qtFit Documentation

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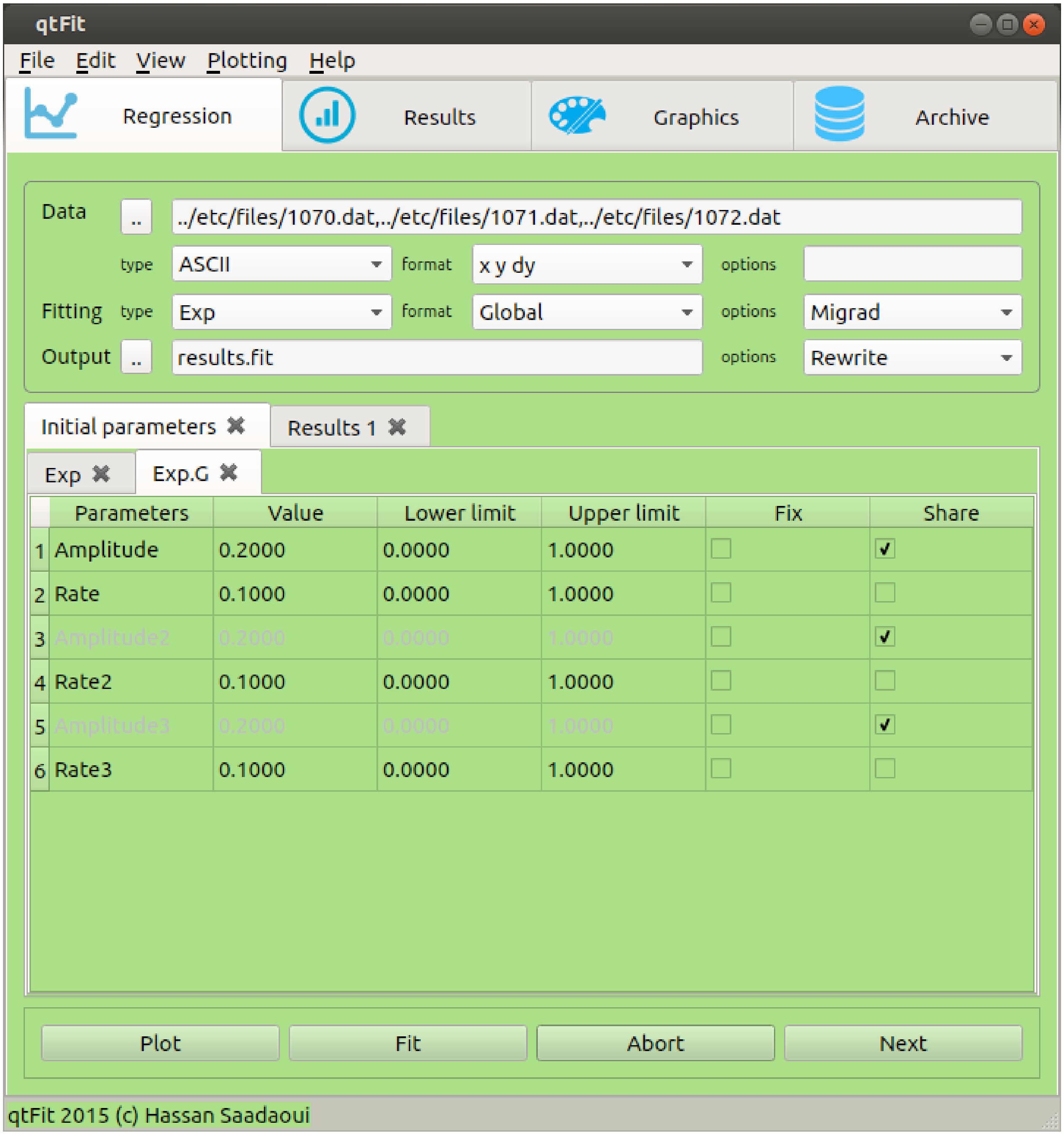
Abstract

qtFit is a program used to fit ASCII data. The graphical user interface (GUI) of qtFit is designed using QT software. The regression is done using CERN's MINUIT routine and plotting is perfomed with the QCustomPlot library. This document is a manual of the qtFit program, and includes instructions about installation, features description, and how-to-use examples.

Contents

1 Introduction

qtFit is used to search, view, and analyze ASCII data. It can be extended by the user to read any type of data. This program is developed by Hassan Saadaoui and is maintained as needed. It is open source and released under the General Public License (GPL). No warranty or guarantee of the results is implied. Please acknowledge the author if you are using this program. For any questions, please email at saadaoui@triumf.ca.



Data .. ../etc/files/1070.dat,../etc/files/1071.dat,../etc/files/1072.dat

type ASCII format x y dy options

Fitting type Exp format Global options Migrad

Output .. results.fit options Rewrite

	Parameters	Value	Lower limit	Upper limit	Fix	Share
1	Amplitude	0.2000	0.0000	1.0000	□	☑
2	Rate	0.1000	0.0000	1.0000	□	□
3	Amplitude2	0.2000	0.0000	1.0000	□	☑
4	Rate2	0.1000	0.0000	1.0000	□	□
5	Amplitude3	0.2000	0.0000	1.0000	□	☑
6	Rate3	0.1000	0.0000	1.0000	□	□

Figure 1: Regression page of the qtFit graphical user interface.

