Exercise/Hands-on #4

- Scientific Data Analysis Lab. course -

Introduction to the ROOT/RooFit toolkit

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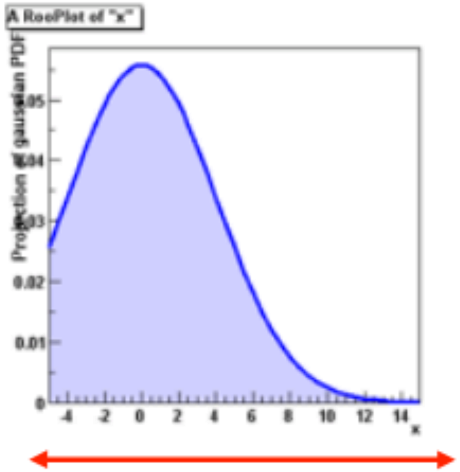
[*] Credits go to V.Werkerke, L.Lista & L.Moneta

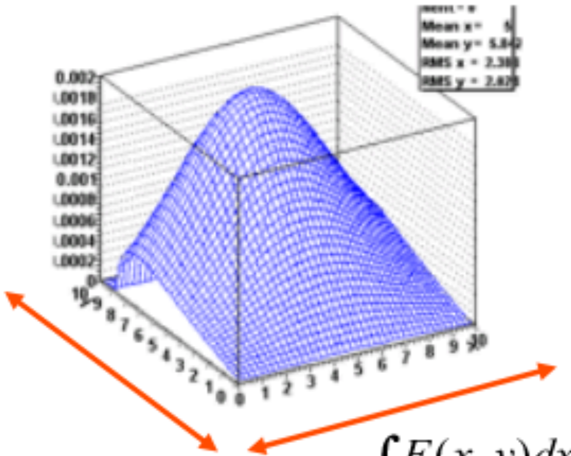
- Toolkit for data modeling
  - developed by *W. Verkerke and D. Kirkby*
- model distribution of observable $\boldsymbol{x}$ in terms of parameters $\boldsymbol{p}$
  - probability density function (pdf): $\mathcal{P}$`(x;p)`
- pdf are normalized over allowed range of observables $\boldsymbol{x}$ with respect to the parameters $\boldsymbol{p}$

- Probability Density Functions describe probabilities, thus
  - All values most be >0
  - The total probability must be 1 *for each* *p*, i.e.
  - Can have any number of dimensions

$$\int_{\vec{x}_{\min}}^{\vec{x}_{\max}} g(\vec{x}, \vec{p})\, d\vec{x} \equiv 1$$



$\int F(x)dx \equiv 1$



$\int F(x,y)dxdy \equiv 1$

- Note distinction in role between *parameters* (p) and *observables* (x)
  - Observables are measured quantities
  - Parameters are degrees of freedom in your model

- ROOT function framework can handle complicated functions
  - but require writing large amount of code
- Normalization of p.d.f. not always trivial
  - RooFit does it automatically
- In complex fit, computation performance important
  - need to optimize code for acceptable performance
  - built-in optimization available in RooFit
    - evaluation only when needed
- Simultaneous fit to different data samples
- Provide full description of model for further use

- RooFit provides functionality for building the pdf's
  - complex model building from standard components
  - composition with addition product and convolution
- All models provide the functionality for
  - maximum likelihood fitting
  - toy MC generator
  - visualization

