LAB Fit: Summarized Tutorial (Curve Fitting)

Note: if you do not want to see this quick tutorial at startup, in the “Help” menu, uncheck this option.

General Information

The **LAB Fit** is a software for Windows developed aiming the **treatment and the analysis of experimental data**. At **LAB Fit** you are able to:

1) Treat similar data (grouped and ungrouped dataset, one or two samples);

2) Treat non-similar data (each measurement given by a mean and its uncertainty);

3) Calculate probabilities for many distributions (Gaussian, t-Student, Fisher-Snedecor, Chi-Square and Correlation Coefficient);

4) Determine propagated error (error propagation up to eight independent variables);

5) Plot 2D and 3D graphs (normal, parametric, imported dataset, contour of maps);

6) Execute several calculations: system of linear equations, roots of function, nonlinear equation, ordinary differential equation (ODE up to fifth order), system of ordinary differential equations (first order ODE, up to five equations), approximate function for ODE solution, calculator, etc;

7) Extract data (x;y) from a 2D graph (digitizing);

8) **Curve Fitting** (nonlinear regression - least squares method, Levenberg-Marquardt algorithm -, almost 500 functions at the library with one or two independent variables, functions finder, there is an option that let you write your own fitting function with up to 150 characters, 6 independent variables and 10 parameters).

The **LAB Fit** has a menu for curve fitting and the main programs of this menu use nonlinear regression. The **LAB Fit** fits functions of one or several independent variables (from 1 up to 6), allowing uncertainties at the dependent variable (Y) and also at the independent variables (X). In case of uncertainties in X and in Y a pre-fit is made, not considering the uncertainties in X, that later on are transferred to Y by error propagation. At the **LAB Fit** library there are more than 200 functions with one independent variable and almost 280 functions with two independent variables. The user disposes of a functions finder program. If necessary, there is an option for the user to be able to write the own fit function. Once determined the fit parameters, it's possible to extrapolate the fit function and, for the 2D and 3D cases, the graph of the obtained function is shown. For the 2D case, beyond the extrapolation possibility, the user can even include error bars and confidence bands to the graph. The **LAB Fit** has also a menu destined to the treatment of similar data, non-similar data and error propagation. Beyond that, there is a third menu with general tools like one that allows to plot a function informed by the user and many other types of calculations are also included.

1 – Data Information: choose one among the options

To **create** a new data file (up to 500 points) click on the "New" button. Select the adequate options at the "**Data: general information**" dialog box and, if you want to inform your data **manually**, click on "OK". At the **box of data acquisition** inform all the values of X and click on "OK" (inform also sigmax, if there is any). At next, inform all the values of Y and click on "OK" (inform also sigmay, if there is any). When the browser appears, give a name (without blank spaces) to the file and click on "Save".

To **paste** data in columns (from **Excel**, for example, or other software), with up to 300 points, select and copy them. Then, click on the "New" button and paste the data directly into the **LAB Fit** using the "Paste" button on the **"Data: general information"** dialog box (the last column must be the dependent variable or the uncertainty of the dependent variable).

To **extract** data (graph digitizing) from a 2D graph within a bitmap file, with up to 1500 points, click on the "New" button. At the "**Data: general information**" dialog box, click on the "xyExtract" button. **Attention**: After the reading process, if there are more than 500 points, **LAB Fit** will select approximately the 500 most representative points to perform the analysis.

To **import** data from a **non formatted** file (txt, for example), with any amount of points, click on the "Imp" button. Specify the file type in columns at the **"Import Data File in Columns"** dialog box and click on "OK" (the last column must be the dependent variable or the uncertainty of the dependent variable). Select the file with the data in columns at the browser and click on "Open". If the data is not formatted, they will be read and a new file will be formed using the **LAB Fit** data file pattern. **Attention**: After the reading process, if there are more than 500 points, **LAB Fit** will select approximately the 500 most representative points to perform the analysis. **<= Main approach for data supply.**

EXCEL Import: select the data from **Excel**, copy it, paste it on the NOTEPAD and save. The "txt" file can then be imported.

Attention: data in columns, up to 300 points, can be copied (from **Excel**, for example) and pasted directly into the **LAB Fit** using the "Paste" button on the **"Import Data File in Columns"** dialog box (the last column must be the dependent variable or its uncertainty).

To **save** the file generated through one of the options defined previously, when the browser appears, give a **name** (up to 40 characters) to the new file and click on "Save".

