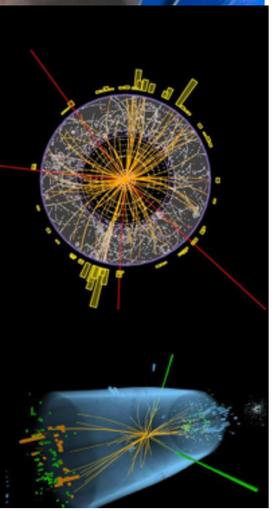
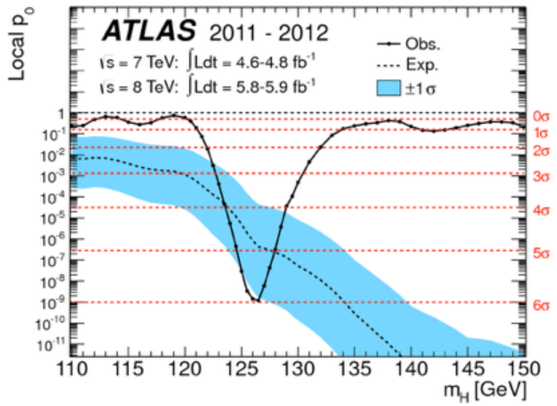
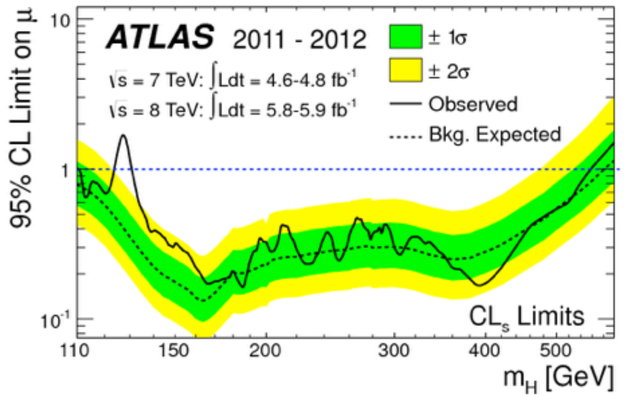


ROOT and Statistic Tutorial at UERJ

5. Advanced Statistical Analysis with RooStats





Rio de Janeiro, 24 November 2015

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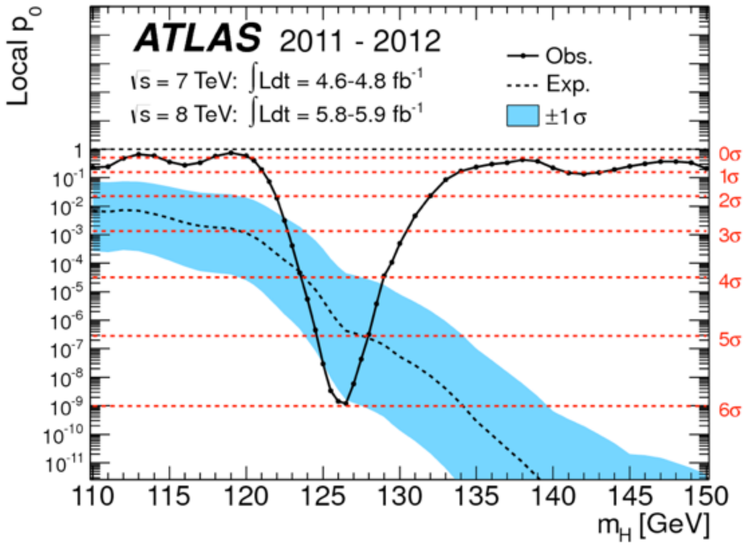
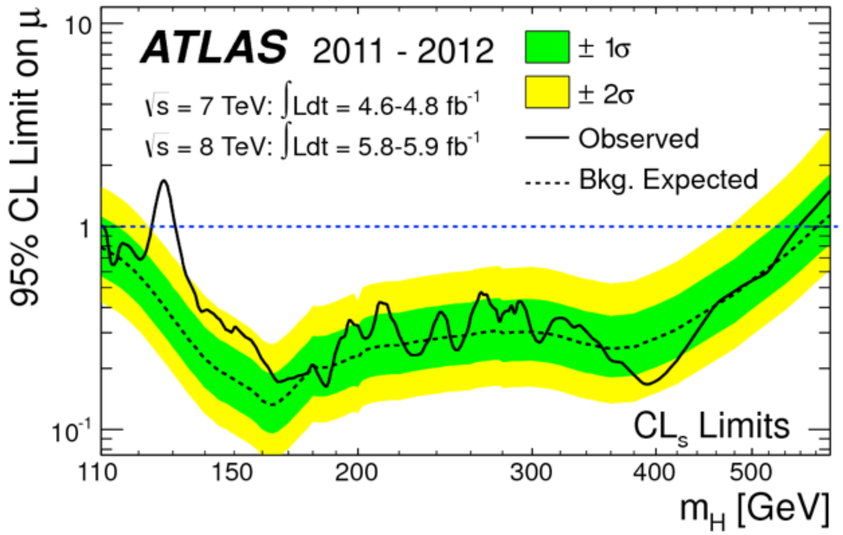
Introduction

- We have seen yesterday:
  - Parameter Estimation methods
    - Histogram Fitting
    - Maximum Likelihood methods
  - Introduction to RooFit
    - model building with RooFit
      - how to build composite models
- What we will see today:
  - Interval estimation:
    - Confidence interval based on Likelihood
    - Frequentist (Neyman) intervals
    - Bayesian (credible) intervals

Outline (2)

- To understand better confidence intervals and hypothesis testing
  - see practical examples of estimating frequentist and bayesian intervals using RooStats software package
  - e.g. how to make p0 or Brazilian (limit) plots with RooStat
- Exercises on interval/limit estimation and discovery significance (hypothesis test)



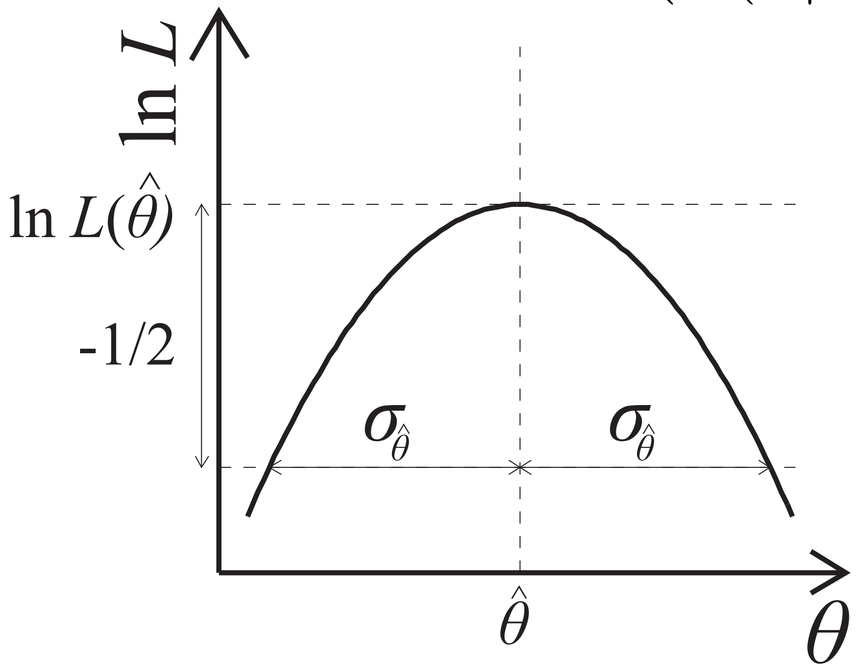


Parameter Estimation with Maximum Likelihood

- The ML estimate of the parameter are those who maximise the likelihood function

$$L(\vec{x}_1, ..., \vec{x}_N|\theta) = \prod_{i=1}^{N} f(\vec{x}_i, \theta)$$

$$\text{Best Estimate } \hat{\theta} \longleftarrow \text{Max}(L(x|\theta))$$



ML is the preferred estimator given its good properties:
- consistent
- asymptotically unbiased
- efficient

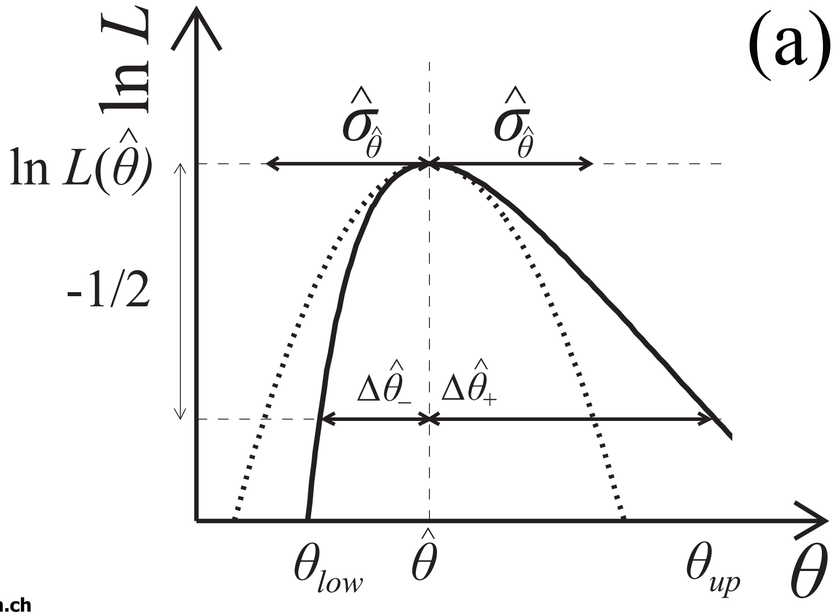
Parameter Estimation with Maximum

– Asymptotically the parameter estimates are normally distributed. The estimated variance is then:

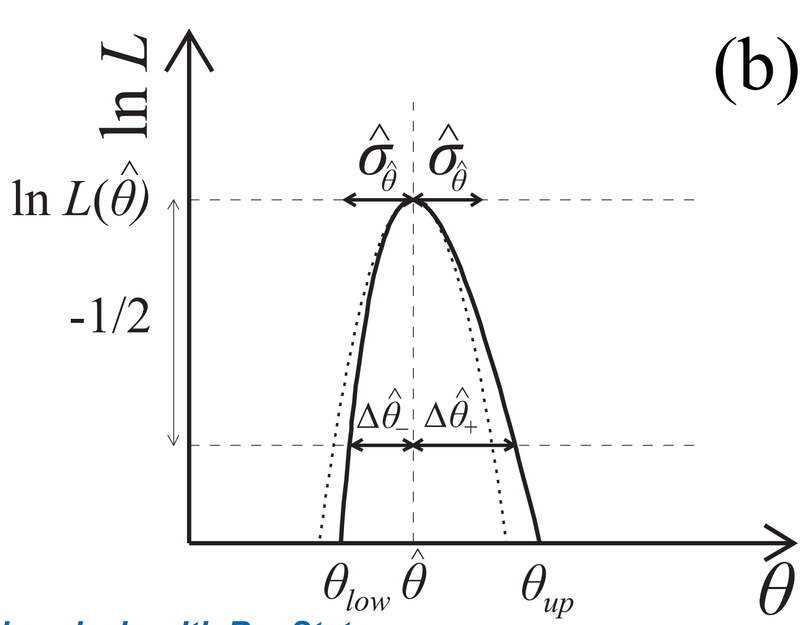
$$\hat{\mathbf{V}}(\hat{\boldsymbol{\theta}}) = \left[\left(-\frac{\partial^2 \ln L(\mathbf{x};\boldsymbol{\theta})}{\partial^2 \boldsymbol{\theta}} \right)_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}} \right]^{-1} = \mathbf{H}^{-1}$$

Exponential decay fit

2 events



8 events

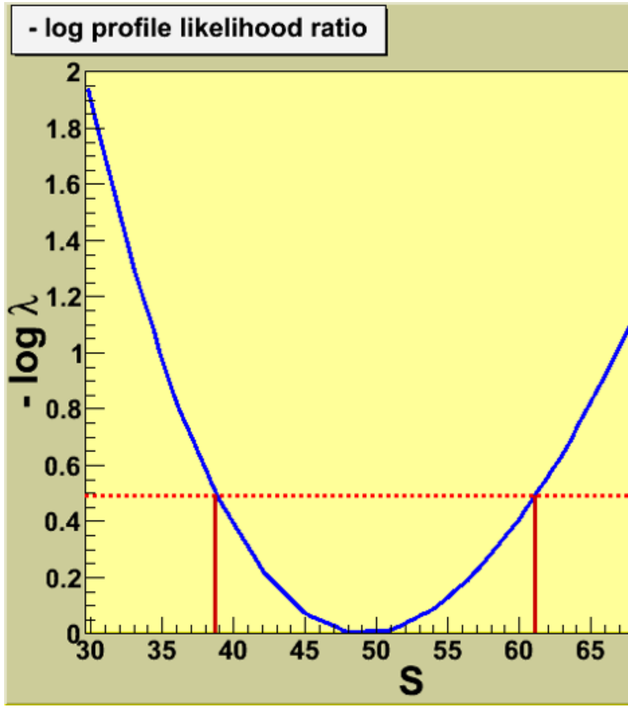


Confidence Interval using Likelihood Ratio

$$\lambda(\theta) = \frac{L(x|\theta)}{L(x|\hat{\theta})}$$

Function of parameter θ

Maximum Likelihood value

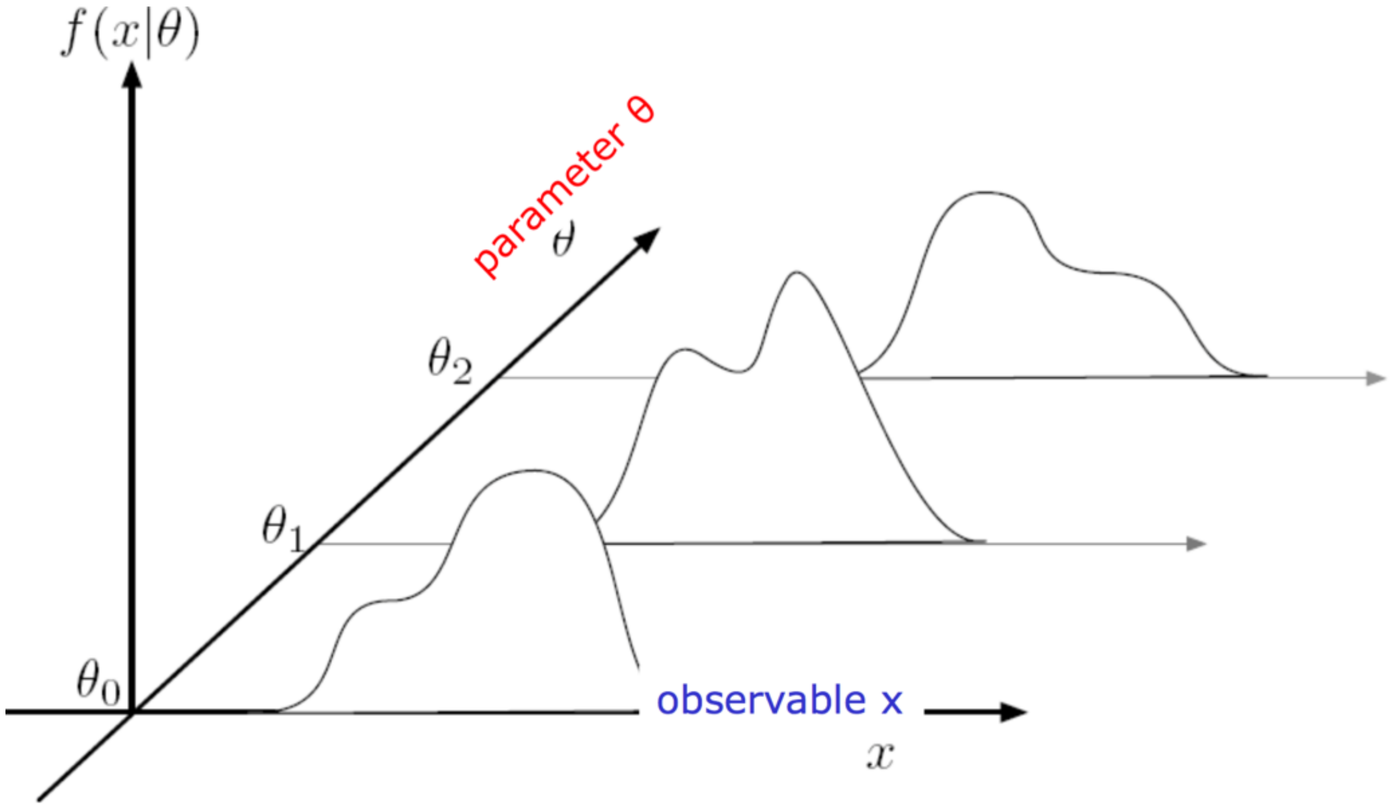


$$-2\log\lambda(\theta) \sim \chi^2 \text{distribution}$$

$$-\log\lambda(\theta_{low} \equiv \hat{\theta} - \delta\hat{\theta}_-) = -\log\lambda(\theta_{up} \equiv \hat{\theta} + \delta\hat{\theta}_+) = \frac{1}{2}F^{-1}_{\chi^2}(0.68, 1) = 0.5$$

Newman Construction of Confidence Intervals

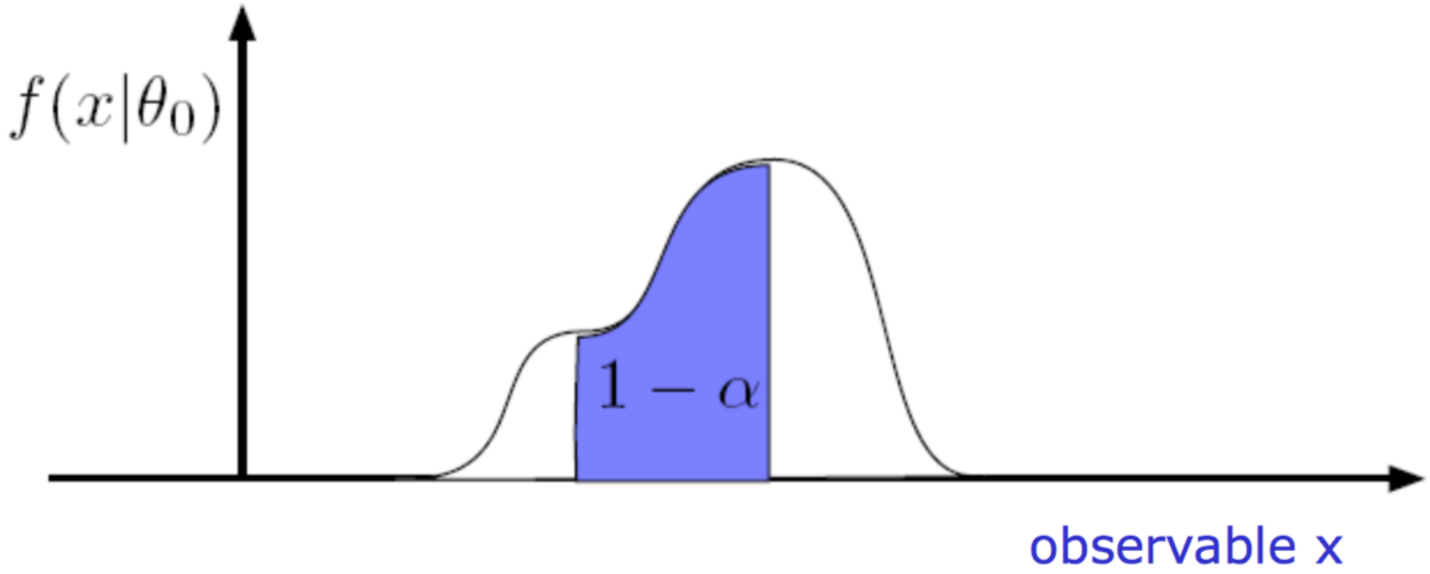
- Simplest case: one measurement (x) and one parameter θ
- For each θ one has a distribution in observable (x)



