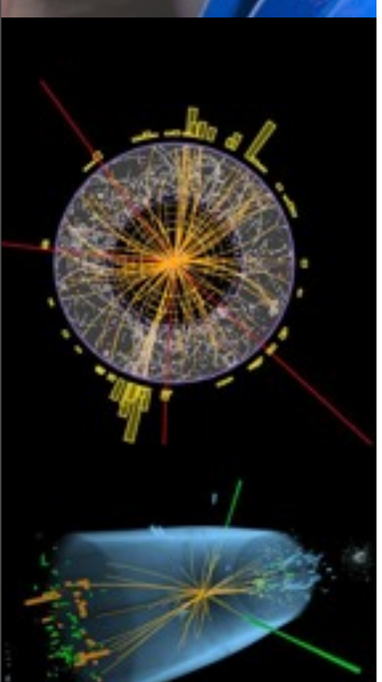
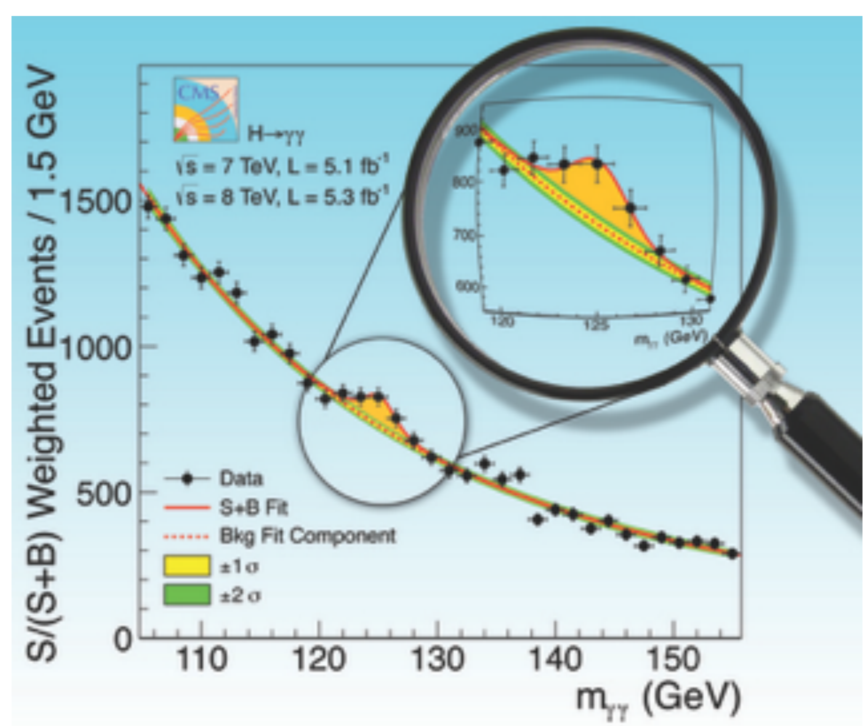


Fitting and Parameter Estimation in ROOT

ROOT Training at IRMM

26th February 2013



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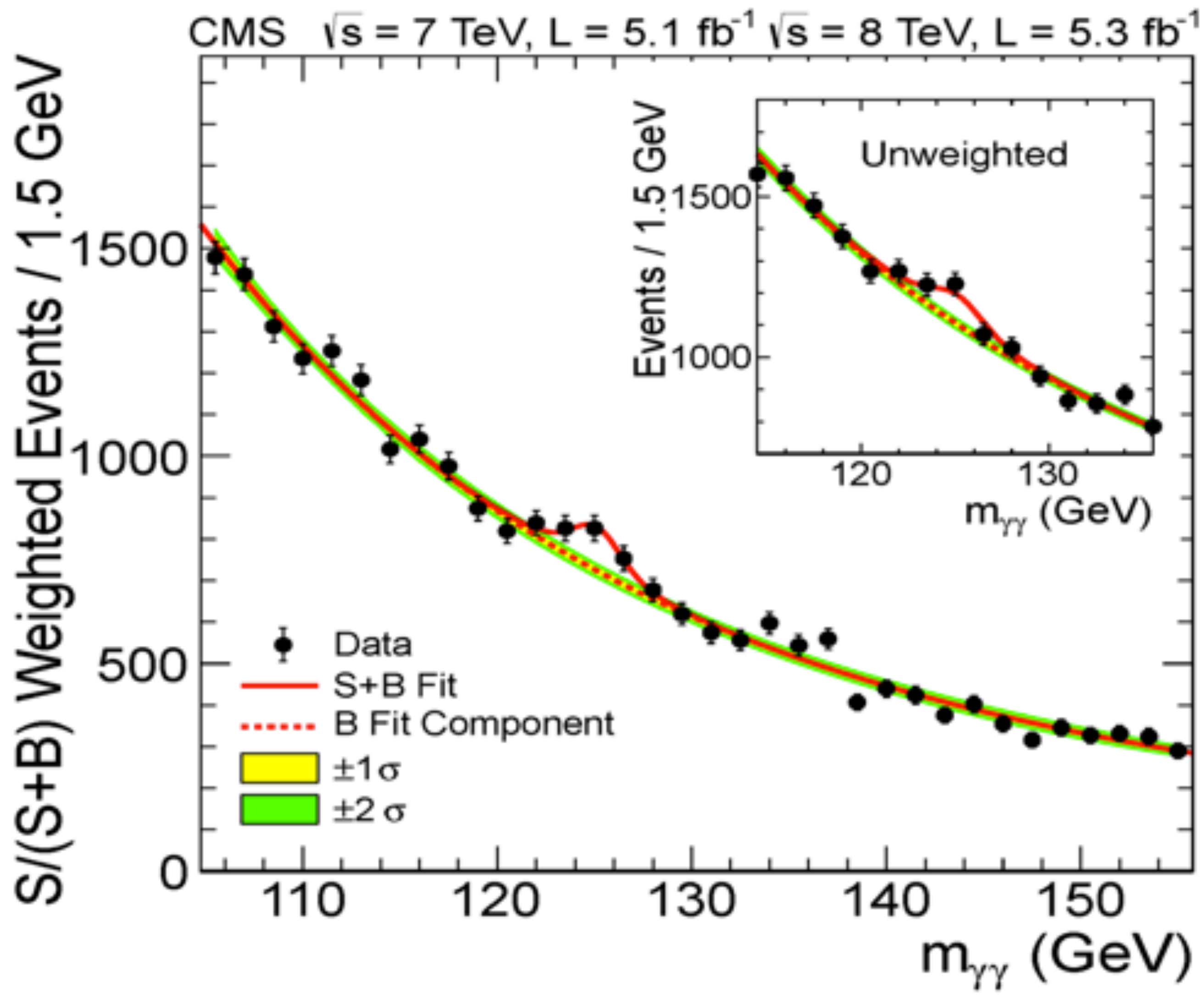
Outline

- Introduction to Fitting:
  - what is fitting,
  - how to fit a histogram in ROOT,
  - how to retrieve the fit result.
- Building complex fit functions in ROOT.
- Interface to Minimization.
- Common Fitting problems.
- Using the ROOT Fit GUI (Fit Panel).
- Random number generations in ROOT.
- How to generate random numbers from distributions.

What is Fitting ?

