

# FITTING TUTORIAL

Using ROOT, TMinuit and RooFit for fitting.

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**Uses ROOT 5.12.00** 

#### **OVERVIEW**

- 3 tutorials over the next two days:
  - Introduction:
    - Introduction to ROOT.
  - Multi Variate Analysis:
    - Training Neural Networks
    - Tools to calculate fisher discriminants, train neutral networks and boosted decision trees.
  - Fitting:

```
Fitting in ROOT (1): writing your own PDF to fit to.
```

(2): Using TMinuit

(3): RooFit

#### Aims of this Tutorial

- Lean how to define a user function for fitting within ROOT
- Learn how to set up a fit using TMinuit directly.
- Learn how to set up a fit using RooFit.
  - There is insufficient time for this tutorial to cover the use of RooFit, however there is self study material on this subject.

http://www.pp.rhul.ac.uk/~cowan/stat\_yeti.html http://www.ph.qmul.ac.uk/~bevan/yeti/index.html



Examples can be downloaded from theses URLs or the YETI program page

### Fitting in ROOT

- You saw how to use the ROOT Fit Panel to fit a pre-defined function to a histogram.
- What if the function you need to fit is not predefined within ROOT?
  - Define a function to use in ROOT.
  - Write the function to minimise and use TMinuit directly to minimise the function.
  - Use a higher level fitting package to build a more complicated fit model (e.g. RooFit).

### Defining a function to fit in ROOT

Several steps involved

See Chapter 5 of the ROOT 5.12 User Guide for more details

- Write the fit function.
- Instantiate a TF1 object for a 1D fit.
  - Note you can also define 2D (3D) fit function using a TF2 (TF3). If you need to perform a higher dimensional fit, then you need to consider using TMinuit, RooFit or an equivalent fit method.
- Set the initial parameter values, limits etc for the fit object
- Fit the data.
  - You can choose between a  $\chi^2$  fit (default) or a  $-\ln \mathcal{L}$  fit.

 Sometimes a Gaussian function is insufficient to model both the core and outlier parts of a peaking distribution.
 The sum of more than one Gaussian might give a better χ<sup>2</sup> than a single Gaussian model.

$$G3(x, N, \mu_1, \sigma_1, \mu_2, \sigma_2, \mu_3, \sigma_3) = N \left\{ f_1 e^{-(x-\mu_1)^2/2\sigma_1^2} + f_2 e^{-(x-\mu_2)^2/2\sigma_2^2} + \left(1 - f_1 - f_2\right) e^{-(x-\mu_3)^2/2\sigma_3^2} \right\}$$

- Variables to fit are:
  - N, the overall normalisation.
  - Three means and widths of the Gaussian functions  $(\mu_i, \sigma_i)$ .
  - Two fractions: f<sub>1</sub> and f<sub>2</sub>.

#### Write the fit function for

$$G3(x, N, \mu_1, \sigma_1, \mu_2, \sigma_2, \mu_3, \sigma_3) = N \left\{ f_1 e^{-(x-\mu_1)^2/2\sigma_1^2} + f_2 e^{-(x-\mu_2)^2/2\sigma_2^2} + \left(1 - f_1 - f_2\right) e^{-(x-\mu_3)^2/2\sigma_3^2} \right\}$$

```
* Define the fit function to determine the parameters of the
* sum of three Gaussians
* parameter
                                     description
                                Normalisation. The value of this parameter is dependent on the
                                                fit range and choice of histogram binning.
             mu1
                                mean of Gaussian 1
              siqma1
                                width of Gaussian 1
              mu2
                                mean of Gaussian 2
                                width of Gaussian 2
* 4
              sigma2
              mu3
                                mean of Gaussian 3
              sigma3
                                width of Gaussian 3
* 7
              frac1
                                fraction of Gaussian 1
              frac2
                               fraction of Gaussian 2
*/
Double t fitFunc(Double t * x, Double t * par)
 Double t PDF
                  = 0.0:
 Double t q1
                 = 0.0;
 Double t g2
                 = 0.0;
 Double t q3
                  = 0.0;
```

It's a good idea to keep track of the parameter Names when writing the fit function.

Calculate the value of the function G3

return PDF;

Return the calculated value

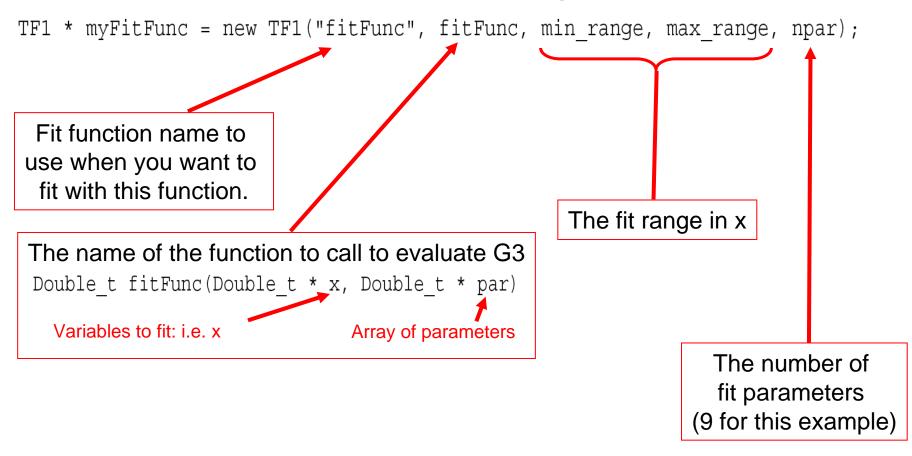
// Calculate the exponents of the Gaussians

