

#### RooFit

A tool kit for data modeling in ROOT (W. Verkerke, D. Kirkby)

#### RooStats

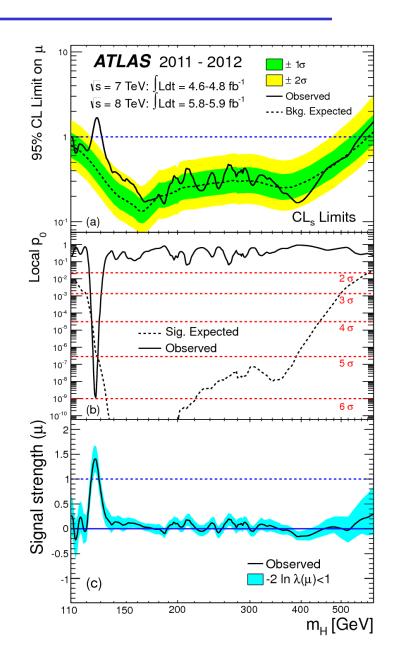
A tool kit for statistical analysis (K. Cranmer, L. Moneta, S. Kreiss, G. Kukartsev, G. Schott,

G. Petrucciani, W. Verkerke)

Wouter Verkerke (NIKHEF)

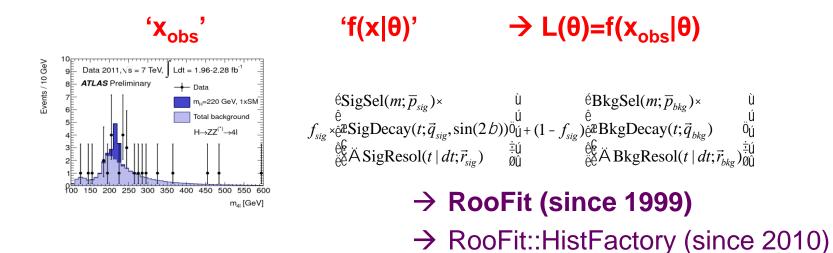
#### Introduction

- Statistical data analysis is at the heart of all (particle) physics experiments.
- Techniques deployed in HEP get more and more complicated
   → Hunting for 'difficult signals' (Higgs)
  - → Desire to control systematic uncertainties through simultaneous fits to control measurements
- Nowadays discoveries entail simultaneous modeling of hundreds of distributions with models with over a 1000 parameters → Well beyond ROOTs 'TF1' function classes



#### A structured approach to computational statistical analysis

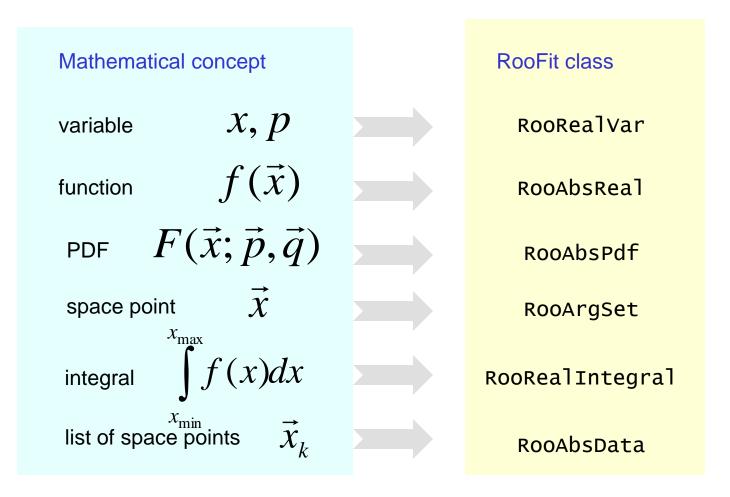
- A structured approach is needed to be able to describe and use data models needed for modern HEP analyses
- 1 Data modeling: construct a model f(x|θ)



- 2 Statistical inference on θ, given x<sub>0</sub> and f(x|θ)
  - Parameter estimation ' $\theta$ ' & variance estimation ( $V(\theta)$ )  $\rightarrow$  MINUIT
  - Confidence intervals:  $[\theta_-, \theta_+]$ ,  $\theta_- \times 10^{-7}$  And  $\theta_- \times 10^{-7}$  RooStats (since 2007) hypothesis testing etc:  $\theta_- \times 10^{-7}$  RooStats (since 2007)

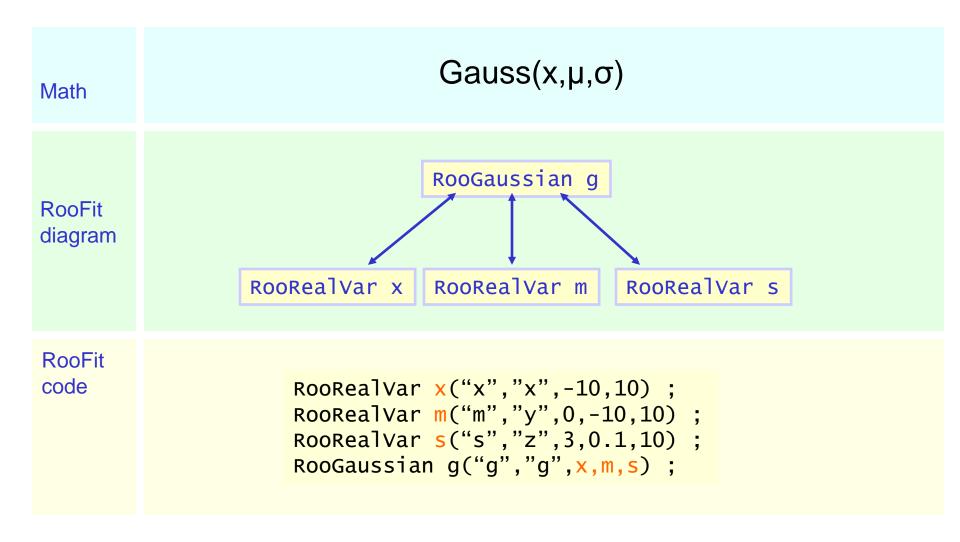
#### RooFit – a toolkit to formulate probability models in C++

 Key concept: represent individual elements of a mathematical model by separate C++ objects



# RooFit core design philosophy

 Functions objects are always 'trees' of objects, with pointers (managed through proxies) expressing relations



#### RooFit: complete model functionality, e.g. sampling (un)binned data

Example: generate 10000 events from Gaussian p.d.f and show distribution

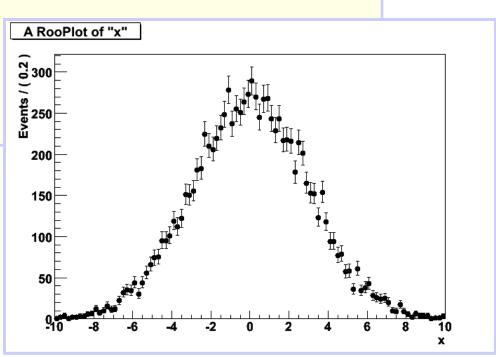
```
// Generate an unbinned toy MC set
RooDataSet* data = gauss.generate(x,10000) ;

// Generate an binned toy MC set
RooDataHist* data = gauss.generateBinned(x,10000) ;

// Plot PDF
RooPlot* xframe = x.frame() ;
data->plotOn(xframe) ;
ARooPlot of "x"
```

