

# roofit tutorial

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## references

<http://roofit.sourceforge.net/quicktour/first.html>

<https://www.slideserve.com/denna/statistical-methods-for-data-analysis-parameter-estimates-with-roofit>

<https://www.slideserve.com/gomer/deviations-from-exponential-decay>

## RooFit: Your toolkit for data modeling

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### What is it?

- A powerful toolkit for modeling the expected distribution(s) of events in a physics analysis
- Primarily targeted to high-energy physicists using ROOT
- Originally developed for the BaBar collaboration by Wouter Verkerke and David Kirkby.
- Included with ROOT v5.xx

### Documentation:

- <http://root.cern.ch/root/Reference.html> – for latest class descriptions. RooFit classes start with "Roo".
- <http://roofit.sourceforge.net> – for documentation and tutorials

### Tutorials:

- Dig \$ROOTSYS/tutorials/rootfit

# Math – The Likelihood estimator

- **Definition** of Likelihood

- given  $\mathbf{D}(\vec{x})$  and  $\mathbf{F}(\vec{x}; \vec{p})$

Functions used in likelihoods must be Probability Density Functions:

$$\int F(\vec{x}; \vec{p}) d\vec{x} \equiv 1, \quad F(\vec{x}; \vec{p}) > 0$$

$$L(\vec{p}) = \prod_i F(\vec{x}_i; \vec{p}), \quad \text{i.e.} \quad L(\vec{p}) = F(x_0; \vec{p}) \cdot F(x_1; \vec{p}) \cdot F(x_2; \vec{p}) \dots$$

- For convenience the **negative log of the Likelihood** is often used

$$-\ln L(\vec{p}) = -\sum_i \ln F(\vec{x}_i; \vec{p})$$

- Parameters are estimated by maximizing the Likelihood, or equivalently minimizing  $-\log(L)$

$$\left. \frac{d \ln L(\vec{p})}{d\vec{p}} \right|_{p_i = \hat{p}_i} = 0$$

Wouter Verkerke, NIKHEF

# Math – Variance on ML parameter estimates

- **Estimator** for the **parameter variance** is

$$\hat{\sigma}(p)^2 = \hat{V}(p) = \left( \frac{d^2 \ln L}{d^2 p} \right)^{-1}$$

- I.e. variance is estimated from 2<sup>nd</sup> derivative of  $-\log(L)$  at minimum
- Valid if estimator is **efficient** and **unbiased!**

From Rao-Cramer-Frechet inequality

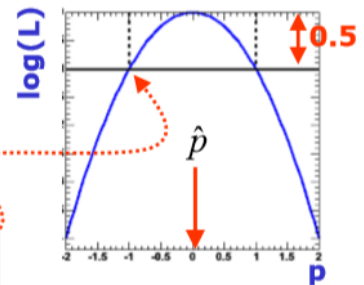
$$V(\hat{p}) \geq 1 + \frac{db}{dp} \left/ \left( \frac{d^2 \ln L}{d^2 p} \right) \right.$$

$b$  = bias as function of  $p$ , inequality becomes equality in limit of efficient estimator

- **Visual interpretation** of variance estimate

- Taylor expand  $-\log(L)$  around minimum

$$\begin{aligned} \ln L(p) &= \ln L(\hat{p}) + \left. \frac{d \ln L}{dp} \right|_{p=\hat{p}} (p - \hat{p}) + \frac{1}{2} \left. \frac{d^2 \ln L}{d^2 p} \right|_{p=\hat{p}} (p - \hat{p})^2 \\ &= \ln L_{\max} + \left. \frac{d^2 \ln L}{d^2 p} \right|_{p=\hat{p}} \frac{(p - \hat{p})^2}{2} \\ &= \ln L_{\max} + \frac{(p - \hat{p})^2}{2\hat{\sigma}_p^2} \Rightarrow \ln L(p \pm \sigma) = \ln L_{\max} - \frac{1}{2} \end{aligned}$$



Wouter Verkerke, NIKHEF

## RooFit core design philosophy

- Mathematical objects are represented as C++ objects

Mathematical concept			RooFit class
variable	$x$	→	<code>RooRealVar</code>
function	$f(x)$	→	<code>RooAbsReal</code>
PDF	$f(x)$	→	<code>RooAbsPdf</code>
space point	$\vec{x}$	→	<code>RooArgSet</code>
integral	$\int_{x_{\min}}^{x_{\max}} f(x) dx$	→	<code>RooRealIntegral</code>
list of space points		→	<code>RooAbsData</code>