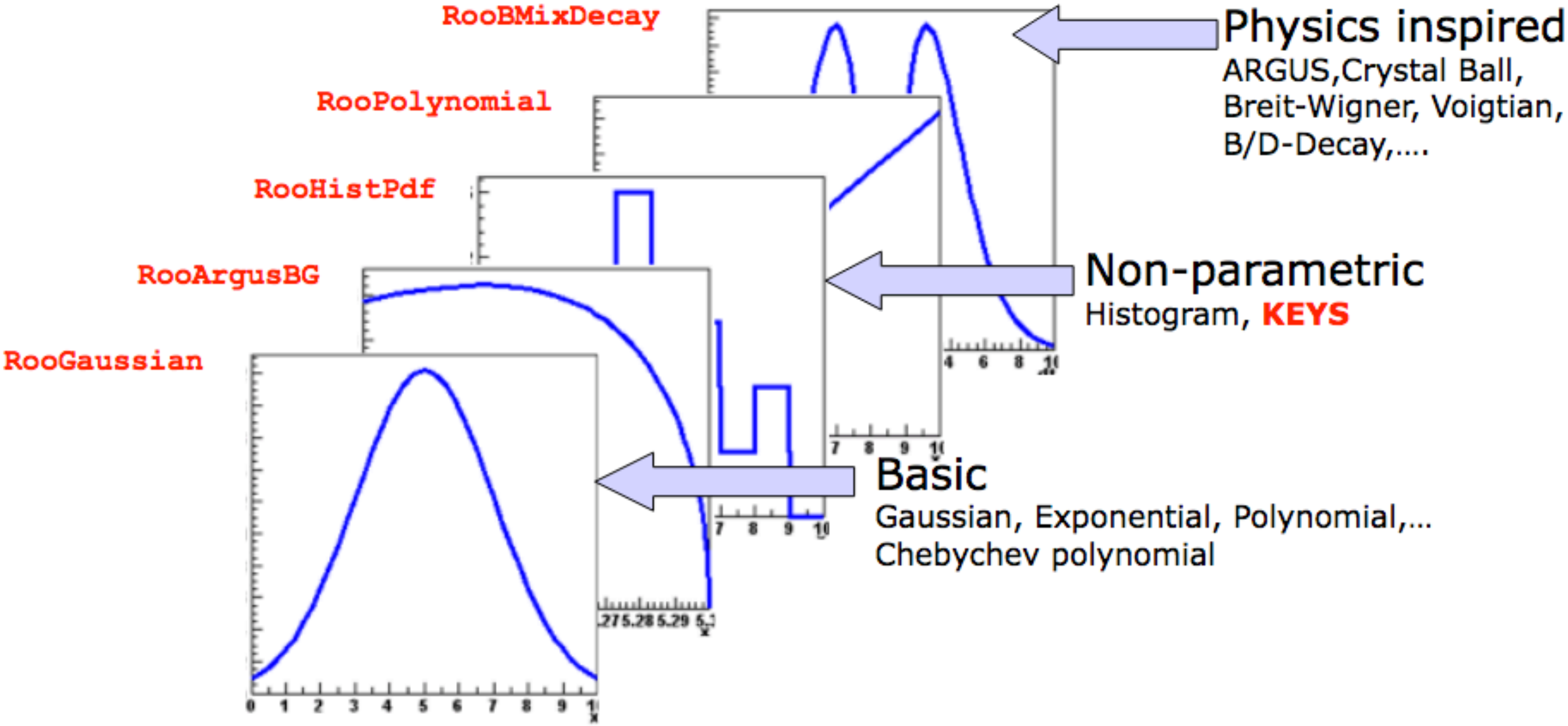
Mathematical concepts are represented as C++ objects

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

- List of most frequently used pdfs and their factory spec

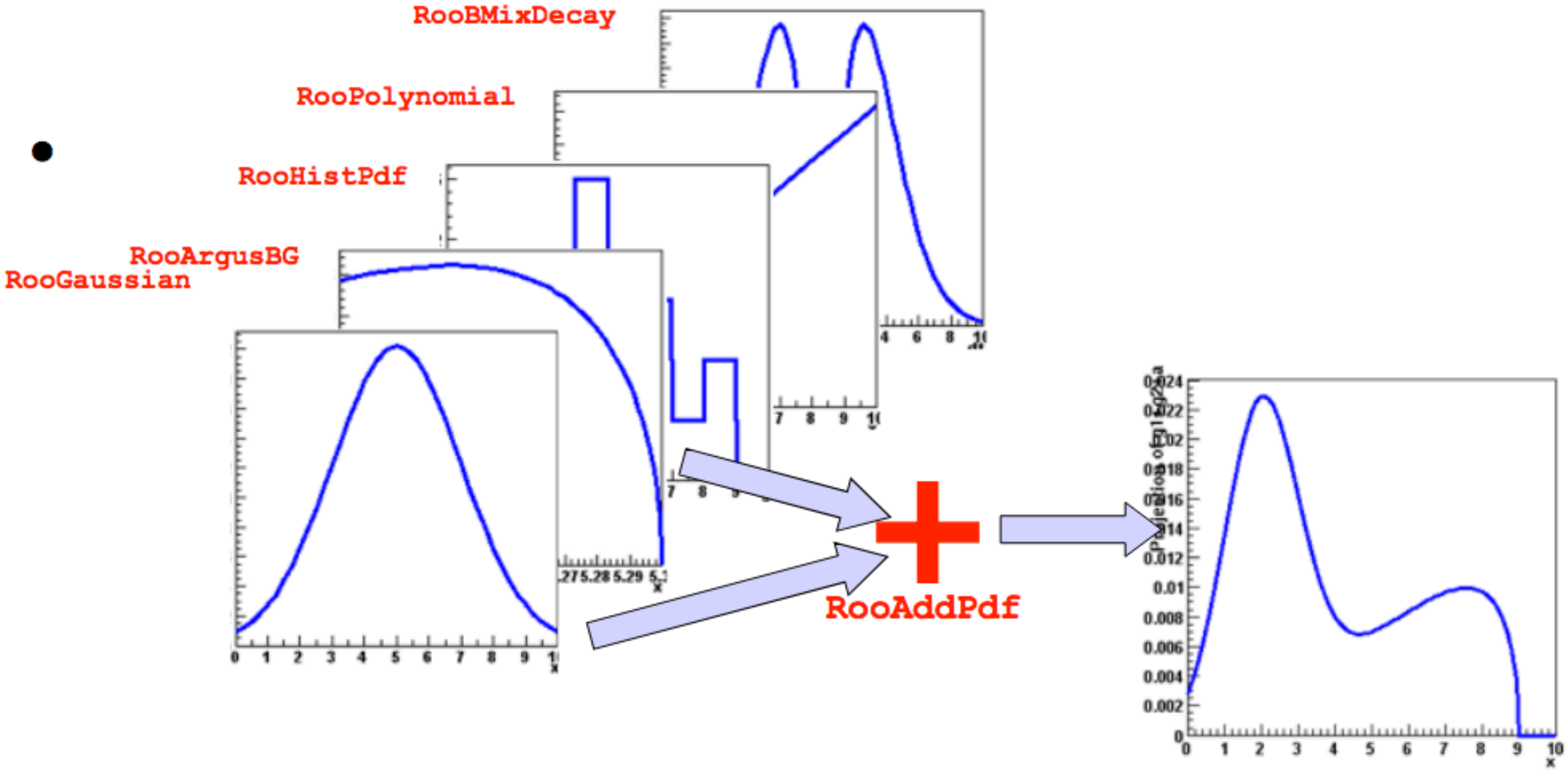
Gaussian	`Gaussian::g(x,mean,sigma)`
Breit-Wigner	`BreitWigner::bw(x,mean,gamma)`
Landau	`Landau::l(x,mean,sigma)`
Exponential	`Exponential::e(x,alpha)`
Polynomial	`Polynomial::p(x,{a0,a1,a2})`
Chebychev	`Chebychev::p(x,{a0,a1,a2})`
Kernel Estimation	`KeysPdf::k(x,dataSet)`
Poisson	`Poisson::p(x,mu)`
Voigtian (=BW⊗G)	`Voigtian::v(x,mean,gamma,sigma)`