// add each Gaussian contribution to the PDF

g1 = exp(-0.5\*arg1\*arg1)/(par[2]\*sqrt(2.0\*TMath::Pi()));
g2 = exp(-0.5\*arg2\*arg2)/(par[4]\*sqrt(2.0\*TMath::Pi()));
g3 = exp(-0.5\*arg3\*arg3)/(par[6]\*sqrt(2.0\*TMath::Pi()));
PDF = par[0]\*(par[7]\*g1 + par[8]\*g2 + (1-par[7]-par[8])\*g3);

Double\_t arg1 = (par[2] != 0.0) ? (x[0] - par[1])/(par[2]) : 0.0;Double\_t arg2 = (par[4] != 0.0) ? (x[0] - par[3])/(par[4]) : 0.0;Double\_t arg3 = (par[6] != 0.0) ? (x[0] - par[5])/(par[6]) : 0.0;

Set up the TF1 object for fitting



Set up the TF1 object for fitting

```
TF1 * myFitFunc = new TF1("fitFunc", fitFunc, min range, max range, npar);
```

Define the parameters, and give initial values

```
myFitFunc->SetParName(0, "norm");
myFitFunc->SetParName(1, "mu1");
myFitFunc->SetParName(2, "sigma1");
myFitFunc->SetParName(3, "mu2");
myFitFunc->SetParName(4, "siqma2");
myFitFunc->SetParName(5, "mu3");
myFitFunc->SetParName(6, "sigma3");
myFitFunc->SetParName(7, "frac1");
myFitFunc->SetParName(8, "frac2");
  parameter number
                              parameter name
myFitFunc->SetParameters(1500.0, 5, 0.5, 6, 1.5, 5, 5, 0.4, 0.3);
```

Ordered list of initial parameter values

#### Set parameter limits

```
myFitFunc->SetParLimits(0, 0.0, 2500.0);
myFitFunc->SetParLimits(1, 0.01, 10.0);
myFitFunc->SetParLimits(2, 0.0, 5);
myFitFunc->SetParLimits(3, 0.01, 10.0);
myFitFunc->SetParLimits(4, 0.0, 5);
myFitFunc->SetParLimits(5, 0.01, 10.0);
myFitFunc->SetParLimits(6, 0.0, 10.);
myFitFunc->SetParLimits(7, 0.0, 1.0);
myFitFunc->SetParLimits(8, 0.0, 1.0);
```

parameter number

parameter limits (min, max)

#### Fix any required parameters before fitting

```
myFitFunc->FixParameter(5, 5.0);
myFitFunc->FixParameter(6, 5.0);

parameter number
    parameter value
```

- Generate a dataset & fit
  - A quick way to do this is to get ROOT to generate a data set by filling a histogram

TH1F data\_hist("data\_hist", "", 50, min\_range, max\_range);
data\_hist.FillRandom(fitFunc, 1500);

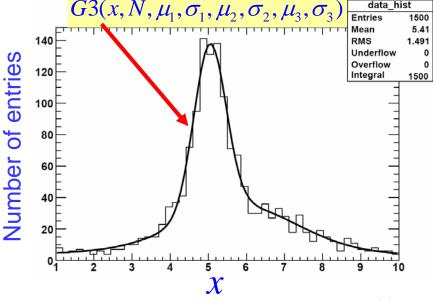
Your fit function

The number of entries to generate

Then you can do a likelihood fit to the data

data\_hist.Fit("fitFunc", "L");
The name of your
fit function Fit options

 You can also fit to a variable in a tree using this function.



#### The full list of possible fit options is:

- W Set all errors to 1
- I Use integral of function in bin instead of value at bin center
- L Use Loglikelihood method (default is chisquare method)
- LL Use Loglikelihood method and bin contents are not integers)
- U Use a User specified fitting algorithm (via SetFCN)
- Q Quiet mode (minimum printing)
- V Verbose mode (default is between Q and V)
- E Perform better Errors estimation using Minos technique
- B Use this option when you want to fix one or more parameters and the fitting function is like "gaus", "expo", "poln", "landau".
- M More. Improve fit results
- R Use the Range specified in the function range
- N Do not store the graphics function, do not draw
- O 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, any previous function is deleted)

### Exercises: Triple Gaussian

- Using the f\_triple\_gaussian.cc macro
  - 1. Run the macro and note the output parameter values.
  - 2. Change the fit option to be "" to perform a  $\chi^2$  fit. What happens to the parameters and convergence status, and why do you think this happens?
  - 3. Do the same using MINOS (E) and the Improve solution (M) options & note differences. What option gives the best fit  $\chi^2$ /degree of freedom?
    - Hint:

```
 \begin{array}{lll} \chi 2 \; can \; be \; calculated \; using \\ v \; (\#degrees \; of \; freedom) & myFitFunc->GetChisquare(); \\ P(\chi 2, \, v) \; can \; be \; calculated \; using \\ \end{array}
```

### Exercises: Triple Gaussian

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    - Hint:

```
\chi 2 can be calculated using myFitFunc->GetChisquare(); \nu (#degrees of freedom) myFitFunc->GetNDF(); P(\chi 2, \nu) can be calculated using myFitFunc->GetProb();
```

4. You can print the covariance and correlation matrices by adding the following line at the end of the macro:

```
gMinuit->mnmatu(1);
```

Make this alteration and re-run the fit. What does this tell you about the fit parameters?