## Likelihood function

- Given a sample of  $N$  events each with variables  $(x_1, \dots, x_n)$ , the likelihood function expresses the probability density of the sample, as a function of the unknown parameters:

$$L = \prod_{i=1}^N f(x_1^i, \dots, x_n^i; \theta_1, \dots, \theta_m)$$

- Sometimes the used notation for parameters is the same as for conditional probability:

$$f(x_1, \dots, x_n | \theta_1, \dots, \theta_m)$$

- If the size  $N$  of the sample is also a random variable, the extended likelihood function is also used:

$$L = p(N; \theta_1, \dots, \theta_m) \prod_{i=1}^N f(x_1^i, \dots, x_n^i; \theta_1, \dots, \theta_m)$$

- Where  $p$  is most of the times a Poisson distribution whose average is a function of the unknown parameters

- In many cases it is convenient to use  $-\ln L$  or  $-2 \ln L$ :  $\prod_i \rightarrow \sum_i$



# Example



```
RooRealVar x("x","x",-10,10) ;
RooRealVar mean("mean","mean of gaussian",0,-10,10);
RooRealVar sigma("sigma","width of gaussian",3);

RooGaussian gauss("gauss","gaussian PDF",x,mean,sigma);

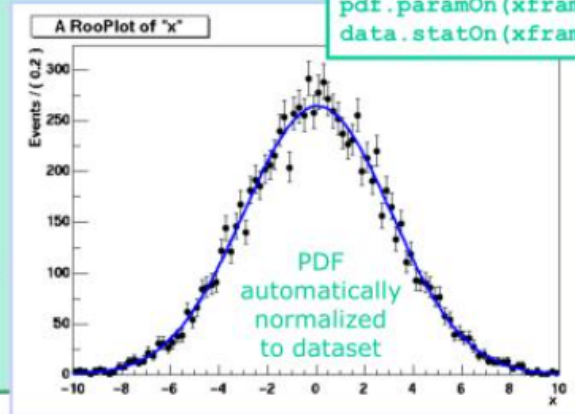
RooDataSet* data = gauss.generate(x,10000);

// ML fit is the default
gauss.fitTo(*data);

mean.Print();
// RooRealVar::mean =
// 0.0172335 +/- 0.0299542
sigma.Print();
// RooRealVar::sigma =
// 2.98094 +/- 0.0217306

RooPlot* xframe = x.frame();
data->plotOn(xframe);
gauss.plotOn(xframe);
xframe->Draw();
```

```
Further drawing options:
pdf.paramOn(xframe,data);
data.statOn(xframe);
```



## Extended ML fits



- Specify extended ML fit adding one extra parameter:

```
pdf.fitTo(*data,
          RooFit::Extended(kTRUE));
```

# Import external data sets



- Read a ROOT tree:

```
RooRealVar x("x","x",-10,10);
RooRealVar c("c","c",0,30);
RooDataSet data("data","data",inputTree,
               RooArgSet(x,c));
```

– Automatic removal of entries out of variable range

- Read an ASCII file:

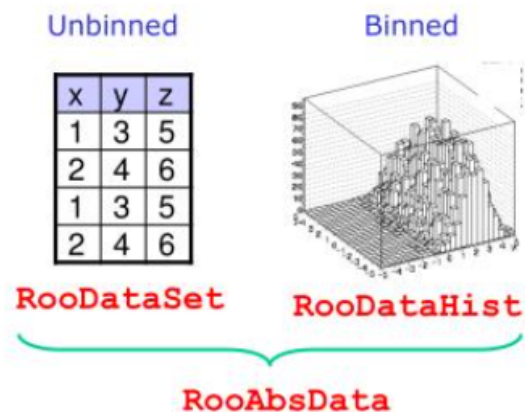
```
RooDataSet* data =
  RooDataSet::read("ascii.file",
                 RooArgList(x,c));
```

– One line per entry; variable order given by argument list

# Histogram fits



- Use a binned data set:
  - **RooDataHist** instead of **RooDataSet**
- Fit with binned model



