ok** button to accept the changes you have made.

Do a Preliminary Analysis

When you are dealing with data that may not be well described by the fitting function a large number of iterations may be required before ***FitAll*** converges to the final result. To begin, keep the maximum number of iterations small, for example 10, and the termination criterion large, for example 0.01.

> **NOTE:**
> The 'Maximum iterations' and 'Termination criterion' settings are on the Function tab of the 'Analyze Setup' dialog box which appears when you select Analyze > Setup 91 or click the  toolbar button.

Once you have tried the analysis, increase the maximum allowable iterations and/or decrease the value of the termination criterion to obtain more precise final parameter values.

do Batch Mode Analyses

Batch Mode Analysis is used to analyze many sets of experimental data to the same function. It is most useful when a series of experiments are done using a variety of conditions that are expected to yield data that can be described by the same function.

> **For example:**
> When investigating the rate of a chemical reaction, the effectiveness of a corrosion inhibitor or how acid rain might affect the performance of a solar cell, one might do a series of experiments that are identical in all respects, except that the acidity (pH) of the medium in which the experiment is done differs from experiment to experiment.
>
> Under such circumstances one would expect that the data from each experiment should be described by the same function (equation).
>
> If the above is the case, it would be useful to 'automatically' analyze each of the data sets and record the results of the analyses in another data file that can be viewed and further analyzed.
>
> This is what 'Batch Mode Analysis' (also known as Monte Carlo Analysis) does.

Create the Data Sets

To create data sets that can be used in batch mode analyses:

1. Do a set of experiments that are expected to be fitted to the same function.

2. Save each experiment's data in a file that is named: **<basefilename>ddddddd.dta,** in which all of the data files are named so that the names only differ in the number at the end of the name.

   The numbers can range from 1 to 2,000,000 and up to seven digits in length.

Analyzing Batch Mode Data Sets

To analyze a group of data sets do the following:

1. Confirm that your data sets have file names like "basenamedddddd.dta", in which the ddddd are numbers from 0000001 to 2000000 and that all of the files are in the same directory (folder).

   NOTES:

   1. The numbers in the file name do not have to be contiguous.

      When a number in the sequence is missing ***FitAll*** will skip the missing file and continue analyzing the data in the files that are present.

   2. The numbers in the filenames can be up to seven digits long. That is, the numbers may have fewer than seven digits.

2. Load the first file; for example the file named abcd00001.dta.

3. Fit the data using an appropriate function; for example, Function 0001 with 1 term in the background polynomial and use a weighting factor of $1/(0.1*Y)^2$.

4. Choose Analyze > Setup 91 menu selections.

In the 'Analysis Setup' dialog box that appears do the following:

5. On the Function 62 tab:

   - Choose function 0001 (with 1 term in the background polynomial).
   - Confirm that the analysis range is the same as you used to analyze the first data set.
   - Uncheck the '**Force automatic initial estimates**' checkbox, if you want ***FitAll*** to use the analysis results obtained from analyzing the first data set as the starting point for all subsequent analyses. This is what normally should done when doing Monte Carlo analyses.

     Check the '**Force automatic initial estimates**' checkbox, if you want ***FitAll*** to automatically make the initial parameter estimates for each data set that it processes. This is what normally should be done when doing 'batch mode 154' analyses.

   - Check the "**Monte Carlo (Analyze multiple data sets)** checkbox. NOTE that a new tab, the 'Monte Carlo' tab, appears.

6. On the Monte Carlo 100 tab:

   - Use the **'First file...**' button to locate the first data file that should be analyzed. For example, 'abcd00001.dta'.
   - Use the '**Last file...**' button to locate the last data file that should be analyzed. For example, 'abcd00025.dta'.
   - Use the 'Results:, **Data file...**' button to create a file in which the results of the analyses should be saved. For example: 'abcdResults.dta' in the same file directory (folder) as the data files that are to be analyzed.
   - Use the 'Results: **Title** and **Sub-Title**' edit boxes to enter a title and sub-title for the results data

set. For example: 'Results of abcd analyses with Ftn0001'.

7. Click the **OK** button

8. Select Analyze > Analyze MonteCarlo data sets 105, press **Alt+N** or click the f button.

   FitAll will do the analyses, store the results in the results data file 202 and load the results file into memory.

9. Select View > Standard stats 119 to see a summary of the results of the analyses.

Results Data File Structure

The results data file, created when doing a Monte Carlo (or Batch Mode) analysis, contains 2*NTerms+3 columns of data when the nlls or nlad analysis methods are used and 2*NTerms+2 columns of data when the lls analysis method is used. Nterms is the number of parameters in the analysis function.

For example, if the fitting function contains three parameters, the results data file will contain eight or nine columns.

The columns contained in the results data file are:

- **File Num**: The number from the file name of the data file that was analyzed to get the reported results.
- **Parameter 1**: The resolved value of the function's first parameter
- **EE_Parameter 1**: The estimated error in parameter 1. If the nlls or lls analysis methods were used, this corresponds to the estimated standard deviation of parameter 1. If the nllad analysis method was used, this corresponds to the estimated average deviation of parameter 1.
- ... etc. ...
- ... etc. ...
- **Parameter Last**
- **EE_Last Parameter**
- **SD_Fit**: The standard deviation of the fit.
- **Iterations**: The number of iterations required to do the fit.

  This column is not present when the fitting function is linear in its parameters; that is, when the lls method is used to analyze the data.

CAUTION:
When the number of iterations is the same as the Max. Iterations 96 setting it is likely that ***FitAll*** has stopped before the final best fit was obtained.

[This is more likely to occur when doing 'batch mode' analyses rather than Monte Carlo analyses].

If this occurs, the best thing to do is:

- Individually re-analyze the data set(s) in question using the 'normal' analysis type, and / or
- Re-analyze all of the data sets using a larger value for the Max. Iterations setting.

NOTE:
The beginning of the file may contain a Byte Order Marker, BOM, which specifies the type of encoding that is used.

do Monte Carlo Simulation and Analyses

Monte Carlo Simulation and Analysis is used to estimate the error and probability distribution of the resolved parameters.

To do this:

1. Open the data set that you are interested in and fit the data using an appropriate function.

2. Generate many simulated data sets with the same values of the independent variable(s), X, and the resolved parameter values and add random errors to the resulting dependent variable, Y.

> **NOTE:**
> ***FitAll***'s Monte Carlo simulation (data generation) feature uses the currently loaded data set as the source of the X values.

3. Analyze the generated data sets using the same function and analysis method that was used to analyze the original data set.

4. The variation and distribution of the resolved parameters can then be used to estimate the errors (and error distribution) associated with each of the resolved parameters.

> **NOTE:**
> ***FitAll***'s Monte Carlo analysis feature also can be used to analyze up to a million data sets to the same function in 'batch mode 154'.

Simulation

To generate the simulated data sets do:

1. Load the file named 'ABCDTST0.DTA' into memory. (This file contains 100 data points).

2. Fit the data using Function 0001 with 1 term in the background polynomial and a weighting factor of $1/(0.1*Y)^2$.

3. Choose the Edit > Generate Monte Carlo data sets 61 menu selection.

In the 'Generate Monte Carlo data sets' dialog box that appears do the following:

4. On the Function 62 tab:

   - Choose function 0001 (with 1 term in the background polynomial).
   - Enter a Title and Sub-Title that will be saved with each generated data set; for example, "abcdtest0 Monte Carlo Test".

5. On the Noise 65 tab:

   - Check the 'Add random errors (noise) to Y' check box.
   - Select the 'Add noise to Y as: "N * 0.10 * Y"' radio button.
   - Set the 'Std. Dev. of the Noise (NSD)' to 1.0.
   - Check the 'Average Noise Value' checkbox and set its value to 0, zero.

- Uncheck the 'Y Value Limit' checkbox.

6. On the Monte Carlo 67 tab:

   - Use the 'Browse' button to select the directory in which you want the generated data files to be saved.

   - Enter a 'Base file name'; for example, "abcd". ***FitAll*** will name the generated data files "Base file namedddddd.dta", in which ddddd is a five digit number; for example: abcd00001.dta, abcd00002.dta, ..., and abcd00025.dta.

   - Use the 'First and Last file number' spin-edit boxes to enter the first and last numbers that should be used. For example, if the first and last file numbers are 1 and 25, twenty-five data sets will be generated.

7. Click the **OK** button. The data sets will be generated and saved to disk.

Analyzing Monte Carlo Data Sets

To analyze a group of data sets do the following:

1. Confirm that your data sets have file names like "basenameddddd.dta", in which the ddddd are numbers from 0000001 to 2000000 and that all of the files are in the same directory (folder).

> **NOTES:**
>
> 1. The numbers in the file name do not have to be contiguous.
>
>   When a number in the sequence is missing ***FitAll*** will skip the missing file and continue analyzing the data in the files that are present.
>
> 2. The numbers in the filenames can be up to seven digits long. That is, the numbers may have fewer than seven digits.

2. Load the first file; for example the file named abcd00001.dta.

3. Fit the data using an appropriate function; for example, Function 0001 with 1 term in the background polynomial and use a weighting factor of $1/(0.1*Y)^2$.

4. Choose Analyze > Setup 91 menu selections.

In the 'Analysis Setup' dialog box that appears do the following:

5. On the Function 62 tab:

   - Choose function 0001 (with 1 term in the background polynomial).
   - Confirm that the analysis range is the same as you used to analyze the first data set.
   - Uncheck the '**Force automatic initial estimates**' checkbox, if you want ***FitAll*** to use the analysis results obtained from analyzing the first data set as the starting point for all subsequent analyses. This is what normally should done when doing Monte Carlo analyses.

     Check the '**Force automatic initial estimates**' checkbox, if you want ***FitAll*** to automatically make the initial parameter estimates for each data set that it processes. This is what normally should be done when doing 'batch mode 154' analyses.

   - Check the "**Monte Carlo (Analyze multiple data sets)** checkbox. NOTE that a new tab, the 'Monte Carlo' tab, appears.

6. On the Monte Carlo 100 tab:

   - Use the **'First file...**' button to locate the first data file that should be analyzed. For example, 'abcd00001.dta'.
   - Use the '**Last file...**' button to locate the last data file that should be analyzed. For example, 'abcd00025.dta'.
   - Use the 'Results:, **Data file...**' button to create a file in which the results of the analyses should be saved. For example: 'abcdResults.dta' in the same file directory (folder) as the data files that are to be analyzed.
   - Use the 'Results: **Title** and **Sub-Title**' edit boxes to enter a title and sub-title for the results data

set. For example: 'Results of abcd analyses with Ftn0001'.

7. Click the **OK** button

8. Select Analyze > Analyze MonteCarlo data sets 105, press **Alt+N** or click the  button.

   FitAll will do the analyses, store the results in the results data file 202 and load the results file into memory.

9. Select View > Standard stats 119 to see a summary of the results of the analyses.

Results Data File Structure

The results data file, created when doing a Monte Carlo (or Batch Mode) analysis, contains 2*NTerms+3 columns of data when the nlls or nlad analysis methods are used and 2*NTerms+2 columns of data when the lls analysis method is used. Nterms is the number of parameters in the analysis function.

For example, if the fitting function contains three parameters, the results data file will contain eight or nine columns.

The columns contained in the results data file are:

- **File Num**: The number from the file name of the data file that was analyzed to get the reported results.
- **Parameter 1**: The resolved value of the function's first parameter
- **EE_Parameter 1**: The estimated error in parameter 1. If the nlls or lls analysis methods were used, this corresponds to the estimated standard deviation of parameter 1. If the nllad analysis method was used, this corresponds to the estimated average deviation of parameter 1.
- ... etc. ...
- ... etc. ...
- **Parameter Last**
- **EE_Last Parameter**
- **SD_Fit**: The standard deviation of the fit.
- **Iterations**: The number of iterations required to do the fit.

  This column is not present when the fitting function is linear in its parameters; that is, when the lls method is used to analyze the data.

> **CAUTION:**
> When the number of iterations is the same as the Max. Iterations 96 setting it is likely that ***FitAll*** has stopped before the final best fit was obtained.
>
> [This is more likely to occur when doing 'batch mode' analyses rather than Monte Carlo analyses].
>
> If this occurs, the best thing to do is:
>
> - Individually re-analyze the data set(s) in question using the 'normal' analysis type, and / or
> - Re-analyze all of the data sets using a larger value for the Max. Iterations setting.

> **NOTE:**
> The beginning of the file may contain a Byte Order Marker, BOM, which specifies the type of encoding that is used.

Histogram for One Parameter

When inspecting the results of a Monte Carlo analysis, it may be desirable to see a histogram of the deviation of a parameter's values from its average.

To do this:

1. Retrieve (File > Open 11) the results data file.

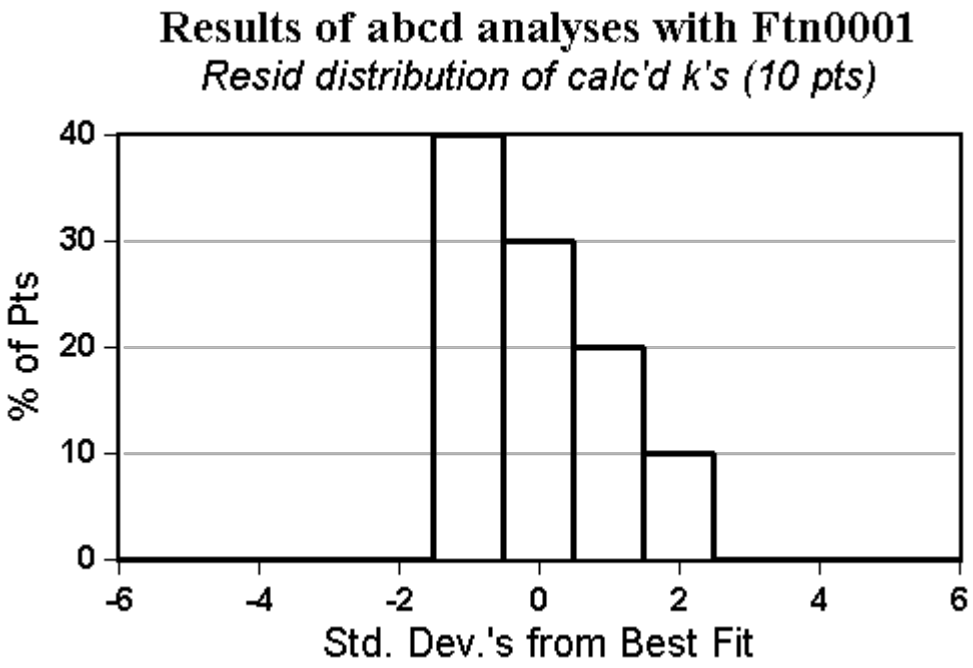
2. Use the Edit > column Move 54 menu selection to move the column containing the parameter of interest to the second last column position. (In ***FitAll*** data sets, this column corresponds to the Y-values).

