Contents

Chapter 1

Fitting Histograms

To fit a histogram you can use the Fit Panel on a visible histogram via the context menu, or you can use the `TH1::Fit` method. The Fit Panel, which is limited, is best for prototyping. The histogram needs to be drawn in a pad before the Fit Panel is invoked. The method `TH1::Fit` is more powerful and is used in scripts and programs.

1.1 The Fit Method

The Fit method is implemented in ROOT for the histogram classes `TH1`, the sparce histogram classes, `THnSparse`, the graph classes, `TGraph`, `TGraph2D` and `TMultiGraph` for fitting a collection of Graphs with the same function.

1.1.1 The TH1::Fit Method

To fit a histogram programmatically, you can use the `TH1::Fit` method. Here is the signatures of `TH1::Fit` and an explanation of the parameters:

```
TFitResultPtr Fit(TF1 *function, Option_t *option, Option_t *goption,
        Axis_t xxmin, Axis_t  xxmax)
```

- `function` a pointer to the fitted function (the fit model) object. One can also use the function name. This name may be one of ROOT pre-defined function names or a user-defined function. See the next paragraph for the list of pre-defined functions.

- `*option:` The second parameter is the fitting option. Here is the list of fitting options:

  - "`W`" Set all weights to 1 for non empty bins; ignore error bars

  - "`WW`" Set all weights to 1 including empty bins; ignore error bars

  - "`I`" Use integral of function in bin instead of value at bin center

  - "`L`" Use log likelihood method (default is chi-square method). To be used when the histogram represents counts

  - "`WL`" Weighted log likelihood method. To be used when the histogram has been filled with weights different than 1.

  - "`P`" Use Pearson chi-square method, using expected errors instead of the observed one given by `TH1::GetBinError` (default case). The expected error is instead estimated from the the square-root of the bin function value.

  - "`Q`" Quiet mode (minimum printing)

  - "`V`" Verbose mode (default is between Q and V)

  - "`S`" The result of the fit is returned in the `TFitResultPtr`.

  - "`E`" Perform better errors estimation using the Minos technique

  - "`M`" Improve fit results, by using the *IMPROVE* algorithm of TMinuit.

  - "`R`" Use the range specified in the function range

  - "`N`" Do not store the graphics function, do not draw

- "0" Do not plot the result of the fit. By default the fitted function is drawn unless the option "N" above is specified.

- "+" Add this new fitted function to the list of fitted functions (by default, the previous function is deleted and only the last one is kept)

- "B"Use this option when you want to fix one or more parameters and the fitting function is a predefined one, like `polN`, `expo`, `landau`, `gaus`. Note that in case of pre-defined functions some default initial values and limits are set.

- "C"In case of linear fitting, don't calculate the chisquare (saves time).

- "F"If fitting a linear function (e.g. `polN`), switch to use the default minimizer (e.g. `Minuit`). By default, `polN` functions are fitted by the linear fitter.

- *goption:The third parameter is the graphics option that is the same as in the `TH1::Draw` (see the chapter Draw Options).

- `xxmin`, `xxmax`:Thee fourth and fifth parameters specify the range over which to apply the fit.

By default, the fitted function object is added to the histogram and is drawn in the current pad.

1.1.2   The TGraph::Fit Method

The signature for fitting a TGraph is exactly the same as for the `TH1`. Only some options apply only for fitting histograms, these are the options "L", "WL" and "I". These options apply instead only for `TGraph::Fit`, the rest of options (appart from "L", "WL" and "I" are the same)

- `TGraph` specific *options*

  - "EX0" When fitting a `TGraphErrors` or a `TgraphAsymErrors` the errors on the coordinates are not used in the fit

  - "ROB" in case of linear fitting use the Robust fitting. Compute the LTS regression coefficients (robust (resistant) regression), using the default fraction of good points.

  - "ROB=0.x" as above, but compute the LTS regression coefficients, using 0.x as a fraction of good points.

1.2   The TF1 function class

Here we will show how to create the `TF1` class that is used for fitting histograms and graphs.

1.2.1   Fit with a Predefined Function

To fit a histogram with a predefined function, simply pass the name of the function in the first parameter of `TH1::Fit`. For example, this line fits histogram object `hist` with a Gaussian.

```
root[] hist.Fit("gaus");
```

The initial parameter values (and eventual limits) for pre-defined functions are set automatically. For overriding the default limits values use the fit option B.

The list of pre-defined functions that can be used with the `Fit` method is the following:

- "gaus" Gaussian function with 3 parameters: `f(x) = p0*exp(-0.5*((x-p1)/p2)^2)`

- "expo"An Exponential with 2 parameters: `f(x) = exp(p0+p1*x)`

- "pol*N*" A polynomial of degree *N*, where N is a number between 0 and 9: `f(x) = p0 + p1*x + p2*x2 +...`

- "chebyshev*N*" A Chebyshev polynomial of degree *N*, where N is a number between 0 and 9: `f(x) = p0 + p1*x + p2*(2*x2-1) +...`

- "landau" Landau function with mean and sigma. This function has been adapted from the `CERNLIB` routine `G110 denlan` (see `TMath::Landau`).

- "gausn Normalized form of the gaussian function with 3 parameters `f(x) = p0*exp(-0.5*((x-p1)/p2)^2)/(p2 *sqrt(2PI))`

1.2.2 Creating User-Defined Functions (TF1)

You can create a **TF1** object and use it in the call the **TH1::Fit**. The parameter in to the **Fit** method is the NAME of the **TF1** object. There are three ways to create a **TF1**.

- Using C++ expression using x with a fixed set of operators and functions defined in **TFormula**.
- Same as first one, with parameters
- Using a function that you have defined. This can be a free function or a functor object or a particular member function of a class.

1.2.2.1 Creating a TF1 with a Formula

Let's look at the first case. Here we call the **TF1** constructor by giving it the formula: `sin(x)/x`.

```
root[] TF1  *f1 = new TF1("f1","sin(x)/x",0,10)
```

You can also use a **TF1** object in the constructor of another **TF1**.

```
root[] TF1  *f2 = new TF1("f2","f1*2",0,10)
```

1.2.2.2 Creating a TF1 with Parameters

The second way to construct a **TF1** is to add parameters to the expression. Here we use two parameters:

```
root[] TF1 *f1 = new TF1("f1","[0]*x*sin([1]*x)",-3,3);
```
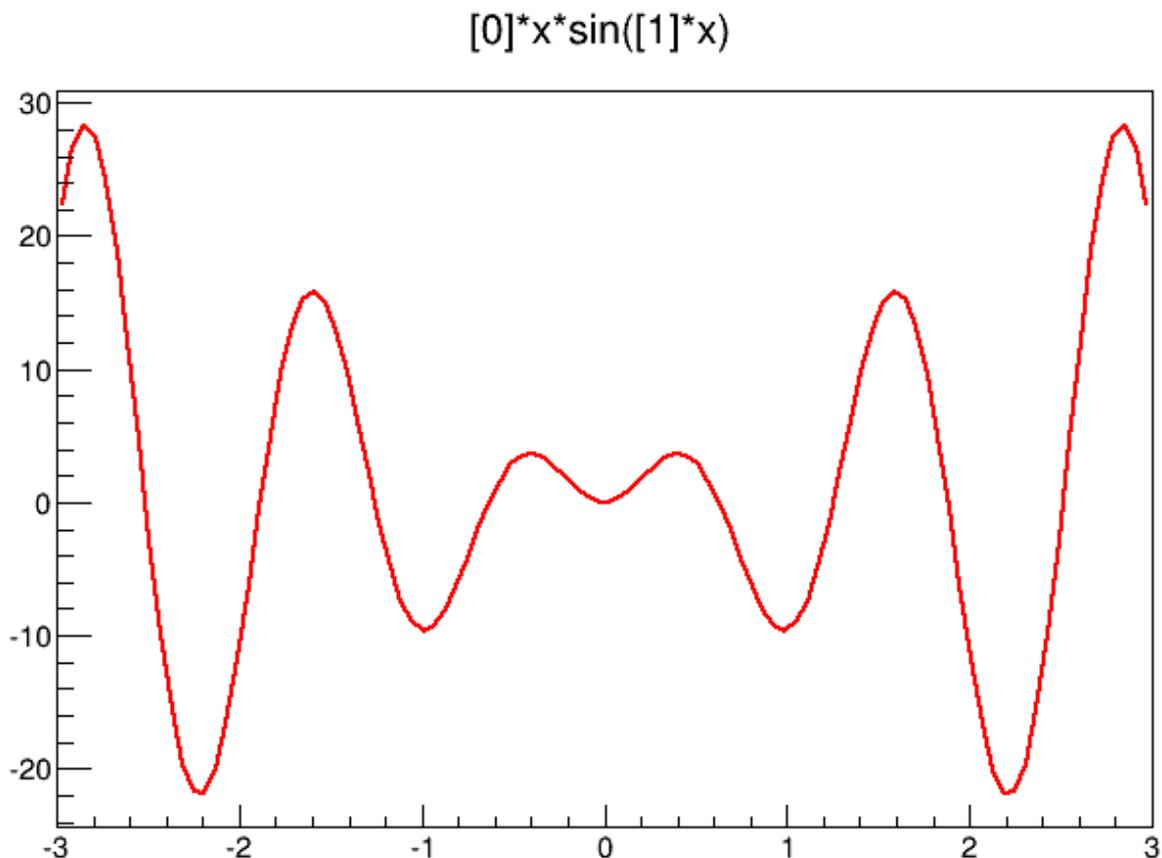

Figure 1.1: The function `x*sin(x)`

The parameter index is enclosed in square brackets. To set the initial parameters explicitly you can use:

```
root[] f1->SetParameter(0,10);
```

This sets parameter 0 to 10. You can also use **SetParameters** to set multiple parameters at once.

```
root[] f1->SetParameters(10,5);
```

This sets parameter 0 to 10 and parameter 1 to 5. We can now draw the `TF1`:

```
root[] f1->Draw()
```

1.2.2.3   Creating a TF1 with a User Function

The third way to build a `TF1` is to define a function yourself and then pass the function pointer to the constructor. A function for a `TF1` constructor needs to have this exact signature:

```
Double_t fitf(Double_t *x,Double_t *par)
```

The two parameters are:

- `x` a pointer to the dimension array. Each element contains a dimension. For a 1D histogram only `x[0]` is used, for a 2D histogram `x[0]` and `x[1]` is used, and for a 3D histogram `x[0]`, `x[1]`, and `x[2]` are used. For histograms, only 3 dimensions apply, but this method is also used to fit other objects, for example an ntuple could have 10 dimensions.

- `par` a pointer to the parameters array. This array contains the current values of parameters when it is called by the fitting function.