- What is Fitting ?
  - It is the process used to estimate parameters of an hypothetical distribution from the observed data distribution



Example

Higgs search in CMS ($H \rightarrow \gamma\gamma$)

We fit for the expected number of Higgs events and for the Higgs mass

What is Fitting (2)

- A histogram (or a graph) represents an estimate of an underlying distribution (or a function).
- The histogram or the graph can be used to infer the parameters describing the underlying distribution.
- Assume a relation between the observed variables y and x:
  - $y = f (x | \theta)$
    - $f (x | \theta)$ is the fit (model) function
    - for an histogram y is the bin content

- One typically minimizes the deviations between the observed y and the predicted function values:
  - Least square fit (χ^2) :
    - minimize square deviation
    - weighted by the observed errors
      - $\sigma = \sqrt{N}$ for the histograms

$$\chi^2 = \sum_i \frac{(Y_i - f(X_i, \theta))^2}{\sigma_i^2}$$

ML Fit of an Histogram

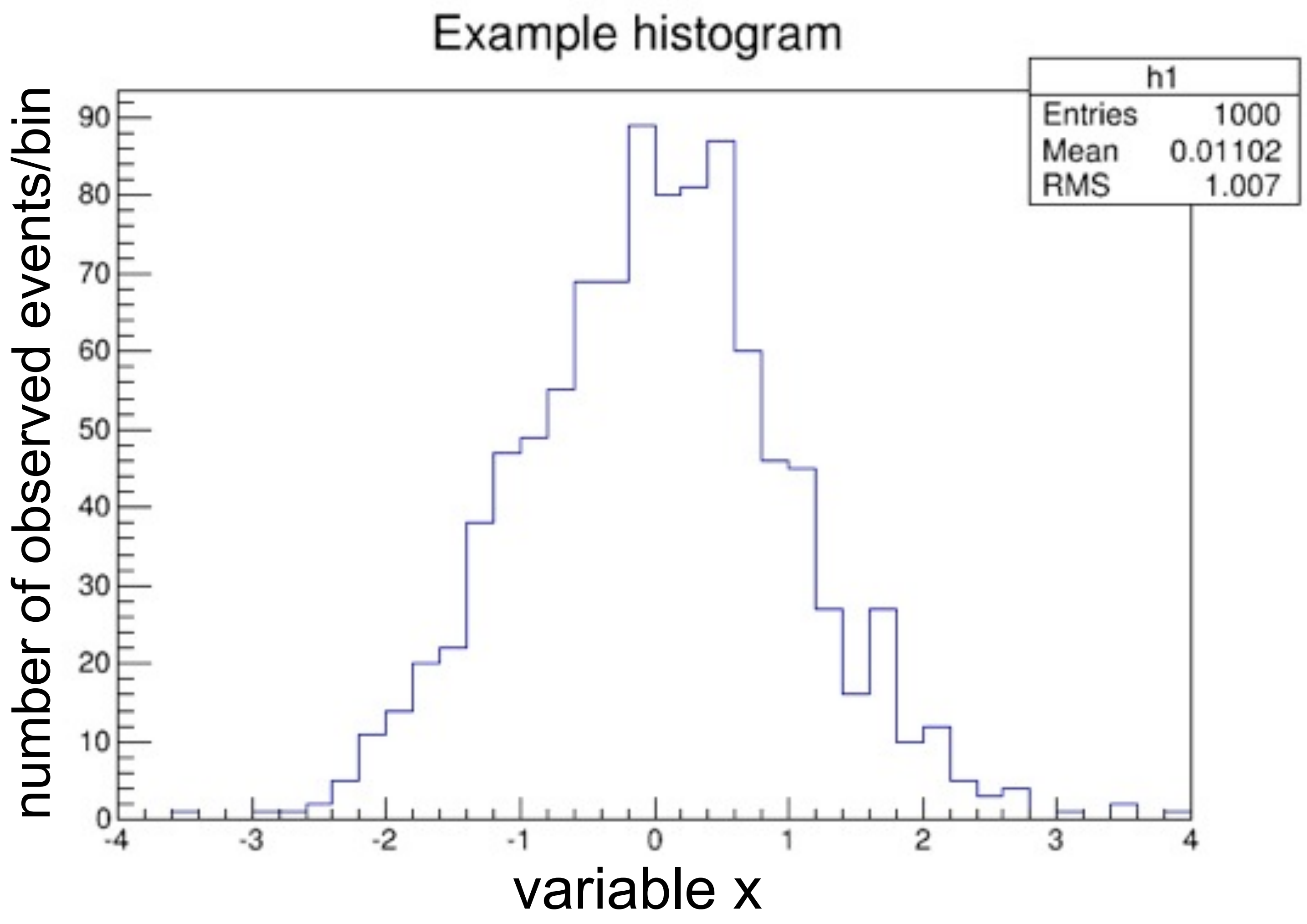
- Maximum Likelihood (ML) Fit:
  - The parameters are estimated by finding the maximum of the likelihood function (or minimum of the negative log-likelihood function).
  - Likelihood: $$L(x|\theta) = \prod_i P(x_i|\theta)$$
- The Likelihood for a histogram is obtained by assuming a Poisson distribution in every bin:
  - `Poisson(` n_{obs} | n_{exp} `)`
    - n_{obs} is the observed bin content.
    - n_{exp} is the expected bin content, which can be obtained from the fit model function (the underlying distribution of the histogram)
      - $n_{exp} = f(x_c|\theta)$, where x_c is the bin center, assuming a linear function within the bin. Otherwise it is obtained from the integral of the function in the bin.
- The least-square fit and the maximum likelihood fit are equivalent when the distribution of observed events in each bin is normal.
  - This is true only for large histogram statistics (large bin contents).
- For low histogram statistics the ML method is the correct one !

Fitting in ROOT

- How do we do fit in ROOT:
  - Create first a parametric function object, `TF1`, which represents our model, *i.e.* the fit function.
  - Set the initial values of the function parameters.
  - Fit the data object (Histogram or Graph):
    - call the `Fit` method on the Histogram or Graphs passing the function object as parameter
      - various options are possibles (see the `TH1::Fit` documentation)
        - » e.g select type of fit : least-square (default) or likelihood (option “L”)
      - the resulting fit function is then drawn on top of the Histogram or the Graph.
  - Examine result:
    - get parameter values;
    - get parameter errors (e.g. their confidence level);
    - get parameter correlation;
    - get fit quality.

Simple Gaussian Fitting

- Recalling our previous histogram:
  - suppose we do not know how it was generated;
  - we want to estimate the mean and sigma of the underlying gaussian distribution.