# Minuit function MIGRAD



- Purpose: find minimum

```

*****
** 13 **MIGRAD      1000      1
*****
(some output omitted)
MIGRAD MINIMIZATION HAS CONVERGED.
MIGRAD WILL VERIFY CONVERGENCE AND ERROR MATRIX
COVARIANCE MATRIX CALCULATED SUCCESSFULLY
FCN=257.304 FROM MIGRAD      STATUS=CONVERGED      31 CALLS      32 TOTAL
                        EDM=2.36773e-06      STRATEGY= 1      ERROR MATRIX ACCURATE

EXT PARAMETER
NO.  NAME      VALUE      ERROR      STEP      FIRST
      NAME      VALUE      ERROR      SIZE      DERIVATIVE
  1  mean      8.84225e-02  3.23862e-01  3.58344e-04 -2.24755e-02
  2  sigma     3.20763e+00  2.39540e-01  2.78628e-04 -5.34724e-02
                        ERR DEF= 0.5

EXTERNAL ERROR MATRIX.      NDIM= 25      NPAR= 2      ERR DEF=0.5
1.049e-01  3.338e-04
3.338e-04  5.739e-02

PARAMETER CORRELATION COEFFICIENTS
NO.  GLOBAL      1      2
  1  0.00430      1.000  0.004
  2  0.00430      0.004  1.000
    
```

Progress information, watch for errors here

Parameter values and approximate errors reported by MINUIT

Error definition (in this case 0.5 for a likelihood fit)

Luca Lista

Statistical Methods

# Minuit function MIGRAD



- Purpose: find minimum

```

*****
** 13 **MIGRAD
*****
(some output omitted)
MIGRAD MINIMIZATION HAS CONVERGED.
MIGRAD WILL VERIFY CONVERGENCE AND ERROR MATRIX.
COVARIANCE MATRIX CALCULATED SUCCESSFULLY
FCN=257.304 FROM MIGRAD      STATUS=CONVERGED      31 CALLS      32 TOTAL
                        EDM=2.36773e-06      STRATEGY= 1      ERROR MATRIX ACCURATE

EXT PARAMETER
NO.  NAME      VALUE      ERROR      STEP      FIRST
      NAME      VALUE      ERROR      SIZE      DERIVATIVE
  1  mean      8.84225e-02  3.23862e-01  3.58344e-04 -2.24755e-02
  2  sigma     3.20763e+00  2.39540e-01  2.78628e-04 -5.34724e-02
                        ERR DEF= 0.5

EXTERNAL ERROR MATRIX.      NDIM= 25      NPAR= 2      ERR DEF=0.5
1.049e-01  3.338e-04
3.338e-04  5.739e-02

PARAMETER CORRELATION COEFFICIENTS
NO.  GLOBAL      1      2
  1  0.00430      1.000  0.004
  2  0.00430      0.004  1.000
    
```

Value of  $\chi^2$  or likelihood at minimum

(NB:  $\chi^2$  values are not divided by  $N_{d.o.f}$ )

Approximate Error matrix And covariance matrix

Luca Lista

Statistical Methods for Data Analysis

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# Minuit function MIGRAD



- Purpose: find minimum

**Status:**  
Should be 'converged' but can be 'failed'

**Estimated Distance to Minimum**  
should be small  $O(10^{-6})$

**Error Matrix Quality**  
should be 'accurate', but can be 'approximate' in case of trouble

```

*****
** 13 **MIGRAD          1000
*****
(some output omitted)
MIGRAD MINIMIZATION HAS CONVERGED
MIGRAD WILL VERIFY CONVERGENCE AND COMPUTE A MATRIX.
COVARIANCE MATRIX CALCULATED SUCCESSFULLY
FCN=257.304 FROM MIGRAD      STATUS=CONVERGED      31 CALLS      32 TOTAL
EDM=2.36773e-06      STRATEGY= 1      ERROR MATRIX ACCURATE

EXT PARAMETER
NO.  NAME      VALUE      ERROR      STEP      FIRST
    1  mean      8.84225e-02  3.23862e-01  3.58344e-04 -2.24755e-02
    2  sigma      3.20763e+00  2.39540e-01  2.78628e-04 -5.34724e-02
                                ERR DEF= 0.5

EXTERNAL ERROR MATRIX.      NDIM= 25      NPAR= 2      ERR DEF=0.5
1.049e-01  3.338e-04
3.338e-04  5.739e-02
PARAMETER CORRELATION COEFFICIENTS
NO.  GLOBAL      1      2
  1  0.00430      1.000  0.004
  2  0.00430      0.004  1.000
    
```