Can generate both binned and unbinned datasets

xframe->Draw() ;



#### RooFit model functionality – max.likelihood parameter estimation

% 300

A RooPlot of "x"

**PDF** 

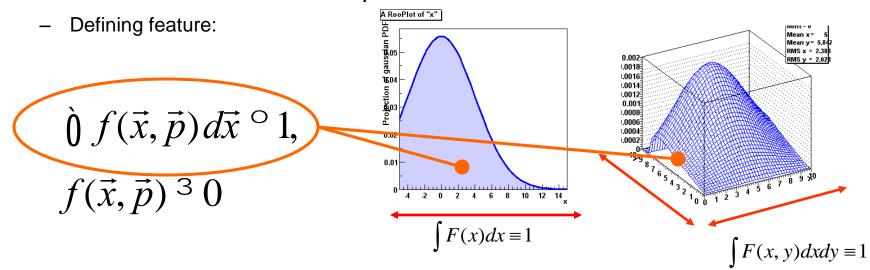
automatically normalized

to dataset

```
200
// ML fit of gauss to data
                                   150
w::gauss.fitTo(*data);
(MINUIT printout omitted)
                                   100
                                    50
// Parameters if gauss now
// reflect fitted values
mean.Print() ;
sigma.Print();
RooRealVar::mean = 0.0172335 + - 0.0299542
RooRealVar::sigma = 2.98094 + - 0.0217306
// Plot fitted PDF and toy data overlaid
RooPlot* xframe = x.frame() :
data->plotOn(xframe) ;
gauss.plotOn(xframe) ;
```

# RooFit implements normalized probability models

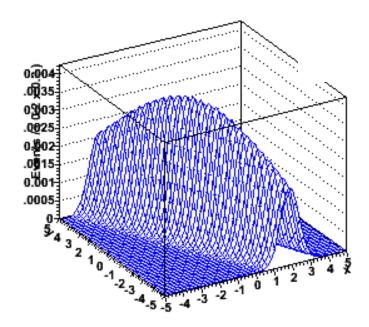
Normalized probability (density) models are the basis of all fundamental statistical techniques



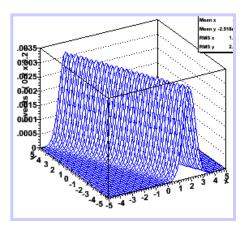
- Normalization guarantee introduces extra complication in calculation, but has important advantages
  - Directly usable in fundamental statistical techniques
  - Easier construction of complex models (will shows this in moment)
- RooFit provides built-in support for normalization, taking away downside for users, leaving upside
  - Default normalization strategy relies on numeric techniques, but user can specify known (partial) analytical integrals in pdf classes.

# The power of conditional probability modeling

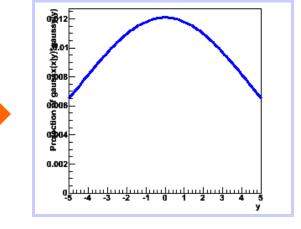
 Take following model f(x,y): what is the analytical form?



 Trivially constructed with (conditional) probability density functions! Gauss f(x|a\*y+b,1)



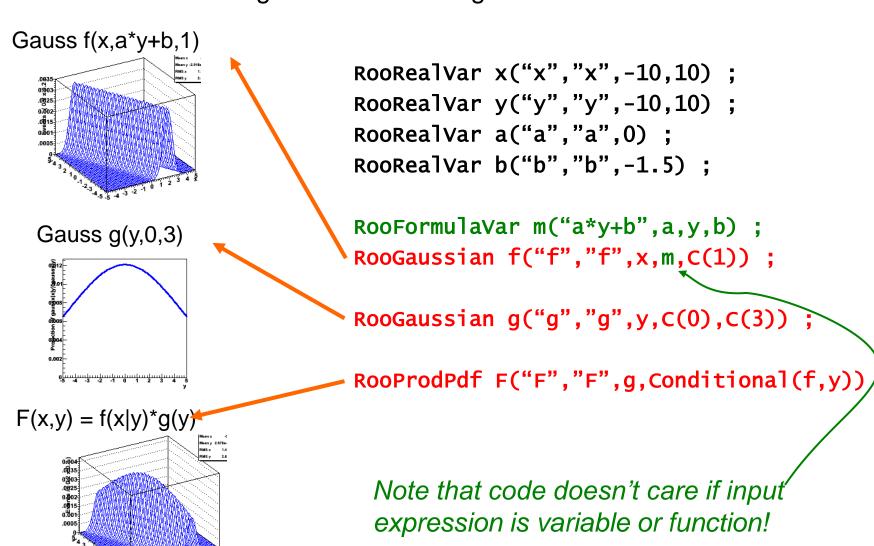
Gauss g(y,0,3)



$$F(x,y) = f(x|y)^*g(y_y)_{e, NIKHEF}$$

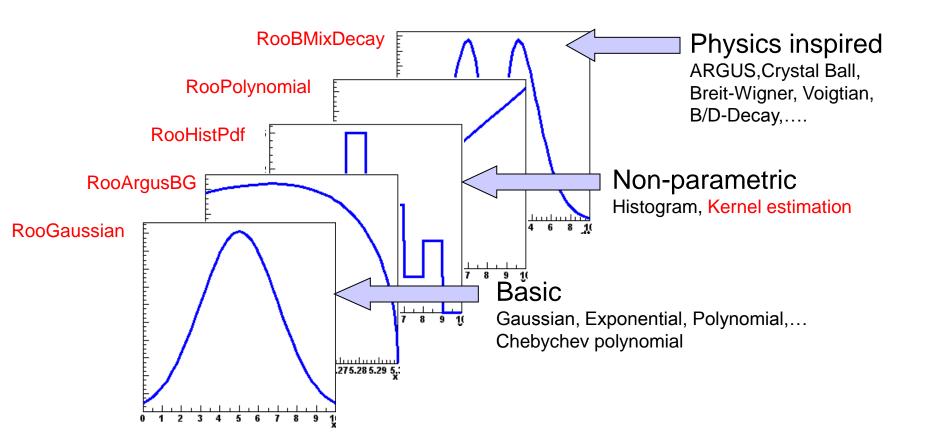
# Coding a conditional product model in RooFit

