

A Basic Introduction to QtiPlot

1 Introduction

What is QtiPlot: a program that could: 1) represent data graphically; 2) do data analysis.

2 Installation

Steps for installing QtiPlot:

- Go to this link: <http://www.qtiplot.com/download.html> (This is the demo version, to a complete version for windows only, please go to this link and choose “qtiplot_0.9.8.3-3-Unofficial-win.zip”)
- Under “QtiPlot evaluation/demo”, choose the one fitting to laptop/computer
- Extract and open the executable “qtiplot”

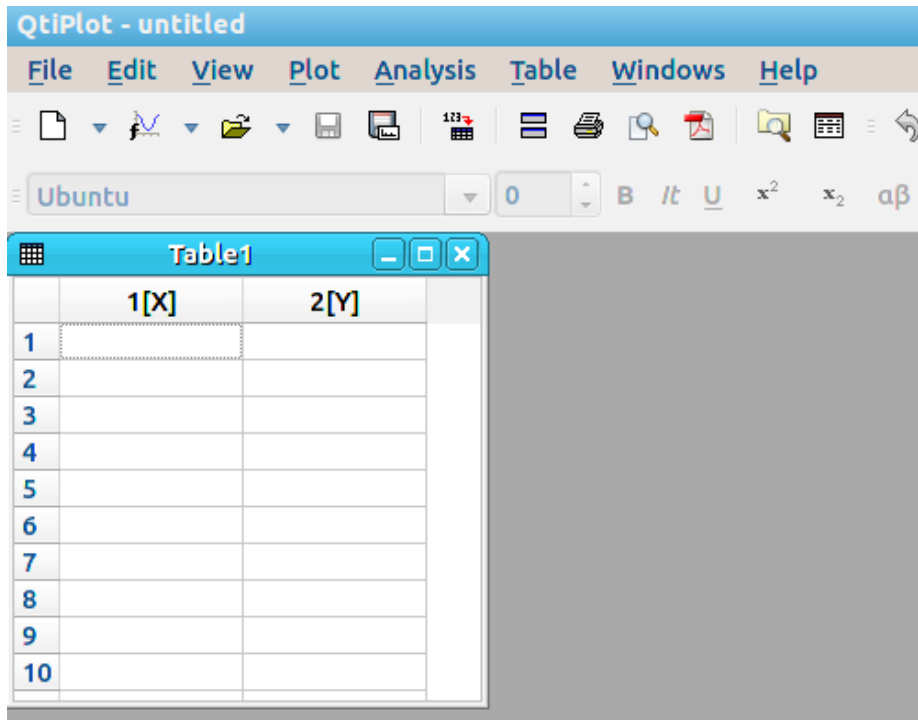
Caution:

- This is a demo version. You can't use it for more than 30 minutes once you opened it → so be quick: record the result on your notebook or export the result to some .txt file quickly!
- You can't save a project. A project simply means the whole work you've done in the program. So you should complete the work in one try: you can't save and continue next time!

