™WinFit 1.22

WinFit - A Non-Linear-Least-Squars Fitting program for windows 3.1

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About WinFit

A general purpose Non Linear Weighted Least Squares Fitting program for windows 3.x The program can load X, Y, Error data from a file plot the data and fit it to several built in functions and to a user define function.

Features

New to this version

- Data fitting region can be selected from the plot.
- User defined equations can be saved in the winfit.ini file.
- Parameters file can be save and restored.
- Added Ionrentzian equation for resonance shape fitting.

Other

- Reads a simple ASCII file, space or tab delimited of X Y with an optional Y-error data.
- The data can be plotted with log axis options.
- The program uses Levenberg-Marquardt fitting method.
- There are some built in functions and the a user-defined function.
- The program can generate weights that improve fitting performance for some problems.
- This version can read up to 5000 data points and fit up to 10 parameters.
- The program provides a REPORT file and the plot can be copied to the clipboard.
- The program will calculate and display the COVARIANCE and CURVATURE matrixes

Using WinFit

In order to use a non linear fitting algorithm the user must start the fitting session with an initial guess for the parameters to be fitted. If this guess is good enough the program will converge to a "good" fit.

- 1. Prepare your data file (with notepad for example) and save it with .DAT extension. Open the file with the <u>File Open</u> menu command. A sample data file FIT.DAT is provided with the program.
- 2. If your file is not simple (column 1 is X and Column 2 is Y) specify the columns in the FIle Open window also specify the Y-error column. The Y-error should represent one standard deviation in the value of Y.
- 3. As an indication that the file was read correctly you should check the **No. of Points** in the WinFit window, it will show the number of data points in your file.
- 4 You are ready to plot your data so you can click the \underline{Plot} button. You can also view the numbers with the Data \underline{View} menu.
- 5. Next, select an <u>Equation</u> from the WinFit window, if you are in the <u>Plot</u> window click the FIT window to go back. When you select an equations the parameters windows will appear (a simple linear function is provided as a test to be used with the file FIT.DAT).
- 6. Change the initial parameters and click the <u>Plot</u> button. Repeat that process until you see the fitted curve plotted with your data. This should provide a good initial guess for the WinFit start fitting.
- 7. From the WinFit window click the FIT button.

Equations

Equations can be selected from the WinFit window there are several built in equations and a user-defined equation entry windows. The built in equations will perform best in speed of calculations an fit converges this is because the equations are coded to WINFIT.DLL and the analytical form of the derivative is used.

The user-defined equations are interpreted from left to write without the normal calculation order therefore you must enforce the correct order by using parenthesis. The equations can be save to the WINFIT.INI file. Use the **ADD** command in the Equation window to add a new equation. **UPDATE** to update a change in an equation and **DELETE** to delete an equation. You must also enter the number of parameters in the equation.

Plot

The plot windows has two main functions: the first is to display the data and the second is to select the data range to be fitted. The data range can be selected by the scroll bars; lower and upper limits cab be set in this way.

The data and the fit can be plotted on linear or log scale. The fitted curve is calculated by default at every data point the can be change by changing the number in the **Fit Plot Points** box, increasing this number will result in a smother curve.

The Results

The results of the fits will appear in the parameter window with the standard deviation of each parameter. During the fitting process the message window will give information about the fitting process. An iteration starting with a + (plus) sign is a successful iteration (the chisquare was minimized).

The program will iterate until the number of iterations is equal to the number in the Max iteration box (you can change this number) or the %-Error is equal or less then value in the Chisq % Error box (you can change this value).

The COVARIANCE and CURVATURE Matrixes can be viewed by choosing this option in the <u>Prameters</u> menu.

Methods and Math

- 2. The reduced chisq is defined by rchisq=chisq/(N-Nfit) where Nfit is the number of fitted parameters. (parameters that are kept variable during the fit).
- 3. The Percent Error in chi-square is Defined: %Error=100(1-chisq/ochisq) where ochisq is the value of chi-square in the previous iteration.
- 4. In Some problems a better fit is obtained if the data is weighted. A simple way for generate the weights (if they are not available in the data file) is to use the <u>Data</u> menu and choose Set Weights this will set the value of sigYi (see note 1).

Guarantee

None, the author is not responsible to any damage that may be caused by the program or by the use of the program results. The responsibility is of the user alone.

<u>Menu</u>

<u>File</u>

<u>Parameters</u>

<u>Data</u>

<u>Help</u>

File

Open Data

This menu will prompt you for the ASCII file name where the X,Y data is stored. The file should be organized columns of X, Y or X,Y and the Y-Error. The numbers could be delimited by tab or space. If the file contains more than 3 columns, by default WinFit will read only the first 2, however you can specify the which column is the X, Y or Y-Error.

Save Report As

Save a report of the fit parameters in a text file.

Open Param

Opens a paramter File (see Save Param As)

Save Param As

This command can save the fitting session. The data is saved to a text file in the following format:

- 1. Function number.
- 2. Number of terms in the equation.
- 3. The parameters.
- 4. The data file name.
- 5. The data columns to read.
- 6. The data range to be fitted.

When a parameter file is restored fitting the data with 1 iteration will generate the covariance matrix.

Exit

Exits WinFit

Paramenters

Show

Displays the fit parameters form, you must select an equation first.

View Covariance Matrix

Displays the covariance matrix obtained from the fit. The elements on the diagonal are the variances in each fitted parameter.

View Curvature Matrix

Displays the Curvature matrix.

<u>Data</u>

Set Weights

Allows to set the weights as a simple power function of the Y values; W=A*Y**B This can help in some fitting problems to force the fit to a specific region of the un-weighted data.

View

Displays the X, Y, Y-Error and the Y(x) which is the fitted-Y value.

<u>Help</u>

HelpHelp for using WinFit

About

Details on WinFit

Revisions

Version 0.99

■ First release

Version 1.0

■ 3D-look

Versions 1.0a, 1.0b

■ Fix Various bugs and reduce DLL size (minor speed improvements in user defined equation).

Version 1.1

- Improve Interface
- New Help File
- Add small markers to Plot.
- Add registration code.

Version 1.2 May 1993

- Save user equations.
- Save and load parameter files, allows saving and restoring the fit session.
- Allow to fit a data region. using 'live' data selection from the plot.
- Improved plotting, parameters can now be printed on the plot.
- Data Reader; Read X,Y point from plot.

Version 1.22 May 1993

■ Pressing the FIT button in any window will start the fit session.

Registration

If you use WinFit for more than 30 days (or you liked it much sooner) you should register it by sending \$15 to:

Yaron Danon 14 Beman Lane Troy, NY 12180

A registered user will receive a user code that resisters this version of WinFit. This user code will also work with future releases of WinFit. This enables the registered user to download any future release of WinFit and register it without any communication with the author. This gives the user a fast way of updating WinFit.

<u>Suggestions</u>

Suggestions and comments are welcomed and can be E-Mail to:

Danony@rpi.edu

Digitize

Also Avilable is Digitize:

Digitize is an Un-Graphing program, it can import a scanned X,Y plot and digitize it to end up with a text file (or clipboard data) containing the X,Y points.

This program is written in Visual Basic so you need the **VBRUN200.DLL**, you would probably also need a scanner to scan your plots and save it as a bitmap file (BMPor PCX). Digitize also accepts bitmaps pasted from the clipboard.