Construct each ingredient with a single line of code



#### Building power – most needed shapes already provided

RooFit provides a collection of compiled standard PDF classes



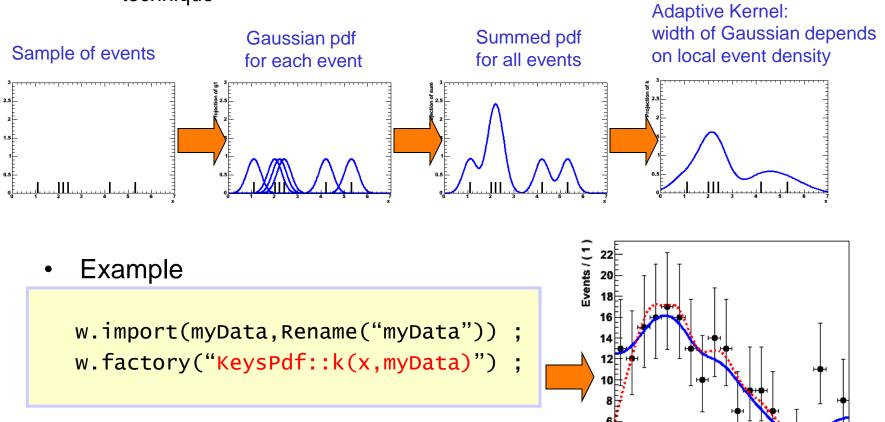
Easy to extend the library: each p.d.f. is a separate C++ class

#### Individual classes can encapsulate powerful algorithms

Example: a 'kernel estimation probability model'

Construct smooth pdf from unbinned data, using kernel estimation

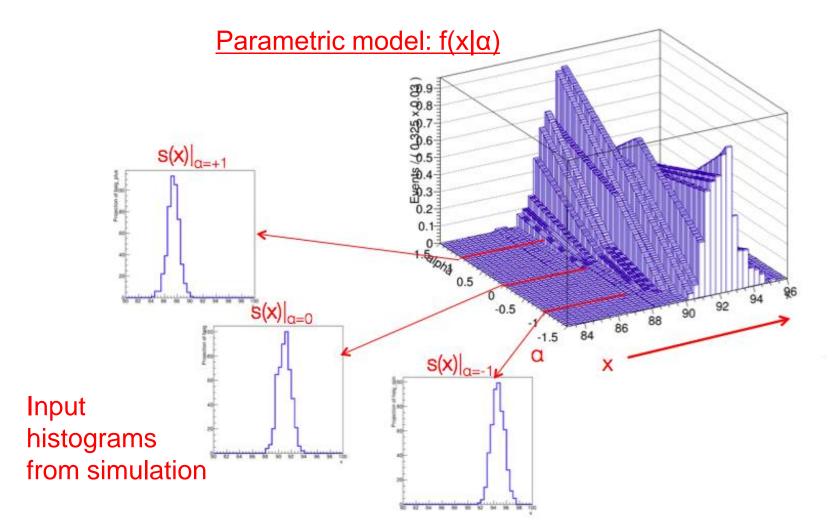
technique



Also available for n-D data

# Advanced modeling building – template morphing

 At LHC shapes are often derived from histograms, instead of relying on analytical shapes. Construct parametric from histograms using 'template morphing' techniques



# Code example – template morphing

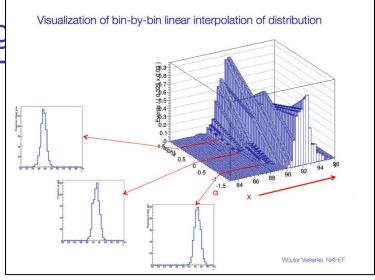
 Example of template morphing systematic in a binned likelihood

$$s_{i}(a,...) = \int_{0}^{n} s_{i}^{0} + a \times (s_{i}^{+} - s_{i}^{0}) \quad "a > 0$$

$$f \quad s_{i}^{0} + a \times (s_{i}^{0} - s_{i}^{-}) \quad "a < 0$$

$$L(\vec{N} \mid a, \vec{s}^{-}, \vec{s}^{0}, \vec{s}^{+}) = \tilde{O}P(N_{i} \mid s_{i}(a, s_{i}^{-}, s_{i}^{0}, s_{i}^{+})) \times G(0 \mid a, 1)$$

$$bins$$

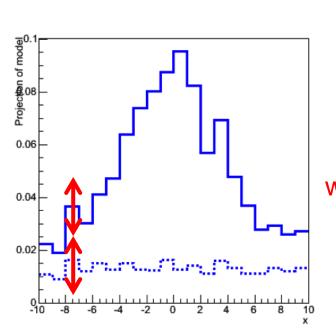


Class from the HistFactory project (K. Cranmer, A. Shibata, G. Lewis, L. Moneta, W. Verkerke)

```
// Construct template models from histograms
w.factory("HistFunc::s_0(x[80,100],hs_0)");
w.factory("HistFunc::s_p(x,hs_p)");
w.factory("HistFunc::s_m(x,hs_m)");
// Construct morphing model
w.factory("PiecewiseInterpolation::sig(s_0,s_,m,s_p,alpha[-5,5])");
// Construct full model
w.factory("PROD::model(ASUM(sig,bkg,f[0,1]),Gaussian(0,alpha,1))");
```

# Advanced model building – describe MC statistical uncertainty

- Histogram-based models have intrinsic uncertainty to MC statistics...
- How to express corresponding shape uncertainty with model params?
  - Assign parameter to each histogram bin, introduce Poisson 'constraint' on each bin
  - 'Beeston-Barlow' technique. Mathematically accurate, but introduce results in complex models with many parameters.



$$L(\vec{N}) = \tilde{\bigcirc} P(N_i \mid \tilde{s}_i + \tilde{b}_i)$$
 Binned likelihood with rigid template 
$$L(\vec{N} \mid \vec{s}, \vec{b}) = \tilde{\bigcirc} P(N_i \mid s_i + b_i) \tilde{\bigcirc} P(\tilde{s}_i \mid s_i) \tilde{\bigcirc} P(\tilde{b}_i \mid b_i)$$
 bins bins bins bins

Response function w.r.t. s, b as parameters

Subsidiary measurements of s ,b from s~,b~

$$L(\vec{N} \mid \vec{g}_{s}, \vec{g}_{b}) = \widetilde{\bigcap}_{bins} P(N_{i} \mid g_{s,i} \tilde{s}_{i} + g_{b,i} \tilde{b}_{i}) \widetilde{\bigcap}_{bins} P(\tilde{s}_{i} \mid g_{s,i} \tilde{s}_{i}) \widetilde{\bigcap}_{bins} P(\tilde{b}_{i} \mid g_{b,i} \tilde{b}_{i})$$

Normalized NP model (nominal value of all γ is 1)

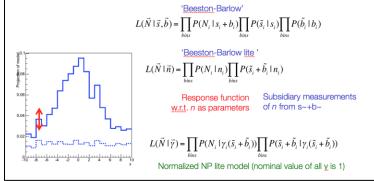
#### Code example – Beeston-Barlow

 Beeston-Barlow-(lite) modeling of MC statistical uncertainties

$$L(\vec{N} | \vec{g}) = \widetilde{O}_{bins} P(N_i | g_i(\tilde{s}_i + \tilde{b}_i)) \widetilde{O}_{bins} P(\tilde{s}_i + \tilde{b}_i | g_i(\tilde{s}_i + \tilde{b}_i))$$