5. Is there a better way to write the PDF?

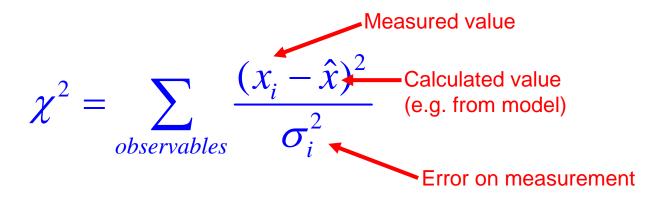
### **Using TMinuit**

Many logical steps involved:

See Chapter 5 of the ROOT 5.12 User Guide for more details

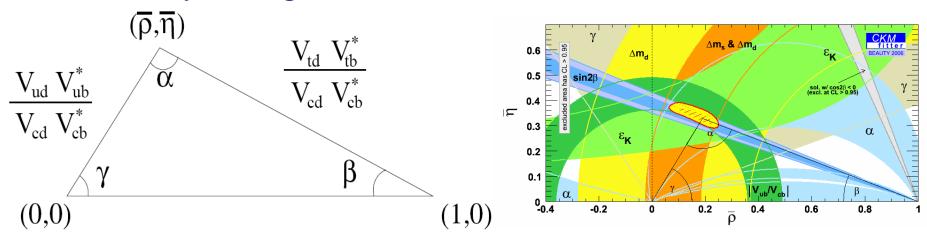
- Write the function to minimise.
- Define the global data to fit to.
- Set up a TMinuit object for fitting.
  - Need to specify parameters (and ranges) to use in the fit.
    - Are parameters allowed to vary in the fit?
    - Are parameters fixed to a constant value in the fit?
  - Need to specify what type of fit to do.
    - MIGRAD?
    - HESSE?
    - MINOS?
- Recall the results (and test statistic at the fit minimum) for interpretation. [can be read from file or screen]

- Define the problem to solve.
  - Write down the equations to solve and calculate the function to minimise (e.g. a  $\chi^2$ ):



- Then code into a function with a specific prototype.
- Measured values should be declared with global scope (i.e. outside any function & before they are used).

Two independent variables define the shape of the Unitarity Triangle:  $\bar{\rho}, \bar{\eta}$ 



And the B-factories have produced measurements of the angles (and sides of this triangle). e.g.

#### Measurements

$$\alpha = (92 \pm 7)^{\circ}$$
$$\beta = (21.2 \pm 1)^{\circ}$$

$$\beta = (21.2 \pm 1)^{\circ}$$

Relation to apex co-ordinate 
$$\alpha = \operatorname{atan}\left(\frac{\overline{\rho}}{\overline{\eta}}\right) + \operatorname{atan}\left(\frac{1-\overline{\rho}}{\overline{\eta}}\right)$$
$$\beta = \operatorname{atan}\left(\frac{\overline{\eta}}{1-\overline{\rho}}\right)$$

• So we can write the  $\chi^2$  to calculate for a given value of the apex co-ordinates:

$$\chi^{2} = \frac{\left(\alpha_{meas} - \alpha(\bar{\rho}, \bar{\eta})\right)^{2}}{\sigma_{\alpha_{meas}}^{2}} + \frac{\left(\beta_{meas} - \beta(\bar{\rho}, \bar{\eta})\right)^{2}}{\sigma_{\beta_{meas}}^{2}}$$

- Need to write a function that calculates the  $\chi^2$  for a given set of values of the parameters  $\overline{\rho}$  and  $\overline{\eta}$ .
- This fit is coded up in the file yeti07/TMinuit/FitUT.cc.
- To compile & run the program:

```
cd yeti07/TMinuit/
gmake
./FitUT
```

Declare the global data: measurements of  $\beta$  and  $\alpha$  (with their uncertainties)

```
double deg2rad = M PI/180.0;
double beta meas = 21.2*deq2rad;
double dbeta meas = 1.0*deg2rad;
double alpha meas = 95.8*deq2rad;
double dalpha meas = 7.0*deg2rad;
```

An array of the parameters defined in the fit  $(\overline{\rho}, \overline{\eta})$ 

Write the function to minimise

```
extern void chi2(Int t &npar, Double t *gin, Double t &f, Double t *par, Int t iflag)
 double thechi2 = 0.0;
 // calculate the alpha chi2 contribution for a given set of rhobar and etabar
  double alpha_arg1(0), alpha_arg2(0);
  if(par[1]!= 0.0) \{ alpha\_arg1 = par[0]/par[1]; \}
                 alpha_arg2 = (1-par[0])/par[1];
  double alpha_chi2 = (alpha_meas - ( atan(alpha_arg1) + atan(alpha_arg2) ))/dalpha_meas;
 double beta arg = 0.0;
  if ((1-par[0]) != 0.0) beta arg = par[1]/(1-par[0]);
 double beta chi2 = (beta meas - atan(beta arg))/dbeta meas;
  // add the chi2 contributions together and set the return value
  thechi2 += alpha chi2*alpha chi2;
  thechi2 += beta chi2*beta chi2;
                                       Equate the variable f with the value of the
  f= thechi2;
```