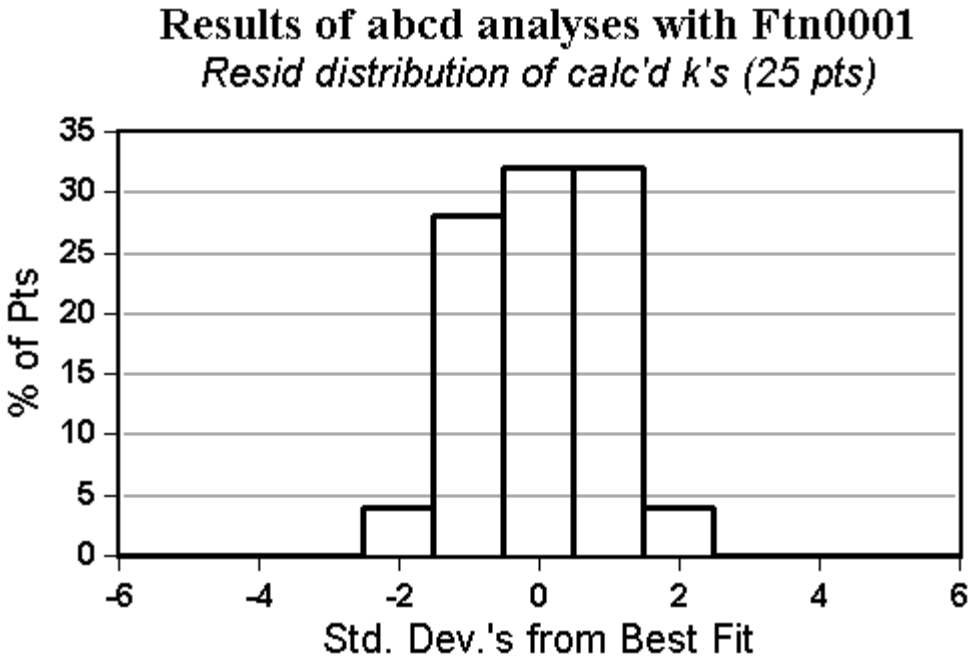
3. Fit the data using the Polynomial_1 function.

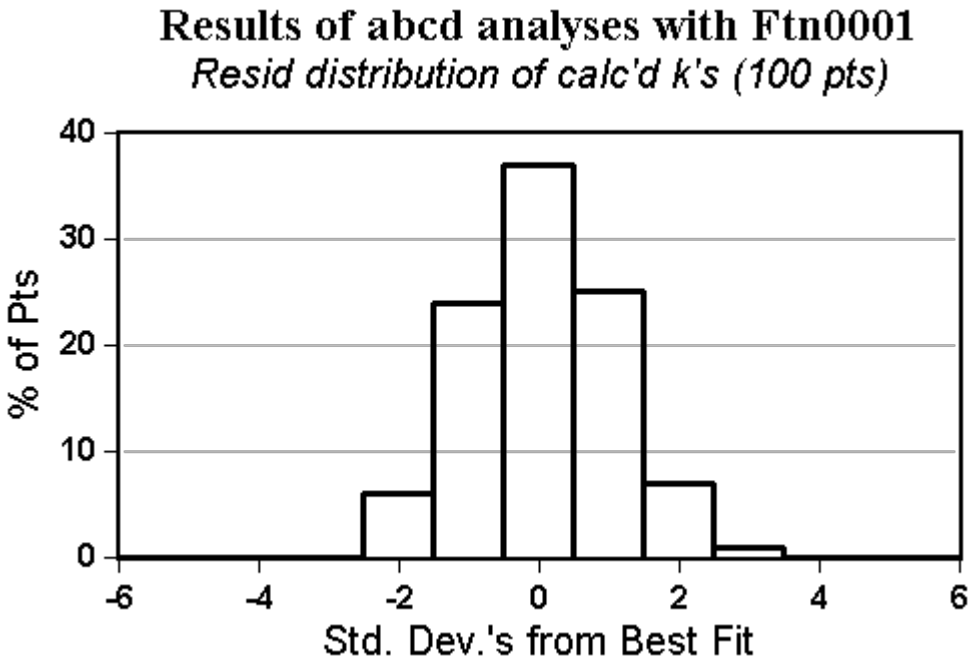
   Set both the 'Smallest exponent in polynomial' and the 'Largest exponent in polynomial' to zero. By doing this, the data will be fit to the equation: Y = A; that is, the 'best fit' value is the average value. Also, use a weighting factor of 1.

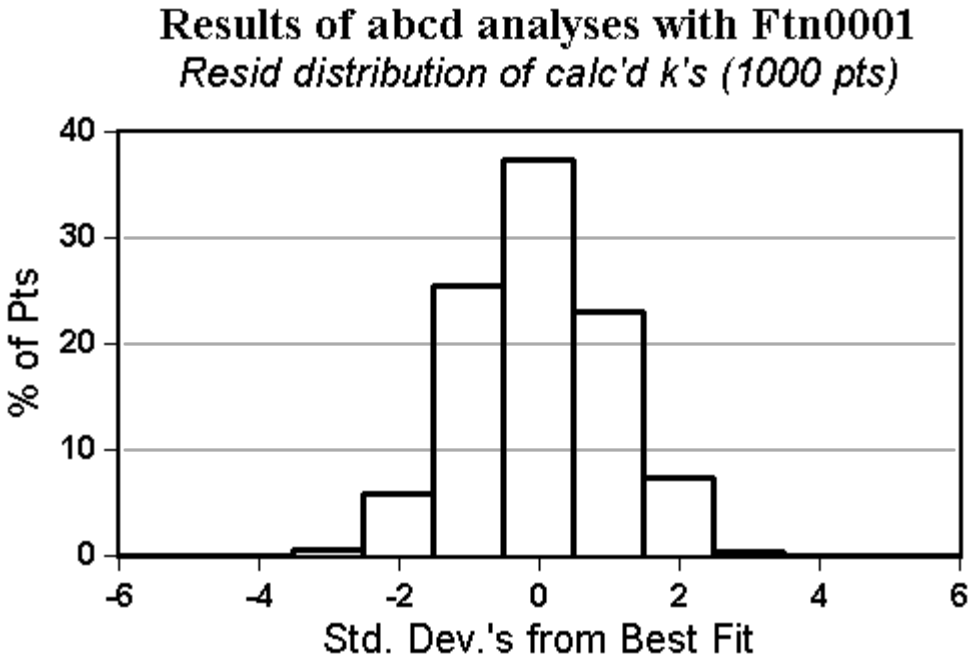
4. Use the View > residuals distribution graph 111 menu selections to plot the histogram.

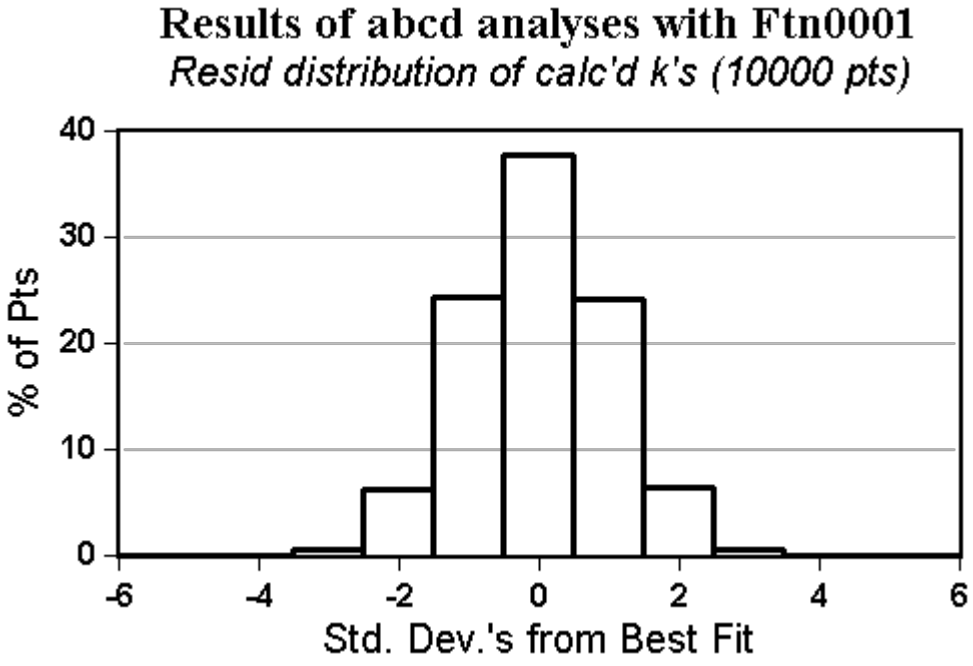
Here are some examples of what the graph may look like:




Results of abcd analyses with Ftn0001
Resid distribution of calc'd k's (25 pts)
% of Pts
35
30
25
20
15
10
5
0
-6
-4
-2
0
2
4
6
Std. Dev.'s from Best Fit


Results of abcd analyses with Ftn0001
Resid distribution of calc'd k's (100 pts)
% of Pts
40
30
20
10
0
-6
-4
-2
0
2
4
6
Std. Dev.'s from Best Fit





NOTE:
The greater the number of data sets analyzed the more likely that the residuals distribution histogram will look like a "normal" or "Gaussian" curve.

do Multi-Fit Analyses

Multi-Fit analyses are used to fit one set of data to many different forms (variations) of a single function.

The goal is to identify the variation (form) of the function that provides the best fit.

> **NOTE:**
> In ***FitAll*** version 8 and later the functions 0024 (Multiple Linear_2), 0208 and 0209 (DNA-Drug Binding) are Multi-Fit enabled.

To do Multi-Fit analyses:

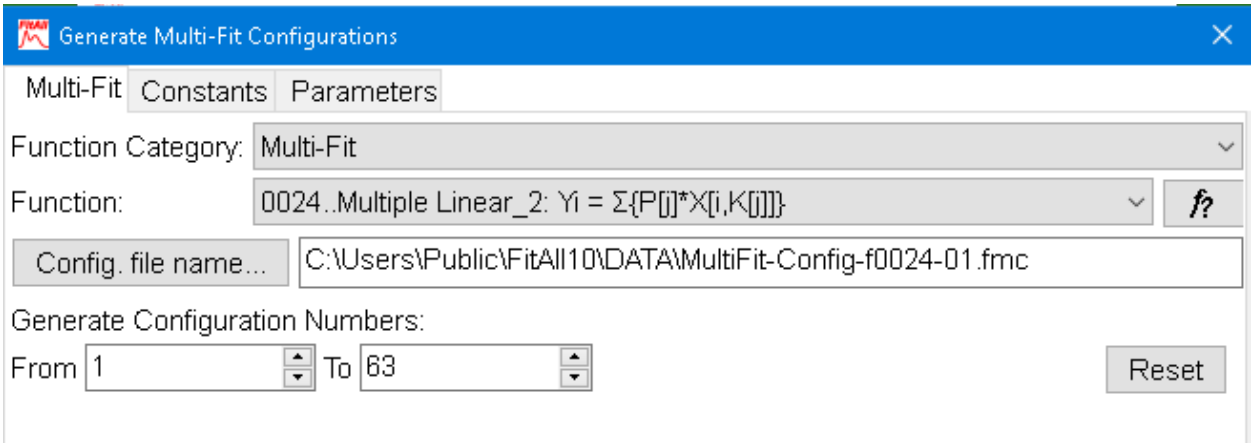
1. Load (File > Open) the data file that you want to analyze using Multi-Fit analysis.
2. Generate a file containing the configurations (variations) of the function that are to be analyzed (Edit > Generate Multi-Fit Configs... 69).

> **NOTE:**
> The types of configurations that can be generated depend on the function being used.
>
> Read the documentation for the function that you are using to get an understanding of what kinds of configurations (variations) can be generated.

3. Setup the Multi-Fit analysis (Analyze > Setup, Multi-Fit 102).
   When setting up the analysis, it is necessary to identify both the file that contains the configurations and the file into which the results should be saved.
4. Do the analyses (Analyze > Analyze 105).
5. Review the Multi-Fit results.

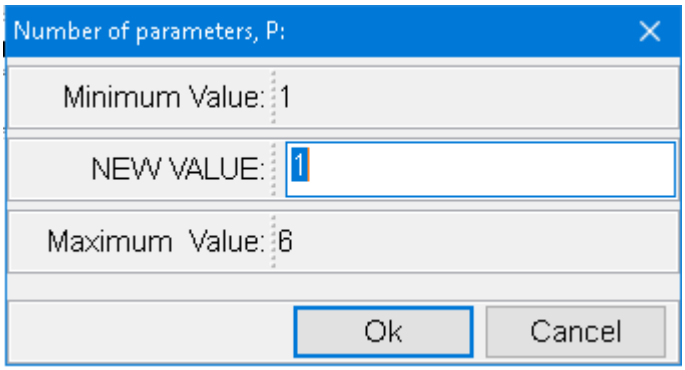
Generate Multi-Fit Configuration File

1. Retrieve the file named F0024TST01.DTA.
2. Choose Analyze > Setup and select function 0024.
3.
4. Choose Edit > Generate Multi-Fit Configs... 69
5. Edit the Generate Multi-Fit Configurations dialog box so that it looks like this:



4. On the Function tab:

   - Choose function 0024..Multiple Linear_2 from the Function drop-down list.
   - When the 'Number of parameters' dialog box that appears after the function is selected, click the **OK** button.



   - Click the Config. file name... button to create (or locate) a file that will contain the configuration information. For example, the file could be named 'C:\Users\Public\FitAll10\DATA\MultiFit-Config-f0024-01.fmc.

> **NOTE:**
> You can name the file whatever you like as long at the file name extension is '.fmc', which is an acronym for ***FitAll*** Multi-fit Configuration file.

5. In the 'Generate Configuration Numbers' **From** and **To** spin-edit boxes enter one, **1**, and a number that is large enough to include all of the possible configurations, for example, **1000**.

> **NOTE:**
> The data file F0024TST01.DTA has six (6) columns of independent variables as well as the Y and SigmaY columns.
>
> Function 0024's Generate Multi-Fit Configurations procedure creates all of the possible configurations for one to six parameters.
>
> Although the contents of the '.fmc' file can be viewed with a text editor such as Notepad++, it is most unlikely that you will find this to be a useful endeavour.