The following script `$ROOTSYS/tutorials/fit/myfit.C` illustrates how to fit a 1D histogram with a user-defined function. First we declare the function.

```
// define a function with 3 parameters
Double_t fitf(Double_t *x,Double_t *par) {
   Double_t arg = 0;
   if (par[2]!=0) arg = (x[0] - par[1])/par[2];
   Double_t fitval = par[0]*TMath::Exp(-0.5*arg*arg);
   return fitval;
}
```

Now we use the function:

```
// this function used fitf to fit a histogram
void fitexample() {

   // open a file and get a histogram
   TFile *f = new TFile("hsimple.root");
   TH1F *hpx = (TH1F*)f->Get("hpx");

   // Create a TF1 object using the function defined above.
   // The last three parameters specify the number of parameters
   // for the function.
   TF1 *func = new TF1("fit",fitf,-3,3,3);
   // set the parameters to the mean and RMS of the histogram
   func->SetParameters(500,hpx->GetMean(),hpx->GetRMS());

   // give the parameters meaningful names
   func->SetParNames ("Constant","Mean_value","Sigma");

   // call TH1::Fit with the name of the TF1 object
   hpx->Fit("fit");
}
```

You can create a TF1 also from a C++ function object (functor) with parameters A TF1 can be created from any C++ class implementing this member function:

```
double operator()(double *x, double *p)
```

The advantage of the function object is that it can have a state and reference therefore what-ever other object the user needs, without using globals. This is an example to define first the function object

```
class  MyFunctionObject {
 public:
  // use constructor to customize your function object
  MyFunctionObject(......) { ......}

   double operator() (double *x, double *p) {
```

```
        // function implementation using class data members
    }
};
```

and then use it to create the `TF1`:

```
    MyFunctionObject fobj(....);        // create the function object
    TF1 * f = new TF1("f",fobj,xmin,xmax,npar);    // create TF1 class with n-parameters and range [xmin,xm
```

If using C++11, one can create a `TF1` also from a C++ `lambda` function:

```
// create TF1 class with 2 parameters and range [xmin,xmax] using a lambda
TF1 * f = new TF1("f",[](double*x,double*p){return p[0] + p[1]*x[0];},xmin,xmax,2);
```

1.3 Configuring the Fit

We will show here some configuration actions that can or must be done when fitting histogram or graph using the `Fit` method.

1.3.1 Fixing and Setting Parameters' Bounds

Parameters must be initialized before invoking the `Fit` method. The setting of the parameter initial values is automatic for the predefined functions: `poln`, `exp`, `gaus`, and `landau`. You can fix one or more parameters by specifying the "B" option when calling the `Fit` method. When a function is not predefined, the fit parameters must be initialized to some value as close as possible to the expected values before calling the fit function.

To set bounds for one parameter, use `TF1::SetParLimits`:

```
    func->SetParLimits(0,-1,1);
```

When the lower and upper limits are equal, the parameter is fixed. Next two statements fix parameter 4 at 10.

```
    func->SetParameter(4,10);
    func->SetParLimits(4,10,10);
```

However, to fix a parameter to 0, one must call the `FixParameter` function:

```
    func->SetParameter(4,0);
    func->FixParameter(4,0);
```

Note that you are not forced to set the limits for all parameters. For example, if you fit a function with 6 parameters, you can:

```
    func->SetParameters(0,3.1,1.e-6,-1.5,0,100);
    func->SetParLimits(3,-10,4);
    func->FixParameter(4,0);
```

With this setup, parameters 0->2 can vary freely, parameter 3 has boundaries [-10, 4] with initial value -1.5, and parameter 4 is fixed to 0.

1.3.2 Fitting Sub Ranges

By default, `TH1::Fit` will fit the function on the defined histogram range. You can specify the option "R" in the second parameter of `TH1::Fit` to restrict the fit to the range specified in the `TF1` constructor. In this example, the fit will be limited to -3 to 3, the range specified in the `TF1` constructor.

```
root[] TF1 *f1 = new TF1("f1","[0]*x*sin([1]*x)",-3,3);
root[] hist->Fit("f1","R");
```

You can also specify a range in the call to `TH1::Fit`:

```
root[] hist->Fit("f1","","",-2,2)
```

See macros `$ROOTSYS/tutorials/fit/myfit.C` and `multifit.C` as more completed examples.

1.3.3   Fitting Multiple Sub Ranges

The script for this example is `$ROOTSYS/tutorials/fit/multifit.C`. It shows how to use several Gaussian functions
with different parameters on separate sub ranges of the same histogram. To use a Gaussian, or any other ROOT built
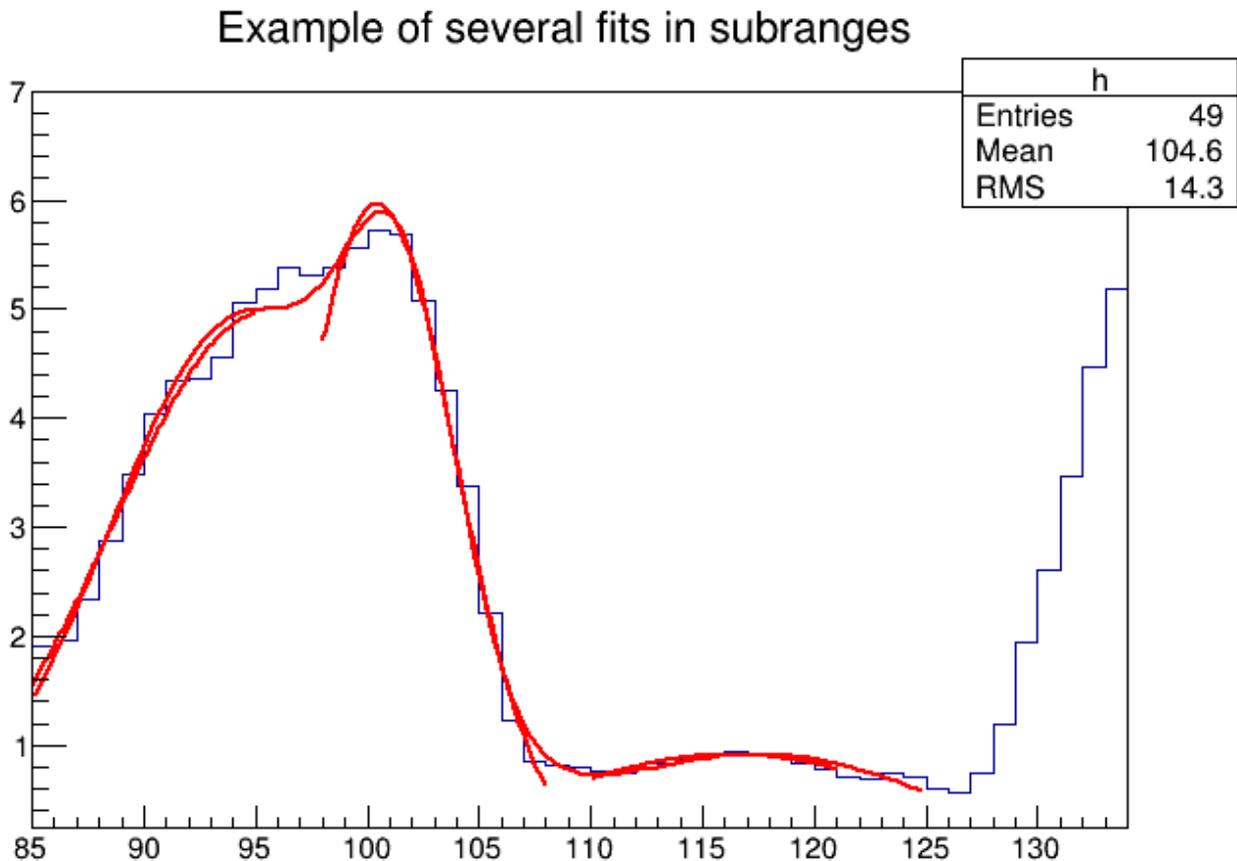in function, on a sub range you need to define a new `TF1`. Each is 'derived' from the canned function `gaus`.

Figure 1.2: Fitting a histogram with several Gaussian functions

First, four TF1 objects are created - one for each sub-range:

```
g1 = new TF1("m1","gaus",85,95);
g2 = new TF1("m2","gaus",98,108);
g3 = new TF1("m3","gaus",110,121);
// The total is the sum of the three, each has 3 parameters
total = new TF1("mstotal","gaus(0)+gaus(3)+gaus(6)",85,125);
```

Next, we fill a histogram with bins defined in the array x.

```
// Create a histogram and set it's contents
h = new TH1F("g1","Example of several fits in subranges",
             np,85,134);
h->SetMaximum(7);
for (int i=0; i<np; i++) {
   h->SetBinContent(i+1,x[i]);
}
// Define the parameter array for the total function
Double_t par[9];
```

When fitting simple functions, such as a Gaussian, the initial values of the parameters are automatically computed by
ROOT. In the more complicated case of the sum of 3 Gaussian functions, the initial values of parameters must be set.
In this particular case, the initial values are taken from the result of the individual fits. The use of the "+" sign is
explained below:

```
// Fit each function and add it to the list of functions
h->Fit(g1,"R");
h->Fit(g2,"R+");
```

```
h->Fit(g3,"R+");

// Get the parameters from the fit
g1->GetParameters(&par[0]);
g2->GetParameters(&par[3]);
g3->GetParameters(&par[6]);

// Use the parameters on the sum
total->SetParameters(par);
h->Fit(total,"R+");
```

1.3.4 Adding Functions to the List

The example `$ROOTSYS/tutorials/fit/multifit.C` also illustrates how to fit several functions on the same histogram. By default a Fit command deletes the previously fitted function in the histogram object. You can specify the option "+" in the second parameter to add the newly fitted function to the existing list of functions for the histogram.

```
root[] hist->Fit("f1","+","",-2,2)
```

Note that the fitted function(s) are saved with the histogram when it is written to a ROOT file.

1.4 Example of fit: Combining Functions

You can combine functions to fit a histogram with their sum as it is illustrated in the macro `FitDemo.C` (`$ROOTSYS/tutorials/fit/FittingDemo.C`). We have a function that is the combination of a background and Lorentzian peak. Each function contributes 3 parameters:

$$y(E) = a_1 + a_2E + a_3E^2 + \frac{A_p(\frac{G}{2p})}{(E-m)^2 + (\frac{G}{2})^2}$$

BackgroundLorentzian Peak

`par[0]` $= a_1$ `par[0]` $= A_p$

`par[1]` $= a_2$ `par[1]` $= G$

`par[2]` $= a_3$ `par[2]` $= m$

The combination function (`fitFunction`) has six parameters:

`fitFunction = background(x,par) + LorentzianPeak(x,&par[3])`

`par[0]=`a_1 `par[1]=`a_2 `par[2]=`a_3 `par[3]=`A_p `par[4]=`G `par[5]=`m

This script creates a histogram and fits it with the combination of two functions. First we define the two functions and the combination function:

```
// Quadratic background function
Double_t background(Double_t *x, Double_t *par) {
    return par[0] + par[1]*x[0] + par[2]*x[0]*x[0];
}

// Lorentzian Peak function
Double_t lorentzianPeak(Double_t *x, Double_t *par) {
    return (0.5*par[0]*par[1]/TMath::Pi()) / TMath::Max(1.e-10,
    (x[0]-par[2])*(x[0]-par[2])+ .25*par[1]*par[1]);
}

// Sum of background and peak function
Double_t fitFunction(Double_t *x, Double_t *par) {
    return background(x,par) + lorentzianPeak(x,&par[3]);
}

void FittingDemo() {
// bevington exercise by P. Malzacher, modified by R. Brun
```

```cpp
const int nBins = 60;
Stat_t data[nBins] = {  6, 1,10,12, 6,13,23,22,15,21,
23,26,36,25,27,35,40,44,66,81,
75,57,48,45,46,41,35,36,53,32,
40,37,38,31,36,44,42,37,32,32,
43,44,35,33,33,39,29,41,32,44,
26,39,29,35,32,21,21,15,25,15};
TH1F *histo = new TH1F("example_9_1",
"Lorentzian Peak on Quadratic Background",60,0,3);

for(int i=0; i < nBins;  i++) {
   // we use these methods to explicitly set the content
   // and error instead of using the fill method.
   histo->SetBinContent(i+1,data[i]);
   histo->SetBinError(i+1,TMath::Sqrt(data[i]));
}
// create a TF1 with the range from 0 to 3 and 6 parameters
TF1 *fitFcn = new TF1("fitFcn",fitFunction,0,3,6);

// first try without starting values for the parameters
// this defaults to 1 for each param.
histo->Fit("fitFcn");
// this results in an ok fit for the polynomial function however
// the non-linear part (Lorentzian
```
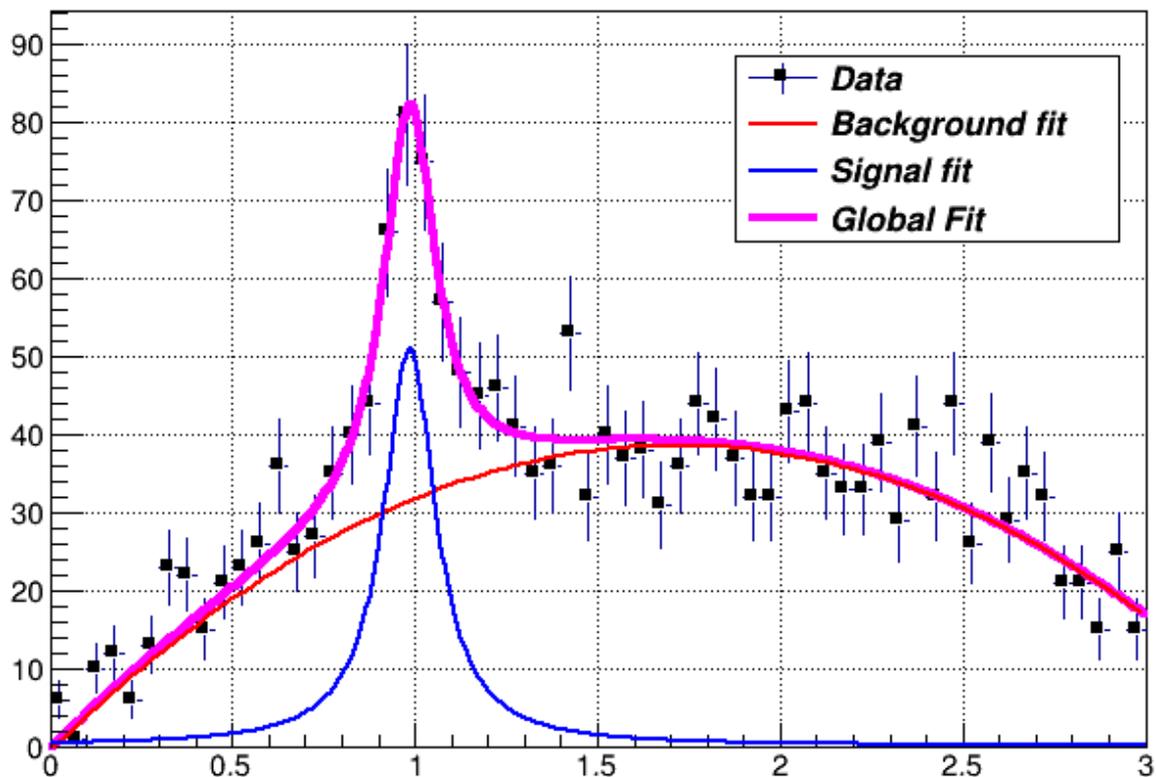

Figure 1.3: The output of the FittingDemo() example

1.5   Result of the fit

Here we will show how to obtain the result of the fit (fitted function, parameter values, errors and eventually the covariance and correlation matrix).

1.5.1   Associated Function

One or more objects (typically a `TF1`*) can be added to the list of functions (`fFunctions`) associated to each histogram. A call to `TH1::Fit` adds the fitted function to this list. Given a histogram `h`, one can retrieve the associated function with:

```
TF1 *myfunc = h->GetFunction("myfunc");
```

1.5.2   Access to the Fit Parameters and Results

If the histogram (or graph) is made persistent, the list of associated functions is also persistent. Retrieve a pointer to the function with the `TH1::GetFunction()`method. Then you can retrieve the fit parameters from the function (**TF1'**) with calls such as:

```
root[] TF1 *fit = hist->GetFunction(function_name);
root[] Double_t chi2 = fit->GetChisquare();
// value of the first parameter
root[] Double_t p1 = fit->GetParameter(0);
// error of the first parameter
root[] Double_t e1 = fit->GetParError(0);
```

Using the fit option `S` one can access the full result of the fit including the covariance and correlation matrix. See later the paragraph `TFitResult`.

1.5.3   Associated Errors

By default, for each bin, the sum of weights is computed at fill time. One can also call `TH1::Sumw2` to force the storage and computation of the sum of the square of weights per bin. If Sumw2 has been called, the error per bin is computed as the `sqrt(sum of squares of weights)`; otherwise, the error is set equal to the `sqrt(bin content)`. To return the error for a given bin number, do:

```
Double_t error = h->GetBinError(bin);
```

Empty bins are excluded in the fit when using the Chi-square fit method. When fitting an histogram representing counts (i.e with Poisson statistics) it is recommended to use the Log-Likelihood method (option 'L' or "WL"), particularly in case of low statistics. When the histogram has been filled with weights different than one, a weighted likelihood method can be used and the errors retrieved from the fit are corrected following a procedure described in paragraph 8.5.2 of the book, *F. James, Statistical Methods in Experimental Physics, 2nd Edition.*

1.5.4   Fit Statistics

You can change the statistics box to display the fit parameters with the `TStyle::SetOptFit(mode)` method. This parameter has four digits: `mode = pcev (default = 0111)`

- `p = 1` print probability
- `c = 1` print Chi-square/number of degrees of freedom
- `e = 1` print errors (if `e=1`, `v` must be 1)
- `v = 1` print name/values of parameters

For example, to print the fit probability, parameter names/values, and errors, use:

```
gStyle->SetOptFit(1011);
```

1.6   The Fit Panel

To display the Fit Panel right click on a histogram to pop up the context menu, and then select the menu entry Fit Panel.

The new Fit Panel GUI is available in ROOT v5.14. Its goal is to replace the old Fit Panel and to provide more user friendly way for performing, exploring and comparing fits.

By design, this user interface is planned to contain two tabs: "General" and "Minimization". Currently, the "General" tab provides user interface elements for setting the fit function, fit method and different fit, draw, print options. The "Minimization tab" provides the option to set the Minimizer to use in the fit and its specific options.
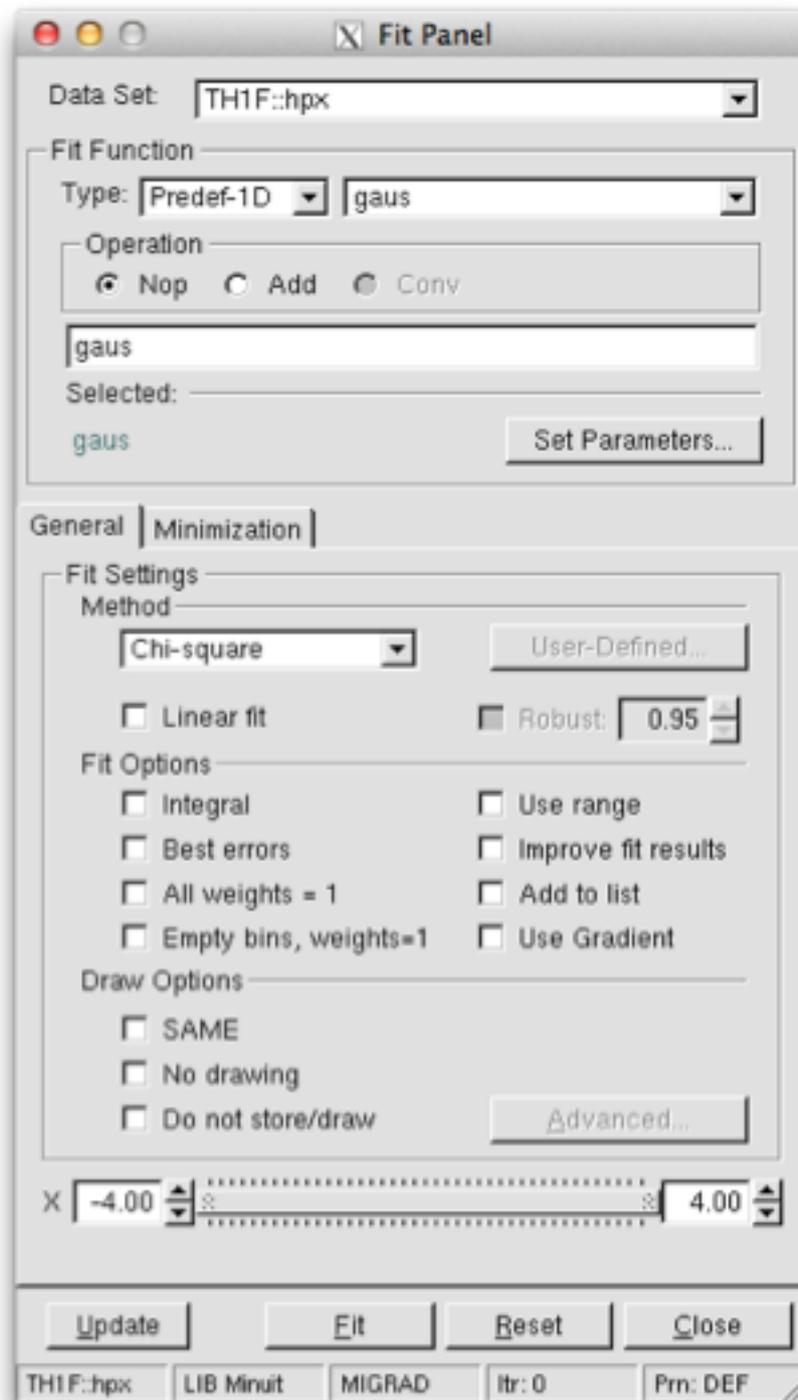
Figure 1.4: The Fit Panel

The new fit panel is a modeless dialog, i.e. when opened, it does not prevent users from interacting with other windows. Its first prototype is a singleton application. When the Fit Panel is activated, users can select an object for fitting in the usual way, i.e. by left-mouse click on it. If the selected object is suitable for fitting, the fit panel is connected with this object and users can perform fits by setting different parameters and options.

1.6.1   Function Choice and Settings

'Predefined' combo box - contains a list of predefined functions in ROOT. You have a choice of several polynomials, a Gaussian, a Landau, and an Exponential function. The default one is Gaussian.

'Operation' radio button group defines the selected operational mode between functions:

Nop - no operation (default);

Add - addition;

Conv - convolution (will be implemented in the future).

Users can enter the function expression into the text entry field below the 'Predefined' combo box. The entered string is checked after the Enter key was pressed and an error message shows up, if the function string is not accepted.

'Set Parameters' button opens a dialog for parameters settings, which will be explaned later.

1.6.2   Fitter Settings

'Method' combo box currently provides only two fit model choices: Chi-square and Binned Likelihood. The default one is Chi-square. The Binned Likelihood is recomended for bins with low statistics.

'Linear Fit' check button sets the use of Linear fitter when is selected. Otherwise the minimization is done by Minuit, i.e. fit option "F" is applied. The Linear fitter can be selected only for functions linears in parameters (for example - `polN`).

'Robust' number entry sets the robust value when fitting graphs.

'No Chi-square' check button switch On/Off the fit option "C" - do not calculate Chi-square (for Linear fitter).

'Integral' check button switch On/Off the option "I" - use integral of function instead of value in bin center.

'Best Errors' sets On/Off the option "E" - better errors estimation by using Minos technique.

'All weights = 1' sets On/Off the option "W"- all weights set to 1 excluding empty bins; error bars ignored.

'Empty bins, weights=1' sets On/Off the option "WW" - all weights equal to 1 including empty bins; error bars ignored.

'Use range' sets On/Off the option "R" - fit only data within the specified function range. Sliders settings are used if this option is set to On. Users can change the function range values by pressing the left mouse button near to the left/right slider edges. It is possible to change both values simultaneously by pressing the left mouse button near to the slider center and moving it to a new position.

'Improve fit results' sets On/Off the option "M"- after minimum is found, search for a new one.

