
Version 6.2

FitAll

nonlinear regression analysis

Getting Started Guide



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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](#) ³

[FitAll Basics](#) ¹¹

[FitAll Fundamentals](#) ¹⁹

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What's New

[New In FitAll version 6.2](#) 

[New In FitAll version 6.1](#) 

[New In FitAll version 6.0](#) 

New In FitAll version 6.2

FitAll version 6.2 has been enhanced to include the following new features:

1. The Research Edition of *FitAll* version 6.2 can act as an ActiveX (COM / Automation) server.

This means that other programs, such as data acquisition programs written in languages like C, Delphi, LabView and Visual Basic, can start *FitAll*, transfer data to *FitAll*, have *FitAll* do the regression analysis and retrieve the analysis results from *FitAll*.

A client application, **FaClient**, that demonstrates how *FitAll* can be controlled by other programs is included with *FitAll Research Edition*.

2. User defined **FitAll Function Libraries**, FFLs, can now be created using Delphi 5 to 2010 and **Free Pascal**, an open source compiler available from www.freepascal.org.

3. A **Check for Updates** selection is now available under *FitAll*'s Help menu as well as under MS Windows' menu selections Start, Programs, FitAll62.

This makes it easier for you to check for updates and to keep your copy of *FitAll* up to date.

Note: This feature is disabled in the Evaluation Edition of *FitAll*.

4. By default, *FitAll* is now installed in a directory that is accessible to all users of the computer. This is especially important on systems that are running MS Windows Vista or MS Windows 7.

Note: To install or uninstall *FitAll* a user with "Administrator Permissions" is still required.

5. A new selection, Pearson's R, has been added under the View menu.

Selecting this item will display a table containing the values of Pearson's R, which is also known as the Linear Correlation Coefficient, for each pair of data columns in the current data set.

6. Several minor bug fixes, such as ensuring that the colour of grid lines in a graph are properly saved and restored when the graph window is closed and then reopened.

New In FitAll version 6.1

FitAll version 6.1 has been enhanced to include the following new features:

1. *FitAll* can now do **Multi-Fit** analyses.

For **Multi-Fit enabled** functions, such as the multiple linear function

$$Y = \sum_j P_j * X_{i,K[j]}$$

FitAll can:

- Create a file that contains the possible function variation descriptions. -- In some cases there can be *millions* of variations.
- Analyze one set of data using each of the possible function variations and save the results in a file that can be viewed and further analyzed.

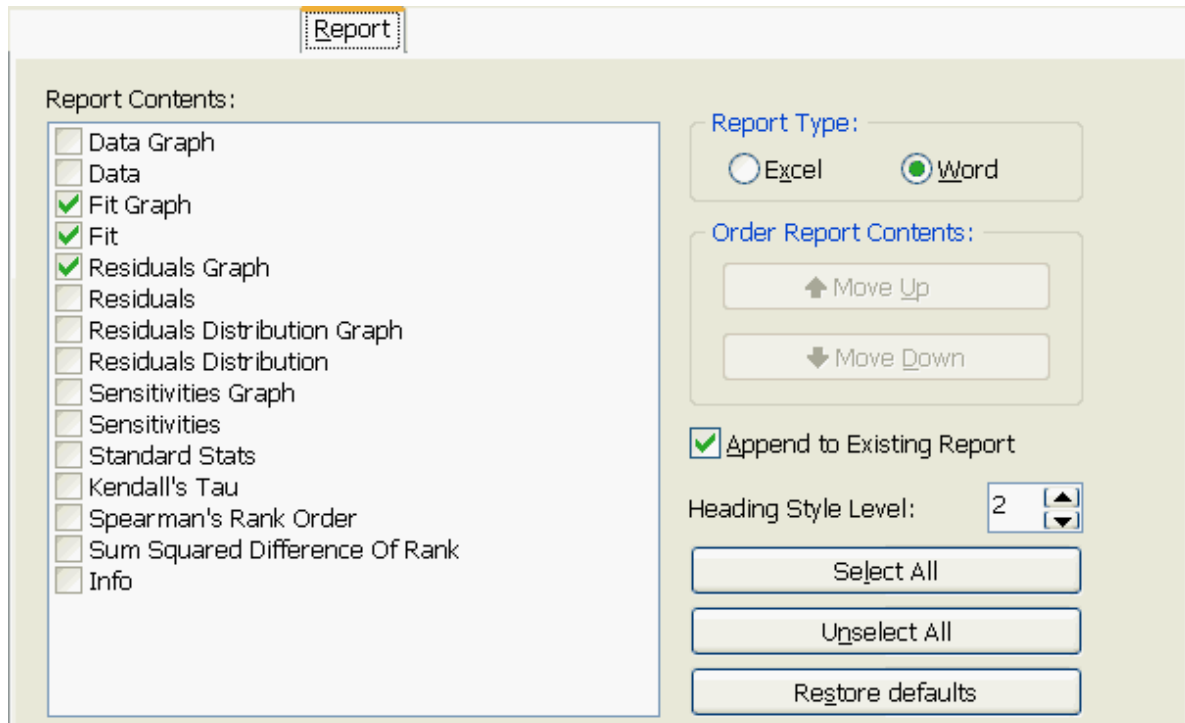
This capability is particularly useful in situations in which you would like to determine which of many independent variables are the most important predictors of the function's value.

For example, *FitAll* can now help you to answer a question such as: "Which of the independent variables: lot size, street frontage, number of stories, floor area, number of bedrooms, number of bathrooms, proximity to mass transit, proximity to schools, proximity to hospitals, proximity to shopping centers or proximity to recreational venues are the most reliable predictors of a residential property's assessed value?".

2. *FitAll* can now create **MS Word and MS Excel reports**.

The reports:

- Can include the information in any or all of *FitAll*'s windows and you can customize the order in which the information is presented.



- Can be appended to the end of an open, existing Word or Excel document. This makes it very easy to create one document that has the results from several analyses. Of course, if you so choose, a new document can be created for each report.
 - Can be created after every successful regression analysis. When doing Monte Carlo / Batch Mode or Multi-Fit analyses. This is a convenient way to automatically document all of the results that are generated.
3. The Monte Carlo analysis procedure has been generalized to facilitate **batch mode analysis** of data sets that may contain differing numbers of data points. This makes it easy to analyze tens, hundreds or even thousands of data sets to the same function and save all of the results in to another data file that can be viewed and further analyzed.
 4. A new **Multi-Fit enabled Multiple Linear** function has been added to the **Basic Functions Library**.
 5. Four new **Solar Cell Light I-V** functions have been added to the **Solar Cell Functions Library**.
 6. **FitAll** now can be configured to load the last used data file when it is started.

New In FitAll version 6.0

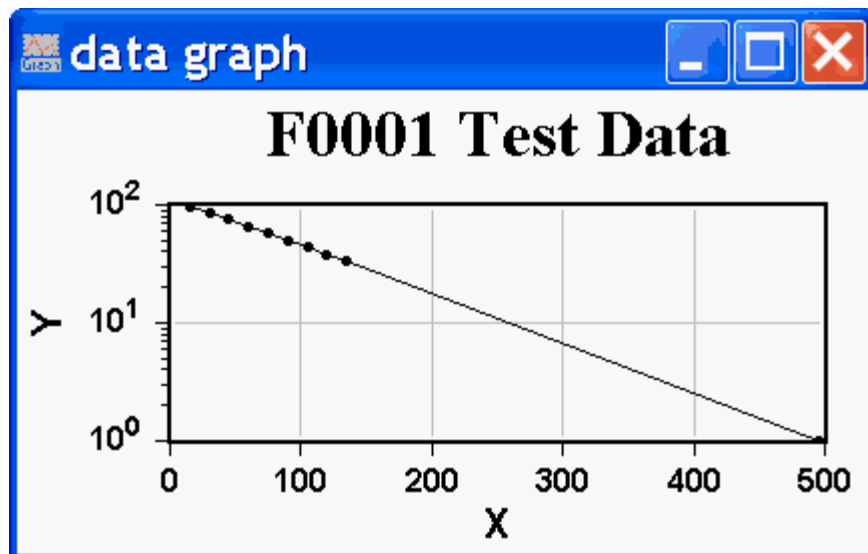
FitAll version 6.0 has been completely re-written and enhanced to take better advantage of the capabilities of Windows 98SE/2K/XP.