Creating the Fit Function

- To create a parametric function object (a `TF1`) :
  - we can use the available functions in ROOT library

```
TF1 * f1 = new TF1("f1","[0]*TMath::Gaus(x,[1],[2])");
```

  - or we can use pre-defined functions defined in `TFormula` (see `TFormula` documentation for the list of them):

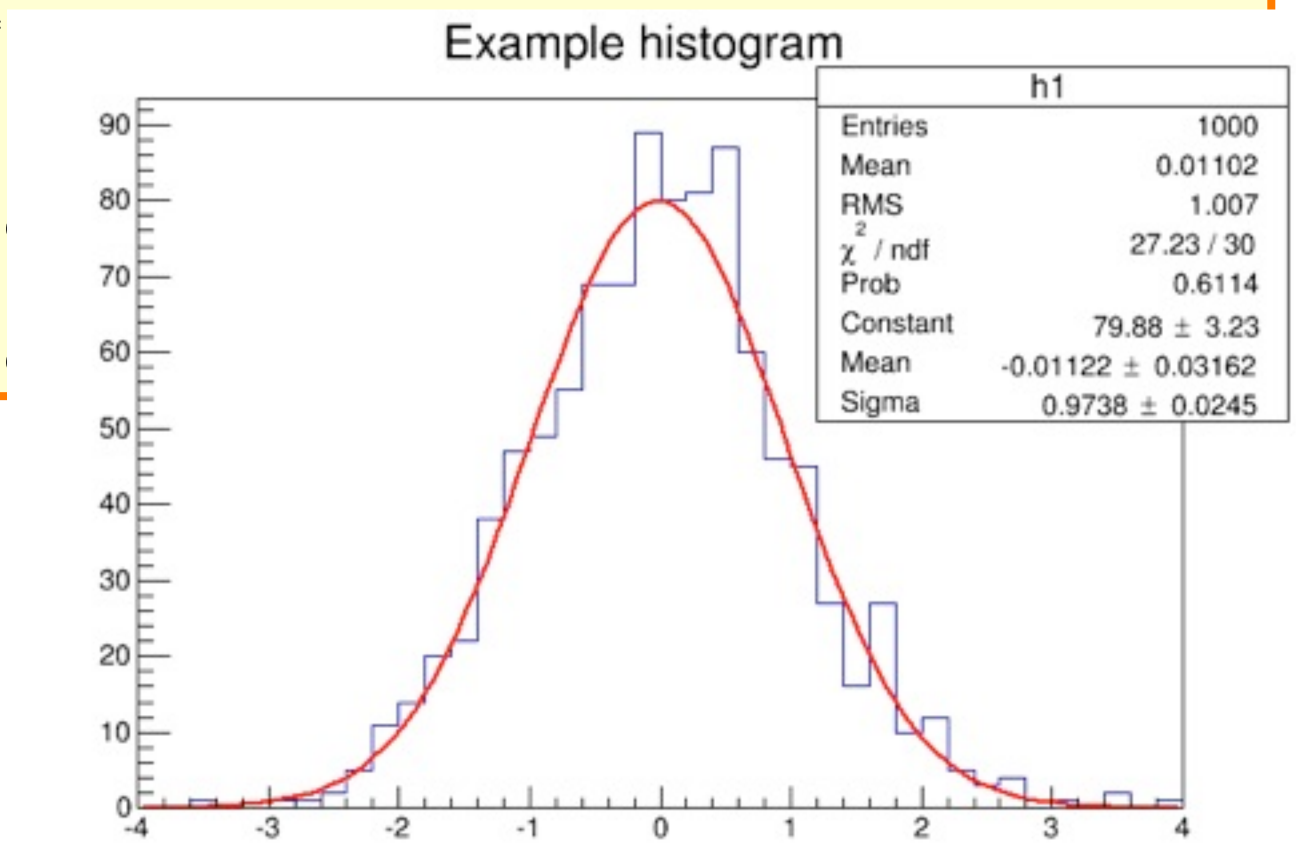
```
TF1 * f1 = new TF1("f1","gaus");
```

    - using pre-defined functions we have the parameter name automatically set to meaningful values.
    - initial parameter values are estimated whenever possible.
  - We will see later in general how to build a more complex function objects
    - e.g. by using other functions

Fitting Histogram

- How to fit the histogram:
  - after creating the function one needs to set the initial value of the parameters
  - then we can call the `Fit` method of the histogram class

```
root [] TF1 * f1 = new TF1("f1","gaus");
root [] f1->SetParameters(1,0,1);
root [] h1->Fit(f1);
 FCN=27.2252 FROM MIGRAD    STATUS=CONVERGED      60 CALLS          61 TOTAL
                      EDM=1.12393e-07    STRATEGY=
  EXT PARAMETER
  NO.   NAME      VALUE            ERROR
   1  Constant     7.98760e+01   3.22882e+00   6.
   2  Mean        -1.12183e-02   3.16223e-02   8.
   3  Sigma        9.73840e-01   2.44738e-02   1.
```



For displaying the fit parameters:

```
gStyle->SetOptFit(1111);
```

Retrieving The Fit Result

- The main results from the fit are stored in the fit function, which is attached to the histogram; it can be saved in a file (except for customized C/C++ functions).
- The fit function can be retrieved using its name:
  - ```
    TF1 * fitFunc = h1->GetFunction("f1");
    ```
- The parameter values using their indices (or their names):
  - ```
    fitFunc->GetParameter(par_index);
    ```
- The parameter errors:
  - ```
    fitFunc->GetParError(par_index);
    ```
- It is also possible to access the `TFitResult` class which has all information about the fit, if we use the fit option "S":

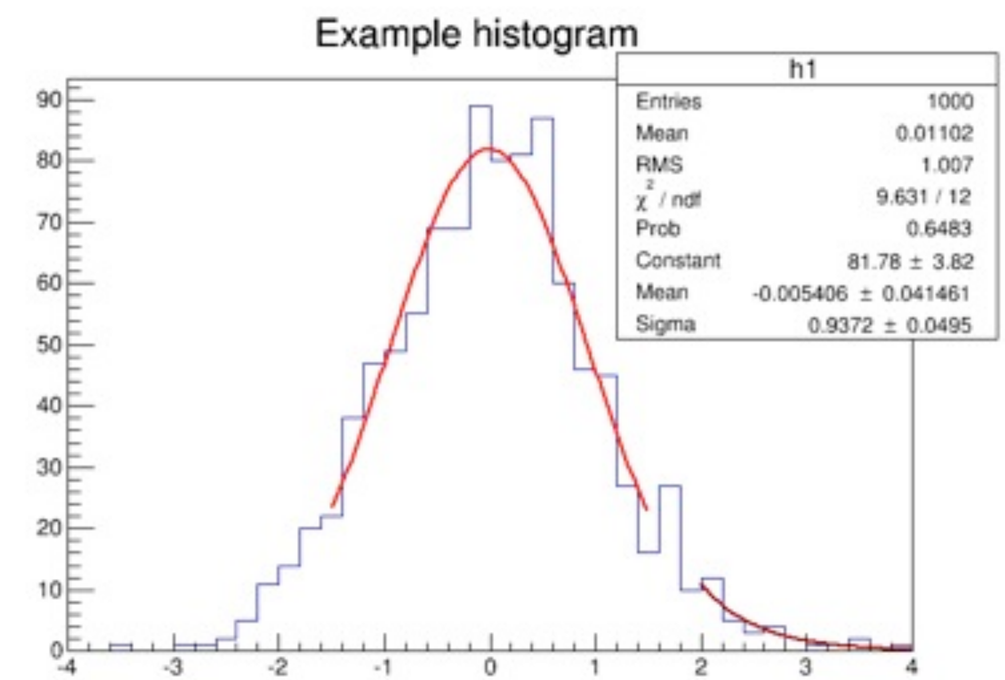
```
TFitResultPtr r = h1->Fit(f1,"S");
r->Print();
TMatrixDSym C = r->GetCorrelationMatrix();
```

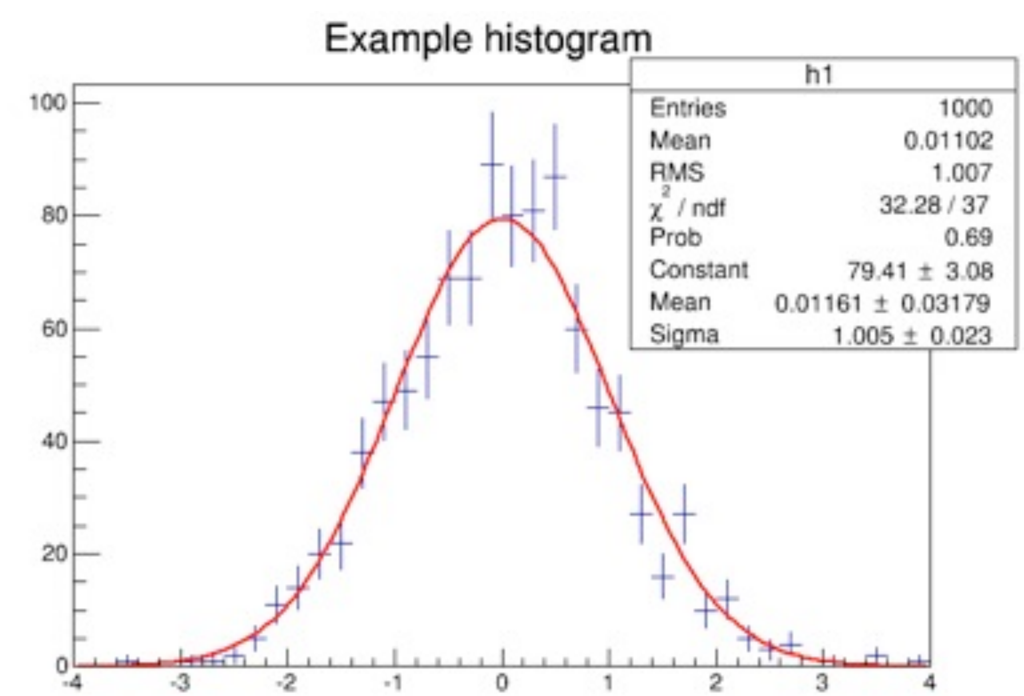
C++ Note: the TFitResult class is accessed by using operator-> of TFitResultPtr
```

