Version 10

FitAll

nonlinear regression analysis

Getting Started Guide

Published by

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Contents

Introduction

This ***FitAll*** Getting Started Guide provides an introduction to What's New in this version of ***FitAll*** and how to get started using ***FitAll***.

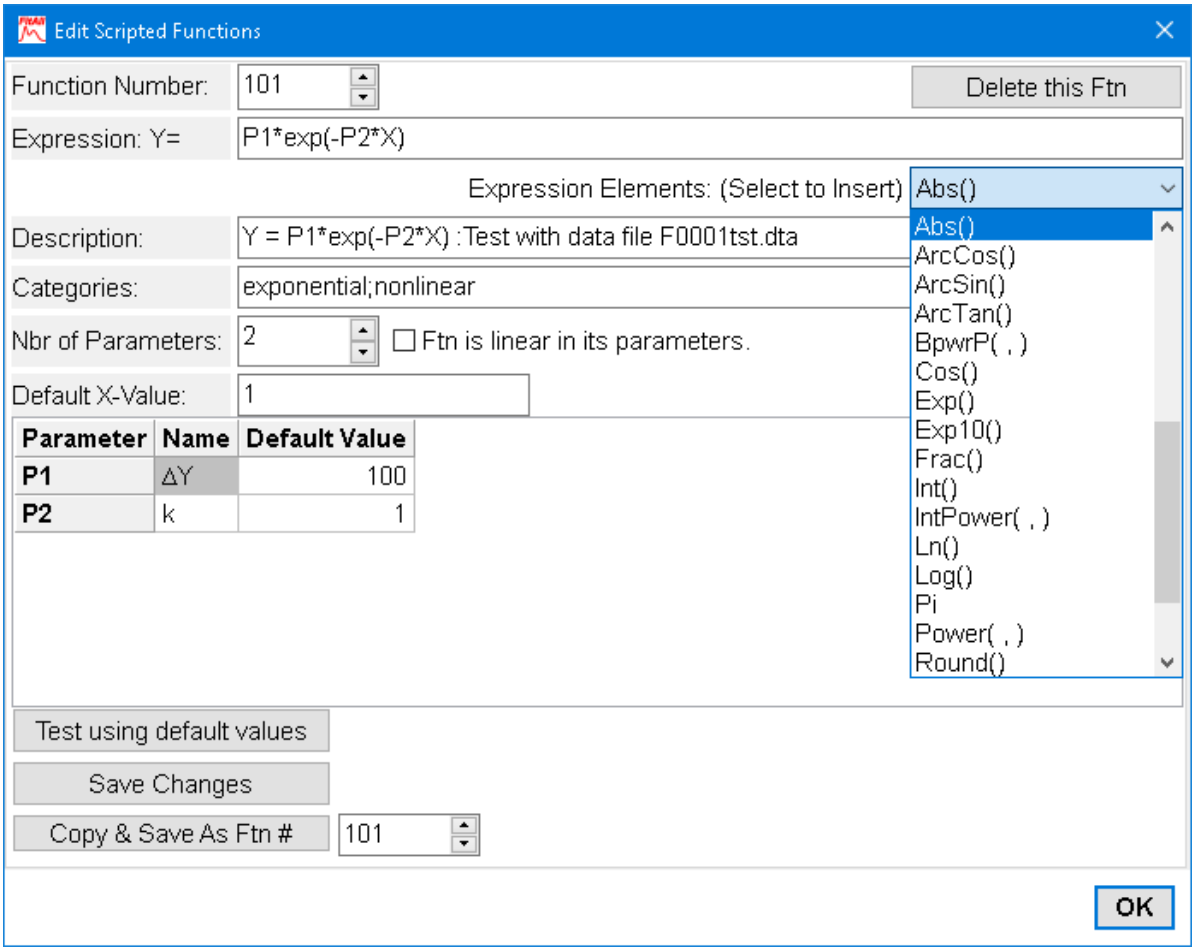
For more complete and detailed information consult the ***FitAll Reference Guide***.

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

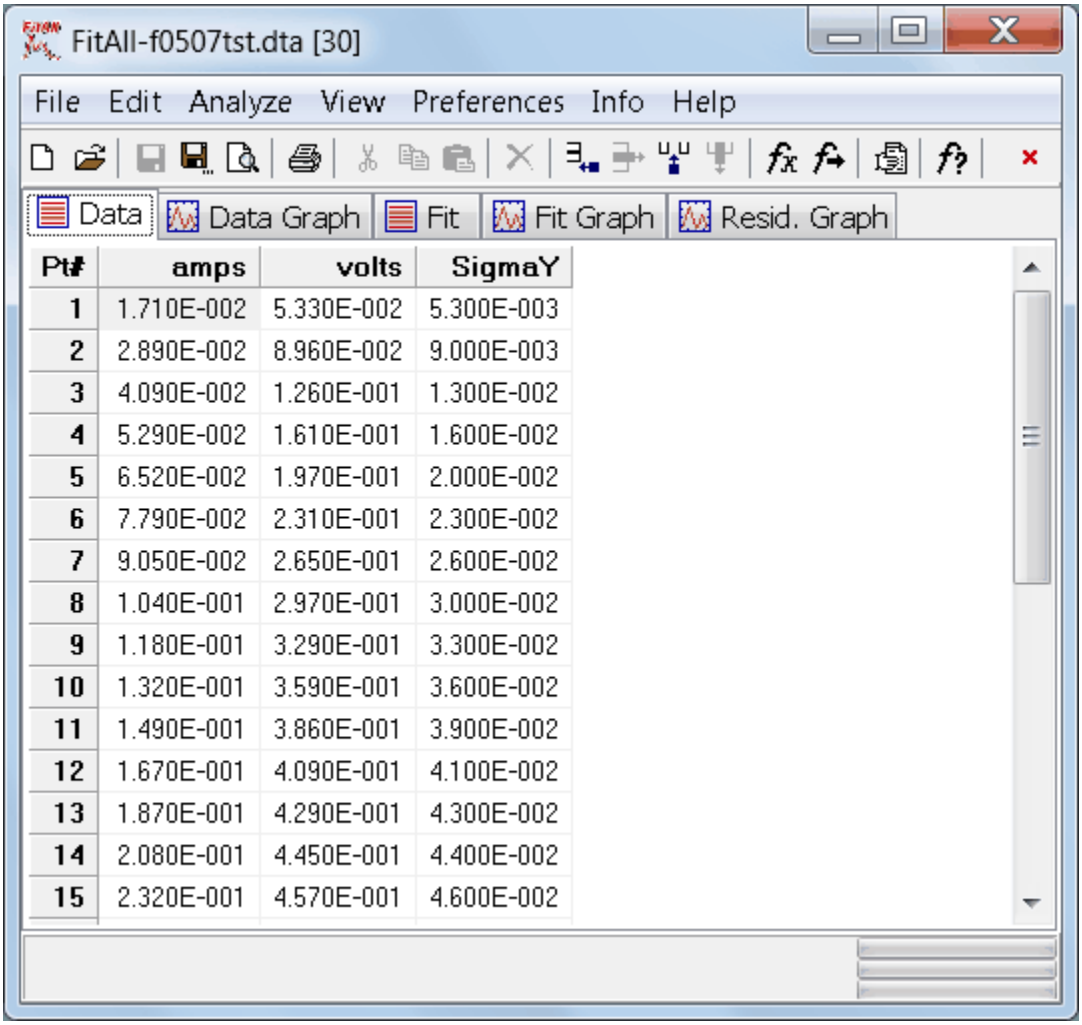
- Support for MS Windows XP has been discontinued.

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.

FitAll Basics

What FitAll Does

FitAll is a general-purpose, nonlinear regression analysis (curve fitting) program that can be used to fit a set of experimental data to any of the defined functions (models).

The 'best fit' is obtained by one of three methods:

- Linear Least Squares (lls): minimizes the sum of the squares of the deviations between the observed and calculated values of a function that is linear in its parameters. (For more information see: Linear Least Squares Method in the ***FitAll*** Reference Guide).
- Nonlinear Least Squares (nlls): minimizes the sum of the squares of the deviations between the observed and calculated values. (For more information see: Nonlinear Least Squares Method in the ***FitAll*** Reference Guide).
- Nonlinear Least Absolute Deviations (nlad): minimizes the absolute deviations between the observed and calculated values. (For more information see: Nonlinear Least Absolute Deviations Method in the ***FitAll*** Reference Guide)

FitAll is a tool to use in analyzing data that characterize all kinds of phenomena studied by scientists, engineers and students.

Some of the areas in which ***FitAll*** is being used are:

- biochemistry.
- biomedical research.
- cancer research.
- chemistry.
- corrosion.
- electrochemistry.
- enzymology.
- metallurgy.
- oceanography.
- pharmacology.
- petroleum research.
- reaction kinetics.
- semiconductor diode research.
- solar cell research.

FitAll fits data to continuous, single-valued:

functions with the general form:

$$Y_i = \boldsymbol{f}(X_{ij}, K_K, P_P)$$

and

implicit functions with the general form:

$$Y_i = \boldsymbol{f}(\mathbf{Y}_i, X_{ij}, K_K, P_P)$$

in which:

- Y_i is the dependent variable (measured value of the function for the i^{th} data point).
- X_{ij} is the set of j *in*dependent variables for the i^{th} data point.
- K_k is a set of k constants.
- P_p is the set of p parameters that are evaluated by ***FitAll***.

FitAll can use weighting factors in the analysis.

FitAll provides two methods (Boxcar and Fourier transform) for smoothing data.

FitAll reports the standard deviation of the overall fit and of each parameter that it resolves.

FitAll makes two-dimensional graphs of the:

- original data.
- calculated curve.
- residuals (that is, the difference between the actual and the calculated values).
- parameter sensitivities.
- residual distribution.

FitAll automatically scales the graphs for you or you can specify the axis limits and the number of tic-marks that should be used.

Graphs created by ***FitAll*** can be:

- displayed on the computer's screen.
- copied to the Windows Clipboard.
- printed.
- saved to a disk file in several different graphics formats.

FitAll creates tables containing:

- the original data.
- the data and the corresponding calculated values.

- the resolved parameter values.
- the parameter sensitivities.
- the residual distribution.
- nonparametric statistics, such as, Kendall's tau and the sum squared difference of ranks.

Tables generated by ***FitAll*** can be:

- displayed on the computer's screen.
- copied to the Windows' Clipboard.
- printed.
- saved to disk as text files.

> **NOTE:**
> ***FitAll*** can, at the click of a button, create MS Word and Libre Office Writer reports that can contain any or all of its graphs and tables.

What FitAll Cannot Do

- ***FitAll*** can tell you which function gives the best fit; however, it cannot tell you which function is most appropriate for your use. You must make that judgment.

- ***FitAll*** cannot guarantee that the results it produces are physically meaningful. You must make that judgment based on your knowledge of the processes involved.

What You Need to Use FitAll

To use ***FitAll*** you need the following:

1. A MS Windows 7 or later capable computer.
2. A hard disk with at least twenty megabytes (20 MB) of available space.
3. 256 MB of memory (1 GB or more recommended).
4. The ***FitAll*** program.