Here are just some of the enhancements and additions to *FitAll*:

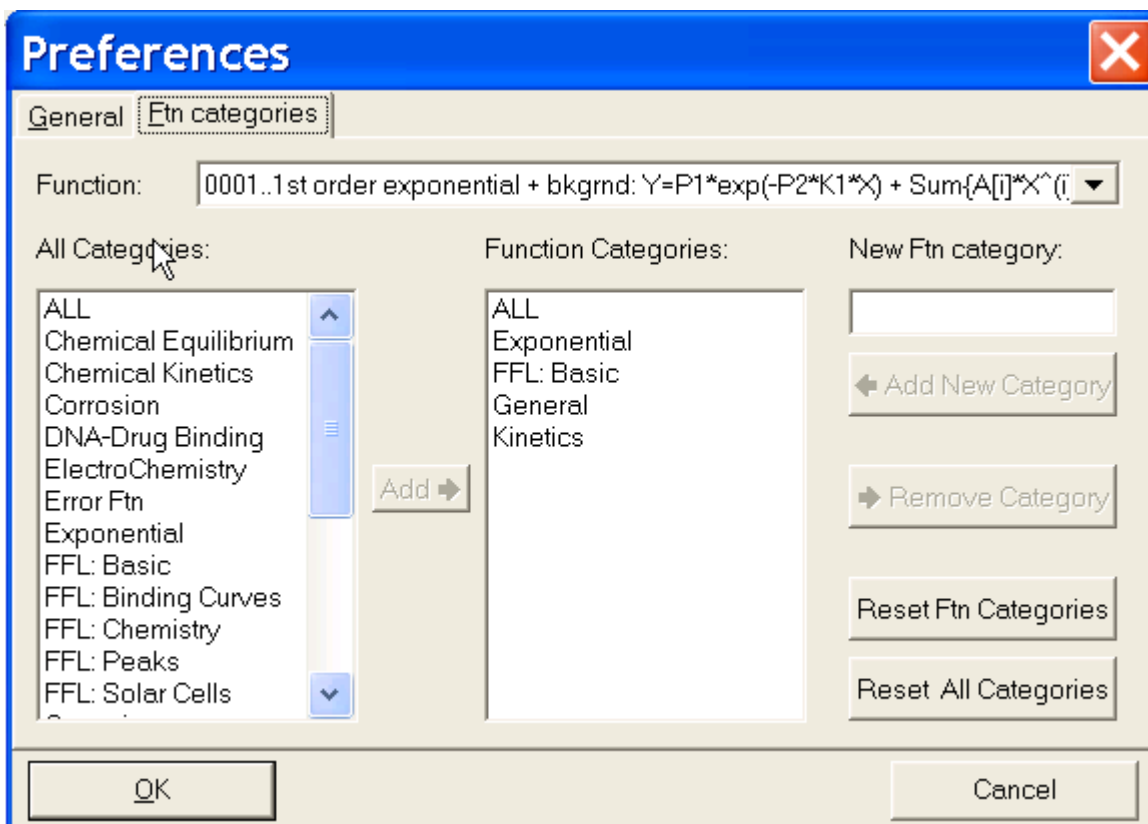
- The 'analysis set up' can be saved and recalled at a later time. If you have data sets that you want to analyze with the same function and settings, you now can do it quickly and easily.

Most settings are automatically saved so that when the same window is displayed, the last group of settings are used. -- This can be a real time-saver!

- All graphs have more 'properties' that you can use to customize them. For example, you can now change the background colour, the line width, the format of the numbers that are displayed on the axes, the width of the calculated lines and much more. Here's an example of a data graph with a logarithmic axis:



- *FitAll* now uses '*FitAll* Function Libraries' -- that means that adding functions to *FitAll* is easier, because changes to the *FitAll* program, itself, are not required. Instead, you can purchase additional function libraries from **MTR Software**, have **MTR Software** create a custom function library for you or you can create your own user defined *FitAll* Function Library.
- The available functions are now grouped into categories. This means that if you are looking for an exponential function, you can filter the function selection list by that category and, consequently, the list of functions from which to choose will be shorter. -- This makes it easier for you to identify and select the function that you want.
- You even can add categories of your own!

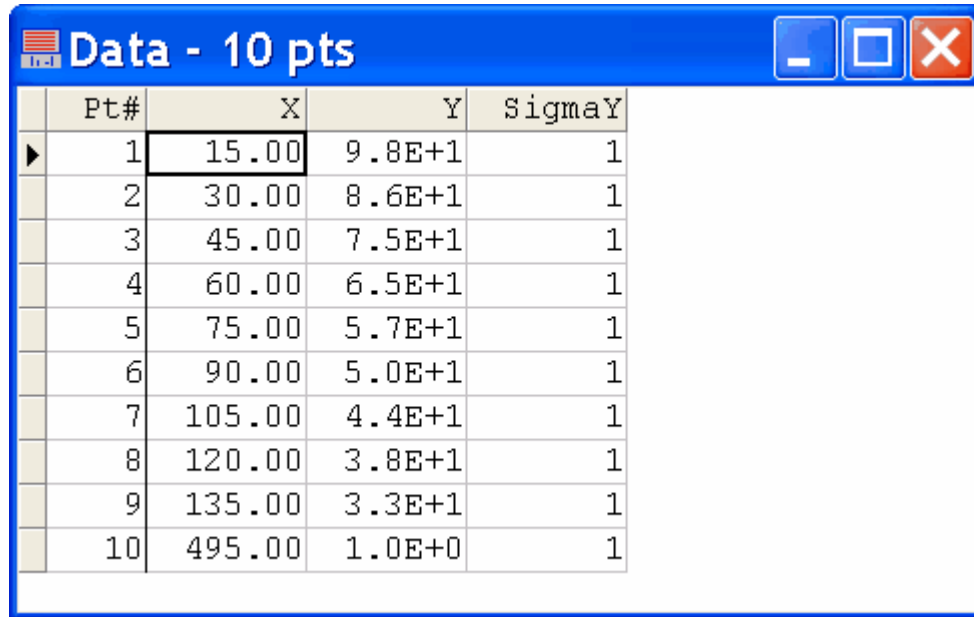


FitAll can save a graph in several graphics formats, including:

- as an Enhanced Meta file (*.emf),
- as a JPEG (*.jpg) file,
- as a bitmap (*.bmp), or
- as a Windows' Meta file (*.wmf).

This provides you with more flexibility in sharing graphs of your data and fits with other applications. -- For example, JPEG files can easily be included in internet web pages.

- It is now possible to format each column of numbers in the 'data window'. For example, the data window could look like this:



Pt#	X	Y	SigmaY
1	15.00	9.8E+1	1
2	30.00	8.6E+1	1
3	45.00	7.5E+1	1
4	60.00	6.5E+1	1
5	75.00	5.7E+1	1
6	90.00	5.0E+1	1
7	105.00	4.4E+1	1
8	120.00	3.8E+1	1
9	135.00	3.3E+1	1
10	495.00	1.0E+0	1

- Linear least squares regression analysis is now used to fit a function that is linear in its parameters. This speeds up the regression analysis of these functions.

FitAll Basics

[What FitAll Does](#) ¹²

[What FitAll Cannot Do](#) ¹⁵

[What You Need to Use FitAll](#) ¹⁶

[How to Install FitAll](#) ¹⁷

[How to Uninstall FitAll](#) ¹⁸

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:

$$Y_i = f(X_{ij}, K_k, P_p)$$

and

implicit functions with the general form:

$$Y_i = f(Y_i, X_{ij}, K_k, P_p)$$

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 independent 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 MS Excel 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 2000, XP, Vista or 7 capable computer.
2. MS Windows 2000, XP, Vista or 7.
3. A hard disk with at least twenty megabytes (20 MB) of available space.
4. 128 MB of memory (512 MB or more recommended).
5. The **FitAll** program.

Optional equipment:

1. MS Office 2000, 2002 or 2007 to generate the MS Excel and MS Word reports that can be created by **FitAll**.
2. A MS Windows compatible printer to print the tables and graphs created by **FitAll**.

To add your own functions to **FitAll**:

1. **FitAll Research Edition**.
2. **Delphi** version 5 to 2010 or **Free Pascal**, which is available from www.freepascal.org.

How to Install FitAll

1. Put the FitAll CD in the CD drive or, when purchased on-line, download the file to a directory of your choice.
2. Use Windows Explorer to locate the file named Fa06???.EXE; for example, Fa062.EXE.
3. Double click on the Fa06???.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, FitAll62, Uninstall FitAll .

1. In Windows 2K / XP / Vista:
Click Start, Settings, Control Panel.

In Windows 7:
Click Start, Control Panel.

2. In Windows 2K / XP
Double-click:
Add/Remove Programs

In Windows Vista:
Double-click Programs and Features.

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

3. Click on the **FitAll** item to select it.
4. Click the Ok or Change/Remove button or in MS Windows Vista and 7 double-click on the **FitAll** item.
5. Follow the on-screen instructions.

FitAll Fundamentals

[Starting FitAll](#) ²⁰

[Opening a Data File](#) ²²

[Graphing the Data](#) ²⁵

[Setting up the Analysis](#) ²⁸

[Analyzing the Data](#) ³¹

[Printing the Results](#) ³³

[Plotting the Fit](#) ³⁴

[Printing a Graph](#) ³⁵

[Saving a Graph as a Picture](#) ³⁷


[Generating a Report](#) ³⁸

[Entering and Editing Data](#) ³⁹

[Creating a Data Set](#) ⁴³

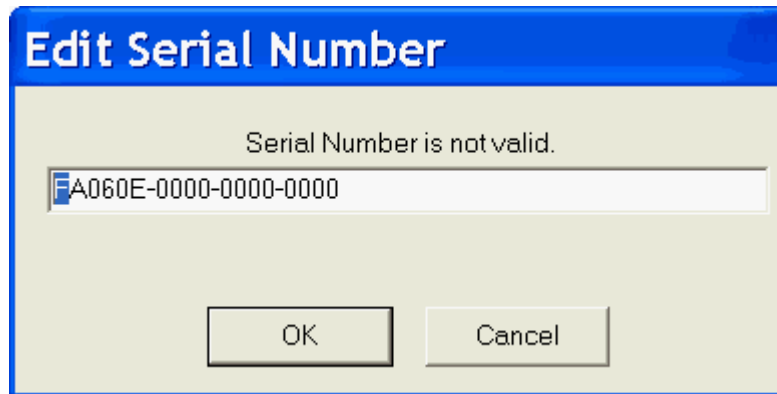
Starting FitAll

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, FitAll62, FitAll.