6. Click the **OK** button to generate the configurations.

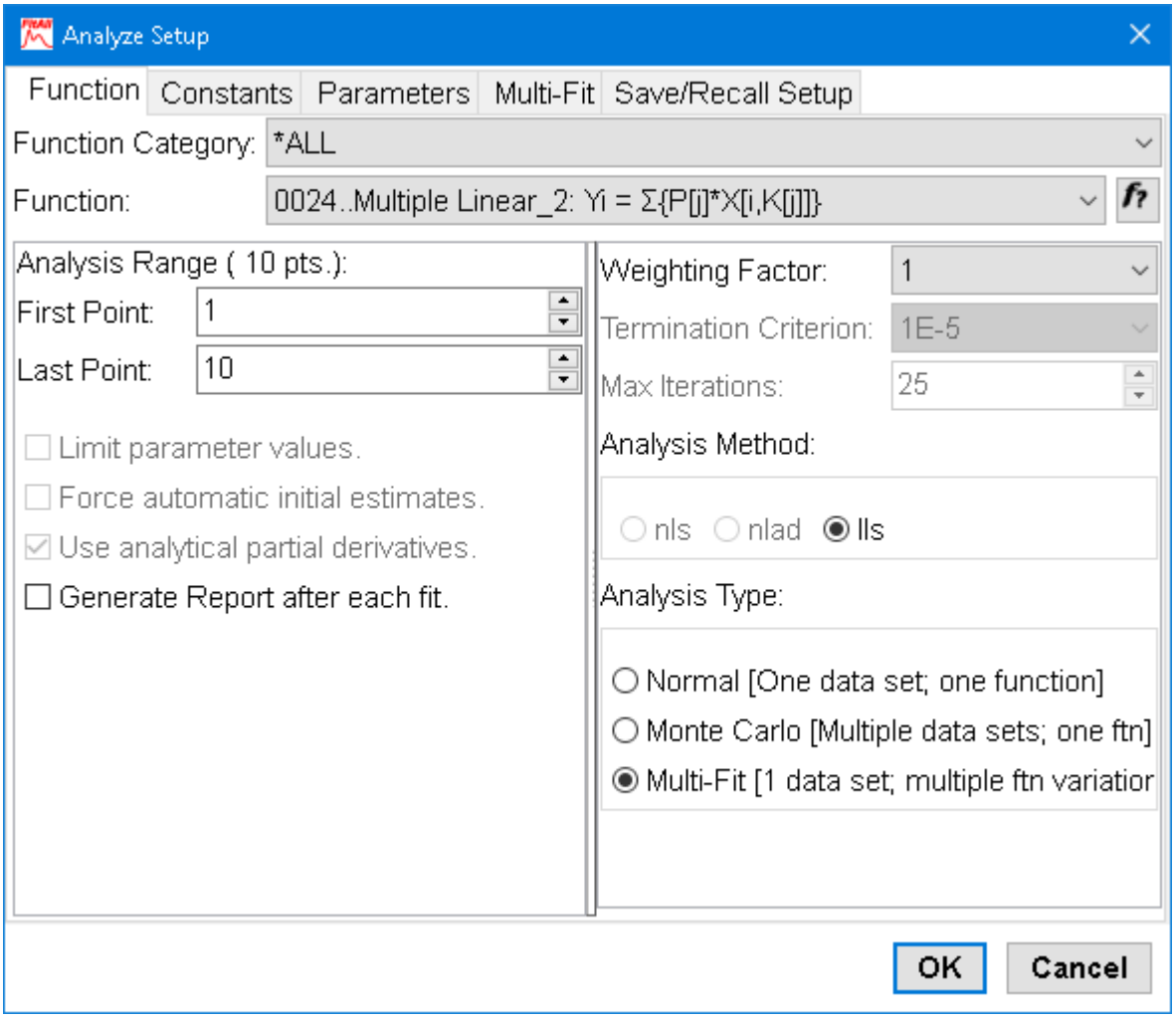
Analyze Multi-Fit Configurations

To do the Multi-Fit analysis of the configuration were generated in the previous section:

1. Retrieve the file named F0024TST01.DTA.

2. Choose Analyze > Setup....

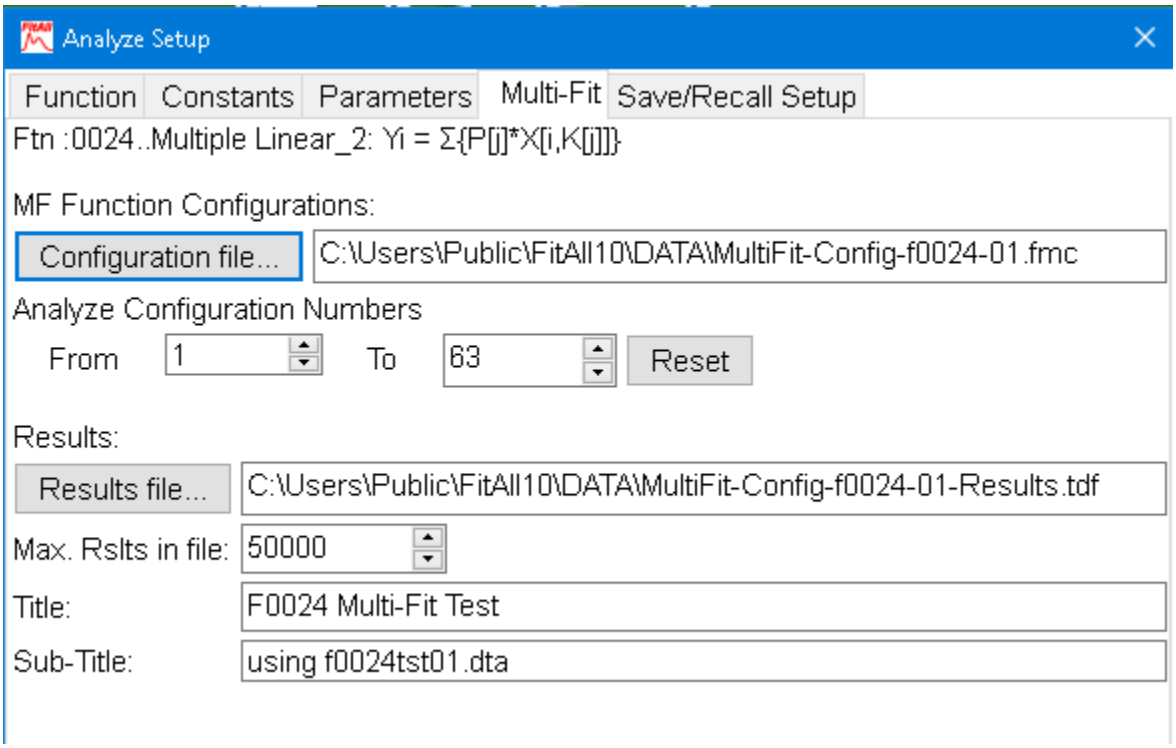
   The Analyze Setup dialog the appears, it looks like this:



3. On the **Function** tab:

   - Choose function 0024.
   - Set the analysis range to include all of the data points.
   - Set the Analysis Type to Multi-Fit.

4. On the **Multi-Fit** tab:



   - Click the Configuration file... button and select the previously created file that contains the Multi-Fit configurations.
   - In the Analyze Configuration Numbers **From** and **To** spin-edit boxes enter one, **1**, and a number large enough to include all of the configurations. FitAll normally enters the appropriate values.
   - Click the Results file... button select or create / open the file into which the results should be saved; for example, C:\Users\Public\FitAll10\DATA\MultiFit-Config-f0024-01-Results.tdf.

     NOTE:
     Because the results file has a file name extension of **.tdf**, the results file will be saved as a tab-delimited file.

   - Enter a **Title** and **Sub-Title** for the results data file.

5. Click the **OK** button.

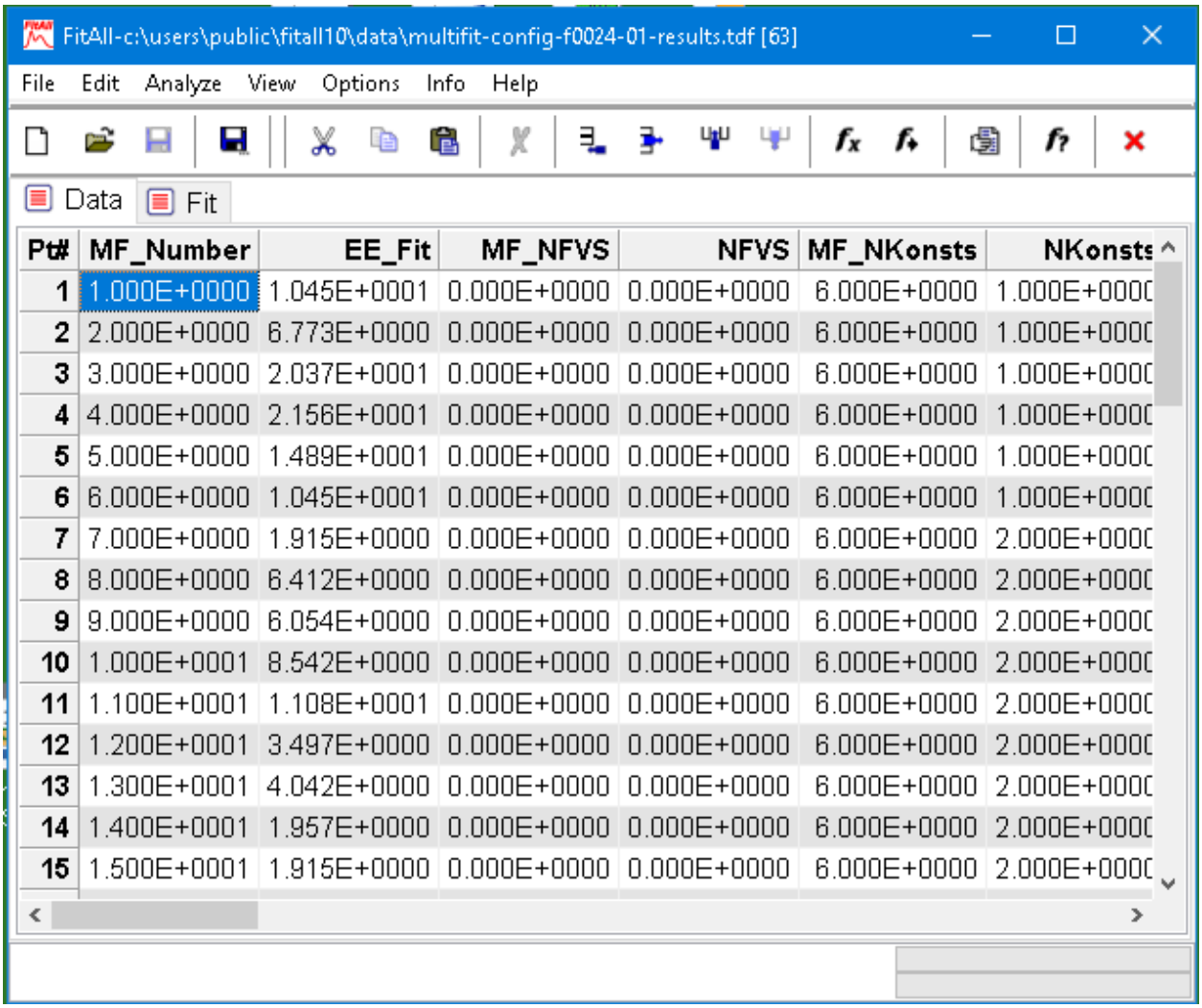
6. Choose Analyze > Analyze Multi-Fit or click the f_x button to do the Multi-Fit analyses. The results will be saved in the results file and be opened by ***FitAll***.

Review Multi-Fit Results

The Multi-Fit results file should have been automatically opened in ***FitAll***. If it wasn't or you are reviewing the results at a later open the results file using the menu selections File > Open.

In this 'How To', the results file only contains 63 results so it can be opened in ***FitAll***. Here's what to do:

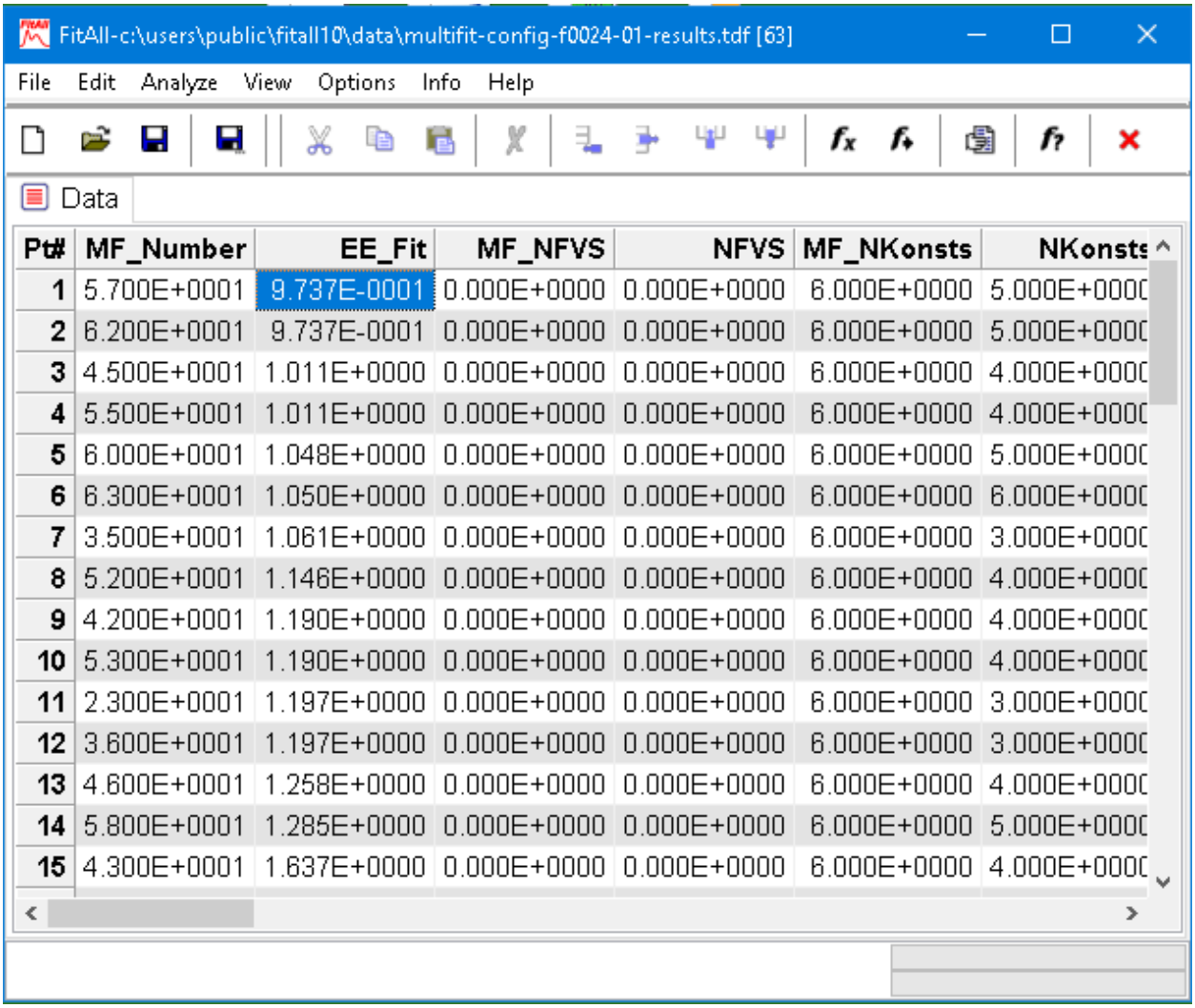
1. The data window should look like this:



Pt#	MF_Number	EE_Fit	MF_NFVS	NFVS	MF_NKonsts	NKonsts
1	1.000E+0000	1.045E+0001	0.000E+0000	0.000E+0000	6.000E+0000	1.000E+000
2	2.000E+0000	6.773E+0000	0.000E+0000	0.000E+0000	6.000E+0000	1.000E+000
3	3.000E+0000	2.037E+0001	0.000E+0000	0.000E+0000	6.000E+0000	1.000E+000
4	4.000E+0000	2.156E+0001	0.000E+0000	0.000E+0000	6.000E+0000	1.000E+000
5	5.000E+0000	1.489E+0001	0.000E+0000	0.000E+0000	6.000E+0000	1.000E+000
6	6.000E+0000	1.045E+0001	0.000E+0000	0.000E+0000	6.000E+0000	1.000E+000
7	7.000E+0000	1.915E+0000	0.000E+0000	0.000E+0000	6.000E+0000	2.000E+000
8	8.000E+0000	6.412E+0000	0.000E+0000	0.000E+0000	6.000E+0000	2.000E+000
9	9.000E+0000	6.054E+0000	0.000E+0000	0.000E+0000	6.000E+0000	2.000E+000
10	1.000E+0001	8.542E+0000	0.000E+0000	0.000E+0000	6.000E+0000	2.000E+000
11	1.100E+0001	1.108E+0001	0.000E+0000	0.000E+0000	6.000E+0000	2.000E+000
12	1.200E+0001	3.497E+0000	0.000E+0000	0.000E+0000	6.000E+0000	2.000E+000
13	1.300E+0001	4.042E+0000	0.000E+0000	0.000E+0000	6.000E+0000	2.000E+000
14	1.400E+0001	1.957E+0000	0.000E+0000	0.000E+0000	6.000E+0000	2.000E+000
15	1.500E+0001	1.915E+0000	0.000E+0000	0.000E+0000	6.000E+0000	2.000E+000

2. The first column of the results data file 204 contains the Multi-Fit configuration number and the second column contains the estimated error of the fit; that is, the standard deviation of the fit.