- RooFit provides a collection of compiled standard PDF classes



Easy to extend the library: each p.d.f. is a separate C++ class

- Most realistic models are constructed as the sum of one or more p.d.f.s (e.g. signal and background)
- Facilitated through operator p.d.f RooAddPdf
-



Syntax for `RooAddPdf`

- Additions of PDF (using fractions)

```
SUM::name(frac1*PDF1,PDFN)
```

```
SUM::name(frac1*PDF1,frac2*PDF2,...,PDFN)
```

  - Note that last PDF does not have an associated fraction

$$F(x) = f \times S(x) + (1-f)B(x) \quad ; \quad N_{exp} = N$$

- PDF additions (using expected events instead of fractions)

```
SUM::name(Nsig*SigPDF,Nbkg*BkgPDF)
```

$$F(x) = \frac{N_S}{N_S + N_B} \times S(x) + \frac{N_B}{N_S + N_B} B(x) \quad ; \quad N_{exp} = N_S + N_B$$

  - the resulting model will be extended
  - the likelihood will contain a Poisson term depending on the total number of expected events (Nsig+Nbkg)

$L(x \mid p) \rightarrow L(x|p)Poisson(N_{obs},N_{exp})$

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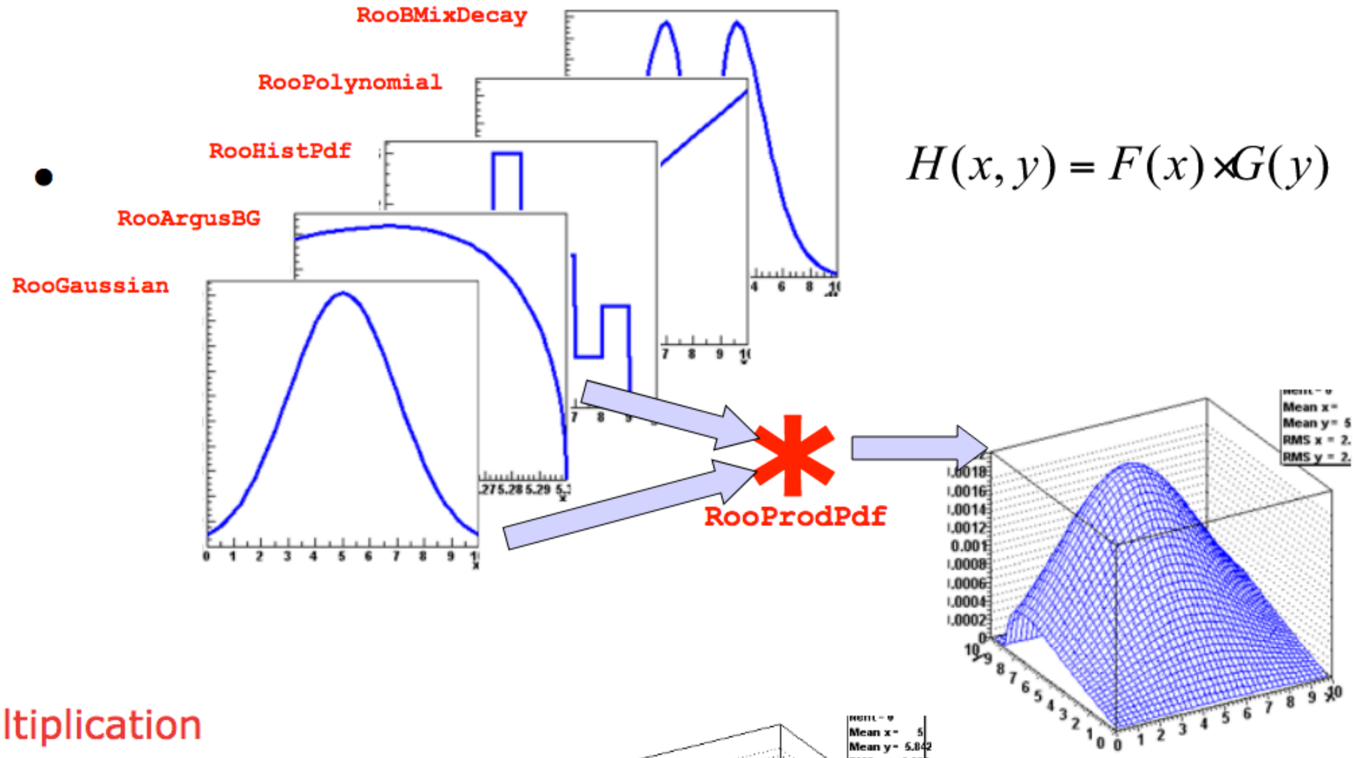