3 Data

Data is represented in the form of table

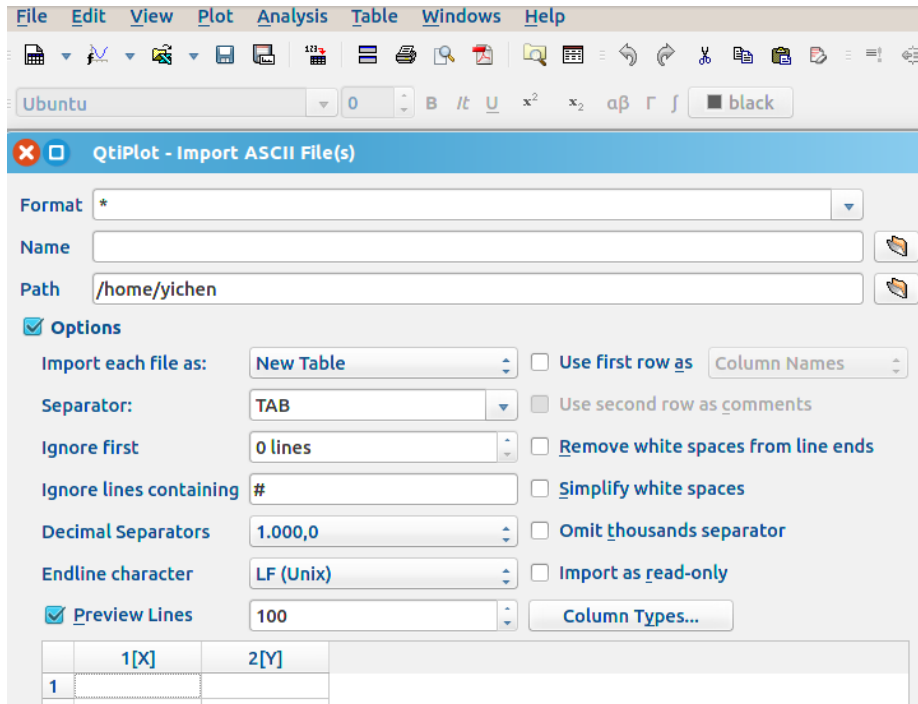
- An empty table is automatically opened once you double clicked “qtiplot”, see figure below
- 2-D table is the default and the one you will use in the lab course, although higher dimensional table is possible



To make/fill a table:

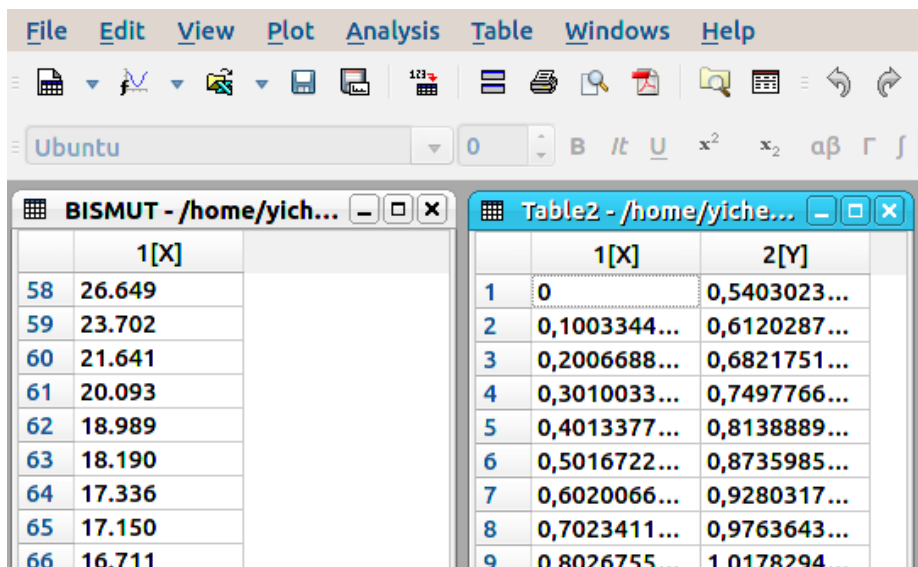
- Type numbers into the table directly from keyboard (straightforward)
- read from an ASCII file

Read from an ASCII file: “File“ → “Import” → “Import ASCII”. A window will pop out. Then choose the file you want to import by click the “folder” icon



Two examples:

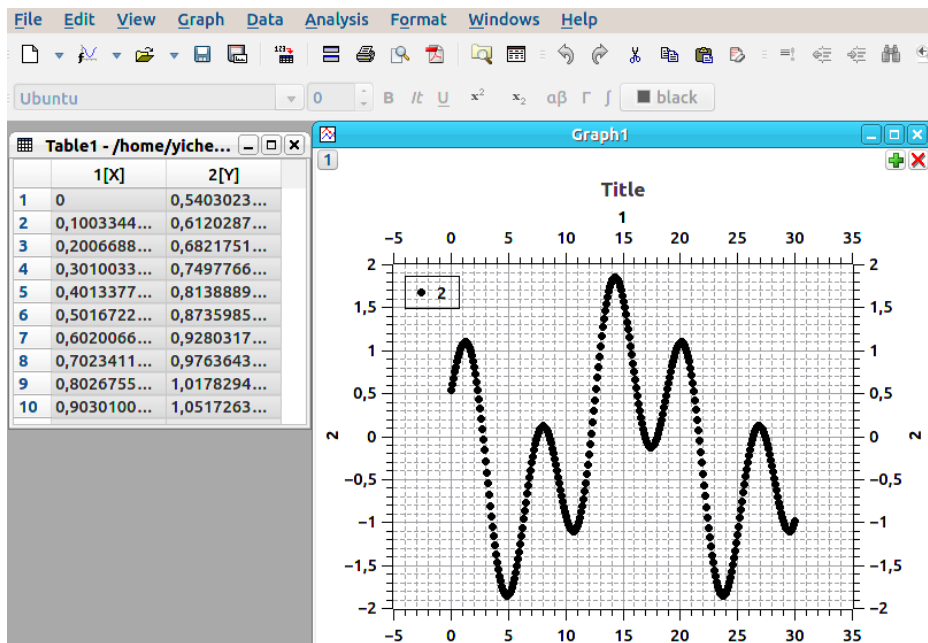
- Left table from 1-D ASCII file.
- Right table from 2-D ASCII file



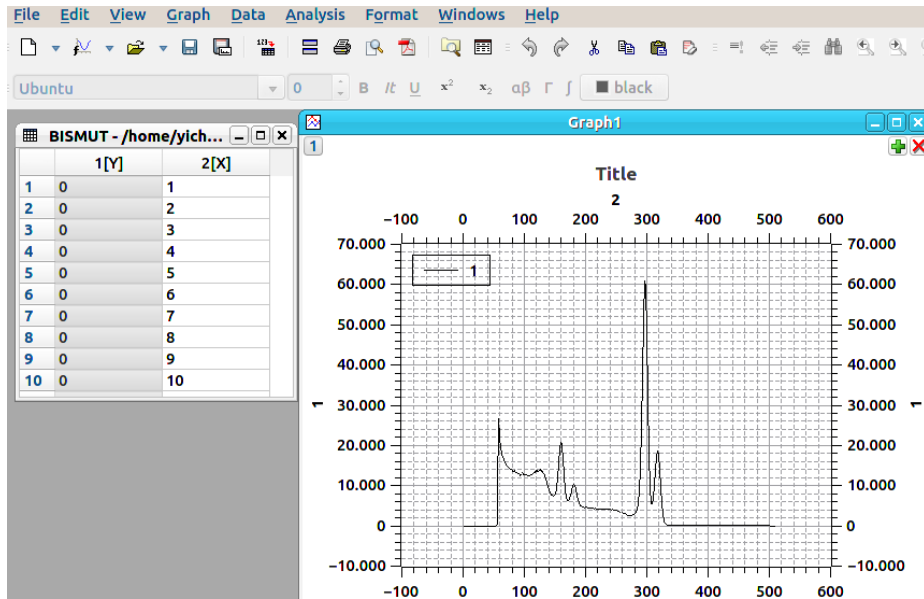
4 Visualization of Data

Visualization means make plots on x-y frame from the data (which is the table).

- For 2-D table, it's easy
 - Hold the “Ctrl” button and left click on the titles of the two columns: one with “[x]” in the title denoting that it is for the x-axis and the other with “[y]” for the y-axis.
 - Right click the table, from the “Plot” option, choose the way you like to do the plot. Many styles available. Just try it out.
 - Below is the effect if I choose “Symbol/Scatter”



- For 1-D table, we need to transform it into 2-D table first
 - First, the default axis is x-axis. So we need to change it to y-axis: double click the column title; find “Plot Designation”; change it to “Y (ordinates)”
 - Then, add another column to make the x-axis: right click the empty space and choose “Add Column”; change its plot designation to “X (abscissae)”; right click the title and choose “Set Column Values”; in the empty space where you can input text, type “i”, which is the row index; click “OK”, then this column will be filled with “i” in each of its row
 - Now you can do the plot as before. An example is shown below:



Besides, each element in the plot (title, tick, dot, line, etc.) can be double clicked and from the window popped up, you can interact with it to configure the style of that element. Try it out. This helps you to make your plots more appealing.