Newman Interval Construction

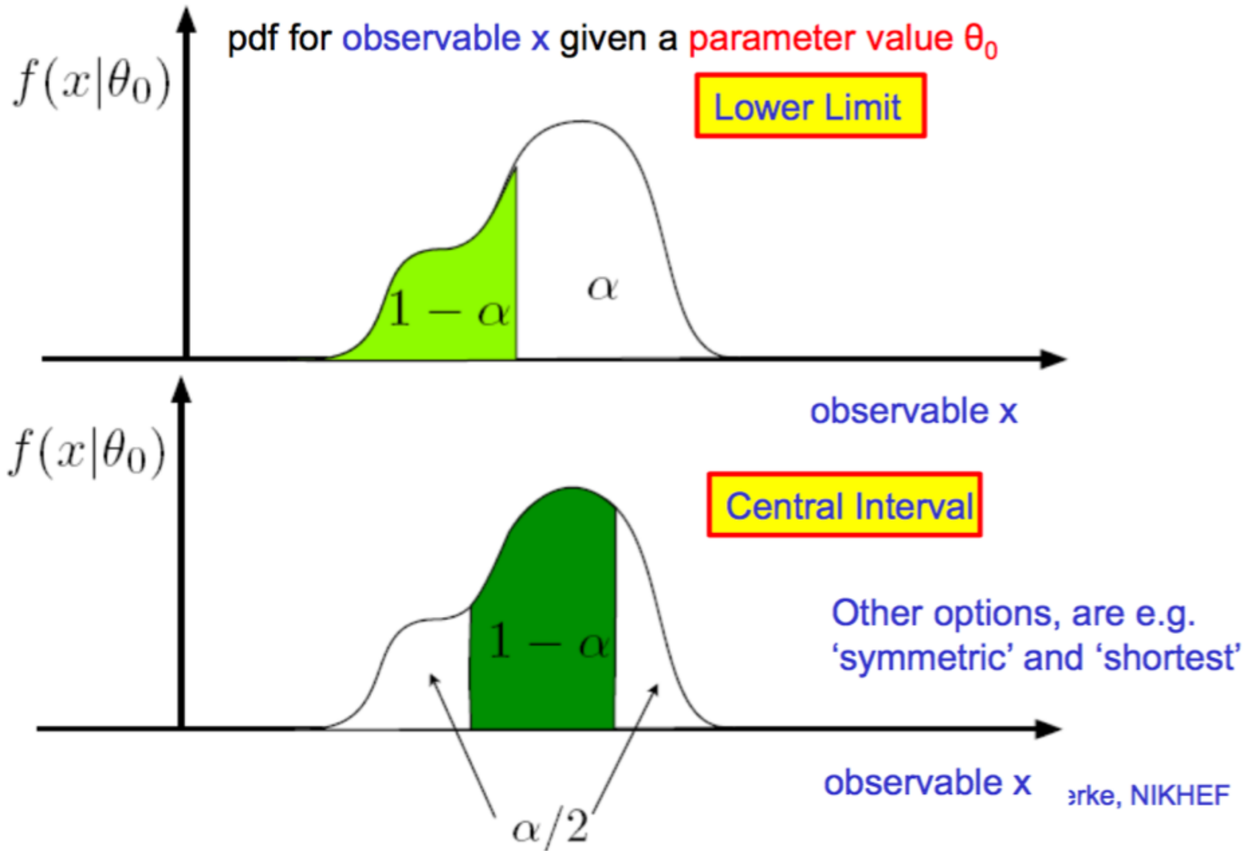
- Focus on a slice in θ
  - For a 1-α% confidence Interval, define ***acceptance interval*** that contains 100%-α% of the distribution

pdf for observable x
given a parameter value θ_0



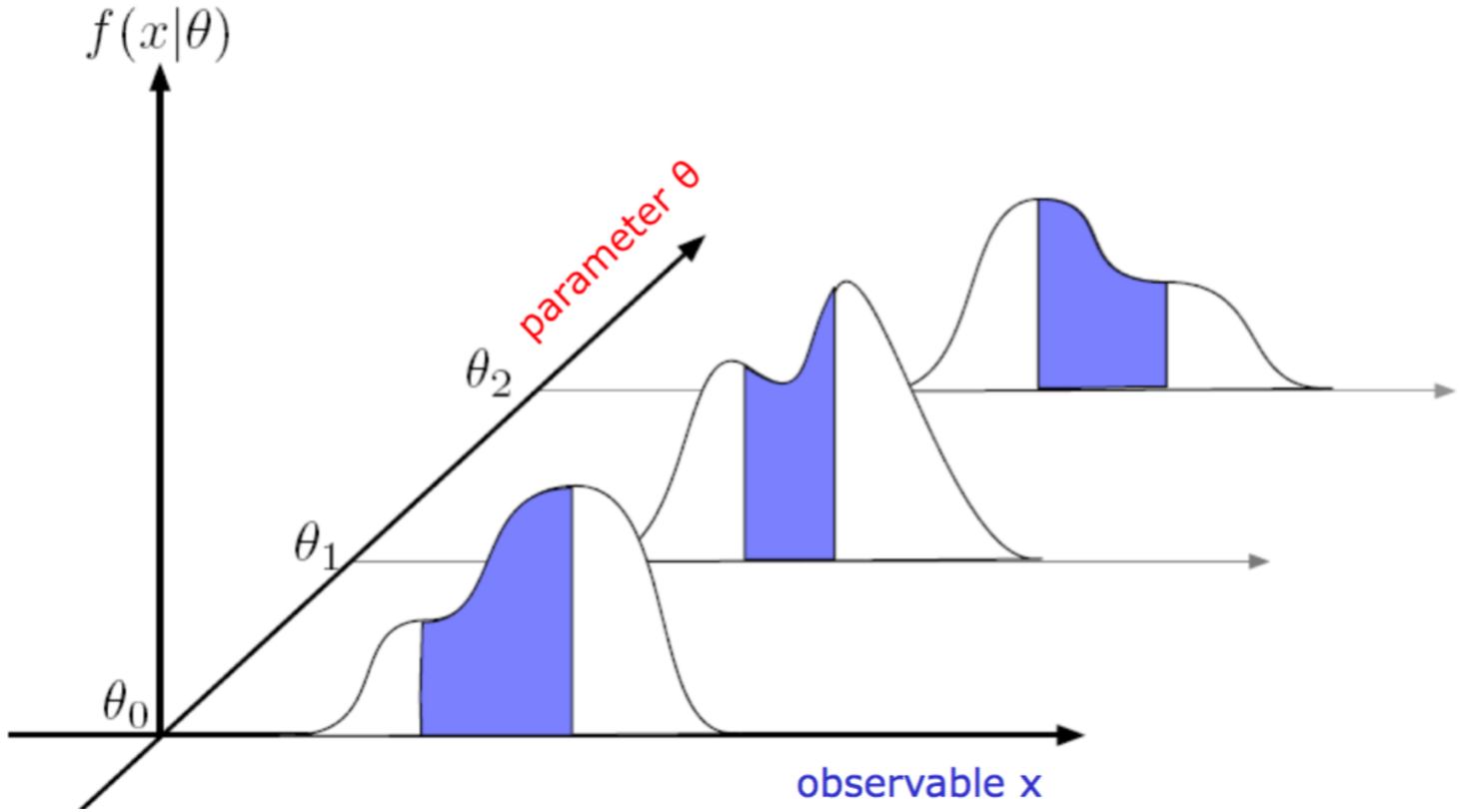
Ordering Rule

- Definition of acceptance interval is not unique
  → Choose shape of interval you want to set here.
  - Algorithm to define acceptance interval is called 'ordering rule'

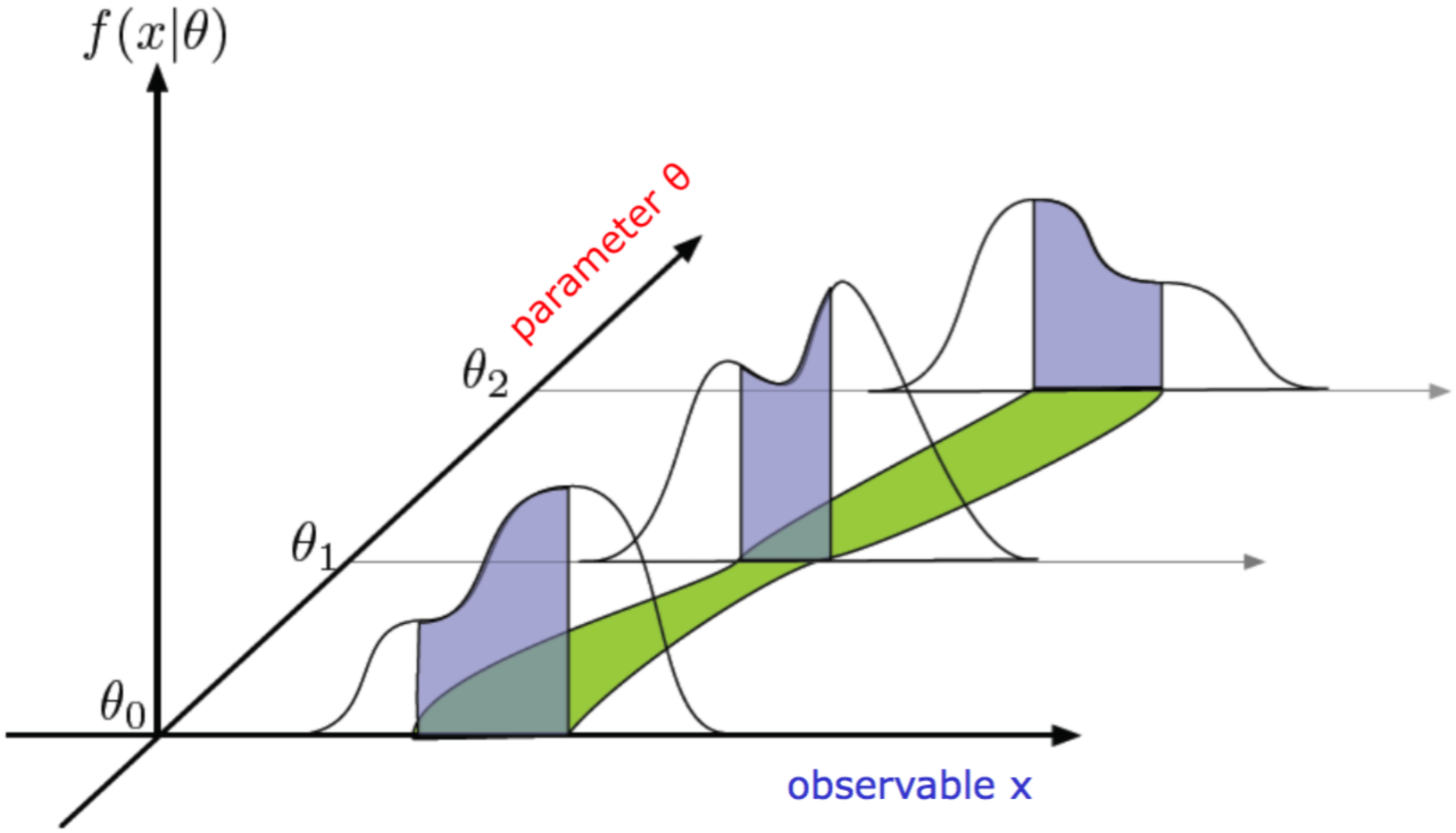


How to construct the interval

- Make an acceptance interval in observable x for each value of parameter θ

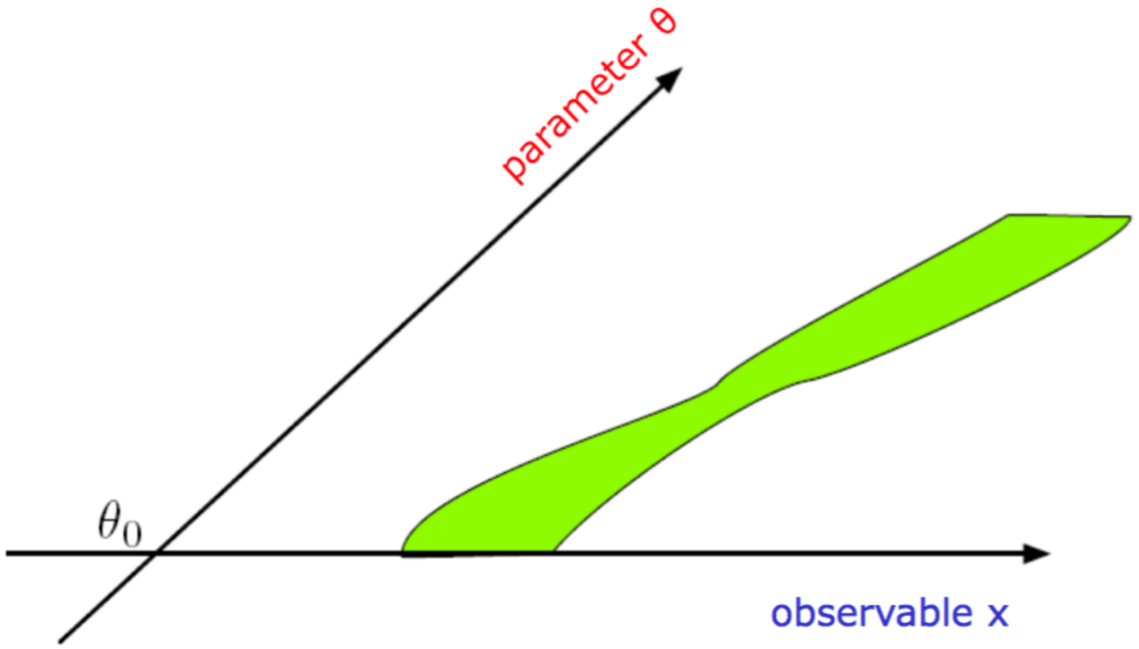


Confidence Belt



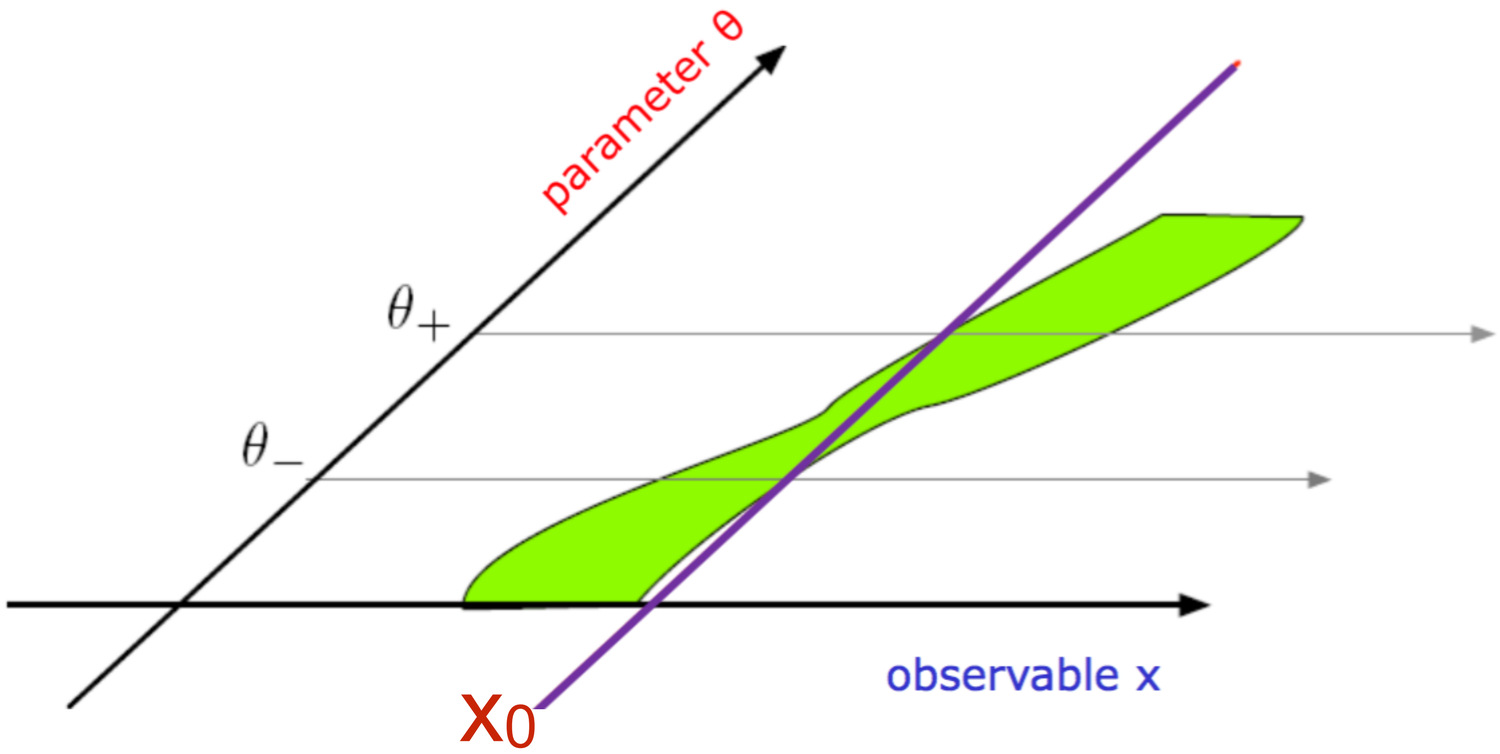
Confidence Belt (2)

- Confidence belt is a property of the model. Can be constructed in advance of any measurement



Interval Construction

- Compare with a given measurement x_0 we can construct the confidence interval $[\theta_+, \theta_-]$
- The interval $[\theta_+, \theta_-]$ has a 68% probability to cover the true value



Meaning of Frequentist Confidence Interval

- A confidence interval is an interval is an interval that contains the true value X% (e.g. 68%) of the time
- Property of the procedure:
  - confidence intervals are a random variable
  - true value is in X% of the intervals in series of repeated measurements (coverage)
- It is not a probability statement on the true value
- In Frequentist statistics the true value is fixed (but unknown)

Interpretation of Confidence Interval

Why isn't everyone a Bayesian ?

My suspicion: it is because most people do not understand the frequentist approach. Frequentist statements and Bayesian statements are thought to be about the same logical concept, and the frequentist statement does not require a prior, so …

A. L. Read, *Presentation of search results: the CL_S technique,* J. Phys. G: Nucl. Part. Phys. **28** (2002) 2693-2704.

nearly all physicists tend to misinterpret frequentist results as statements about the theory given the data.

Frequentist statements are not statements about the model – only about the data in the context of the model. This is not what we wanted to know … At least not the ultimate statement.