$$H(x,y) = F(x) \times G(y)$$

Uncorrelated products – Mathematics and constructors

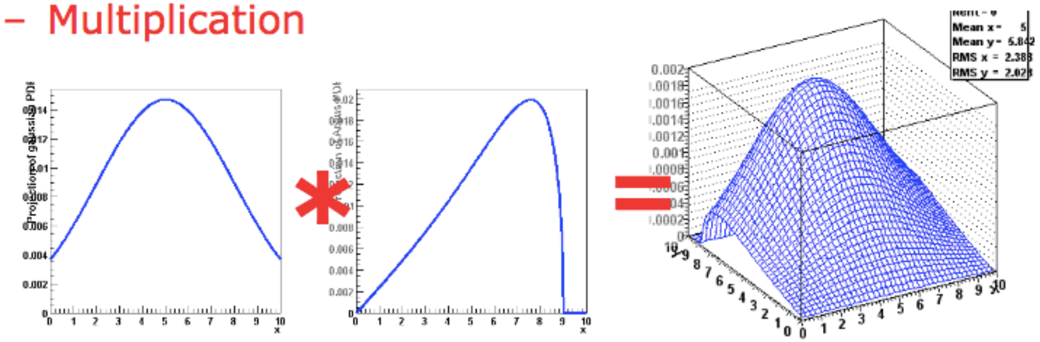
- Mathematical construction of products of uncorrelated p.d.f.s is straightforward

2D $$H(x,y) = F(x) \cdot G(y)$$

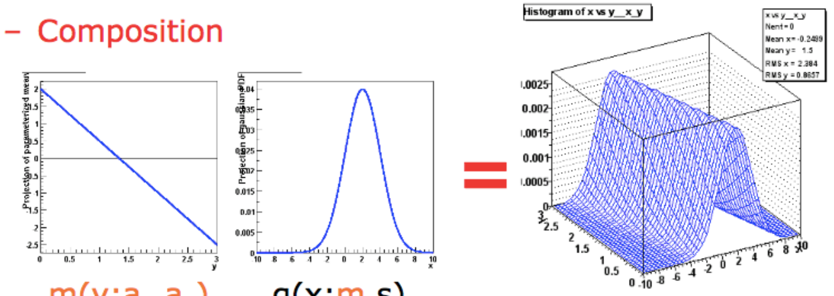
nD $$H(x^{\{i\}}) = \prod_i F^{\{i\}}(x^{\{i\}})$$

– No explicit normalization required → If input p.d.f.s are unit normalized, product is also unit normalized
(this is true *only* because of the absence of correlations)

– Multiplication



– Composition



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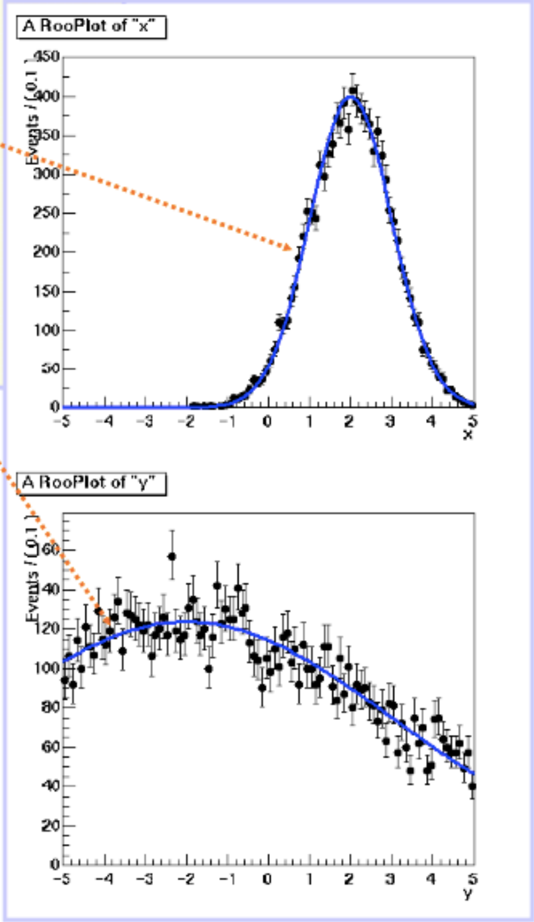
Plotting multi-dimensional PDFs