'Add to list' sets On/Off the option "+"- add function to the list without deleting the previous one. When fitting a histogram, the function is attached to the histogram's list of functions. By default, the previously fitted function is deleted and replaced with the most recent one, so the list only contains one function. Setting this option to On will add the newly fitted function to the existing list of functions for the histogram. Note that the fitted functions are saved with the histogram when it is written to a ROOT file. By default, the function is drawn on the pad displaying the histogram.

1.6.3   Draw Options

'SAME' sets On/Off function drawing on the same pad. When a fit is executed, the image of the function is drawn on the current pad.

'No drawing' sets On/Off the option "0"- do not draw the fit results.

'Do not store/draw' sets On/Off option "N"- do not store the function and do not draw it.

1.6.4 Advances Options

The advance option button is enabled only after having performed the fit and provides additional drawing options that can be used after having done the fit. These new drawing tools, which can be selected by the "Advanced Drawing Tool" panel that pops up when clicking the "Advanced" button, are:

- *Contour*: to plot the confidence contour of two chosen parameters. One can select the number of points to draw the contour (more points might require more time to compute it), the parameters and the desired confidence level .

- *Scan* : to plot a scan of the minimization function (likelihood or chi-squared) around the minimum as function of the chosen parameter.

- *Conf Interval* : to plot the confidence interval of the fitted function as a filled coloured band around its central value. One can select the desired confidence level for the band to be plotted.

1.6.5 Print Options

This set of options specifies the amount of feedback printed on the root command line after performed fits.

'*Verbose'* - prints fit results after each iteration.

'*Quiet'* - no fit information is printed.

'*Default'* - between Verbose and Quiet.

1.6.6 Command Buttons

Fit button - performs a fit taking different option settings via the Fit Panel interface.

Reset - sets the GUI elements and related fit settings to the default ones.

Close - closes the Fit panel window.

1.6.7 Minimization Options

With this tab one can select specific options for minimization. These include

- The minimizer library (*Minuit*, *Minuit2*, *Fumili*, *GSL*, *Genetics*)
- The method (algorithm) for minimization. For example for Minuit one can choose between (*Migrad*, *Simplex* or *Scan*)
- Error definition
- Minimization tolerance
- Number of iterations/function calls
- Print Level: (*Default*, *Verbose* or *Quiet*).

1.7 New ROOT::Fit classes

The fitting of the data objects in ROOT, histograms, graphs and tree is performed via some common classes, which are defined in the `ROOT::Fit` namespace. These classes can be classified in the following groups:

- User classes driving the fit: `ROOT::Fit::Fitter` for executing the fit, `ROOT::Fit::FitConfig` for configuring the fit, `ROOT::Fit::ParameterSettings` to define the properties of the fit parameters (initial values, bounds, etc..), `ROOT::Fit::FitResult` for storing the result of the fit.
- Data classes containing the data sets used in the fitting. These classes are the`ROOT::Fit::BinData`for describing bin data sets, thus data points containing both coordinates and a corresponding value/weight with optionally an error on the value or the coordinate and the `ROOT::Fit::UnBinData` for un-binned data sets, which consisst only of a vector of coordinate values. The coordinate values can be one-dimensional (i.e. one entry per event) or multi-dimensional (N entries per event).
- Function classes defining the type of fit (the objective function used for fitting):
    - `ROOT::Fit::Chi2FCN` for chi2 (least-square fits),
    - `ROOT::Fit::PoissonLikelihoodFCN` for binned likelihood fits of histograms,

– `ROOT::Fit::LogLikelihoodFCN` for generic un-binned likelihood fits. These classes are templated on the type of function interface they implement (see later). User convenient typedefs are also provided. They derive from the common generic interface multi-dimensional for function evaluation, `ROOT::Math::IBaseFunctionMultiDim`.

In addition the fitter classes make uses of the generic interfaces for parametric function evaluations, `ROOT::Math::IParametricFunc` to define the fit model function and use the `ROOT::Math::Minimizer` interface to perform the minimization of the objective function.

More information about the function interface and the multi-dimensional minimization in ROOT is given in the Mathematical Library chapter.

Here we present a detailed description of the `ROOT::Fit` classes and how to use them. Using these classes instead of the interface provided directly in the ROOT data objects, like `TH1::Fit` allow are more fine control to configure and customise the fits. For example, using these classes a combined fit of several histograms can be performed.

To understand how these class work, let's go through a simple example, such as fitting an histogram.

When fitting an histogram, instead of using `TH1::Fit` we will show in the following hot wo use the `ROOT::Fit` classes. We will show how to perform the following different type of fits with the histogram data: * a least square fit using the observed errors (Neyman chi-squared); * a least square fit using the expected errors from the function (Pearson chi-squared); * a binned likelihood fit; * an extended unbinned likelihood fits, if the histogram has been set to store in the buffer the original data used to fill it.

Let's go through all the steps required for performing these fits using the `ROOT::Fit::Fitter` class. These steps are: 1. Create the input fit data object. 2. Create the input model function. 3. Configure the fit. 4. Perform the data fitting. 5. Examine the result.

1.7.1 Creating the input fit data

We have two types of input data, binned data (class `ROOT::Fit::BinData`) used for least square (chi-square) fits of histograms or `TGraph` objects or un-binned data (class `ROOT::Fit::UnBinData`) used for fitting vectors of data points (e.g. from a `TTree`).

1.7.1.1 Using Binned data

Let's suppose we have an histogram, represented as a `TH1` type object (it can be one or multi-dimensional). The following shows how to create and fill a `ROOT:Fit::BinData` object.

```
ROOT::Fit::DataOptions opt;
opt.fIntegral = true;
ROOT::Fit::BinData data(opt);
// fill the bin data using the histogram
// we can do this using the following helper function from the Hist library
TH1 * h1 = (TH1*) gDirectory->Get("myHistogram");
ROOT::Fit::FillData(data, h1);
```

In this code example, we have used the utility function of the *Hist* library, `ROOT::Fit::FillData` to fill the `BinData` object. The `ROOT::Fit::FillData` is defined in the headerfile `HFitInterface.h` and it has a signature for all different ROOT objects, like `TH1`, `THnBase`, `TGraph`, `TGraph2D` and `TMultiGraph` It is possible to specify, when creating the `BinData` object, the data range we want to use and some fitting options we want to apply to fill in the object and later when fitting. The fit data options are controlled by the `ROOT::Fit::DataOptions` class, the range by the `ROOT::Fit::DataRange` class.

Here is an example how to specify the input option to use the integral of the function value in the bin instead of using the function value evaluated at the bin center, when doing the fit and to use a range beween the 'xmin' and 'xmax' values.

```
ROOT::Fit::DataOptions opt;
opt.fIntegral = true;
ROOT::Fit::DataRange range(xmin,xmax);
ROOT::Fit::BinData data(opt,range);
// fill the bin data using the histogram
// we can do this using the following helper function from the Hist library
TH1 * h1 = (TH1*) gDirectory->Get("myHistogram");
ROOT::Fit::FillData(data, h1);
```

The list of possible fit options available is the following:

```
ROOT::Fit::DataOptions opt;
opt.fIntegral = true;       // use integral of bin content instead of bin center (default is false).
opt.fBinVolume = true;      // normalize data by the bin volume (default is false).
                            //  This is for fitting density functions in histograms with variable bin si
opt.fUseRange  =true;       // use the function range when creating the fit data (default is false).
opt.fExpErrors = true;      // use the expected errors estimated from the function values
                            //  assuming Poisson statistics and not the observed errors (default is fals
opt.fUseEmpty = true;       // use empty bins when fitting (default is false). If fExpErrors
                            //  is not set an arbitrary error = 1 is assigned to those bins.
opt.fErrors1 = true;        // Set all measured errors to 1 (default is false).
opt.fCoordErrors = false;   // When available coordinate errors are not used in the fit
                            //  (default is true: the errors are used when they are available,
                            //  e.g. fitting a TGraphErrors).
opt.fAsymErrors = false;    // When available asymmetric errors are considered in the fit
                            //  (default is true, the asymmetric errors are used when they are available
                            //  e.g. fitting a TGraphAsymmErrors).
```

The `ROOT::Fit::DataRange` class supports defining multiple rectangular ranges in each dimension, and supports n-dimension. The function `DataRange::AddRange(icoord,xmin,xmax)` adds a range in the coordinate `icoord` with lower value `xmin` and upper value `xmax`:

```
ROOT::Fit::DataRange range;
range.AddRange(icoordinate, xmin, xmax);
```

1.7.1.2   Using Un-Binned data

The unbinned data sets are represented with the `ROOT::Fit::UnBinData` class. For creating un-binned data sets, a `ROOT::Fit::UnBinData` object, one has two possibilities: 1. Copy the data inside `ROOT::Fit::UnBinData`. One can create an empty `UnBinData` object, iterate on the data and add the data point one by one, or directly create the `UnBinData` object from a data iterator. In this case an input `ROOT::Fit::DataRange` object is passed in order to copy the data according to the given range. 2. Use `ROOT::Fit::UnBinData` as a wrapper to an external data storage. In this case the `UnBinData` object is created from an iterator or pointers to the data and the data are not copied inside. In this case the data cannot be selected according to a specified range. All the data points will be included in the fit.

The `ROOT::Fit::UnBinData` class supports also weighted data. In addition to the data points (coordinates), which can be of arbitrary `k` dimensions, the class can be constructed from a vector of weights. This is an example of taking data from an histogram buffer of a `TH1` object:

```
double * buffer = histogram->GetBuffer();
// number of entry is first entry in the buffer
int n = buffer[0];
// when creating the data object it is important to create with the size of the data
ROOT::Fit::UnBinData data(n);
for (int i = 0; i < n; ++i)
    data.add(buffer[2*i+1]);   // the buffer of 1D histogram contains nevt,x1,w1,x2,w2,......
```

Instead in this example we will create a 2-dim `UnBinData` object with the contents from a ROOT `TTree`

```
TFile * file = TFile::Open("hsimple.root");
TTree *ntuple = 0; file->GetObject("ntuple",ntuple);
// select from the tree the data we want to use for fitting
// we use TTree::Draw  for this
int nevt = ntuple->Draw("px:py","","goff");
double * x = ntuple->GetV1();
double * y = ntuple->GetV2();
ROOT::Fit::UnBinData data(nevt, x, y );
```

1.7.2   Creating the Fit model

In order to fit a data sets we need a model to describe our data, e.g. a probability density function describing our observed data or an hypothetical function describing the relation between the independent variables `X` and the single dependent variable `Y`. We can have an arbitrary number `k` of independent variables. For example, when fitting a k-dimensional histogram, the independent variables `X` are the bin center coordinates and `Y` is the bin weight.

The model function needs to be expressed as function of some unknown parameters. The fitting will find the best parameter value to describe the observed data.

We can use the ROOT `TF1` class, the parametric function class, to describe the model function. However the `ROOT::Fit::Fitter` class, to be independent of the ROOT *Hist* library, takes as input a more general parametric function object, the interface (abstract) class `ROOT::Math::IParametricFunctionMultiDim`, which describe a generic one or multi-dimensional function with parameters. This interface extends the abstract class `ROOT::Math::IBaseFunctionMultiDim`, with methods to set/retrieve parameter values and to evaluate the function given the independent vector of values `X` and vector of parameters `P`. More information about the different `ROOT::Math` function interfaces is available in the Mathematical Library chapter.

An end-user can convert a `TF1` object in a `ROOT::Math::IParametricFunctionMultiDim`, using the wrapper class `ROOT::Math::WrapperMultiTF1`:

```
TF1 * f1 = new TF1("f1","gaus");
ROOT::Math::WrappedMultiTF1 fitFunction(f1, f1->GetNdim() );
ROOT::Fit::Fitter fitter;
fitter.SetFunction( fitFunction, false);
```

When creating the wrapper, the parameter values stored in `TF1` will be copied in the `ROOT::Math::WrappedMultiTF1` object. The function object representing the model function is given to the `ROOT::Fitter` class using the `Fitter::SetFunction` method.