Optional equipment:

1. MS Office 2007 or later to generate the MS Word reports.
2. LibreOffice.org 5.x or later to generate LO Writer reports.
   (LibreOffice is a free, open source office suite available from https://www.libreoffice.org/.)
3. A MS Windows compatible printer to print the tables, graphs and reports created by ***FitAll***.

To add your own functions as compiled ***FitAll*** **Function Libraries**.

1. ***FitAll*** **Research Edition**.
2. **Lazarus / Free Pascal**, which is a free, open source, Pascal compiler and is available from http://www.lazarus.freepascal.org/ .

How to Install FitAll

1. Download the file to a directory of your choice.
2. Use Windows Explorer to locate the file named fa?????.exe; for example, fa010P.exe.
3. Double click on the fa?????.exe file to run it.
4. Follow the on screen instructions.

How to Uninstall FitAll

To uninstall (remove) ***FitAll*** from your computer:

Click on Start, Programs, FitAll70, Uninstall FitAll .

1. In Windows 7:
   Click Start > Control Panel.

   In Windows 10:
   Click Start > Settings

2. In Windows 7:
   Click Programs > Programs and Features > Uninstall a program.

   In Windows 8:
   Double-click the Control Panel desktop icon and then click Uninstall a program.

   In Windows 10:
   Click Apps (uninstall defaults, optional features)

3. Click on the ***FitAll*** item to select it.

4. In Windows 7:
   Click the Ok or Change/Remove button.

   In Windows 10:
   Click the Uninstall button.

5. Follow the on-screen instructions.

FitAll Fundamentals

Starting FitAll

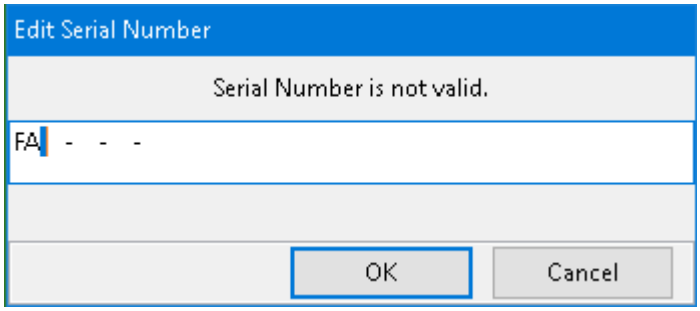
To start ***FitAll***:

Double click on the 

icon. (If you followed the standard setup procedure, the ***FitAll*** icon will be located on your desktop). -- Or select (click): Start > Programs > FitAll10.

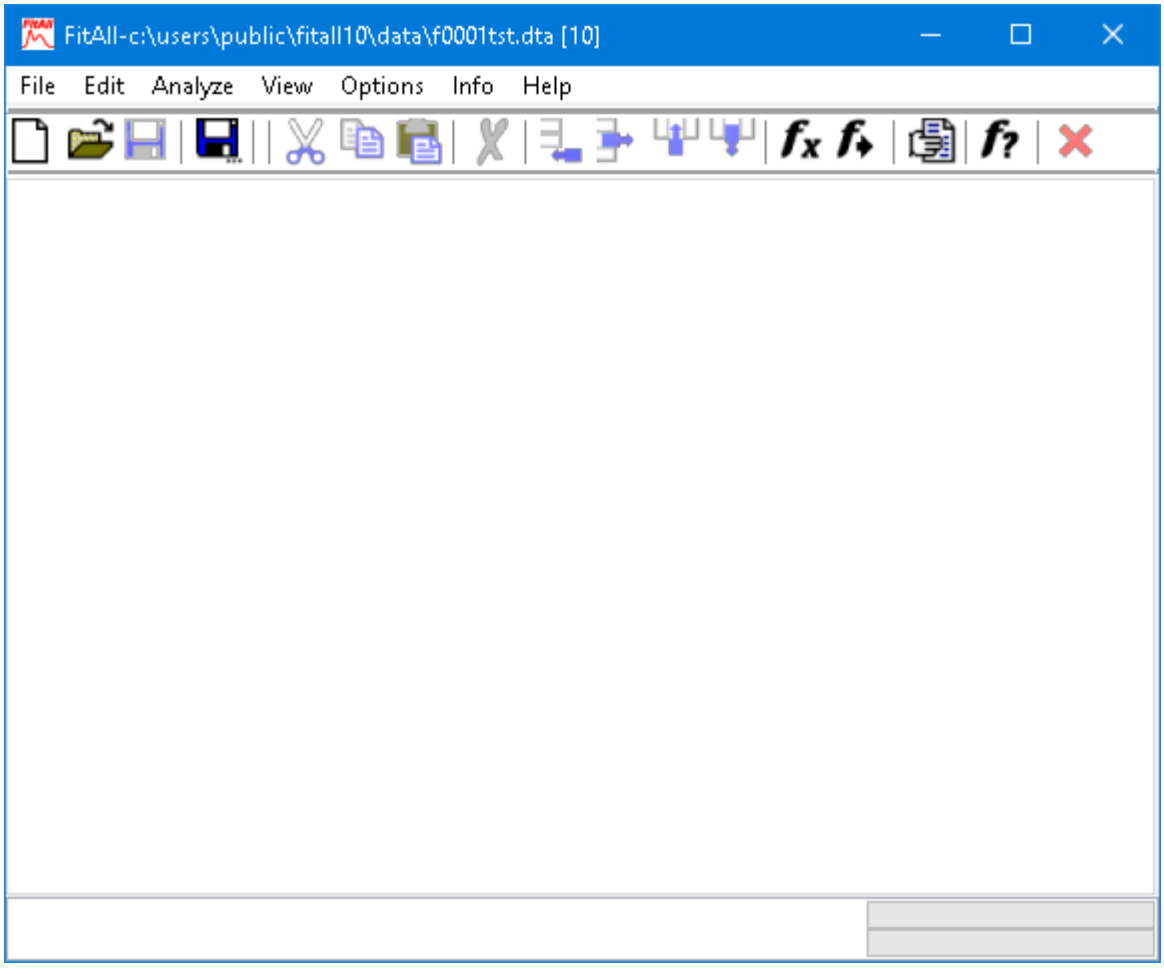
The first time that you start ***FitAll***:

- The 'Edit Serial Number' dialog box *may* appear. It looks like this:



- Enter your serial number.
- Click the OK button.

After a brief pause, ***FitAll***'s main window will appear. It should look like this:



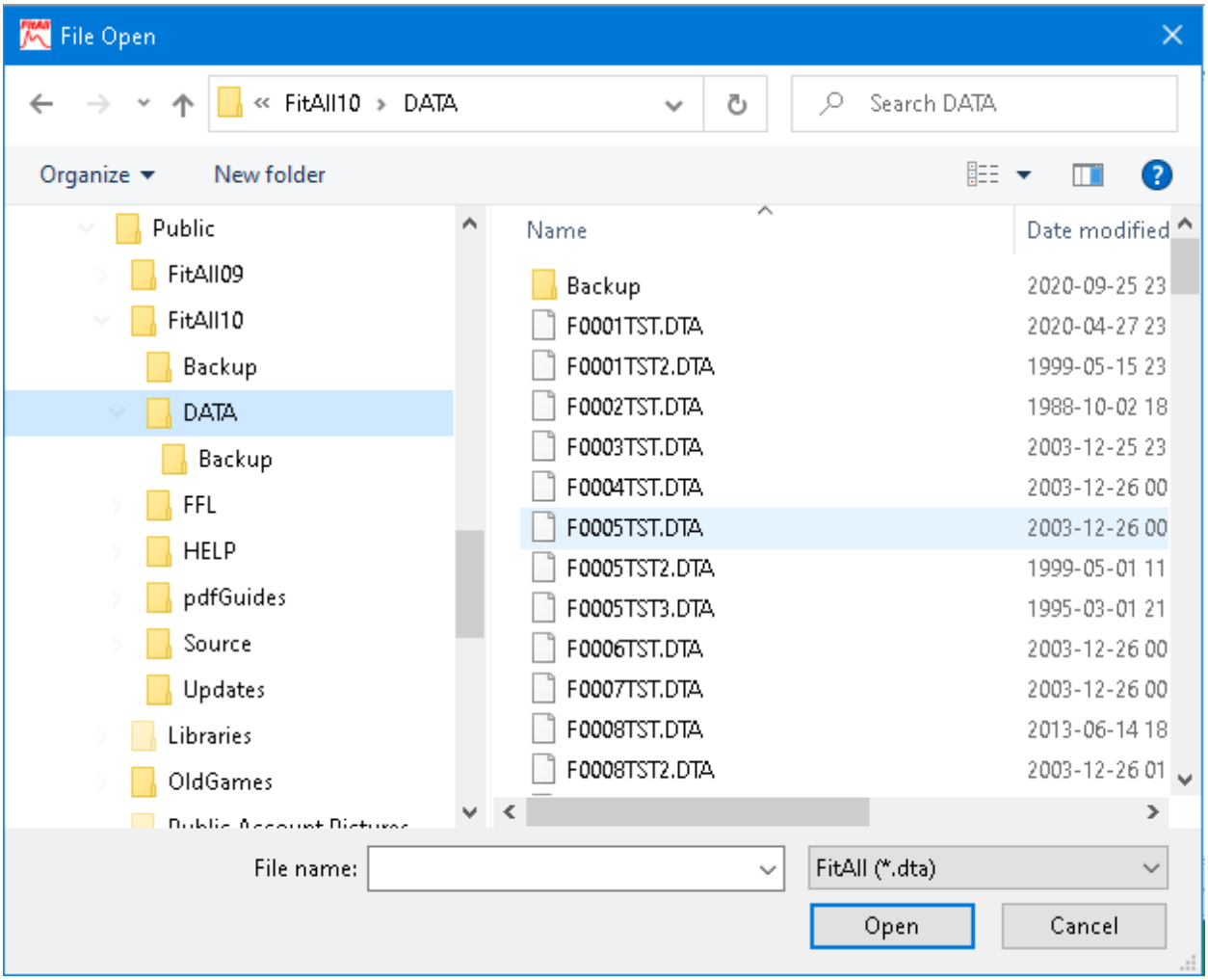
- The main menu is displayed across the top of the window.
- Below the menu is a toolbar, which has buttons representing the most commonly used commands.
- At the bottom of the main window there is a status line in which messages *may* appear.
- On the right side of the status line there are two progress bars.