2 Requirements and structure

The program is written in C++ and QT. The latter is used for general programming as well as the graphical user interface. Version 4.8.x or 5.x is needed. The regression is done using MINUIT minimization routine developed at CERN. This package is originally in Fortran and later converted to C++. It is very powerful and well tested. QCustomPlot library (included within the package) is used for data visualization. In addition to the above requirements, and depending on your system, you may also need other packages such as gcc compiler, and automake. The qtFit package contains 4 sub-folders and 5 files.

- src/: contains the source code, and includes the shared main.cpp, and mainwindow.(cpp,ui,h) and a sub-folder for each page.
- fct/ contains the fitting functions and the script "compile" to execute the codes and create the libraries.
- etc/ for documentation, images, data, scripts and templates, and the resources.qrc file needed by QT.
- bin/ where the execution binary data is dumped.
- qtfit.pro used to generate the makefile.
- AUTHOR for authorship attributions.
- COPYING supplies the GPL agreement.
- README.md for installation instructions.

3 Installation

3.1 QT

Download the QT on-line installer from http://www.qt.io/download-open-source/. You need to install QT 4.X.X or QT 5.x binary and source packages.

3.2 MINUIT

To compile, do the following steps.

1. Download latest Minuit2 located at
   http://seal.web.cern.ch/seal/snapshot/work-packages/mathlibs/minuit/release/download.html
2. Unpack and cd `$ tar -xvf minuit.tar.gz -C ~/`
   `$ cd ~/minuit`
3. To install follow the instructions at
   http://seal.web.cern.ch/seal/snapshot/work-packages/mathlibs/minuit/gettingStarted/autoconf.html
4. Make SURE that the tests in the tutorial are running as described in the link
   http://seal.web.cern.ch/seal/snapshot/work-packages/mathlibs/minuit/gettingStarted/testOutput.html
5. Copy (as superuser) the miniut libraries from
   minuit/src/.lib/liblcg_Minuit.* to /usr/lib/
   `$ sudo cp minuit/src/.lib/liblcg_Minuit.* /usr/lib/`
6. Update ldconfig
   `$ sudo ldconfig`

Extra notes: It is somewhat a challenge to compile Minuit2. These extra notes maybe useful.

- Depending on your system, you may need to modify few codes namely src/MnUserTransformation.cpp to add `#include <cstdio>` or `#include <cstdio.h>` just below `#include <algorithm>` and re-compile.
- Locate where libraries and header files are, hopefully in `/usr/local/include/Minuit2`, and `/usr/local/lib/`
- Add the path `/usr/local/lib/` to `/etc/ld.so.conf` as described here http://stackoverflow.com/questions/1099981/why-cant-python-find-shared-objects-that-are-in-directories-in-sys-path

  ```
  $ export LD_LIBRARY_PATH=/usr/local/lib
  ```
  or
  ```
  $ export LD_LIBRARY_PATH=/usr/local/lib:$LD_LIBRARY_PATH
  ```
- Run ldconfig
  ```
  $ sudo ldconfig
  ```

3.3 qtFit

1. Download the latest `qtFit` from local computers, sourceforge, or github.
   ```
   $ wget https://sourceforge.net/projects/qtfit/files/qtfit.tar.gz/download
   ```
2. Unpack it
   ```
   $tar -xvf qtfit.tar.gz -C ~/
   ```
3. cd to the downloaded package
   ```
   $ cd ~/qtfit
   ```
4. If `QT` binaries are not in your path, set the env (locate where qmake is)
   `$ PATH=/usr/Qt/5.4/gcc_64/bin:$PATH` (change `"/usr/Qt/5.4/gcc_64/bin"` as per your system)
   ```
   $ export PATH
   ```
5. Run qmake
   ```
   $ qmake
   ```
6. Run make and make install (as root)
   ```
   $ make
   $ sudo make install
   ```
7. cd to directory `fct/` and compile all the libraries using the script compile
   ```
   $ cd fct
   $ sudo ./compile
   ```
8. To test the gui, invoke
   ```
   $ qtfit
   ```
   or
   `$ ./qtfit` if not installed as root.

4 Description of the GUI

The GUI has a menu bar at the very top and a tab widget below it. This tab widget contains 4 tabs (pages): `Regression`, `Results`, `Plotting`, and `Archive`. Each of these contains widgets for user input and push buttons for issuing signals. The menu bar and the pages functionalities will be described next.

4.1 Menu bar

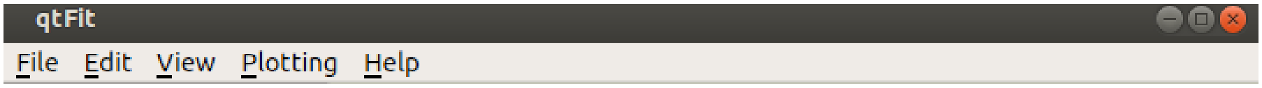


Figure 2: Menubar of the GUI.