The user has also the possibility to provide a function object, which implements the derivatives of the function with respect to the parameters. This information might be useful for some types of fits. In this case he needs to provide the function object as a class deriving from the `ROOT::Math::IParametricGradFunctionMultiDim` interface. Note that the wrapper class `ROOT::Math::WrappedMultiTF1` implements also the gradient interface, using internally `TF1::GradientPar`, which is based on numerical differentiation, apart for the case of linear functions (i.e. when `TF1::IsLinear()` is `true`). The parameter derivatives of the model function can be useful to some minimization algorithms, such as Fumili. However, in general is better to leave the minimization algorithm (e.g. Minuit) to compute the needed derivatives using its own customised numerical differentiation algorithm. In order to not provide to the fitter the parameter derivatives, we explicitly passed in `Fitter::SetFunction` a `false` value.

1.7.3 Fit Configuration

The configuration of the fit is done via the `ROOT::Fit::FitConfig` class and its contained `ROOT::Fit::ParameterSettings` class. These are the possible allowed fit configurations:

- setting the initial values of the parameters;
- setting the parameter step sizes;
- setting eventual parameter bounds;
- setting the minimizer library and the particular algorithm to use;
- setting different minimization options (print level, tolerance, max iterations, etc...)
- setting the type of parameter errors to compute (parabolic error, Minos errors, re-normalize errors using fitted chi2 values)

The initial parameter values can be set directly in the input model function object. However, for setting parameter bounds and step sizes to values different than the automatically computed ones, one needs to use the `ROOT::Fit::ParameterSetting` class. This example code will set the lower/upper bounds for the first parameter and a lower bound for the second parameter

```
fitter.SetFunction( fitFunction, false);
fitter.Config().ParSettings(0).SetLimits(0,1.E6);
fitter.Config().ParSettings(2).SetLowerLimit(0);
```

Note that a `ROOT::Fit::ParameterSettings` objects exists for each fit parameter and it created by the `ROOT::Fit::FitConfig` class, after the model function has been set in the Fitter. Only when the function is set, the number of parameter is known and automatically the `FitConfig` creates the corresponding `ParameterSetting` objects.

When fitting, different minimizer can be used. The can be implemented in different libraries and loaded ar run time by the plug-in manager system of ROOT. Each different minimizer (e.g. *Minuit, Minuit2, Fumili,* etc.) consists of a different implementation of the `ROOT::Math::Minimizer` interface. Within the same minimizer, thus within the same class implementing the `Minimizer` interface, different algorithms can exist. For example in the case of Minuit, we have *Migrad, Simplex* or *Minimize*. The minimizer and its corresponding algorithm, when available, can be set by using the function `FitConfig::SetMinimizer("minimizerName")` or by using directly the `ROOT:Math::MinimizerOptions` class.

If the requested minimizer is not available in ROOT, the default one is used. The default minimizer type and algorithm can be specified by using the static function `ROOT::Math::MinimizerOptions::SetDefaultMinimizer("minimizerName")`

1.7.4 Minimizer Libraries and Algorithms

The list of available minimizer libraries currently available in ROOT, with their corresponding available algorithms is the following one. Some minimizers (e.g. *Minuit*) contain several algorithms that the user can choose. Others are based on a single algorithm (e.g. *Fumili*)

- `Minuit` (library *libMinuit*). Old version of Minuit, based on the `TMinuit` class. The list of possible algorithms are:

  - *Migrad* (default one)
  - *Simplex*
  - *Minimize* (it is a combination of Migrad and Simplex)
  - *MigradImproved*
  - *Scan*
  - *Seek*

- `Minuit2` (library *libMinuit2*). New C++ version of Minuit. The list of possible algorithm is :

  - *Migrad* (default)
  - *Simplex*
  - *Minimize*
  - *Scan*
  - *Fumili* . This is the same algorithm of `TFumili`, but implemented in the Minuit2 library.

- `Fumili`. Implement a dedicated minimization algorithm for least-square and likelihood fits. It has requirements on the type of method function to be used. No specific algorithm exists

- `GSLMultiMin` (library *libMathMore*). Minimizer based on the Multidimensional Minimization routines of the Gnu Scientific Library (GSL). The list of available algorithms is

  - *BFGS2* (default) : second version of the vector Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm;
  - *BFGS* : old version of the vector Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm;
  - *ConjugateFR* : Fletcher-Reeves conjugate gradient algorithm;
  - *ConjugatePR* : Polak-Ribiere conjugate gradient algorithm;
  - *SteepestDescent*: steepest descent algorithm;

- `GSLMultiFit` (library *libMathMore*). Minimizer based on the Non-Linear Least-Square routines of GSL. This minimizer can be used only for least-square fits.

- `GSLSimAn` (library *libMathMore*). Minimizer based on simulated annealing.

- `Genetic` (library *libGenetic*). Genetic minimizer based on an algorithm implemented in the *TMVA* package.

Each minimizer can be configured using the `ROOT::Math::MinimizerOptions` class. The list of possible option that can be set are:

- *Minimizer type* (`MinimizerOptions::SetMinimizerType(const char *)`) .
- *Minimizer algorithm* (`MinimizerOptions::SetMinimizerAlgorithm(const char *)`).
- *Print Level* (`MinimizerOptions::SetPrintLevel(int )`) to set the verbose printing level (default is 0).

- *Tolerance* (`MinimizerOptions::SetTolerance(double )`) tolerance used to control the iterations.
- *Maximum number of function calls* (`MinimizerOptions::SetMaxFunctionCalls(int )`).
- *Maximum number of iterations* (`MinimizerOptions::SetMaxIterations(int )`). Note that this is not used by *Minuit*
- *FCN Upper value for Error Definition* (`MinimizerOptions::SetErrorDef(double )`). Value in the minimization function used to compute the parameter errors. The default is to get the uncertainties at the 68% CL is a value of 1 for a chi-squared function minimization and 0.5 for a log-likelihood function.
- *Strategy* (`MinimizerOptions::SetStrategy(int )`), minimization strategy used. For each minimization strategy *Minuit* uses different configuration parameters (e.g. different requirements in computing derivatives, computing full Hessian (strategy = 2) or an approximate version. The default is a value of 1. In this case the full Hessian matrix is computed only after the minimization.
- *Precision* (`MinimizerOptions::SetPrecision(double )`). Precision value in the evaluation of the minimization function. Default is numerical double precision.

Note that not all the options are implemented by all the minimizers. For example in *Minuit* is possible to set the maximum number of function calls, but not the maximum number of iterations. The Strategy and the Precision options apply instead only for *Minuit* (and *Minuit2*).

The class supports also setting global default values for the options, by using the static functions `MinimizerOptions::SetDefault...` (for example `MinimizerOptions::SetDefaultPrintLevel(int )`). The static functions can be also used to set the minimizer options when using `TH1::Fit` or `TGraph::Fit`. The list of the current option values can be inspected by using `MinimizerOptions::Print`.

```
ROOT::Math::MinimizerOptions() opt;
// print the default minimizer option values
opt.Print();
```

In addition it is possible to provide extra options which might apply for a particular minimizer `MinimizerOptions::SetExtraOptions(const IOptions & )`. See the documentation of the particular minimizer to use for the list of possible additional options available.

1.7.5   Performing the Fit

Here we have now all the required input ingredients for the fit, the data and the function to fit. Depending on these we have now several different way to perform the fit, using the corresponding methods of the `ROOT::Fit::Fitter` class and depending on the type of input data.

1.7.5.1   Available fit methods

- **Least-square fit**: `Fitter::LeastSquare(const BinData & )` or `Fitter::Fit(const Bindata &)`. It requires the user to pass a `BinData` object. It should be used when the data values follow a Gaussian distribution. This fit method is implemented using the class `ROOT::Fit::Chi2FCN`.
- **Binned Likelihood fit** : `Fitter::LikelihoodFit(const Bindata & )`. The user needs to pass a `BinData` object. It should be used when the data values follow a Poisson or a multinomial distribution. The Poisson case (extended fit) is the default and in this case the function normalization is also fit to the data. The Multi-nominal case can be selected by passing the optional *extended* boolean flag as *false*. This method is implemented by the class `ROOT::Fit:::PoissonLikelihoodFCN`.
- **Un-Binned likelihood fit**: `Fitter::LikelihoodFit(const UnBindata &)`. The user needs to pass an `UnBinData` object. By default the fit is not extended (i.e. the normalization is not fitted to the data). As above the user can select an extended likelihood fit by passing the optional *extended* boolean flag as *true*. This methos is implemented using the class `LogLikelihoodFCN`
- **Linear Fit**: A linear fit can be selected (no iterative minimization is needed in this case, but using linear algebra algorithms from the *Matrix* library), if the model function is linear in the parameters.

1.7.5.2   Customised Fit methods

Above we described the pre-defined methods used for fitting. A user can also implement its own fitting methods, thus its version of the chi-square or likelihood function he wants to minimize. In this cas, the user does not really need to build as input a `ROOT::Fit` data set and model function as we described before. He can implements its own version of the method function using on its own data set objects and functions.

In this case `ROOT::Fit::Fitter::SetFCN` is used to set the method function and `ROOT::Fit::FitFCN` is used for fitting. The method function can be passed also in `ROOT::Fit::FitFCN`, but in this case a previously defined fitting configuration is used.

The possible type of method functions that can be bassed in `ROOT::Fit::Fitter::SetFCN` are:

- A generic functor object implementing `operator()(const double * p)` where **p** is the parameter vectors. In this case one needs to pass the number of parameters, the function object and optionally a vector of initial parameter values. Other optional parameter include the size of the data sets and a flag specifying if it is a chi2 (least-square fit). In the last two parameters are given, the `chi2/ndf` can be computed after fitting the data.

```
template <class Function>
bool Fitter::SetFCN(unsigned int npar, Function & f,
                    const double * initialParameters = 0,
                    unsigned int dataSize=0, bool isChi2Fit = false)
```

- A function object implementing the `ROOT::Math::IBaseFunctionMultiDim` interface:

```
bool Fitter::SetFCN(const ROOT::Math::IBaseFunctionMultiDim  & f,
                    const double * initialParameters = 0,
                    unsigned int dataSize=0, bool isChi2Fit = false)
```

- A function object implementing the `ROOT::Math::FitMethodFunction` interface. This is an interface class extending the `ROOT::Math::IBaseFunctionMultiDim` with some extra functionality which can be used when fitting. This extra functionality is required by dedicated fitting algorithms like *Fumili* or *GSLMultiFit*.

```
bool Fitter::SetFCN(const ROOT::Math::FitMethodFunction  & f,
                    const double * initialParameters = 0, unsigned int dataSize=0)
```

- A old-Minuit like FCN interface (i.e. a free function with the signature `fcn(int &npar, double *gin, double &f, double *u, int flag)`.

```
typedef void(* MinuitFCN)(int &npar, double *gin, double &f, double *u, int flag)
bool Fitter::SetFCN(MinuitFCN fcn, int npar,
                    const double * initialParameters = 0,
                    unsigned int dataSize=0, bool isChi2Fit = false)
```

1.7.6   Fit Result

The result of the fit is contained in the `ROOT::Fit::Result` object. A reference to the result object is obtained with the function `Fitter::Result()`. The `ROOT::Fit::FitResult` class provides an API for retrieving parameter values, errors, covariance and correlation matrix from the fit, minimum chi2/likelihood values, etc. . .

A `FitResult::Print` method is also available to print the result of the fit.

The class has a self-explanatory API so, see its reference documentation for the possible information available after the fit.