5 Analysis of Data

We always assume the data is sampled from a given distribution but with unknown parameters

$$f(x|a, b, \dots)$$

The task of data analysis is to guess the parameter values from the data set we observed. This process is also called “fit”. It is done automatically in QtiPlot.

We will introduce 4 types of fit:

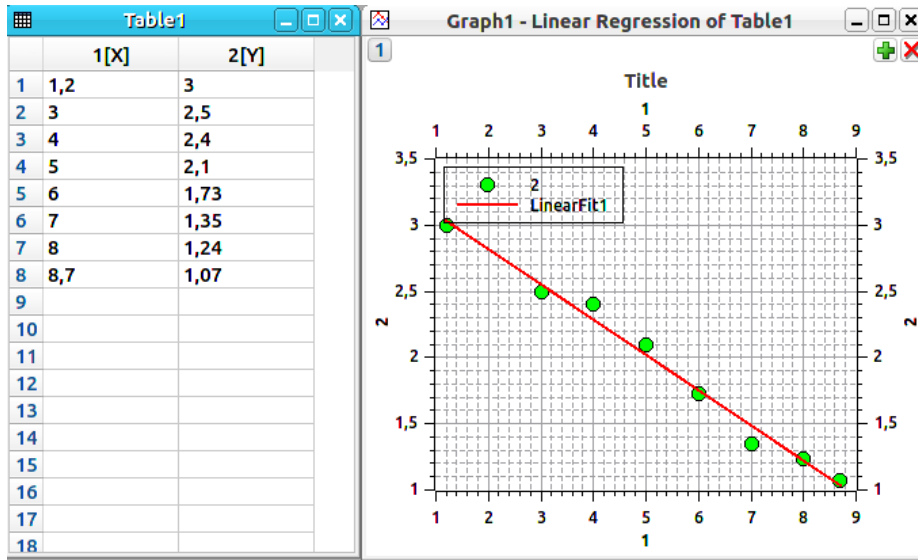
- Linear function, used more often in economics, simple
- Exponential decay function, used to describe isotope activity
- Gaussian function, used to describe error distribution or resonance peak
- Gaussian plus linear function, used to describe resonance peak superimposed on a linear background

5.1 Linear Fit

We have a data set consisted of 8 points, as shown in the figure left below. The points look like to form a straight line. So we can try to fit the points with a linear function

$$f(x|a, b) = a \cdot x + b$$

- Select the two columns in the table as before. Then right click the table and select “Analysis/Fit Linear”
- A graph will be shown including the data presented as dots and the fitted function, as in the figure right below
- Details of the fit will be shown in another dialog



Results Log

```

[02.11.16 13:22      Plot: "Graph1"]
Linear Regression of dataset: Table1_2, using function: A*x+B
Sort: No
Weighting Method: No weighting
From x = 1,2000000000000e+00 to x = 8,7000000000000e+00 (8 data points)
-----
B (y-intercept) = 3,3516794617910e+00 +/- 7,4249329783872e-02
A (slope) = -2,6628055231533e-01 +/- 1,2638069370074e-02
-----
Chi^2/df = 7,3597346933239e-03
R^2 = 0,9866646811465
Adjusted R^2 = 0,9813305536051
RMSE (Root Mean Squared Error) = 0,08578889609573
RSS (Residual Sum of Squares) = 0,04415840815994
  
```

Information shown in the “Results Log”