#### Reducing the number NPs - Beeston-Barlow 'lite'

- Another approach that is being used is called 'BB' lite
- Premise: effect of statistical fluctuations on sum of templates is dominant → Use one NP per bin instead of one NP per component per bin



```
// Import template histogram in workspace
w.import(hs);

// Construct parametric template models from histograms
// implicitly creates vector of gamma parameters
w.factory("ParamHistFunc::s(hs)");

// Product of subsidiary measurement
w.factory("HistConstraint::subs(s)");

// Construct full model
w.factory("PROD::model(s,subs)");
```

#### Code example: BB + morphing

 Template morphing model with Beeston-Barlow-lite MC statistical uncertainties

$$s_{i}(\partial,...) = \int_{i}^{i} s_{i}^{0} + \partial \times (s_{i}^{+} - s_{i}^{0})$$
 "  $\partial > 0$   
 $s_{i}(\partial,...) = \int_{i}^{0} s_{i}^{0} + \partial \times (s_{i}^{0} - s_{i}^{-})$  "  $\partial < 0$ 

$$L(\vec{N} \mid \vec{s}, \vec{b}) = \underbrace{\tilde{O}}_{bins} P(N_i \mid g_i \times [s_i(a, s_i^-, s_i^0, s_i^+) + b_i]) \underbrace{\tilde{O}}_{bins} P(\tilde{s}_i + \tilde{b}_i \mid g_i \times [\tilde{s}_i + \tilde{b}_i]) G(0 \mid a, 1)$$

The interplay between shape systematics and MC systematics

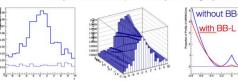
• Commonly chosen practical solution 
$$s_{i}(\alpha,...) = \begin{cases} s_{i}^{0} + \alpha \cdot (s_{i}^{*} - s_{i}^{0}) & \forall \alpha > 0 \\ s_{i}^{0} + \alpha \cdot (s_{i}^{0} - s_{i}^{-}) & \forall \alpha < 0 \end{cases}$$

$$L(\vec{N} \mid \vec{s}, \vec{b}) = \prod_{bloc} P(N_{i} \mid \gamma_{i} \cdot [s_{i}(\alpha, s_{i}^{-}, s_{i}^{0}, s_{i}^{*}) + b_{i}]) \prod_{bloc} P(\tilde{s}_{i} + \tilde{b}_{i} \mid \gamma_{i} \cdot [\tilde{s}_{i} + \tilde{b}_{i}]) G(0 \mid \alpha, s_{i}^{-}, s_{i}^{0}, s_{i}^{0}) = \frac{1}{2} \left[ \frac{1} \left[ \frac{1}{2} \left[ \frac{1}{2} \left[ \frac{1}{2} \left[ \frac{1}{2} \left[ \frac{1}{2} \left[ \frac{1}$$

Morphing & MC response function

Subsidiary measurements

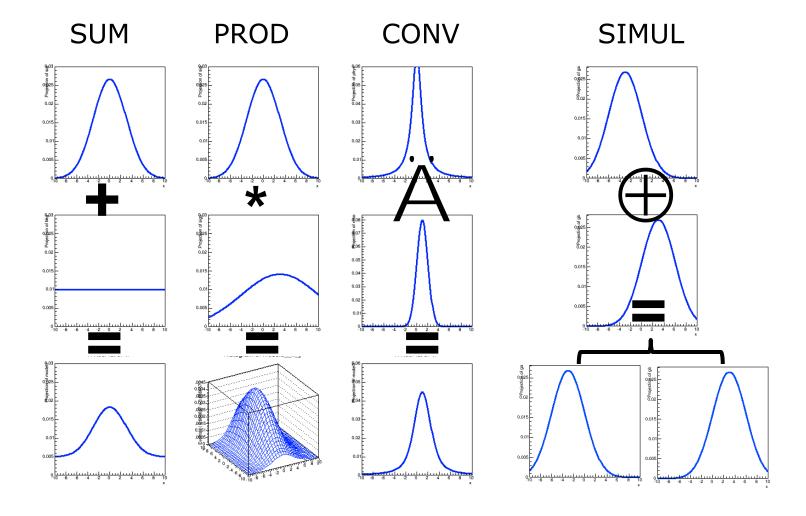
Models relative MC rate uncertainty for each bin w.r.t the nominal MC yield, even if morphed total yield is slightly different



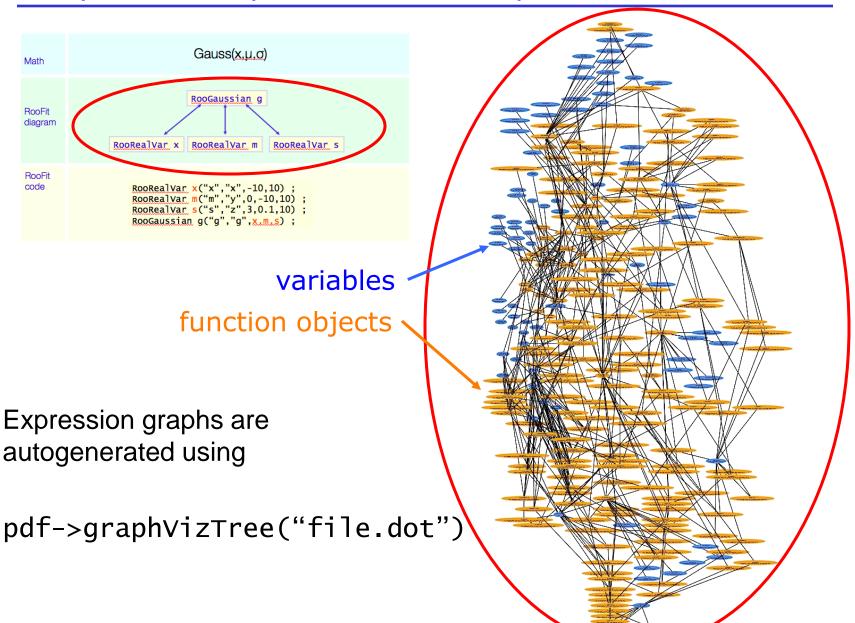
- Approximate MC template statistics already significantly improves influence of MC fluctuations on template morphing
  - Because ML fit can now 'reweight' contributions of each bin

# From simple to realistic models: composition techniques

 Realistic models with signal and bkg, and with control regions built from basic shapes using addition, product, convolution, simultaneous operator classes