SOS 12

Recap: Bayesian Theorem

- Bayesian Theorem

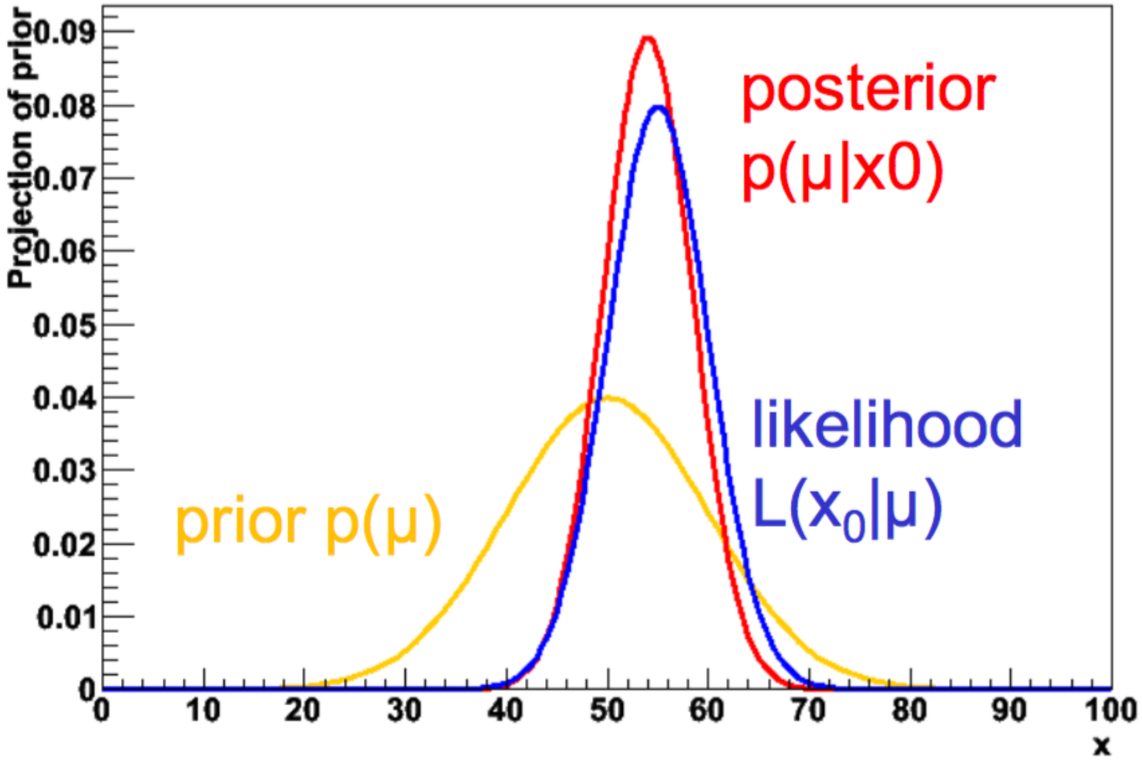
posterior

likelihood

prior

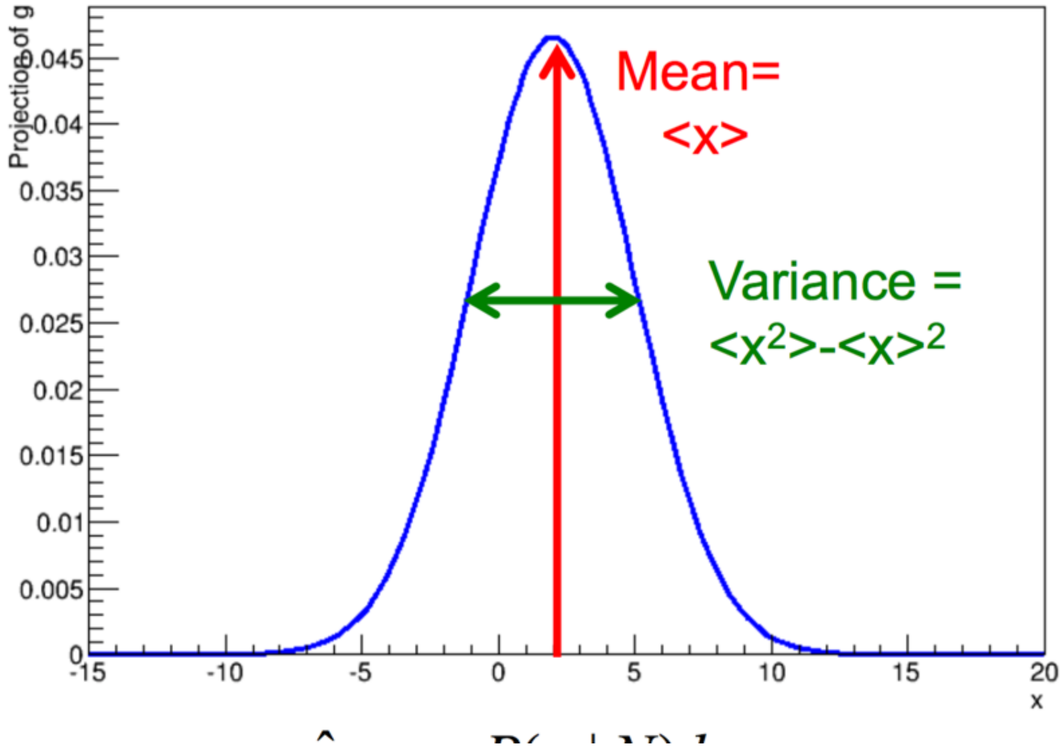
$$f(\theta|x) = \frac{L(x|\theta)p(\theta)}{\int \mathrm{d}\theta L(x|\theta)p(\theta)}$$

normalisation term

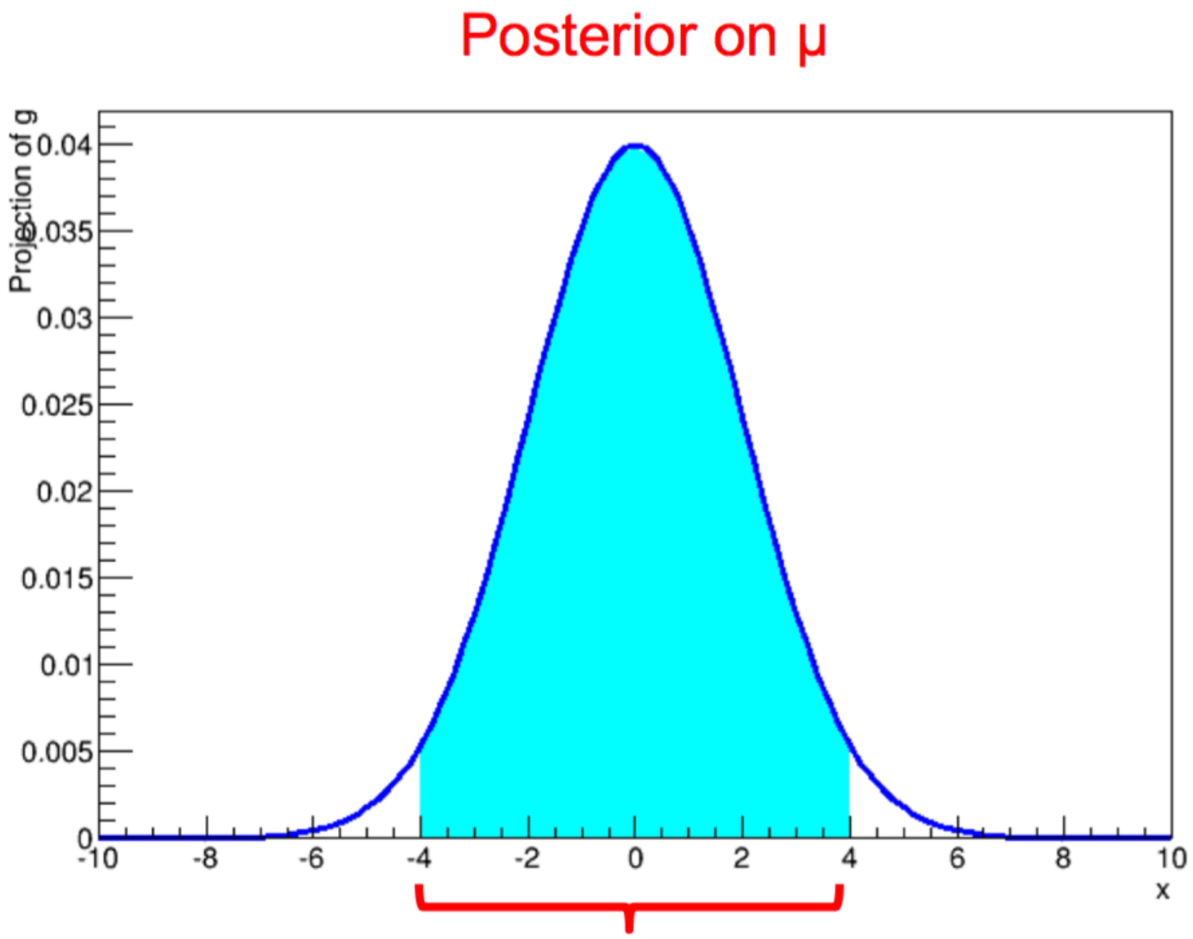


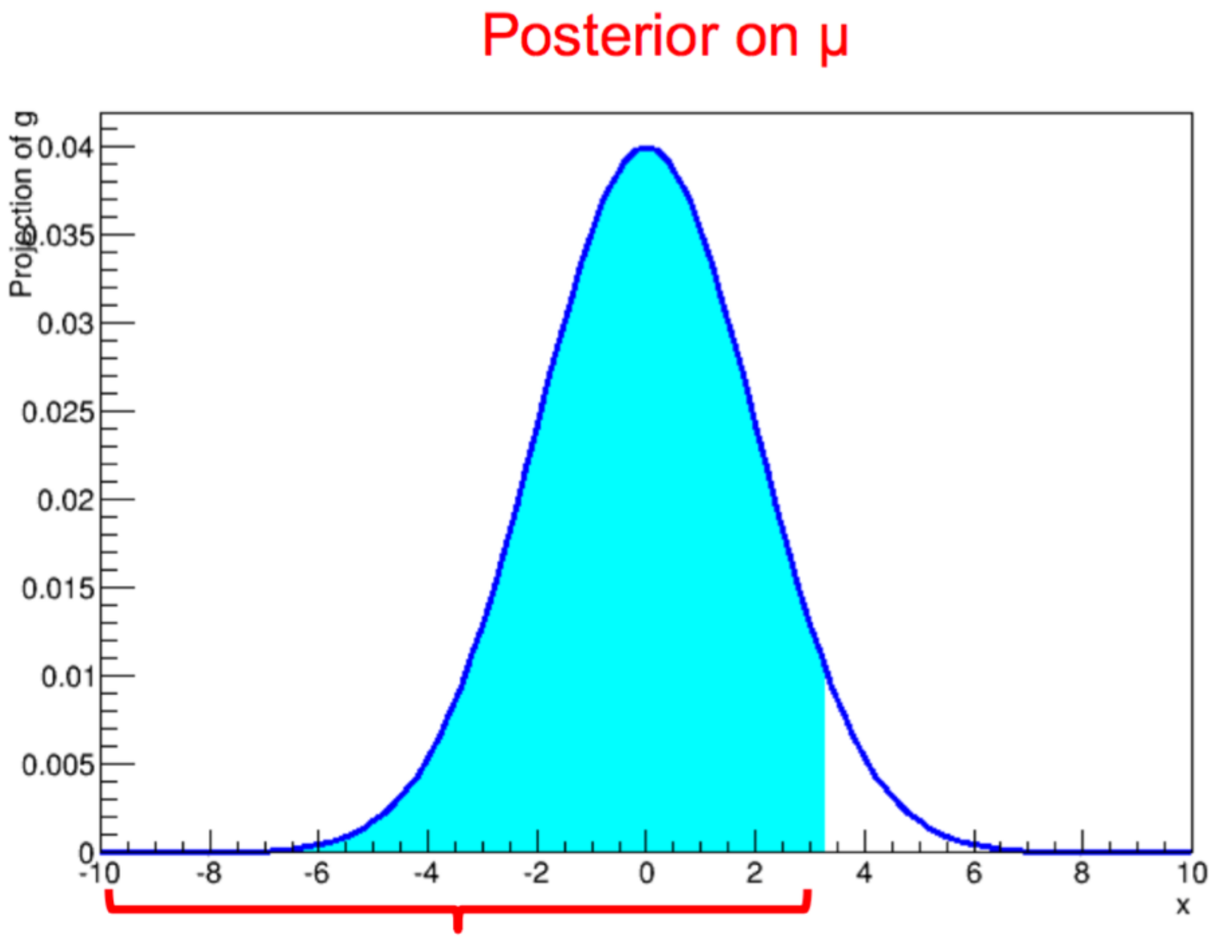
Bayesian Parameter Estimation

- A possible Bayesian parameter estimation is the posterior mean (one could also use posterior mode)
  - Bayesian variance is posterior variance



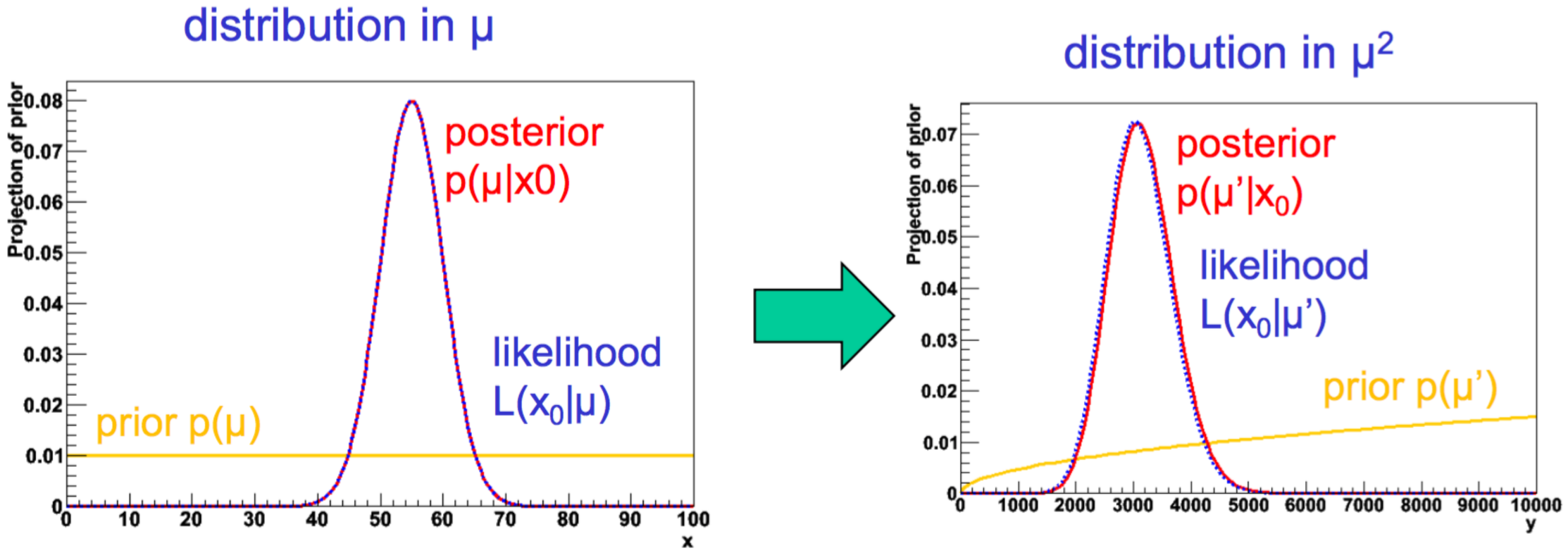
Bayesian Credible Intervals





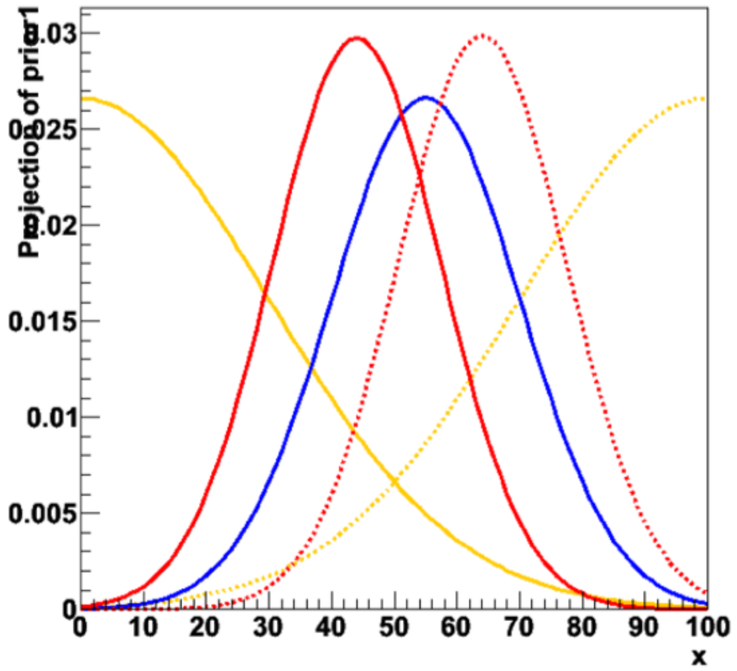
Problem with flat prior

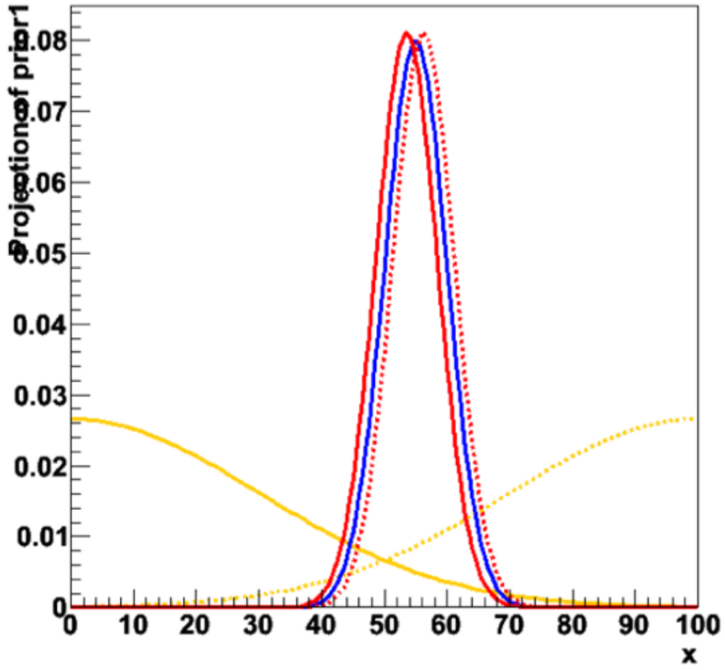
- A prior flat in x is not anymore flat in log(x)

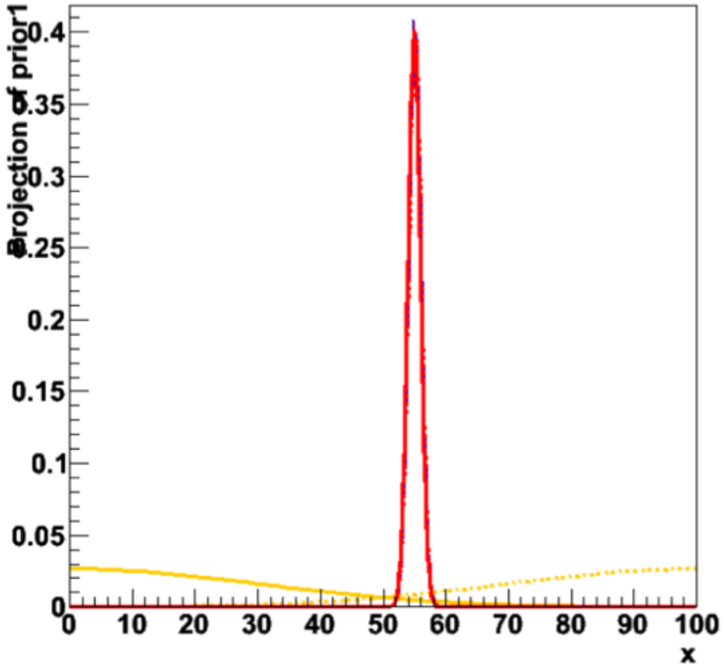


Prior Dependence

- Sensitivity of analysis to prior distributions
  - study result for different prior distributions
  - prior dependence decreases for increasing precision (large statistics)