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

c->cd(2) ;
RooPlot* yframe = y.frame() ;
data->plotOn(yframe) ;
prod->plotOn(yframe) ;
yframe->Draw() ;
```

$$f(x) = \int pdf(x,y)dy$$

$$f(y) = \int pdf(x,y)dx$$



-Plotting a dataset D(x,y) versus x represents a *projection over y*

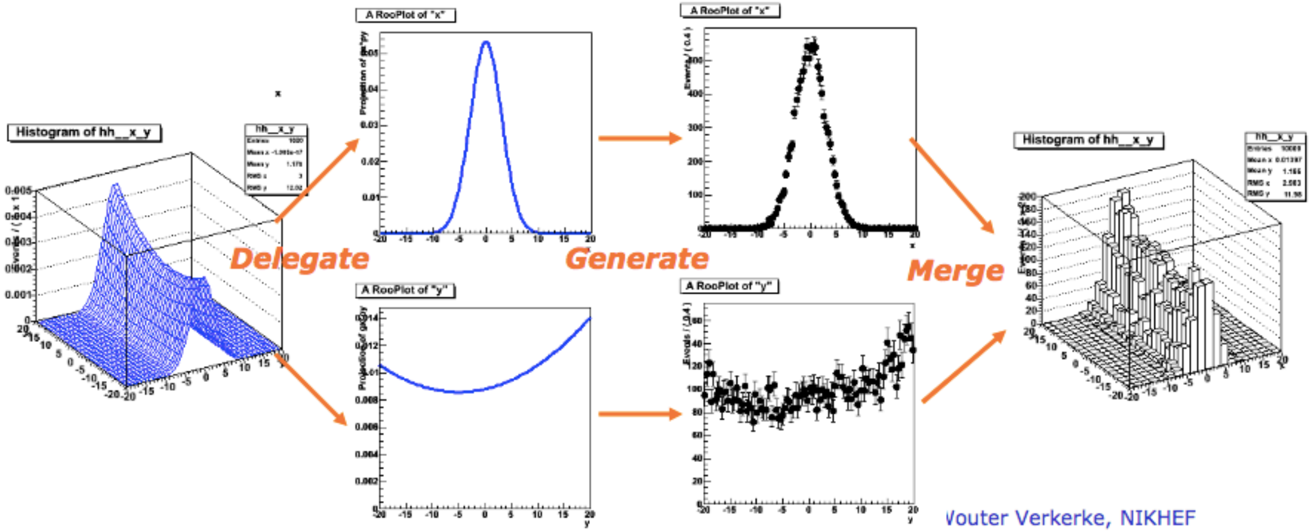
-To overlay PDF(x,y), you must plot *Int(dy)PDF(x,y)*

-RooFit automatically takes care of this!

- RooPlot remembers dimensions of plotted datasets

How it work – event generation on uncorrelated products

- If p.d.f.s are uncorrelated, each observable can be generated separately
  - Reduced dimensionality of problem (important for e.g. accept/reject sampling)
  - Actual event generation delegated to component p.d.f (can e.g. use internal generator if available)
  - **`RooProdPdf`** just aggregates output in single dataset



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Function minimization: minimization algorithm - I

- Common interface class (`ROOT::Math::Minimizer`)
- Existing implementations available as plug-ins:
  - **Minuit** (based on class `TMinuit`, direct translation from Fortran code)
    - with Migrad, Simplex, Minimize algorithms
  - **Minuit2** (new C++ implementation with OO design)
    - with Migrad, Simplex, Minimize and Fumili2
  - **Fumili** (only for least-square or log-likelihood minimizations)
  - **GSLMultiMin**: conjugate gradient minimization algorithm from GSL (Fletcher-Reeves, BFGS)
  - **GSLMultiFit**: Levenberg-Marquardt (for minimizing least square functions) from GSL
  - **Linear** for least square functions (direct solution, non-iterative method)
  - **GSLSimAn**: Simulated Annealing from GSL
  - **Genetic**: based on a genetic algorithm implemented in TMVA
- All these are available for ROOT fitting and in RooFit/RooStats
- Possible to combine them (e.g. use Minuit and Genetic)
- Easy to extend and add new implementations
  - e.g. minimizer based on NagC exists in the development branch (see here)

L.Moneta's slide

Function minimization: `Minuit` functionality - II

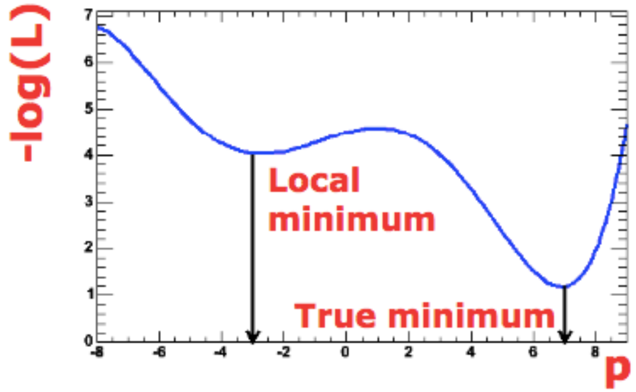
- MIGRAD
  - Find function minimum. Calculates function gradient, follow to (local) minimum, recalculate gradient, iterate until minimum found
    - To see what MIGRAD does, it is very instructive to do RooMinuit::setVerbose(1). It will print a line for each step through parameter space
  - Number of function calls required depends greatly on number of floating parameters, distance from function minimum and shape of function
- HESSE
  - Calculation of error matrix from 2^{nd} derivatives at minimum
  - Gives symmetric error. Valid in assumption that likelihood is (locally parabolic)

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

  - Requires roughly N^2 likelihood evaluations (with N = number of floating parameters)

- MINOS
  - Calculate errors by explicit finding points (or contour for >1D) where Δ-log(L)=0.5
  - Reported errors can be asymmetric
  - Can be very expensive in with large number of floating parameters
- CONTOUR
  - Find contours of equal Δ-log(L) in two parameters and draw corresponding shape
  - Mostly an interactive analysis tool

- For all but the most trivial scenarios it is not possible to automatically find reasonable starting values of parameters
  - So you need to supply 'reasonable' starting values for your parameters



Reason: There may exist multiple (local) minima in the likelihood or χ^2

  - You may also need to supply 'reasonable' initial step size in parameters. (A step size 10x the range of the above plot is clearly unhelpful)
  - Using RooMinuit, the initial step size is the value of `RooRealVar::getError()`, so you can control this by supplying initial error values

GETTING CONFIDENCE WITH … FUNCTION PLOTTING & HISTOGRAM HANDLING

Function minimization: `Migrad` - IV

- 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                                   STEP         FIRST
 NO.   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)

- Purpose: find minimum