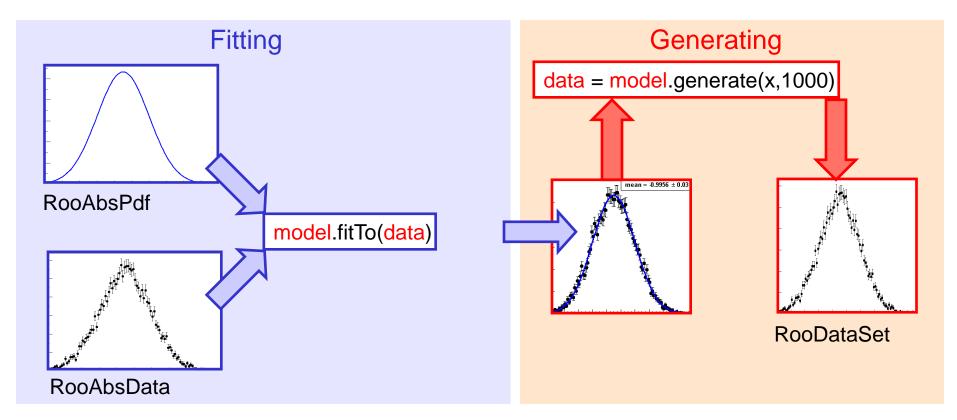


# Graphical example of realistic complex models



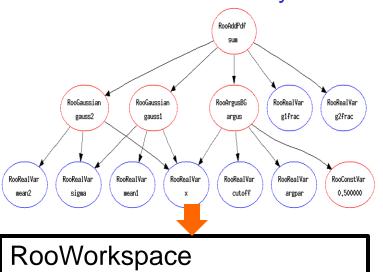
# Abstracting model building from model use - 1

- For universal statistical analysis tools (RooStats), must be have universal functionality of models (independent of structure and complexity)
- Was already possible in RooFit since 1999



# Abstracting model building from model use - 2

- Must be able to practically separate model building code from statistical analysis code.
- Solution: you can persist RooFit models of arbitrary complexity in 'workspace' containers
- The workspace concept has revolutionized the way people share and combine analyses!



# RooWorkspace Roofsdard Var Roofsda

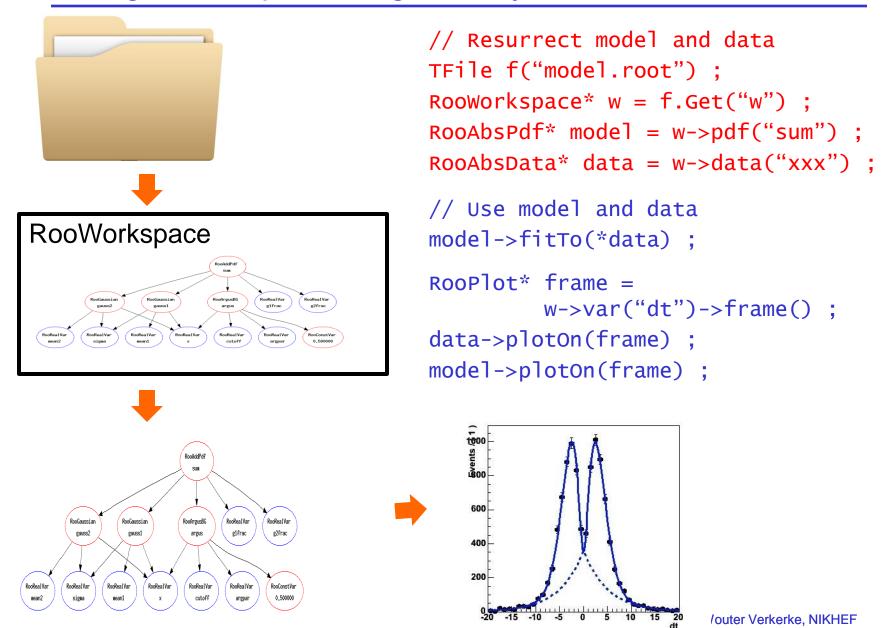
#### Realizes complete and practical

factorization of process of building and using likelihood functions!

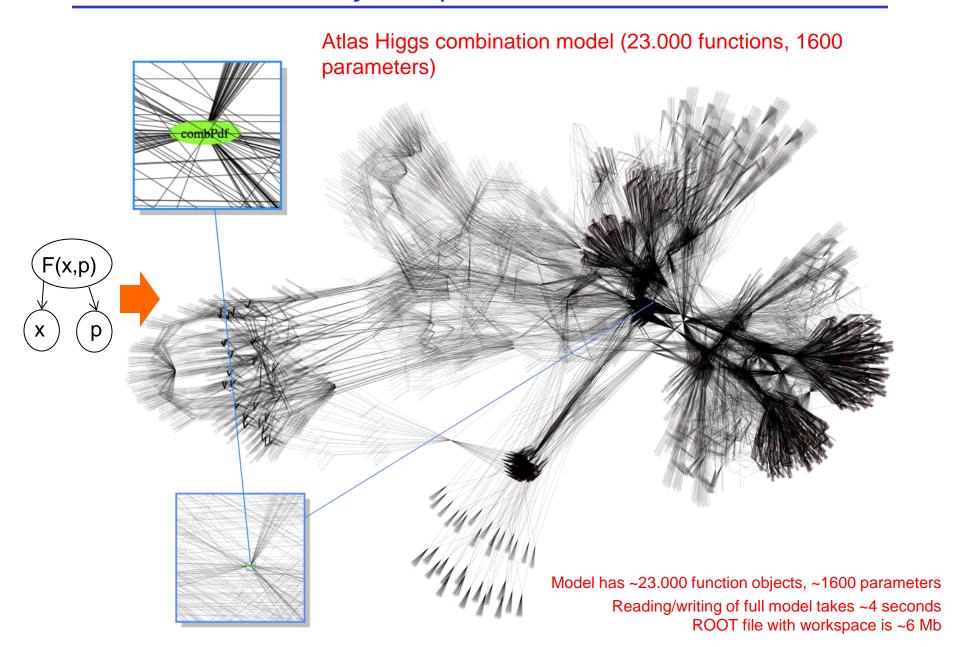
```
RooWorkspace w("w");
w.import(sum);
w.writeToFile("model.root");
model.root
```



# Using a workspace file given to you...



# Persistence of *really* complex models works too!



# An excursion – Collaborative analyses with workspaces

- Workspaces allow to share and modify very complex analyses with very little technical knowledge required
- Example: Higgs coupling fits

-1

0 +1 Signal strength (μ)

ATLAS Preliminary Confidence  $\sqrt{s} = 7 \text{ TeV}, \int Ldt = 4.6-4.8 \text{ fb}^{-1}$  $\sqrt{s} = 8 \text{ TeV}, \int Ldt = 13-20.7 \text{ fb}^{-1}$ intervals ---- 95% CL Full on Higgs Higgs fermion, model boson couplings 0.8 0.9 1.1 ATLAS Preliminary m<sub>u</sub> = 125.5 GeV  $W,Z H \rightarrow bb$  $\sigma(gg \to H) * BR(H \to \gamma\gamma)$ vs = 8 TeV: Ldt = 13 fb-1 Signal √s = 7 TeV: ∫Ldt = 4.6 fb<sup>-1</sup>  $\kappa_V^2 \cdot \kappa_\gamma^2(\kappa_F, \kappa_V)$ Reparametrize vs = 8 TeV: ∫Ldt = 13 fb  $\sigma(qq' \rightarrow qq'H) * BR(H \rightarrow \gamma\gamma) \sim$ strength  $H \rightarrow WW^{(*)} \rightarrow lvlv$ √s = 8 TeV: ∫Ldt = 13 fb in terms of in 5  $\sigma(gg \to H) * \mathrm{BR}(H \to ZZ^{(*)}, H \to WW^{(*)}) ~\sim~$ fermion, boson channels  $\sigma(qq' \to qq'H) * BR(H \to ZZ^{(*)}, H \to WW^{(*)}) \sim$ scale factors  $\sigma(qq' \to qq'H, VH) * \text{BR}(H \to \tau\tau, H \to b\bar{b}) ~\sim ~ \frac{\kappa_V^2 \cdot \kappa_F^2}{0.75 \cdot \kappa_F^2 + 0.25 \cdot}$  $\mu=1.43\pm0.21$ vs = 7 TeV: Ldt = 4.6 - 4.8 fb vs = 8 TeV: ∫Ldt = 13 - 20.7 fb