Frequentist vs Bayesian Intervals

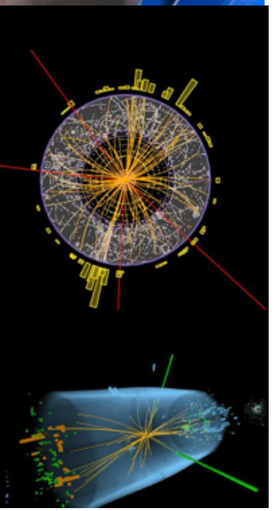
- Interpretation of parameter errors:
  - $\theta = \theta^{est} \pm \delta$
  - $\theta = \theta^{est} {}^{+\delta 2}_{-\delta 1}$

  $\Rightarrow$

  $\theta \in [\theta^{est} - \delta, \theta^{est} + \delta]$

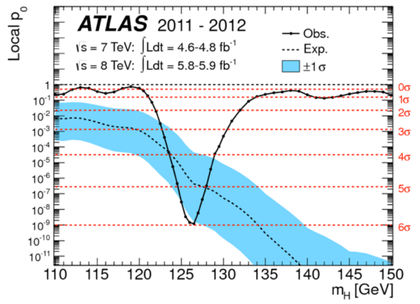
  $\theta \in [\theta^{est} - \delta_1, \theta^{est} + \delta_2]$

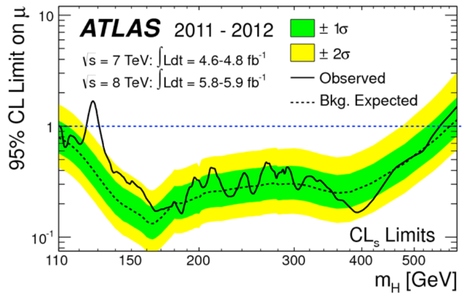
- Frequentist approach:
  - Knowing a parameter within some error means that a large fraction (68% or 95%, usually) of the experiments contain the (fixed but unknown) true value within the quoted confidence interval: $[\theta^{est} - \delta_1, \theta^{est} + \delta_2]$
- Bayesian approach:
  - The posterior PDF for θ is maximum at θ^{est} and its integral is 68% within the range $[\theta^{est} - \delta_1, \theta^{est} + \delta_2]$
- The choice of the interval, i.e.. δ_1 and δ_2 can be done in different ways, e.g: same area in the two tails, shortest interval, symmetric error, …
- Note that both approaches provide the same results for a Gaussian model using a uniform prior, leading to possible confusions in the interpretation



Introduction to RooStats

- Interval estimation tools (Likelihood/Bayesian)
- Hypothesis tests
- Frequentist interval/limit calculator (CLs)
- Exercises on interval/limit estimation and discovery significance (hypothesis test)





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Introduction to RooStats

- Collaborative project to provide and consolidate advanced statistical tools needed by LHC experiments
- Joint contribution from ATLAS, CMS, ROOT and RooFit
  - developments over-sighted by ATLAS and CMS statistics committees
  - initiated from previous code developed in ATLAS and CMS
  - used by both collaborations

RooStats Goal

- Common framework for statistical calculations
  - work on arbitrary models and datasets
    - factorize modeling from statistical calculations
  - implement most accepted techniques
    - frequentists, Bayesian and likelihood based tools
  - possible to easy compare different statistical methods
  - provide utility for combinations of results
  - using same tools across experiments facilitates the combinations of results

Statistical Applications

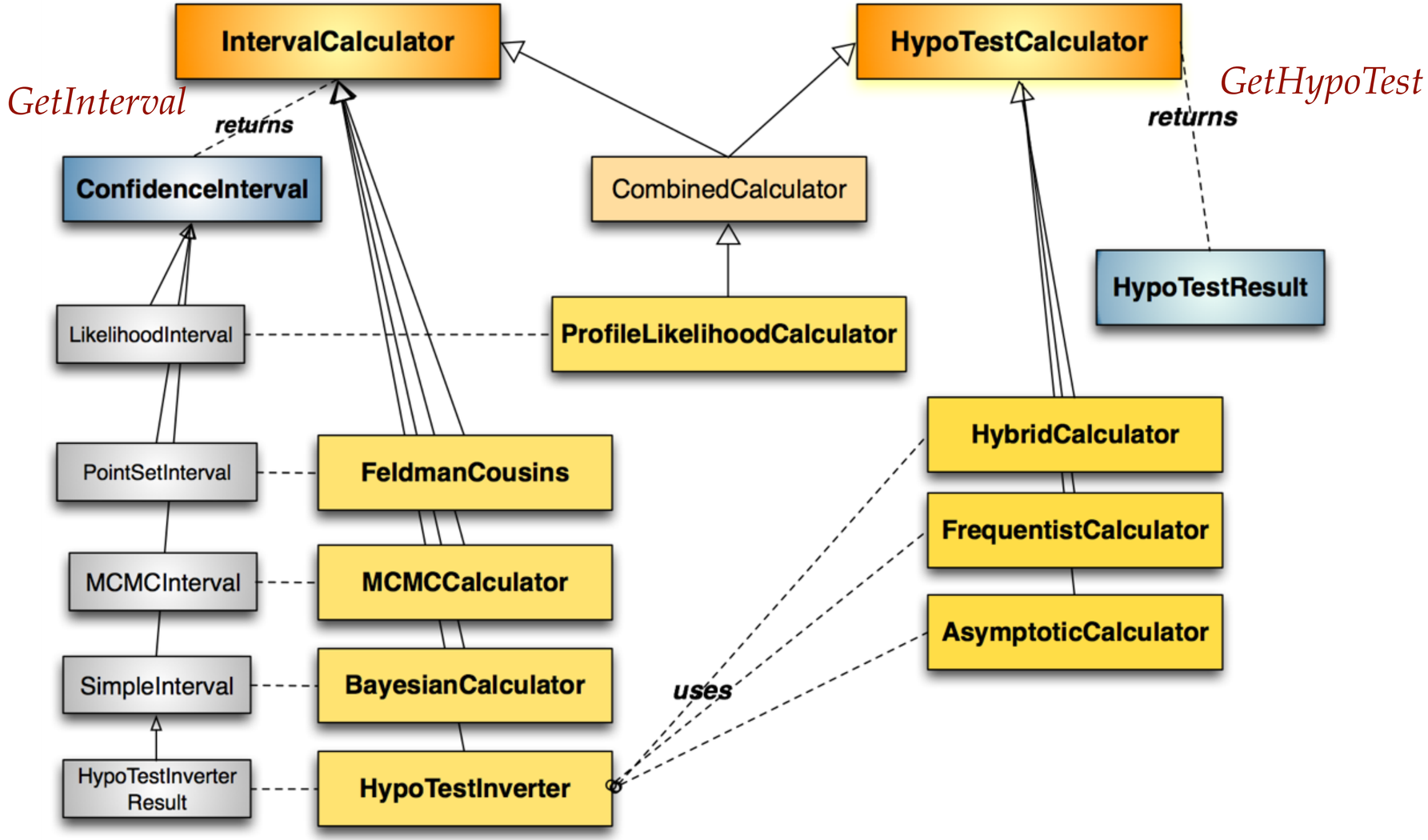
- Statistical problems:
  - point estimation (covered by RooFit)
  - estimation of confidence (credible) intervals
  - hypothesis tests
  - goodness of fit (not yet addressed)

RooStats Technology

- Built on top of RooFit
  - generic and convenient description of models (probability density function or likelihood functions)
  - provides *workspace* (RooWorkspace)
    - container for model and data and can be written to disk
    - inputs to all RooStats statistical tools
    - convenient for sharing models (e.g digital publishing of results)
  - easily generation of models (workspace factory and HistFactory tool)
  - tools for combinations of model (e.g. simultaneous pdf)
- Use of ROOT core libraries:
  - minimization (e.g. Minuit), numerical integration, etc...
  - additional tools provided when needed (e.g. Markov-Chain MC)

RooStats Design

- C++ interfaces and classes mapping to real statistical concepts



RooStats Calculator classes

Interval Calculators

- ProfileLikelihoodCalculator
  - interval estimation using asymptotic properties of the likelihood function
- BayesianCalculator
  - interval estimation based on Bayes theorem using adaptive numerical integration
- MCMCCalculator
  - Bayesian calculator using Markov-Chain Monte Carlo

- HypoTestInverter
  - invert hypothesis test results to estimate an interval
    - CLs limits, FC interval
- NeymanConstruction and FeldmanCousins
  - frequentist interval calculators

HypoTest Calculators

- HybridCalculator, FrequentistCalculator
  - frequentist hypothesis test calculators using toy data (difference in treatment of nuisance parameters)
- AsymptoticCalculator
  - hypothesis tests using asymptotic properties of likelihood function

ModelConfig Class

- **`ModelConfig`** class input to all Roostats calculators
  - contains a reference to the RooFit workspace class
  - provides the workspace meta information needed to run RooStats calculators
    - pdf of the model stored in the workspace
    - what are observables (needed for toy generations)
    - what are the parameters of interest and the nuisance parameters
    - global observables (from auxiliary measurements) for frequentist calculators
    - prior pdf for the Bayesian tools
  - ModelConfig can be imported in workspace for storage and later retrieval

Building ModelConfig Class

- ModelConfig must be built after having the workspace
- Identify all the components which are present in the workspace

```
//specify components of model for statistical tools
ModelConfig  modelConfig("G(xlmu,1)");
modelConfig.SetWorkspace(workspace);
//set components using the name of ws objects
modelConfig.SetPdf( "normal");
modelConfig.SetParameterOfInterest("poi");
modelConfig.SetObservables("obs");
```

- Some tools (Bayesian) require to specify prior pdf

```
//Bayesian tools would also need a prior
modelConfig.SetPriorPdf( "prior");
```

- ModelConfig can be imported in workspace to be then stored in a file

```
//can import modelConfig into workspace too
workspace.import(*modelConfig);
```

Profile Likelihood Calculator

- Method based on properties of the likelihood function
- Profile likelihood function:

$$\lambda(\mu) = \frac{L(x|\mu, \hat{\hat{\nu}})}{L(x|\hat{\mu}, \hat{\nu})}$$

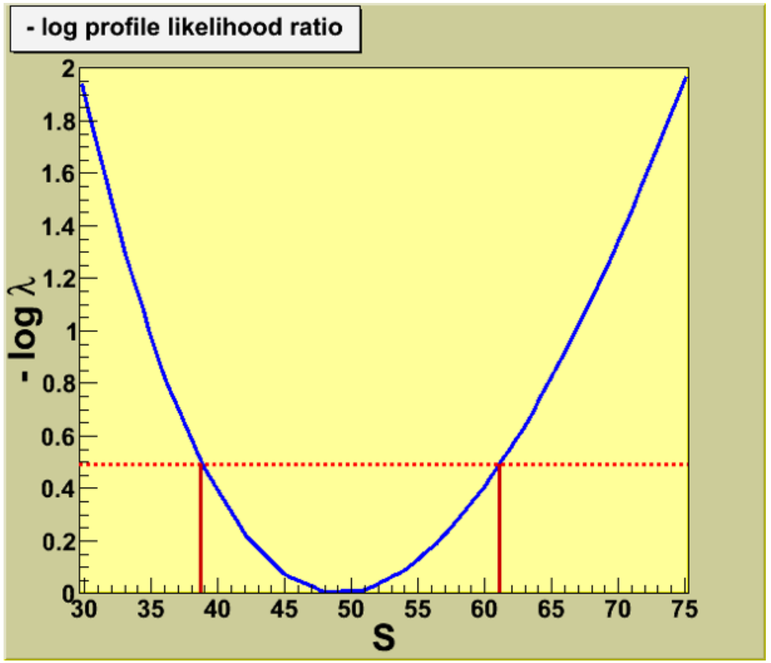
→ maximize w.r.t nuisance parameters ν and fix POI μ

→ maximize w.r.t. all parameters

λ is a function of only the parameter of interest μ

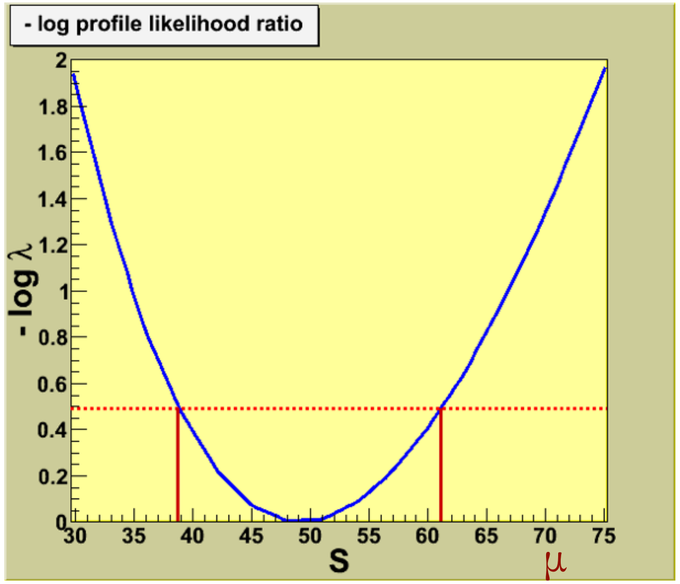
- Uses asymptotic properties of λ based on Wilks' theorem:
- from a Taylor expansion of $\log\lambda$ around the minimum:
  - ➔ $-2\log\lambda$ is a parabola (λ is a gaussian function)
  - ➔ interval on μ from $\log\lambda$ values

- Method of MINUIT/MINOS
  - lower/upper limits for 1D
  - contours for 2 parameters



Using the Profile Likelihood

- For one-dimensional intervals:
  - 68% CL (1 σ) interval : $\Delta \log \boldsymbol{\lambda} = 0.5$
  - 95% CL interval : $\Delta \log \boldsymbol{\lambda} = 1.96$
- **`LikelihoodIntervalPlot`** can plot the 2D contours




```
// 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();
double lowerLimit = interval->LowerLimit(*mu);
double upperLimit = interval->UpperLimit(*mu);

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

Bayesian Analysis in RooStats

- **RooStats** provides classes for
  - marginalize posterior and estimate credible interval

$$P(\mu|x) = \frac{\int L(x|\mu,\nu)\Pi(\mu,\nu)d\nu}{\underbrace{\iint L(x|\mu,\nu)\Pi(\mu,\nu)d\mu d\nu}_{\text{normalisation term}}}$$

posterior probability: $P(\mu|x)$ (POI: μ, data: x)

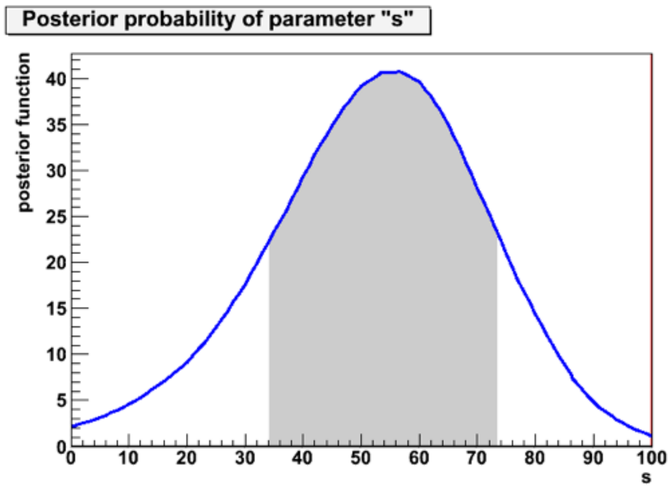
likelihood function: $L(x|\mu,\nu)$

prior probability: $\Pi(\mu,\nu)$

nuisance parameters marginalization: $\int \ldots d\nu$

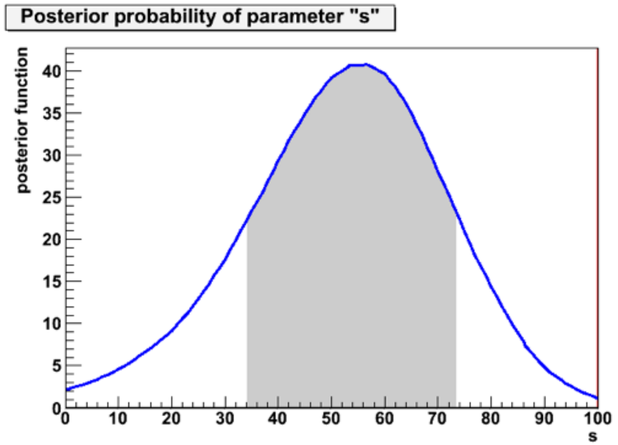
Bayesian Theorem

  - support for different integration algorithms:
    - adaptive (numerical)
    - MC integration
    - Markov-Chain
  - can work with models with many parameters (e.g few hundreds)



Bayesian Classes

- **`BayesianCalculator`** class
  - posterior and interval estimation using numerical integration
  - working only for one parameter of interest but can integrate (marginalize) many nuisance parameters
  - support for different integration algorithms, using **`BayesianCalculator::SetIntegrationType`**
    - adaptive numerical (default type), working only for few nuisances (< 10)
    - Monte Carlo integration (PLAIN, MISER, VEGAS)
    - TOYMC : average from toys where the nuisance parameters are sampled from a given p.d.f. (nuisance pdf), but can work in model with many parameters
  - can compute:
    - central interval
    - one-sided interval (upper limit)
    - a shortest interval
  - provide plot of posterior and interval

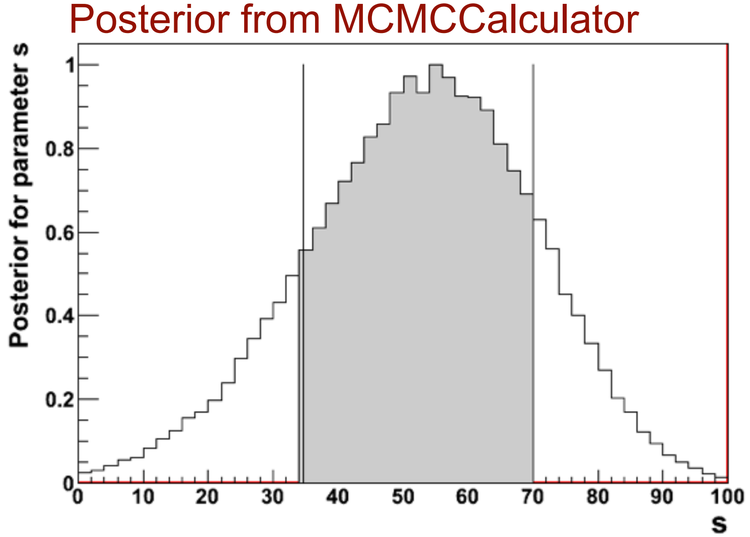


Example: 68% CL central interval

```
BayesianCalculator bc(data, model);
bc.SetConfidenceLevel(0.683);
bc.SetLeftSideTailFraction(0.5);
bc.SetIntegrationType("ADAPTIVE");
SimpleInterval* interval = bc.GetInterval();
double lowerLimit = interval->LowerLimit();
double upperLimit = interval->UpperLimit();
RooPlot * plot = bc.GetPosteriorPlot();
plot->Draw();
```

MCMC Calculator

- **`MCMCCalculator`** class
  - integration using Markov-Chain Monte Carlo (Metropolis Hastings algorithm)
  - can deal with more than one parameter of interest
  - can work with many nuisance parameters
    - e.g. used in Higgs combination with more than 300 r
  - possible to specify ProposalFunction
    - multivariate Gaussian from fit result
    - Sequential proposal
  - can visualize posterior and also the chain result