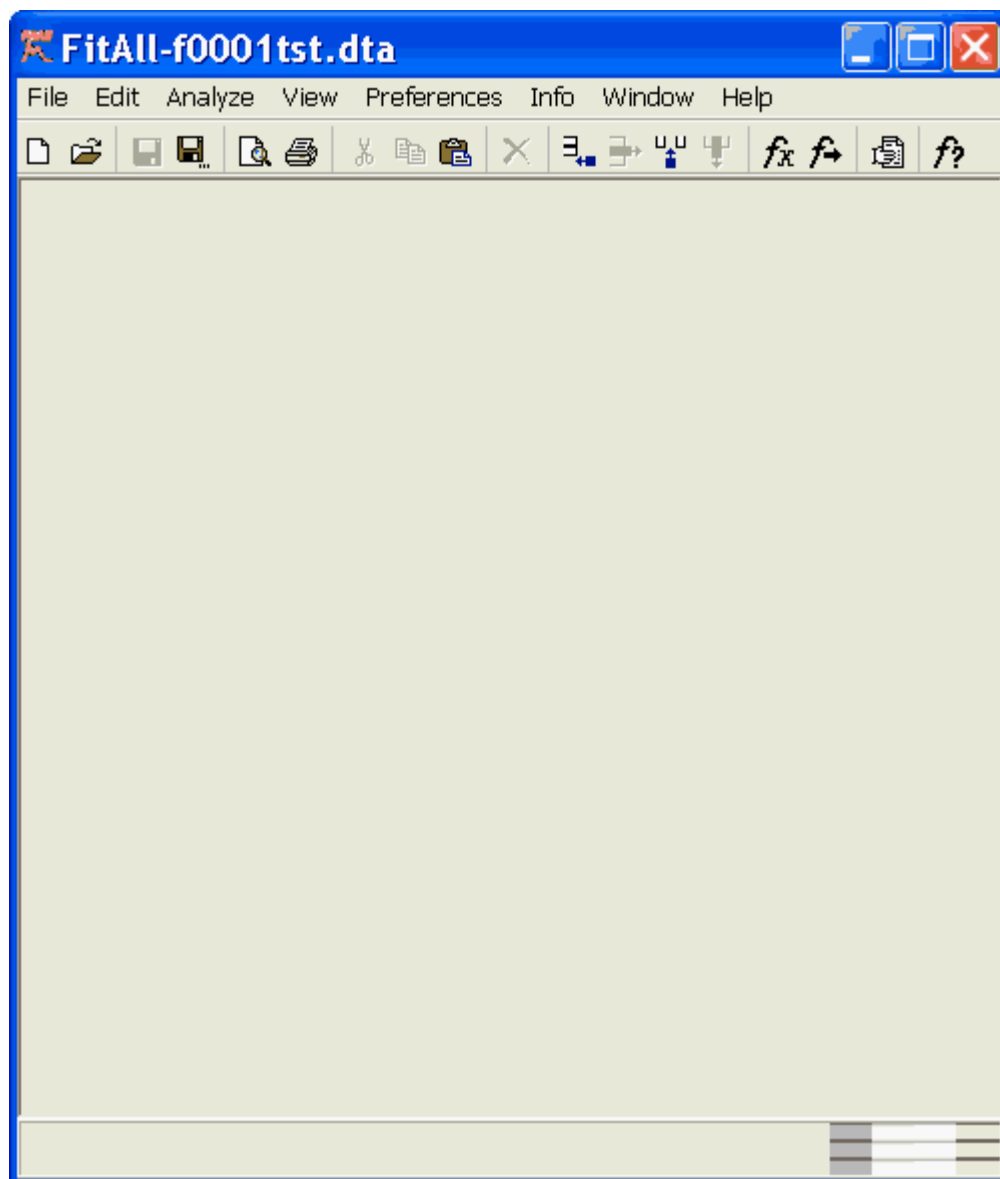
The first time that you start *FitAll*:

- 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:



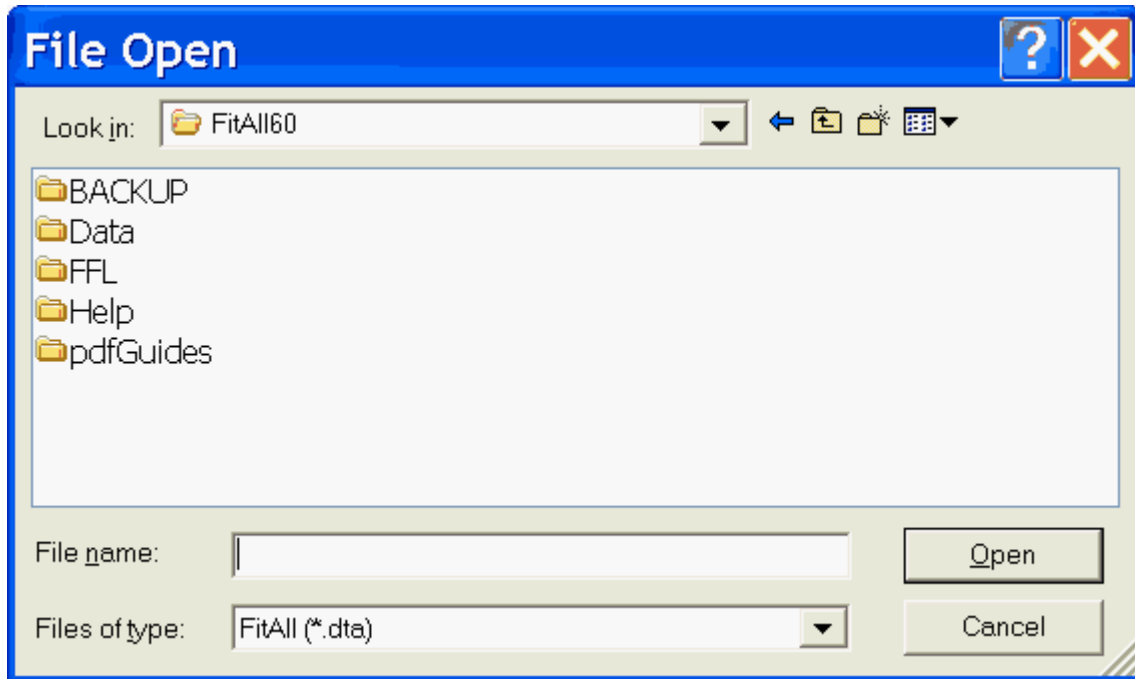
- The main menu is displayed across the top of the window.
- Below the menu is a toolbar, which has buttons representing the most commonly used commands.
- At the bottom of the main window there is a status line in which messages *may* appear.
- On the right side of the status line there are three progress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

Opening a Data File

To retrieve an existing set of data:

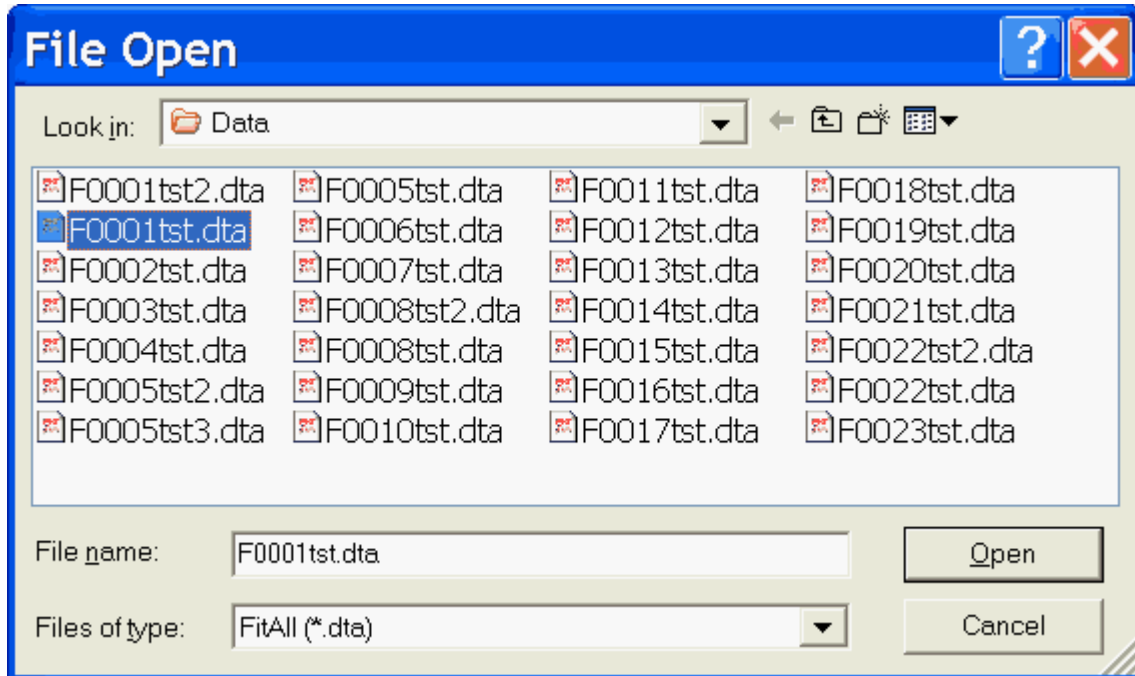
Click the File, Open menu selections, press Ctrl+O or click the  button.