```
**********
**   13 **MIGR
**********
(some output o
MIGRAD MINIMIZ
MIGRAD WILL VERI… 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                                      STEP         FIRST
 NO.   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: χ^2 values are not divided by $N_{d.o.f}$)

Approximate Error matrix And covariance matrix

- Purpose: find minimu

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

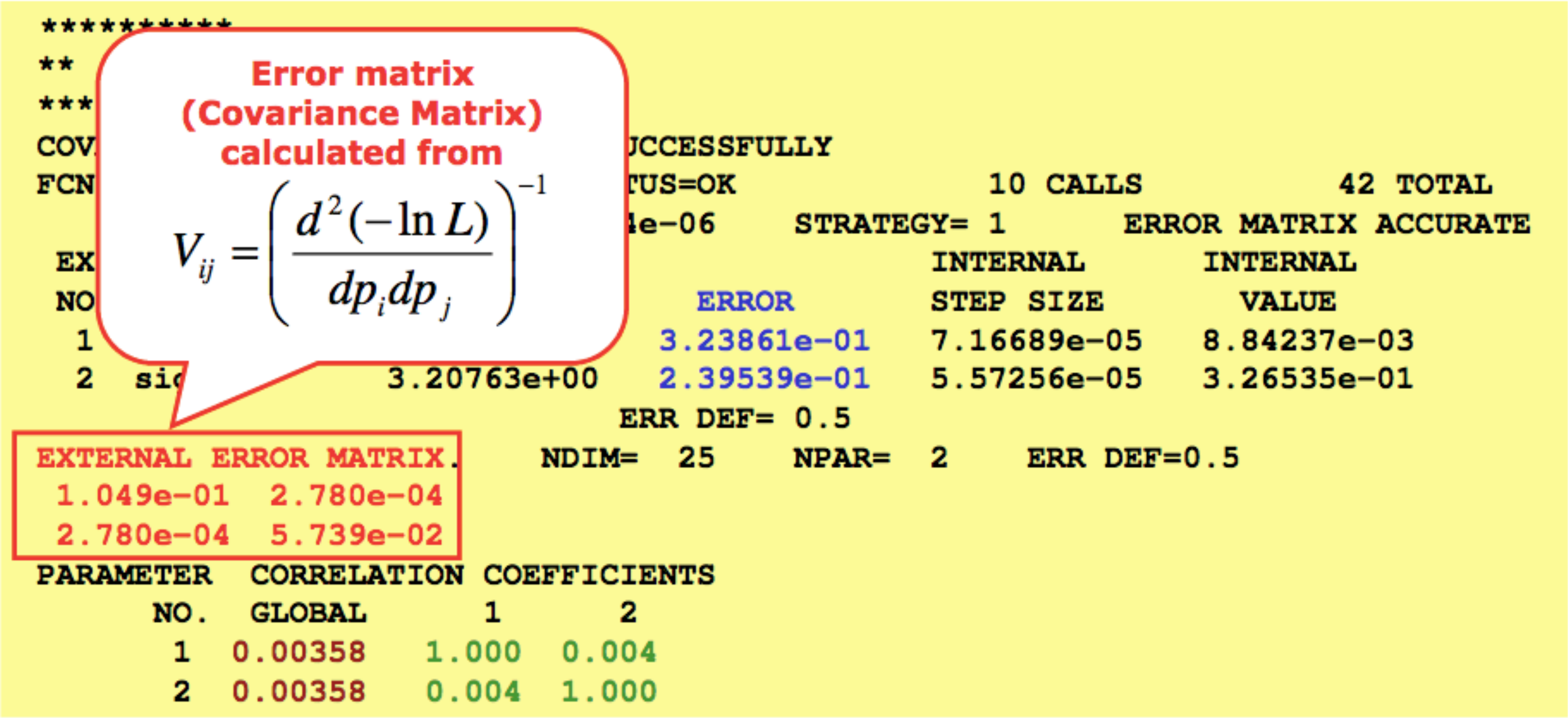
```
**********
**   13 **MIGRAD        1000
**********
(some output omitted)
MIGRAD MINIMIZATION HAS CONVERGE
MIGRAD WILL VERIFY CONVERGENCE AND E     MATRIX.
COVARIANCE MATRIX CALCULATED SUCCESSFULLY
FCN=257.304 FROM MIGRAD    STATUS=CONVERGED      31 CALLS         32 TOTAL
                    EDM=2.36773e-06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

 EXT PARAMETER                                   STEP          FIRST
 NO.   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
```