Opening a Data File

To retrieve an existing set of data:

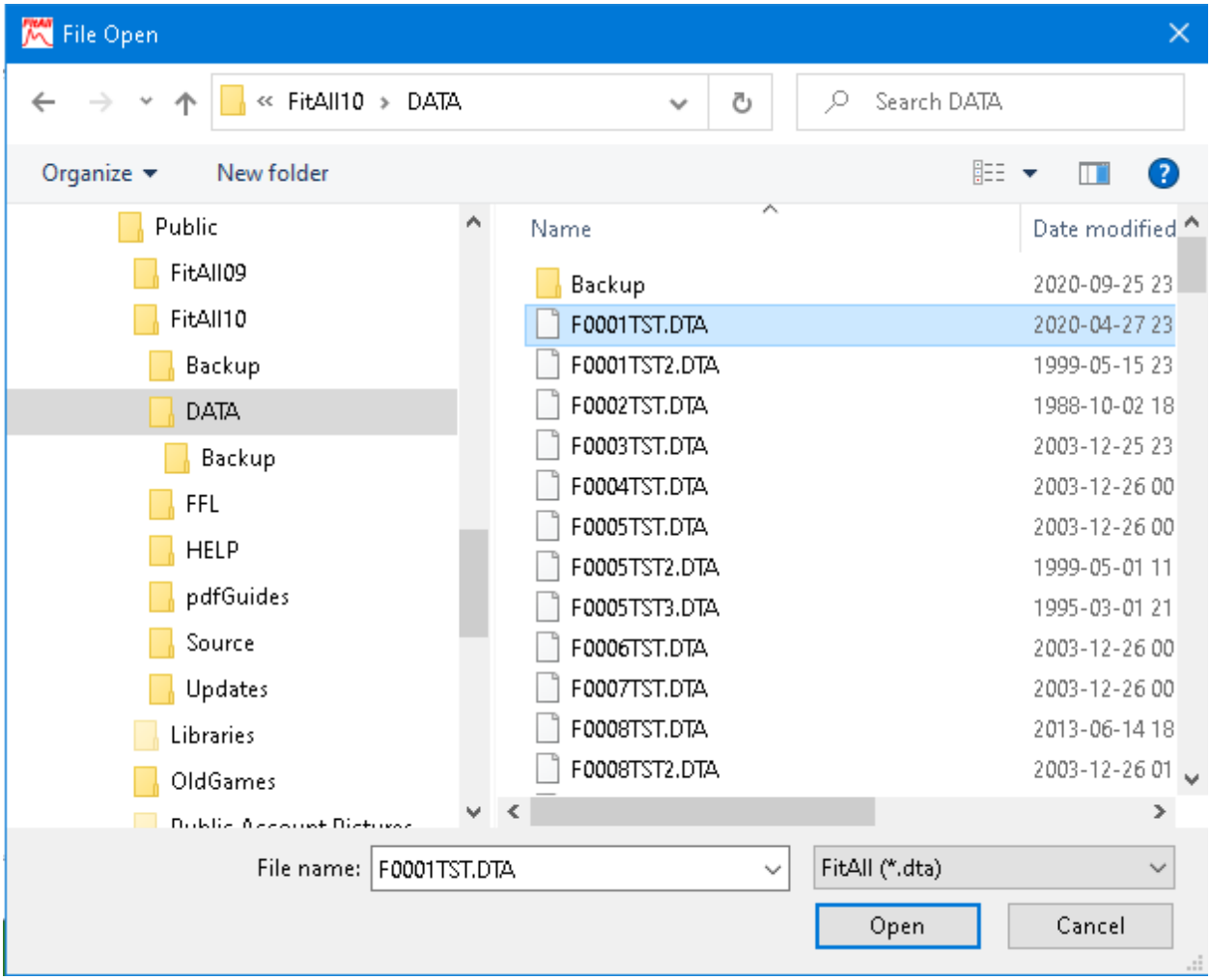
Click the File > Open menu selections, press Ctrl+O or click the button.

The File Open dialog box will appear. It should look like this:



Navigate to the Data directory and click on 'f0001tst.dta' to select this file as the one to open.

Your screen should look like this:

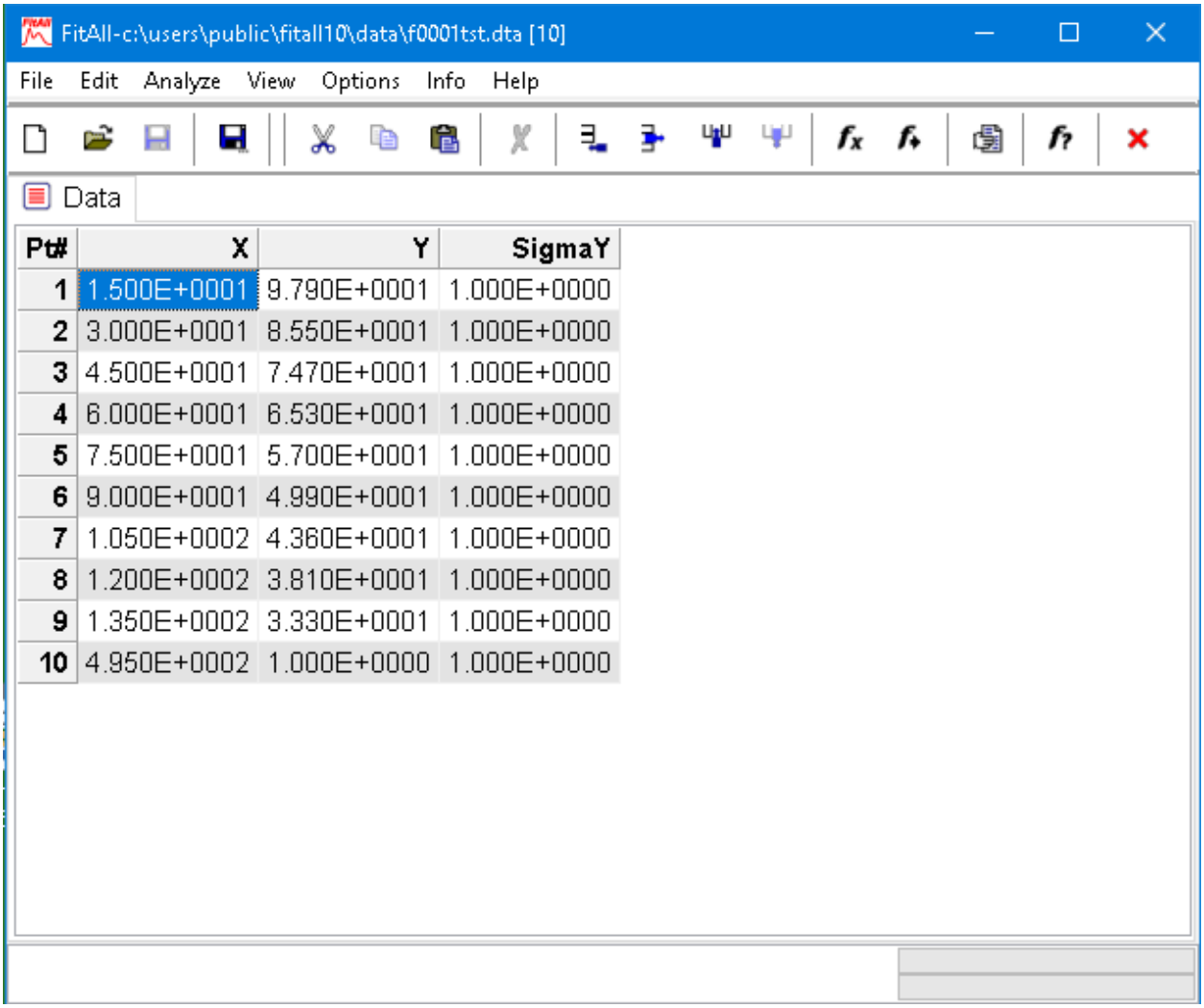


NOTE:
FitAll normally expects data files to have the file name extension ".DTA".

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' in the ***FitAll*** **Reference Guide**).

Click the Open button.

FitAll will retrieve the data and place it in its 'Data' window. Your screen should look like this:

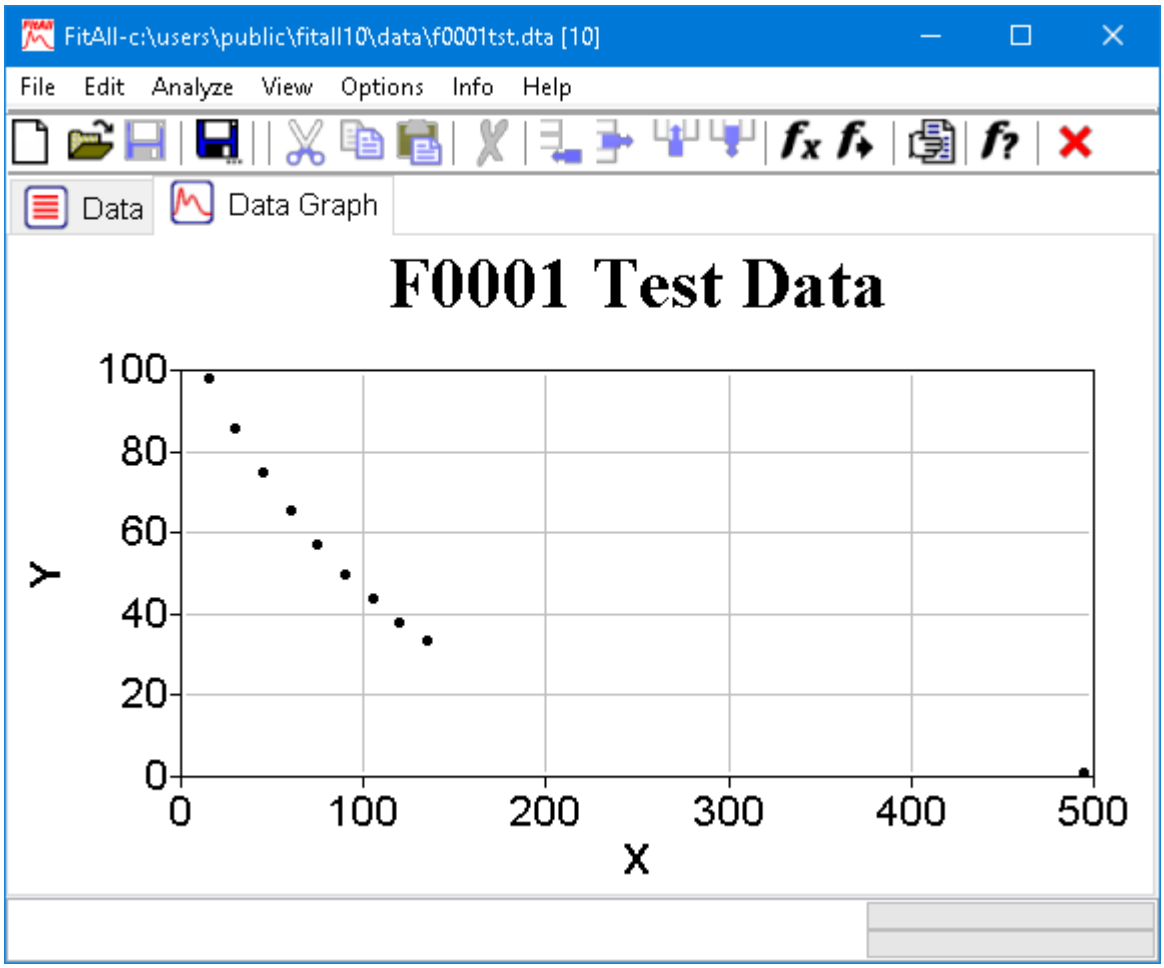


Pt#	X	Y	SigmaY
1	1.500E+0001	9.790E+0001	1.000E+0000
2	3.000E+0001	8.550E+0001	1.000E+0000
3	4.500E+0001	7.470E+0001	1.000E+0000
4	6.000E+0001	6.530E+0001	1.000E+0000
5	7.500E+0001	5.700E+0001	1.000E+0000
6	9.000E+0001	4.990E+0001	1.000E+0000
7	1.050E+0002	4.360E+0001	1.000E+0000
8	1.200E+0002	3.810E+0001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