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:

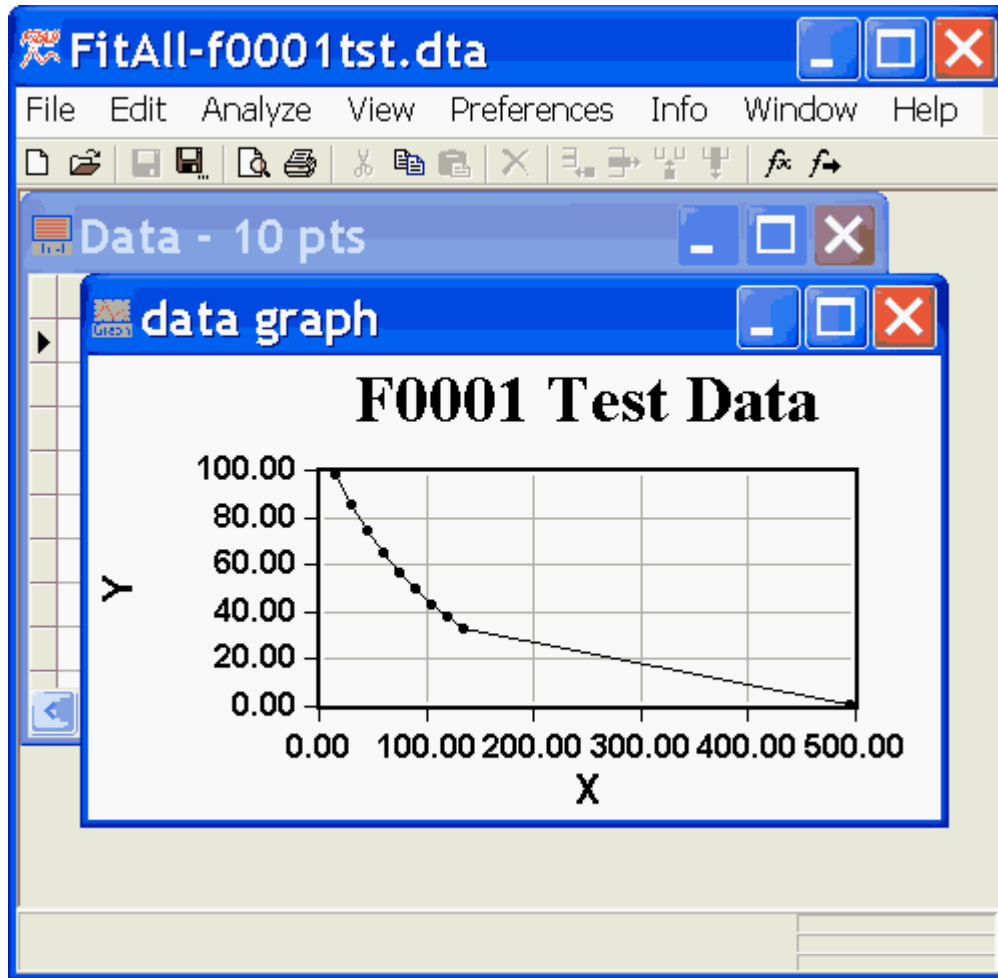
The screenshot shows the FitAll software interface. The main window is titled "FitAll-f0001tst.dta" and has a menu bar with "File", "Edit", "Analyze", "View", "Preferences", "Info", "Window", and "Help". Below the menu bar is a toolbar with various icons for file operations and analysis. A secondary window titled "Data - 10 pts" is open, displaying a table of data points. The table has four columns: "Pt#", "X", "Y", and "S". The data points are as follows:

Pt#	X	Y	S
1	1.500E+0001	9.790E+0001	1.000E
2	3.000E+0001	8.550E+0001	1.000E
3	4.500E+0001	7.470E+0001	1.000E
4	6.000E+0001	6.530E+0001	1.000E
5	7.500E+0001	5.700E+0001	1.000E
6	9.000E+0001	4.990E+0001	1.000E
7	1.050E+0002	4.360E+0001	1.000E
8	1.200E+0002	3.810E+0001	1.000E
9	1.350E+0002	3.330E+0001	1.000E
10	1.500E+0002	2.920E+0001	1.000E

Graphing the Data

To see a graph of the data:

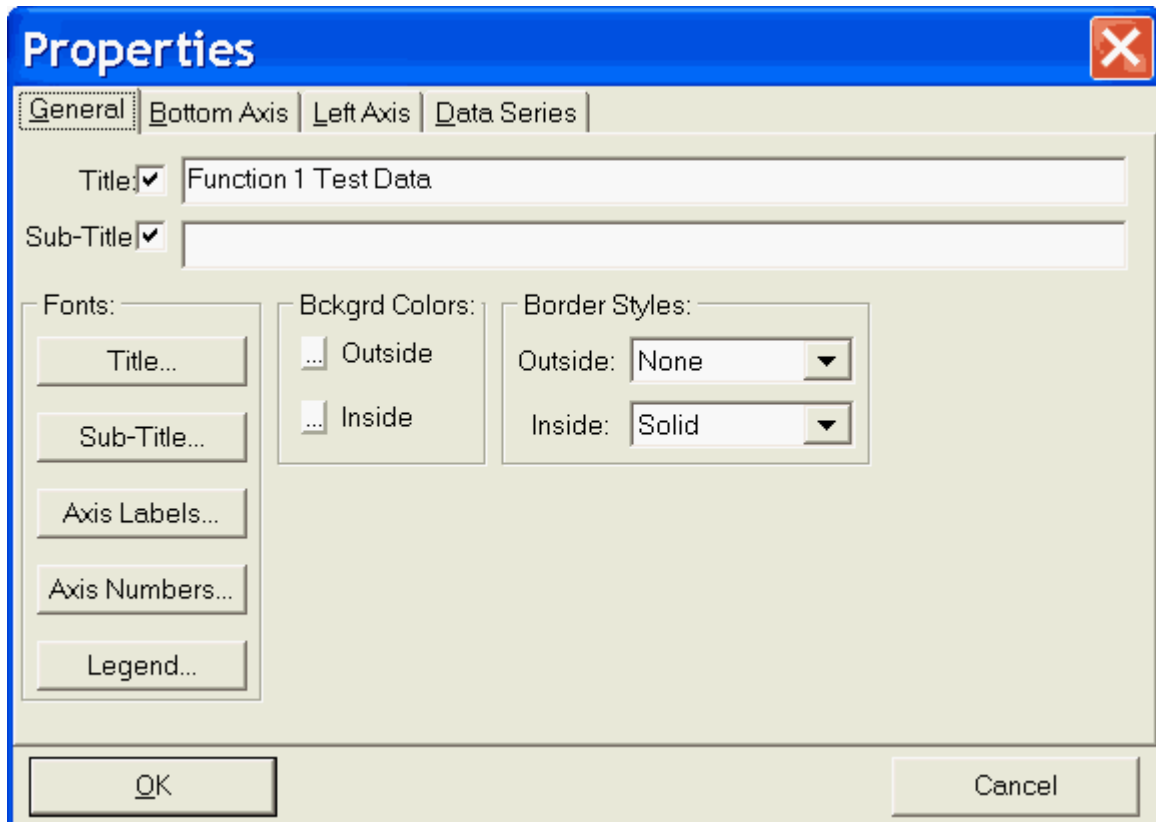
- Click the View, data graph menu selections.
- **FitAll** will open its 'data graph' window and place the graph in it. Your screen should look like this:



To change the appearance of the data graph:

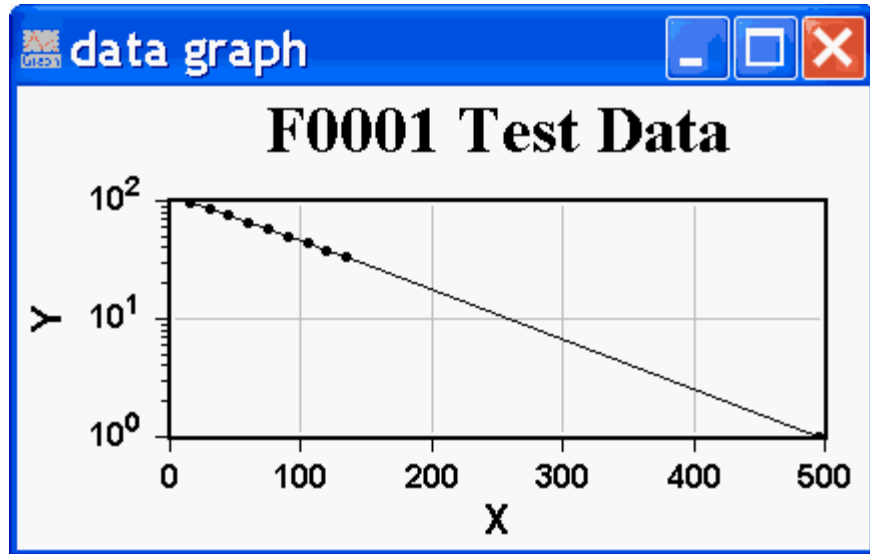
- Select the menu item Edit, Properties... or right-click anywhere in the data graph window and select the Properties... item on the resulting popup menu.