```
MCMCCalculator mc(data, model);
mc.SetConfidenceLevel(0.683);
mc.SetLeftSideTailFraction(0.5);
SequentialProposal sp(0.1);
mc.SetProposalFunction(sp);
mc.SetNumIters(1000000);
mc.SetNumBurnInSteps(50);
MCInterval* interval = bc.GetInterval();
RooRealVar * s = (RooRealVar*)
model.GetParametersOfInterest()->find("s");
double lowerLimit = interval->LowerLimit(*s);
double upperLimit = interval->UpperLimit(*s);
MCMCIntervalPlot plot(*interval);
plot.Draw();
```

Running RooStats

- RooStats provides standard tutorials taking all as input workspace, ModelConfig and data set names
  - StandardProfileLikelihoodDemo.C

run ProfileLikelihoodCalculator - get interval and produce plot

root[]StandardProfileLikelihoodDemo("ws.root","w","ModelConfig","data")

  - StandardBayesianNumericalDemo.C

run Bayesiancalculator: get a credible interval and produce plot of posterior function

root[]StandardBayesianNumericalDemo("ws.root","w","ModelConfig","data")

  - StandardBayesianMCMCDemo.C

run bayesian MCMCCalculator: get a credible interval and produce plot of posterior function

root[]StandardBayesianMCMCDemo("ws.root","w","ModelConfig","data")

RooStats (Part 2)

- Hypothesis tests in RooStats using toys and asymptotic formulae
- Hypothesis test inversion
  - Limit and interval calculators
    - CLs, Feldman-Cousins

Hypothesis Test

- H_0 : null hypothesis
  - the hypothesis we want to prove that is false
  - e.g. the data contains only background (no Higgs signal)
- H_1 : alternate hypothesis
  - e.g. the data contains signal (Higgs) and background
- α : significance level: probability to reject H_1 if true (error of first kind)
  - α = 1 - selection efficiency
- β : probability to reject H_0 if true (error of second kind)
  - power (probability to reject H0 if H1 is true) = 1 - β
  - β= misidentification probability

Frequentist Hypothesis Tests

- Ingredients:
  - Null Hypothesis: the hypothesis being tested (e.g. $\theta = \theta_0$), assumed to be true and one tries to reject it
  - Alternate Hypothesis: the competitive hypothesis (e.g. $\theta \neq \theta_0$)
  - w is the critical region, a subspace of all possible data:
    - size of test : $\alpha = P(X \in w \mid H_0)$
    - power of test : $1- \beta = P(X \in w \mid H_1)$
  - Test statistics: a function of the data, t(X) ,used for defining the critical region in multidimensional data: $X \in w \rightarrow t(X) \in w_t$

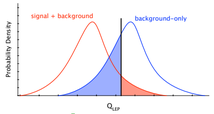
Test Statistics

- Test statistics maps multidimensional space in one, in a way relevant to the hypothesis being tested

RooStats has the three common test statistics used in the field (and more)

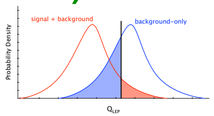
- simple likelihood ratio (used at LEP, nuisance parameters fixed)

$$Q_{LEP} = L_{s+b}(\mu = 1)/L_b(\mu = 0)$$



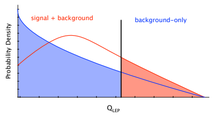
- ratio of profiled likelihoods (used commonly at Tevatron)

$$Q_{TEV} = L_{s+b}(\mu = 1, \hat{\hat{\nu}})/L_b(\mu = 0, \hat{\hat{\nu}}')$$



- profile likelihood ratio (related to Wilks's theorem)

$$\lambda(\mu) = L_{s+b}(\mu, \hat{\hat{\nu}})/L_{s+b}(\hat{\mu}, \hat{\nu})$$



- preferred choice is profile likelihood ratio which has known asymptotic distribution

Likelihood Ratio

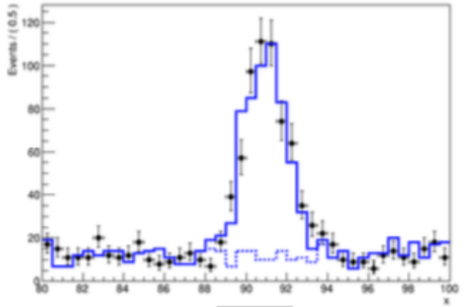
- We make the ratio of likelihoods defined in the two hypotheses:

$$Q = \frac{L_s(x_1, \cdots, x_n)}{L_b(x_1, \cdots, x_n)}$$

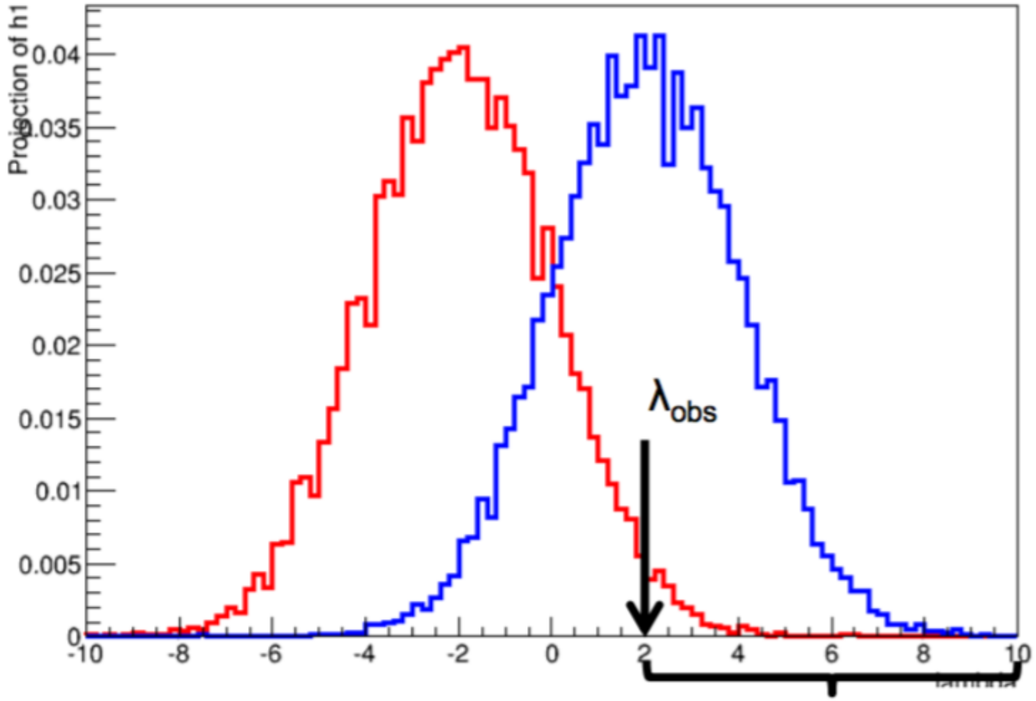
- Q may also depend on a number of unknown parameters $(\theta_1,\ldots,\theta_N)$
- Best discriminator, if the multi-dimensional likelihood is perfectly known (Neyman-Pearson lemma)

p-value

- p-value with likelihood ratio test statistics



$$\lambda(\vec{N}) = \frac{L(\vec{N} \mid H_{s+b})}{L(\vec{N} \mid H_b)}$$



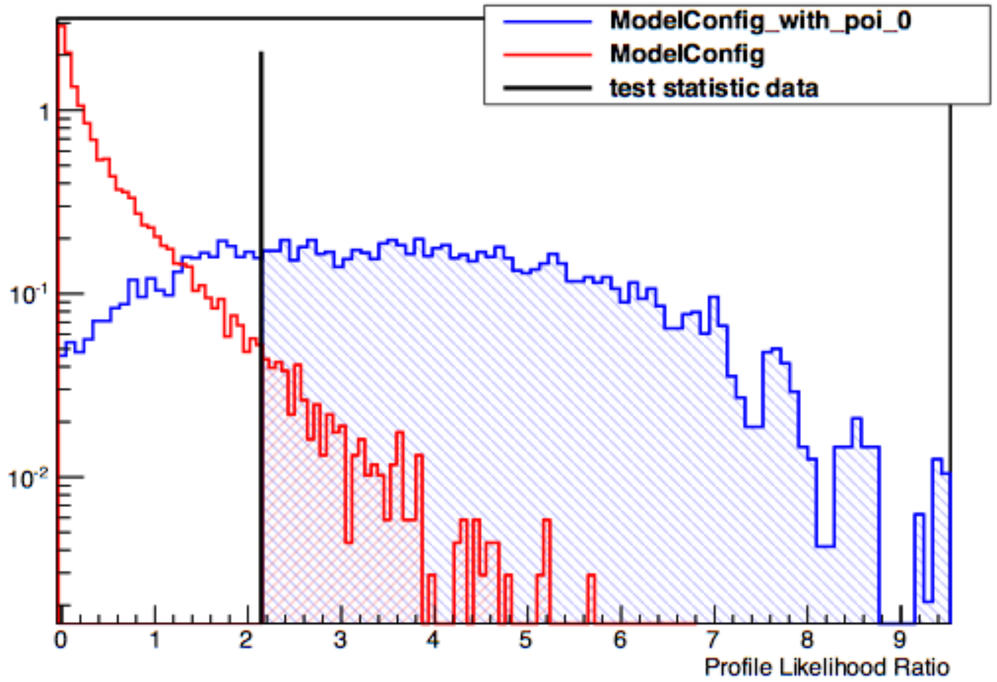
$$p \quad value = \quad f(\quad \mid H_b)$$

obs

- *Except that we generally don't know distribution f(λ)…*

RooStats Hypothesis Test

- Define null and alternate model using ModelConfig
  - can use ModelConfig::SetSnapshot(const RooArgSet &) to define parameter values for the null in case of a common model (e.g. μ = 0 for the B model)
- Select test statistics to use
- Select calculator
  - Use toys or asymptotic formula to get sampling distribution of test statistics
  - FrequentistCalculator or HybridCalculator have different treatment of nuisance parameters



FrequentistCalculator

- Generate toys using nuisance parameter at their conditional ML estimate ($\theta = \theta_{\mu}$) by fitting them to the observed data
- Treat constraint terms in the likelihood (e.g. systematic errors) as auxiliary measurements
  - introduce global observables which will be varied (tossed) for each pseudo-experiment
  - $L = Poisson(n_{obs} | \mu + b) \; Gaussian(b_0 | b, \sigma_b)$
    - b_0 is a global observables, varied for each toys but it needs to be considered constant when fitting
    - n_{obs} is the observable which is part of the data set
    - μ is the parameter of interest (poi)
    - b is the nuisance parameter

HybridCalculator

- Nuisance parameters are integrated using their pdf (the constraint term) which is interpreted as a Bayesian prior
  - integration is done by generating for each toys different nuisance parameters values
  - need to have a pdf for the nuisance parameters (often it can be derived automatically from the model)

$$L = \text{Poisson}(n_{obs} \mid \mu + b) \, \text{Gaussian}(b \mid b_0, \sigma_b)$$

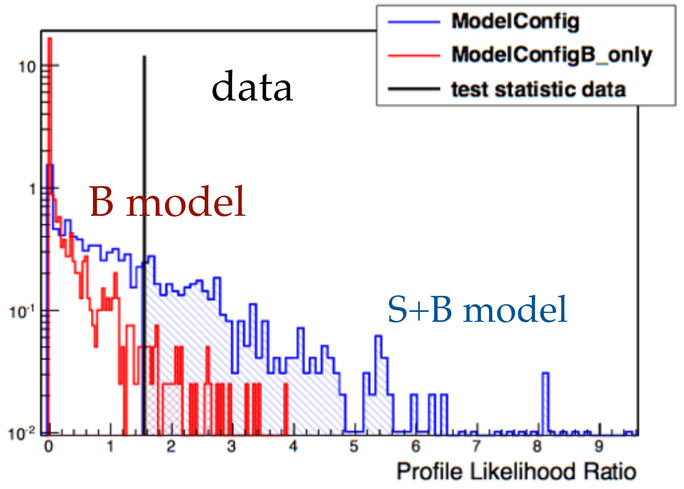
$$L = \int \text{Poisson}(n_{obs} \mid \mu + b) \, \text{Gaussian}(b \mid b_0, \sigma_b) \, db$$

Example: FrequentistCalculator

- Define the models
  - N.B for discovery significance null is B model and alt is S+B

```
// create first HypoTest calculator (data, alt model , null model)
FrequentistCalculator fcalc(*data, *sbModel, *bModel);

// create the test statistics
ProfileLikelihoodTestStat profll(*sbModel->GetPdf());
// use one-sided profile likelihood for discovery tests
profll.SetOneSidedDiscovery(true);

// configure  ToyMCSampler and set the test statistics
ToyMCSampler *toymcs = (ToyMCSampler*)fcalc.GetTestStatSampler();
toymcs->SetTestStatistic(&profll);

fcalc.SetToys(1000,1000);  // set number of toys for (null, alt)

// run the test
HypoTestResult * r = fcalc.GetHypoTest();
r->Print();

// plot test statistic distributions
HypoTestPlot * plot = new HypoTestPlot(*r);
plot->Draw();
```