Calculate the  $\chi^2$ 

 $\chi^2$  before returning from the function

Set up a TMinuit object in the main function

```
Initialise Minuit with a maximum of 2 parameters to minimise

// set the function to minimise with minuit.
gMinuit->SetFCN(chi2);

Double_t arglist[10];
arglist[0] = 1;
gMinuit->mnexcm("SET ERR", arglist, 1, iflag);

Set the '1o' tolerance for the change in FCN
That determines when a function has been minimised
```

Set up a TMinuit object in the main function

Initialise Minuit with a maximum of TMinuit \*qMinuit = new TMinuit(2); 2 parameters to minimise // set the function to minimise with minuit. Set the function to minimise qMinuit->SetFCN(chi2); Double t arglist[10]; arglist[0] = 1;gMinuit->mnexcm("SET ERR", arglist, 1, iflag); ← Interprets command Set the '1 $\sigma$ ' tolerance for the change in FCN That determines when a function has been minimised Set the parameters gMinuit->mnparm(0, "rhobar", 0.2, .1, 0.0, 0.5, iflag); qMinuit->mnparm(1, "etabar", 0.3, .1, 0.0, 0.5, iflag); used in the fit mnparam(Int tiPar, TString name, Double\_t startval, Double\_t stepval, Double\_t min, Double\_t max, Int\_t &errFlag) Allowed limits Parameter number (start counting from zero) Step size for parameter Parameter name OK if zero Start value for the parameter

Set up a TMinuit object in the main function

```
Initialise Minuit with a maximum of
TMinuit *qMinuit = new TMinuit(2);
                                                   2 parameters to minimise
// set the function to minimise with minuit.
                                                         Set the function to minimise
qMinuit->SetFCN(chi2); ←
Double t arglist[10];
arglist[0] = 1;
gMinuit->mnexcm("SET ERR", arglist, 1, iflag); ←
                                                                  Interprets command
Set the '1\sigma' tolerance for the change in FCN
That determines when a function has been minimised
                                                              Set the parameters
gMinuit->mnparm(0, "rhobar", 0.2, .1, 0.0, 0.5, iflag);
gMinuit->mnparm(1, "etabar", 0.3, .1, 0.0, 0.5, iflag);
                                                              used in the fit
gMinuit->mnexcm("CALL FCN", arglist, 1, iflag);
Call the user defined function, to calculate the value
FCN, and print the result out to the screen.
```

Set up a TMinuit object in the main function

Initialise Minuit with a maximum of TMinuit \*qMinuit = new TMinuit(2); 2 parameters to minimise // set the function to minimise with minuit. Set the function to minimise qMinuit->SetFCN(chi2); ← Double t arglist[10]; arglist[0] = 1;gMinuit->mnexcm("SET ERR", arglist, 1, iflag); ← Interprets command Set the ' $1\sigma$ ' tolerance for the change in FCN That determines when a function has been minimised Set the parameters qMinuit->mnparm(0, "rhobar", 0.2, .1, 0.0, 0.5, iflag); gMinuit->mnparm(1, "etabar", 0.3, .1, 0.0, 0.5, iflag); used in the fit qMinuit->mnexcm("CALL FCN", arglist, 1, iflag); Run the minimisation qMinuit->mnexcm("MIGRAD", arglist,2, iflag); Using MIGRAD

#### MIGRAD vs. HESSE vs. MINOS

#### MIGRAD

 Performs a local function minimization using a modified version of the Davidson-Fletcher-Powell switching method described in Fletcher, Comp.J. 13,317 (1970).

#### HESSE

 Calculates the full second-derivative matrix of the user function FCN using a finite difference method. This is often used to improve upon the result obtained by MIGRAD.

#### MINOS

- Performs a MINOS error analysis. This can result in different errors than obtained using MIGRAD or HESSE methods. In general one obtains asymmetry errors from MINOS.
- You should use (at least) HESSE after MIGRAD to obtain reliable errors for a given fit result. MINOS will give the best estimate of the errors of a given set of parameters.

- Using the FitUT program
  - 1. Run the program and note the output values of the apex coordinates and errors.
  - 2. Run with the –hesse and –minuit options and note how the fitted values and errors change, and what the different options are doing.
  - 3. What is the significance of the correlation between the two fit parameters?
  - 4. What do you do when the fit fails to converge?

- Using the FitUT program
  - 1. Run the program and note the output values of the apex coordinates and errors.
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- Try extending the program to include  $\gamma = (82\pm20)^{\circ}$ .