Graphing the Data

To see a graph of the data:

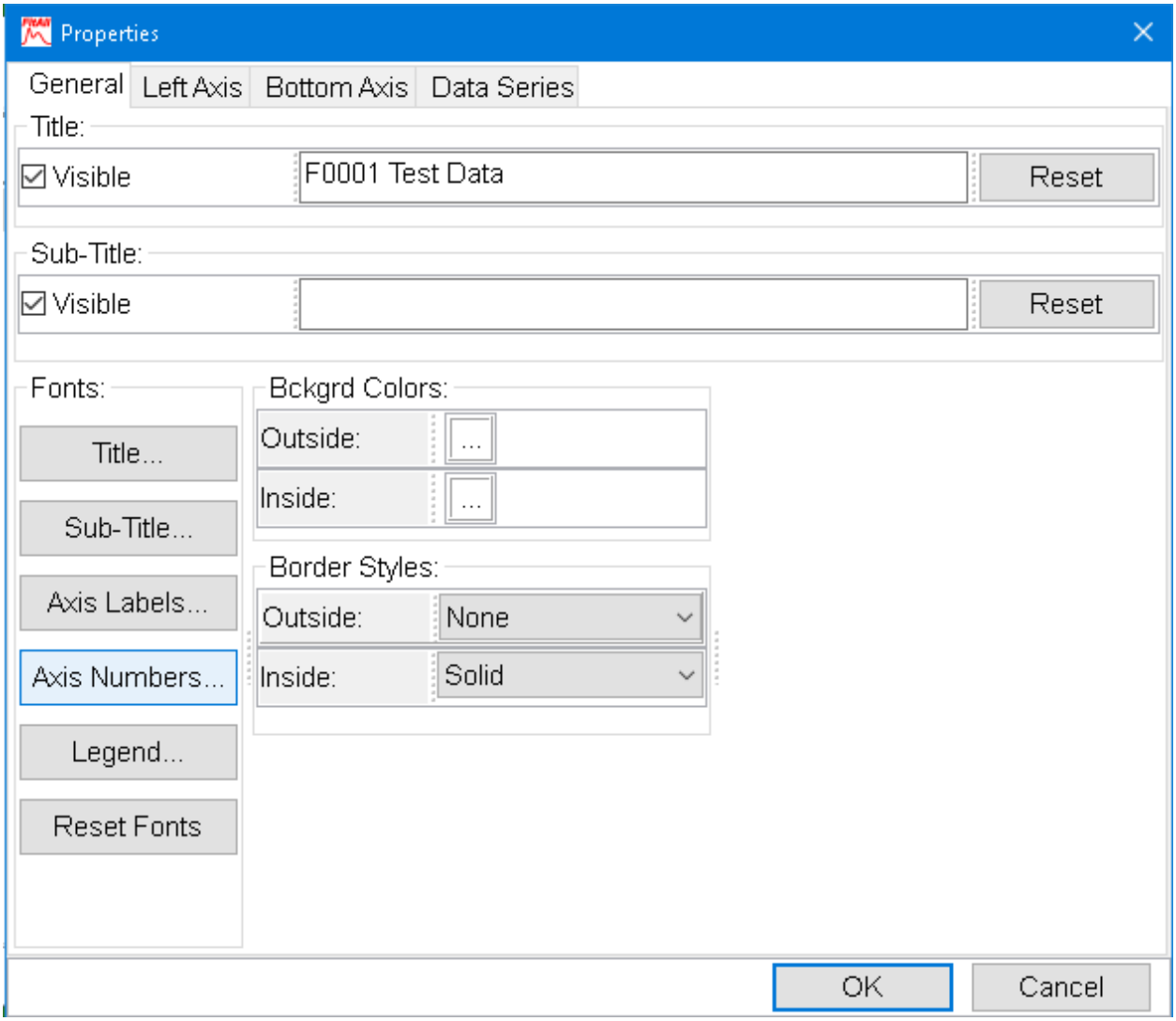
- Click the View > data graph menu selections.
- ***FitAll*** will open its 'data graph' window and place the graph in it. Your screen should look like this:



To change the appearance of the data graph:

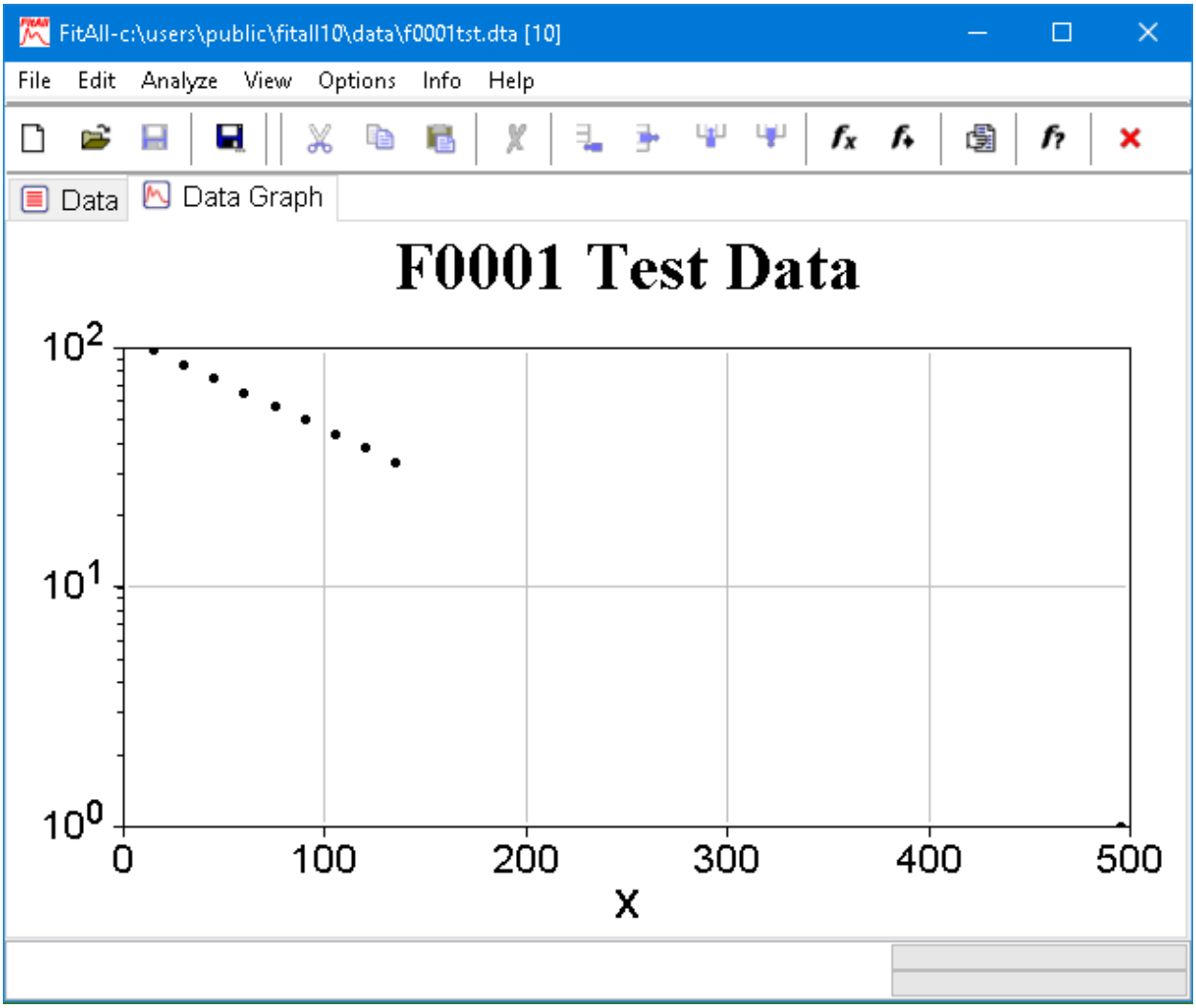
- Select the menu item Edit > Properties... or right-click anywhere in the data graph window and select the Properties... item on the resulting context menu.

The Properties dialog will appear. It should look like this:



- Make whatever changes you want and click the Ok button. For example, do the following:
  - Click on the 'Bottom Axis' tab.
  - Use the 'Label Fmt:' drop down list to change the format from '0.00' to '0'.
  - Click on the 'Left Axis' tab.
  - In the Scale Style group box, click the 'Log' radio button.
  - Click the Ok button.

The graph window should now look like this:



The Properties dialog box provides many other options for changing the appearance of the graph.

Most of the settings are saved when the window is closed and are used again when the same window is next displayed.

Setting up the Analysis

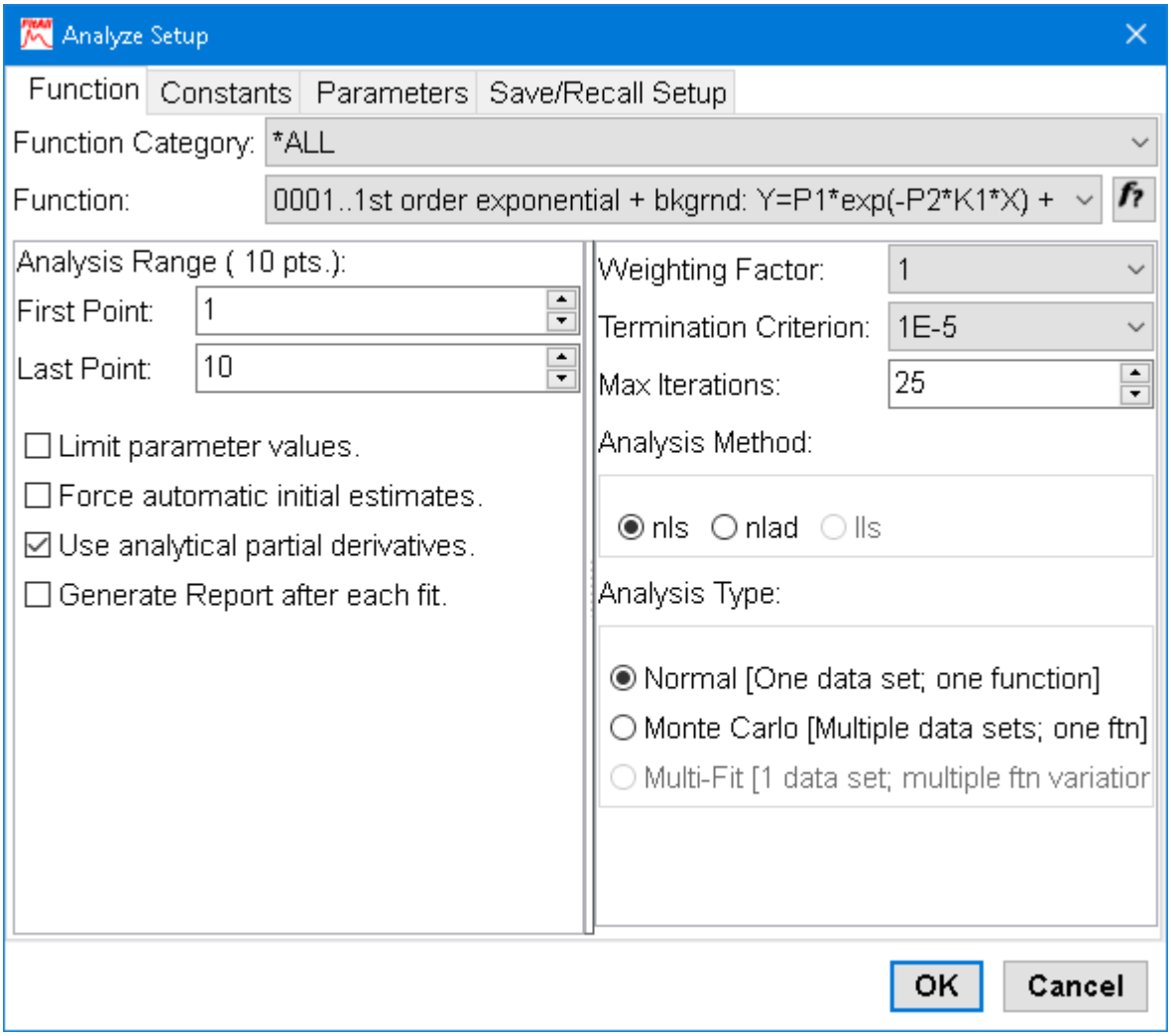
Before ***FitAll*** can analyze the data, it must be told a number of things, including:

- Which function to use.
- Which weighting factor to use.
- Which data points to use.