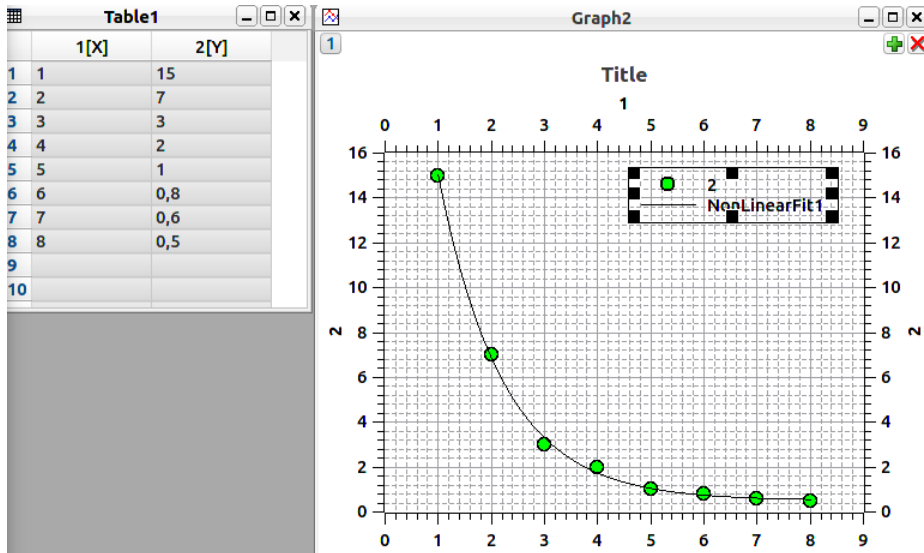
- The dataset and function form used are shown at the beginning
- The fitted values of the parameters together with their uncertainties are shown in the middle
- The bottom shows some nuisance results of the fit

5.2 Exponential Fit

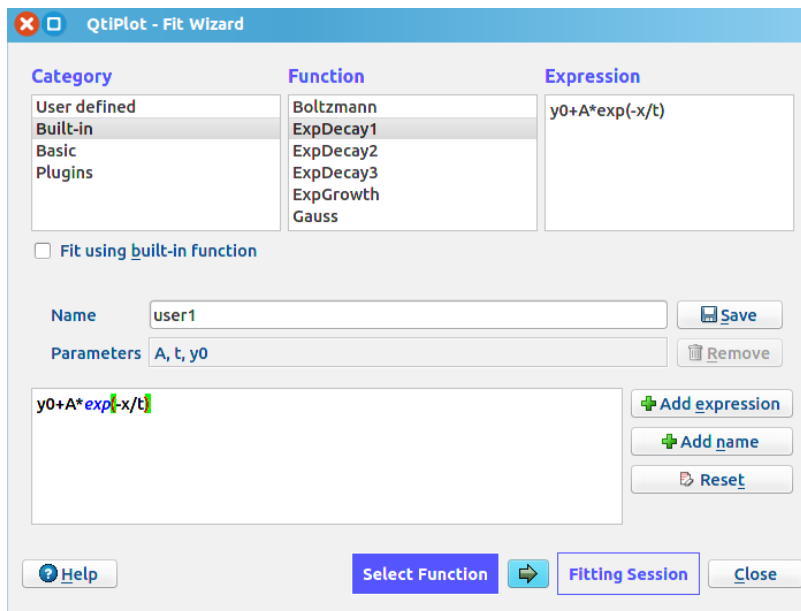
The idea is similar as for linear fit. So I just give the general function form