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

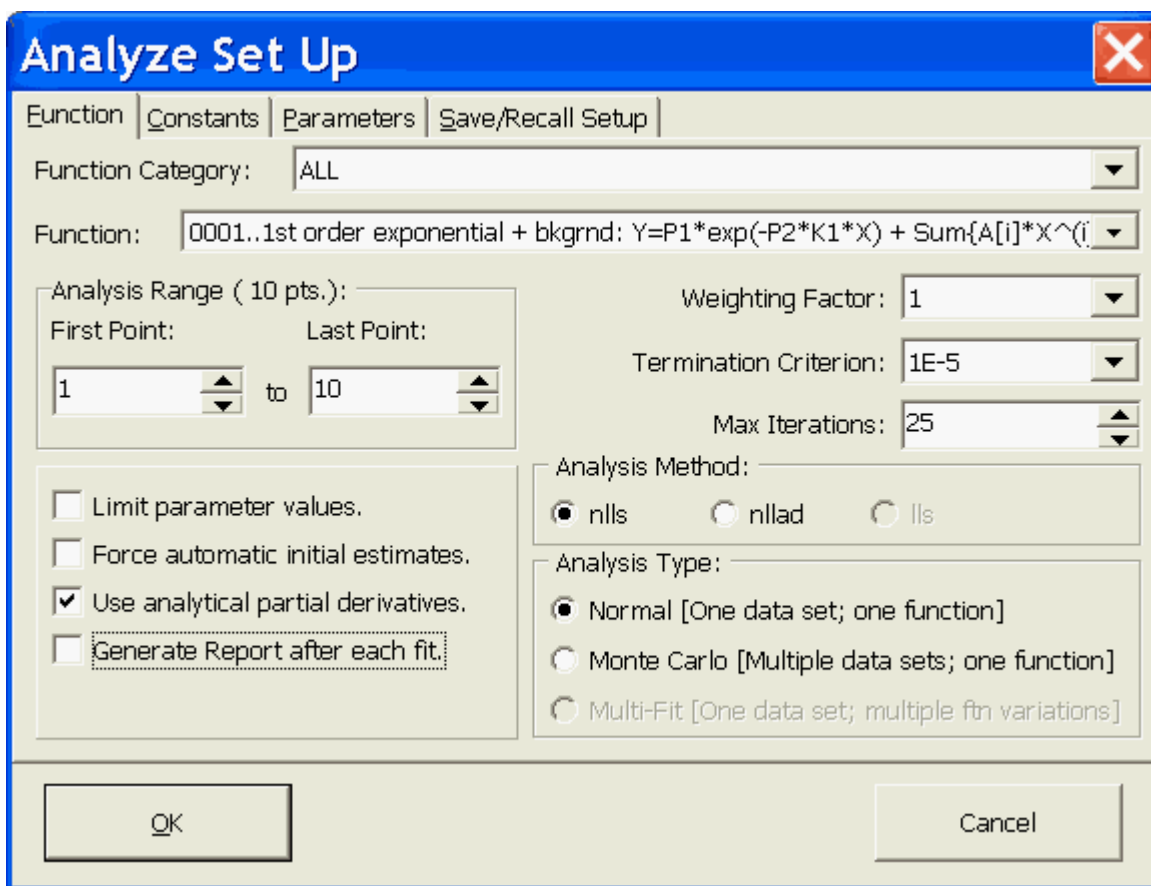
Before **FitAll** can analyze the data, it must be told a number of things, including:

- 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  button, located on the toolbar under the main menu.

The 'Analyze Set Up' 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.

Number of terms in background p...

Minimum Value: 0

NEW VALUE: 1

Maximum Value: 3

Ok

Cancel

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:

Analyze Set Up

Function | Constants | Parameters | Save/Recall Setup

Ftn: 0001..1st order exp decay+bkgnd: $Y=P1*\exp(-P2*K1*X) + \text{Sum}\{A[i]*X^{(i)}\}$


Parameter	Name	Value (Est'd)
P1	Yo-Yinf	96.9
P2	k	0.007311037708820
P3	Yinf	1

OK Initial Estimates Cancel

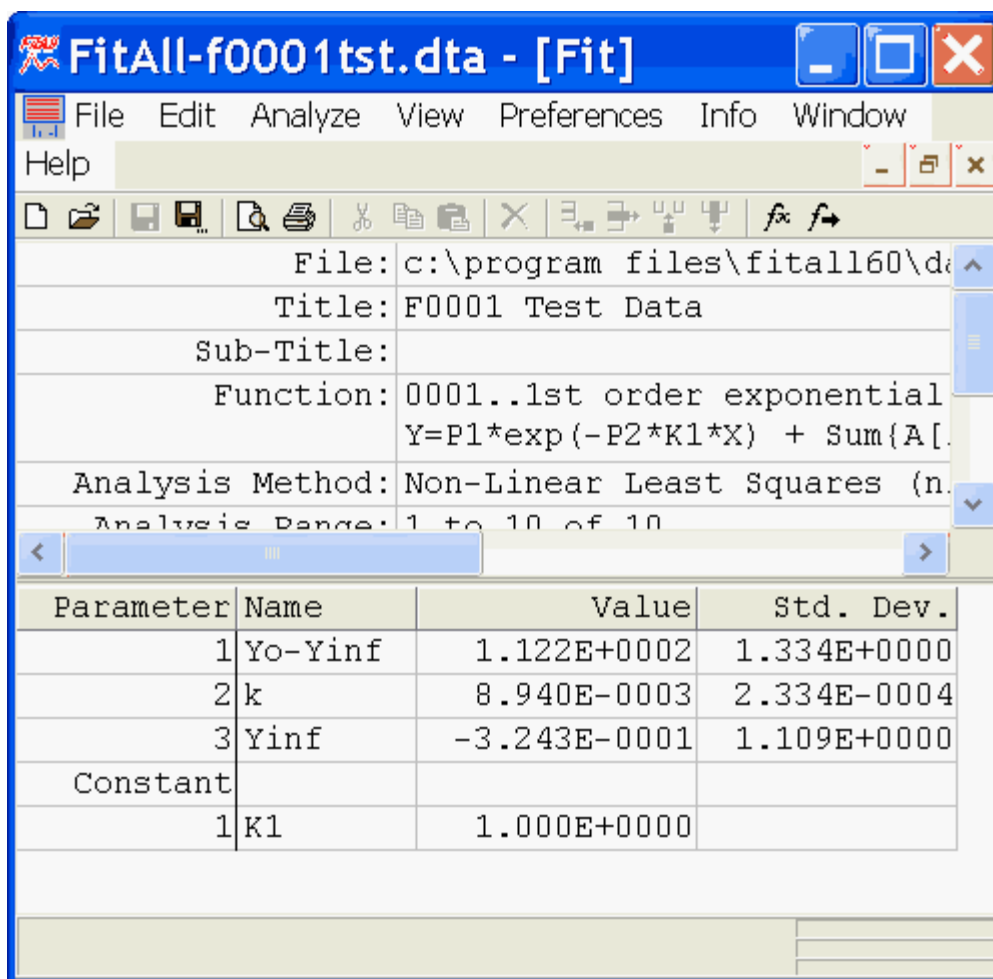
- Click the **OK** button.

Analyzing the Data

To analyze the current data with the function and other settings selected in the 'Analyze, Set Up' 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.

Click the 'maximize button' on the 'Fit' window's title bar so that the window is larger. Your screen should look like this:



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 (nlls, 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.
- The names and values of all constants.
- If parameter limits were used, the upper and lower limiting values for each of the parameters.

Printing the Results

Make sure that the 'Fit' window is the active window. If it is not, click anywhere in it or click the View, Fit menu selections.

Click the File, Print menu selections, press Ctrl+P or click the  button, located on the toolbar under the main menu.