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

```
**********
**   18 **HESSE          1000
**********
COVARIANCE MATRIX CALCULATED SUCCESSFULLY
FCN=257.304 FROM HESSE      STATUS=OK                              OTAL
                    EDM=2.36534e-06     STRAT                          CURATE
 EXT PARAMETER                                        I  ERNAL        INTERNAL
 NO.   NAME        VALUE            ERROR           STEP SIZE        VALUE
  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
```

Symmetric errors calculated from 2nd derivative of –ln(L) or χ^2



```
**********
**
***
COV                                      UCCESSFULLY
FCN                                      TUS=OK                10 CALLS              42 TOTAL
                                         4e-06     STRATEGY= 1         ERROR MATRIX ACCURATE
 EX                                                          INTERNAL          INTERNAL
 NO                                        ERROR             STEP SIZE           VALUE
  1                                      3.23861e-01       7.16689e-05       8.84237e-03
  2   si                   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
```

Error matrix (Covariance Matrix) calculated from

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

```
**********
**   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          8.84225e-02                                 8.84237e-03
  2  sigma         3.20763e+00                                 3.26535e-01

EXTERNAL ERROR MATRIX.    NDIM                               F=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
```

Correlation matrix ρ_{ij} calculated from

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

```
**********
**   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                                2     ERR DEF=0.5
 1.049e-01  2.
 2.780e-04  5.739e-
PARAMETER  CORRELA    N 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

```
**********
**   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

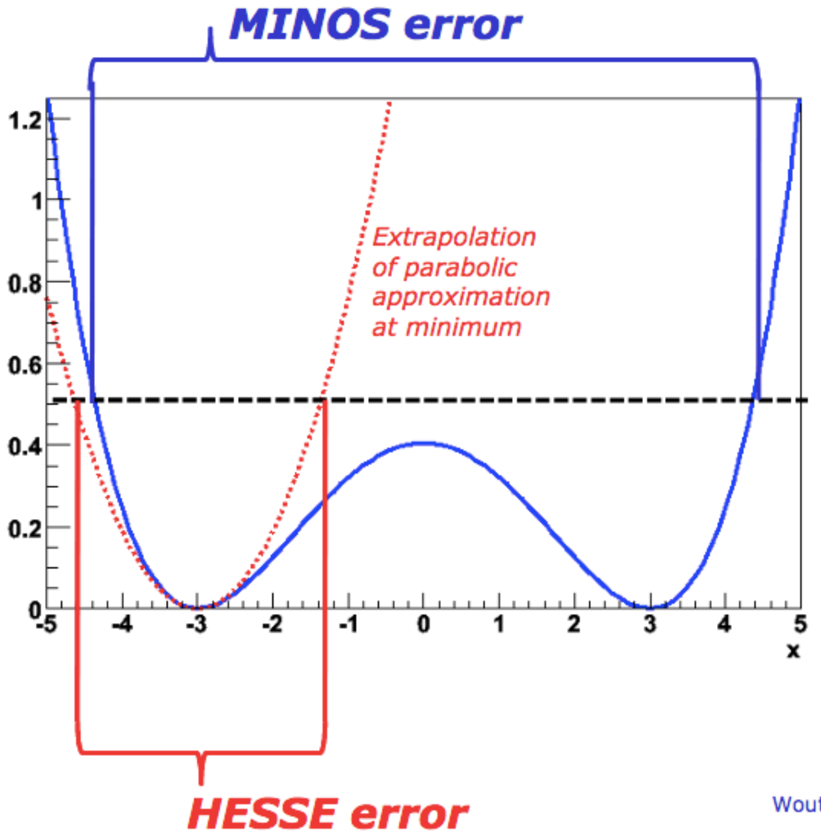
(repeated result from HESSE)