$$f(x|y_0, A, t) = y_0 + A \cdot e^{-x/t}$$

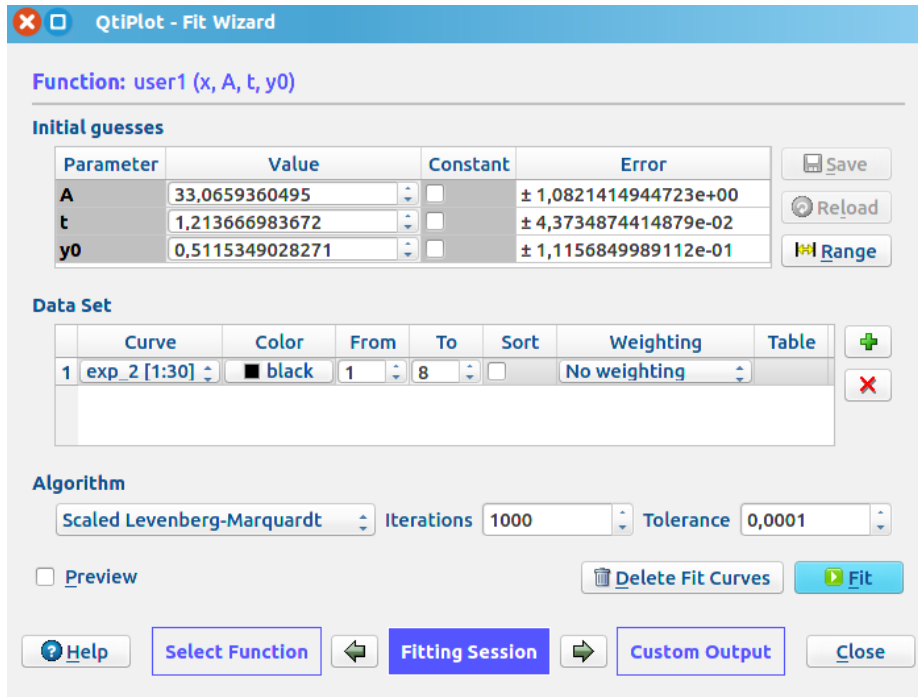
And a simple example below:



But, this function is not directly available from the menu popped out when you right click. Instead you need to select “Analysis/FitWizard”. From the window (shown below), in the “Category” of “Built-in”, find the “Function” of ”ExpDecay1”, and then click “Add expression”.



Now you are ready to do the fit: click the green arrow in the bottom to go to the fitting session (see below). You can click the “Fit” button to perform the fit. Similar results as in linear fit will be shown.



5.3 Gaussian Fit

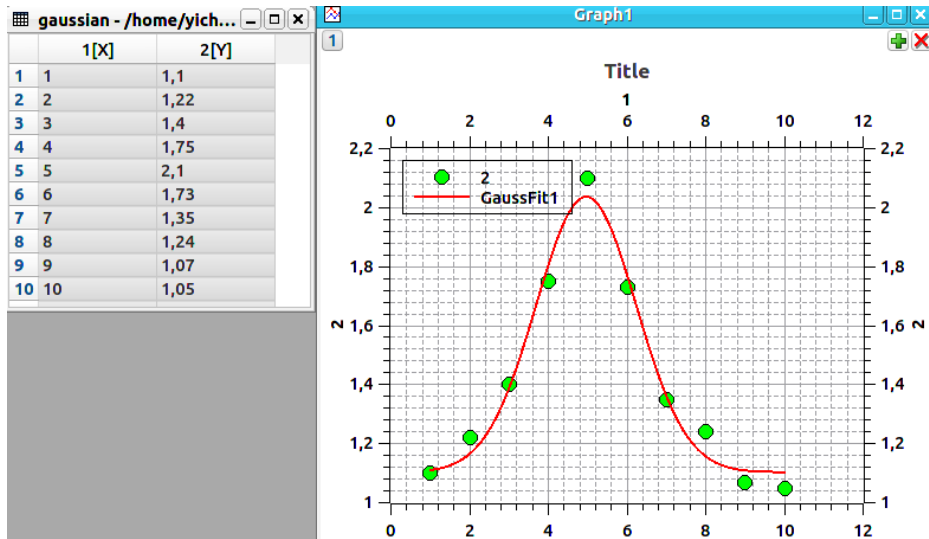
Again, the method is similar as the exponential fit. So I just give the general function form

$$f(x|y_0, x_c, w, A) = y_0 + A \cdot \sqrt{2/\pi}/w \cdot e^{-2(\frac{x-x_c}{w})^2}$$

And a simple example below:

Caution:

- The Gaussian defined in QtiPlot is not the same one we introduced before. It’s a generalized Gaussian. If you want to use the usual Gaussian, you can go to “User defined” to write down the formula by yourself.
- Sometimes the fit won’t work: e.g. the fitted curve shown on the plot doesn’t describe the data points at all. In this case it might be an impropereate initial values for the parameters. You can try to alter the initial values, e.g. the center of the distribution, then try again.