3. To identify the configuration that gave the best fit, find the row with the smallest value in the EE_Fit column. The easiest way to do this is to sort the data on the second column. The result of sorting the results on the EE_Fit column is:

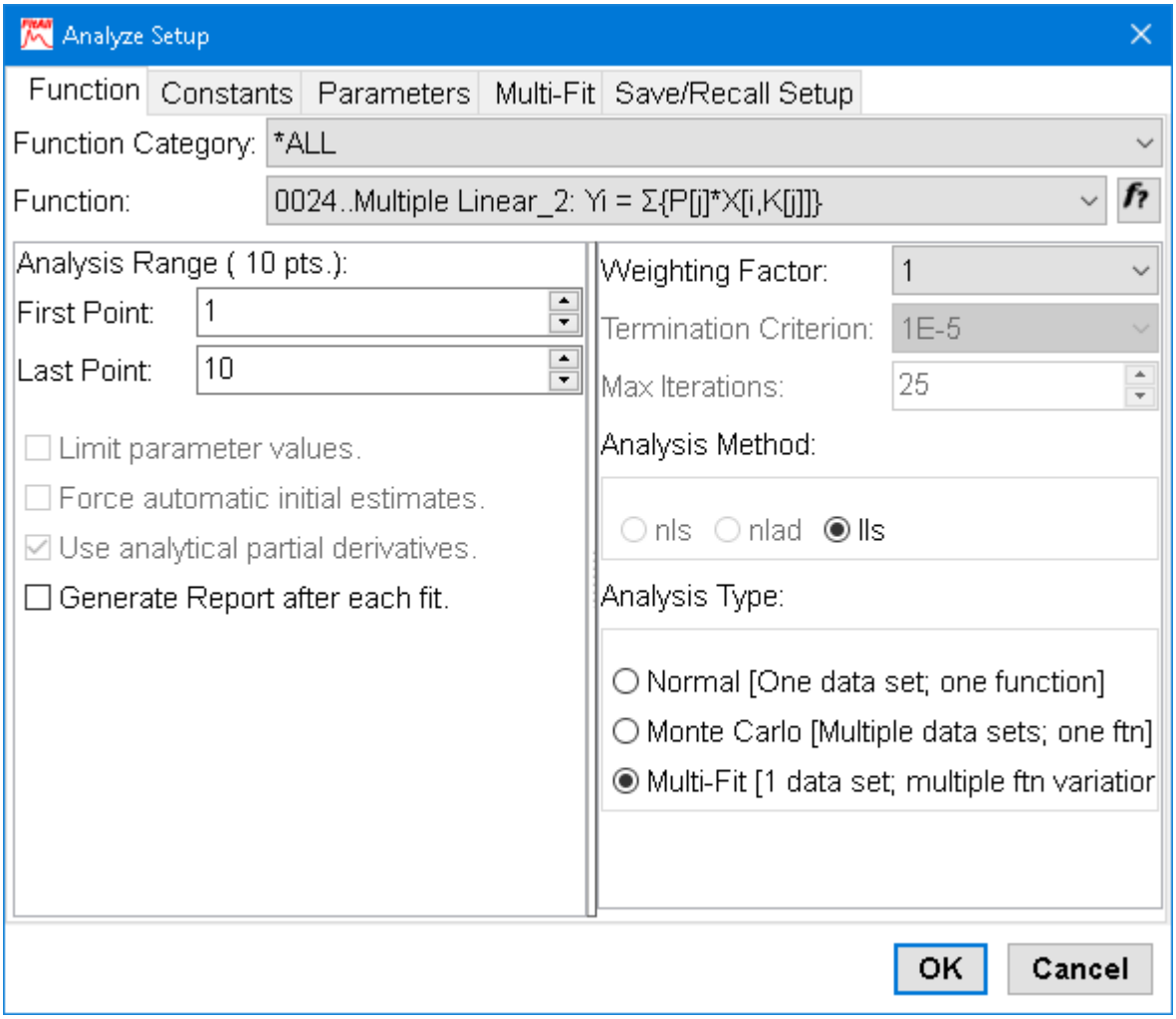


Pt#	MF_Number	EE_Fit	MF_NFVS	NFVS	MF_NKonsts	NKonsts
1	5.700E+0001	9.737E-0001	0.000E+0000	0.000E+0000	6.000E+0000	5.000E+0000
2	6.200E+0001	9.737E-0001	0.000E+0000	0.000E+0000	6.000E+0000	5.000E+0000
3	4.500E+0001	1.011E+0000	0.000E+0000	0.000E+0000	6.000E+0000	4.000E+0000
4	5.500E+0001	1.011E+0000	0.000E+0000	0.000E+0000	6.000E+0000	4.000E+0000
5	6.000E+0001	1.048E+0000	0.000E+0000	0.000E+0000	6.000E+0000	5.000E+0000
6	6.300E+0001	1.050E+0000	0.000E+0000	0.000E+0000	6.000E+0000	6.000E+0000
7	3.500E+0001	1.061E+0000	0.000E+0000	0.000E+0000	6.000E+0000	3.000E+0000
8	5.200E+0001	1.146E+0000	0.000E+0000	0.000E+0000	6.000E+0000	4.000E+0000
9	4.200E+0001	1.190E+0000	0.000E+0000	0.000E+0000	6.000E+0000	4.000E+0000
10	5.300E+0001	1.190E+0000	0.000E+0000	0.000E+0000	6.000E+0000	4.000E+0000
11	2.300E+0001	1.197E+0000	0.000E+0000	0.000E+0000	6.000E+0000	3.000E+0000
12	3.600E+0001	1.197E+0000	0.000E+0000	0.000E+0000	6.000E+0000	3.000E+0000
13	4.600E+0001	1.258E+0000	0.000E+0000	0.000E+0000	6.000E+0000	4.000E+0000
14	5.800E+0001	1.285E+0000	0.000E+0000	0.000E+0000	6.000E+0000	5.000E+0000
15	4.300E+0001	1.637E+0000	0.000E+0000	0.000E+0000	6.000E+0000	4.000E+0000

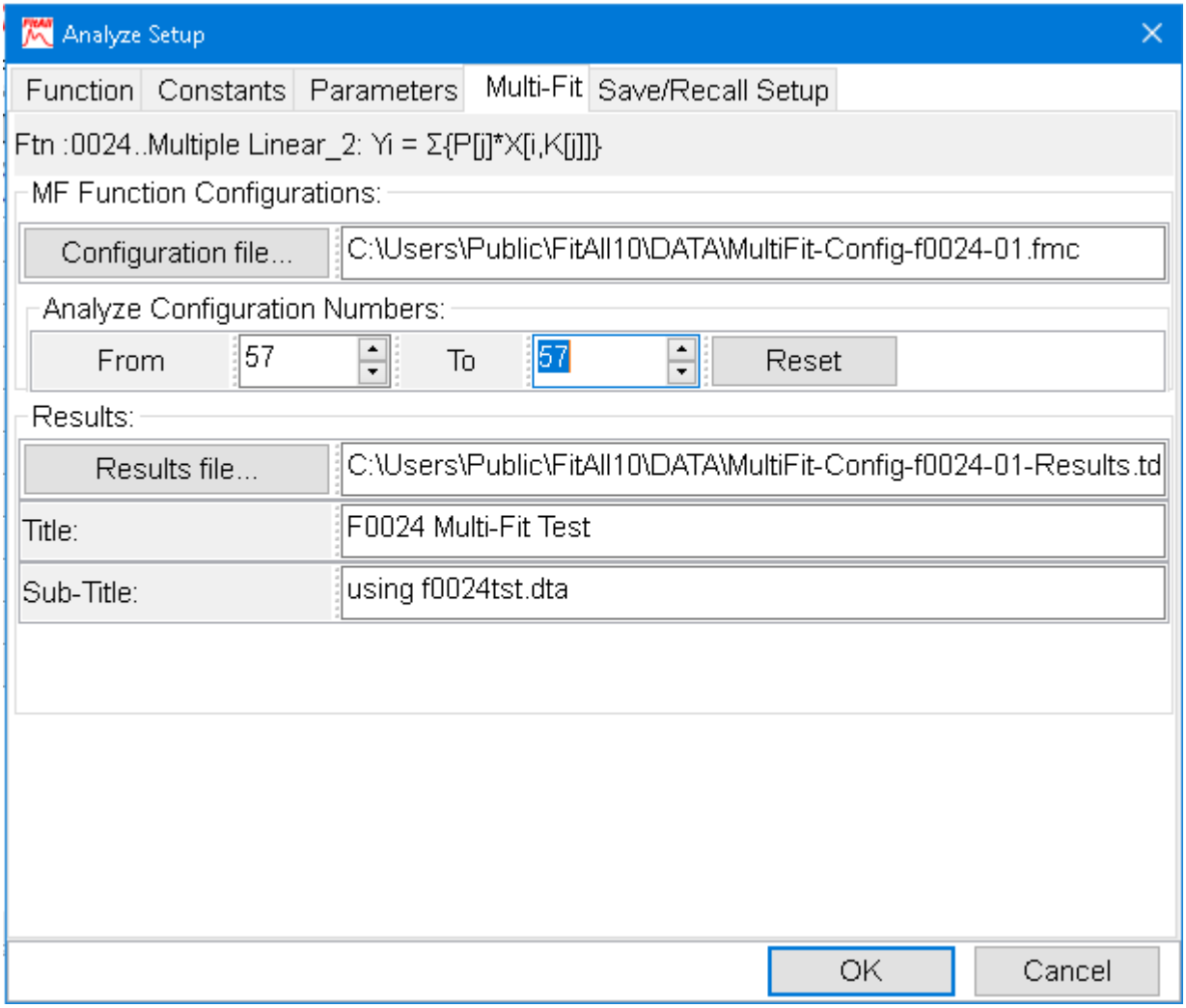
Inspection of the sorted results shows that configurations, MF_Number, 57 and 62 gave the best fit.

4. To view the results of the fit for configuration number 57 in detail, do the following:

   - Retrieve (File > Open) the data file (F0024TST01.DTA) that was analyzed.
   - Choose Analyze > Setup... and select function 0024, if it is not already selected. The Function tab of the Analyze Setup dialog box should look like this:



- On the Multi-Fit tab set the 'Configuration file' and set both the **From** and **To** Analyze Configuration Numbers to **57**, because this configuration number corresponds to the best fit. The Multi-Fit tab should look like this:



NOTE:
When the **From** and **To** Analyze Configuration Numbers fields are equal, ***FitAll*** will retrieve the configuration information and analyze the data, but it will not save the results to the results file and will not load the results file.

- Click the **OK** button.
- Choose Analyze > Analyze Multi-Fit or click the $f_{\rightarrow}$ speed-button to do the analysis.

5. The resulting 'Fit Window' should look like this:

Data | Fit

File:	c:\users\public\fitall10\data\f0024tst01.dta
Title:	F0024: Multi-Fit
Sub-Title:	
Function:	0024..Multiple Linear_2: Yi = Σ{P[j]*X[i,K[j]]}
Analysis Method:	Linear Least Squares (lls)
Analysis Range:	1 to 10 of 10
Weighted as:	1
Variance:	0.948066223214934
Std. Dev. of Fit:	0.973686922585969

Parameter	Name	Value	Std. Dev.	RSD /%
1	P1	1.669E+0000	9.167E-0001	54.93
2	P2	9.979E-0002	8.840E-0003	8.86
3	P3	-1.443E+0000	1.191E+0000	82.53
4	P4	-1.535E-0003	4.440E-0004	28.92
5	P5	3.822E+0000	1.919E+0000	50.21
Constant				
1	K1	1.000E+0000		

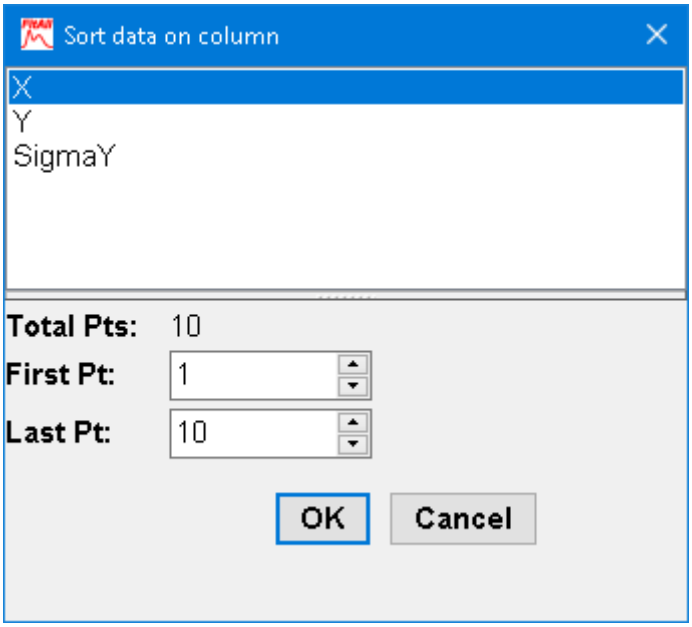
Sort Data

When ***FitAll*** does automatic initial estimates of the parameter values it normally expects the data to be sorted on the first, X, data column.

To sort your data:

- Make the 'Data' window the active window by clicking anywhere in it or by choosing the View > Data 113 menu selections.
- Choose Edit > Sort 48 data from the main menu or right click in the data window and choose data Sort from the context menu.

The 'Sort data on column' dialog box will appear. It looks like this:



- Click the name of the column on which you want to sort the data.
- Click the **OK** button.

Spot Data Entry Errors

After entering all or part of a data set, plot it using the View > data graph 108 menu selections.

Often it will be easy to see if a value was entered incorrectly.

If a data entry error was made, make the 'Data' window the active window and edit the appropriate value.

Verify the Appropriateness of Initial Estimates

After you have selected the function (see, Analyze > Setup 91) and estimated the initial parameter values (see: Analyze > Setup - Parameters tab 99) plot the fit (see View > fit graph 109) to see if the initial estimates generate a calculated curve that is reasonably close to the data.

