Statistical Methods for Data Analysis

Parameter estimates with RooFit

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Fits with RooFit

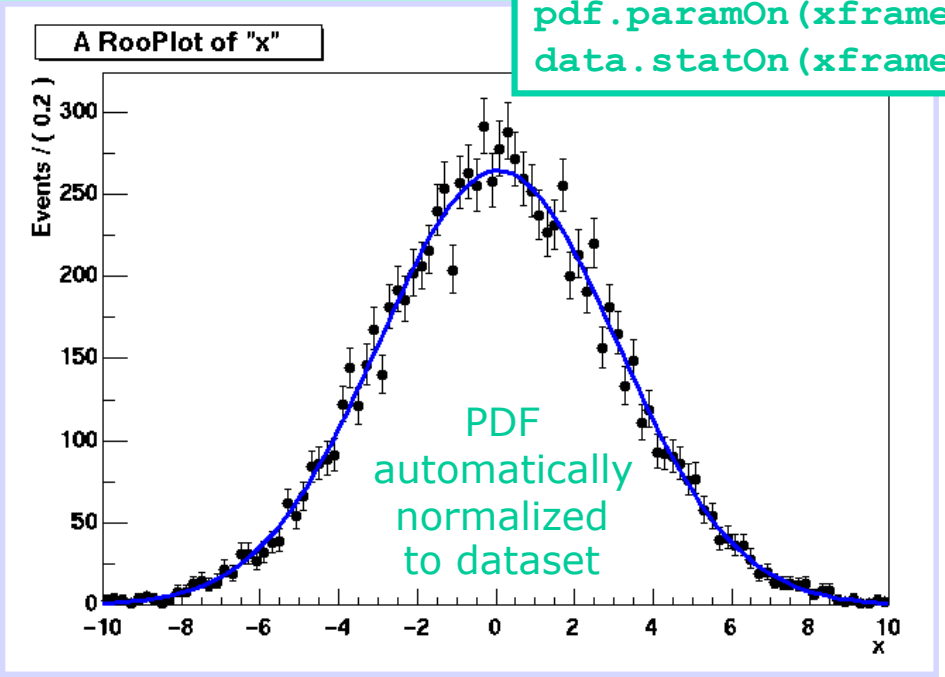
- Get data sample (or generate it, for Toy Monte Carlo)
- Specify data model (PDF's)
- Fit specified model to data set with preferred technique (ML, Extended ML, …)

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));
```

  - Une line per entry; variable order given by argument list

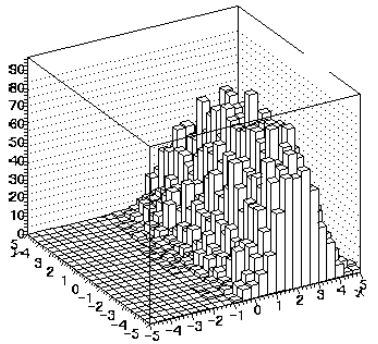
Histogram fits

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

Unbinned

x	y	z
1	3	5
2	4	6
1	3	5
2	4	6

Binned



`RooDataSet` **`RooDataHist`**

`RooAbsData`

Import external histograms

- From ROOT TH1/TH2/TH3:

```
RooDataHist bdata1("bdata","bdata",RooArgList(x),histo1d);
RooDataHist bdata2("bdata","bdata",RooArgList
   (x,y),histo2d);
RooDataHist bdata3("bdata","bdata",RooArgList
   (x,y,z),histo3d);
```

- Binning an unbinned data set:

```
RooDataHist* binnedData = data->binnedClone();
```

- Specifying binning:

```
x.setBins(50);
RooDataHist binnedData("binnedData", "data", RooArgList
   (x), *data);
```

Discrete variables

- Define categories
- E.g.: b-tag:

```
RooCategory b0flav("b0flav", "B0 flavour");
b0flav.defineType("B0",    -1);
b0flav.defineType("B0bar", 1);
```

Indices automatically assigned if omitted

- Several tools defined to combine categories (`RooSuperCategory`) and analyze data according to categories
  - See Root user manual for more details…
- Switch between PDF's based on a category can be implemented for simultaneous fits of multiple categories:

```
RooSimultaneous simPdf("simPdf","simPdf", categoryType);
simPdf.addPdf(pdfA,"A");
simPdf.addPdf(pdfB,"B");
```

Explicit Minuit minimization

- Build negative log-Likelihood finction (NLL)

```
// Construct function object representing -log(L)
RooNLLVar nll("nll", "nll", pdf, data);