5.4 Gaussian Plus Linear Fit

This belongs to a more general type of fit where there are more than one function forms involved. Which means the data set is sampled from a distribution that is a combination of several sub-distributions:

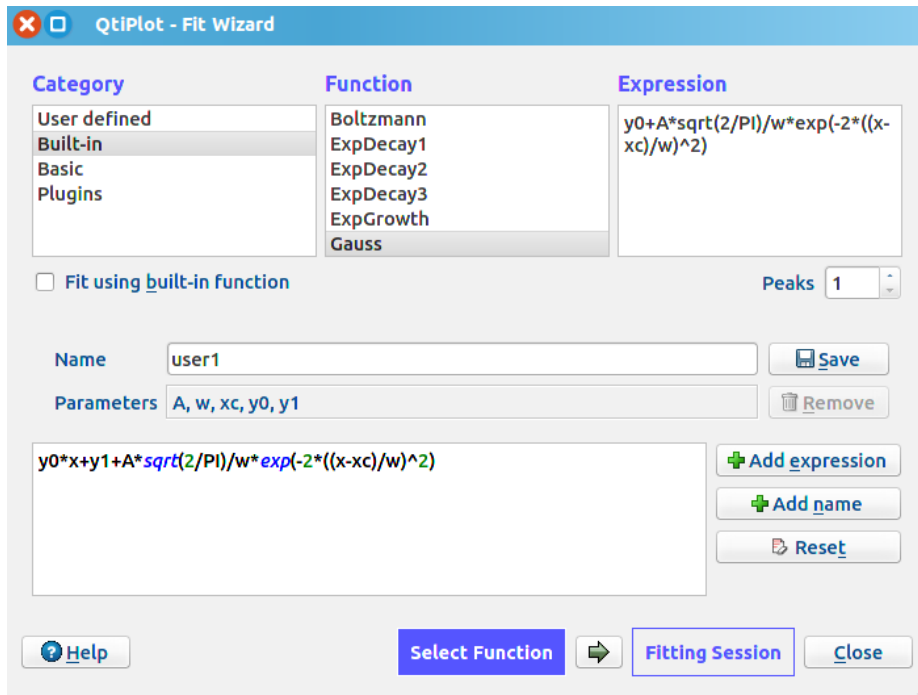
$$f(x|a1, b1, a2, b2, \dots) = a1 \cdot f_1(x|b1, \dots) + a2 \cdot f_2(x|b2, \dots) + \dots$$

Actually, the previous example, which is the generalized Gaussian is already a combined function: a constant y_0 combined with a normal Gaussian.

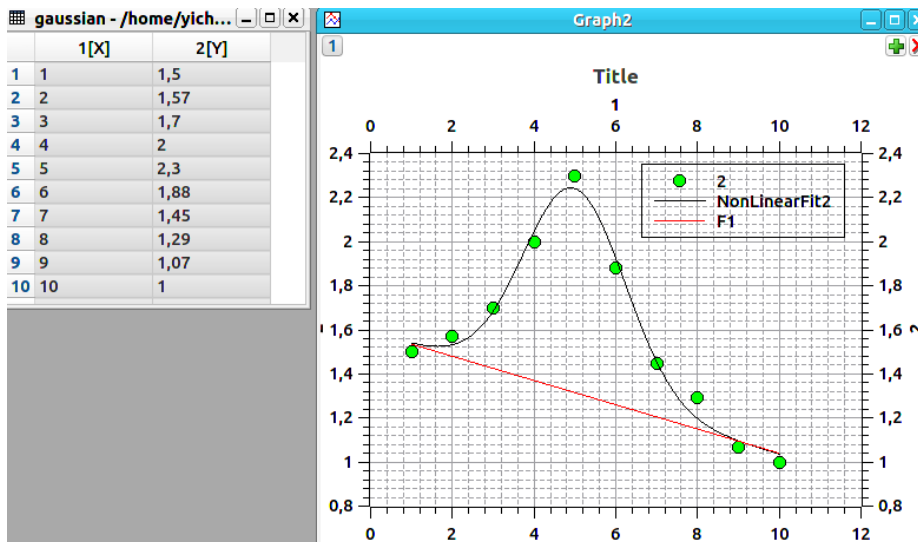
Now let's take a look at an example fit of Gaussian plus linear functions

$$f(x|y_0, y_1, x_c, w, A) = \underbrace{y_0 * x + y_1}_{linear} + \underbrace{A \cdot \sqrt{2/\pi}/w \cdot e^{-2(\frac{x-x_c}{w})^2}}_{Gaussian}$$

This can be constructed directly from the previous Gaussian (see below)



And the fit results can be achieved as usual.