Some Fitting Options

- Fitting in a Range
  - ```
    h1->Fit(“gaus”,””,””,-1.5,1.5);
    ```
- Fitting more functions to an histogram (option “+”)
  - ```
    h1->Fit(“expo”,”+”,””,2.,4);
    ```
- Quite / Verbose:
  - option “Q”/”V”.
- Likelihood fit:
  - option “L” for count histograms;
  - option “LW” in case of weighted counts.
- Return a fit result class:
  - option “S”
- Plotting options for the histogram can be passed as well:

```
h1->Fit(“gaus”,”L”,”E”);
```





Time for Exercises!

Put in practice the concepts to which you were just exposed: read the instructions here

https://twiki.cern.ch/twiki/bin/view/Main/RootIRMMTutorial2013FittingExercises

and solve exercise 1

Building More Complex Functions

- It is possible to write some complex formulae and pass as string in the constructor of `TF1`
  - but difficult and prone to error
- Better to write directly the functions in C/C++
- A parametric `TF1` can be constructed from
  - a general free function with parameters:

```
double function(double *x, double *p){
   return p[0]*TMath::Gaus(x[0],p[0],p[1]);
}
TF1 * f1 = new TF1("f1",function,xmin,xmax,npar);
```

  - any C++ object implementing `double operator() (double *x, double *p)`

```
struct Function {
   double operator()(double *x, double *p){
      return p[0]*TMath::Gaus(x[0],p[0],p[1]);}
};
Function func;
TF1 * f1 = new TF1("f1",&func,xmin,xmax,npar,"Function");
```

Minimization

- The fit is done by minimizing the least-square or likelihood function.
- A direct solution exists only in case of linear fitting
  - it is done automatically in such cases (e.g fitting polynomials).
- Otherwise an iterative algorithm is used:
  - Minuit is the minimization algorithm used by default
    - ROOT provides two implementations: Minuit and Minuit2
    - other algorithms exists: Fumili, or minimizers based on GSL, genetic and simulated annealing algorithms
  - To change the minimizer:

```
ROOT::Math::MinimizerOptions::SetDefaultMinimizer("Minuit2");
```

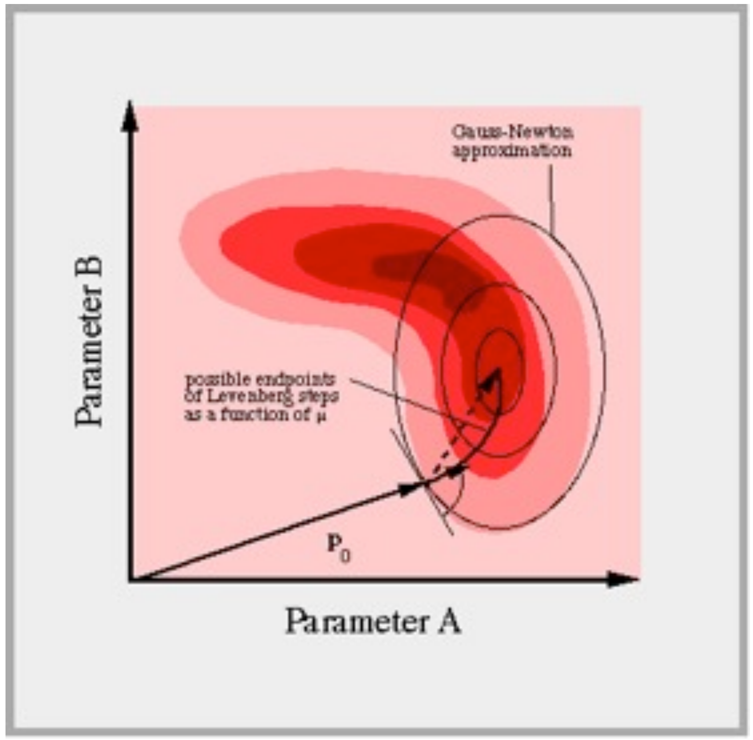
  - Other commands are also available to control the minimization:

```
ROOT::Math::MinimizerOptions::SetDefaultTolerance(1.E-6);
```

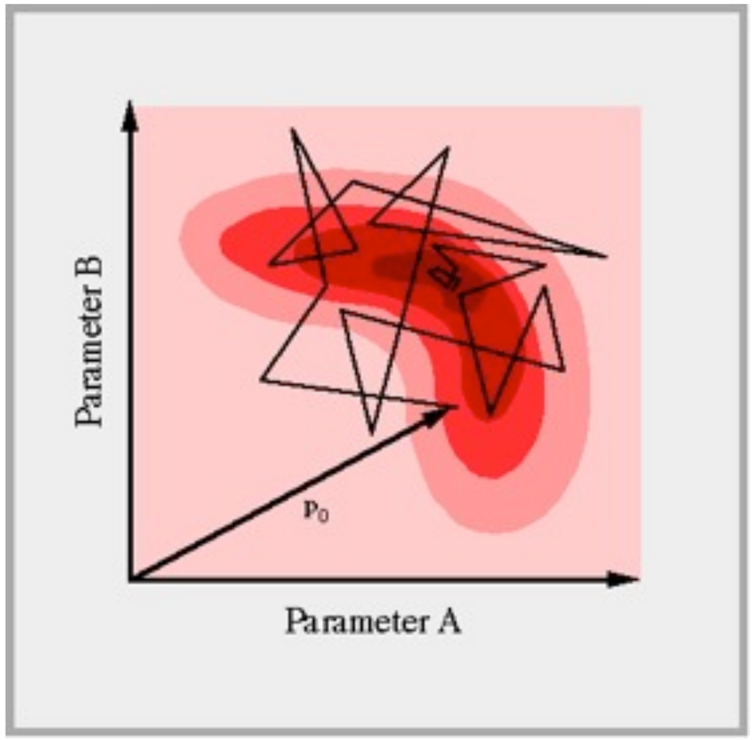
Minimization Techniques

- Methods like Minuit based on gradient can get stuck easily in local minima.
- Stochastic methods like simulated annealing or genetic algorithms can help to find the global minimum.