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# An excursion – Collaborative analyses with workspaces

- How can you reparametrize existing Higgs likelihoods in practice?
- Write functions expressions corresponding to new

$$\sigma(gg \to H) * BR(H \to \gamma \gamma) \sim \frac{\kappa_F^2 \cdot \kappa_\gamma^2(\kappa_F, \kappa_V)}{0.75 \cdot \kappa_F^2 + 0.25 \cdot \kappa_V^2}$$

Edit existing model

```
w.import(mu_gg_func);
w.factory("EDIT::newmodel(model,mu_gg=mu_gg_gunc)");
```

Top node of *modified*Higgs combination pdf

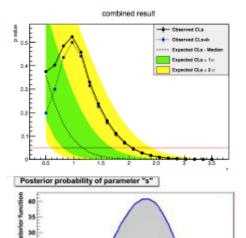
Top node of *original* Higgs combination pdf

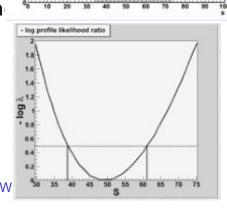
Modification prescription: replace parameter mu\_gg with function mu\_gg\_func everywhere

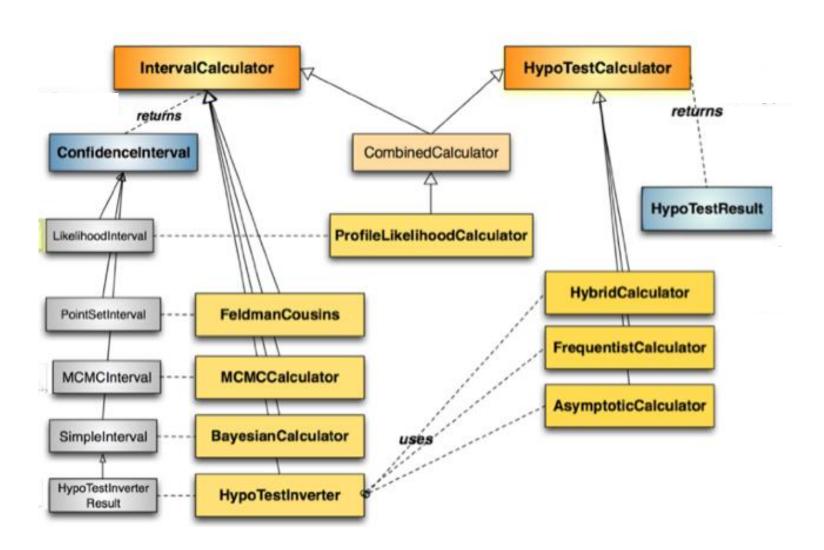
# RooStats – Statistical analysis of RooFit models

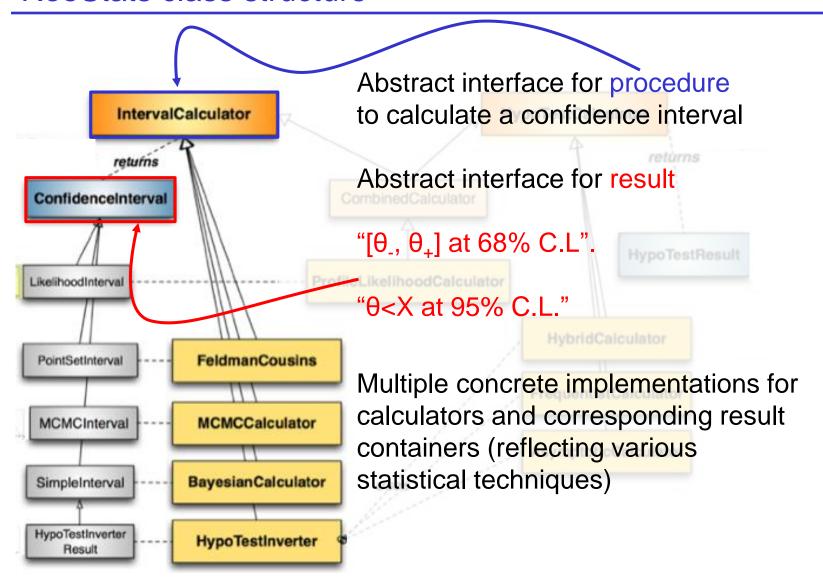
- With RooFits one has (almost) limitless possibility to construct probability density models
  - With the workspaces one also has the ability to deliver such models to statistical tools that are completely decoupled from the model construction code.
     Will now focus on the design of those statistical tools
- The RooStats projected was started in 2007 as a joint venture between ATLAS, CMS, the ROOT team and myself.
  - <u>Goal</u>: to deliver a series of tools that can calculate intervals and perform hypothesis tests using a variety of statistical techniques
    - Frequentist methods (confidence intervals, hypothesis testing)
    - Bayesian methods (credible intervals, odd-ratios)
    - Likelihood-based methods

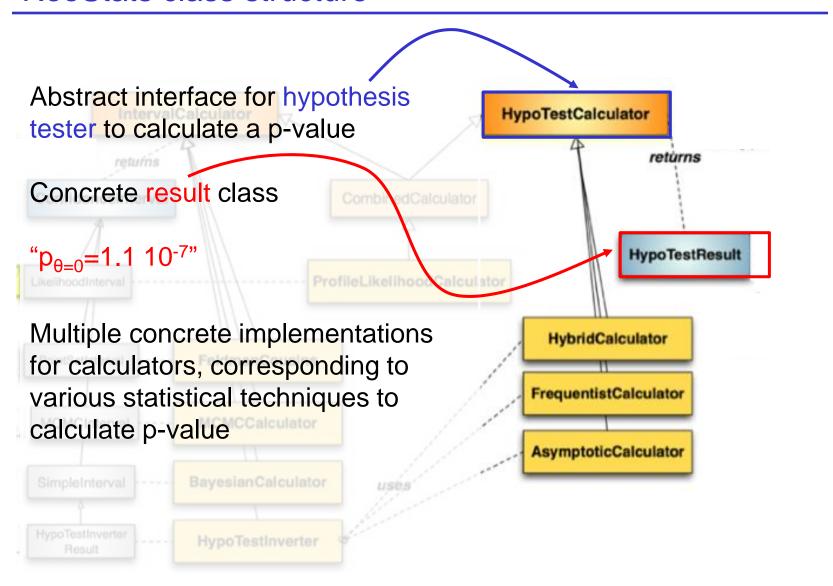
Confidence intervals:  $[\theta_{-}, \theta_{+}]$ , or  $\theta < X$  at 95% C.L. Hypothesis testing:  $\rightarrow p(data|\theta=0) = 1.10^{-7}$ 