If the calculated curve does not come close to the data points:

- Choose the Analyze > Setup 91 menu item.
- Click on the Parameters 99 tab.
- Edit the parameter values.
- Click the **OK** button.

Once the calculated curve is approximately the same as the data, the actual analysis can be done (see: Analyze > Analyze 105).

> **NOTE:**
> The 'Force automatic initial estimates 94' check box in the 'Analyze Setup' dialog on the Function tab sheet should not be checked when you do the analysis. If it is, your manually adjusted initial estimates will be recalculated before the regression analysis is done.

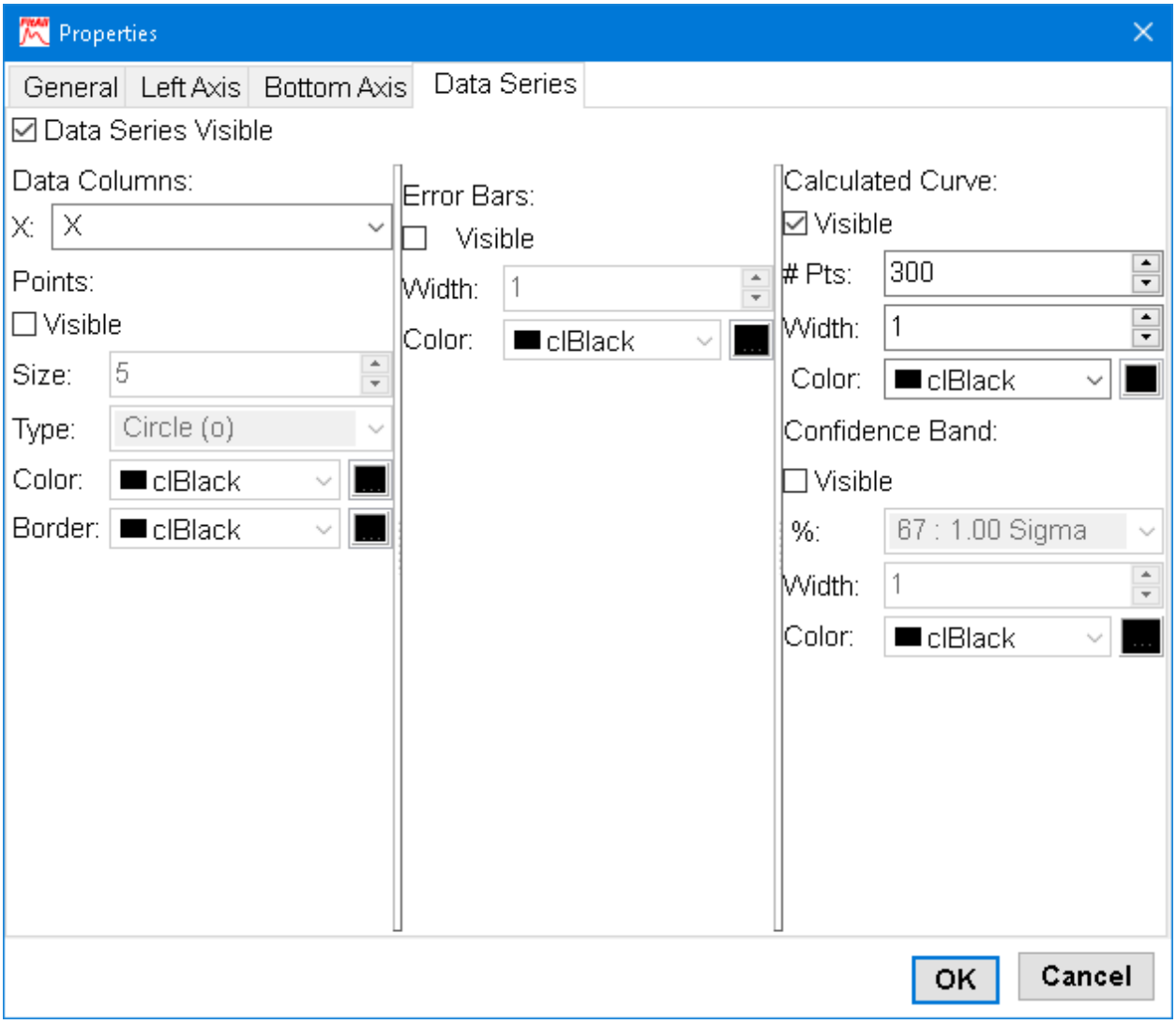
Make Calibration Curves

A calibration curve is a graph of the 'fit' that does not display the data points.

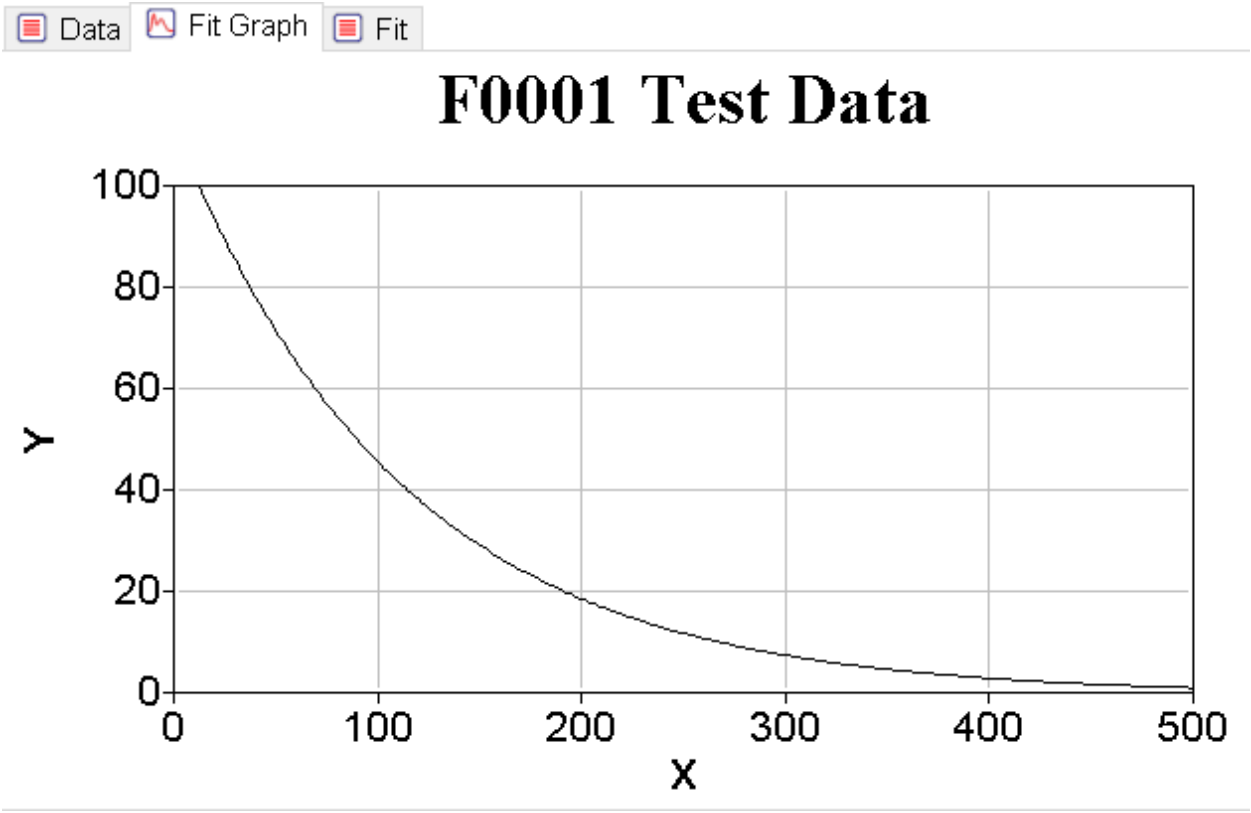
Here's how to do it:

- Retrieve a set of data and analyze it using an appropriate function or use the Edit > Generate data 55 menu choice to create a set of data with the function that you want to use to create the calibration curve.
- Select View > fit graph 109.
- Select Edit > Properties 81 (or right click in the fit graph window and click the Properties item on context menu).
- Click on the "data series 86" tab in the Properties dialog box.
- Uncheck the "Points Visible", "Error Bars Visible" and "Confidence Band Visible" checkboxes.

The "data series" tab sheet should look like this:



- Click the **OK** button. The resulting calibration graph might look like this:



NOTES:

1. You can adjust many of the graph's other properties to customize its appearance. (See: Edit > Properties, Graph Window 81).

2. You also can evaluate the function at a single point using the Analyze > One point 106 menu selection.

Make Graphs with Total and Sub-Component Curves

Some of the functions available in ***FitAll*** are the sum of several 'sub-functions' or components.

For example, function number 0302 is the sum of one to five Gaussian curves.

When such a function is analyzed (de-convoluted), the resulting parameters describe each of the component Gaussian curves that make up the total.

Sometimes, for example in spectroscopy, it may be desirable to plot a graph that shows the total curve as well as the component curves.

Although ***FitAll*** can only plot one calculated curve and one set of data at a time, it is possible to construct a graph that shows the calculated curve as well as the component curves that make it up.

General Procedure 181

An Example 182

General Procedure

Here's how to construct a graph that shows the calculated curve along with the sub-component curves.

1. Retrieve a set of data.
2. Analyze it using the desired function.
3. Record or print the result of the analysis.
4. Use the Edit > Generate data 55 menu option to create a set of data in which only the component of interest contributes to the function's value.

   To do this, adjust the parameter values so that only one of the components contributes to the calculated values.
5. Save the generated data for each of the components in a data file.
6. Use the menu options File > Open 11 and File > Join 17 to create a new data set that contains the data for all of the components.
7. Use the Analyze > Setup > Analysis Range 93 option to set the analysis range so that it includes all of the data points in the new data set.
8. Use the Analyze > Setup > Parameters 99 option to manually set the parameter values to the values that were obtained in step 2 and recorded in step 3.
9. Use the View > fit graph 109 and Edit > Properties 81 options to manually scale the graph and set the plot symbol.

The resulting graph will consist of a solid line for the overall function and a dotted line for each of the component curves. The spacing between the dots in the dotted lines is determined by the number of data points that were generated for each component.

An Example

This example:

- Uses function 0302 to analyze a sample data set, F0302TST.DTA, which is described by and can be fitted to the sum of two Gaussian curves.
- Creates a graph that displays the overall calculated curve and the two sub-component Gaussian curves.

Here's what to do:

1. Retrieve the data set named F0302TST.DTA using the File > Open 11 menu option.

2. Analyze it using function number 0302.
   When doing the analysis, you should fit the first 20 points to the function using one Gaussian curve, then redo the fit using two Gaussians and all of the data.

> **NOTE:**
> When a function has more than one form, it will be necessary to 're-select' the function from the function tab in the Analyze > Setup 92 dialog.

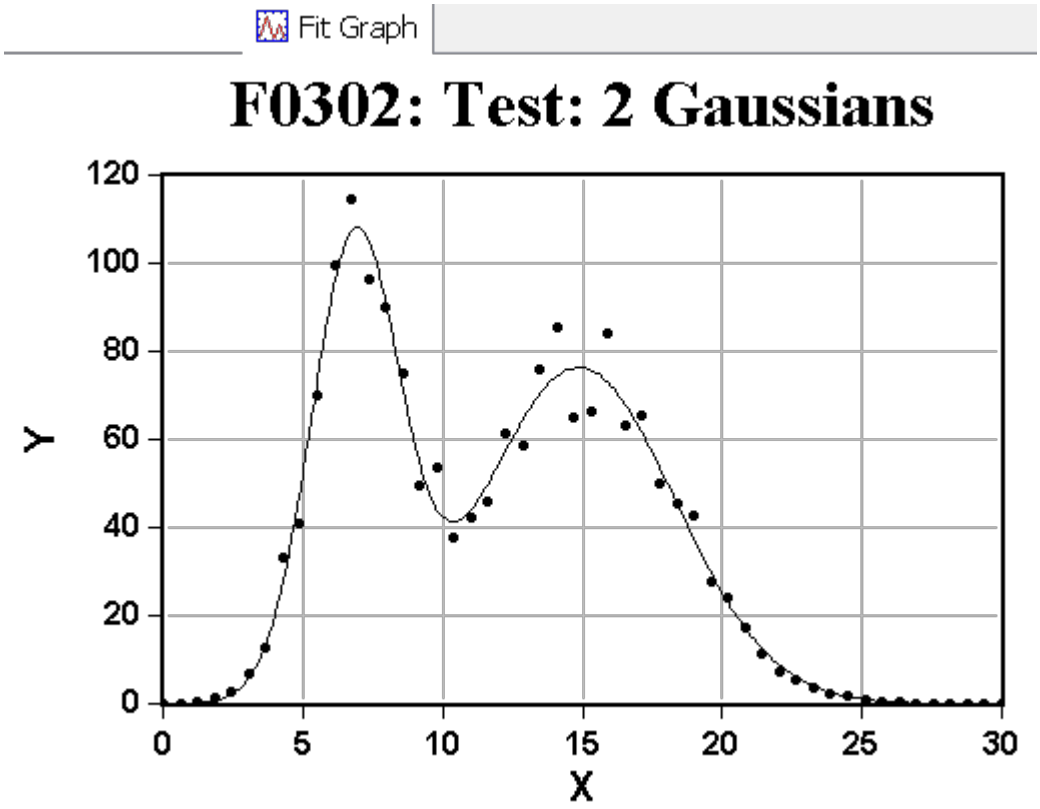
3. Record or print the results of the analysis.
   The results of the analysis should be:

File:	c:\Users\Public\fitall10\data\f0302tst.dta
Title:	Ftn0302 Test Data: 2 Gaussians
Sub-Title:	
Function:	0302..Sum of Gaussians: Y=∑{P[3*I-2]*exp[-2.77*{(X-P[3*I-1])/P[3*I]}^{2}] }
Analysis Method:	Nonlinear Least Squares (nls)
Analysis Range:	1 to 50 of 50
Weighted as:	1/SigmaY^2
Variance:	6.73101600438054E-7
Std. Dev. of Fit:	0.000820427693607458 after 4 iterations

Parameter	**Name**	**Value**	**Std. Dev.**
1	Ypeak1	9.902E+0001	5.658E-0001
2	Xpeak1	6.973E+0000	1.220E-0002
3	FWHH1	3.991E+0000	1.013E-0002