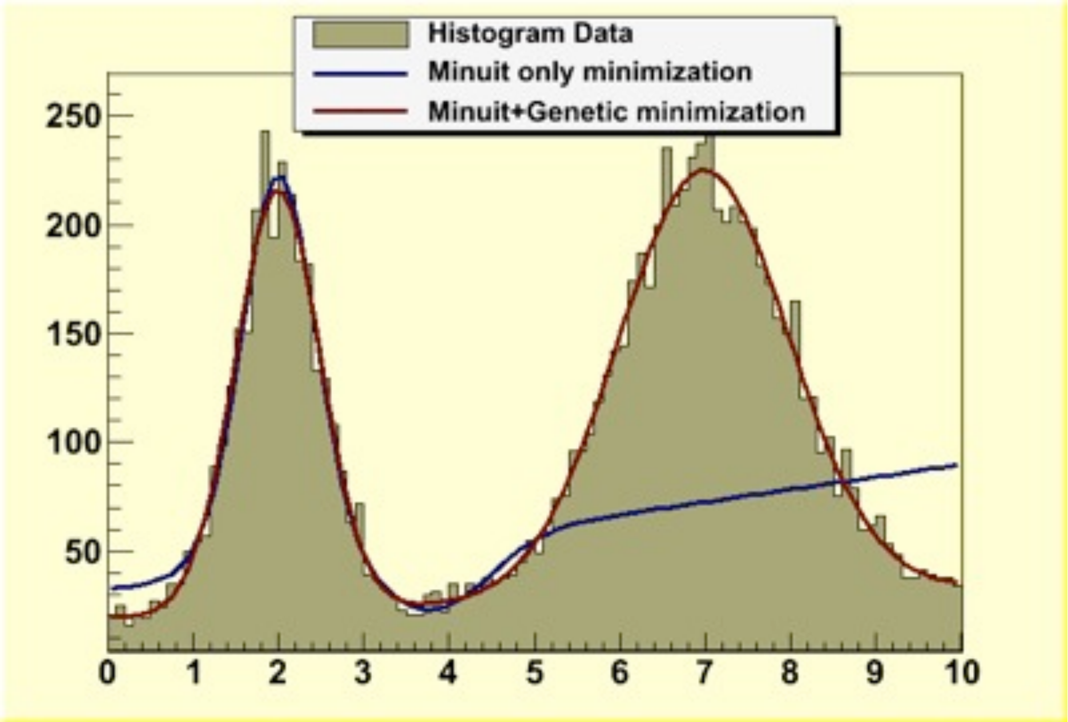
Quadratic Newton



Simulated Annealing



Example: Fitting 2 peaks in a spectrum



Interface to Minimization

- A common interface for all ROOT Minimizer algorithms exists: class `ROOT::Math::Minimizer`
- All minimizers in ROOT (Minuit, Minuit2, Fumili, GSL minimizers, simulated annealing, genetic) implement this interface
- Using the ROOT plug-in manager it is possible to change the implementation at run-time
- The interface can be used for fitting user defined likelihood or least-square functions
  - see ROOT `tutorial fit/NumericalMinimization.C` on how to use this interface

Comments on Minimization

- Sometimes fits converge to a wrong solution
  - Often is the case of a local minimum which is not the global one.
  - This is often solved with better initial parameter values. A minimizer like Minuit is able to find only the local best minimum using the function gradient.
  - Otherwise one needs to use a genetic or simulated annealing minimizer (but it can be quite inefficient, e.g. many function calls).
- Sometimes fit does not converge :

```
Warning in <Fit>: Abnormal termination of minimization.
```

  - can happen because the Hessian matrix is not positive defined
    - e.g. there are no minimum in that region →wrong initial parameters;
  - numerical precision problems in the function evaluation
    - need to check and re-think on how to implement better the fit model function;
  - highly correlated parameters in the fit. In case of 100% correlation the point solution becomes a line (or an hyper-surface) in parameter space. The minimization problem is no longer well defined.

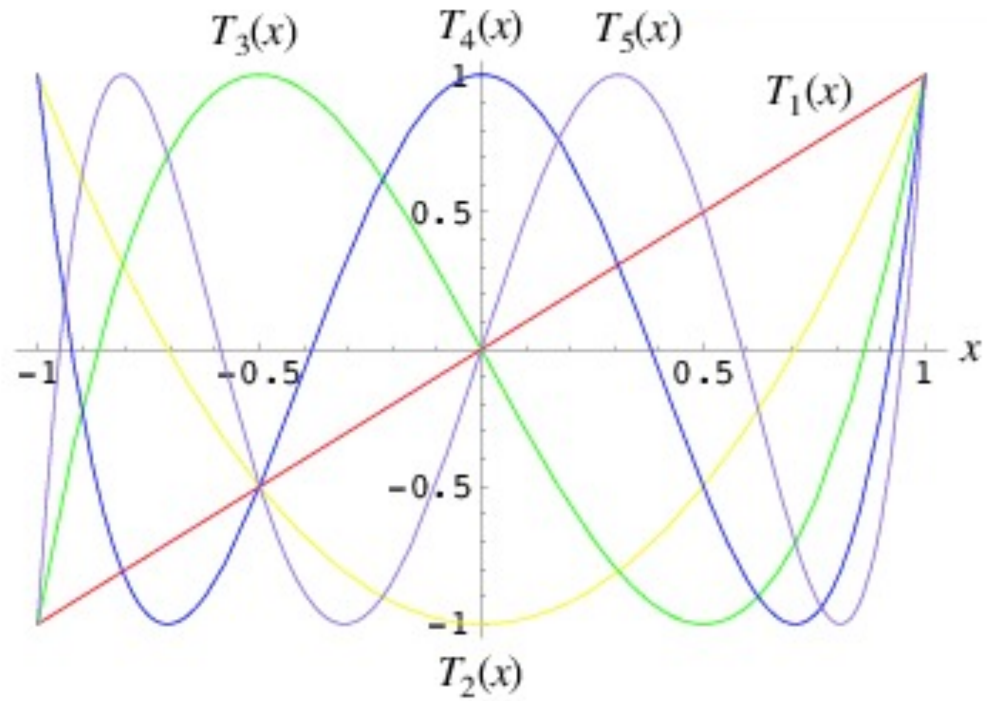
```
PARAMETER  CORRELATION COEFFICIENTS
      NO.  GLOBAL      1      2
        1  0.99835   1.000  0.998
        2  0.99835   0.998  1.000
```

Signs of trouble...