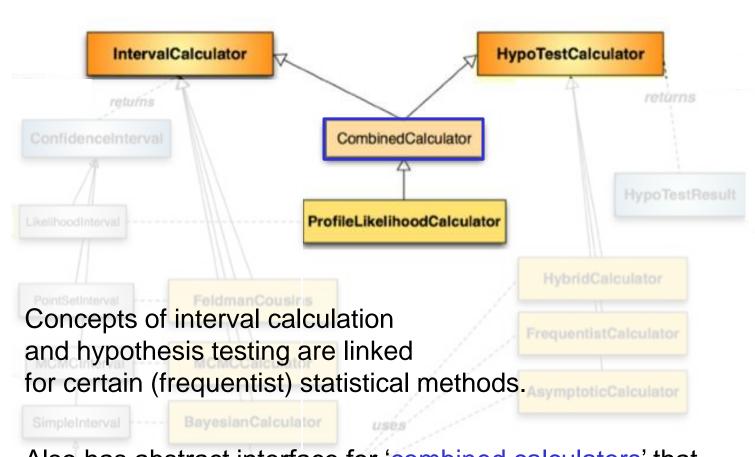












Also has abstract interface for 'combined calculators' that can perform both types of calculations

# Working with RooStats calculators

- Calculators interface to RooFit via a 'ModelConfig' object
- ModelConfig completes f(x|θ) from workspace with additional information to become an unambiguous statistical problem specification (together with x<sub>obs</sub>)
  - E.g. which of parameters  $\theta$  are 'of interest' which are 'nuisance parameters'.
  - For certain types of complex models, additional info is needed

```
// create the class using data and model
ProfileLikelihoodCalculator plc(data, model);

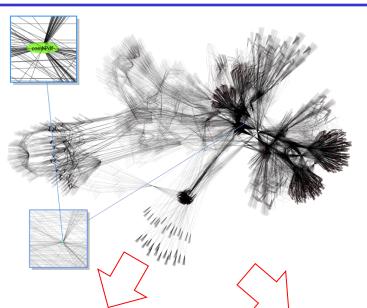
// set the confidence level
plc.SetConfidenceLevel(0.683);

// compute the interval
LikelihoodInterval* interval = plc.GetInterval();

// plot the interval
LikelihoodIntervalPlot plot(interval);
plot.Draw();
```

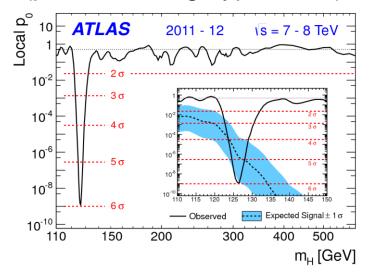
Calculator works for any model, no matter how complex

#### Some famous RooFit/RooStats results

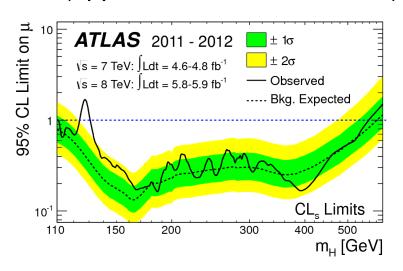


Atlas Higgs combination model (23.000 functions, 1600 parameters)

RooStats hypothesis testing (p-value of bkg hypothesis)



RooStats interval calculation (upper limit intervals at 95%)



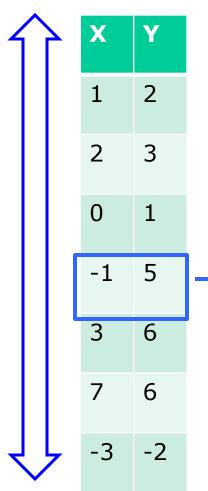
#### Performance considerations

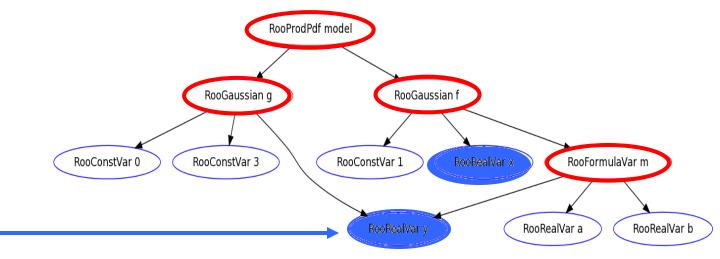
- While functionality is (nearly) universal, good computational performance for all models requires substantial work behind the scenes.
  - Will highlight three techniques that are used to boost performance
- Heuristic constant-expression detection
  - Identify (highest)-level constant expression in user expression in a given use context and prevent unnecessary recalculation of these
- (Pseudo)-vectorization
  - Reorder calculations to approach concept of vectorization
- Parallelization
  - Exploit pervasive ability of CPU farms and multi-core host to parallelize calculations that intrinsically of a repetitive nature
- The boundary condition of all optimizations is that user code should not need to accommodate these.
  - User probability models are often already complex, must be kept in 'most readable' representation
  - Use RooFit model introspection to reorganize user functions 'on the fly' in vectorization-friendly order

# Optimization of likelihood calculations

Likelihood evaluates pdf at all data points, essentially a 'loop' call

$$-\log L(\vec{p}) = - \mathop{\mathring{\text{o}}}_{i=0\dots n} \log f(\vec{x}_i, \vec{p})$$

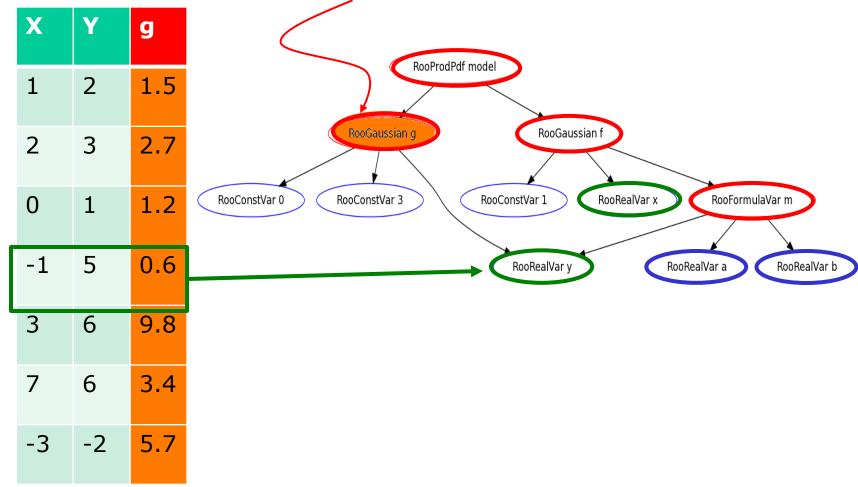




As written by user, the p.d.f is a scalar expression that is *unaware* of underlying repeated calculation of likelihood

#### Level-1 optimization of likelihood calculation

 RooFit can heuristically detect constant terms (depends only on observables, not on parameters) are pre-calculated, cached with likelihood dataset. Calculation tree modified to omit recalculation of



#### Level-2 optimization of likelihood calculation

Can also apply caching strategy to all functions nodes, instead of just constant nodes\_ Depends on m Depends on a,b X g RooProdPdf model 1.5 1 2 RooGaussian g RooGaussian f 3 RooConstVar 0 RooConstVar 3 RooConstVar 1 RooRealVar x RooFormulaVar m 1 0 -1 5 0.6 RooRealVar y RooRealVar a RooRealVar b To ensure correct calculation: 3 6 9.8 Value cache of non-constant function objects will be invalidated if dependent parameters 3.4 6 changed 5.7 -2 Faster than level-1 if non-constant cache

miss rate <100%

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#### What is the value cache miss rate for non-constant objects?