- Using the FitUT program
  - Run the program and note the output values of the apex coordinates and errors.
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  - What is the significance of the correlation between the two fit parameters?
  - 4. What do you do when a fit fails to converge?
- Try extending the program to include  $\gamma = (82\pm20)^{\circ}$ .
  - So add the  $\chi^2$  term:

So add the 
$$\chi^2$$
 term: 
$$\chi^2 = \frac{\left(\gamma_{meas} - \gamma(\bar{\rho}, \bar{\eta})\right)^2}{\sigma_{\gamma_{meas}}^2}$$
 where  $\gamma = \operatorname{atan}\left(\frac{\bar{\eta}}{\bar{\rho}}\right)$ 

where 
$$\gamma = \operatorname{atan}\left(\frac{\overline{\eta}}{\overline{\rho}}\right)$$

#### Possible commands for mnexcm

void <a href="mailto:mnexcm">mnexcm</a>(const char \*command, <a href="Double\_t">Double\_t</a> \*plist, <a href="mailto:lnt\_t">Int\_t</a> llist, <a href="Int\_t">Int\_t</a> &ierflg)

equivalent TMinuit function call

#### mnexcm command **MIGrad** Call MIGRAD for minimisation **HESse** Call HESSE for minimisation **MINOs** Call MINOS for minimisation **MINImize** Call MIGRAD for minimisation SEEk Use a Monte Carlo method to minimise with a 3 $\sigma$ hypercube Use a simplex method for minimisation SIMplex Set the values of configurable options for Minuit SET xxx Display covariance matrix, value of FCN etc. SHOw xxx Fix the specified parameter in the fit FIX Restore fixed parameters to variable status REStore RELease Allow the specified parameter to vary in the fit Scan the value of the user function for a parameter SCAn CONtour Trace contour lines between parameters SAVe Write output to file TOP of pag Set output to top of file Given a fit minimum, search for additional local minima **IMProve** CALI fcn Call the specified user function STAndard Do nothing END Signals the end of a fit Calculate final parameters and exit from minuit EXIt RETurn Return from Minuit to the calling function CLEar Reset all parameters and values to undefined **HELP** Access the Minuit help interface Calculate the $N_{\sigma}$ contour between two parameters MNContour STOp Same as EXIT **aMUL** Jump to a new point to continue minimisation COVARIANCE Obsolete PRINTOUT Obsolete, please use SET PRInt GRADIENT Obsolete, please use SET GRAdient MATOUT Obsolete, please use SHOW COVar ERROR DEF Obsolete, please use SET ERRordef

Obsolete, please use SET LIMits Obsolete please use SAVe

LIMITS

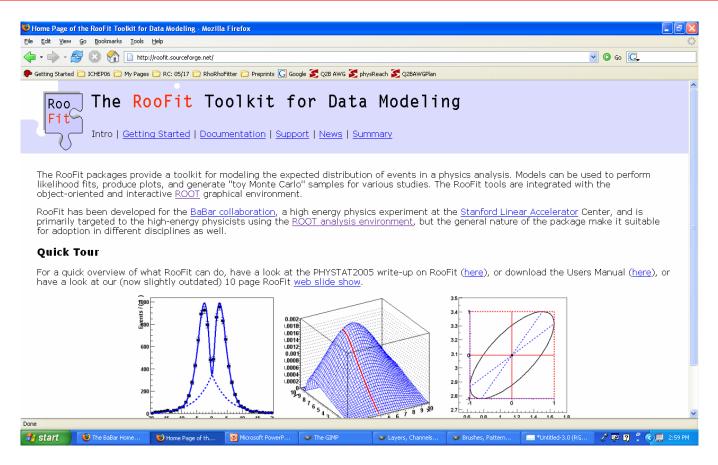
PUNCH

9th January 2007

```
Migrad()
    Migrad()
    mnseek()
    mnsimp()
    mnset()
    mnset()
    FixParameter(Int t iPar)
    Release(Int tiPar)
    mnscan()
    Contour(Int t npoints=10, Int+t pa1=0, Int t pa2=1)
    mnsave()
   mnimpr()
Eval(Int t npar, Double t *grad, Double t &val, Double t &fval, Double t *par, Int t flag)
    mncler()
    mnhelp(), mnhelp(TString command)
    Contour(Int t npoints=10, Int+t pa1=0, Int t pa2=1)
```

#### RooFit

**Synopsis:** A fitting package to facilitate complex likelihood fits within the HEP community. This is an extremely flexible and an extendible set of tools.



More information is available at http://roofit.sourceforge.net

See the sourceforge website for examples, tutorials and a user guide.

### **Basic Types**

#### RooRealVar

- Used for discriminating variables (x,y,...).
- Used for shape parameters (Gaussian width and mean etc.).
- Probability Density Function types (e.g. RooPolynomial and RooGaussian)
  - See the RooFit web site for examples and a user guide listing other available PDF types.

#### RooDataSet

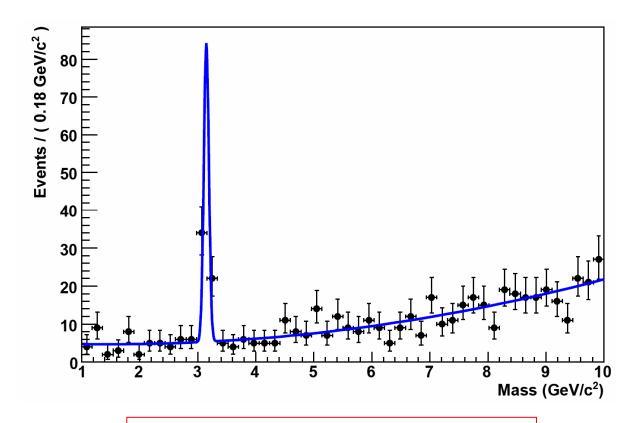
- Data container that stores information on an entry by entry basis.
- Can get a TTree from a RooDataSet.