File has 2 options; (i) invoke a new window, and (ii) quit/close the window.

Edit is empty for now, not finished...zzz.

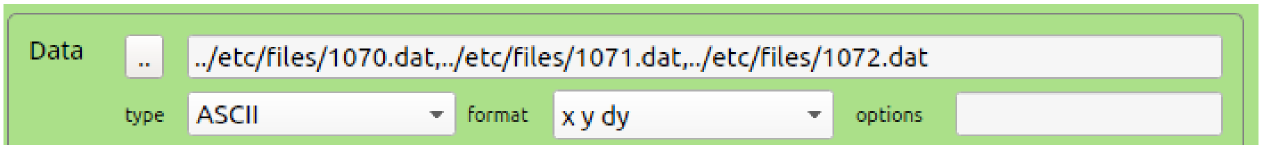
View to change the widget type of the GUI (default is `fuse`+), and its color (default is `"Green-white"`).

Plotting not finished...zzzz.

Help This contains the `"About"` dialog for authorship and version of the current GUI, `"Tips"` dialog which does nothing but remind the user that by hovering the mouse index onto labels one can get the tool-tips for each widget. `"Tutorial"` invokes an HTML page with these instructions.

4.2 Regression

Data input



Data ../etc/files/1070.dat,../etc/files/1071.dat,../etc/files/1072.dat

type ASCII format x y dy options

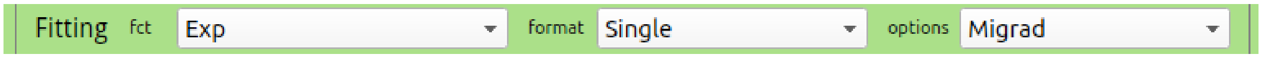
Figure 3: Data input of the regression page.

The user can choose to fit either ASCII text data or something else, for now it is only ASCII. The user can locate the data using the tool button next to Data for ASCII files. The data file must reside in the working directory, otherwise its full name with path should be given. Filenames of the data to fit should be either given in the lineEdit (direct method); or using a file of `.list` or `.inf` suffix, and the user specifies the name of this file (eg: example.list or example.inf) in the lineEdit.

- Direct input, the user can write in the lineEdit "Data" something like `"file1.txt,file2.txt,file3.txt"`
- Indirect input, the user can write in the lineEdit "Data" something like `example.list`, and this file has nothing but a single ascii line like `"file1.txt,file2.txt,file3.txt"`
- Indirect input, the user can write in the lineEdit "Data" something like `example.inf`, and this file contains the columns
```
filenames year variable
file1.txt 2015 100
file2.txt 2014 200
file3.txt 2015 300
```

The inner format of the ASCII file must be set in the field `format`. The file must be in column format separated by space and no other characters than numbers. The limits of xmin and xmax values can be set in the options (settings) field. These must be numbers separated by commas.

Fitting selection



fct Exp
format Single
options Migrad

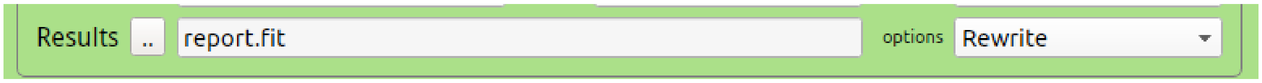
Figure 4: Fitting functions input.

The user can select the function to use, the mode of fitting (single or global) and type of errors. The functions are defined in the folder `fct/` and the user can add new ones by invoking the selection `"Create New"` in the functions comboBox. The user must follow the instructions in the pop-up window and then select `"Update"` from the comboBox. This will add the newly defined function to the list.

For the global method the user can choose to show all parameters for each run or not. These settings can be changed by double clicking on the initial parameters tab-widget.

The errors are defined by `MINUIT` routine, and are symmetric (Migrad) or asymmetric (Minos) errors. The latter are heavy to compute and the program may become unresponsive for sometime while the computation is ongoing. For further details read `http://seal.web.cern.ch/seal/documents/minuit/mnerror.pdf`.

Results output



report.fit
options Rewrite

Figure 5: Fitting results output.

The fitting results are written to this file. The user must specify a name, or browse for an old file. The results can be either appended (using `Append`) to the old file keeping its content (useful for doing run by run fitting), or the old file is overwritten using `Rewrite`.