Mitigating fit stability problems

- When using a polynomial parametrization:
  - $a_0+a_1x+a_2x^2+a_3x^3$ nearly always results in strong correlations between the coefficients.
    - problems in fit stability and inability to find the right solution at high order
- This can be solved using a better polynomial parametrization:
  - e.g. Chebychev polynomials

$$
\begin{aligned}
T_0(x) &= 1\\
T_1(x) &= x\\
T_2(x) &= 2x^2-1\\
T_3(x) &= 4x^3-3x\\
T_4(x) &= 8x^4-8x^2+1\\
T_5(x) &= 16x^5-20x^3+5x\\
T_6(x) &= 32x^6-48x^4+18x^2-1.
\end{aligned}
$$



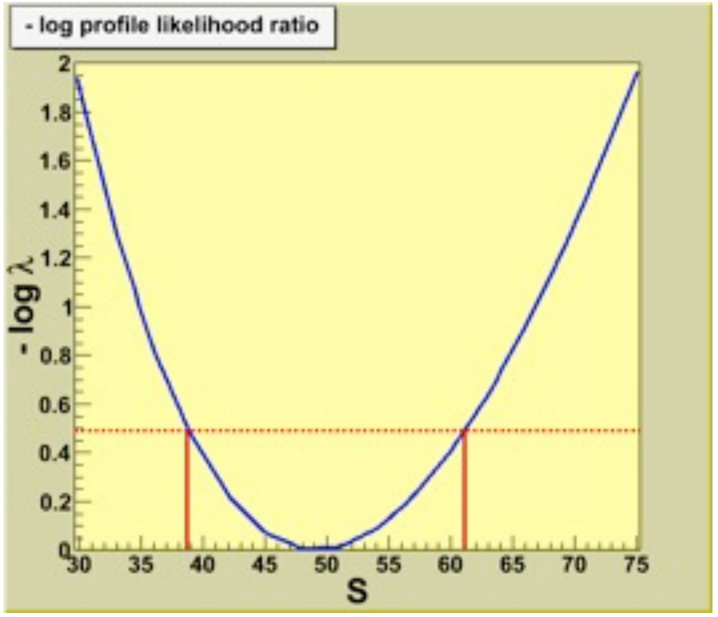
Parameter Errors

- Errors returned by the fit are computed from the second derivatives of the likelihood function
  - Asymptotically the parameter estimates are normally distributed. The estimated correlation matrix is then:

$$\hat{\mathbf{V}}(\hat{\boldsymbol{\theta}}) = \left[\left(-\frac{\partial^2 \ln L(\mathbf{x};\boldsymbol{\theta})}{\partial^2 \boldsymbol{\theta}} \right)_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}} \right]^{-1} = \mathbf{H}^{-1}$$

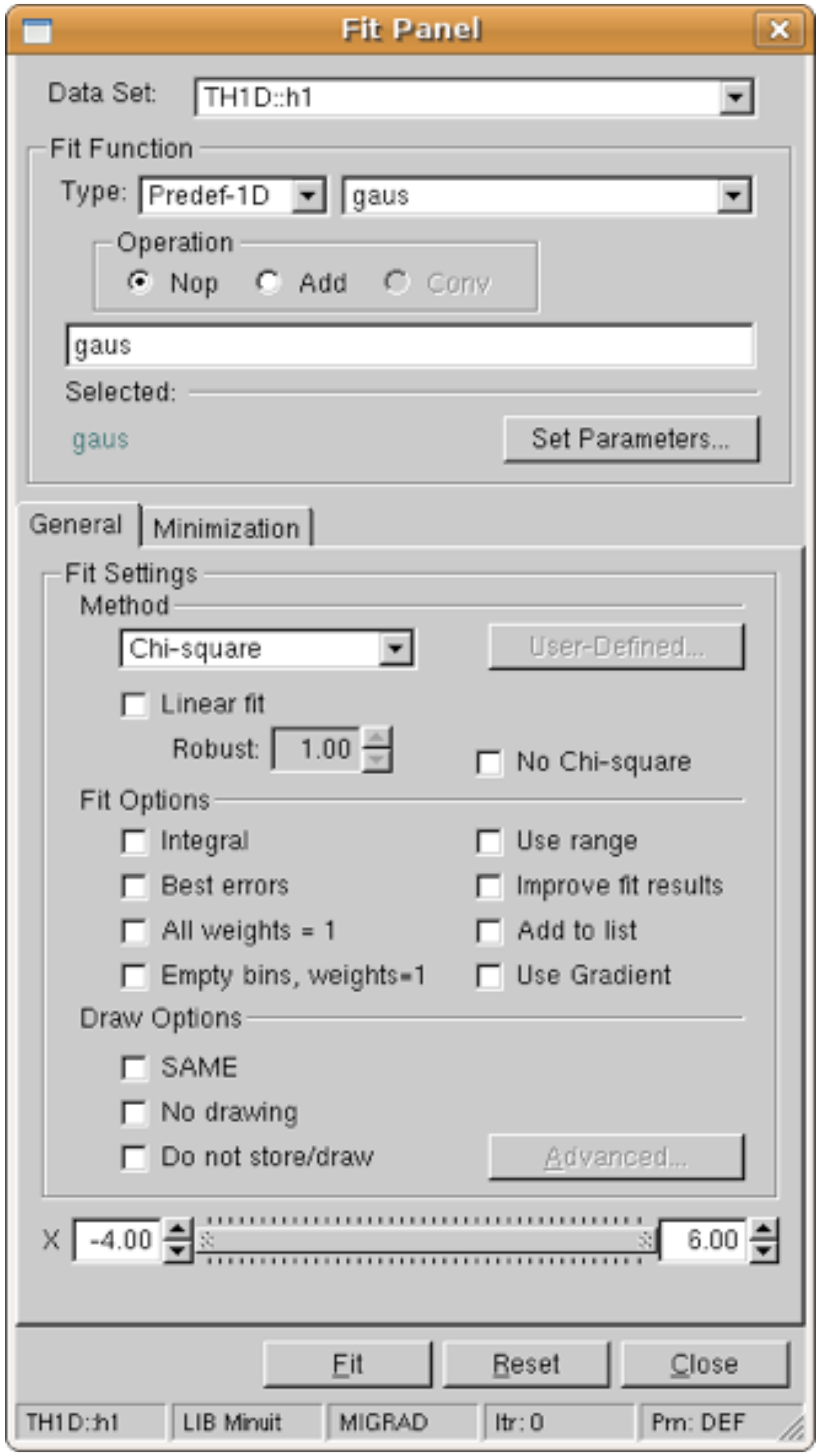
- A better approximation to estimate the confidence level in the parameter is to use directly the log-likelihood function and look at the difference from the minimum.
  - Method of Minuit/Minos (Fit option “E”)
    - obtain a confidence interval which is in general not symmetric around the best parameter estimate

```
TFitResultPtr r = h1->Fit(f1,”E S”);
r->LowerError(par_number);
r->UpperError(par_number);
```