# Minuit function HESSE



- Purpose: calculate error matrix from  $\frac{d^2L}{dp^2}$

**Symmetric errors**  
calculated from 2<sup>nd</sup>  
derivative of  $-\ln(L)$  or  $\chi^2$

```

*****
** 18 **HESSE          1000
*****
COVARIANCE MATRIX CALCULATED SUCCESSFULLY
FCN=257.304 FROM HESSE      STATUS=OK
EDM=2.36534e-06      STRAT
INTERNAL      INTERNAL      TOTAL
CURATE

EXT PARAMETER
NO.  NAME      VALUE      ERROR      STEP      INTERNAL      INTERNAL
    1  mean      8.84225e-02  3.23861e-01  7.16689e-05  8.84237e-03
    2  sigma      3.20763e+00  2.39539e-01  5.57256e-05  3.26535e-01
                                ERR DEF= 0.5

EXTERNAL ERROR MATRIX.      NDIM= 25      NPAR= 2      ERR DEF=0.5
1.049e-01  2.780e-04
2.780e-04  5.739e-02
PARAMETER CORRELATION COEFFICIENTS
NO.  GLOBAL      1      2
  1  0.00358      1.000  0.004
  2  0.00358      0.004  1.000
    
```

# Minuit function HESSE



- Purpose: calculate error matrix from  $\frac{d^2L}{dp^2}$

```

*****
**
***
COV SUCCESSFULLY
FCN STATUS=OK 10 CALLS 42 TOTAL
EDM=2.36534e-06 STRATEGY= 1 ERROR MATRIX ACCURATE
INTERNAL INTERNAL
ERROR STEP SIZE VALUE
1 8.84237e-03
2 sigma 3.20763e+00 2.39539e-01 5.57256e-05 3.26535e-01
ERR DEF= 0.5
NDIM= 25 NPAR= 2 ERR DEF=0.5

EXTERNAL ERROR MATRIX.
1.049e-01 2.780e-04
2.780e-04 5.739e-02

PARAMETER CORRELATION COEFFICIENTS
NO. GLOBAL 1 2
1 0.00358 1.000 0.004
2 0.00358 0.004 1.000
    
```

**Error matrix (Covariance Matrix) calculated from**

$$V_{ij} = \left( \frac{d^2(-\ln L)}{dp_i dp_j} \right)^{-1}$$

**EXTERNAL ERROR MATRIX.**

PARAMETER NO.	GLOBAL	1	2
1	0.00358	1.000	0.004
2	0.00358	0.004	1.000

# Minuit function HESSE



- Purpose: calculate error matrix from  $\frac{d^2L}{dp^2}$

```

*****
** 18 **HESSE 1000
*****
COVARIANCE MATRIX CALCULATED SUCCESSFULLY
FCN=257.304 FROM HESSE STATUS=OK 10 CALLS 42 TOTAL
EDM=2.36534e-06 STRATEGY= 1 ERROR MATRIX ACCURATE
INTERNAL INTERNAL
EXT PARAMETER NAME VALUE ERROR STEP SIZE VALUE
1 mean 8.84225e-02 8.84237e-03
2 sigma 3.20763e+00 2.39539e-01 5.57256e-05 3.26535e-01
ERR DEF= 0.5
NDIM= 25 NPAR= 2 ERR DEF=0.5

EXTERNAL ERROR MATRIX.
1.049e-01 2.780e-04
2.780e-04 5.739e-02

PARAMETER CORRELATION COEFFICIENT
NO. GLOBAL 1 2
1 0.00358 1.000 0.004
2 0.00358 0.004 1.000
    
```