### **Example: Peak finding**

 Fit for a Gaussian peak of known mass on a polynomial background.

#### Need the following:

- Signal
  - Shape (PDF)
  - Yield
- Background
  - Shape (PDF)
  - Yield
- Data or Monte Carlo simulated data (to fit and plot result of)



The ROOT macro for this exercise is yeti07/fitting/rf\_fit\_for\_peak.cc

# Peak finding: Signal PDF

Need to define the discriminating variable:

RooRealVar mass("mass", "Mass", 1, 10, "GeV/c $^{2}$ ");

Allowed range for the parameter mass

Then define the signal PDF

Parameter fixed to 3.15

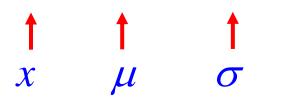
```
RooRealVar sig_mu("sig_mu", "mean", 3.15);
RooRealVar sig_sigma("sig_sigma", "width", 0.05, 0.0, 0.1);
```

Parameter set to 0.05

range

RooGaussian sig\_pdf("sig\_pdf", "signal pdf", mass, sig\_mu, sig\_sigma);

$$G(x,\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}}e^{-(x-\mu)^2/2\sigma^2}$$



# Peak finding: Background PDF

- Use the same discriminating variable as the signal
- Define the background PDF

```
RooRealVar bg_pol1("bg_pol1", "linear coefficient", 0.01, -10, 10.);
RooRealVar bg_pol2("bg_pol2", "quadratic coefficient", 0.05, -10, 10);
```

```
P = ax + bx^2 + C RooArgList bgCoefList; bgCoefList.add(bg_pol1); bgCoefList.add(bg_pol2); C is determined from the automatic PDF normalisation in RooFit
```

RooPolynomial bg\_pdf("bg\_pdf", "background pdf", mass, bgCoefList);

RooFit defines a polynomial of order n (Pn) as

$$Pn = \sum_{i=1}^{n} a_i x^i + C$$

### Peak finding: Total PDF

Need to define signal and background yields

```
RooRealVar signalYield("signalYield", "", 50.0, -10.0, 150.0);
RooRealVar backgroundYield("backgroundYield", "", 500.0, 0.0, 15000.0);
```

 And make the total PDF that corresponds to the extended likelihood that we want to fit

```
RooArgList pdfList;
pdfList.add(sig_pdf);
pdfList.add(bg_pdf);
RooArgList coefList;
coefList.add(signalYield);
coefList.add(backgroundYield);
```

- Need to respect the order that you Add the PDFs and the yields.
- •If the number of entries added to the pdfList match the number for the coefList, RooFit will automatically set up an extended likelihood fit.

RooAddPdf TotalPdf("TotalPdf", "Extended PDF", pdfList, coefList);

$$TotalPdf = N_{signal} \left[ \frac{1}{\sigma \sqrt{2\pi}} e^{-(x-\mu)^2/2\sigma^2} \right] + N_{background} \left[ ax + bx^2 + C \right]$$

#### Peak finding: Generate & fit a toy data sample

Use TotalPdf to generate a data set

```
Int_t nToGen = (Int_t)( signalYield.getVal() + backgroundYield.getVal() );
RooDataSet * data = (RooDataSet*)TotalPdf.generate(RooArgSet(mass), nToGen);
```



Then fit...

The set of discriminating variables to generate

```
RooFitResult * result = TotalPdf.fitTo(*data, "etr");
```

#### **AVAILABLE FIT OPTIONS:**

```
"m" = MIGRAD only (no MINOS)
```

"s" = Estimate step size with HESSE

"h" = Run HESSE after MIGRAD

"e" = Perform extended -InL fit

"0" = Run MIGRAD with strategy MINUIT 0 (don't calculate correlation matrix – not valid if running HESSE or MINOS)

"q" = Switch off verbose mode

"I" = Save log file with values at each MINUIT step

"v" = Show change in parameters at each step

"t" = Time the fit

"r" = Save the fit output in a RooFitResult object.

#### Peak finding: Looking at the data and fit result

The fit result obtained is printed to the screen:

```
Fit worked and
  23 **MINOS
                2500
                                                             errors are sensible
FCN=-1817.09 FROM MINOS STATUS SUCCESSFUL 511 CALLS
         EDM=3.55819e-06 STRATEGY= T ERROR MATRIX ACCURATE
                            PARABOLIC
                                            MINOS ERRORS
EXT PARAMETER
                  VALUE
                              ERROR
                                         NEGATIVE
NO. NAME
                                                    POSITIVE
1 backgroundYield 5.02392e+02 2.25756e+01 -2.22056e+01 2.29511e+01
2 bg_pol1
                -1.37144e-01 1.00305e-01 -8.06255e-02 1.34265e-01
              4.53396e-02 7.60813e-03 -7.33347e-03 8.40973e-03
3 bg_pol2
               4.32667e-02 5.39951e-03 -5.07501e-03 5.83116e-03
4 sig sigma
5 signalYield
                4.75675e+01 7.39504e+00 -7.07024e+00 7.75175e+00
```