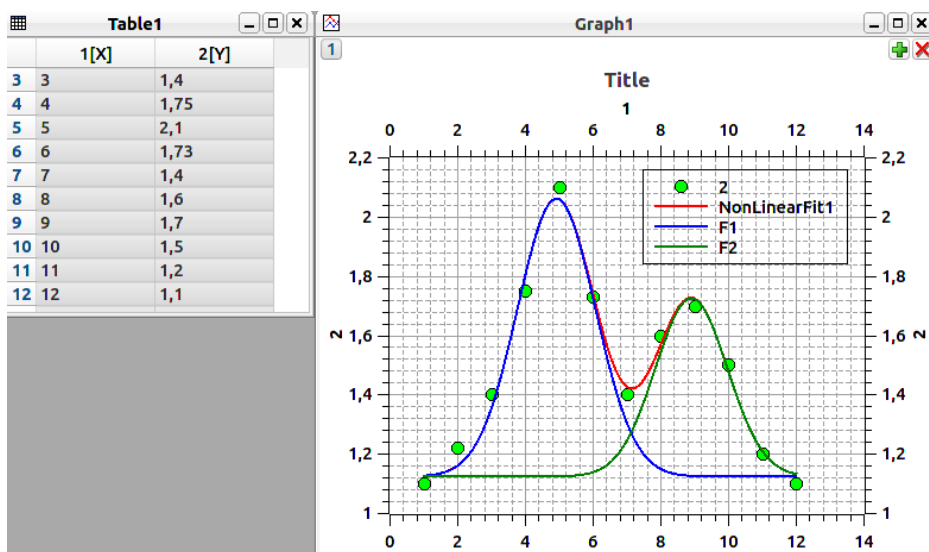


In the above plot, the background model which is the linear function is obviously shown. This is done by right click the panel and select “Add/Add Function”. Then select the linear function and in the window popped out, set the parameters of the linear function to those from the fit results you get in the Gaussian + linear fit.

5.5 Multi-peak Fit

If there are several peaks simultaneously shown on the data, as the left plot below, you would like to fit them in one step. This can be done via

- Go to “Fit Wizard”, select “Built-in/Gauss”. At the right margin, there is a option to control the number of peaks. In this case make it 2
- Then in the “Fitting Session”, input the positions of the two peaks (give values to “xc1” and “xc2”. Then click “Fit”
- You can plot the two peaks separately by adding two more Gaussian onto the plot, where the parameters of the two Gaussian can be found from “Results Log”
- The final effect is shown below on the right



5.6 A Real Example

Below is some real data distribution, what if we want to fit the right most two peaks ? (which means we want to know their exact positions and widths)

- First we need to define the functions to perform the fit. As the example before, we can use the Gaussian with 2 peaks. But it's obvious that the left peak is sitting on some slop. Here we can model this slop using linear function. So the final function will be two Gaussian plus a linear function. So go to “Fit Wizard” and define these functions
- There is another problem: we don't want to fit the whole range of data but just the stretch where the two peaks located. This can be done in the “Fitting Session” panel by choosing the “From” and “To” values of the fit in the “Data Set” category. Let's choose 260 and 340
- Again we need to guess a good initial peak position. In this case, we even might need to adjust the initial widths.

- Now fit and you can get the result shown in the plot below. As usual you can shown each Gaussian and the linear function explicitly. (not done here)
- Finally, you can adjust the range of the x-axis to be presented by double clicking the x-axis and set the parameters in the “scale” category