**Correlation matrix  $\rho_{ij}$  calculated from**

$$V_{ij} = \sigma_i \sigma_j \rho_{ij}$$

PARAMETER NO.	GLOBAL	1	2
1	0.00358	1.000	0.004
2	0.00358	0.004	1.000



# Minuit function HESSE



- Purpose: calculate error matrix from  $\frac{d^2L}{dp^2}$

```
*****
** 18 **HESSE          1000
*****
COVARIANCE MATRIX CALCULATED SUCCESSFULLY
FCN=257.304 FROM HESSE      STATUS=OK          10 CALLS          42 TOTAL
                                EDM=2.36534e-06  STRATEGY= 1      ERROR MATRIX ACCURATE

EXT PARAMETER          INTERNAL          INTERNAL
NO.  NAME              VALUE              ERROR          STEP SIZE          VALUE
  1  mean              7.16689e-05      8.84237e-03
  2  sigma             5.57256e-05      3.26535e-01

EXTERNAL ERROR
1.049e-01  2.780e-04
2.780e-04  5.739e-01

PARAMETER CORRELATION COEFFICIENTS
NO.  GLOBAL      1      2
  1  0.00358     1.000  0.004
  2  0.00358     0.004  1.000
```

Global correlation vector:  
correlation of each parameter  
with all other parameters

# Minuit function MINOS



- Error analysis through  $\Delta nll$  contour finding

```
*****
** 23 **MINOS          1000
*****
FCN=257.304 FROM MINOS  STATUS=SUCCESSFUL     52 CALLS          94 TOTAL
                                EDM=2.36534e-06  STRATEGY= 1      ERROR MATRIX ACCURATE

EXT PARAMETER          PARABOLIC          MINOS ERRORS
NO.  NAME              VALUE              ERROR          NEGATIVE          POSITIVE
  1  mean              8.84225e-02      3.23861e-01    -3.24688e-01     3.25391e-01
  2  sigma             3.20763e+00      2.39539e-01    -2.23321e-01     2.58893e-01

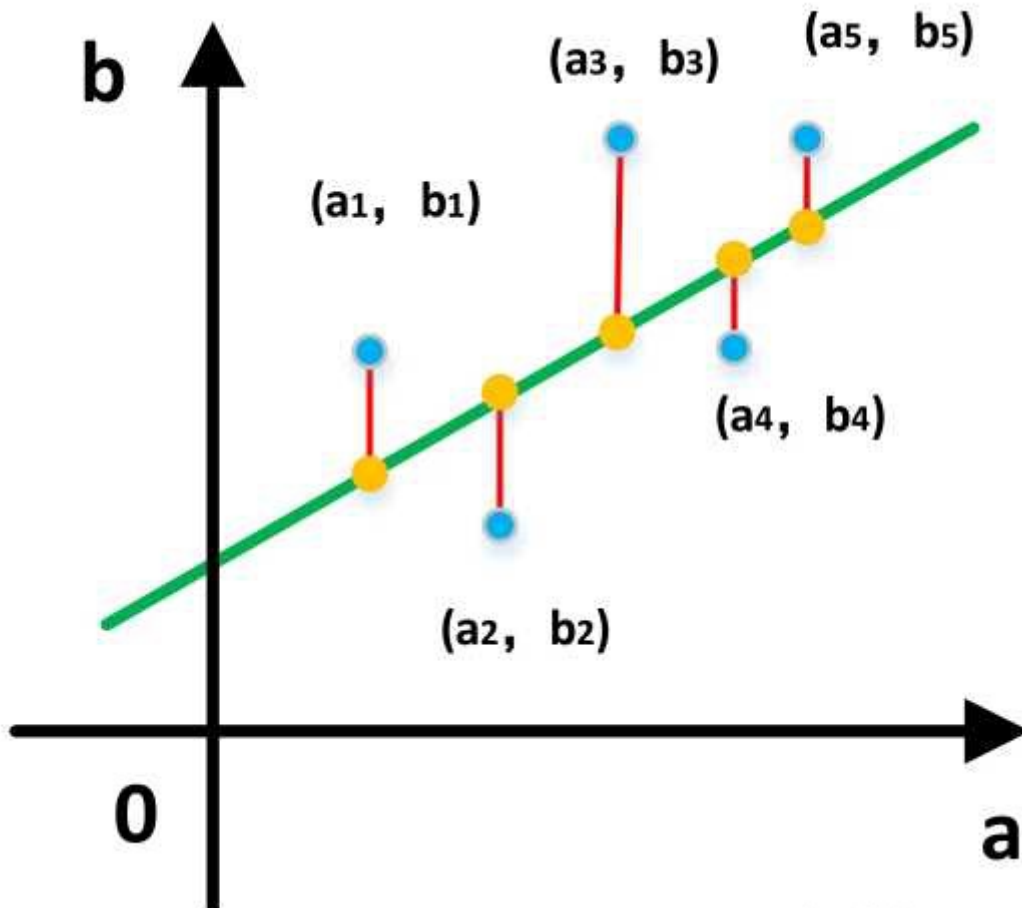
ERR DEF= 0.5
```