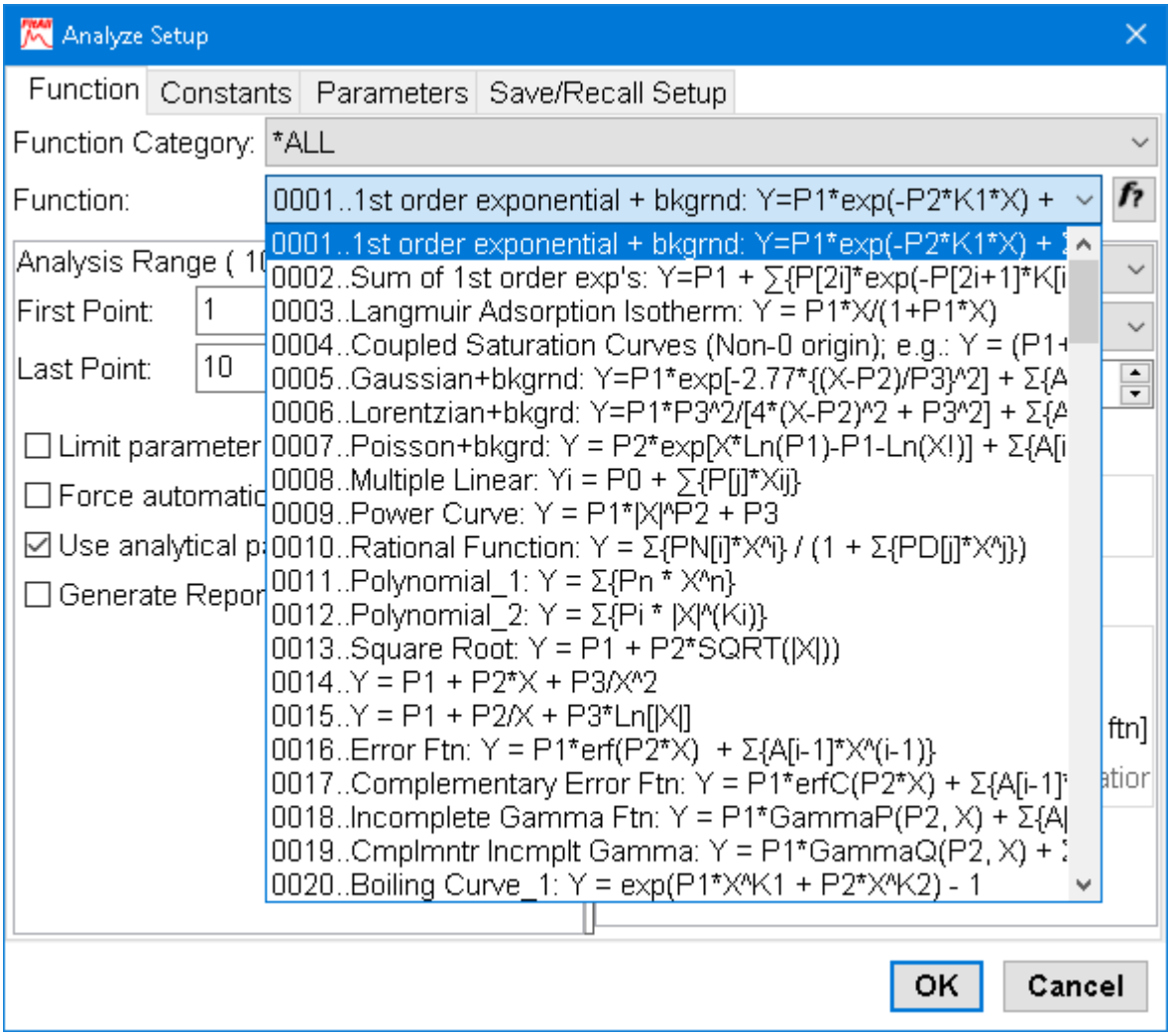
Here's how to do it:

- Click the Analyze > Setup menu selections, press Alt+S or click the f_x button, located on the toolbar under the main menu.

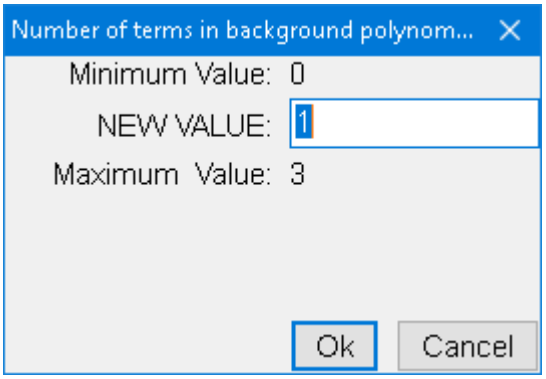
  The 'Analyze Setup' dialog box will appear. It should look like this:



- Use the Function drop-down listbox to choose function number 0001.



- When the 'Number of terms in background polynomial' dialog box appears, change the value to one and click the **OK** button.

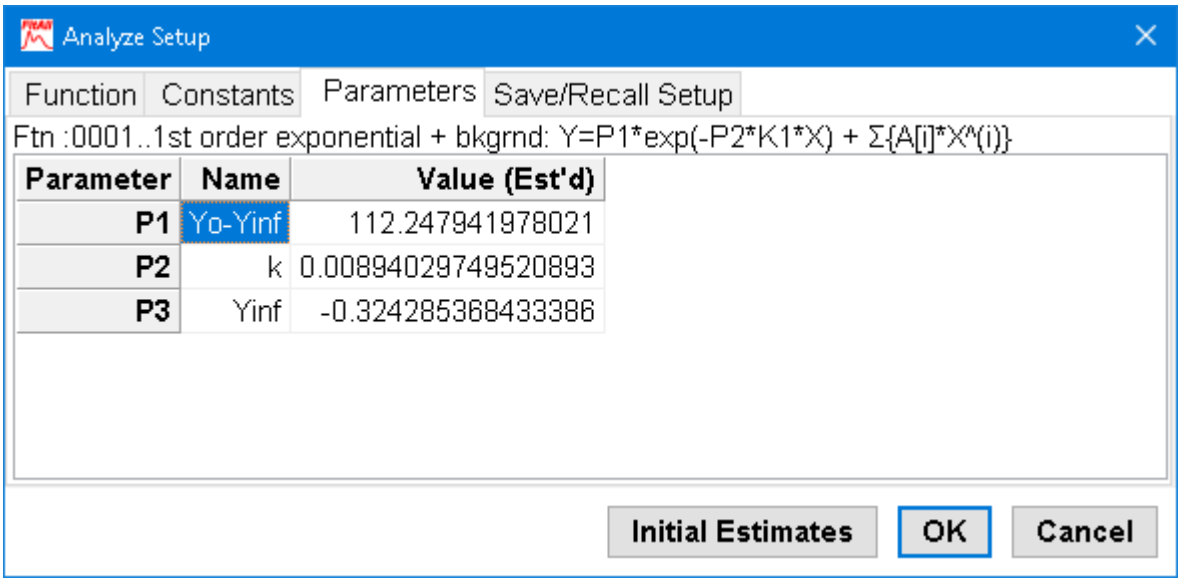


NOTE:
When more than one variation of a function is available, one or more dialog boxes may appear requesting additional information.

- Confirm that the 'Force automatic initial estimates' and 'Limit parameters' check boxes are *not* checked, that the 'Analysis Range' is 1 to 10, the 'Analysis Method' is nlls and the 'Monte Carlo' checkbox is *not* checked.

- Click on the 'Parameters' tab.

Click the 'Initial Estimates' button. The SetUp dialog's 'Parameters' page should look like this:



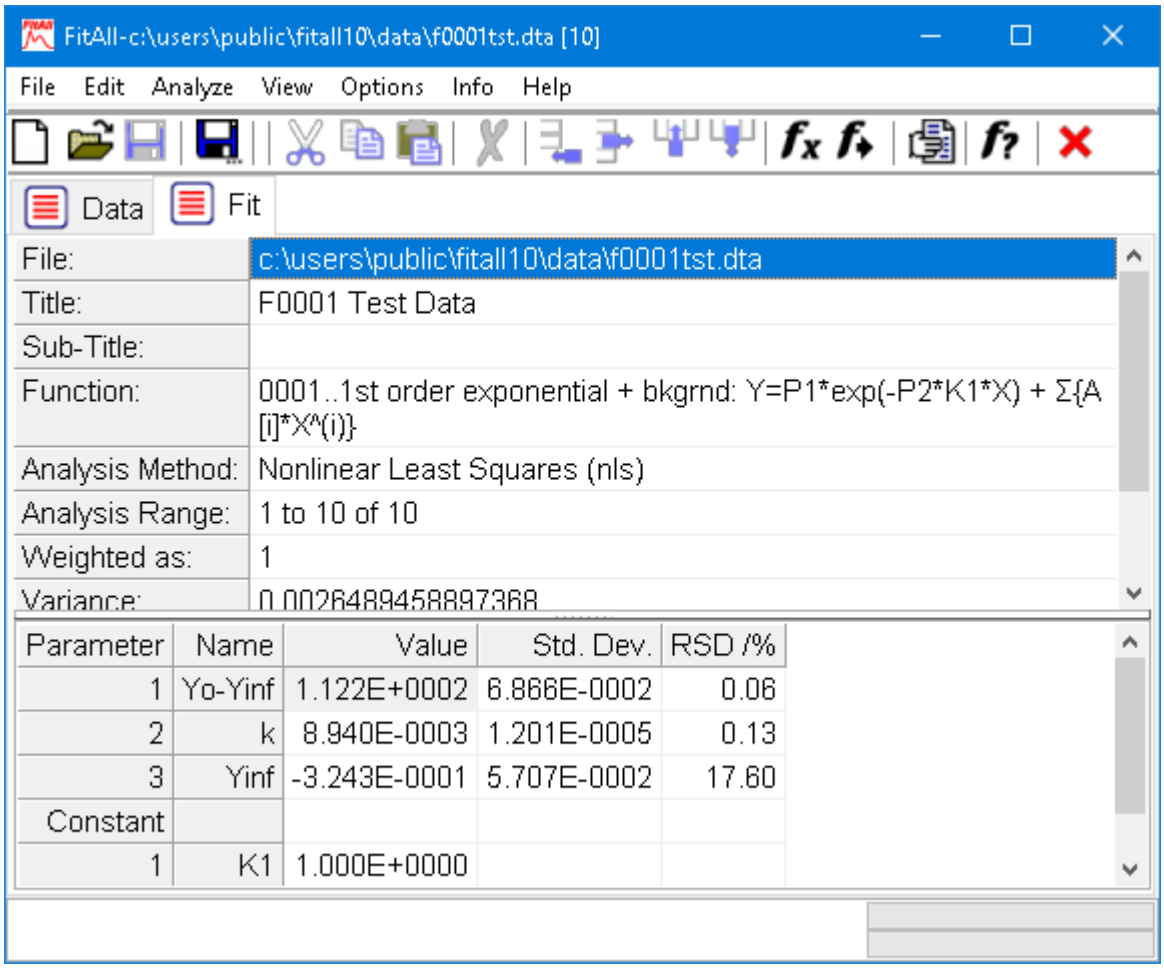
- Click the **OK** button.