MINOS error Can be asymmetric

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

Illustration of difference between HESSE and MINOS errors

- 'Pathological' example likelihood with multiple minima and non-parabolic behavior



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Practical estimation – Fit converge problems

- Sometimes fits don't converge because, e.g.
  - MIGRAD unable to find minimum
  - HESSE finds negative second derivatives (which would imply negative errors)
- Reason is usually numerical precision and stability problems, but
  - The underlying cause of fit stability problems is usually by **highly correlated parameters** in fit
- HESSE correlation matrix in primary investigative tool

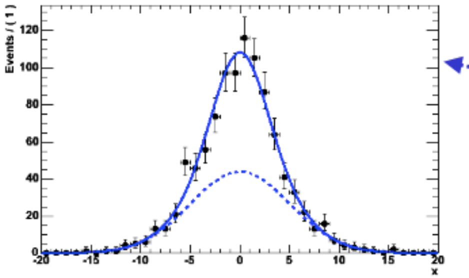
PARAMETER NO.	CORRELATION GLOBAL	COEFFICIENTS 1	2
1	0.99835	1.000	0.998
2	0.99835	0.998	1.000

Signs of trouble…

  - In limit of 100% correlation, the usual point solution becomes a line solution (or surface solution) in parameter space. Minimization problem is no longer well defined

- Strategy I – More orthogonal choice of parameters
  - Example: fitting sum of 2 Gaussians of similar width

$$F(x; f, m, s_1, s_2) = fG_1(x; s_1, m) + (1-f)G_2(x; s_2, m)$$



HESSE correlation matrix

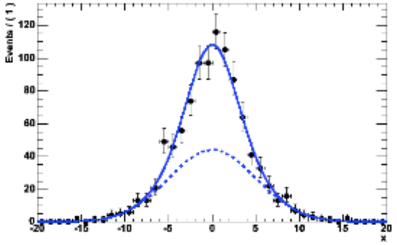
Widths s_1,s_2 strongly correlated fraction f

PARAMETER NO.	CORRELATION COEFFICIENTS GLOBAL	[f]	[m]	[s1]	[s2]
[f]	0.96973	1.000	-0.135	0.918	0.915
[m]	0.14407	-0.135	1.000	-0.144	-0.114
[s1]	0.92762	0.918	-0.144	1.000	0.786
[s2]	0.92486	0.915	-0.114	0.786	1.000

- Different parameterization:

$$fG_1(x; s_1, m_1) + (1-f)G_2(x; s_1 \cdot s_2, m_2)$$

PARAMETER NO.	CORRELATION COEFFICIENTS GLOBAL	[f]	[m]	[s1]	[s2]
[f]	0.96951	1.000	-0.134	0.917	-0.681
[m]	0.14312	-0.134	1.000	-0.143	0.127
[s1]	0.98879	0.917	-0.143	1.000	-0.895
[s2]	0.96156	-0.681	0.127	-0.895	1.000



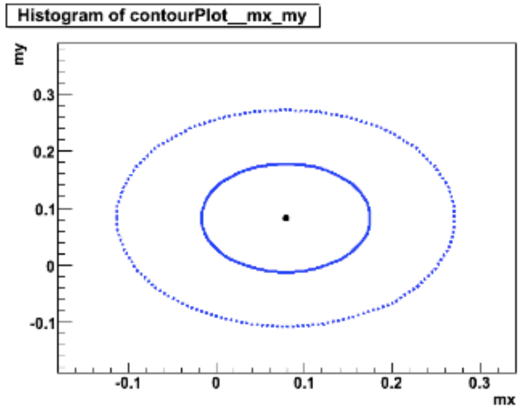
- Correlation of width s2 and fraction f reduced from 0.92 to 0.68
- Choice of parameterization matters!

- Strategy II – Fix all but one of the correlated parameters
  - If floating parameters are highly correlated, some of them may be redundant and not contribute to additional degrees of freedom in your model

- Sometimes is it desirable to bound the allowed range of parameters in a fit
  - Example: a fraction parameter is only defined in the range [0,1]

Minuit CONTOUR tool also useful to examine 'bad' correlations

- Example of 1,2 sigma contour of two uncorrelated variables
  - Elliptical shape. In this example parameters are uncorrelation



- Example of 1,2 sigma contour of two variables with problematic correlation
  - Pdf = f·G1(x,0,3)+(1-f)·G2(x,0,s) with s=4 in data