Symmetric error  
(repeated result  
from HESSE)

MINOS error  
Can be asymmetric  
(in this example the 'sigma' error  
is slightly asymmetric)

## 最小二乘法和最大似然法

最小二乘法



代表: hist->Fit(f1);

最大似然法

## Likelihood function

- Given a sample of  $N$  events each with variables  $(x_1, \dots, x_n)$ , the likelihood function expresses the probability density of the sample, as a function of the unknown parameters:

$$L = \prod_{i=1}^N f(x_1^i, \dots, x_n^i; \theta_1, \dots, \theta_m)$$

- Sometimes the used notation for parameters is the same as for conditional probability:

$$f(x_1, \dots, x_n | \theta_1, \dots, \theta_m)$$

- If the size  $N$  of the sample is also a random variable, the extended likelihood function is also used:

$$L = p(N; \theta_1, \dots, \theta_m) \prod_{i=1}^N f(x_1^i, \dots, x_n^i; \theta_1, \dots, \theta_m)$$

- Where  $p$  is most of the times a Poisson distribution whose average is a function of the unknown parameters

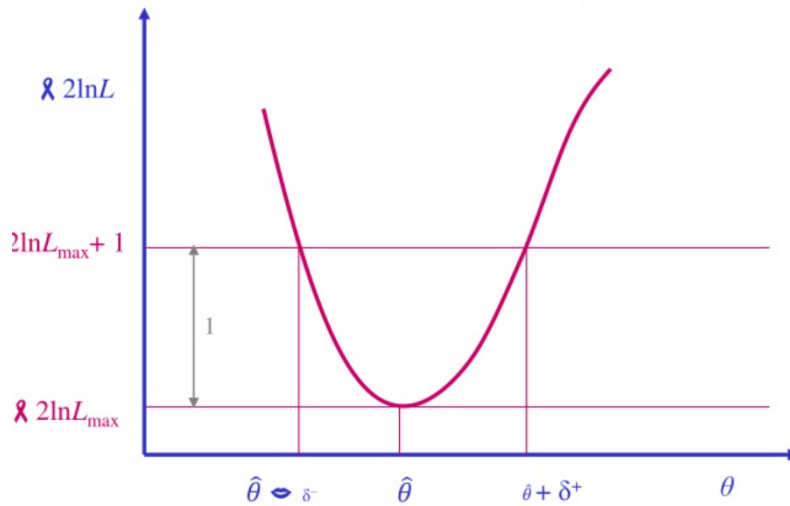
- In many cases it is convenient to use  $-\ln L$  or  $-2\ln L$ :  $\prod_i \rightarrow \sum_i$

# Asymmetric errors

按 Esc 即可退出全屏模式



- Another approximation alternative to the parabolic one may be to evaluate the excursion range of  $\chi^2 2\ln L$ .
- Error ( $n\sigma$ ) determined by the range around the maximum for which  $\chi^2 2\ln L$  increases by +1 ( $+n^2$  for  $n\sigma$  intervals)



- Errors can be asymmetric
- For a Gaussian PDF the result is identical to the 2<sup>nd</sup> order derivative matrix
- Implemented in Minuit as MINOS function

roofit是一个容易进行最大似然拟合的框架

roofit也可以进行最小二乘拟合 (rf602\_chi2fit.C)

```
66
67 // Construct a chi^2 of the data and the model.
68 // When a p.d.f. is used in a chi^2 fit, the probability density scaled
69 // by the number of events in the dataset to obtain the fit function
70 // If model is an extended p.d.f, the expected number events is used
71 // instead of the observed number of events.
72 model.chi2FitTo(*dh) ;
73 return;
```

root 的Fit是常用的最小二乘拟合手段,

但是调用minuit方法, 也可以进行最大似然拟合