// Minimize nll w.r.t its parameters
RooMinuit m(nll);
m.migrad();
m.hesse();
```

- Extra arguments: specify extended likelihood:

```
RooNLLVar nll("nll","nll",pdf,data,Extended());
```

- Chi-squared functions (only accepts `RooDataHist`):

```
RooNLLVar chi2("chi2","chi2",pdf,data);
```

Drive converging process

```
// Start Minuit session on above nll
RooMinuit m(nll);

// MIGRAD likelihood minimization
m.migrad();

// Run HESSE error analysis
m.hesse();

// Set sx to 3, keep fixed in fit
sx.setVal(3);
sx.setConstant(kTRUE);

// MIGRAD likelihood minimization
m.migrad();

// Run MINOS error analysis
m.minos();

// Draw 1,2,3 'sigma' contours in sx,sy
m.contour(sx, sy);
```

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                                   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)

Minuit function MIGRAD

- Purpose: find minimum

```
**********
**    13 **MIGR
**********
(some output c
MIGRAD MINIMIZ
MIGRAD WILL VERIF     ERGENCE 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 χ^2 or likelihood at minimum

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

Approximate Error matrix And covariance matrix

Minuit function MIGRAD

- Purpose: find minimu

```
**********
**    13 **MIGRAD        1000
**********
(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
```

***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

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                                  OTAL
                    EDM=2.36534e-06    STRATI                      CCURATE
 EXT PARAMETER                                          NTERNAL      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

Minuit function HESSE

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

Error matrix (Covariance Matrix) calculated from

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

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

Minuit function HESSE

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

```
**********
**   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                           STEP SIZE       VALUE
  1   mean         8.84225e-02                                  8.84237e-03
  2   sigma        3.20763e+00                                  3.26535e-01

EXTERNAL ERROR MATRIX.    NDIM=
 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 ρ_{ij} calculated from

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

Minuit function HESSE

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

```
**********
**    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                                  2    ERR DEF=0.5
 1.049e-01  2.780e
 2.780e-04  5.739e-
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 Δnll 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)

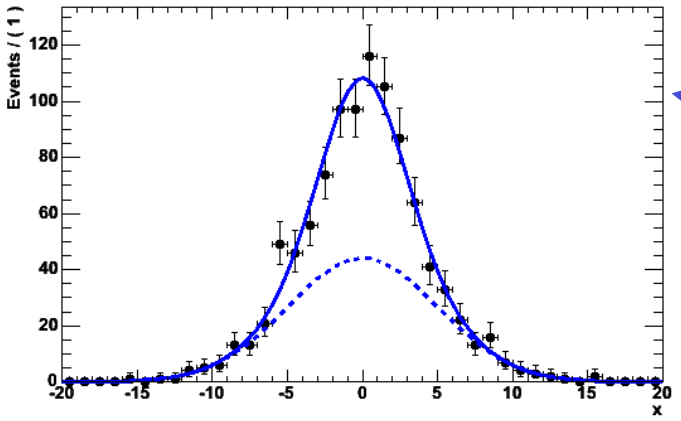
MINOS error
Can be asymmetric

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

Mitigating fit stability problems

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

$$F(x; f, m, s_1, s_2) = f\, G_1(x; s_1, m) + (1 - f) G_2(x; s_2, m)$$



HESSE correlation matrix

PARAMETER	CORRELATION COEFFICIENTS				
NO.	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

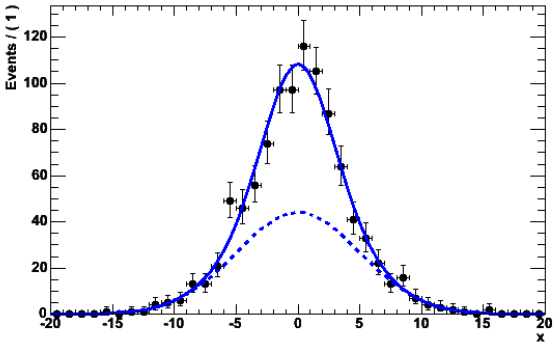
Widths s_1,s_2 strongly correlated fraction f