#### Get a RooPlot

Add the data to the plot

```
RooPlot * frame = mass.frame(50);
data->plotOn(frame);
```

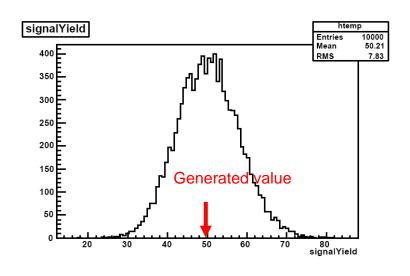
 Add the fitted PDF to the plot with correct normalisation

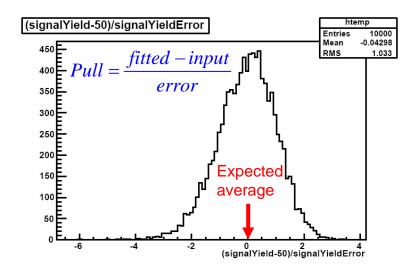
```
TotalPdf.plotOn(frame);
```

Display the result on-screen frame->Draw();

# Peak finding: Validating the fit

- $\chi^2$  and likelihood fits are intrinsically biased. So the fit needs to be validated before you can trust the result.
  - The first step in validating a fit is to run ensembles of toy MC simulations and compare the results with the fit to data.
  - Then check the pull distribution.

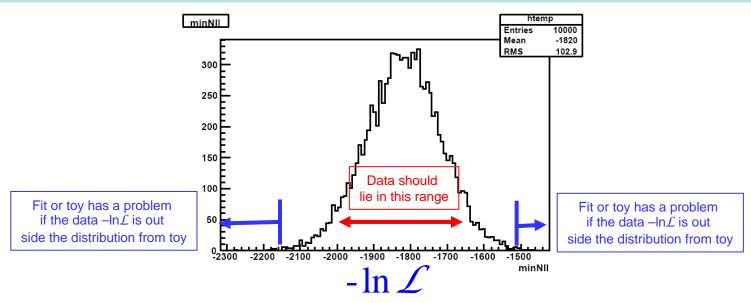




# Peak finding: Validating the fit

- If the fit works then you can compare the value of −ln £ you obtain in data with that of the ensemble of toy MC experiments that you run.
  - -In £ from data should be compatible with the toys or you have a problem!

$$\mathcal{L} = e^{-(N_{signal} + N_{background})} \prod_{i=1}^{n} N_{signal} PDF_{signal} + N_{background} PDF_{background}$$



### **Exercises: Peak Finding**

- 1. Run the macro yeti07/fitting/rf\_fit\_for\_peak.cc and look at the resulting plot and fit result.
- 2. Change the signal yield from 50 events and see what happens.
- 3. Increase the background yield by a factor of 10, 20, 100 and see what happens to the error on the signal yield.

### **Exercises: Peak Finding**

- 1. Run the macro yeti07/fitting/rf\_fit\_for\_peak.cc and look at the resulting plot and fit result.
- 2. Change the signal yield from 50 events and see what happens.
- 3. Increase the background yield by a factor of 10, 20, 100 and see what happens to the error on the signal yield.
- 4. Run the macro yeti07/fitting/rf\_toy\_mc.cc
  - 1. What are the mean  $(\mu)$  and width  $(\sigma)$  of the pull distribution when you fit a Gaussian to them?
  - 2. If you increase the number of toy MC studies run to 1000 toys what happens to  $\mu$  and  $\sigma$ ?

### Summary

- You have seen
  - How to do simple fits using ROOT.
    - Fitting a user defined PDF to a histogram (or data from a TTree).
  - How to write a program that uses TMinuit to solve a problem.
    - Fitting for model parameters given the results of measurements from experiment.
  - How to write a fit using RooFit, and how to use ensembles of toy Monte Carlo simulated data to check that the fit is unbiased.
    - Hunting for a particle of known mass, sitting on a slowly varying background.
- More information on fitting using ROOT and RooFit is available on the web:

http://root.cern.ch

http://roofit.sourceforge.net

http://www.pp.rhul.ac.uk/~cowan/stat\_yeti.html

http://www.ph.qmul.ac.uk/~bevan/yeti/index.html

### **Answers**

### Exercises: Triple Gaussian

1. The fit output is: (likelihood fit using MINOS)

```
STATUS=SUCCESSFUL 1633 CALLS
FCN=279.841 FROM MINOS
         EDM=1.03679e-07 STRATEGY= 1 ERROR MATRIX ACCURATE
EXT PARAMETER
                       PARABOLIC
                                      MINOS ERRORS
                        ERROR NEGATIVE
NO. NAME VALUE
                                             POSITIVE
1 norm
          2.99283e+02 1.21244e+01 -1.30126e+01 1.17130e+01
2 mu1
          5.05660e+00 3.13761e-02 -3.16178e-02 3.12311e-02
3 sigma1 5.47804e-01 3.52334e-02 -3.45777e-02 3.61277e-02
4 mu2
          5.96774e+00 1.88659e-01 -1.68086e-01 2.22287e-01
5 sigma2 1.83507e+00 2.85564e-01 -2.55416e-01 3.39584e-01
6 mu3
          5.00000e+00 fixed
7 sigma3 5.00000e+00 fixed
          4.48193e-01 3.40095e-02 -3.48849e-02 3.36606e-02
8 frac1
9 frac2
          3.01842e-01 8.24768e-02 -7.44924e-02 1.04531e-01
```