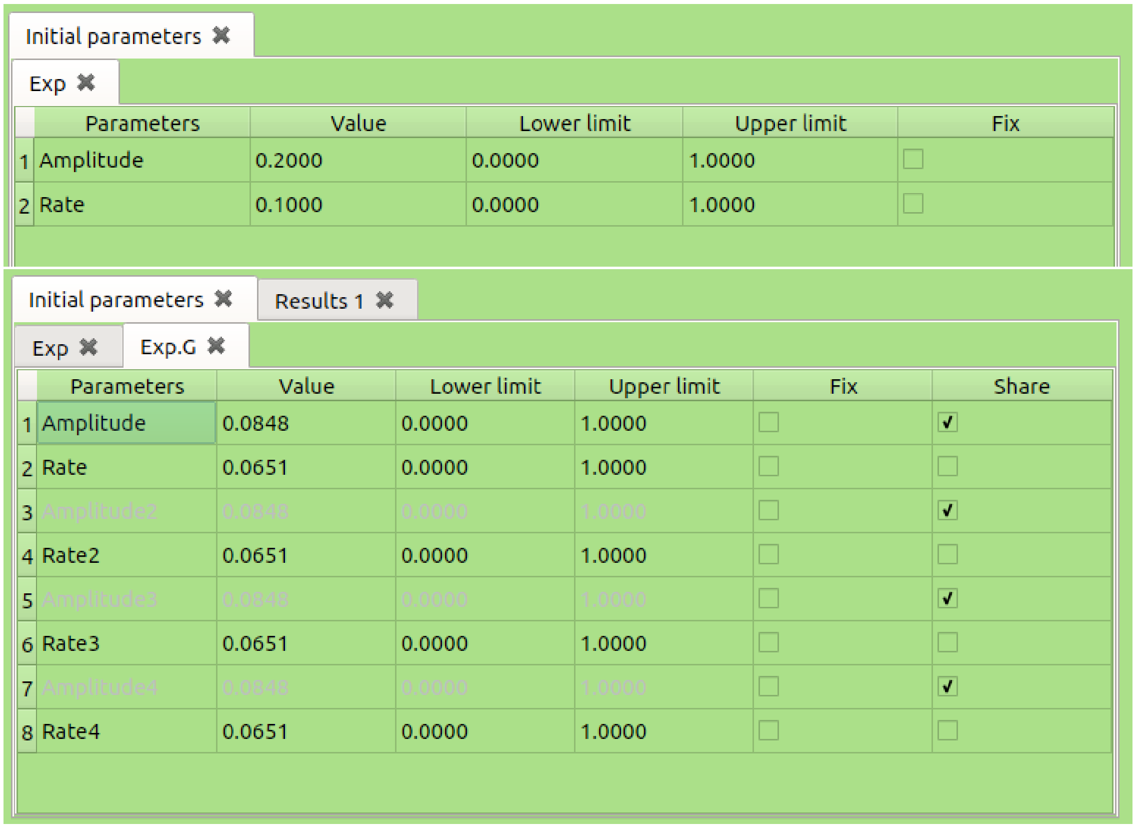
Parameters input

The initial parameters are read from the function library. The table contains 5 columns for the single method, and 6 columns for the global method. These columns are; (1) parameter name, (2) initial value of the parameter, (3) lower limit, (4) upper limit, (5) fix the parameter checkBox, and (6) share the parameter checkBox.

These parameters can be changed, and saved in a template for future use by right-clicking on the specific table and then choose `"save as a template"`. This creates a text file template with a prefix `".tab"`. The user can change this text file as required, and the template can be loaded later for a similar function.

Parameters output

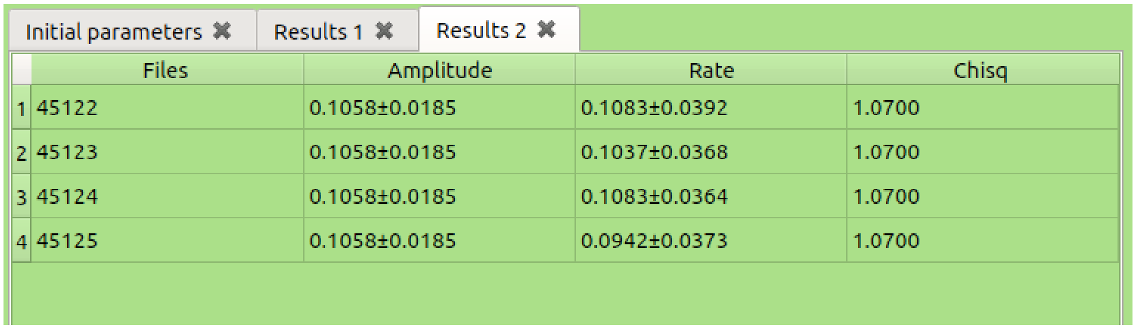
This prints out the output of the fit. The number of significant figures can be set by double-clicking on the results tab. One can also change the number of errors to show, and the way the filename is displayed.



	Parameters	Value	Lower limit	Upper limit	Fix
1	Amplitude	0.2000	0.0000	1.0000	☐
2	Rate	0.1000	0.0000	1.0000	☐

	Parameters	Value	Lower limit	Upper limit	Fix	Share
1	Amplitude	0.0848	0.0000	1.0000	☐	☑
2	Rate	0.0651	0.0000	1.0000	☐	☐
3	Amplitude2	0.0848	0.0000	1.0000	☐	☑
4	Rate2	0.0651	0.0000	1.0000	☐	☐
5	Amplitude3	0.0848	0.0000	1.0000	☐	☑
6	Rate3	0.0651	0.0000	1.0000	☐	☐
7	Amplitude4	0.0848	0.0000	1.0000	☐	☑
8	Rate4	0.0651	0.0000	1.0000	☐	☐

Figure 6: Input parameters for (a) single and (b) global fits. (a) The fit starts from this table for each file, or from the results of the last file in the sequence enabled by double clicking on the `"initial parameters"`. (b) If a parameter is shared between files, only the parameter of the first run is active and the same parameter for other files becomes inactive.