```
Results HypoTestCalculator_result:
 - Null p-value = 0.034 +/- 0.00573097
 - Significance = 1.82501 sigma
 - Number of Alt toys: 1000
 - Number of Null toys: 1000
```

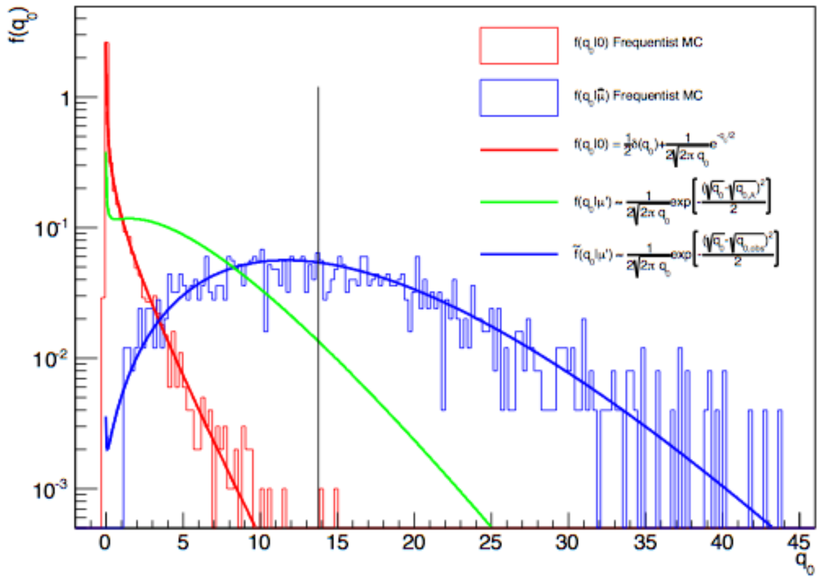


AsymptoticCalculator

- Use the asymptotic formula for the test statistic distributions
- one-sided profile likelihood test statistic:
  - null model ($\mu = \mu_{TEST}$)
    - half X^2 distribution
  - alt model ($\mu \neq \mu_{TEST}$)
    - non-central X^2
    - use Asimov data to get the non centrality parameter $\Lambda = (\mu - \mu_{TEST})/\sigma$
- p-values for null and alternate can be obtained without generating toys

$$\lambda(\mu) = \frac{L(x|\mu, \hat{\hat{\nu}})}{L(x|\hat{\mu}, \hat{\nu})}$$

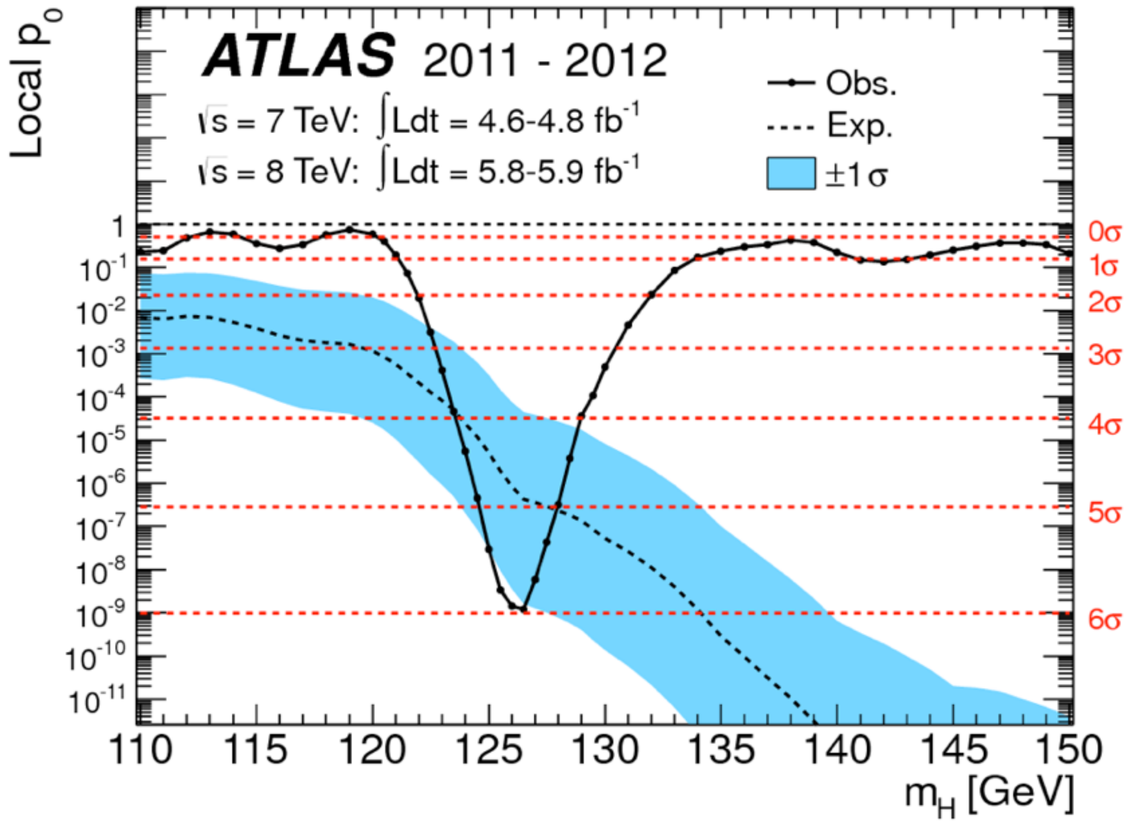
$\lambda(\mu) = 0$ for
$\hat{\mu} < 0$ (discovery)
$\hat{\mu} < \mu_{TEST}$ (limits)



➡ see Cowan, Cranmer, Gross, Vitells, arXiv:1007.1727,EPJC 71 (2011) 1-1

Example: Discovery Significance

- Performing the tests for different mass hypotheses (*i.e* different signal models):



Inversion of Hypothesis Tests

- one-to-one mapping between hypothesis tests and confidence intervals

Table 20.1 Relationships between hypothesis testing and interval estimation

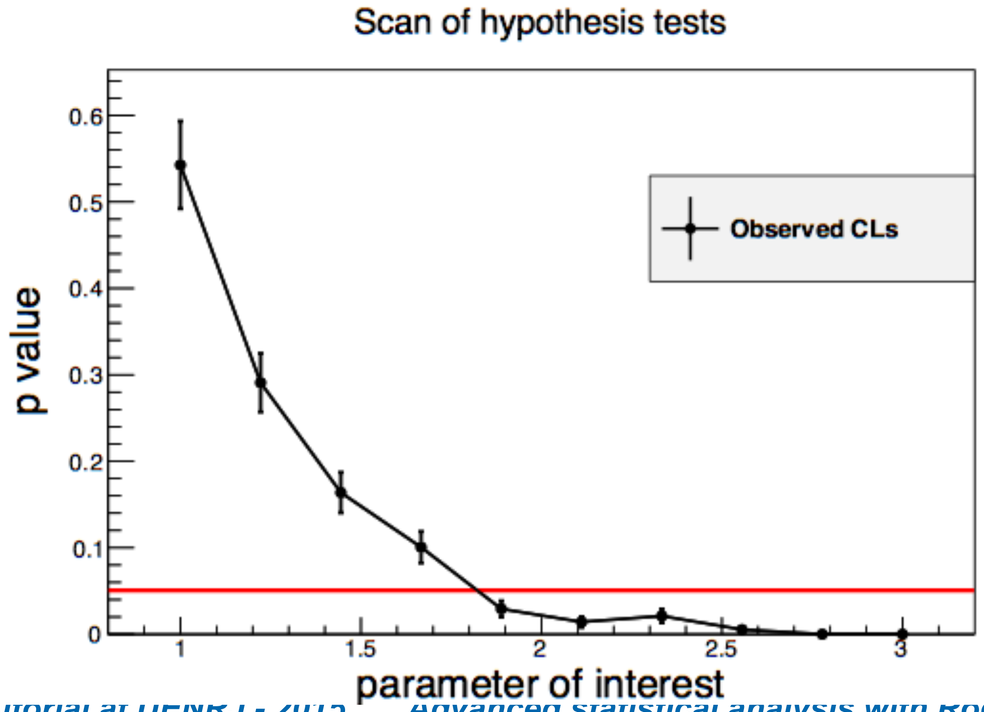
Property of test	Property of corresponding confidence interval
Size $= \alpha$	Confidence coefficient $= 1 - \alpha$
Power = probability of rejecting a false value of $\theta = 1 - \beta$	Probability of not covering a false value of $\theta = 1 - \beta$
Most powerful	Uniformly most accurate
$\longleftarrow$	$\left\{ \begin{array}{c} \textit{Unbiased} \\ 1 - \beta \geq \alpha \end{array} \right\}$ $\longrightarrow$
Equal-tails test $\alpha_1 = \alpha_2 = \frac{1}{2}\alpha$	Central interval

from G. Feldman visiting Harvard statistics department

They explained that in statistical theory there is a one-to-one correspondence between a hypothesis test and a confidence interval. (The confidence interval is a hypothesis test for each value in the interval.) The Neyman-Pearson Theorem states that the likelihood ratio gives the most powerful hypothesis test. Therefore, it must be the standard method of constructing a confidence interval.

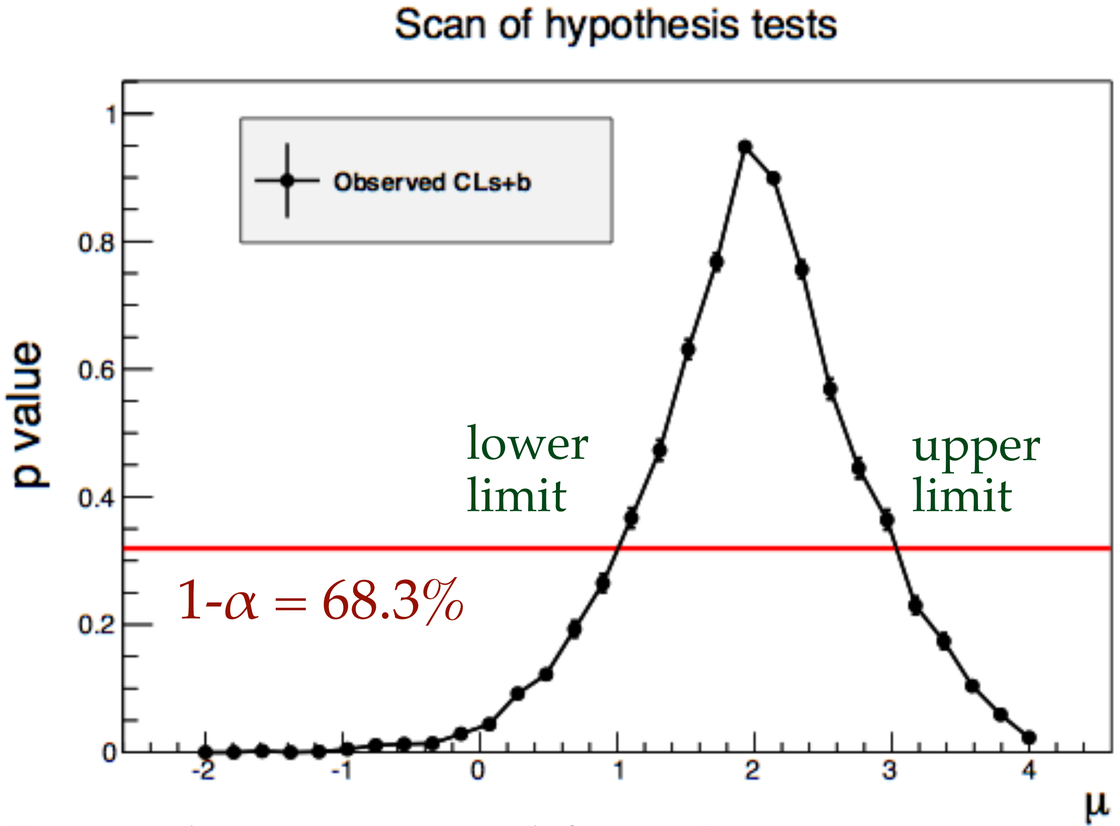
Hypothesis Test Inversion

- Performing an hypothesis test at each value of the parameter
- Interval can be derived by inverting the p-value curve, function of the parameter of interest (μ)
  - value of μ which has p-value α (e.g. 0.05), is the upper limit of 1-α confidence interval (e.g. 95%)



Hypothesis Test Inversion

- use one-sided test for upper limits (e.g. one-side profile likelihood test statistics)
- use two-sided test for a 2-sided interval



Example: 1-σ interval for a Gaussian measurement

HypoTestInverter class

- Input is an Hypothesis Test calculator:
  - Frequentist/Hybrid/AsymptoticCalculator
  - possible to customize test statistic, number of toys, etc..
    - N.B: null model is S+B, alternate is B only model
- Compute an Interval (result is a **`ConfInterval`** object):
  - scan given interval of μ and perform hypothesis tests
  - compute upper/lower limit from scan result
    - can use $CL_s = CL_{s+b} / CL_b$ for the p-value
  - result (**`HypoTestInverterResult`**) contains all the hypothesis test results for each scanned μ value
  - can compute expected limits and bands

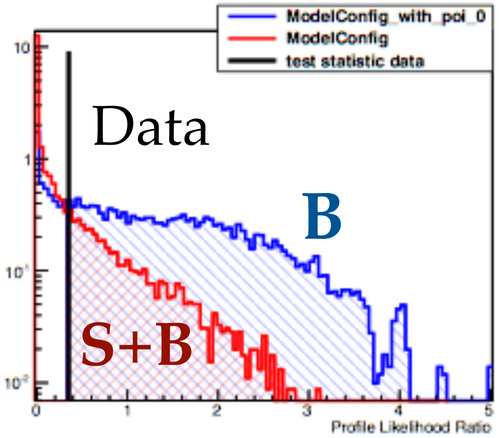
HypoTestInverter

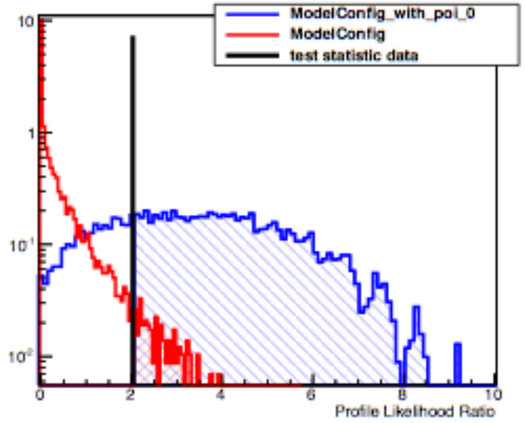
- **`HypoTestInverter`** class in RooStats

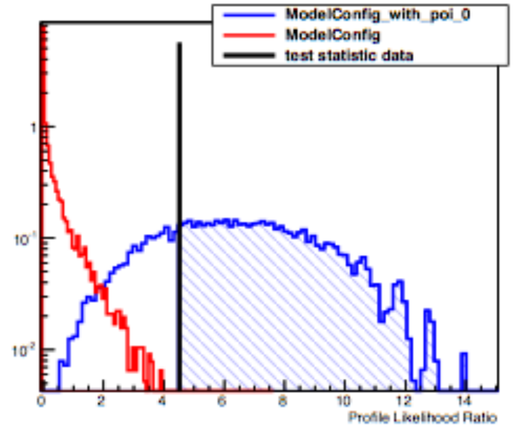
```
// create first HypoTest calculator (N.B null is s+b model)
FrequentistCalculator fc(*data, *bModel, *sbModel);

HypoTestInverter calc(*fc);
calc.UseCLs(true);

// configure  ToyMCSampler and set the test statistics
ToyMCSampler *toymcs = (ToyMCSampler*)fc.GetTestStatSampler();

ProfileLikelihoodTestStat profll(*sbModel->GetPdf());
// for CLs (bounded intervals) use one-sided profile likelihood
profll.SetOneSided(true);
toymcs->SetTestStatistic(&profll);

// configure and run the scan
calc.SetFixedScan(npoints,poimin,poimax);
HypoTestInverterResult * r = calc.GetInterval();

// get result and plot it
double upperLimit = r->UpperLimit();
double expectedLimit = r->GetExpectedUpperLimit(0);

HypoTestInverterPlot *plot = new HypoTestInverterPlot("hi","",r);
plot->Draw();
```

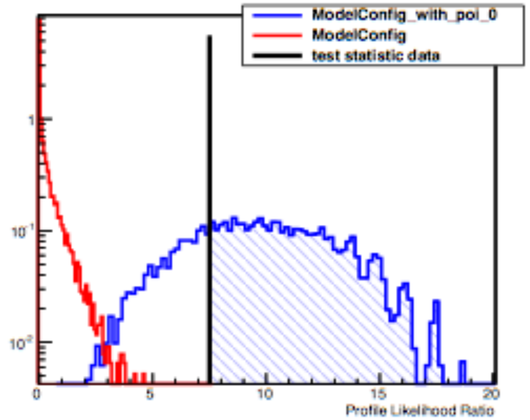
Running the HypoTestInverter

Hypothesis test results for each scanned point





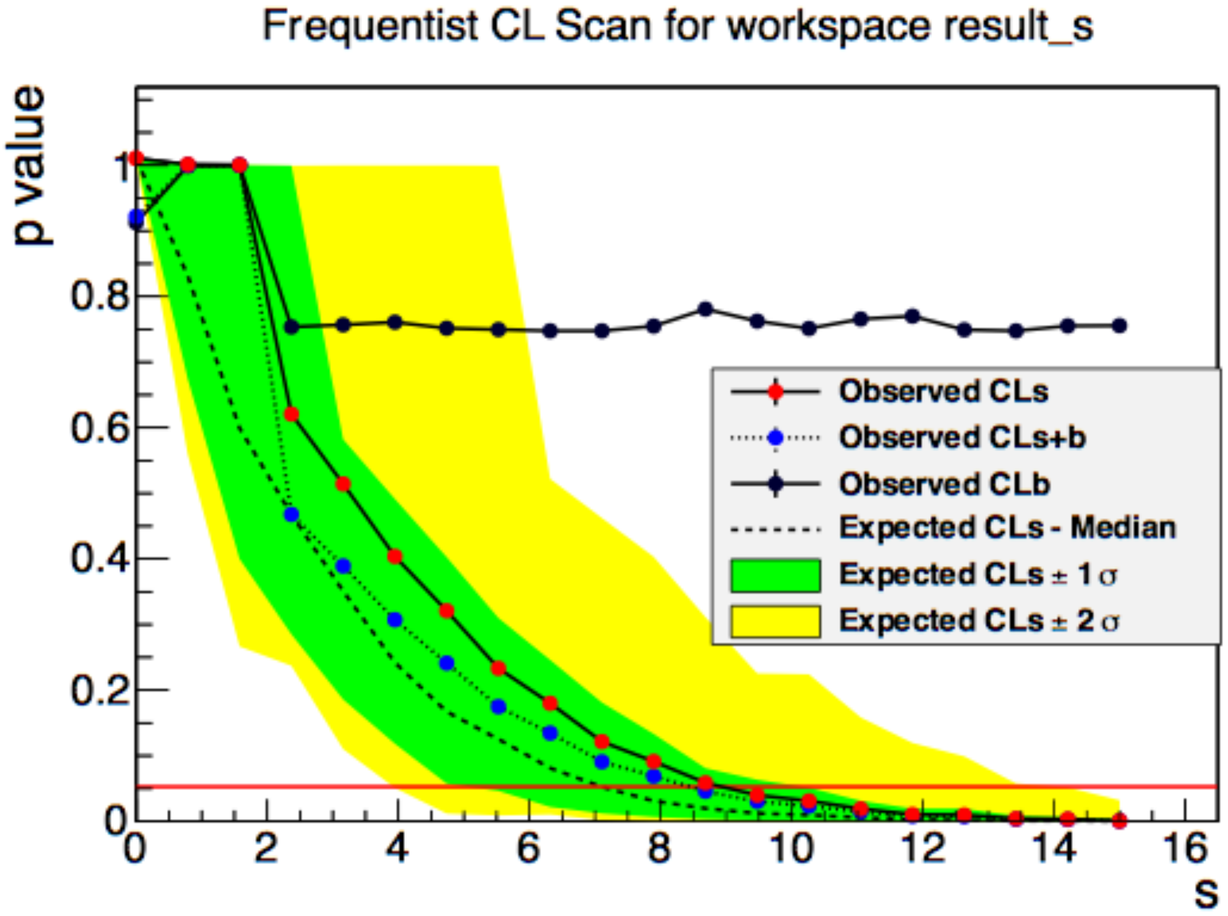




p-value, CL_{s+b} (or CL_b) is integral of S+B (or B) test statistic distribution from data value

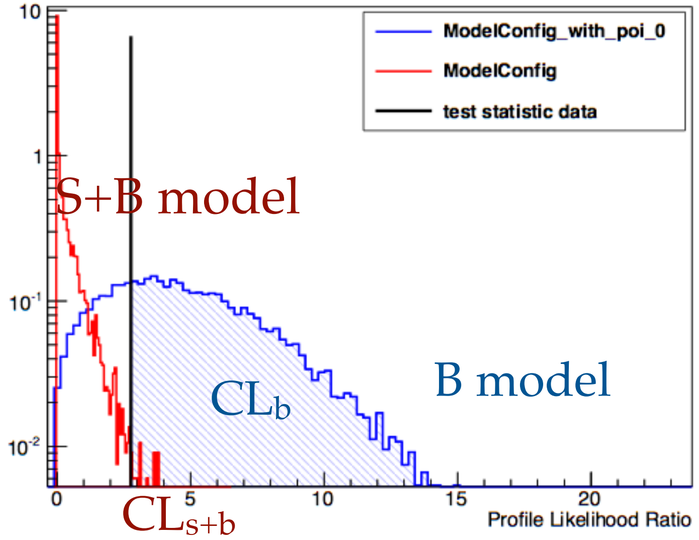
Running the HypoTestInverter (2)

Scan result



How expected limit and bands are obtained ?

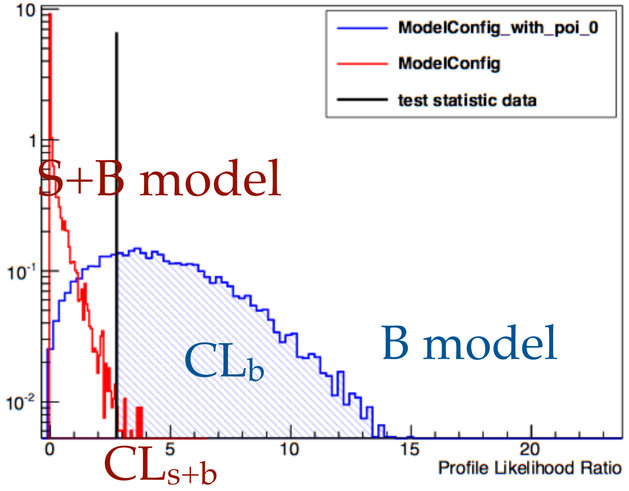
- compute p-value for quantiles (median, +/1,2 sigma) of the B model test statistic distribution (*i.e.* use quantile as the observed value)

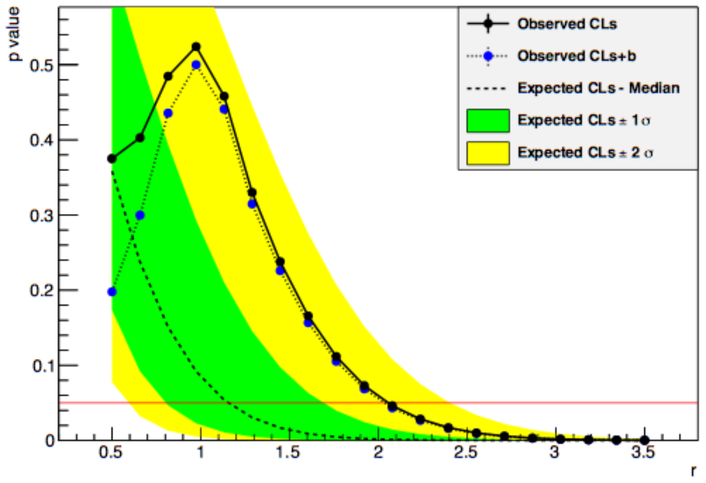


Asymptotic Limits

- **`AsymptoticCalculator`** class for HypoTestInverter
  - use the asymptotic formula for the test statistic distributions
    - χ^2 approximation for the profile likelihood ratio
      - see G. Cowan *et al.*, arXiv:1007.1727,EPJC 71 (2011) 1-1
  - p-values CL_{s+b} (null) and CL_b (alt) obtained without generating toys
  - also expected limits from the alt distribution

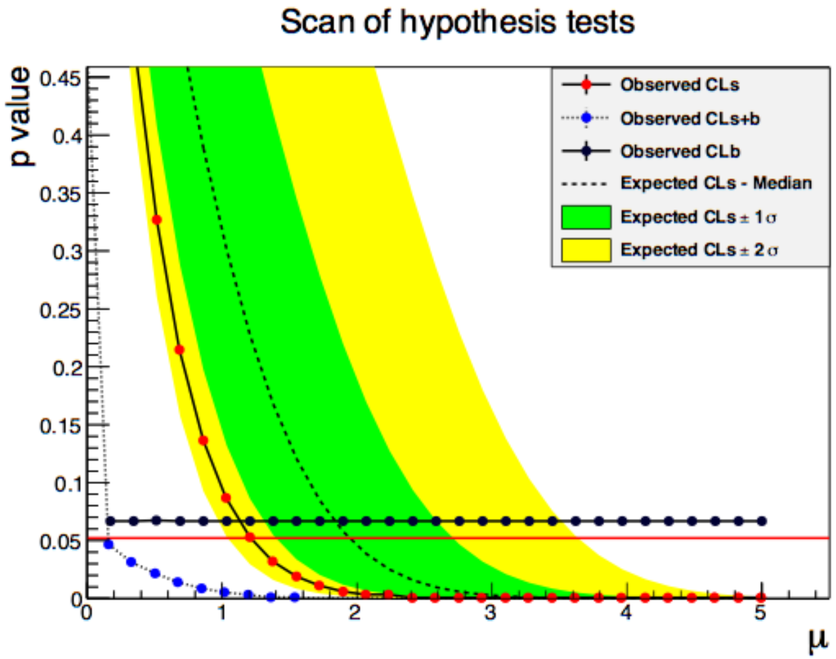
```
// create first HypoTest calculator (N.B null is s+b model)
AsymptoticCalculator ac(*data, *bModel, *sbModel);