One extra functionality offered by `ROOT::Fit::FitResult` is the possibility to compute the confidence intervals of the function after the fit. The function `ROOT::Fit::FitResult::GetConfidenceInterval` given an input data sets (e.g. a `BinData` object) and a confidence level value (e.g. 68%) computes the lower/upper band values of the model function at the given data points.

1.7.7   TFitResult

`TFitResult` is a class deriving from `ROOT::Fit::Result` and providing in addition some convenient methods to return a covariance or correlation matrix as a `TMatrixDSym` object. In addition `TFitResult` derives from `TNamed` and can be conveniently stored in a file.

When fitting an histogram (a `TH1` object) or a graph (a `TGraph` object) it is possible to return a `TFitResult` via the `TFitResultPtr` object, which behaves as a smart pointer to a `TFitResult`. `TFitResultPtr` is the return object by `TH1::Fit` or `TGraph::Fit`. By default the TFitResultPtr contains only the status of the fit and can be obtained by an automatic conversion of the TFitResultPtr to an integer.

If the fit option *S* is instead used, `TFitResultPtr` contains the `TFitResult` and behaves as a smart pointer to it. This is an example:

```
int fitStatus =  hist->Fit(myFunction);     // TFitResultPtr contains only the fit status

TFitResultPtr r = hist->Fit(myFunction,"S"); // TFitResultPtr contains the TFitResult
TMatrixDSym cov = r->GetCovarianceMatrix();  //  to access the covariance matrix
Double_t chi2   = r->Chi2();                 // to retrieve the fit chi2
Double_t par0   = r->Parameter(0);           // retrieve the value for the parameter 0
Double_t err0   = r->ParError(0);            // retrieve the error for the parameter 0
r->Print("V");                               // print full information of fit including covariance matrix
r->Write();                                  // store the result in a file
```

1.8   The Minimization packages

As explained before various minimization packages can be used when fitting in ROOT. We have seen before how to configure the `Fitter` class to use different minimization packages and different minimization options. When using the `Fit` method the minimization package (and its options) can be selected using the static methods of the `ROOT::Math::MinimizerOptions` class. For example to select `Minuit2` instead of `Minuit` for fitting an histogram do:

```
ROOT::Math::MinimizerOptions::SetDefaultMinimizer("Minuit2");
// fit the histogram histo with the gaussian pre-defined function
histo->Fit("gaus");
```

In the following we will give some brief description of the minimization packages. The packages all implement the `ROOT::Math::Minimizer` interface which can be use for finding the minimum of a multi-dimensional function. The interface is documented in the Mathematical Library Chapter.

In addition packages like Minuit or Minuit2 provide their own interfaces.

1.9 MINUIT (Old TMInuit Version)

This package was originally written in FORTRAN by Fred James and part of `PACKLIB` (patch D506). It has been converted to a C++ class by René Brun. The current implementation in C++ is a straightforward conversion of the original FORTRAN version. The main changes are:

- The variables in the various `Minuit` labeled common blocks have been changed to the **TMinuit** class data members

- The internal arrays with a maximum dimension depending on the maximum number of parameters are now data members' arrays with a dynamic dimension such that one can fit very large problems by simply initializing the **TMinuit** constructor with the maximum number of parameters

- The include file `Minuit.h` has been commented as much as possible using existing comments in the code or the printed documentation

- The original `Minuit` subroutines are now member functions

- Constructors and destructor have been added

- Instead of passing the `FCN` function in the argument list, the addresses of this function is stored as pointer in the data members of the class. This is by far more elegant and flexible in an interactive environment. The member function `SetFCN` can be used to define this pointer

- The ROOT static function `Printf` is provided to replace all format statements and to print on currently defined output file

- The functions `SetObjectFit/GetObjectFit` can be used inside the `FCN` function to set/get a referenced object instead of using global variables

- By default `fGraphicsMode` is true. When calling the `Minuit` functions such as `mncont`, `mnscan`, or any `Minuit` command invoking `mnplot`, `TMinuit::mnplot()` produces a **TGraph** object pointed by `fPlot`. One can retrieve this object with **TMinuit::GetPlot()**. For example:

```
h->Fit("gaus");
gMinuit->Command("SCAn 1");
TGraph *gr = (TGraph*)gMinuit->GetPlot();
gr->SetMarkerStyle(21);
gr->Draw("alp");
```

- To set `Minuit` in no graphics mode, call

```
gMinuit->SetGraphicsMode(kFALSE);
```

1.9.1 Basic Concepts of Minuit

The `Minuit` package acts on a multi parameter FORTRAN function to which one must give the generic name `FCN`. In the ROOT implementation, the function `FCN` is defined via the `Minuit SetFCN` member function when an histogram fitting is invoked. The value of `FCN` will in general depend on one or more variable parameters.

1.9.2 The Transformation of Limited Parameters

For variable parameters with limits, `Minuit` uses the following transformation:

```
Pint = arcsin(2((Pext-a)/(b-a))-1)
```

```
Pext = a+((b-a)/(2))(sinPint+1)
```

so that the internal value `Pint` can take on any value, while the external value Pext can take on values only between the lower limit a and the ext upper limit b. Since the transformation is necessarily non-linear, it would transform a nice linear problem into a nasty non-linear one, which is the reason why limits should be avoided if not necessary. In addition, the transformation does require some computer time, so it slows down the computation a little bit, and more importantly, it introduces additional numerical inaccuracy into the problem in addition to what is introduced in the numerical calculation of the FCN value. The effects of non-linearity and numerical round off both become more important as the external value gets closer to one of the limits (expressed as the distance to nearest limit divided by distance between limits). The user must therefore be aware of the fact that, for example, if they put limits of (0, 1010) on a parameter, then the values 0.0 and 1. 0 will be indistinguishable to the accuracy of most machines.

The transformation also affects the parameter error matrix, of course, so Minuit does a transformation of the error matrix (and the ''parabolic" parameter errors) when there are parameter limits. Users should however realize that the transformation is only a linear approximation, and that it cannot give a meaningful result if one or more parameters is very close to a limit, where $\frac{\partial Pext}{\partial Pint} \neq 0$. Therefore, it is recommended that:

- Limits on variable parameters should be used only when needed in order to prevent the parameter from taking on unphysical values

- When a satisfactory minimum has been found using limits, the limits should then be removed if possible, in order to perform or re-perform the error analysis without limits

1.9.3   How to Get the Right Answer from Minuit

`Minuit` offers the user a choice of several minimization algorithms. The `MIGRAD` algorithm is in general the best minimized for nearly all functions. It is a variable-metric method with inexact line search, a stable metric updating scheme, and checks for positive-definiteness. Its main weakness is that it depends heavily on knowledge of the first derivatives, and fails miserably if they are very inaccurate.

If parameter limits are needed, in spite of the side effects, then the user should be aware of the following techniques to alleviate problems caused by limits:

1.9.3.1   Getting the Right Minimum with Limits

If MIGRAD converges normally to a point where no parameter is near one of its limits, then the existence of limits has probably not prevented `Minuit` from finding the right minimum. On the other hand, if one or more parameters is near its limit at the minimum, this may be because the true minimum is indeed at a limit, or it may be because the minimized has become ''blocked" at a limit. This may normally happen only if the parameter is so close to a limit (internal value at an odd multiple of $\pm\frac{\pi}{2}$ that `Minuit` prints a warning to this effect when it prints the parameter values. The minimized can become blocked at a limit, because at a limit the derivative seen by the minimized $\frac{\partial F}{\partial Pint}$ is zero no matter what the real derivative $\frac{\partial F}{\partial Pext}$ is.

$$\left(\frac{\partial F}{\partial Pint}\right) = \left(\frac{\partial F}{\partial Pext}\right)\left(\frac{\partial Pext}{\partial Pint}\right) = \left(\frac{\partial F}{\partial Pext}\right) = 0$$

1.9.3.2   Getting the Right Parameter Errors with Limits

In the best case, where the minimum is far from any limits, `Minuit` will correctly transform the error matrix, and the parameter errors it reports should be accurate and very close to those you would have got without limits. In other cases (which should be more common, since otherwise you would not need limits), the very meaning of parameter errors becomes problematic. Mathematically, since the limit is an absolute constraint on the parameter, a parameter at its limit has no error, at least in one direction. The error matrix, which can assign only symmetric errors, then becomes essentially meaningless.

1.9.3.3   Interpretation of Parameter Errors

There are two kinds of problems that can arise: the reliability of `Minuit`'s error estimates, and their statistical interpretation, assuming they are accurate.

1.9.3.4 Statistical Interpretation

For discussion of basic concepts, such as the meaning of the elements of the error matrix, or setting of exact confidence levels see the articles:

- F.James. Determining the statistical Significance of experimental Results. Technical Report DD/81/02 and CERN Report 81-03, CERN, 1981

- W.T.Eadie, D.Drijard, F.James, M.Roos, and B.Sadoulet. *Statistical Methods in Experimental Physics. North-Holland, 1971*

1.9.4 Reliability of Minuit Error Estimates

`Minuit` always carries around its own current estimates of the parameter errors, which it will print out on request, no matter how accurate they are at any given point in the execution. For example, at initialization, these estimates are just the starting step sizes as specified by the user. After a `HESSE` step, the errors are usually quite accurate, unless there has been a problem. `Minuit`, when it prints out error values, also gives some indication of how reliable it thinks they are. For example, those marked `CURRENT GUESS ERROR` are only working values not to be believed, and `APPROXIMATE ERROR` means that they have been calculated but there is reason to believe that they may not be accurate.

If no mitigating adjective is given, then at least `Minuit` believes the errors are accurate, although there is always a small chance that `Minuit` has been fooled. Some visible signs that `Minuit` may have been fooled:

- Warning messages produced during the minimization or error analysis

- Failure to find new minimum

- Value of EDM too big (estimated Distance to Minimum)

- Correlation coefficients exactly equal to zero, unless some parameters are known to be uncorrelated with the others

- Correlation coefficients very close to one (greater than 0.99). This indicates both an exceptionally difficult problem, and one which has been badly parameterized so that individual errors are not very meaningful because they are so highly correlated

- Parameter at limit. This condition, signaled by a `Minuit` warning message, may make both the function minimum and parameter errors unreliable. See the discussion above 'Getting the right parameter errors with limits'

The best way to be absolutely sure of the errors is to use ''independent''calculations and compare them, or compare the calculated errors with a picture of the function. Theoretically, the covariance matrix for a''physical'' function must be positive-definite at the minimum, although it may not be so for all points far away from the minimum, even for a well-determined physical problem. Therefore, if `MIGRAD` reports that it has found a non-positive-definite covariance matrix, this may be a sign of one or more of the following:

1.9.4.1 A Non-physical Region

On its way to the minimum, `MIGRAD` may have traversed a region that has unphysical behavior, which is of course not a serious problem as long as it recovers and leaves such a region.

1.9.4.2 An Underdetermined Problem

If the matrix is not positive-definite even at the minimum, this may mean that the solution is not well defined, for example that there are more unknowns than there are data points, or that the parameterization of the fit contains a linear dependence. If this is the case, then `Minuit` (or any other program) cannot solve your problem uniquely. The error matrix will necessarily be largely meaningless, so the user must remove the under determinedness by reformulating the parameterization. `Minuit` cannot do this itself.

1.9.4.3 Numerical Inaccuracies

It is possible that the apparent lack of positive-definiteness is due to excessive round off errors in numerical calculations (in the user function), or not enough precision. This is unlikely in general, but becomes more likely if the number of free parameters is very large, or if the parameters are badly scaled (not all of the same order of magnitude), and correlations are large. In any case, whether the non-positive-definiteness is real or only numerical is largely irrelevant, since in both cases the error matrix will be unreliable and the minimum suspicious.