The Fit Panel

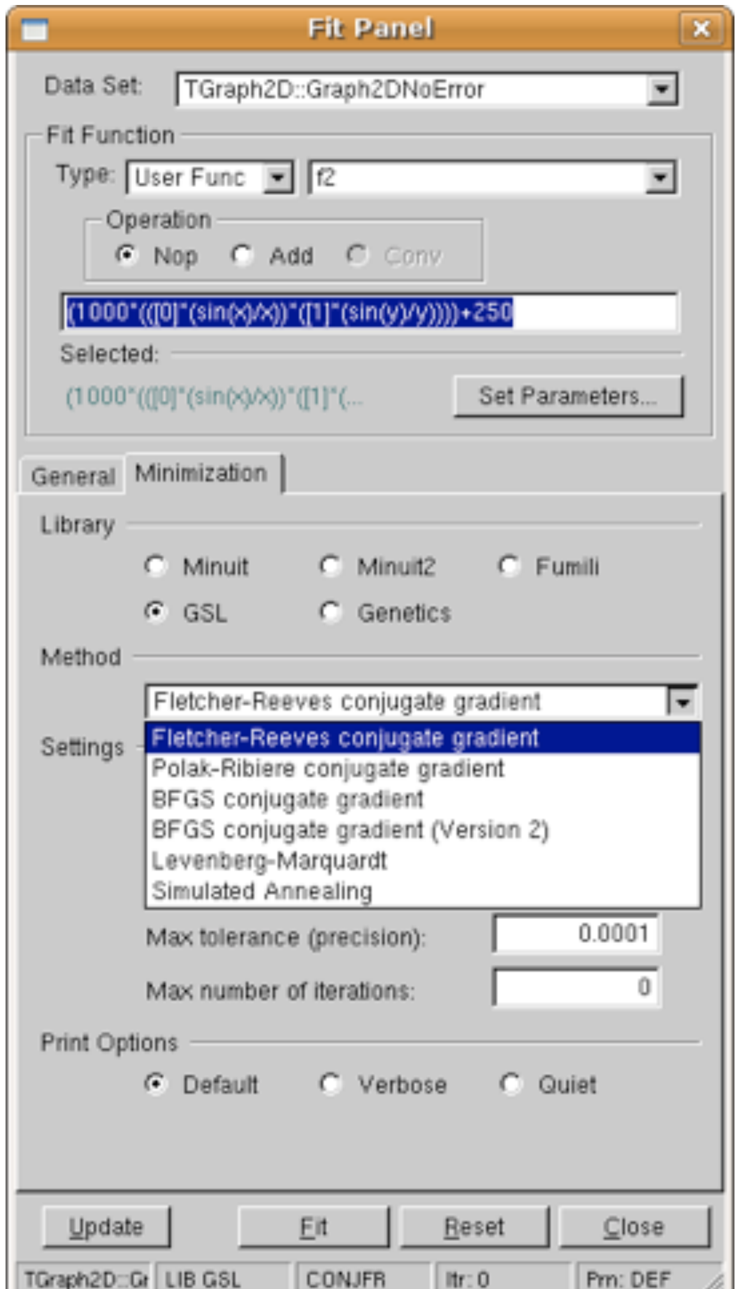
- The fitting in ROOT using the FitPanel GUI
  - GUI for fitting all ROOT data objects (histogram, graphs, trees)
- Using the GUI we can:
  - select data object to fit
  - choose (or create) fit model function
  - set initial parameters
  - choose:
    - fit method (likelihood, chi2)
    - fit options (e.g Minos errors)
    - drawing options
  - change the fit range



Fit Panel (2)

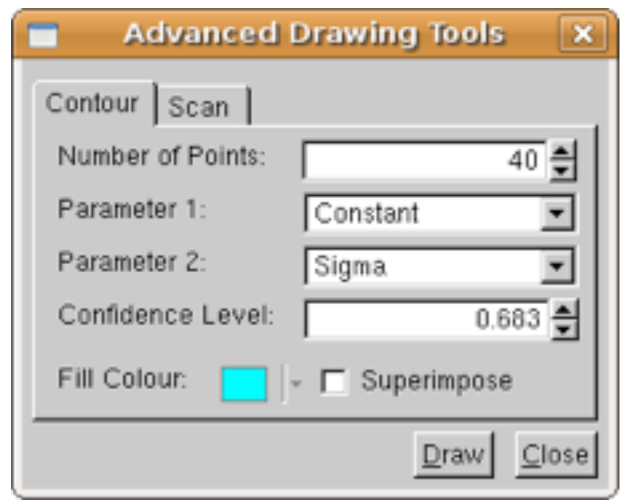
- The Fit Panel provides also extra functionality:

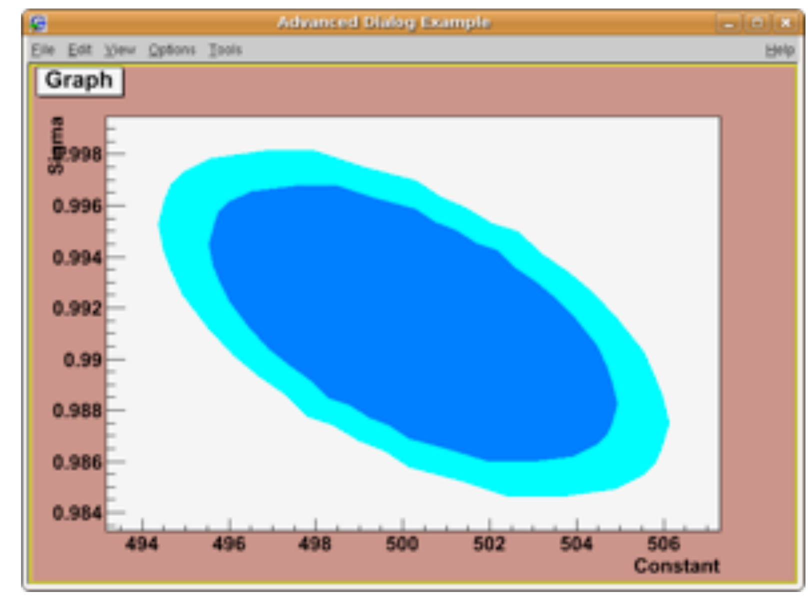
Control the minimization



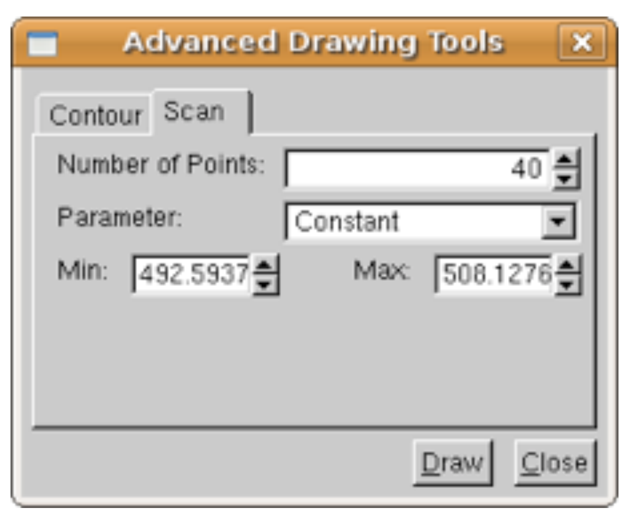
Advanced drawing tools

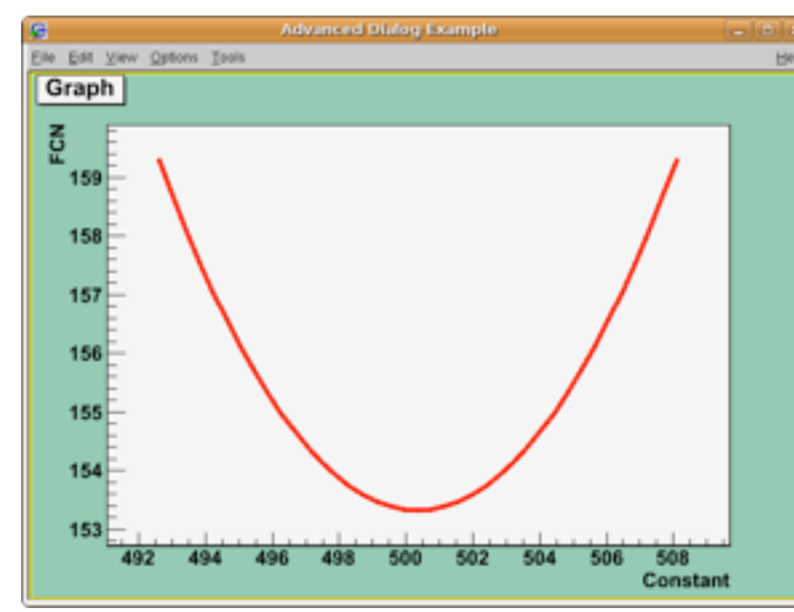
Contour plot





Scan plot of minimization function





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and solve exercises 2 and 3

Generating Pseudo Data

- Random number generation in ROOT is done using the `TRandom` classes
  - Three psudo-random number generator exists, `TRandom1`, `TRandom2` and `TRandom3`. `TRandom` is the base class.
    - `TRandom3` (a Mersenne-Twister generator) is used by default (it has a very long period, ~ 10^{6000} and it is very fast).
    - Random numbers can be generated using the global static variable `gRandom`

```
root [0] gRandom->Rndm()
(Double_t)9.99741748906672001e-01
```

    - `TRandom::Rndm()` generates uniform number in the [0,1] range.
    - Seeding is controlled using `TRandom::SetSeed( seed)`.
    - When using seed = 0, independent random streams can be generated (the seed is based on a UUID number).

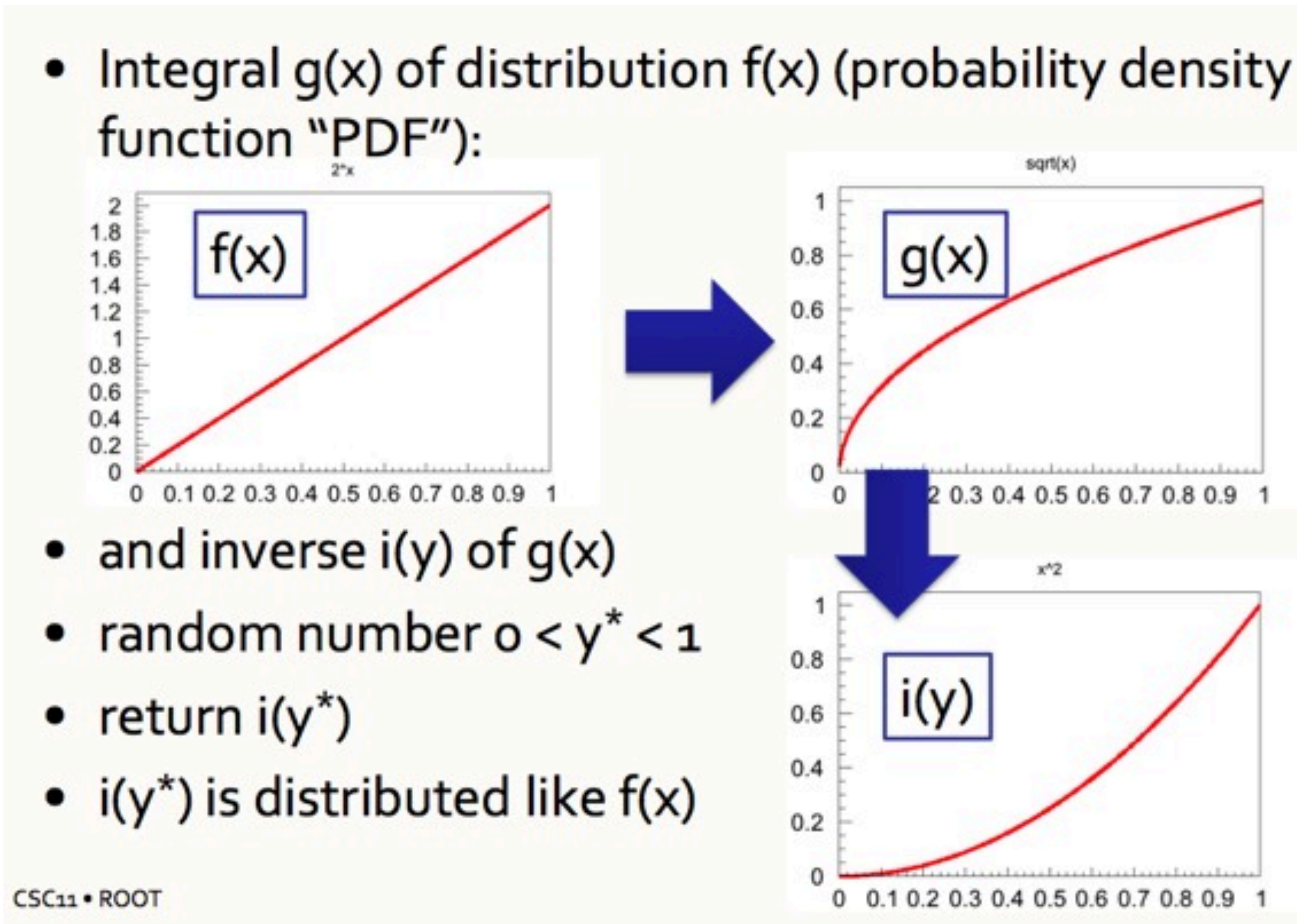
Random Number Distributions

- The class `TRandom` provides methods to generate numbers according to some pre-defined distributions

Distributions	Description
`Double_t Uniform(Double_t x1,Double_t x2)`	Uniform random numbers between `x1,x2`
`Double_t Gaus(Double_t mu,Double_t sigma)`	Gaussian random numbers. Default values: `mu=0, sigma=1`
`Double_t Exp(Double_t tau)`	Exponential random numbers with mean tau.
`Double_t Landau(Double_t mean,Double_t sigma)`	Landau distributed random numbers. Default values: `mean=0, sigma=1`
`Double_t BreitWigner(Double_t mean, Double_t gamma)`	Breit-Wigner distributed random numbers. Default values `mean=0, gamma=1`
`Int_t Poisson(Double_t mean)` `Double_t PoissonD(Double_t mean)`	Poisson random numbers
`Int_t  Binomial(Int_t ntot,Double_t prob)`	Binomial Random numbers
`Circle(Double_t &x,Double_t &y,Double_t r)`	Generate a random 2D point `(x,y)` in a circle of radius `r`
`Sphere(Double_t &x,Double_t &y, Double_t &z,Double_t r)`	Generate a random 3D point `(x,y,z)` in a sphere of radius `r`
`Rannor(Double_t &a,Double_t &b)`	Generate a pair of Gaussian random numbers with `mu=0` and `sigma=1`

Random Number Distributions (2)

- Random numbers can be generated according to what-ever distribution using accept-rejection techniques (often not very efficient) or by using the inverse of the cumulative (integral) distribution



- ROOT has the method `TF1::GetRandom()`, which uses this technique to generate random numbers from a generic function object

Time for Exercises!

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https://twiki.cern.ch/twiki/bin/view/Main/RootIRMMTutorial2013FittingExercises

and solve exercise 4

Summary

- We have learned:
  - the concept of fitting,
  - how to fit a histogram in ROOT.

- We have also learned:
  - how to generate random numbers and distributions which can be used to test and validate the fitting procedure.

- We will see later the fitting in practice using some data from IRMM.
- We will see also how fitting can be facilitate by using a tool like RooFit.
- How it can be extended in a statistical framework (RooStats).