Analyzing the Data

To analyze the current data with the function and other settings selected in the 'Analyze > Setup' dialog box do the following:

- Click the Analyze > Analyze menu selections, press Alt+N or click the  button, located on the toolbar under the main menu.
- ***FitAll*** will do the analysis and place the results in its 'Fit' window.

Your screen should look like this:



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		

The 'Fit window' contains two grids.

The upper grid lists the following information:

- The data file that was analyzed.
- The data set's title.
- The data set's sub-title.
- The name of the function used to analyze the data.

- The analysis method used (nls, nlad or lls).
- The analysis range; i.e., the data points used.
- The weighting factor that was used.
- The variance of the fit.
- The standard deviation of the fit.
- The number of iterations required to obtain the fit.

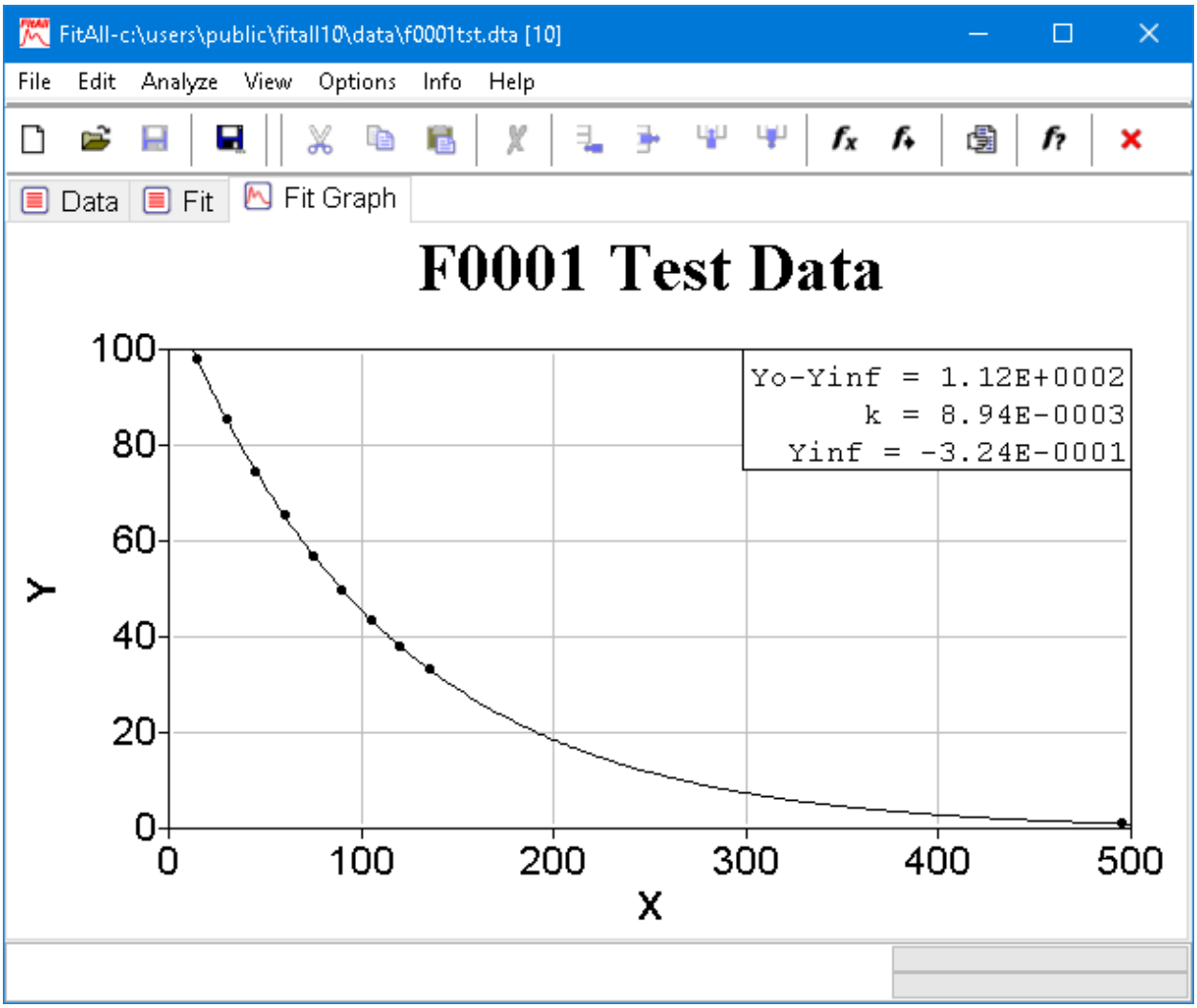
The bottom grid lists the following information:

- The names of the resolved parameters.
- The values of the resolved parameters.
- The standard deviations of the resolved parameters.
- Optionally, the relative standard deviation. RSD%, of the resolved parameters
- The names and values of all constants.
- If parameter limits were used, the upper and lower limiting values for each of the parameters.

Plotting the Fit

To see a graph of the fit:

- Click the View > fit graph menu selections.
- ***FitAll*** will open its 'fit graph' window and place the graph in it. Your screen should look like this:



The appearance of the fit graph can be changed by setting its properties in the same way that the data graph's appearance [22] is changed.

Saving a Graph as a Picture

To save the fit graph as an image, do the following:

- Make sure that the window containing the graph you want to save as a picture is the active window. If it is not, click the appropriate tab.
- Click the File > Save as... menu selections or click the  button located on the tool bar.
- When the 'Save as...' dialog box appears, enter a name for the graph in the 'File Name' edit field.
- Use the 'Save as Type' drop-down list to choose the type of graphic file to create. ***FitAll*** can save a graph as:
    - a Bitmap file (*.bmp).
    - a JPEG image file (*.jpg).
    - a Portable Network Graphics file (*.png).
- Click the **OK** button.

Copying a Graph to the Clipboard

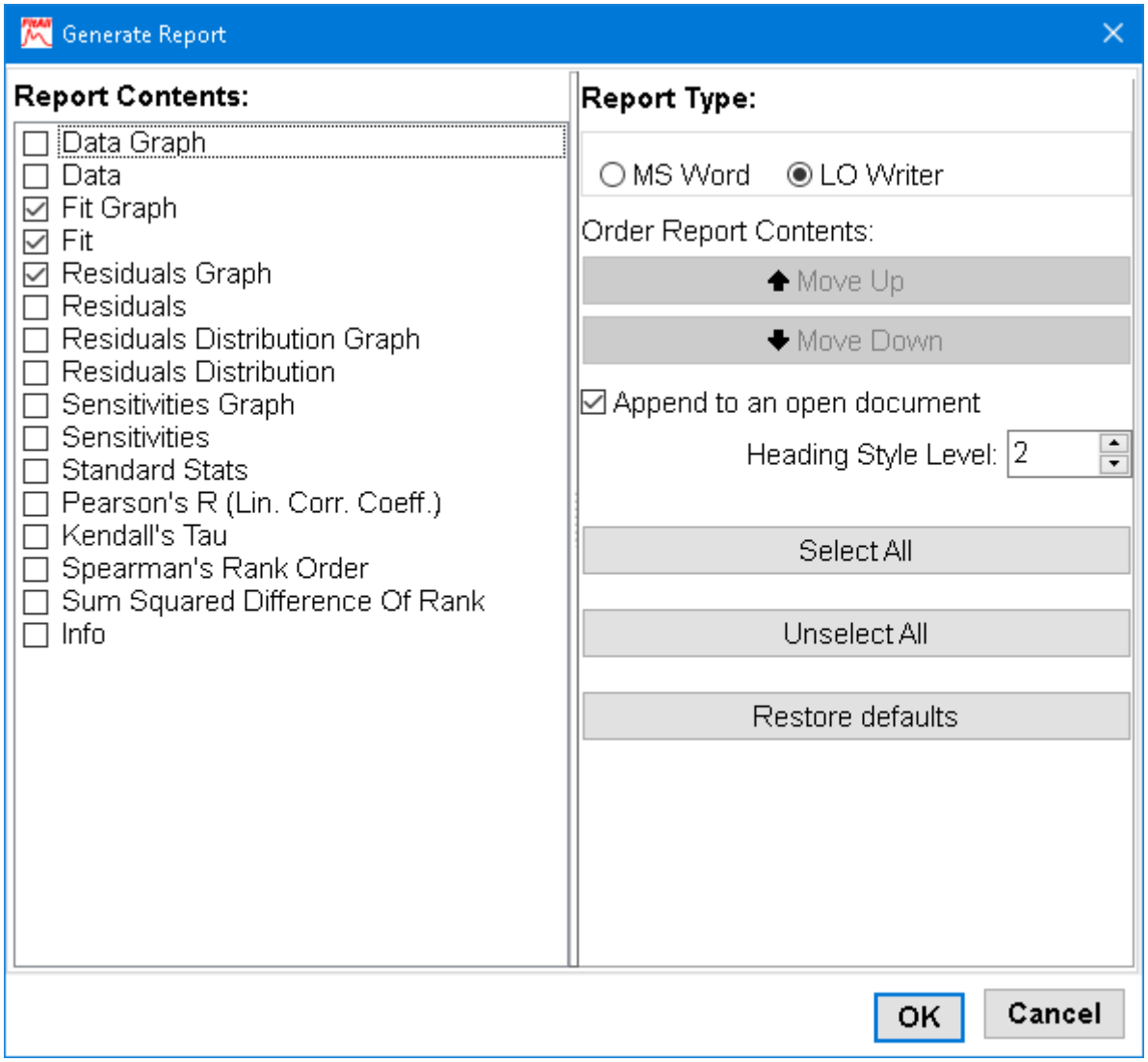
To copy the fit graph as an image to the clipboard so that it can be pasted into other programs, do the following:

- Make sure that the window containing the graph you want to copy is the active window. If it is not, click the appropriate tab.
- Click the File > Print to clipboard or the Edit > Copy menu selections.
- The graph will be copied to the clipboard as a bitmap.