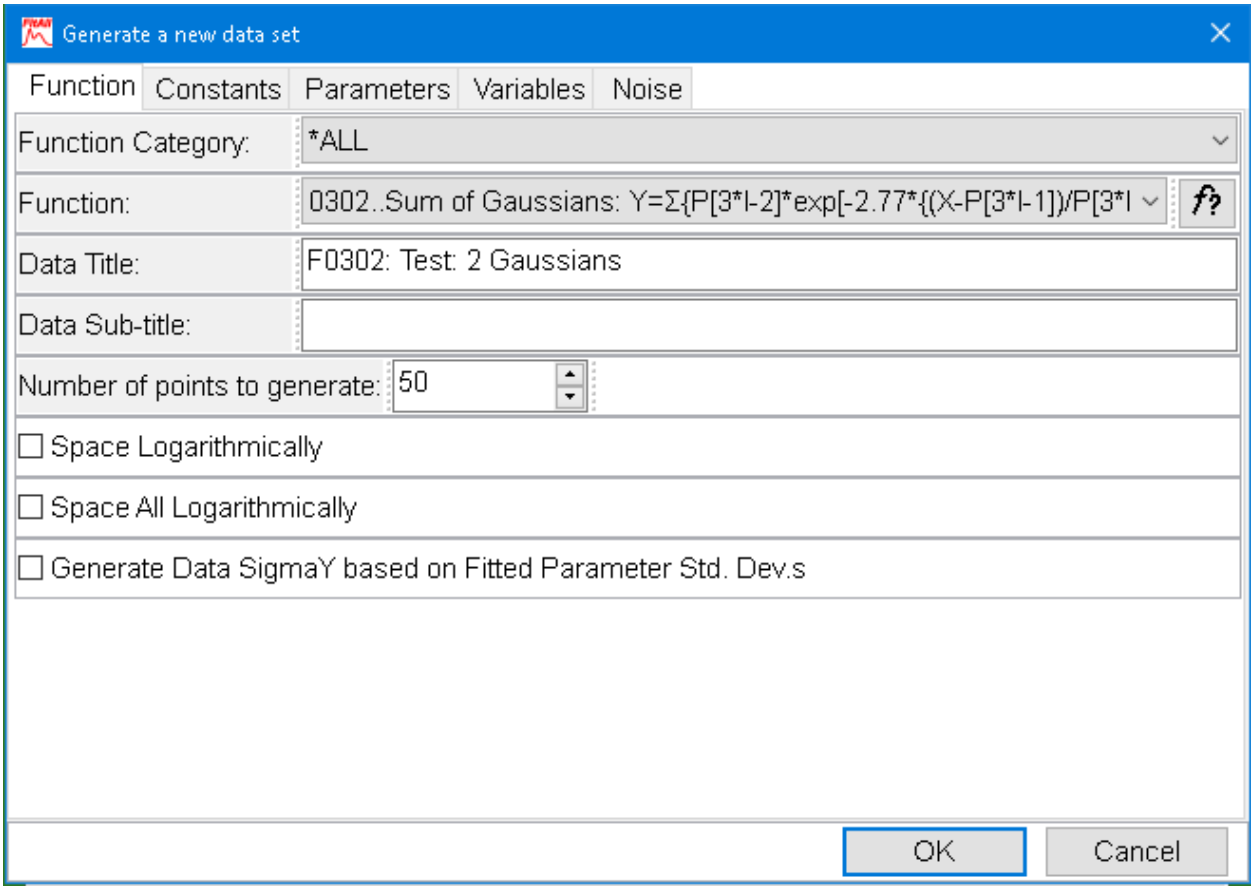
Parameter	Name	Value	Std. Dev.
4	Ypeak2	7.428E+0001	4.188E-0001
5	Xpeak2	1.499E+0001	9.231E-0003
6	FWHH2	8.010E+0000	5.089E-0003

4. Plot a graph of the fit using the View > fit graph 109 menu selections.
The graph should look like this:



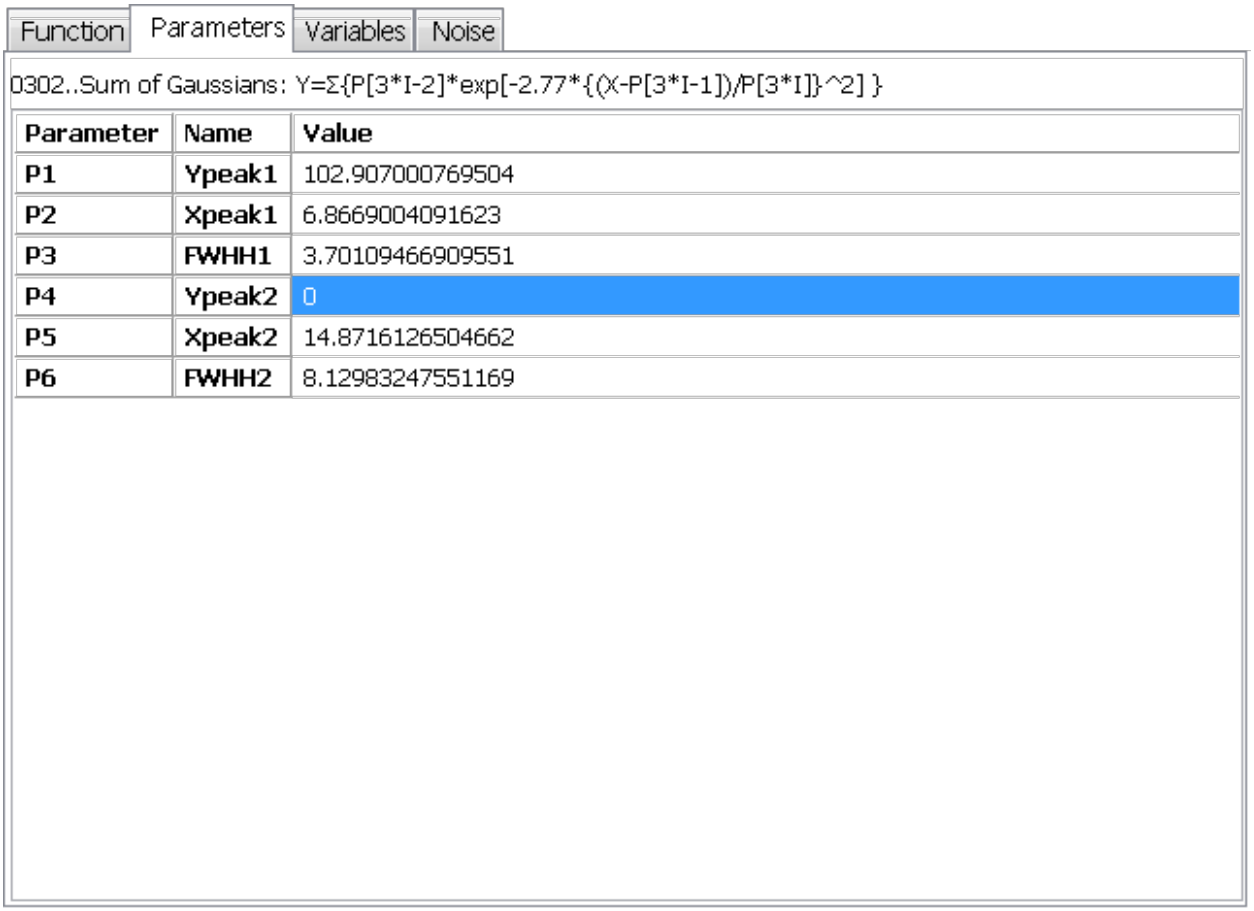
5. Before generating the component data sets, note that:
   - If parameter P1, Ypeak1, is set to zero, the first Gaussian will not contribute to the function's value.
   - If parameter P4, Ypeak2, is zero, the second Gaussian will not contribute to the function's value.
6. Click the Edit > Generate data 55 menu option.
7. Click the Function tab, if it is not already selected.
8. Select function 00302, if it is not already selected.

   If, and when, the 'Number of Gaussians' dialog box appears, enter two, 2, and click the **OK** button.
9. Change the 'Number of points to generate' spin-edit box to 50.



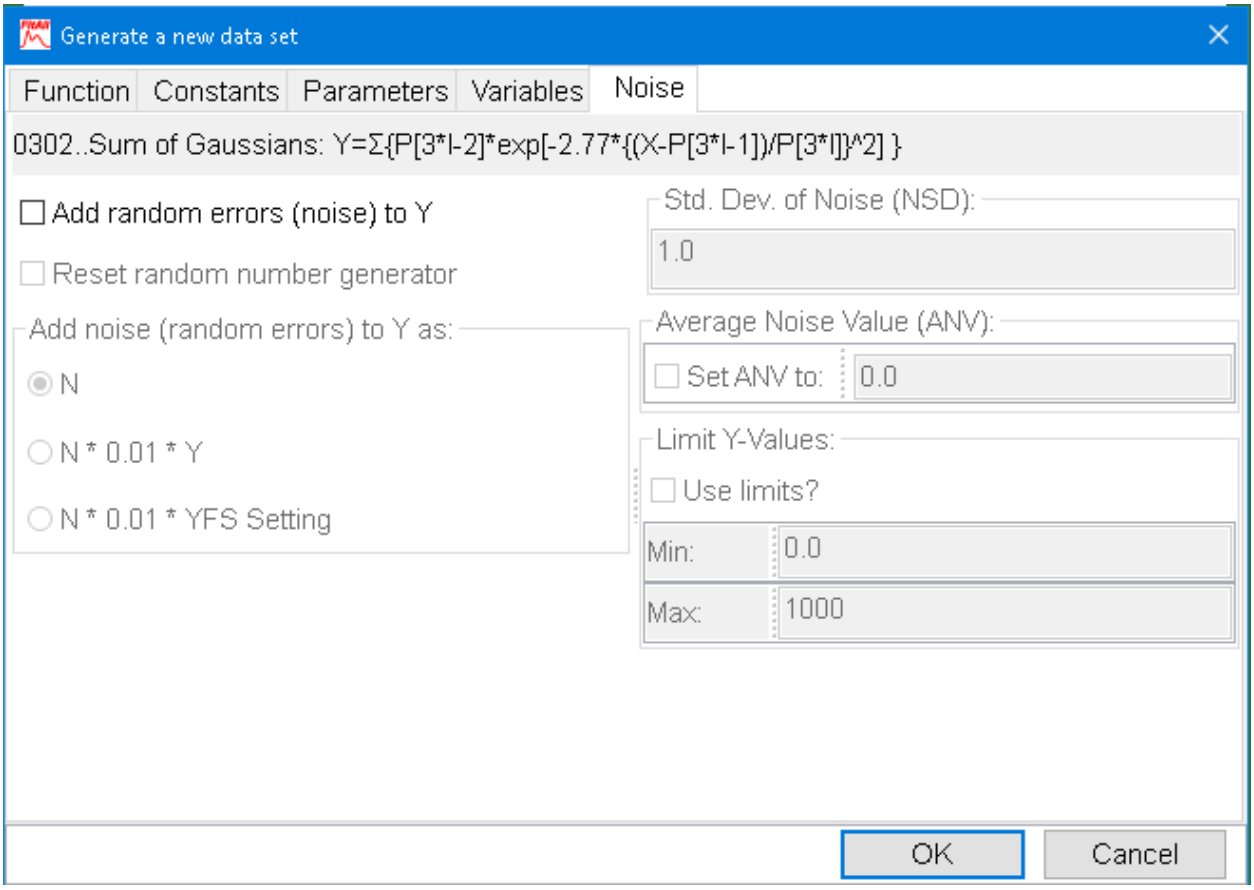
10. Click on the Parameters 57 tab.

    Change the value of parameter P4 to 0, zero.



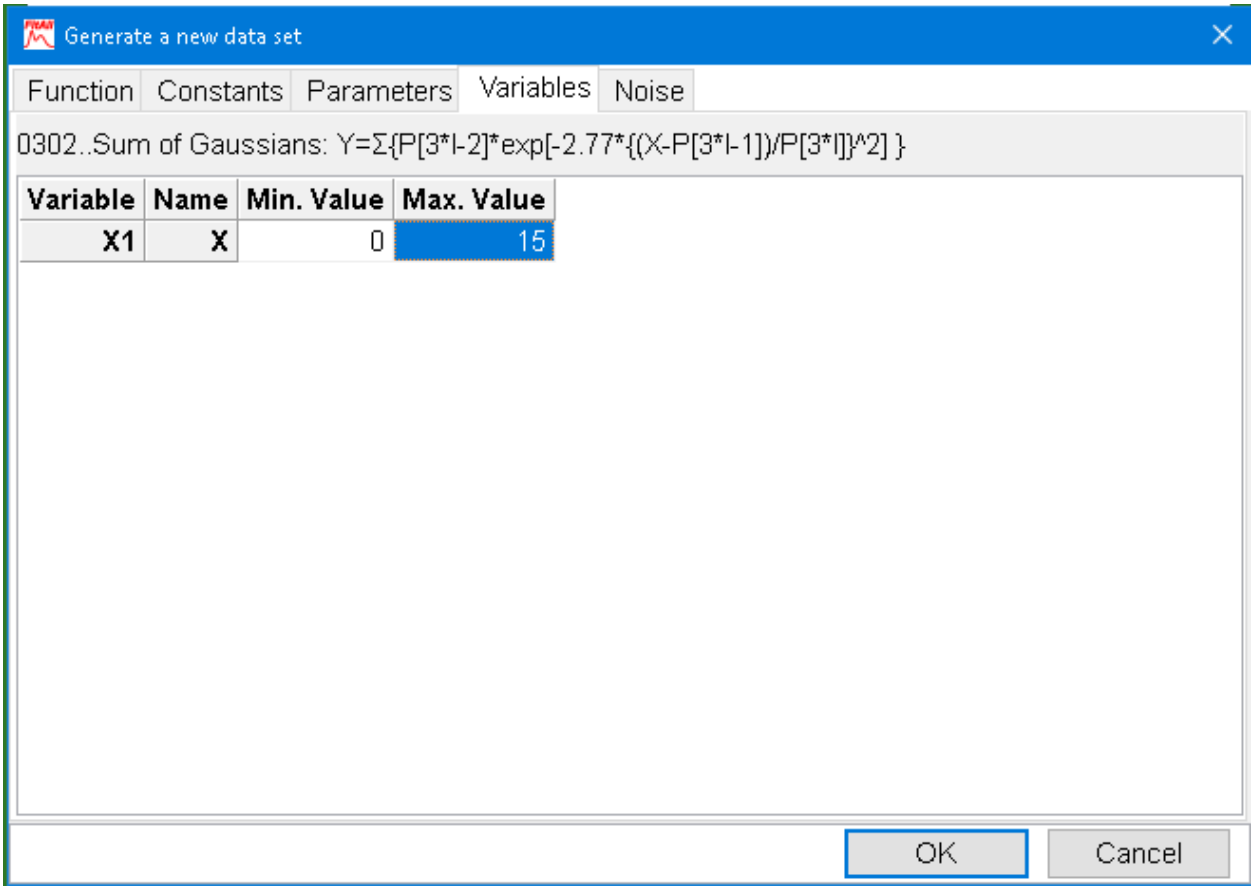
11. Click on the Noise tab.

    Ensure the 'Add random errors' check box is not checked.