To **open** a data set click on the "Open" button. Select the data file at the browser and after click on "Open". The values of X will be shown. If there are any corrections to be made, they must be done now. With everything ok, when "OK" is clicked, the other data (sigmax or Y or sigmay) will also be shown at the **box of data acquisition**.

2 – Curve fit: choose one among the three options

In case the user does not know **which** is the most appropriate function for the fit, the "Find" button can be clicked and the **LAB Fit will select the functions** from its library that best adapt themselves to the data. To do so, when the **"Conditions"** dialog box appears, the number of parameters of the functions that are going to be tested must be selected. When "OK" is clicked, the selection process is initiated and, after some time, the best results will be shown on screen. So, the user can perform the complete fit of the function that was chosen.

To **fit a function of the library** the user must click on the "Libr" button. Right after, a dialog box with a list of the available functions will appear, with 1 or 2 independent variables, according to the case. The user must, then, select the fitting function and click on "OK". Then, a dialog box will appear with the initial values of the parameters to be determined, the maximum number of iterations and the tolerance. After the inspection, "OK" must be clicked. A dialog box called **"Power"** will then appear. At the most simple fittings, the user should click on the "Fit" button (but it can be written 20 or 50, for safety). The **"Results"** dialog box with the fitting results will then appear (mean value and uncertainty of the parameters). The complete results (including covariance matrix) are available through the "Details" button. The evaluation of the fitting function for x values is performed by clicking on the "Evaluate" button and the analysis of the experimental points is available through the "Rejection" button.

To **fit any function** the user must click on the "User" button that, right after, a dialog box will appear where the user must write, using Fortran standard for writting mathematical expressions, the fitting function (up to 150 characters) and the number of parameters of the function (up to 10 parameters, written in alphabetical order, starting by **A**). When "OK" is clicked, a dialog box with the initial values of the parameters to be determined, the maximum number of iterations and the tolerance will appear. If the user makes an approximate idea of the initial values of the parameters, they must be written. If not, after the inspection, just click on "OK". A dialog box called **"Power"** will then appear. For the simplest fittings, the user should just click on the "Fit" button (but it can be written 100 or 200, for safety). The **"Results"** dialog box will then appear with the fitting results (mean value and parameters uncertainty). The complete results (including covariance matrix) are available through the "Details" button. The evaluation of the fitting function for x values is performed by clicking on the "Evaluate" button and the analysis of the experimental points is available through the "Rejection" button.

In both cases, when "OK" is clicked at this **"Results"** dialog box, the function graph will be drawn.

3 – Graph of the fitting function

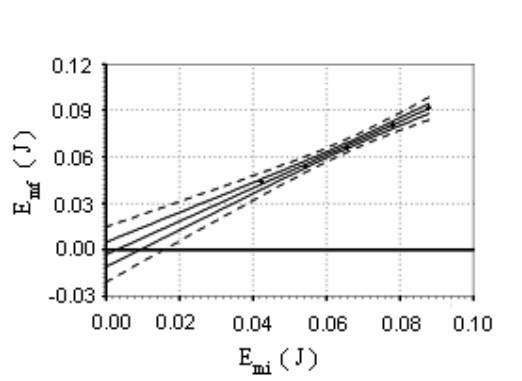
Before the graph be drawn; some information about it is required at a dialog box, that includes details about the extrapolation of the fit function. After that, the graph will be drawn and, to print it, there are two options currently available.

To use the **first option**, the "Print Window" item must be clicked, at the "File" menu, but this option only works to print a **sketch**, because the printing is not of good quality: the printed picture will have the same resolution shown on screen.

The **second option** makes possible to print a graph of **better quality than the previous one**, which can be done by clicking on the "Superzoom in" item at the "Graph" menu. The graph will be, then, drawn again, but with a resolution much higher than the original one, occupying a much bigger space than the available screen size. After that, at the "File" menu, the user must click on "Print graph (superzoom)".

To **paste** a graph into a document the user must choose, at the "Edit" menu, the "Select All" option and after, at the same "Edit" menu, "Copy" must be clicked. Then, it's just a matter of opening the document, and pasting the image that was stored at the clipboard.