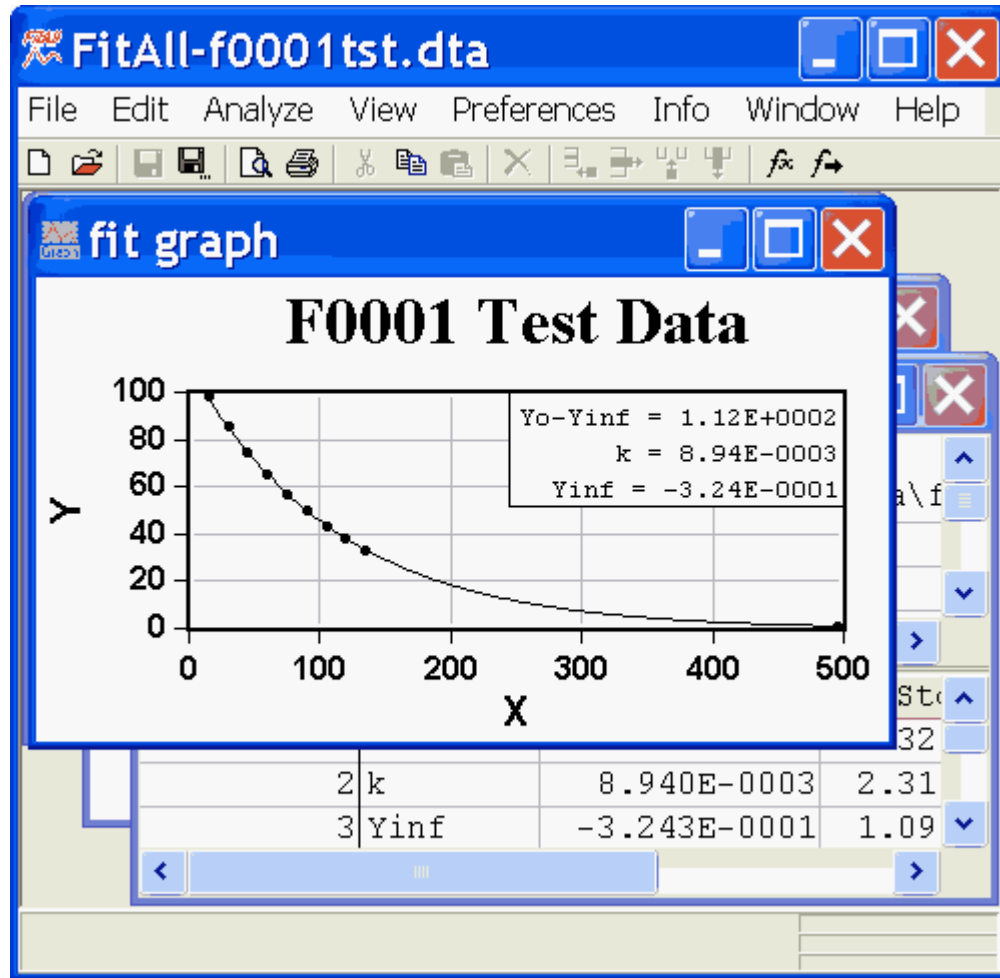
The contents of the 'Fit' window will be printed on your default Windows' printer.

To change the font and margin settings click the File, Page setup... menu selections or right click in the Fit window and choose the Page setup... item on the popup menu.

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:

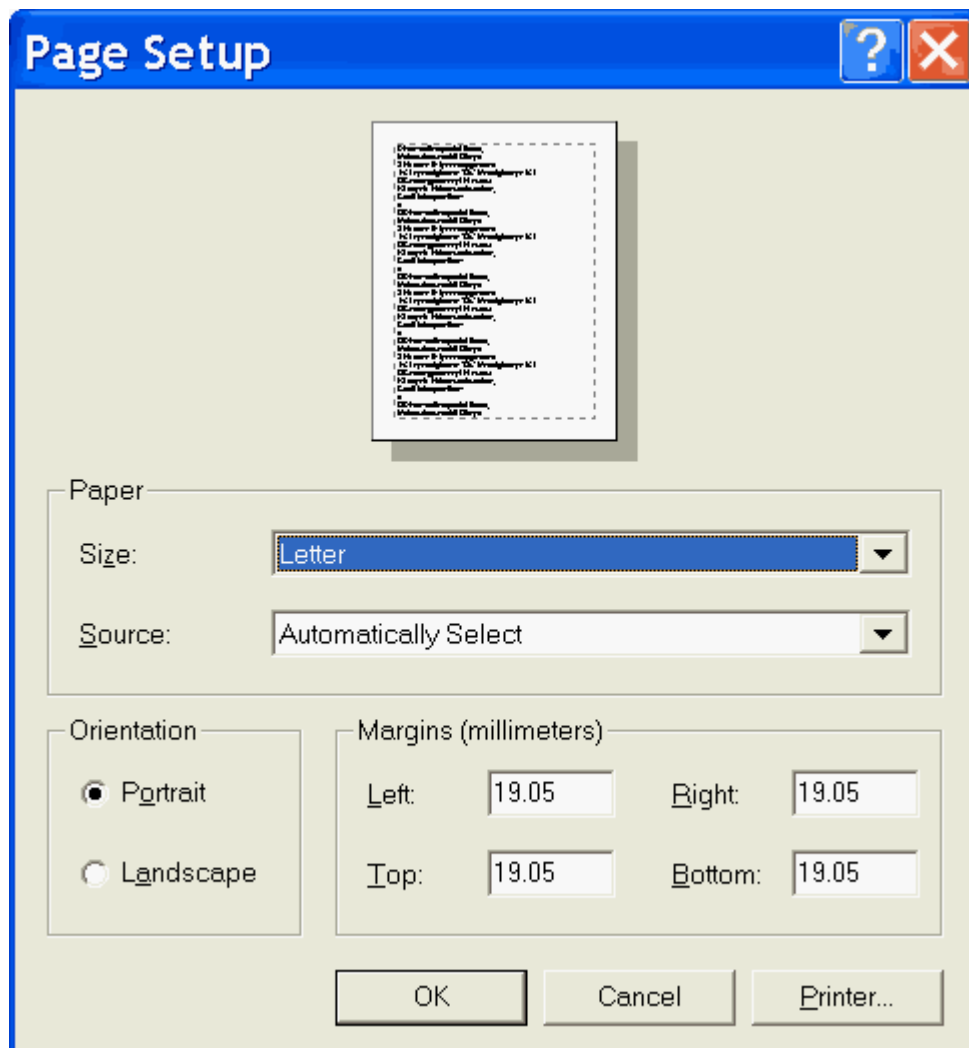


The appearance of the fit graph can be changed by setting its properties in the same way that the [data graph's appearance](#)^[25] is changed.

Printing a Graph

To print a graph:

- Make sure that the 'fit graph' window is the active window. If it is not, click anywhere in it or click the View, fit graph menu selections.
- Click the File, Print menu selections, press Ctrl+P or click the  button located on the toolbar under the main menu.
- The contents of the 'fit graph' window will be printed on your default Windows' printer.
- To change the margin settings or the page's orientation click the File, Page setup... menu selections or right click in the 'fit graph' window and choose the Page setup... item on the popup menu.
- The 'Page Setup' dialog will appear. It looks like this:



NOTE:
When a graph is printed, the image is expanded to fill the space inside the page's


margins, while maintaining the same relative height and width (aspect ratio) as is present on your computer's screen. To change the size of the printed image, use the File, Page setup menu item to change the page margins.

The resolution of the graph is determined by the resolution and size of the image on your computer's screen and the size of the graph window when the graph was originally created. To see how this works try the following:

- Maximize **FitAll's** main window.
- Maximize the fit graph window.
- Close the fit graph window. (This is so that **FitAll** will have to re-calculate the graph size).
- Plot the fit graph by selecting the menu items View, fit graph.