 It is quite a bit better than 100% as most MINUIT calls to likelihood vary one parameter at a time (to calculate derivative)
 Computed cached values will often stay valid

```
prevFCN = 5170.289989 FCN=5170.53 FROM MIGRAD STATUS=INITIATE 6 CALLS 7 TOTAL
prevFCN = 4495.931306 a=0.9961, b=0.106, c=0.06274,
prevFCN = 3936.921265 a=0.9967.
                                                Only a changes, caches
prevFCN = 3936.938281 a=0.9954.
                                                depending on b,c remain valid
prevFCN = 3936.907905 a = 0.9965,
prevFCN = 3936.933086 a=0.9956,
prevFCN = 3936.911321 a=0.9961, b=0.108,
prevFCN = 3937.05644 b=0.104,
                                                Only b changes, caches
prevFCN = 3936.790003 b=0.1074,
                                                depending on a,c remain valid
prevFCN = 3937.014478 b=0.1046,
prevFCN = 3936.829929 b=0.106, c=0.06845,
prevFCN = 3936.934463 c=0.05703,
                                                Only c changes, caches
prevFCN = 3936.911648 c=0.06688,
                                                depending on b,c remain valid
prevFCN = 3936.930463 c=0.05861,
prevFCN = 3936.913944 a=1, b=-0.02103, c=0.02074,
prevFCN = 3936.613348 a=0.9982, b=0.04018, c=0.04096,
```

# From level-2 optimization to vectorization

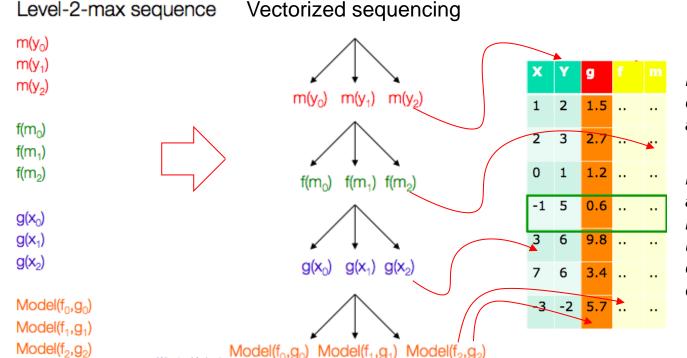
 Note that resequencing of calculation in full level-2 optimization mode results in 'natural ordering' for complete vectorization

```
Level-1 sequence
                                                 Level-2-max sequence
m(y_0)
                                                  m(y_0)
f(m_0)
                                                  m(y_1)
g(x_0)
                                                  m(y_2)
Model(f_0, g_0)
                                                  f(m_0)
m(y_1)
                                                  f(m_1)
f(m_1)
                                                  f(m_2)
g(x_1)
                                                  g(x_0)
Model(f_1,g_1)
                                                  g(x_1)
                                                  g(x_2)
m(y_2)
f(m_2)
                                                  Model(f_0,g_0)
g(x_2)
                                                  Model(f_1,g_1)
Model(f_2,g_2)
                                                  Model(f_2,g_2)
```

#### Work in progress – automatic code vectorization

 Axel noted in his plenary presentation that 'vectorization' is invasive... True, but modular structure of RooFit function expression allows this invasive reorganization to be performed automatically. Aim to vectorize code without making the 'user code' messy!

Construct <u>custom sequence driver</u> on the fly with CLING to eliminate virtual function calls

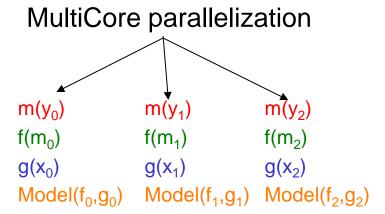


Level-2 optimization ensures all inputs are already in vector form

But, as inputs are already always held in proxies in user code, user code is unaware of scalar/vector nature of inputs

#### Other parallelization techniques – multicore Likelihood calculation

- Parallelization of calculations already introduce at a higher level
- Multi-core calculation of likelihood at the granularity of the event level, rather than the function call level

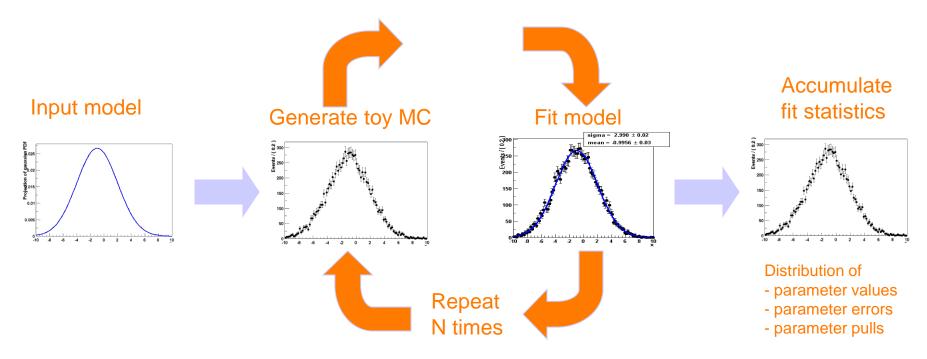


Trivial use invocation make this already popular with users

 But load balancing can become uneven for 'simultaneous fits' (not every event has the same probability model in that case)

# Parallelization using PROOF

- Simple parallelization of likelihood calculation using NumCPU(n) option of RooAbsPdf::fitTo() very popular, but restricted to likelihood calculations
- Another common CPU-intensive task are toy studies



Have generic interface to PROOF(-lite) to parallelize loop tasks.
 Also used by RooStats for sampling procedures

# Summary

RooFit and RooStats allow you to perform advanced statistical data analysis

- LHC Higgs results a prominent example
- RooFit provides (almost) limitless model building facilities
  - Concept of persistable model workspace allows to separate model building and model interpretation
  - HistFactory package introduces structured model building for binned likelihood template models that are common in LHC analyses
- RooStats provide a wide set of statistica tests that can be performed on RooFit models
  - Bayesian, Frequentist and Likelihood-based test concepts
  - Wide range op options (Frequentist test statistics, Bayesian integration methods, asympotic calculators...)