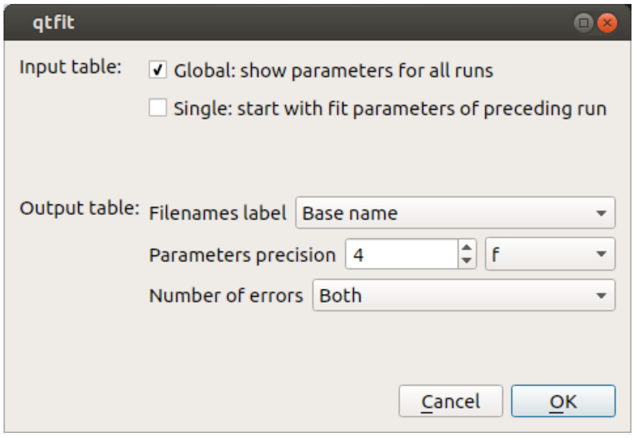


	Files	Amplitude	Rate	Chisq
1	45122	0.1058±0.0185	0.1083±0.0392	1.0700
2	45123	0.1058±0.0185	0.1037±0.0368	1.0700
3	45124	0.1058±0.0185	0.1083±0.0364	1.0700
4	45125	0.1058±0.0185	0.0942±0.0373	1.0700

Figure 7: Results of a global fit where the shared parameter is Amplitude.

Input and output options

The window shown in figure **??** can be invoked by double clicking on the header of the parameters table. In the pop-up window, the user can choose to show the parameters for all files in the case of a global fit, or use a common template for all files. The user can also choose to start the fit with the results of best fitting parameters of the previous file in the sequence (only valid for single fit). For the output table, the user can choose the format of the filename label, parameters precision, and number of errors to display.



Input table: ☑ Global: show parameters for all runs
□ Single: start with fit parameters of preceding run

Output table: Filenames label: Base name
Parameters precision: 4 f
Number of errors: Both

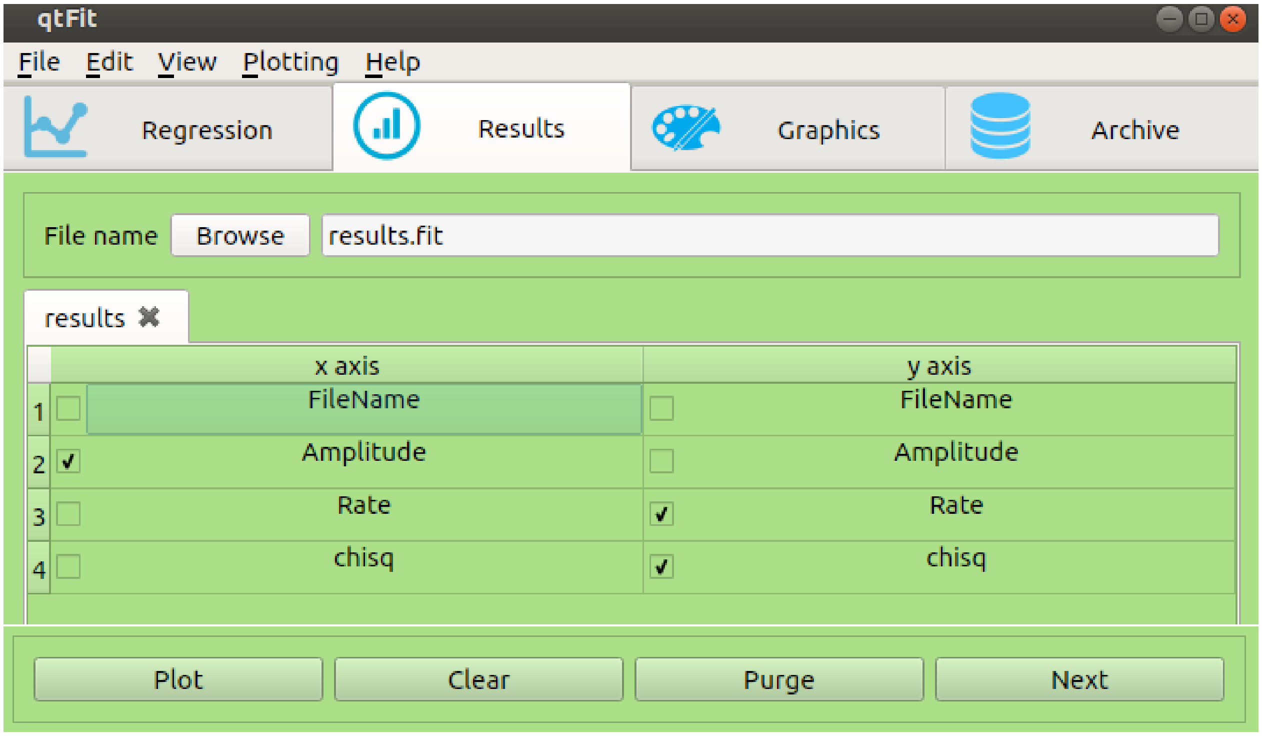
Figure 8: Input and output options.