HypoTestInverter calc(*ac);
// run inverter same as using other calculators
........
```



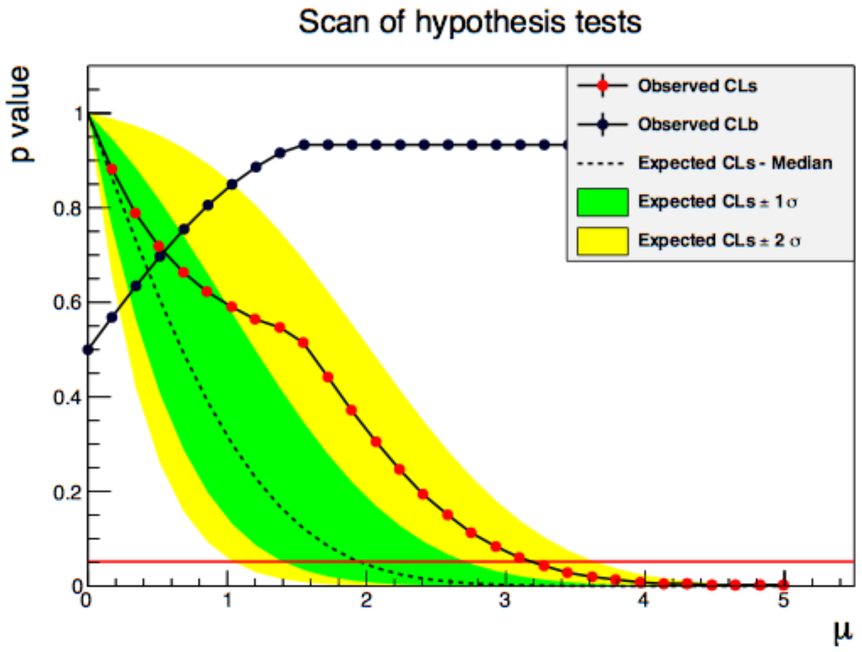


Example of Scan

- 95% CL limit on a Gaussian measurement:
  - Gauss(x,μ,1), with μ≥0



deficit, observation x = -1.5

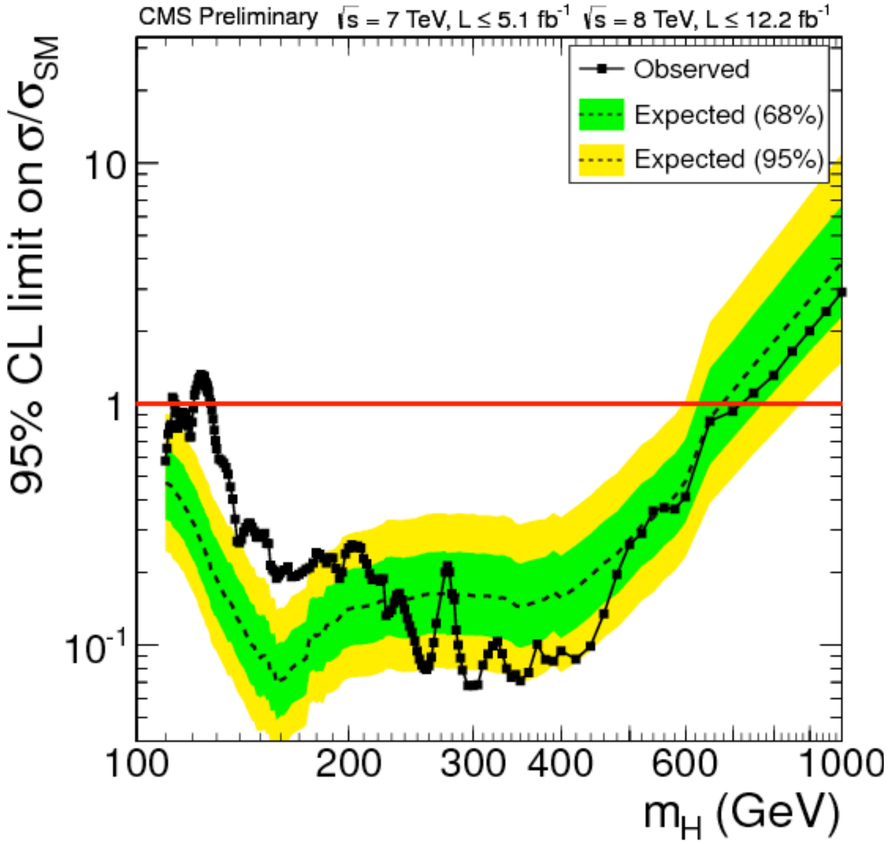


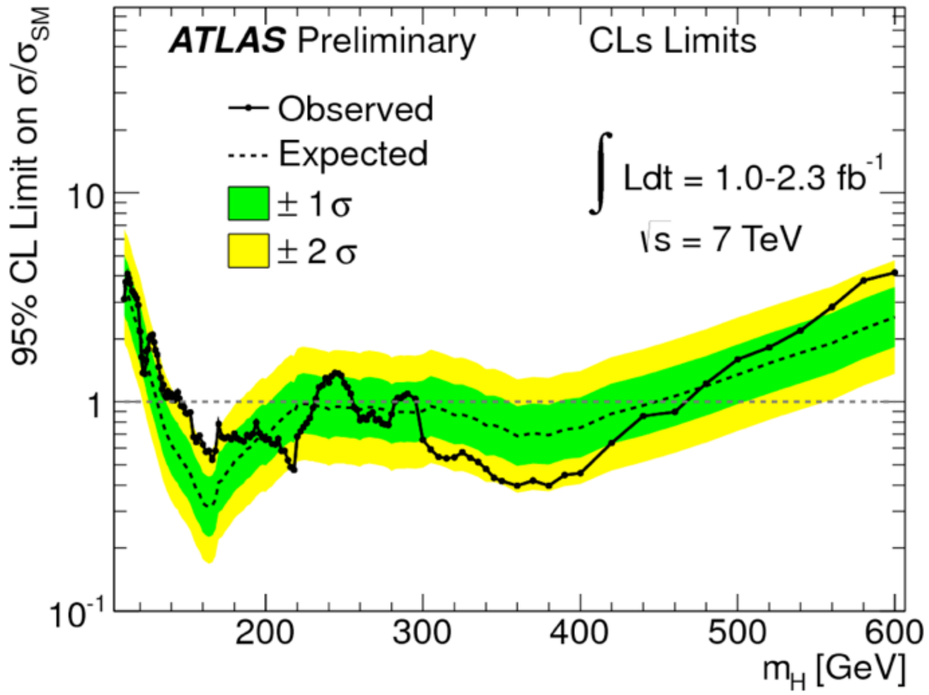
excess, observation x = 1.5

use CL_s as p-value to avoid setting limits which are too good

Example: Computing Limits

- By computing limits for different mass hypothesis:



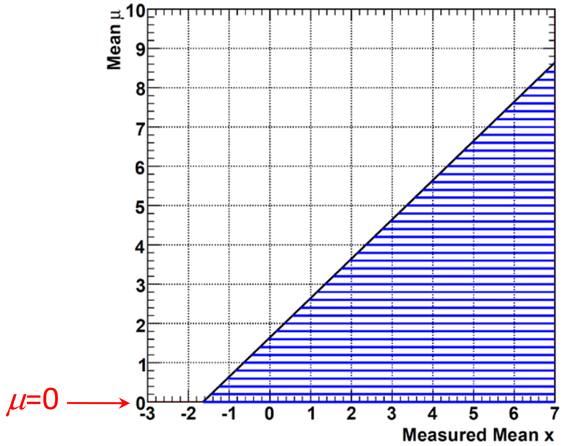


Limits on bounded measurements

from Bob Cousins:

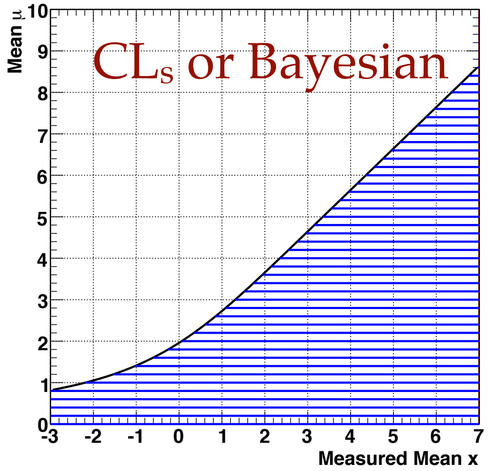
Downward fluctuations in searches for excesses

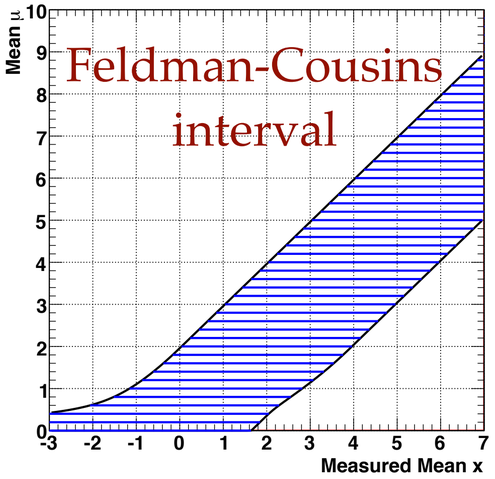
Classic example: Upper limit on mean μ of Gaussian based on measurement *x* (in units of σ).



If μ≥0 in model, as measured x becomes increasingly negative, standard classical upper limit becomes small and then null.

Issue acute 15-25 years ago in expts to measure ν_e mass in (tritium β decay): several measured $m_\nu^2 < 0$.





Frequentist 1-sided 95% C.L. Upper Limits, based on α = 1 – C.L. = 5% (called CL_{sb} at LEP).

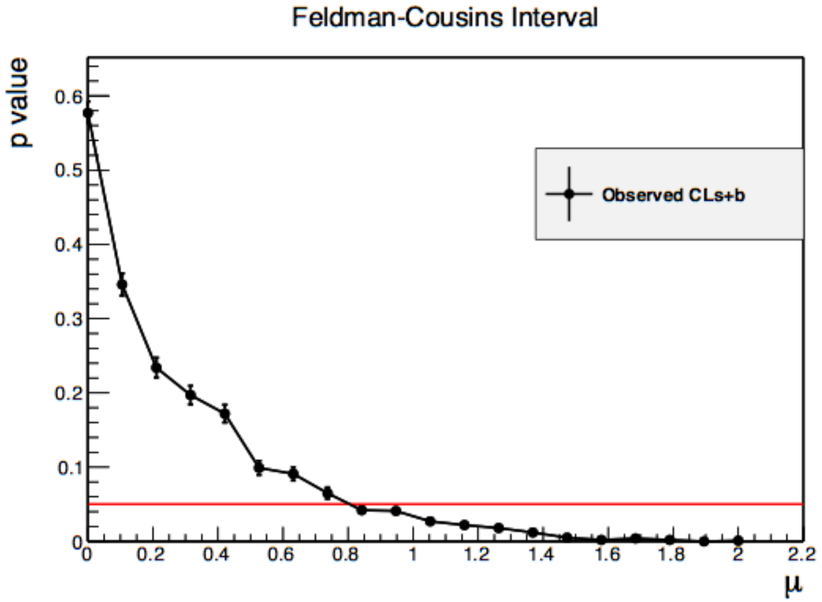
For *x* < –1.64 σ the confidence interval is the *null* set!

Bob Cousins, CMSDAS, 1/2012

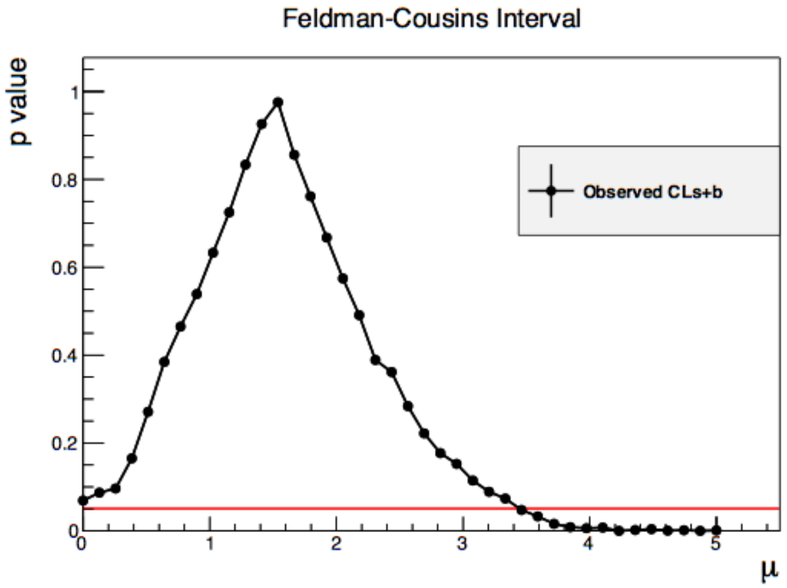
Feldman-Cousins intervals

- HypoTestInverter class can compute also a Feldman-Cousins interval
  - need to use FrequentistCalculator and CL_{s+b} as p-value
  - use the 2-sided profile likelihood test statistic

$$\lambda(\mu) = \frac{L(x|\mu, \hat{\hat{\nu}})}{L(x|\hat{\mu}, \hat{\nu})}$$



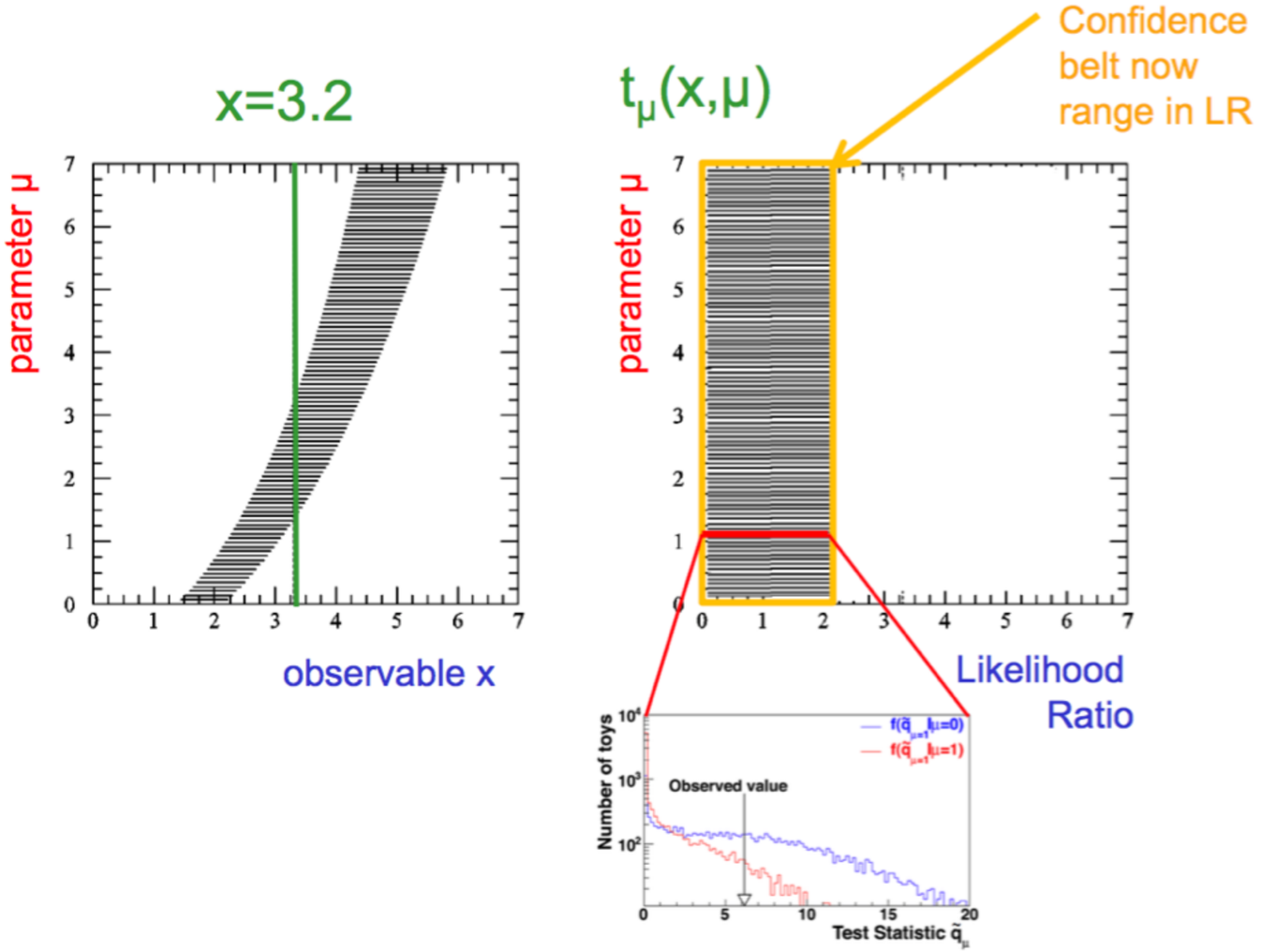
observation x = -1.5



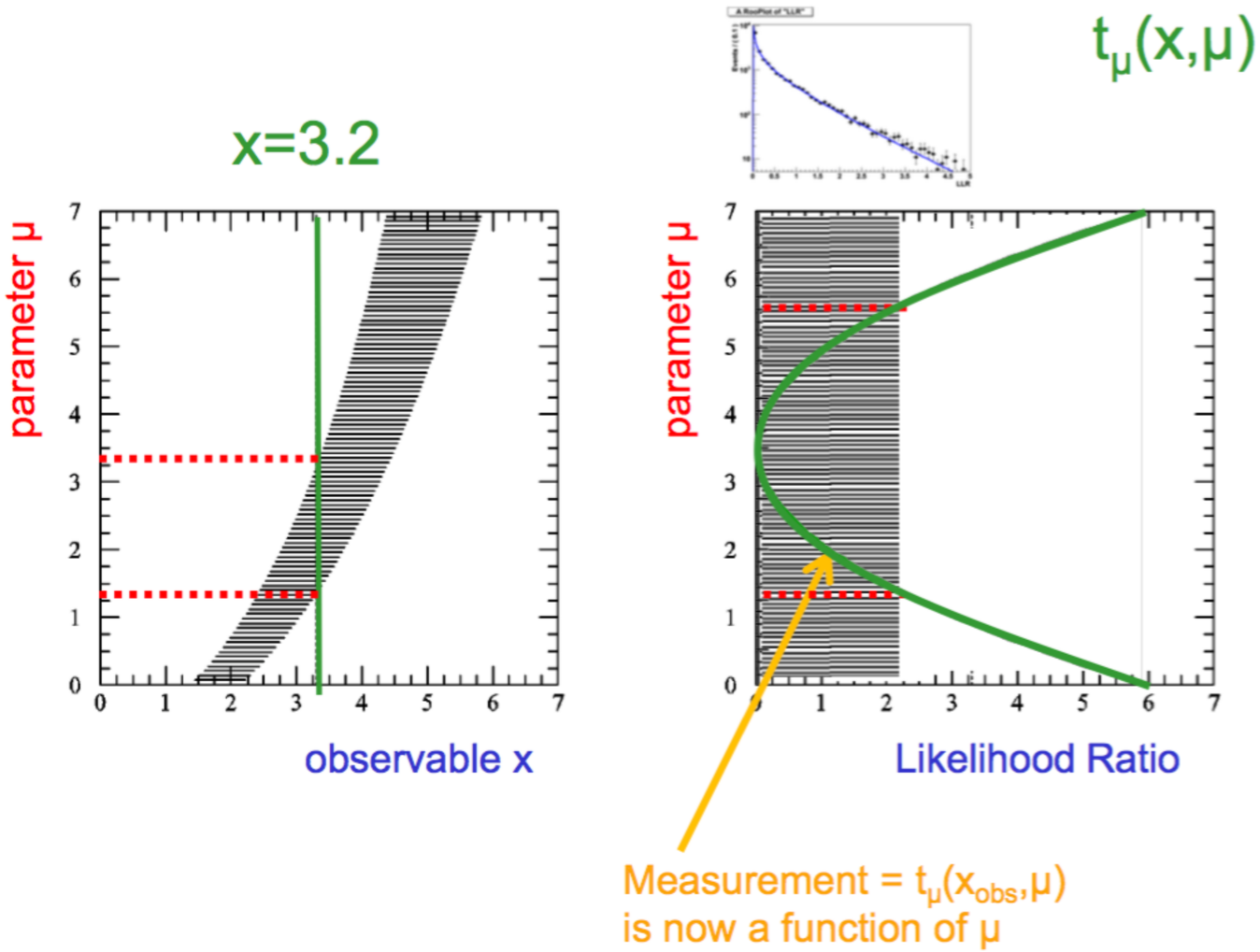
observation x = 1.5

Confidence Interval using the Test Statistic

- Procedure to construct belt with LR is identical:
  obtain distribution of λ for every value of μ to construct belt



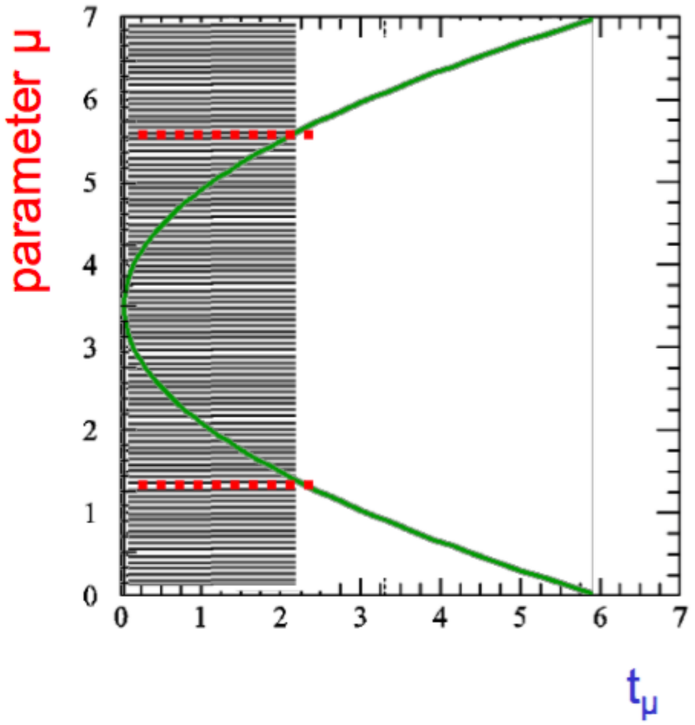
Observed Test Statistic data



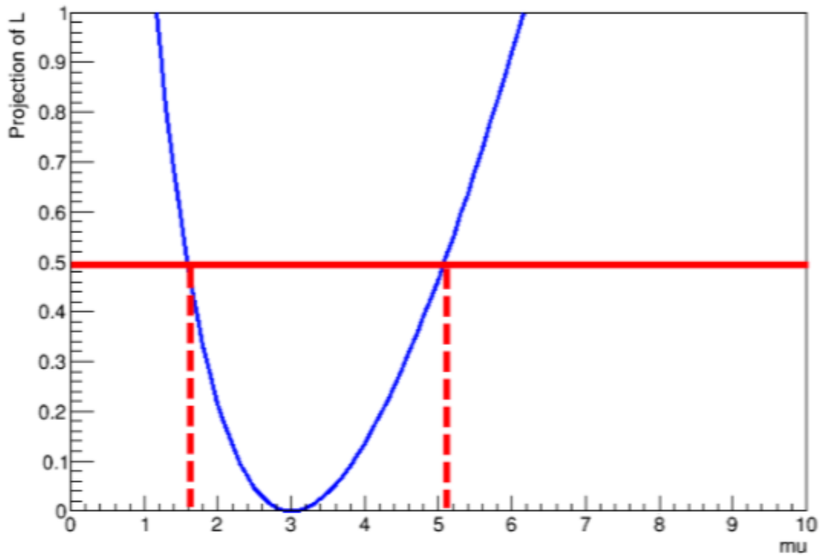
- Ordering based on Likelihood Ratio (Feldman-Cousins interval)

Asymptotic Distribution of Test Statistic

FC interval with Wilks Theorem



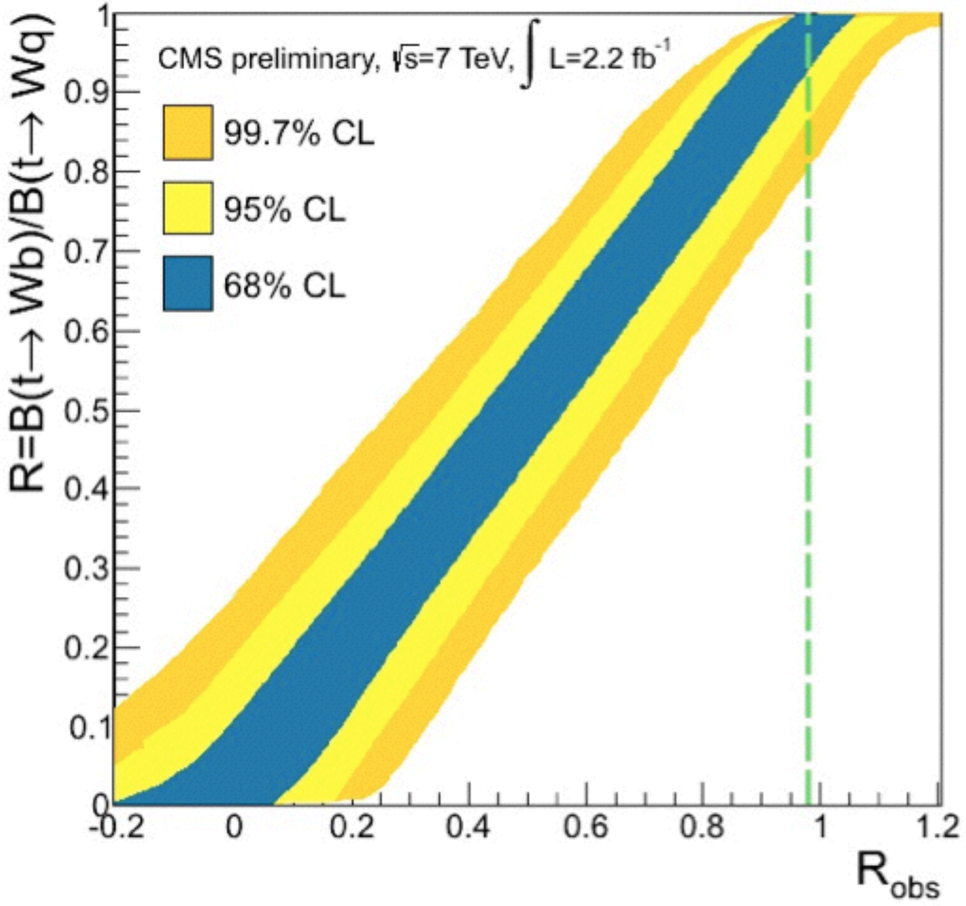
MINOS / Likelihood ratio interval



Wouter Verkerke, NIKHEF

Example: Feldman-Cousins interval

- Same RooStats code but with different configuration can compute also a Feldman-Cousins interval

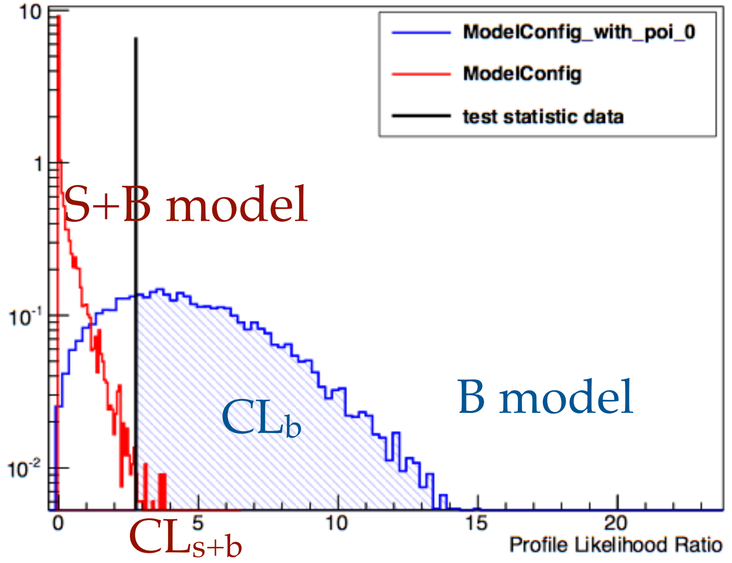


Summary of LR Confidence Interval

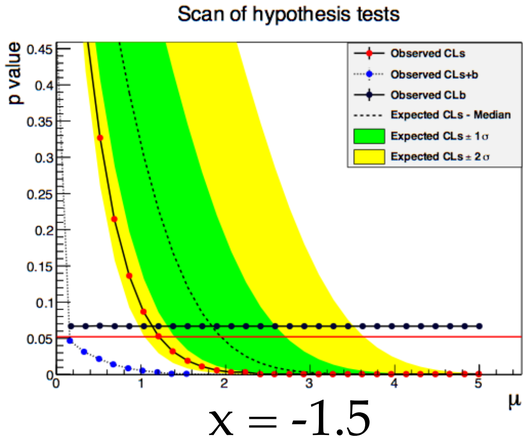
- Upper Limits: based on one-side likelihood-ratio test statistics

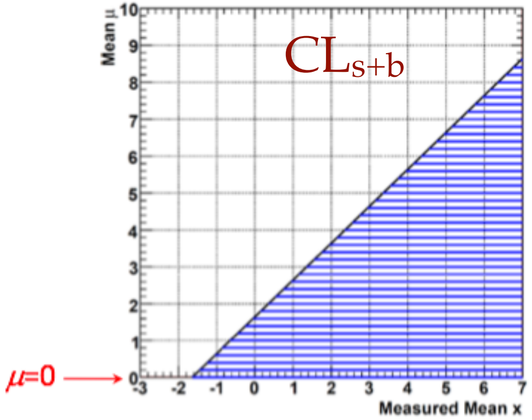
$$\lambda(\mu) = \frac{L(x|\mu, \hat{\hat{\nu}})}{L(x|\hat{\mu}, \hat{\nu})}$$

$\lambda(\mu) = 0$ for
$\mu < \mu_{TEST}$ (limits)

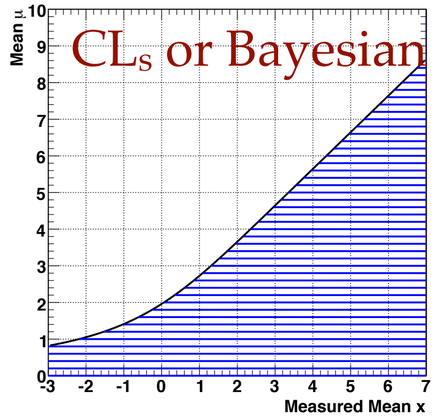


- Use CL_s to avoid empty intervals





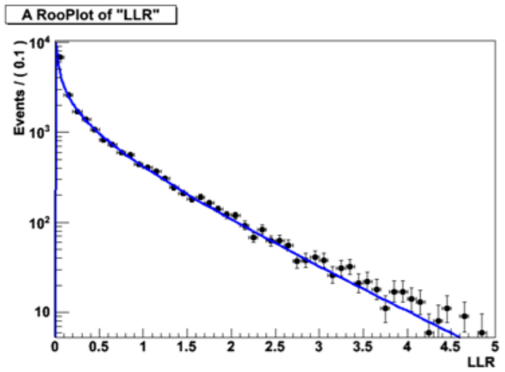
$$CL_s = \frac{CL_{s+b}}{CL_b}$$

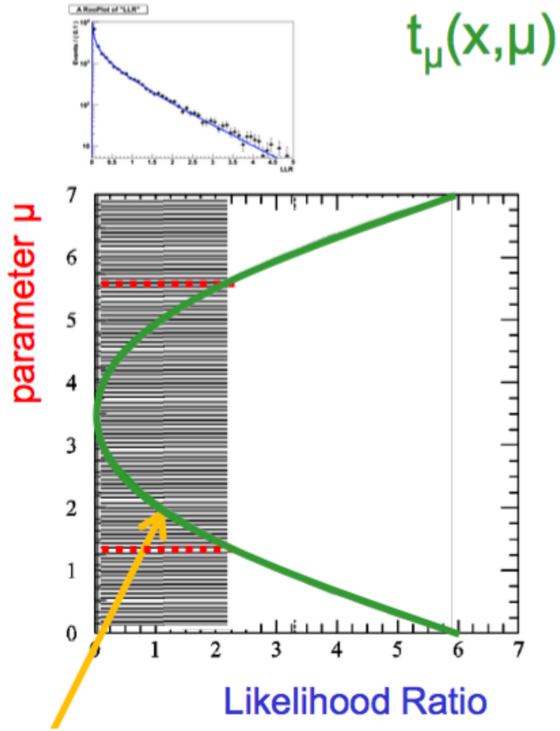


Feldman-Cousins Intervals

- Use normal likelihood-ratio as test statistic

$$\lambda(\mu) = \frac{L(x|\mu, \hat{\hat{\nu}})}{L(x|\hat{\mu}, \hat{\nu})}$$

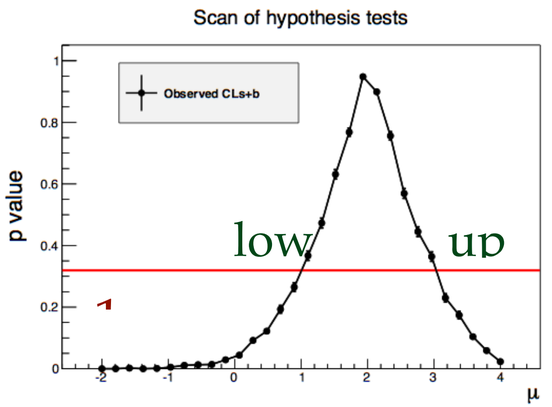


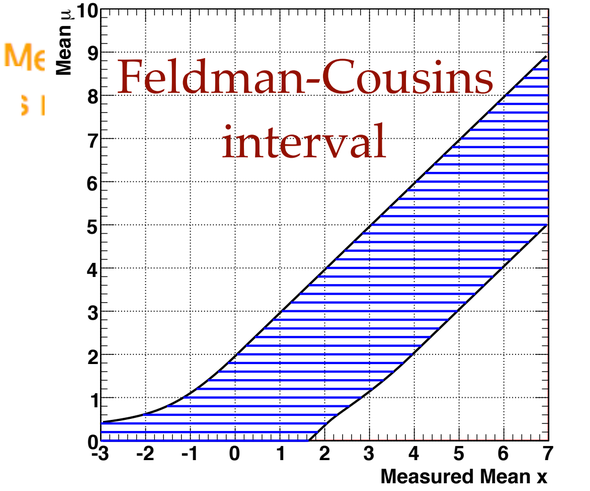


  - order intervals in likelihood-ratio value

    or

  - scan p-value obtained from the two-sided likelihood-ratio test statistic distribution
  - interval is never empty !





StandardHypoTestInvDemo.C

- Standard ROOT macro to run the Hypothesis Test inversion.
- Inputs to the macro:
  - workspace file, workspace name
  - name of S+B model (null) and for B model (alt)
    - if no B model is given, use S+B model with poi = 0
  - data set name
  - calculator type: frequentist (= 0), hybrid (=1), or asymptotic (=2)
  - test statistics
- options:
  - use CL_s or CL_{s+b} for computing limit
  - number of points to scan and min, max of interval