2. The corresponding  $\chi^2$  fit result is

```
FCN=56.4376 FROM MIGRAD STATUS=CONVERGED 421 CALLS
                                                              422 TOTAL
         EDM=1.00695e-07 STRATEGY= 1
                                         ERROR MATRIX ACCURATE
EXT PARAMETER
                                STEP
                                         FIRST
                        ERROR
                                    SIZE DERIVATIVE
NO. NAME VALUE
          2.92910e+02 9.93126e+00 3.54802e-05 -1.74127e-02
1 norm
          5.04437e+00 3.59062e-02 2.11292e-05 1.36630e-02
2 mu1
3 sigma1 5.26065e-01 4.85833e-02 6.13261e-05 -9.31252e-03
4 mu2
          5.70132e+00 1.94817e-01 7.92342e-05 8.87536e-03
5 sigma2 1.40108e+00 2.50419e-01 1.62533e-04 5.24887e-03
6 mu3
          5.00000e+00 fixed
7 sigma3 5.00000e+00 fixed
          4.21881e-01 6.18272e-02 1.31500e-04 -7.82614e-03
8 frac1
          2.74470e-01 5.47831e-02 2.14242e-04 -5.61992e-03
```

where most of the parameter error have increased.

3. The results don't significantly change, but the error is marginally better using these options.

### Exercises: Triple Gaussian

#### 4. The correlation matrix is:

PARAMETER CORRELATION COEFFICIENTS

NO. GLOBAL 1 2 3 4 5 8 9

1 0.63008 1.000 -0.238 -0.186 -0.157 -0.499 -0.340 -0.224

2 0.60735 -0.238 1.000 0.305 0.151 0.539 0.424 -0.106

3 0.85179 -0.186 0.305 1.000 0.711 0.575 0.832 -0.641

4 0.83930 -0.157 0.151 0.711 1.000 0.545 0.792 -0.638

5 0.91961 -0.499 0.539 0.575 0.545 1.000 0.794 -0.118

8 0.95900 -0.340 0.424 0.832 0.792 0.794 1.000 -0.595

9 0.88240 -0.224 -0.106 -0.641 -0.638 -0.118 -0.595 1.000

All off-diagonal elements are non-zero

Diagonal is unity

All of the parameters are correlated with each other. Change one parameter, and the best fit for the all remaining parameters change.

5. Can you write the PDF in a better way? Yes.

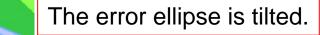
$$G3 = N \left\{ f_1 e^{-(x-\mu_1)^2/2\sigma_1^2} + f_2 e^{-(x-\mu_2)^2/2\sigma_2^2} + \left(1 - f_1 - f_2\right) e^{-(x-\mu_3)^2/2\sigma_3^2} \right\}$$

$$G3 = N \left\{ f_2 \left( f_1 e^{-(x-\mu_1)^2/2\sigma_1^2} + (1-f_1) e^{-(x-\mu_2)^2/2\sigma_2^2} \right) + (1-f_2) e^{-(x-\mu_3)^2/2\sigma_3^2} \right\}$$

The second form of the sum of three Gaussians ranks the contributions from the three Gaussians, which can help the fitter converge to the minimum more quickly than the original implementation of the function. Such a finesse is usually worth making when a function is very heavily used.

- Using the FitUT program
  - 1.  $\bar{\rho} = 0.17 \pm 0.04$ ,  $\bar{\eta} = 0.32 \pm 0.02$
  - 2. HESSE and MINOS give the same errors as MIGRAD to 2d.p.

3. The fit parameter correlation is -0.597, so the parameters are highly correlated.



- 4. What do you do when a fit fails to converge?
  - Try a different start value (in case you are too far from the minimum to converge)
  - b) Try to fix a parameter: If parameters are highly correlated, fixing one to a reasonable value can help improve the convergence property of a fit. Do you need to re-write the fit so that it is simpler (less parameters)?
- Include  $\gamma = (82\pm 20)^{\circ}$ , you should fit

$$\bar{\rho} = 0.15 \pm 0.04, \quad \bar{\eta} = 0.32 \pm 0.02$$

And the correlation changes to -0.554

■ N.B.  $180-\alpha-\beta=63$  degrees, so the shift in fitted parameters comes from a mild discrepancy  $(1\sigma)$  between the three angles.

### **Exercises: Peak Finding**

- If you increase the background yield, the error on the signal yield increases
  - For 10K backround, the error on signal yield is ±13.0 events.
  - For 500 background events, the error on signal yield is ±7.4 events for 500.
- Toys:
  - 100 Toys  $\mu_{pull} = -0.14 \pm 0.10, \ \sigma_{pull} = 0.96 \pm 0.07$
  - 1000 Toys  $\mu_{pull} = -0.06 \pm 0.03$ ,  $\sigma_{pull} = 1.03 \pm 0.02$
  - 10000 Toys  $\mu_{pull} = -0.04 \pm 0.01$ ,  $\sigma_{pull} = 1.03 \pm 0.007$
  - Looks biased.
  - The pull distribution is asymmetric because of the Poisson nature of the signal yield. If you increase the signal yield and repeat the toy experiment this bias will be reduced.