4.3 Results

This page reads the files of fitting parameters created by the analysis page. It displayed a table with two columns, the left column represents the x-axis and the right column the y-axis. Each column contains all fields found in the specified file (as created during the fitting).

The user can check any of the fields, and a matrix of plots of y versus x will be displayed. The user can clear all choices using "Clear", and kill/delete the active table using "Purge".

The plots will be displayed on the Graphics page. Horizontal or vertical error bars are displayed if specified in the chosen parameter.



File name: results.fit

	x axis		y axis
1	□ FileName		□ FileName
2	☑ Amplitude		□ Amplitude
3	□ Rate		☑ Rate
4	□ chisq		☑ chisq

Figure 9: Results page snapshots.

4.4 Graphics

The plots of the regression page and results pages are displayed here. The user can `export` the graphs into png or pdf, or `Purge/Clear` (delete) the active window(s), or go the archive database with `Next`.

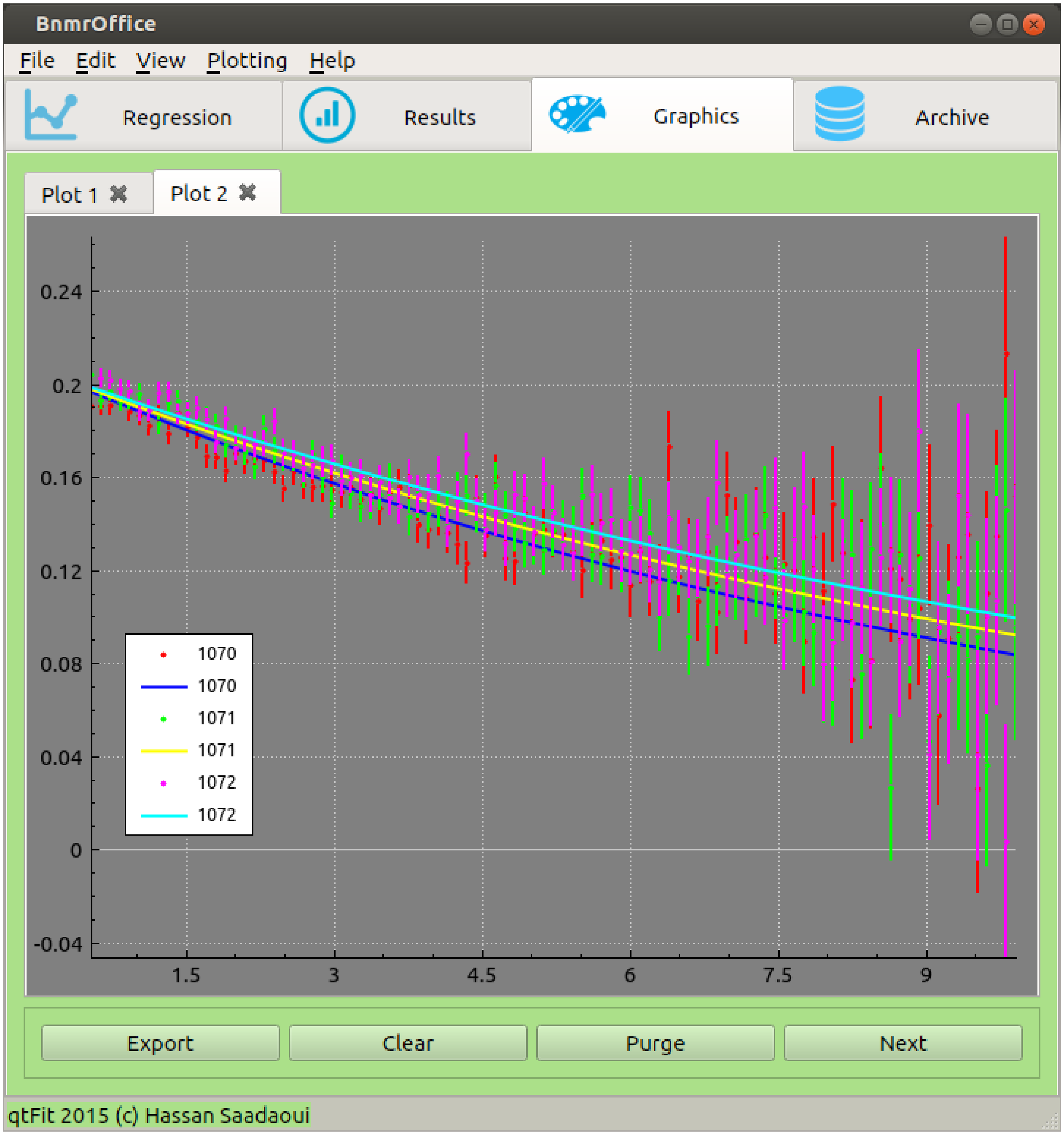
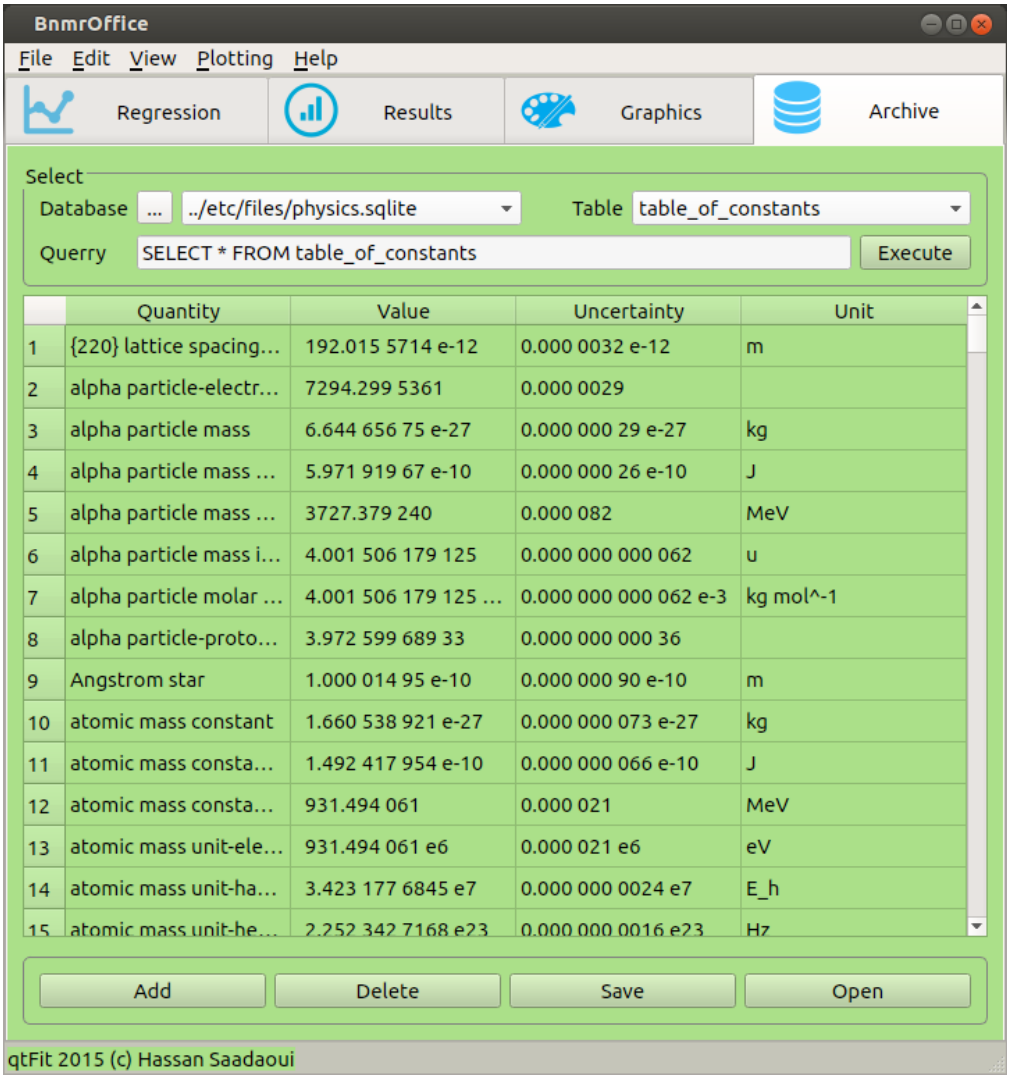