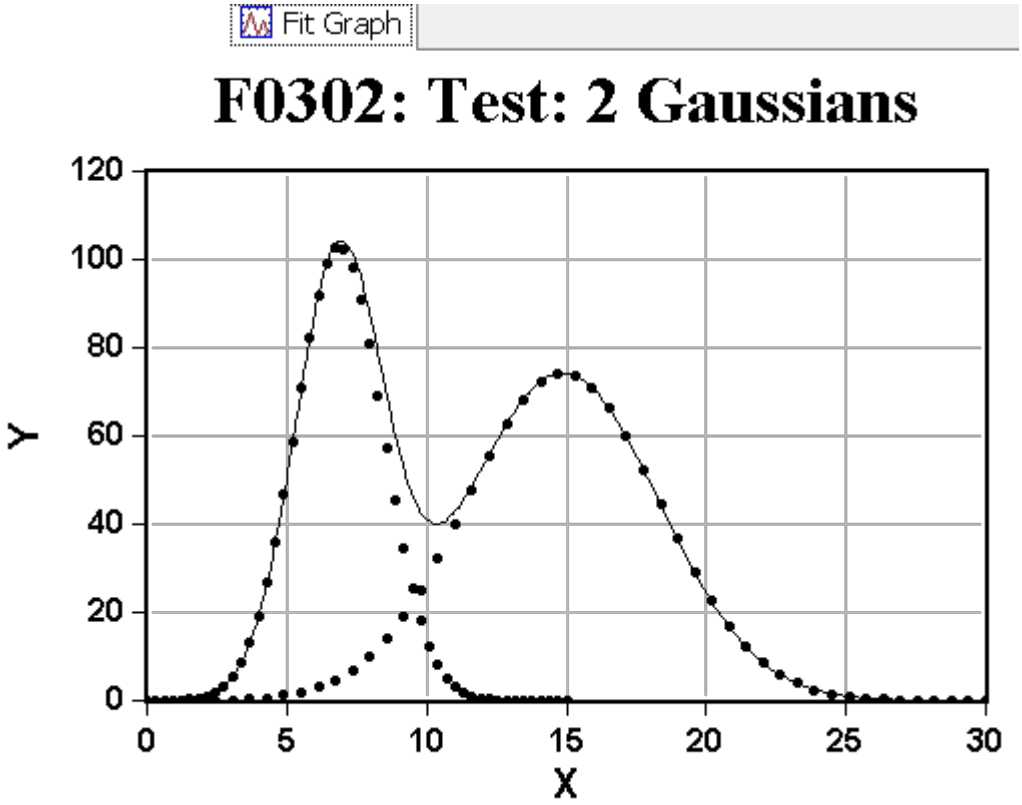
12. Click on the Variables 58 tab.

    Change the Min. and Max. values of the X1 variable to 0 and 15, respectively.



13. Click the **OK** button to generate the data.
14. Use the File > Save as 19 menu selections to save the data in a file named 'TMP1.DTA'.
15. Repeat steps 6 to 13, adjusting the values as follows:
    - The 'Number of points to generate' to 50.
    - The value of parameter P4 to the value saved in step 3.
    - The value of parameter P1 to 0, zero.
    - The Min. and Max. values of the X1 variable to 0 and 30, respectively.
16. Save the data in a file named 'TMP2.DTA'.
17. Use the File > Join 17 menu selections to append the 'TMP1.DTA' data file to the data that is currently in memory.
18. Use the Analyze >, Setup 92 menu selections to set the analysis range to 1 to 100.
19. Use the Analyze > Setup > Parameters 99 tab menu selections to manually set the parameter values to those obtained in steps 3 and 4.

20. Use the View > fit graph menu selections to display the fit graph. It should look like this:



Recast a Function

When you have a function that you wish to fit and it does not seem to be available in ***FitAll***, you should carefully inspect the form of your function and compare it with those in ***FitAll***.

Sometimes it will be possible to rearrange your function so that it is of the same form as one of the functions included in ***FitAll***.

For example, the function:

$$Y = \frac{A - D}{1 + \left(\frac{X}{C}\right)^B} + D$$

does not appear in the list of available functions. It does, however, bare some resemblance to the cooperative saturation curve (Ftn 0204).

In both functions X is raised to a power and the numerator and denominator are the sum of two terms.

The similarity is sufficiently striking that it is worthwhile to rearrange our function to see if it is the same as Ftn 0204.

To do this:

- Multiply the numerator and denominator by C^B to get:

$$Y = \frac{A * C^B - D * X^B}{C^B + X^B} + D$$

- Collect terms using the common denominator ($C^B + X^B$) to get:

$$Y = \frac{A * C^B - D * X^B}{C^B + X^B}$$

- Multiply the numerator and denominator by ($1/C^B$) to get:

$$Y = \frac{A + D * \left(\frac{1}{C^B}\right) * X^B}{1 + \left(\frac{1}{C^B}\right) * X^B}$$

This has exactly the same form as Ftn 0204. The parameters are defined as:

P1 = ($1/C^B$), P2 = D, P3 = A and P4 = B.

In other words, the derivation that resulted in Ftn 0204 defined P1 as the reciprocal of C^B.

Examples of this type are relatively common in physiology, biochemistry, or chemistry where the parameter C^B is referred to as the "50% dose level" or the dissociation constant, while the parameter ($1/C^B$) is called the association or formation constant.

Appendix

Getting Help

To get technical or other assistance from MTR Software you can:

Visit MTR Software's website at:

www.fitall.com

Email MTR Software at:

support@fitall.com

Write to MTR Software at:

MTR Software

77 Carlton Street, Suite 808

Toronto ON Canada

M5B 2J7

Telephone MTR Software at:

416-596-1499

Describe your problem or difficulty as completely as you can. We will try to answer your query quickly and completely.

You should also include your email address as well as your daytime, evening and weekend telephone numbers.

File Structures

DTA Data Files

Files with the ".DTA" extension are normal ***FitAll*** data files. These are UTF-8 or ASCII files that contain the following information:

```
<BOM>Number of columns of data
Title of the data set
Heading for column one
Heading for column two
  .
  .
Heading for last column
X[1,1] X[1,2] ... Y[1] SigmaY[1]
X[2,1] X[2,2] ... Y[2] SigmaY[2]
  .
  .
X[I,1] X[I,2] ... Y[I] SigmaY[I]
  .
  .
X[Npts,1] Xpts,2] ... Y[pts] SigmaY[pts]
```

<BOM> is a "Byte Order Marker" that specifies the type of encoding that has been used. If the data file only contains ASCII characters the BOM is not present.

You can prepare a data file with this format using a word processor (in its non-document or ASCII mode) or a text editor. It will be readable by ***FitAll***.

NOTE:

FitAll usually expects that there will be a minimum of three (3) columns of data, corresponding to the X, Y, and SigmaY values. However, you can create data files that contain only two columns of data using a text editor or similar program.

When ***FitAll*** encounters such a data file, it will automatically creates a third column and assign a value of zero or one to each element of the third column, depending on the Options > Preferences > Set New SigmaY's to 1.0 128 setting. This is particularly useful if you have a data acquisition system that creates data files with only X and Y data.

CSV Data Files

'Comma Separated Values', CSV, data files are assumed to be organized like this:

```
<BOM>"Title of data set"
"Col1 name","Col2 name","Col3 name", ...
X[1,1],X[1,2],...,Y[1],SigmaY[1]
X[2,1],X[2,2],...,Y[2],SigmaY[2]
   .
   .
   .
X[N,1],X[N,2],...,Y[N],SigmaY[N]
```

For example:

```
"Function 1 Test Data"
"X","Y","SigmaY"
1.500E+1,9.790E+1,1.000E+0
3.000E+1,8.550E+1,1.000E+0
4.500E+1,7.470E+1,1.000E+0
6.000E+1,6.530E+1,1.000E+0
7.500E+1,5.700E+1,1.000E+0
9.000E+1,4.990E+1,1.000E+0
1.050E+2,4.360E+1,1.000E+0
1.200E+2,3.810E+1,1.000E+0
1.350E+2,3.330E+1,1.000E+0
4.950E+2,1.000E+0,1.000E+0
```

The first two lines of the data file are optional. If either, or both, of the lines containing the title and the column names is missing, ***FitAll*** will still read in the data correctly.

<BOM> is a "Byte Order Marker" that specifies the type of encoding that has been used. If the data file only contains ASCII characters the BOM is not present.

NOTE:

FitAll usually expects that there will be a minimum of three (3) columns of data, corresponding to the X, Y, and SigmaY values. However, you can create data files that contain only two columns of data using a text editor or similar program.

When ***FitAll*** encounters such a data file, it will automatically creates a third column and assign a value of zero or one to each element of the third column, depending on the Options > Preferences > Set New SigmaY's to 1.0 128 setting. This is particularly useful if you have a data acquisition system that creates data files with only X and Y data.

Also See

XXX Data Files 200

File, Import Text Data ... 12

TDF Data Files

'Tab Delimited File', TDF, files are assumed to be organized like this:

```
<BOM>Title of data set

Col1 name<Tab>Col2 name<Tab>Col3 name<Tab> ...

X[1,1]<Tab>X[1,2]<Tab>...<Tab>Y[1]<Tab>SigmaY[1]

X[2,1]<Tab>X[2,2]<Tab>...<Tab>Y[2]<Tab>SigmaY[2]

   .

X[N,1]<Tab>X[N,2]<Tab>...<Tab>Y[N]<Tab>SigmaY[N]
```

in which <Tab> represents the 'Tab' character.

For example:

```
Function 1 Test Data

X<Tab>Y<Tab>SigmaY

1.500E+1<Tab>9.790E+1<Tab>1.000E+0

3.000E+1<Tab>8.550E+1<Tab>1.000E+0

4.500E+1<Tab>7.470E+1<Tab>1.000E+0

6.000E+1<Tab>6.530E+1<Tab>1.000E+0

7.500E+1<Tab>5.700E+1<Tab>1.000E+0

9.000E+1<Tab>4.990E+1<Tab>1.000E+0

1.050E+2<Tab>4.360E+1<Tab>1.000E+0

1.200E+2<Tab>3.810E+1<Tab>1.000E+0

1.350E+2<Tab>3.330E+1<Tab>1.000E+0

4.950E+2<Tab>1.000E+0<Tab>1.000E+0
```

The first two lines of the data file are optional. If either or both of the lines containing the title and the column names is missing, ***FitAll*** will still read in the data correctly.

<BOM> is a "Byte Order Marker" that specifies the type of encoding that has been used. If the data file only contains ASCII characters the BOM is not present.

> **NOTE:**
>
> ***FitAll*** usually expects that there will be a minimum of three (3) columns of data, corresponding to the X, Y, and SigmaY values. However, you can create data files that contain only two columns of data using a text editor or similar program.

When ***FitAll*** encounters such a data file, it will automatically creates a third column and assign a value of zero or one to each element of the third column, depending on the Options > Preferences > Set New SigmaY's to 1.0 128 setting. This is particularly useful if you have a data acquisition system that creates data files with only X and Y data.

SDF Data Files

'Space Delimited File', SDF, files are assumed to be organized like this:

```
<BOM>Title of data set

Col1_name<Space>Col2_name<Space>Col3_name<Space> ...

X[1,1]<Space>X[1,2]<Space>...<Space>Y[1]<Space>SigmaY[1]

X[2,1]<Space>X[2,2]<Space>...<Space>Y[2]<Space>SigmaY[2]

   .

X[N,1]<Space>X[N,2]<Space>...<Space>Y[N]<Space>SigmaY[N]
```

in which <Space> represents one or more " " characters.

For example:

```
Function 1 Test Data

X<Space>Y<Space>SigmaY

1.500E+1<Space>9.790E+1<Space>1.000E+0

3.000E+1<Space>8.550E+1<Space>1.000E+0

4.500E+1<Space>7.470E+1<Space>1.000E+0

6.000E+1<Space>6.530E+1<Space>1.000E+0

7.500E+1<Space>5.700E+1<Space>1.000E+0

9.000E+1<Space>4.990E+1<Space>1.000E+0

1.050E+2<Space>4.360E+1<Space>1.000E+0

1.200E+2<Space>3.810E+1<Space>1.000E+0

1.350E+2<Space>3.330E+1<Space>1.000E+0

4.950E+2<Space>1.000E+0<Space>1.000E+0
```

The first two lines of the data file are optional. If either or both of the lines containing the title and the column names is missing, ***FitAll*** will still read in the data correctly.

<BOM> is a "Byte Order Marker" that specifies the type of encoding that has been used. If the data file only contains ASCII characters the BOM is not present.

NOTE:

FitAll usually expects that there will be a minimum of three (3) columns of data, corresponding to the X, Y, and SigmaY values. However, you can create data files that contain only two columns of data using a text editor or similar program.

When ***FitAll*** encounters such a data file, it will automatically creates a third column and assign a value of zero or one to each element of the third column, depending on the Options > Preferences > Set New SigmaY's to 1.0 128 setting. This is particularly useful if you have a data acquisition system that creates data files with only X and Y data.

XXX Data Files

There are many types of "CSV", comma separated values, data files.

It is very difficult for a program, such as ***FitAll***, to automatically determine the exact format that has been used by other programs to create a ".csv" data file.

In the vast majority of cases, ".csv" data files are organized as described below for the "XXX data file" data structure.

FitAll's menu selections File, Import Text Data... makes it possible for you to import the data from such files into ***FitAll***.

XXX data files are assumed to be organized like this:

```
<BOM><QuoteChar>Title of data set<QuoteChar>

<QuoteChar>Col1 name<QuoteChar><SepChar><QuoteChar>Col2 name<QuoteChar><SepChar> ...

X[1,1]<SepChar>X[1,2]<SepChar>...<SepChar>Y[1]<SepChar>SigmaY[1]

X[2,1]<SepChar>X[2,2]<SepChar>...,Y[2]<SepChar>SigmaY[2]

   .

   .

   .

X[N,1]<SepChar>X[N,2]<SepChar>...<SepChar>Y[N]<SepChar>SigmaY[N]
```

For example:

```
Function 1 Test Data

X;Y;SigmaY

1<DecChar>500E+1;9<DecChar>790E+1;1<DecChar>000E+0

3,000E+1;8,550E+1;1,000E+0

4,500E+1;7,470E+1;1,000E+0

6,000E+1;6,530E+1;1,000E+0

7,500E+1;5,700E+1;1,000E+0

9,000E+1;4,990E+1;1,000E+0

1,050E+2;4,360E+1;1,000E+0

1,200E+2;3,810E+1;1,000E+0

1,350E+2;3,330E+1;1,000E+0

4,950E+2;1,000E+0;1,000E+0
```

The first two lines of the data file are optional. If either; or both; of the lines containing the title and the column names is missing; ***FitAll*** will still read in the data correctly.

<BOM> is a "Byte Order Marker" that specifies the type of encoding that has been used. If the data file only contains ASCII characters the BOM is not present.

<DecChar>, which separates the integer part from the fraction part of a number, can be a period, [.], or a comma [,] character.

<QuoteChar>, which encloses text items, can be nothing, [], a double quotation mark, ["], or a single quotation mark, ['] character.

<SepChar>, which separates data items, can be a comma, [,], colon, [:], semi-colon, [;], space, [ ] or tab, [»], character.

NOTE:

FitAll usually expects that there will be a minimum of three (3) columns of data, corresponding to the X, Y, and SigmaY values. However, you can create data files that contain only two columns of data using a text editor or similar program.

When ***FitAll*** encounters such a data file, it will automatically creates a third column and assign a value of zero or one to each element of the third column, depending on the Options > Preferences > Set New SigmaY's to 1.0 128 setting. This is particularly useful if you have a data acquisition system that creates data files with only X and Y data.