Generating a Report

To generate a MS Word report do the following:

- 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:



- Check the "Report Contents" items that you want to appear in the report.
- Use the "Move Up" and "Move Down" buttons of change the order of the report items.
- Click the **OK** button to generate the report.

Entering and Editing Data

To add a data point to the data set in memory:

? Make the 'Data' window the active window by clicking 'Data' tab or by choosing the View > Data menu selections.

The 'Data' window might look like this:

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

? Click the Edit > Row Add menu selections, press the Insert key or click the button.

A data point will be appended to the end of the current data set. The values in each column will be zero with the possible exception of the last column. The 'Data' window should now look like this:

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
11	0.000E+0000	0.000E+0000	1.000E+0000

NOTE:
When entering many rows of data it is often useful to allow the pressing Return / Enter key to automatically add a new row when the cursor is on the last cell in the table.

To do this select the menu items Options > Preferences > General 2 and check the "Return / Enter Appends Data Row" checkbox.

? To enter a new value for a number, select the number you want to change by clicking on it or by using the arrow keys to highlight it.

For example, if you want to edit the values in the data point that was just added to the data set, use the arrow keys to highlight the eleventh X-value.

The 'Data' window should now look like this:

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
11	0.000E+0000	0.000E+0000	1.000E+0000

? Type in the new number. (For example: **200**).

When you start to type the new number, the value you are replacing will be deleted.

? Press the Enter key to accept the new value or press the Esc key to cancel it.

? The 'Data' window should look like this:

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
11	2.000E+0002	0.000E+0000	1.000E+0000

? Change the value of Y to **185** for data point number 11 , by typing **185**, and pressing the Enter key.

The 'Data' window should look like this:

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
11	2.000E+0002	1.850E+0002	1.000E+0000

? To save the changed data set, click the menu selections File > Save, press Ctrl + S or click the button on the toolbar.

? To save the changed data with a different name, click the menu selections File > Save as... or click the button on the toolbar.

Creating a New Data Set

What's in a Data Set

Each ***FitAll*** data set consists of a title, at least three (3) columns of numbers and a heading for each of the columns. The three columns of data correspond to the X-values, the Y-values and the SigmaY-values. SigmaY is the value of the measurement error (standard deviation) associated with the Y-value.

For example, if you were keeping a record of the daily noon-time temperature and you had a thermometer that was marked off in one degree intervals, you would record each temperature as a whole (integer) number of degrees even if the actual temperature was between two of the graduation marks. In choosing the number to record, you would choose the lower value if the temperature was closer to it or the higher value if the temperature was nearer to that marker. The net result is that any given temperature could be in error by as much as 0.5 degrees. The value of SigmaY for each temperature that you record would then be 0.5

> **NOTE**:
> This is a simplified example. The actual standard deviation, SigmaY, would be on the order of 0.3.

The errors, SigmaY, can be used by ***FitAll*** to weight the data. The result of the weighting is to de-emphasize those data points that contain large measurement errors so that they do not distort the curve fit by too much.

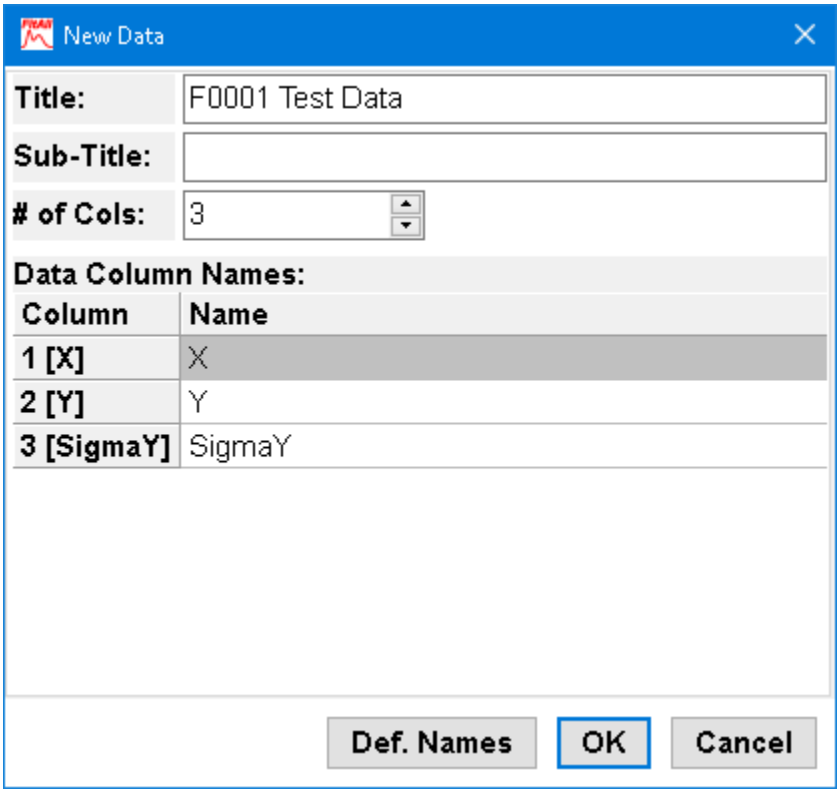
All data sets entered into ***FitAll*** must contain a set of SigmaY values. If these values are not available or are not known, use a value of 1 for SigmaY. The result of entering a value of 1 will be to weight the data equally, even when ***FitAll*** may 'think' that it is using a different weighting scheme.

Creating a Data Set

To create a new data set:

- Click the File > New menu selections, press Ctrl+N or click the  button.

  The 'New Data' dialog box will appear. It should look like this:

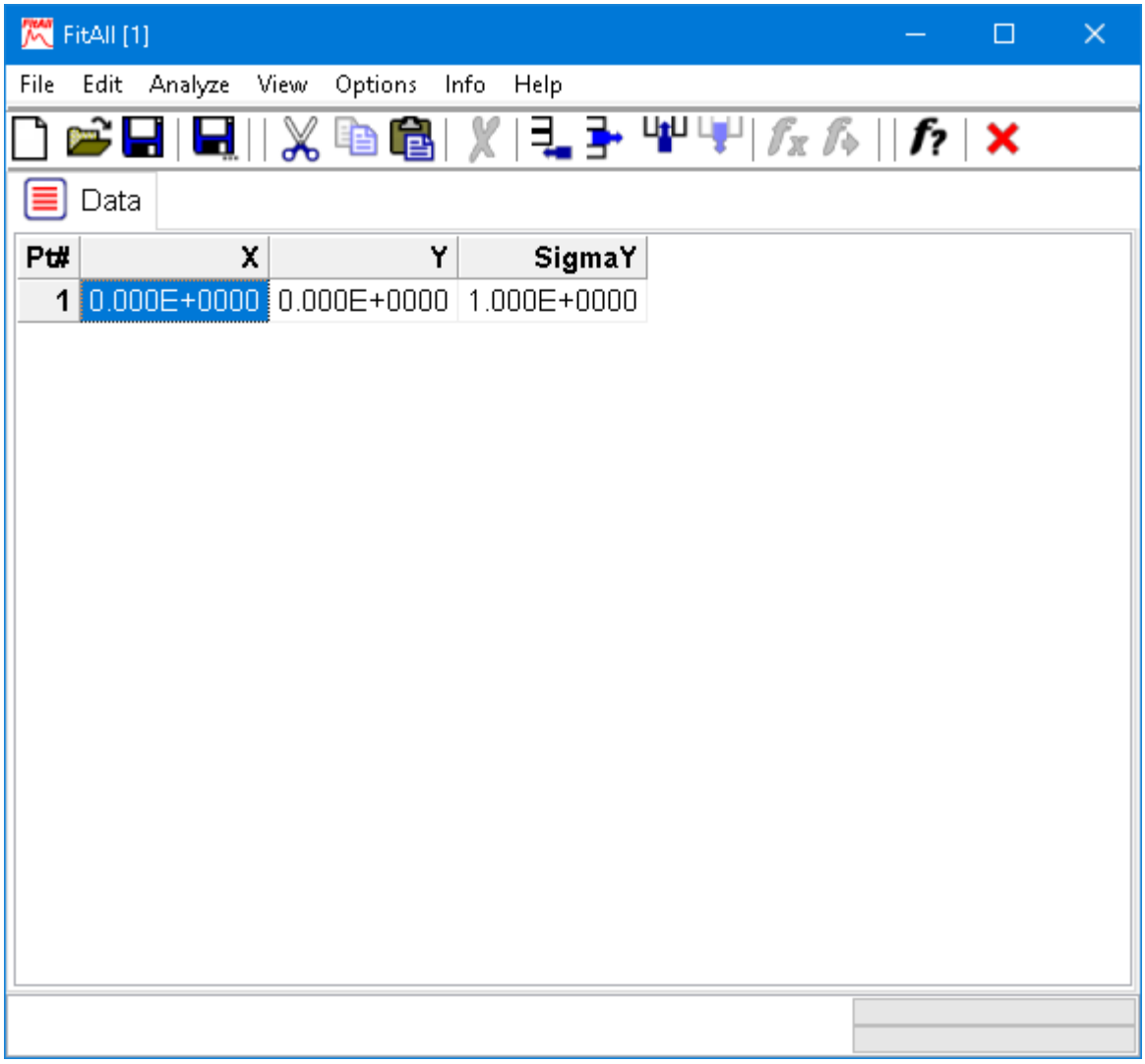


NOTE:
If the current data set has not been saved since it was last modified, you will be asked whether it should be saved before the new data set is created.

If you want to save it, click the **Yes** button, otherwise click the **No** button.

- Click in the 'Title' edit box and type in a title for this data set. For example, type: **My First Data Set**.
- Click in the 'Sub-Title' edit box and type in a sub-title for this data set. For example, type: **My First Sub-Title**.
- Click on the '# of columns' spin-edit box to set the number of data columns that you want.
- Click in the 'Data Column Names' table. Use the up and down arrow keys to highlight the name you want to change. Type in the new column name.
- Press the Enter key to accept the new name or press the Esc key to cancel the entry.
- When you have made all the changes that you want, 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.



- Edit and enter more data points in the same way as explained in 'Entering and Editing Data 34'.