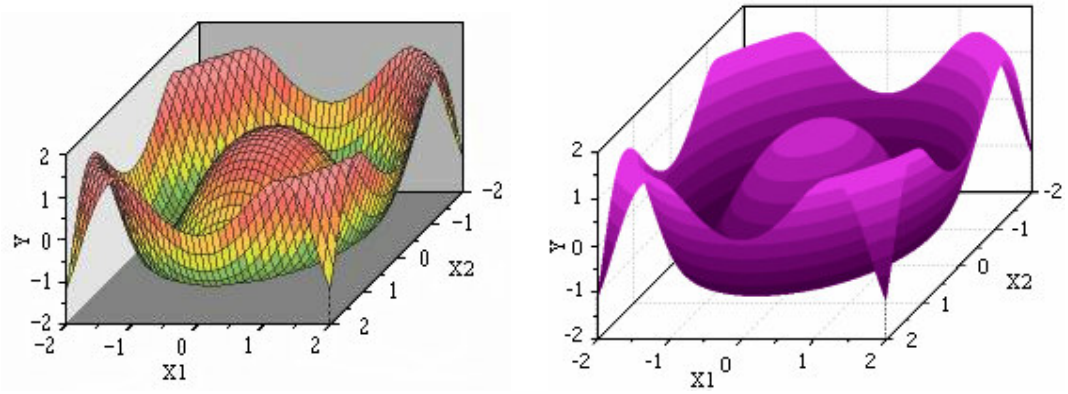
For **publication** purposes, at the "Graph" menu, the user must choose the "Zoom in (+)" option. Then, the user must select and copy the graph. To finish, it must be used an image editing program to reduce and to edit the graph. See an example below (width: 275 pixels) with confidence band, prediction band and extrapolation included:



Attention: all the **image files** generated are available by clicking on the "Files" button. After opening a file, the user can copy and paste the data directly into the cells of a plotting program (**Excel**, for example).

4 – Graph of the user function

See a 3D graph example for the function **Y = cos(X1^2+X2^2) - sin(X1^2+X2^2)**, obtained by clicking on the "G 3D" button:



LAB Fit - Help and Examples Files

You can download help and examples files directly from the LAB Fit home page available at <www.labfit.net> or from the software itself, by clicking on the "Help" button. When the **LAB Fit Help** dialog box appears, click on the "Cancel" button that the software automatically detects the absence (if they are actually absent obviously) of the help and examples files and download them for you. Then install the files into the same location of the **LAB Fit**.

LAB Fit - Certification SRD / NIST

The **LAB Fit** performance has been verified using the Statistical Reference Datasets Project (SRD) of the National Institute of Standards and Technology (NIST). The SRD presents 27 datasets with three levels of difficulty: lower (8 files), average (11 files) and higher (8 files). The results are available at <www.labfit.net> ("Home" button). All the 27 **LAB Fit** results are statistically identical to the certified values.

LICENSE AND DISCLAIMER

Using **LAB Fit** constitutes acceptance of all the terms stated hereafter. Note that care has been taken to prevent errors in the calculation of the curve fittings presented as results by this program. However, any consequences of the use of these results are strictly the responsibility of the user. The authors are not responsible for any consequences of the use of this product. The authors disclaim all warranties, expressed or implied. The authors will assume no liability for damages either from the direct use of this product or as a consequence of the use of this product.

You are hereby granted a license to use **LAB Fit** for an evaluation period of 50 executions, after that you must pay the registration fee (order online or email to the authors) to continue using **LAB Fit**. During the evaluation period the authors grant to you the same rights granted to a registered user (read EULA.txt into the installation directory); including to publish all the results generated by **LAB Fit**. Current fee: USD 0.00

How to Cite the LAB Fit (Presentation and Reference)

... the analyses were performed using LAB Fit [1]. The LAB Fit is a software for Windows developed for the treatment and analysis of experimental data. At the LAB Fit there is the possibility to: treat similar data; treat non-similar data; determine propagated error; plot 2D and 3D graphs; execute calculations (system of equations, roots of function, ordinary differential equations, etc); extract data (x;y) from a 2D graph (digitizing); curve fitting (nonlinear regression - least squares method, Levenberg-Marquardt algorithm -, almost 500 functions at the library, with one and two independent variables, functions finder, option that let you write your own fitting function with up to 150 characters, 6 independent variables and 10 parameters) **...**

[1] Silva, W.P. and Silva, C.M.D.P.S., **LAB Fit Curve Fitting Software (Nonlinear Regression and Treatment of Data Program) V 7.2.48** (1999-2011), online, available at the world wide web at: <www.labfit.net>, date of access: Year-Month-Day.

The software "LAB Fit" is sold as is. Cost USD 0.00

LAB Fit Files

(curve fitting, basic statistics, error propagation, 2D and 3D graph, tools)

- **Lab.exe**
- **Finder_Func.exe**
- **Fit.exe**
- **Graph2D.exe**
- **Graph3D.exe**
- **xyExtract**
- **Res.exe**

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