Mitigating fit stability problems

– Different parameterization:

$$f\,G_1(x;s_1,m_1)+(1-f)G_2(x;s_1\cdot s_2,m_2)$$

```
PARAMETER  CORRELATION COEFFICIENTS
      NO.   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

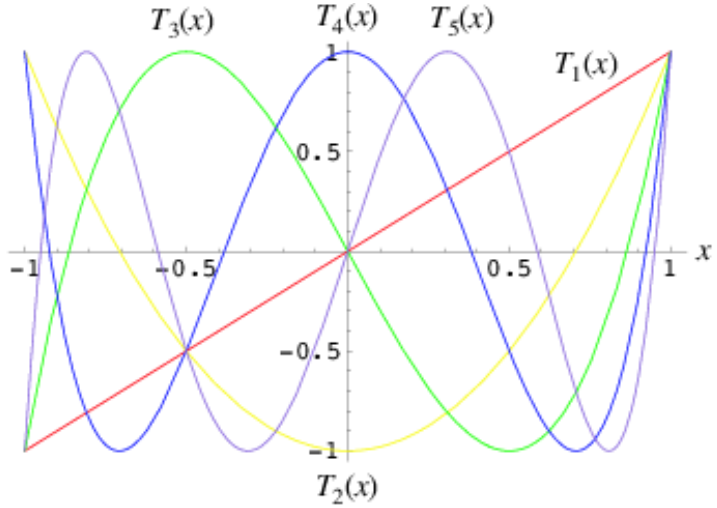
– Choice of parameterization matters!

- 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

Fit stability with polynomials

- **Warning:** Regular parameterization of polynomials $a_0+a_1x+a_2x^2+a_3x^3$ nearly always results in strong correlations between the coefficients a_i.
  - *Fit stability problems, inability to find right solution common at higher orders*
- **Solution:** Use existing parameterizations of polynomials that have (mostly) uncorrelated variables
  - ***Example: Chebychev polynomials***

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



Browsing fit results

- As fits grow in complexity (e.g. 45 floating parameters), number of output variables increases
  - Need better way to navigate output that MINUIT screen dump
- **`RooFitResult`** holds complete snapshot of fit results
  - Constant parameters
  - Initial and final values of floating parameters
  - Global correlations & full correlation matrix
  - Returned from **`RooAbsPdf::fitTo()`** when "**`r`**" option is supplied
- Compact & verbose printing mode

Compact Mode

Constant parameters omitted in compact mode

Alphabetical parameter listing

```
fitres->Print() ;

  RooFitResult: min. NLL value: 1.6e+04, est. distance to min: 1.2e-05

    Floating Parameter    FinalValue +/-  Error
  --------------------  --------------------------
                argpar   -4.6855e-01 +/-  7.11e-02
                g2frac    3.0652e-01 +/-  5.10e-03
                 mean1    7.0022e+00 +/-  7.11e-03
                 mean2    1.9971e+00 +/-  6.27e-03
                 sigma    2.9803e-01 +/-  4.00e-03
```

Browsing fit results

Verbose printing mode

```
fitres->Print("v") ;

  RooFitResult: min. NLL value: 1.6e+04, est. distance to min: 1.2e-05

  Constant Parameter    Value
  --------------------  ------------
                cutoff    9.0000e+00
                g1frac    3.0000e-01

    Floating Parameter  InitialValue    FinalValue +/-  Error      GblCorr.
  --------------------  ------------  --------------------------  --------
                argpar   -5.0000e-01   -4.6855e-01 +/-  7.11e-02  0.191895
                g2frac    3.0000e-01    3.0652e-01 +/-  5.10e-03  0.293455
                 mean1    7.0000e+00    7.0022e+00 +/-  7.11e-03  0.113253
                 mean2    2.0000e+00    1.9971e+00 +/-  6.27e-03  0.100026
                 sigma    3.0000e-01    2.9803e-01 +/-  4.00e-03  0.276640
```

Constant parameters listed separately

Initial,final value and global corr. listed side-by-side

Correlation matrix accessed separately

Browsing fit results

- Easy navigation of correlation matrix
  - Select single element or complete row by parameter name

```
fitres->correlation("argpar","sigma")
(const Double_t)(-9.25606412005910845e-02)

fitres->correlation("mean1")->Print("v")
RooArgList::C[mean1,*]: (Owning contents)
  1) RooRealVar::C[mean1,argpar] :  0.11064 C
  2) RooRealVar::C[mean1,g2frac] : -0.0262487 C
  3) RooRealVar::C[mean1,mean1]  :  1.0000 C
  4) RooRealVar::C[mean1,mean2]  : -0.00632847 C
  5) RooRealVar::C[mean1,sigma]  : -0.0339814 C
```

- **`RooFitResult`** persistable with ROOT I/O
  - Save your batch fit results in a ROOT file and navigate your results just as easy afterwards

References

- RooFit online tutorial
  - http://roofit.sourceforge.net/docs/tutorial/index.html
- Credits:
  - RooFit slides and examples extracted, adapted and/or inspired by original presentations by Wouter Verkerke