Figure 10: Graphics page.

4.5 Database

This page offers a user-friendly interface for databases, and uses SQLite language `http://www.tutorialspoint.com/sqlite/sqlite_overview.htm`. At the start, the user must select a database by clicking on the toolButton next to `"Database"`, or create a new one from the `"Querry"` lineEdit using SQL commands and hitting `"Execute"`. It is advised to use an SQL manager (like the friendly browser extension SQLite manager) to create databases and tables. Then, one can use this interface to add/delete rows and edit cells, interact with the content of the database. But an experienced user can do everything from this page as well by executing the `"Querry"` commands. Te get familiar with the interface, `"physics.sqlite"` is supplied. Each contain several tables. The user can load any of these tables from the comboBox, and a model of the table will be displayed.

The user can execute any query to study the loaded table. Example;
`SELECT * FROM table_of_constants where Unit="kg"` will select all fields in the `table_of_constants` where the unit is in kg. The user must be familiar with SQL to execute from the Query field. Any table can be changed by adding or deleting rows. Also each cell can be edited, or displayed by clicking on `"Open"`. This can be used to display a cell with a lot of text or view the cell as image if the full path of the image was given in that cell.



Database ... ../etc/files/physics.sqlite

Table table_of_constants

Querry SELECT * FROM table_of_constants

	Quantity	Value	Uncertainty	Unit
1	{220} lattice spacing...	192.015 5714 e-12	0.000 0032 e-12	m
2	alpha particle-electr...	7294.299 5361	0.000 0029	
3	alpha particle mass	6.644 656 75 e-27	0.000 000 29 e-27	kg
4	alpha particle mass ...	5.971 919 67 e-10	0.000 000 26 e-10	J
5	alpha particle mass ...	3727.379 240	0.000 082	MeV
6	alpha particle mass i...	4.001 506 179 125	0.000 000 000 062	u
7	alpha particle molar ...	4.001 506 179 125 ...	0.000 000 000 062 e-3	kg mol^-1
8	alpha particle-proto...	3.972 599 689 33	0.000 000 000 36	
9	Angstrom star	1.000 014 95 e-10	0.000 000 90 e-10	m
10	atomic mass constant	1.660 538 921 e-27	0.000 000 073 e-27	kg
11	atomic mass consta...	1.492 417 954 e-10	0.000 000 066 e-10	J
12	atomic mass consta...	931.494 061	0.000 021	MeV
13	atomic mass unit-ele...	931.494 061 e6	0.000 021 e6	eV
14	atomic mass unit-ha...	3.423 177 6845 e7	0.000 000 0024 e7	E_h
15	atomic mass unit-he...	2.252 342 7168 e23	0.000 000 0016 e23	Hz

Figure 11: Database interface loaded with a table of physical constants.

5 Fitting functions

The user can write his own fitting functions in the directory `fct/`. A new function must be written in `C++` but requires minimal programming knowledge of this language. At template of a typical function is as follows:

```
#include <iostream>
#include <fstream>
#include <math.h>
#include <stdio.h>
#include <vector>
#include <sstream>
#include <string.h>
#include <iostream>
using namespace std;
#include "parameters.h"

//Wrap in "C" for the compiler.
extern "C"
{
  //The defalt initial parameters loaded to the table.
  void defaultParameters(Parameters &defaults)
  {
    defaults.addParameter( "Amplitude" , 0.2, 0.001, 0.15, 1.0 );//par[0]
    defaults.addParameter( "Rate"      , 0.1, 0.001, 0.0,  1.0 );//par[1]
  }
  //This must have the same number of parameters as in the default parameters above.
  double function(double x, const std::vector<double> par)
  {
        return par[0]*exp( - par[1]*x);//par[0] is amplitude and par[1] is rate.
  }
}
```

The user must follow these instructions:

- Make a copy of the file `newFunction.cpp` found in `qtfit/etc/files`.
- Rename the file (eg: newfct.cpp) and save it in the folder `qtfit/fct/`.
- cd to the directory `qtfit/fct/`, and run the script `"compile""` as root
  $ `sudo ./compile name` (eg: sudo ./compile newfct.cpp)

This compiles the library and puts a copy in the functions folder (`/usr/local/qtfit/fct/`).

6 How-To-Use examples

6.1 Example 1

1. After the installation is complete, open the qtFit program from a terminal using the command qtfit.
2. Go to the page Regression.
3. To load a data file, click on the toolButton next to the label "Data". Browse the directory qtfit/etc/files and load the files 1070.dat to 1072.dat, (Hold-on Ctrl key to select more than one file).
4. Select ASCII under "type" comboBox, and xydy under format. Leave the Options field empty for now.
5. Under Fitting; select the function Exp (for exponential fit), and format Single (for single fits), and Migrad (symmetric errors) for the type errors.
6. Write an appropriate name for the output file, any name is acceptable, or leave it as default results.fit.
7. Click on Plot pushButton at the bottom of the page to plot and view the selected files.
8. Click on Fit pushButton at the bottom of the page to perform the regression. If the fit converges, the results of the fit will be displayed in a new table. Go to Graphics page to see the plots of the raw data and fitting functions.
9. Click on Next to send the file results.fit to the results page. The columns of this file will be displayed, and the user can choose to plot a column against the other. On the left, check the box of Amplitude as x variable, and on the right-side of the table check the box Rate as y variable. Click on Plot, this will plot Rate versus Amplitude. Go to the page Graphics to see the new plot. If you click on Clear all checkboxes will be unselected. If you click on Purge all shown tables will be deleted. If you click on Next the Graphics window will be shown.

6.2 Example 2

1. To load a ".inf" file, click on the toolButton next to the label "Data". Browse the directory qtfit/etc/files and load the file example.inf. The header of this file looks like this:

   ```
   #FileName             Time(min) Temperature(K)
   ../etc/files/1070.dat 25        10,0.1
   ../etc/files/1071.dat 22        20,0.3
   ```

   In this example, the ".inf" file contains three colums defined in the header (preceded by the sign #): the filename, a variable called Time in units of min, and a variable called Temperature in units of K. The arguments of each columns are given in the next rows. For Temperature, the given value is accompanied by the error. For example, "10,0.1" means Temperature = 10 ± 0.1 K for the file 1070.dat. In all columns (except the filename), the user can specify one or two errors (asymmetric), and all numbers must be separated by a comma. For example, something like "88,0.1,0.2" means Temperature = $[88 - 0.1, 88 + 0.2]$ K.
2. Repeat steps 4 to 9 in example 1.