Saving a Graph as a Picture

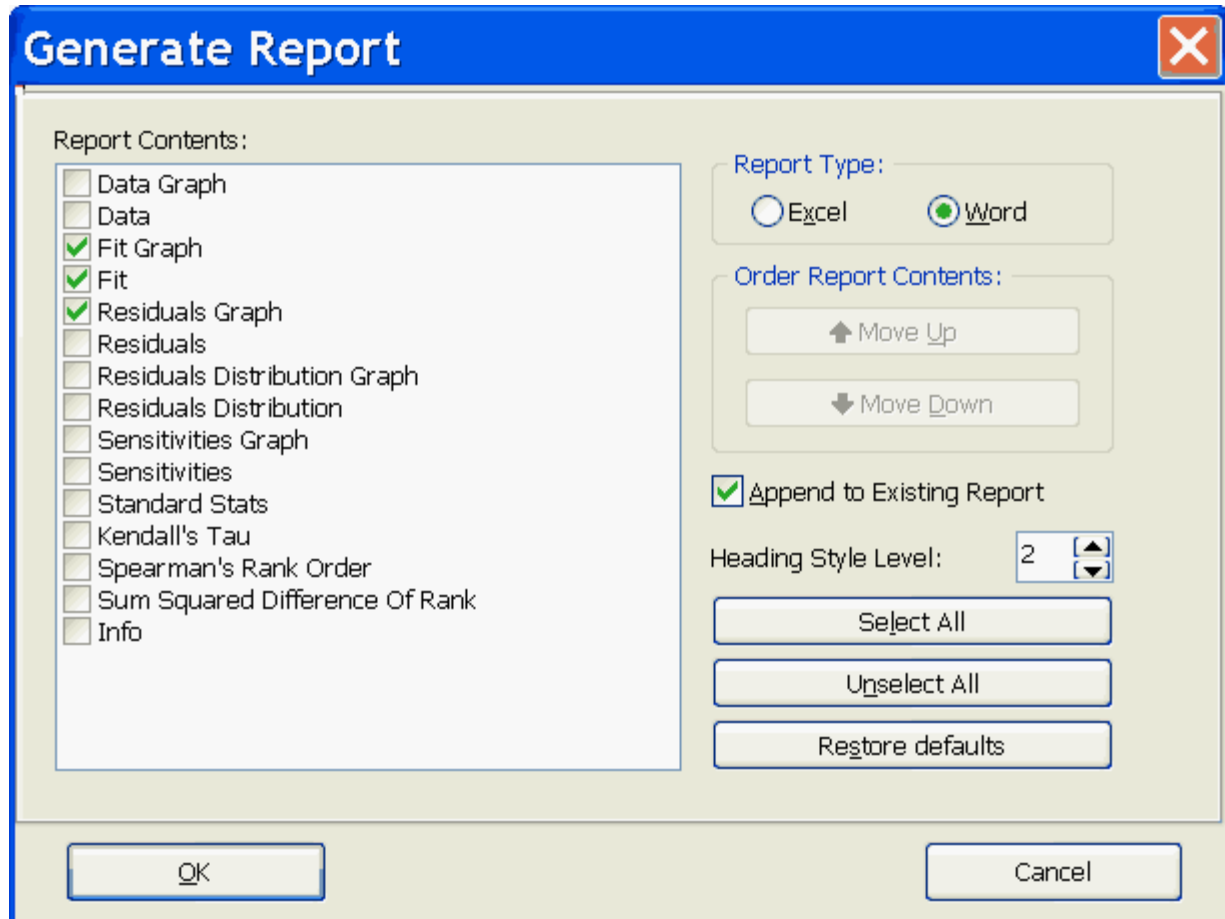
To save the fit graph as an image, do the following:

- Make sure that the window containing the graph you want to save as a picture is the active window. If it is not, click anywhere in it.
- 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).
 - an Enhanced Metafile file (*.emf).
 - a Graphics Interchange Format file (*.gif).
 - a JPEG image file (*.jpg).
 - a Portable Network Graphics file (*.png).
 - a Windows Metafile file (*.wmf).
- Click the **OK** button.

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:



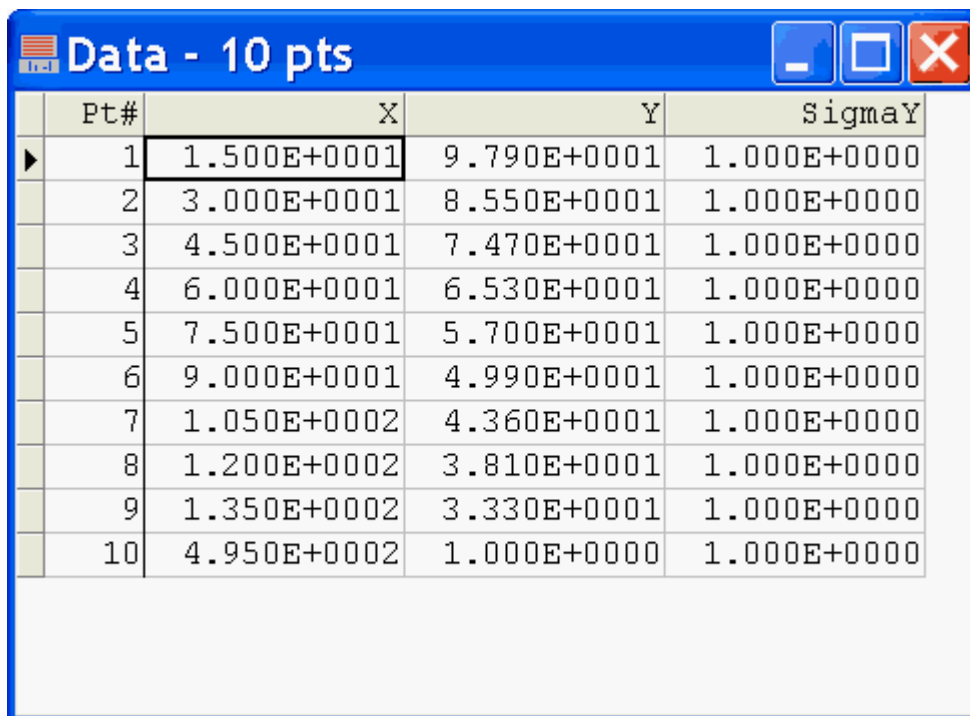
- Check the "Report Contents" items that you want to appear in the report.
- Use the "Move Up" and "Move Down" buttons of change the order of the report items.
- Click the **OK** button to generate the report.

Entering and Editing Data


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

- Make the 'Data' window the active window by clicking anywhere in it or by choosing the View, Data menu selections.

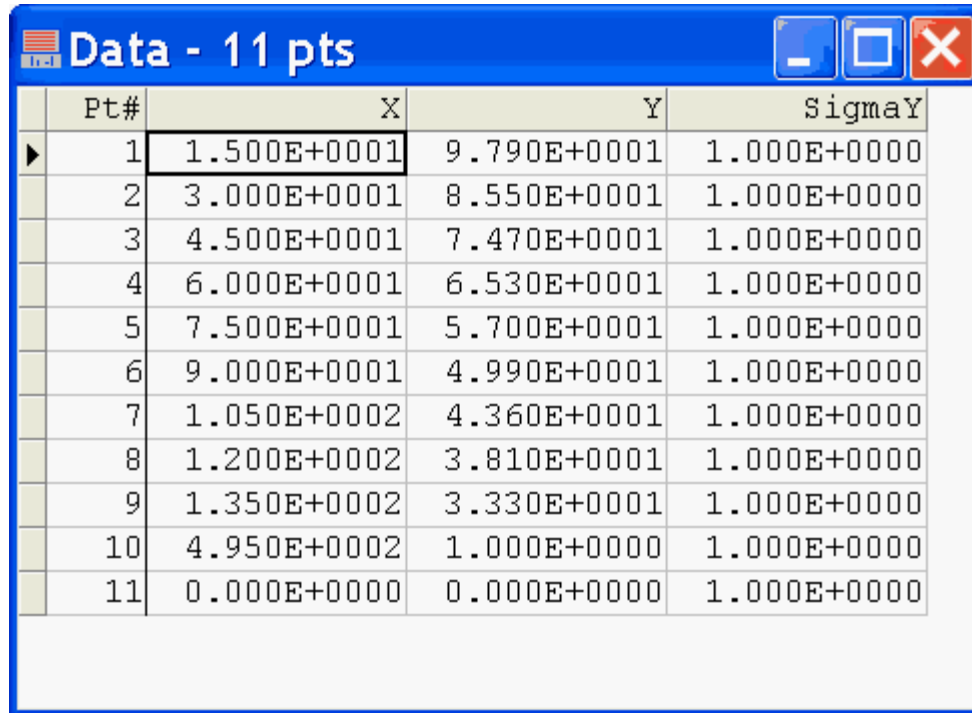
The 'Data' window might look like this:



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

- Click the Edit, Add data 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:

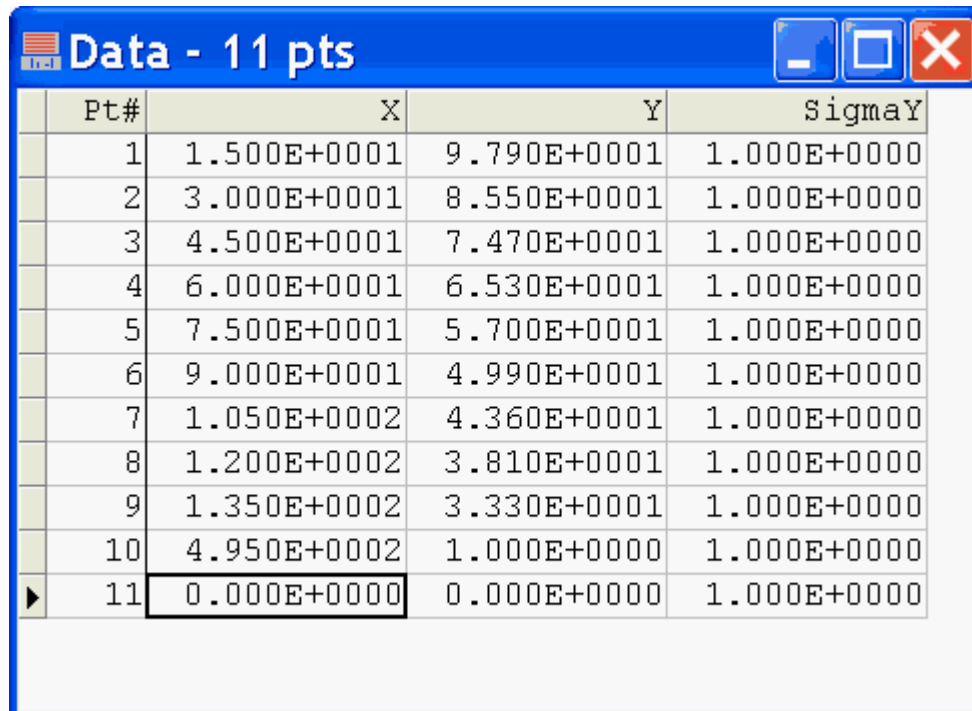


Pt#	X	Y	SigmaY
1	1.500E+0001	9.790E+0001	1.000E+0000
2	3.000E+0001	8.550E+0001	1.000E+0000
3	4.500E+0001	7.470E+0001	1.000E+0000
4	6.000E+0001	6.530E+0001	1.000E+0000
5	7.500E+0001	5.700E+0001	1.000E+0000
6	9.000E+0001	4.990E+0001	1.000E+0000
7	1.050E+0002	4.360E+0001	1.000E+0000
8	1.200E+0002	3.810E+0001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

- 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 move the edit rectangle to 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 move the edit box to the eleventh X-value.