How To

Add Scripted Functions

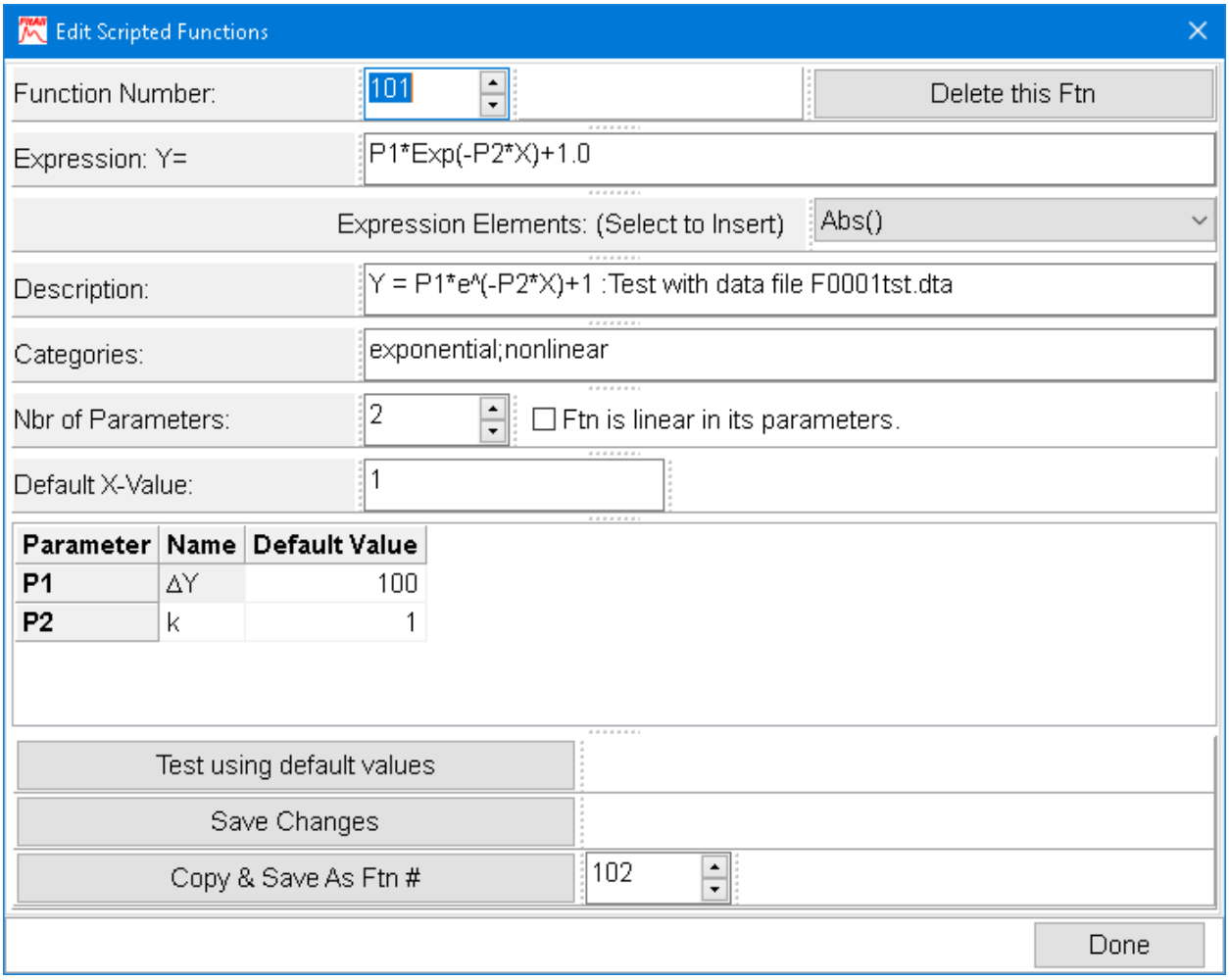
To add your own scripted function to ***FitAll*** do the following:

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.

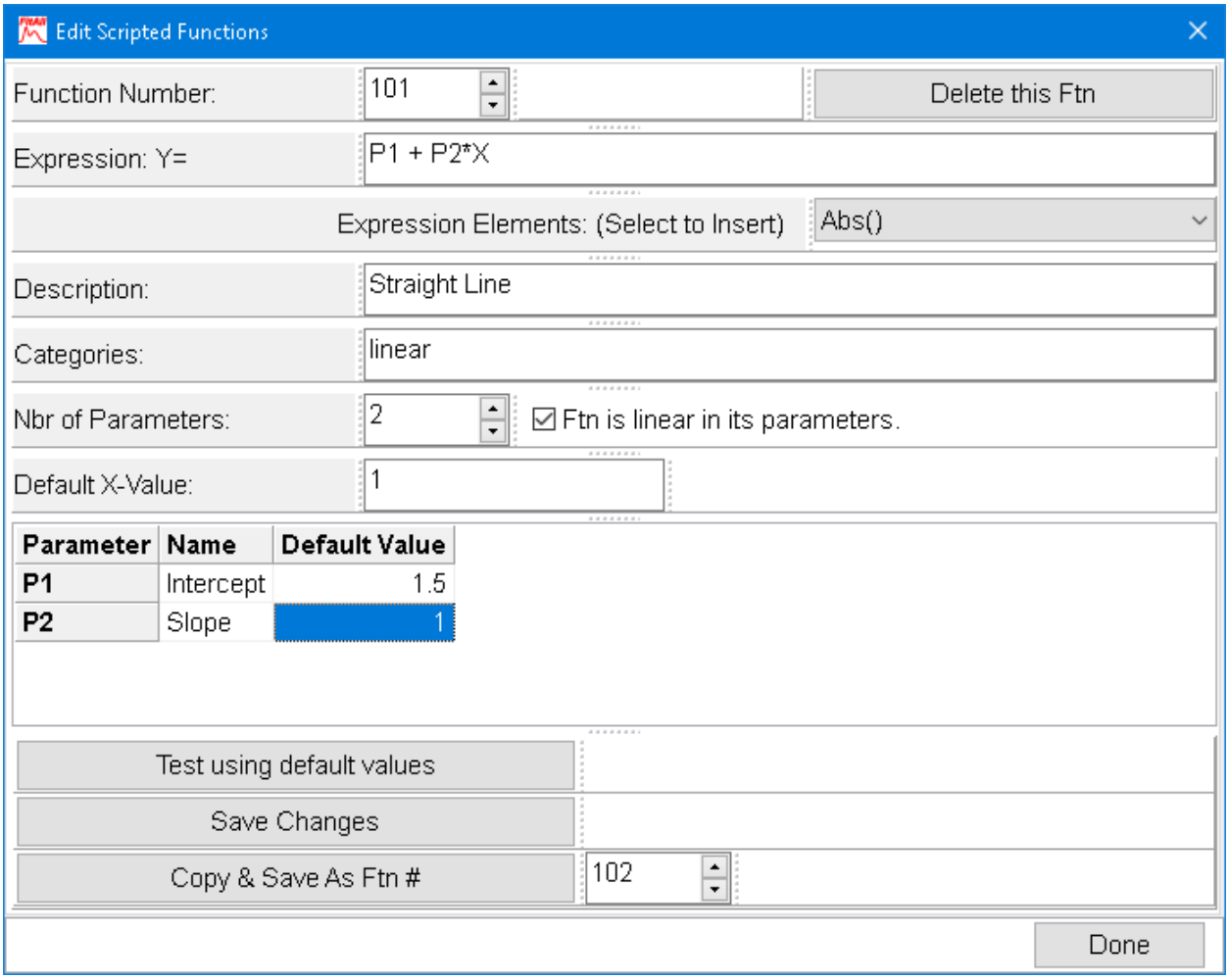
2. Make the menu selection Edit > Scripted Ftns.... The "Edit Scripted Functions" dialog that appears will look like this:



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.

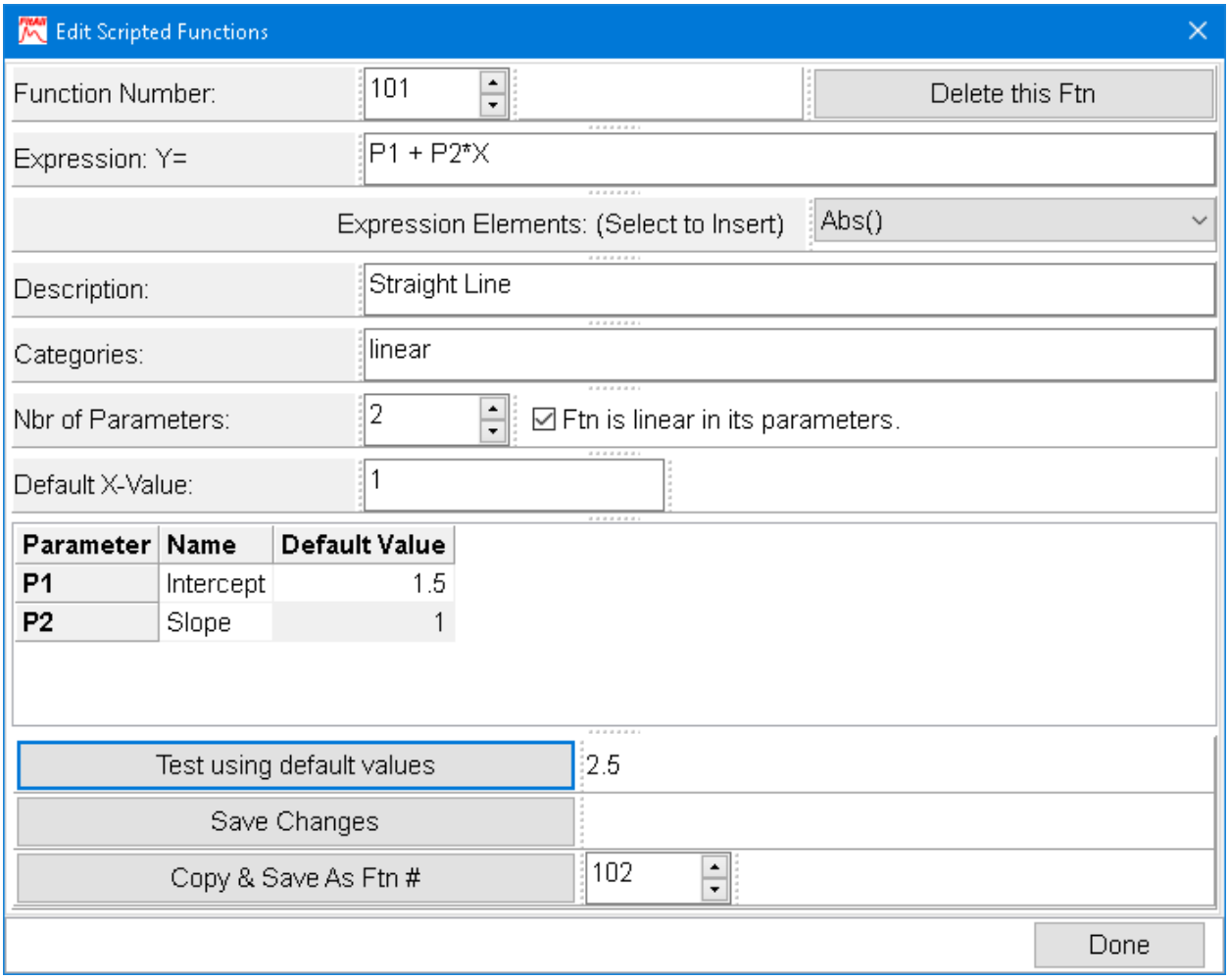
   In this example, edit the definition of function 101.

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.

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.

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**.

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