1.9.4.4 An Ill-posed Problem

For questions of parameter dependence, see the discussion above on positive-definiteness. Possible other mathematical problems are the following:

- Excessive numerical round off - be especially careful of exponential and factorial functions which get big very quickly and lose accuracy.

- Starting too far from the solution - the function may have unphysical local minima, especially at infinity in some variables.

1.10   Minuit2 Package

`Minuit2` is a new object-oriented implementation, written in C++, of the popular `MINUIT` minimization package. Compared with the `TMinuit` class, which is a direct conversion from FORTRAN to C++, `Minuit2` is a complete redesign and re-implementation of the package. This new version provides all the functionality present in the old FORTRAN version, with almost equivalent numerical accuracy and computational performances. Furthermore, it contains some fixes and small improvements and this new functionality: * The possibility to set single side parameter limits * the FUMILI algorithm (see the next paragraph "FUMILI Minimization Package"), which is an optimized method for least square and log likelihood minimizations.

Minuit2 has been originally developed by M. Winkler and F. James in the SEAL project. More information can be found on the MINUIT Web Site and in particular at the following documentation page at http://www.cern.ch/minuit/doc/doc.html.

A detailed User Guide for Minuit2 exists, describing the API of the internal classes. ROOT uses `Minuit2` for fitting via the `Minuit2Minimizer` class which implements the `ROOT::Math::Minimizer` interface.

`Minuit2` is also distributed as an independent package of ROOT and can be built without any other dependency on the ROOT libraries.

Examples on how to use the `Minuit2` and `Fumili2` plug-ins are provided in the tutorials' directory `$ROOTSYS/tutorials/fit`: `minuit2FitBench.C`, `minuit2FitBench2D.C` and `minuit2GausFit.C`. More information on the classes and functions present in `Minuit2` is available at online reference documentation.

Useful information on MINUIT and minimization in general is provided in the following documents:

F. James, *Minuit Tutorial on Function Minimization* (http://seal.cern.ch/documents/minuit/mntutorial.pdf); F. James, *The Interpretation of Errors in Minuit* (http://seal.cern.ch/documents/minuit/mnerror.pdf);

1.11   FUMILI Minimization Package

FUMILI is used to minimize Chi-square function or to search maximum of likelihood function. Experimentally measured values F_i are fitted with theoretical functions $f_i(\vec{x_i}, \vec{\theta})$, where $\vec{x_i}$ are coordinates, and $\vec{\theta}$ - vector of parameters. For better convergence Chi-square function has to be the following form

$$\frac{\chi^2}{2} = \frac{1}{2} \sum_{i=1}^{n} \left(\frac{f_i(\vec{x_i}, \vec{\theta}) - F_i}{\sigma_i} \right)^2$$

where σ_i are errors of the measured function. The minimum condition is:

$$\frac{\partial \chi^2}{\partial \theta_i} = \sum_{j=1}^{n} \frac{1}{\sigma_j^2} \cdot \frac{\partial f_i}{\partial \theta_i} \left[(\vec{x_j}, \vec{\theta}) - F_j \right] = 0, i = 1...m$$

where m is the quantity of parameters. Expanding left part of this equation over parameter increments and retaining only linear terms one gets

$$\left(\frac{\partial \chi^2}{\theta_i} \right)_{\theta = \vec{\theta}^0} + \sum_k \left(\frac{\partial^2 \chi^2}{\partial \theta_i \partial \theta_k} \right)_{\theta = \vec{\theta}^0} \cdot (\theta_k - \theta_k^0) = 0$$

here $\vec{\theta}^0$ is some initial value of parameters. In general case:

$$\frac{\partial^2 \chi^2}{\partial \theta_i \partial \theta_k} = \sum_{j=1}^{n} \frac{1}{\sigma_j^2} \frac{\partial f_j}{\theta_i} \frac{\partial f_j}{\theta_k} + \sum_{j=1}^{n} \frac{(f_j - F_j)}{\sigma_j^2} \cdot \frac{\partial^2 f_j}{\partial \theta_i \partial \theta_k}$$

In FUMILI algorithm for second derivatives of Chi-square approximate expression is used when last term in previous equation is discarded. It is often done, not always wittingly, and sometimes causes troubles, for example, if user wants to limit parameters with positive values by writing down θ_i^2 instead of θ_i. FUMILI will fail if one tries minimize $\chi^2 = g^2(\vec{\theta})$ where g is arbitrary function.

Approximate value is:

$$\frac{\partial^2 \chi^2}{\partial \theta_i \partial \theta_k} \approx Z_{ik} = \sum_{j=1}^{n} \frac{1}{\sigma_j^2} \frac{\partial f_j}{\theta_i} \frac{\partial f_j}{\theta_k}$$

Then the equations for parameter increments are:

$$\left(\frac{\partial \chi^2}{\partial \theta_i} \right)_{\vec{\theta} = \vec{\theta}^0} + \sum_k Z_{ik} \cdot (\theta_k - \theta_k^0) = 0, \qquad i = 1 \ldots m$$

Remarkable feature of algorithm is the technique for step restriction. For an initial value of parameter $\vec{\theta}^0$ a parallelepiped P_0 is built with the center at $\vec{\theta}^0$ and axes parallel to coordinate axes θ_i. The lengths of parallelepiped sides along i-th axis is $2b_i$, where b_i is such a value that the functions $f_j(\vec{\theta})$ are quasi-linear all over the parallelepiped.

FUMILI takes into account simple linear inequalities in the form:

$$\theta_i^{\min} \le \theta_i \le \theta_i^{\max}$$

They form parallelepiped P (P_0 may be deformed by P). Very similar step formulae are used in FUMILI for negative logarithm of the likelihood function with the same idea - linearization of function argument.

1.12 Neural Networks

1.12.1 Introduction

Neural Networks are used in various fields for data analysis and classification, both for research and commercial institutions. Some randomly chosen examples are image analysis, financial movements' predictions and analysis, or sales forecast and product shipping optimization. In particles physics neural networks are mainly used for classification tasks (signal over background discrimination). A vast majority of commonly used neural networks are multilayer perceptrons. This implementation of multilayer perceptrons is inspired from the `MLPfit` package, which remains one of the fastest tools for neural networks studies.

1.12.2 The MLP

The multilayer perceptron is a simple feed-forward network with the following structure showed on the left.

It is made of neurons characterized by a bias and weighted links in between - let's call those links synapses. The input neurons receive the inputs, normalize them and forward them to the first hidden layer. Each neuron in any subsequent layer first computes a linear combination of the outputs of the previous layer. The output of the neuron is then function of that combination with f being linear for output neurons or a sigmoid for hidden layers.

Such a structure is very useful because of two theorems:

1- A linear combination of `sigmoids` can approximate any continuous function.

2- Trained with `output=1` for the signal and 0 for the background, the approximated function of inputs X is the probability of signal, knowing X.
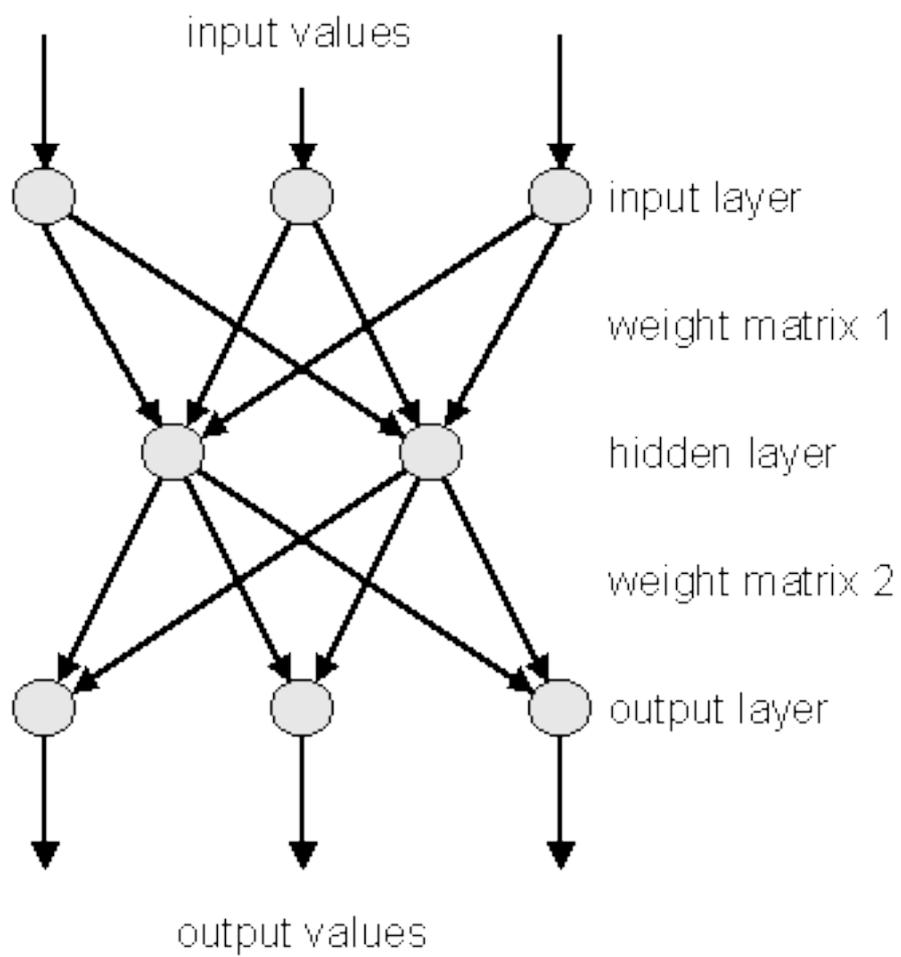
Figure 1.5:

1.12.3 Learning Methods

The aim of all learning methods is to minimize the total error on a set of weighted examples. The error is defined as the sum in quadrate, divided by two, of the error on each individual output neuron. In all methods implemented in this library, one needs to compute the first derivative of that error with respect to the weights. Exploiting the well-known properties of the derivative, one can express this derivative as the product of the local partial derivative by the weighted sum of the outputs derivatives (for a neuron) or as the product of the input value with the local partial derivative of the output neuron (for a synapse). This computation is called "back-propagation of the errors". Six learning methods are implemented.

1.12.3.1 Stochastic Minimization

This is the most trivial learning method. The Robbins-Monro stochastic approximation is applied to multilayer perceptrons. The weights are updated after each example according to the formula:

$$w_{ij}(t+1) = w_{ij}(t) + \Delta w_{ij}(t)$$

with:

$$\Delta w_{ij}(t) = -\eta \left(\frac{\partial e_p}{\partial w_{ij}} + \delta \right) + \epsilon \Delta w_{ij}(t-1)$$

The parameters for this method are `Eta`, `EtaDecay`, `Delta` and `Epsilon`.

1.12.3.2 Steepest Descent With Fixed Step Size (Batch Learning)

It is the same as the stochastic minimization, but the weights are updated after considering all the examples, with the total derivative `dEdw`. The parameters for this method are `Eta`, `EtaDecay`, `Delta` and `Epsilon`.

1.12.3.3 Steepest Descent Algorithm

Weights are set to the minimum along the line defined by the gradient. The only parameter for this method is `Tau`. Lower `Tau` = higher precision = slower search. A value `Tau=3` seems reasonable.

1.12.3.4 Conjugate Gradients With the Polak-Ribiere Updating Formula

Weights are set to the minimum along the line defined by the conjugate gradient. Parameters are `Tau` and `Reset`, which defines the epochs where the direction is reset to the steepest descent (estimated by using the Polak-Ribiere formula).

1.12.3.5 Conjugate Gradients With the Fletcher-Reeves Updating Formula

Weights are set to the minimum along the line defined by the conjugate gradient. Parameters are `Tau` and `Reset`, which defines the epochs where the direction is reset to the steepest descent (estimated by using the Fletcher-Reeves formula).