The 'Data' window should now look like this:

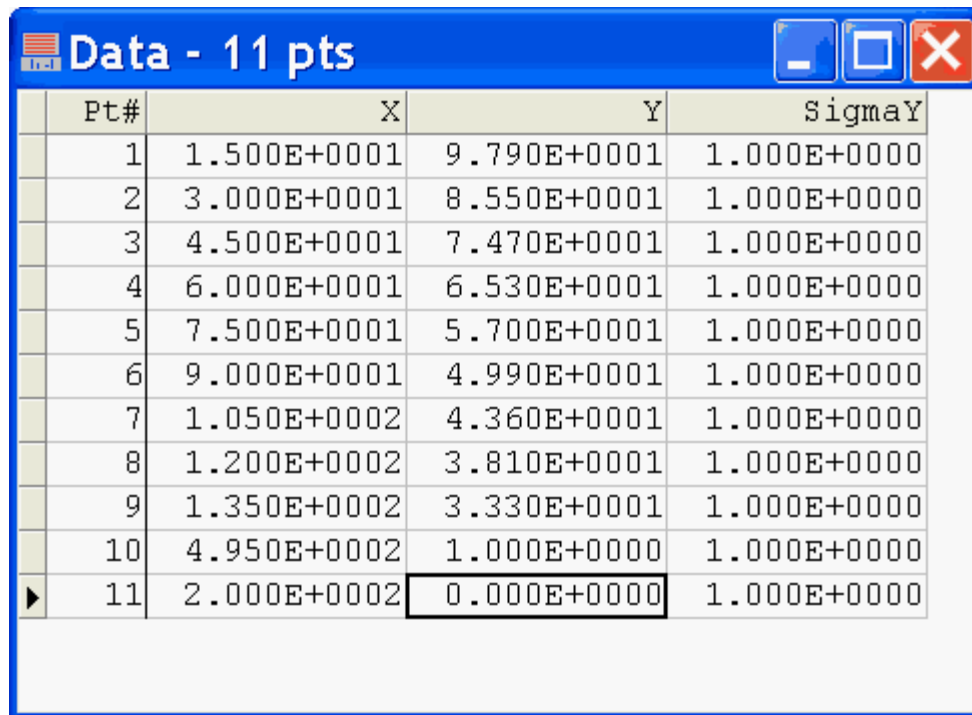


Pt#	X	Y	SigmaY
1	1.500E+0001	9.790E+0001	1.000E+0000
2	3.000E+0001	8.550E+0001	1.000E+0000
3	4.500E+0001	7.470E+0001	1.000E+0000
4	6.000E+0001	6.530E+0001	1.000E+0000
5	7.500E+0001	5.700E+0001	1.000E+0000
6	9.000E+0001	4.990E+0001	1.000E+0000
7	1.050E+0002	4.360E+0001	1.000E+0000
8	1.200E+0002	3.810E+0001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

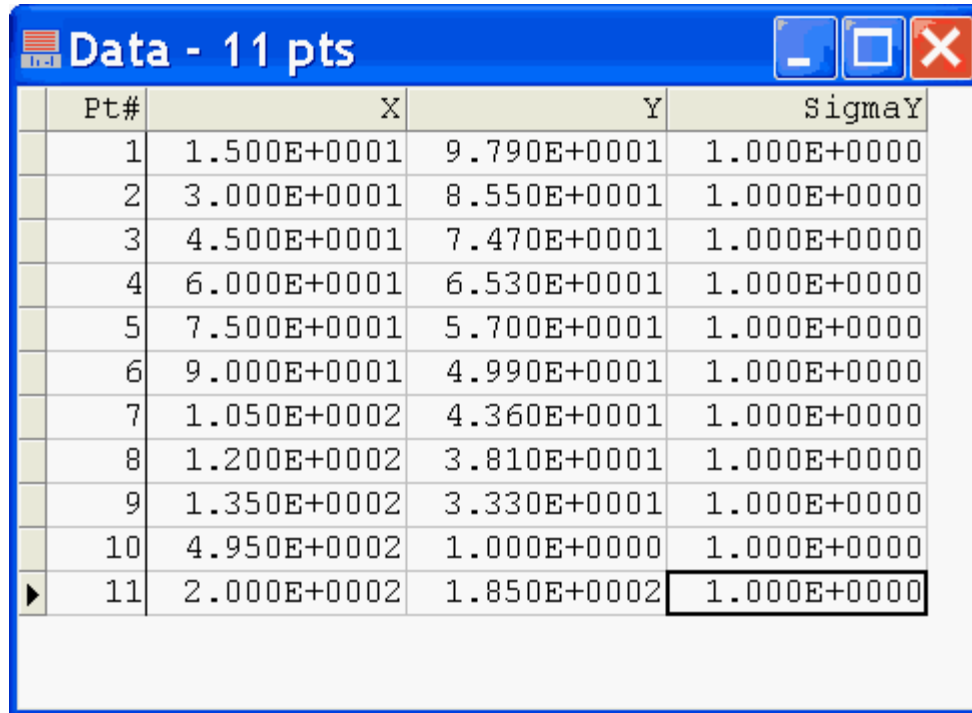
- Press the Enter key to accept the new value or press the Esc key to cancel it.
- The 'Data' window should look like this:





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 , typing **185**, and pressing the Enter key.

The 'Data' window 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
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](#) 

[Creating a 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:

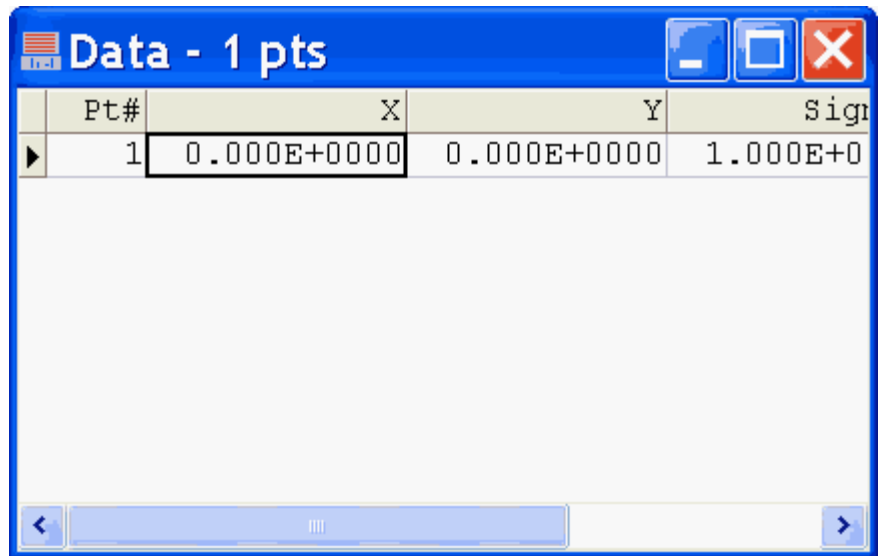
Column	Name
1 [X]	X
2 [Y]	Y
3 [SigmaY]	SigmaY

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.



The screenshot shows a software window titled "Data - 1 pts" with a blue header bar. The window contains a table with the following data:

	Pt#	X	Y	Sign
▶	1	0.000E+0000	0.000E+0000	1.000E+0

The table has a scroll bar at the bottom, and the window includes standard minimize, maximize, and close buttons in the top right corner.

- Edit and enter more data points in the same way as explained in ['Entering and Editing Data'](#)³⁹.

Appendix

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[Adding Functions to FitAll](#)  49

Getting Help

To get technical or other assistance from MTR Software you can:

Visit the FAQ page on MTR Software's web site 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 three ways to add your own specialized functions to *FitAll*.

1. You can contact **MTR Software** to get a quotation on the cost of creating a custom **FitAll Function Library** for you.
2. 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 Delphi versions 5 to 2010 and **Free Pascal**, an open source Pascal compiler, available from www.freepascal.org.
3. You can contact **MTR Software** and request that the function be added to one of *FitAll*'s **Function Libraries**.

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