Also See

CVS Data Files 194

File, Import Text Data ... 12

Monte Carlo and Batch Mode Results Files

The results data file, created when doing a Monte Carlo (or Batch Mode) analysis, contains 2*NTerms+3 columns of data when the nlls or nlad analysis methods are used and 2*NTerms+2 columns of data when the lls analysis method is used. Nterms is the number of parameters in the analysis function.

For example, if the fitting function contains three parameters, the results data file will contain eight or nine columns.

The columns contained in the results data file are:

- **File Num**: The number from the file name of the data file that was analyzed to get the reported results.
- **Parameter 1**: The resolved value of the function's first parameter
- **EE_Parameter 1**: The estimated error in parameter 1. If the nlls or lls analysis methods were used, this corresponds to the estimated standard deviation of parameter 1. If the nllad analysis method was used, this corresponds to the estimated average deviation of parameter 1.
- ... etc. ...
- ... etc. ...
- **Parameter Last**
- **EE_Last Parameter**
- **SD_Fit**: The standard deviation of the fit.
- **Iterations**: The number of iterations required to do the fit.

  This column is not present when the fitting function is linear in its parameters; that is, when the lls method is used to analyze the data.

> **CAUTION:**
> When the number of iterations is the same as the Max. Iterations 96 setting it is likely that ***FitAll*** has stopped before the final best fit was obtained.
>
> [This is more likely to occur when doing 'batch mode' analyses rather than Monte Carlo analyses].
>
> If this occurs, the best thing to do is:
>
> - Individually re-analyze the data set(s) in question using the 'normal' analysis type, and / or
> - Re-analyze all of the data sets using a larger value for the Max. Iterations setting.

> **NOTE:**
> The beginning of the file may contain a Byte Order Marker, BOM, which specifies the type of encoding that is used.

Multi-Fit Configuration Files

The ***FitAll*** Multi-Fit configuration file, with the file name extension '.fmc', is created by selecting Edit, Generate Multi-Fit Configs.... 69.

> **NOTES:**
>
> 1. Although the file can be opened and inspected using almost any text editor, its contents are unlikely to be of interest to most users.
> 2. The file's contents should not be modified.
> 3. The file does not contain a column headings row.

The '.fmc' file is a tab-delimited ASCII file that contains the following columns of data:

- **Configuration Number**: A number assigned by ***FitAll*** to identify the configuration.
- **MF_NFVS**: The maximum number of 'Function Variation Values' used by the function.
- **NFVS**: The actual number of 'Function Variation Values' used by this configuration.
- **MF_NKonsts**: The maximum number of constants, K, used by the function.
- **NKonsts**: The actual number of constants, K, used by this configuration.
- **MF_NTerms**: The maximum number of terms, parameters that are to be resolved, by the function.
- **NTerms**: The actual number of parameters that are resolved (fitted) by this configuration.
- **FtnNum**: The number of the function that was used to generate the configurations and will be used to analyze the data.
- **FVS-Values**: MF_NFVS columns of FVS[] values, beginning with gv.FVS[1]. If NFVS is less than MF_NFVS the values for the last (MF_NFVS - NFVS) columns are assigned a value of zero. If MF_NFVS is zero, no values are written to the file.
- **K-Values**: MF_NKonsts columns of K[] values, beginning with gv.K[1]. If NKonsts is less than MF_NKonsts the values for the last (MF_NKonsts - NKonsts) columns are assigned a value of zero. If MF_NKonsts is zero, no values are written to the file.
- **P-Values**: MF_Terms columns of P[] (parameter) values, beginning with gv.P[1]. These are the initial estimates of the parameters that are used in the regression analyses. If NTerms is less than MF_NTerms the values for the last (MF_NTerms - NTerms) columns are assigned a value of zero.

Multi-Fit Results Files

The Multi-Fit results data file, created when doing Multi-Fit analyses, is a tab- or space-delimited ASCII file.

The type of file created is determined by the file name's extension when the file is created. If the file name extension is '.sdf' a space-delimited ASCII file is created, while a file name extension of '.tdf' creates a tab-delimited file.

Each column in a '.tdf' file is 25 characters wide.

The columns contained in the results data file are:

- **MF_Number**: Multi-Fit configuration number.
- **EE_Fit**: Estimated error of the fit. For nlls and lls fits this corresponds to the standard deviation of the fit. For nlad fits this corresponds to the average absolute deviation of the fit.
- **Iterations**: The number of iterations required to do the nlls or nlad regression analysis.

  This column is not present when the fitting function is linear in its parameters; that is, when the lls method is used to analyze the data.

  > **CAUTION:**
  > When the number of iterations is the same as the Max. Iterations 96 setting it is likely that ***FitAll*** has stopped before the final best fit was obtained.
  >
  > If this occurs, the best thing to do is:
  >
  > - Individually re-analyze the data with the configuration(s) in question using the 'normal' analysis type, and / or
  > - Re-analyze all of the configurations using a larger value for the Max. Iterations setting.

- **MF_FVS**: The maximum number of 'Function Variation Values' used by the function.
- **FVSn**: MF_NFVS columns of FVS[] values, beginning with gv.FVS[1]. If fewer than MF_NFVS FVS's are actually used by this configuration, the values in the 'extra' columns will be zero.
- **MF_NKonst**: The maximum number of constants, K, used by the function. If fewer than MF_NKonsts constants are actually used by this configuration, the values in the 'extra' columns will be zero.
- **Constant**: MF_NKonst columns of the constant, K, values. If fewer than MF_NKonsts constants are actually used by this configuration, the values in the 'extra' columns will be zero.
- **MF_NTerms**: The maximum number of terms, parameters that have been resolved.
- **Parameter**: MF_NTerms columns of the resolved parameter values. If fewer than MF_NTerms parameters are actually used by this configuration, the values in the 'extra' columns will be zero.
- **EE_Parameter**: MF_NTerms columns of the estimated error in the resolved parameter values. If fewer than MF_NTerms parameters are actually used by this configuration, the values in the 'extra' columns will be zero.

Theory Behind FitAll

For functions that are non-linear in their parameters, ***FitAll*** uses a non-linear least-squares, gradient-expansion algorithm developed by Marquardt, which combines the best features of the gradient search and the linearization methods.

- ***FitAll*** also features a unique algorithm for numerically calculating derivatives. This algorithm allows the program to automatically determine the step-size over which the derivative (or slope) should be determined.

- Unlike other nonlinear regression programs, ***FitAll*** does not require you to enter expressions for the derivatives of the function or step-sizes.

The analysis methods used by ***FitAll*** are discussed in the following sections:

Linear Least-Squares Method 206

Nonlinear Least-Squares Method 207

Nonlinear Least Absolute Deviations Method 208

Linear Least-Squares Method

The least-squares method is used to describe the characteristic response, Y, of a system in terms of some other quantity (or quantities), X.

The relationship between the dependent variable, Y, (that is, the response) and the independent variable(s), X, (that is, the stimulus) is expressed in mathematical form by the functional relationship: F = Y = f(X,P), in which the parameters, P, provide the link between X and Y. This relationship (model) ought to have a basis in theory, although it is not uncommon for the function f(X,P) to be arrived at empirically.

The data that is collected consists of various measured values of the response, Y[i], and the corresponding values of the stimulus, X[i].

The sum of the squares of the residuals, S, is given by:

$$S = \sum\left[\left(F_i - Y_i\right)^2\right] = \sum\left[\left(f(X_i,P) - Y_i\right)^2\right] \qquad ..(1)$$

The first step in finding the values of the P's that minimize S in the above equation is to differentiate equation (1) with respect to each of the parameters. This yields a set of equations equal in number to the number of parameters, P_j, present in the original function. The new equations are:

$$\frac{\partial S}{\partial P1} = 2*\sum\left[\left(f(X_i,P) - Y_i\right)*\left(\frac{\partial f(X_i,P)}{\partial P1}\right)\right] = 0 \qquad ..(1.1)$$

$$\frac{\partial S}{\partial P2} = 2*\sum\left[\left(f(X_i,P) - Y_i\right)*\left(\frac{\partial f(X_i,P)}{\partial P2}\right)\right] = 0 \qquad ..(1.2)$$

$$\frac{\partial S}{\partial Pj} = 2*\sum\left[\left(f(X_i,P) - Y_i\right)*\left(\frac{\partial f(X_i,P)}{\partial Pj}\right)\right] = 0 \qquad ..(1.j)$$

When the sum of the squares of the deviations, S, is at a minimum, each of the partial derivatives of S , dS/dP_j, will be equal to zero.

At this point there are j equations in j unknowns, Pj, which can be solved using normal matrix methods.

For functions that are linear in their parameters, P, ***FitAll*** uses the linear least-squares method to determine the parameter values, P.

Nonlinear Least-Squares Method

If the linear least-squares method is applied to a nonlinear function, the equations corresponding to (1.1) through (1.j) will not be solvable.

The way around this problem is to first linearize the original nonlinear function. One general method of linearizing a function is to perform a Taylor expansion to the first order in the parameters, P_j, and defining a new difference function δF = (F - Fo), in which Fo is the value of the original function, F, evaluated using some initial estimated values of the parameters, P_j.

For example, with the nonlinear function:

$$F = A * e^{(-B*X)}, \qquad ..(2)$$

in which A and B are the parameters, the new difference function, dF , is:

$$\delta F = \left(\frac{\partial F}{\partial A}\right) * \delta A + \left(\frac{\partial F}{\partial B}\right) * \delta B \qquad ..(3)$$

Equation (3) is now linear in its (new) parameters, δA and δB. That is, the linearization process transforms the original function, which had the parameters A and B, into a new function, which has the parameters δA and δB.

δA and δB represent the changes that must be made to the initial estimates of the values of A and B.

Since equation (3) is linear in its parameters, δA and δB, it can be fitted using the normal linear least-squares procedure to find values for the new parameters δA and δB.

To obtain the best fit values of the original parameters, A and B, the linear regression must be repeated several times. With each repetition (iteration), new estimates (A' = A + δA and B' = B + δB) of the original parameter estimates are made.

When the estimated parameter values no longer change, or when the sum of the squares of the residuals has reached a minimum, the iterations are halted and the final parameter values are taken to be the best fit values.

For a more complete discussion of the lls and nlls methods, see:

- Marquardt, D.W. "An Algorithm for Least-Squares Estimation of Nonlinear Parameters" J. Soc. Ind. Appl. Math., 1963, vol. 11(number 2), page 431.
- Bevington, P.R. Data Reduction and Error Analysis for the Physical Sciences, McGraw-Hill Book Co., New York, NY, 1969.
- Press, W.H., Flannery, B.P., Teukolsky, S.A., Vetterling, W.T. Numerical Recipes: The Art of Scientific Computing, Cambridge University Press, New York, NY, 1986.

Nonlinear Least Absolute Deviations Method

The non-linear least absolute deviations (nllad) method is very similar to the nonlinear least-squares (nlls) method. The major difference is that the nllad method minimizes the sum of the absolute deviations rather than the sum of the squares of the deviations.

The advantages of the non-linear absolute deviations method over the nonlinear least squares method are:

- The nllad method is less sensitive to the presence of 'outliers'. That is, a few 'bad' data points are less likely to dramatically affect the values of the resolved parameters.
- The nllad method is less sensitive to the measurement error distribution. That is, the nlls method assumes a 'normal' (Gaussian) error distribution, while the nllad method does not.

The disadvantages of the nonlinear absolute deviations method are:

- The nllad method usually requires more iterations to obtain the best-fit values.
- The nllad method may require better initial estimates of the parameter values to prevent it from regressing to a 'false' or 'local' minimum which does not correspond to the 'global' best fit.

For a more complete discussion of the nllad method, see:

- Matheson, I.B.C. "Robust Estimation of Parameters: A Simple Modification to all Non-Linear Fitting Algorithms to Convert From Minimizing the Sum of Squares of Deviations to Minimizing the Sum of the Absolute Deviations" Computers in Chemistry, 1989, vol. 13 (number 4), page 299.
- Matheson, I.B.C. "A Critical Comparison of Least Absolute Deviation Fitting (Robust) and Least Squares Fitting: The Importance of Error Distributions" Computers in Chemistry, 1990, vol. 14 (number 1), page 49.

Adding Functions to FitAll

There are four ways to add your own specialized functions to ***FitAll***.

1. In ***FitAll*** version 10 you can use the new "Scripted Function" feature to add functions that can be defined by a one-line expression and contains one independent variable, X. and up to ten parameters, P.

2. You can contact ***MTR* Software** to get a quotation on the cost of creating a custom ***FitAll* Function Library** for you.

3. The ***FitAll* Programmer's Guide**, which is included with ***FitAll* Research Edition**, explains:

   - how to modify the supplied source code for the User Defined ***FitAll* Function Libraries** and

   - how to compile them using Embarcadero / CodeGear / Borland Delphi version 5 to XE2, **FreePascal** version 2.2 or later and **Lazarus** version 1.0 or later. FreePascal and Lazarus are open source Pascal compilers available from www.freepascal.org and www.lazarus.freepascal.org . Lazarus is highly recommended.

4. You can contact ***MTR* Software** and request that the function be added to one of ***FitAll***'s **Function Libraries**.

Adding UDF Help to FitAll

As of version 9 Update03, ***FitAll*** will display help documents for the User Defined Functions, UDFs.

The help files can be MS Word (*.doc, *.docx), Rich Text Format (*.rtf), Open Document Text (*.odt), Text (*.txt) or Portable Document Format (*.pdf) files.

There are no restrictions on the contents of the help files except those imposed by the document's format and the application that will display it.

Whether a particular document can be displayed depends on what other software is installed on your computer and that an association between the file name extension and the application exists.

For example, a '*.docx' file will normally be displayed by MS Word and a '*.txt' file will normally be displayed by Notepad.

File Names:

The help files must be named like this:

??????**FaHelpUDF-**####??????????**.EXT**

in which #### is a four digit number that corresponds to the function's number.
Note that there is a dash, '-', between the **F** and #### and currently the User Defined Functions are numbered from 5001 to 6000.

The ???'s can be replaced by any text that is acceptable as part of a file name.

Here are some examples of acceptable names for the help file.

- FaHelpUDF-5001.txt
- FaHelpUDF-5001-FirstUDF-Y=AX+B.doc
- CHM101-FaHelpUDF-5001-FirstUDFforChemistry101-Y=AX+B.docx
- CHM101 Lab05-Kinetics-1st-Order Exponential-FaHelpUDF-5001.docx
- MyName-FaHelpUDF-5001-FunctionForFittingMyData-Y=AX+B.pdf
- MyName-FaHelpUDF-5002-A_Better_Function_For_Fitting_My_Data.odt

NOTE:
Help documents can be created and used for both User Defined Functions that are compiled into a ***FitAll*** Function Library and Scripted functions.

The compiled UDFs will have function numbers from 5001 to 6000 and the Scripted functions will have function numbers from 0101 to 0200.

File Location:

The help document must be stored in the <FitAll Installation Directory>\Help directory where ***FitAll*** was installed.

By default this will be 'C:\Users\Public\FitAllxx\Help'.

Sample UDF Help Files:

Several sample help files in different formats are located in the <FitAll Installation Directory>\Help\Samples directory.

Copy and rename any of these files, edit them as appropriate and copy the result to the <FitAll Installation Directory>\Help directory.

THIS IS AN INTENTIONALLY EMPTY PAGE

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