1.12.3.6 The Broyden, Fletcher, Goldfarb, Shanno (BFGS) Method

It implies the computation of a `NxN` matrix, but seems more powerful at least for less than 300 weights. Parameters are `Tau` and `Reset`, which defines the epochs where the direction is reset to the steepest descent.

1.12.4 Using the Network

Neural network are build from a set of "samples". A sample is a set of values defining the inputs and the corresponding output that the network should ideally provide. In ROOT this is a `TTree` entry. The first thing to be decided is the network layout. This layout is described in a string where the layers are separated by semicolons. The input/output layers are defined by giving the expression for each neuron, separated by comas. Hidden layers are just described by the number of neurons.

In addition, input and output layer formulas can be preceded by '@' (e.g. "@out") if one wants to normalize the corresponding value. Also, if the string ends with '!', output neurons are set up for classification, i.e. with a sigmoid (1 neuron) or softmax (more neurons) activation function.

Many questions on the good usage of neural network, including rules of dumb to determine the best network topology are addressed at ftp://ftp.sas.com/pub/neural/FAQ.html

```
// a simple network: 2 inputs, 10 hidden and 1 normalized
// output neuron
TMultiLayerPerceptron network("r,z:10:@Br",tree);
```

Expressions are evaluated as for `TTree::Draw()`.   Input and outputs are taken from the **TTree** associated with the network.   This **TTree** can be given as argument of the constructor or defined later with `TMultiLayerPerceptron::SetData()`.   Events can also be weighted.   The weight expression can be given in the constructor or set later with the method `SetWeight()` of the class **TMultiLayerPerceptron**. Two datasets must be defined before learning the network: a training dataset that is used when minimizing the error, and a test dataset that will avoid bias. Those two datasets can be build aside and then given to the network, or can be build from a standard expression. By default, half of the events are put in both datasets.

```
// a more complex 4:8:1 network
// the ptsumf branch is used as weigh;
// default event lists are explicit
TMultiLayerPerceptron  network("m,pt,acol,acopl:8:type","pt",tree,
                               "Entry$%2","Entry$/2");
```

The method `TMultiLayerPerceptron::SetLearningMethod()` defines the learning method. Learning methods are:

```
TMultiLayerPerceptron::kStochastic,
TMultiLayerPerceptron::kBatch,
TMultiLayerPerceptron::kSteepestDescent,
TMultiLayerPerceptron::kRibierePolak,
TMultiLayerPerceptron::kFletcherReeves,
TMultiLayerPerceptron::kBFGS        // default
```

The training can start with `TMultiLayerPerceptron::Train(Int_t nepoch,Option_t* options)`. The first argument is the number of epochs while option is a string that can contain "**text**" (simple text output), "**graph**" (evaluating graphical training curves), "**update = X**" (step for the text/graph output update) or "**+**" (will skip the randomization and start from the previous values). All combinations are available.

```
network.Train(1000,"text,graph,update=10"); // full output every
                                            // 10 epochs
network.Train(100,"text,+");                // 100 more epochs
//starts with existing weights
```

The weights can be saved to a file (`DumpWeights`) and then reloaded (`LoadWeights`) to a new compatible network. The output can also be evaluated (`Evaluate`) for a given output neuron and an array of double input parameters or the network can be exported (`Export`) as a standalone code. Up to now, this is only as a C++ or PYTHON class, but other languages could be implemented.

1.12.5   Examples

An example of how to use **TMultiLayerPerceptron** is the macro `mlpHiggs.C` in $ROOTSYS/tutorials. Using some standard simulated information that could have been obtained at **LEP**, a neural network is build, which can make the difference between **WW** events and events containing a Higgs boson. Starting with a **TFile** containing two **TTree**s: one for the signal, the other for the background, a simple script is used:

```
void mlpHiggs(Int_t ntrain=100) {
   if (!gROOT->GetClass("TMultiLayerPerceptron"))
   gSystem->Load("libMLP");
   // prepare inputs - the 2 trees are merged into one, and a
   // "type" branch, equal to 1 for the signal and 0 for the
   // background is added
   TFile input("mlpHiggs.root");
   TTree *signal = (TTree *)input.Get("sig_filtered");
   TTree *background = (TTree *)input.Get("bg_filtered");
   TTree *simu = new TTree("MonteCarlo",
```

```
                            "Filtered Monte Carlo Events");
    ...
```

Since the input is a `TTree` and we are starting from two different `TTree`s (with different names), they are first merged into one, and a "`type`" branch is added, that says whether there is a signal or a background event. Those irrelevant details are skipped here.

```
    ...
    TMultiLayerPerceptron *mlp = new TMultiLayerPerceptron(
          "msumf,ptsumf, acolin, acopl:8:type","ptsumf",simu,
          "Entry$%2","Entry$/2");
    mlp->Train(ntrain, "text,graph,update=10");
```

The neural network is instantiated and trained. "`ptsumf`" is used as a weight, and the standard event lists are explicit. The network that is then build has four input neurons, eight additional ones in the only hidden layer and one single output neuron.

```
    // Use the NN to plot the results for each sample
    TH1F *bg = new TH1F("bgh","NN output",50,-.5,1.5);
    TH1F *sig = new TH1F("sigh","NN output",50,-.5,1.5);
    bg->SetDirectory(0);
    sig->SetDirectory(0);
    Double_t params[4];
    for (i = 0; i < background->GetEntries(); i++) {
       background->GetEntry(i);
       params[0] = msumf;    params[1] = ptsumf;
       params[2] = acolin;   params[3] = acopl;
       bg->Fill(mlp->Evaluate(0,params));
    }
    for (i = 0; i < signal->GetEntries(); i++) {
       signal->GetEntry(i);
       params[0] = msumf;
       params[1] = ptsumf;
       params[2] = acolin;
       params[3] = acopl;
       sig->Fill(mlp->Evaluate(0,params));
    }
    TCanvas *cv = new TCanvas("NNout_cv","Neural net output");
    bg->SetFillStyle(3008);
    bg->SetFillColor(kBlue);
    sig->SetFillStyle(3003);
    sig->SetFillColor(kRed);
    bg->SetStats(0);
    sig->SetStats(0);
    bg->Draw();
    sig->Draw("same");
    TLegend *legend = new TLegend(.75,.80,.95,.95);
    legend->AddEntry(bg,"Background(WW)");
    legend->AddEntry(sig,"Signal(Higgs)");
    legend->Draw();
```

The neural net output is then used to display the final difference between background and signal events. The figure "The neural net output" shows this plot.

As it can be seen, this is a quite efficient technique. As mentioned earlier, neural networks are also used for fitting function. For some application with a cylindrical symmetry, a magnetic field simulation gives as output the angular component of the potential vector `A`, as well as the radial and `z` components of the `B` field.

One wants to fit those distributions with a function in order to plug them into the `Geant` simulation code. Polynomial fits could be tried, but it seems difficult to reach the desired precision over the full range. One could also use a `spline` interpolation between known points. In all cases, the resulting field would not be `C`-infinite.

An example of output (for Br) is shown. First the initial function can be seen as the target. Then, the resulting (normalized) neural net output. In order to ease the learning, the "normalize output" was used here. The initial amplitude can be recovered by multiplying by the original RMS and then shifting by the original mean.
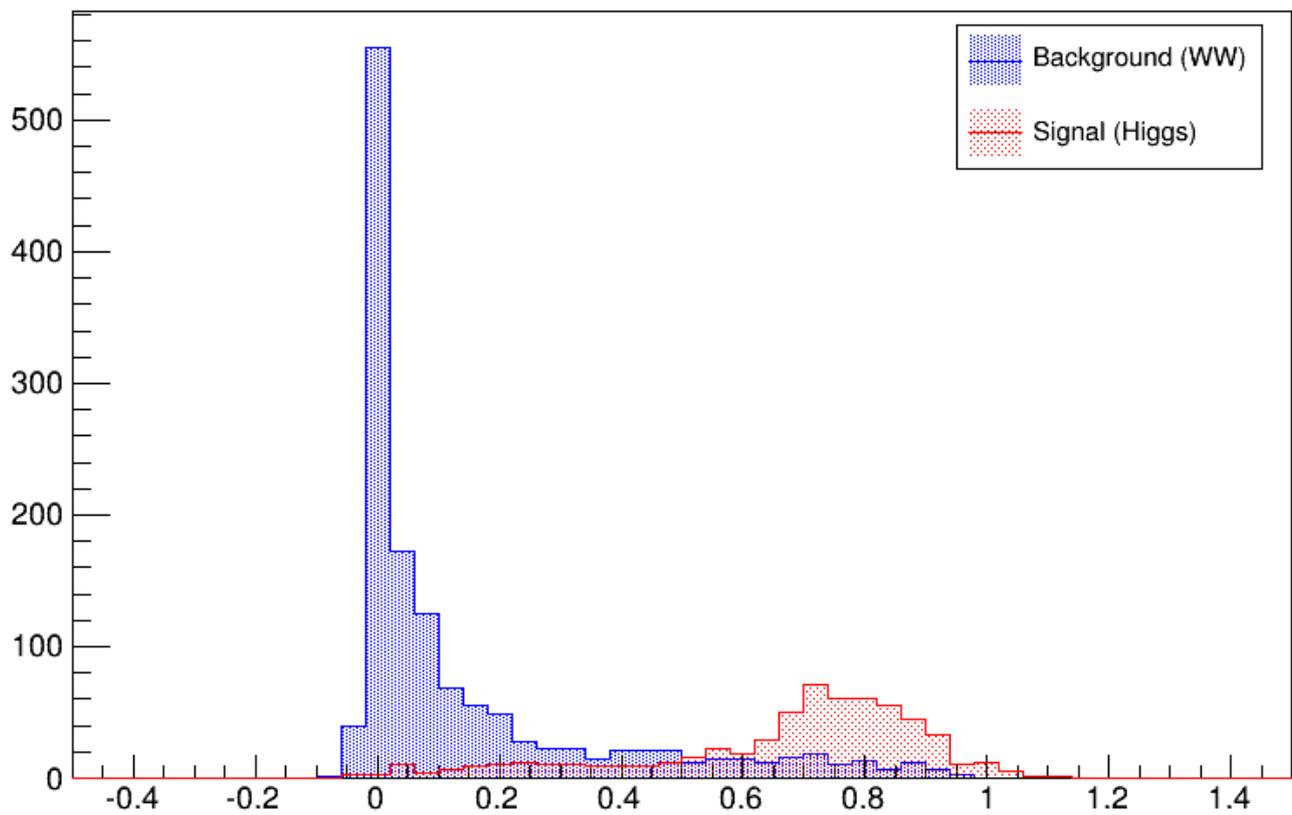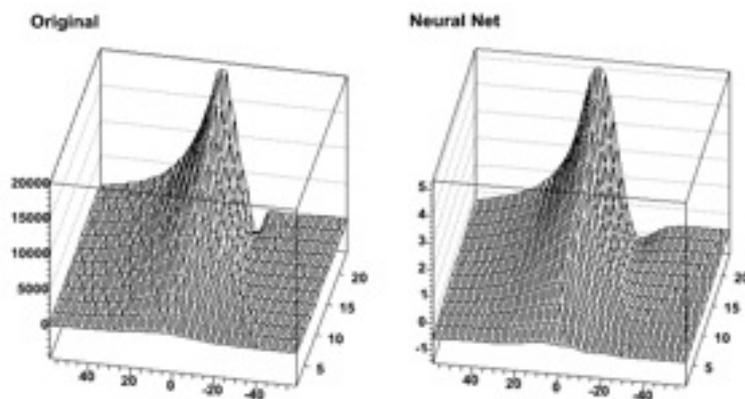
Figure 1.6: The neural net output

Figure 1.7: The original and the neural net for Br