```
load the macro after having created the workspace and saved in file SPlusBExpoModel.root
root[] .L StandardHypoTestInvDemo.C

run for CLs (with  frequentist calculator (type = 0) and one-side PL test statistics (type = 3) scan 10 points in [0,100]

root[] StandardHypoTestInvDemo("SPlusBExpoModel.root","w","ModelConfig","","data",0,3, true, 10, 0, 100)

run for Asymptotic CLs (scan 20 points in [0,100])

root[] StandardHypoTestInvDemo(SPlusBExpoModel.root","w","ModelConfig","","data",2,3, true, 20, 0, 100)

run for Feldman-Cousins  ( scan 10 points in [0,100])

root[] StandardHypoTestInvDemo(SPlusBExpoModel.root","w","ModelConfig","","data",0,2, false, 10, 0, 100)
```

StandardHypoTestInvDemo tutorial

load the macro after having created the workspace and saved in file SPlusBExpoModel.root

```
root[] .L StandardHypoTestInvDemo.C
```

run for CLs (with frequentist calculator (type = 0) and one-side PL test statistics (type = 3) scan 10 points in [0,100]

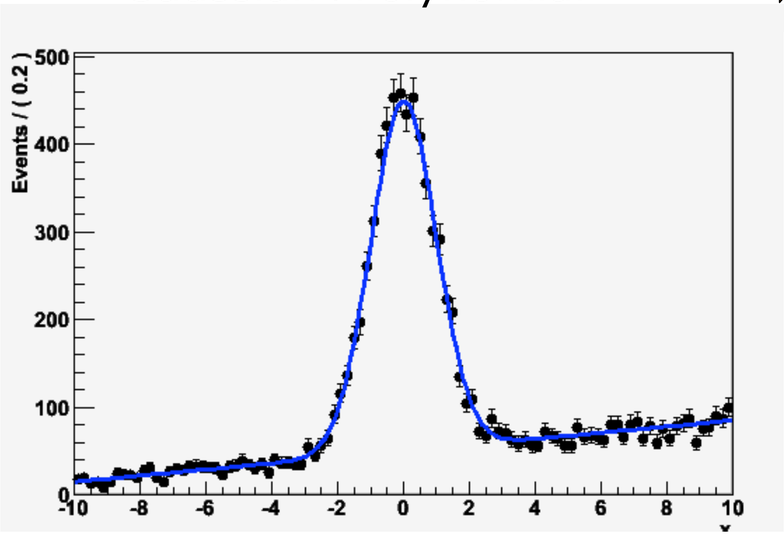
```
root[] StandardHypoTestInvDemo("SPlusBExpoModel.root","w","ModelConfig","","data",0,3, true, 10, 0, 100)
```

```
StandardHypoTestInvDemo(const char * infile = 0,
                        const char * wsName = "combined",
                        const char * modelSBName = "ModelConfig",
                        const char * modelBName = "",
                        const char * dataName = "obsData",
                        int calculatorType = 0,
                        int testStatType = 0,
                        bool useCLs = true ,
                        int npoints = 6,
                        double poimin = 0,
                        double poimax = 5,
                        int ntoys=1000,
                        bool useNumberCounting = false,
                        const char * nuisPriorName = 0)
```

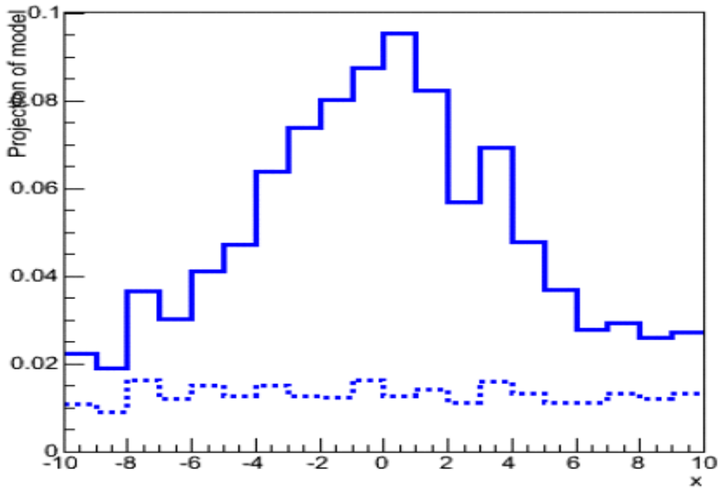
HistFactory – a new class of pdfs

- Focus of RooFit traditionally on analytical models
  - Assumes you can formulate signal/background in an analytical form
  - Often possible in e+e- experiments,
    shapes for hadron colliders cumbersome → **rely on MC simulation**

Analytical form:
Gaussian+Polynomial



Template form:
Histogram (discrete)



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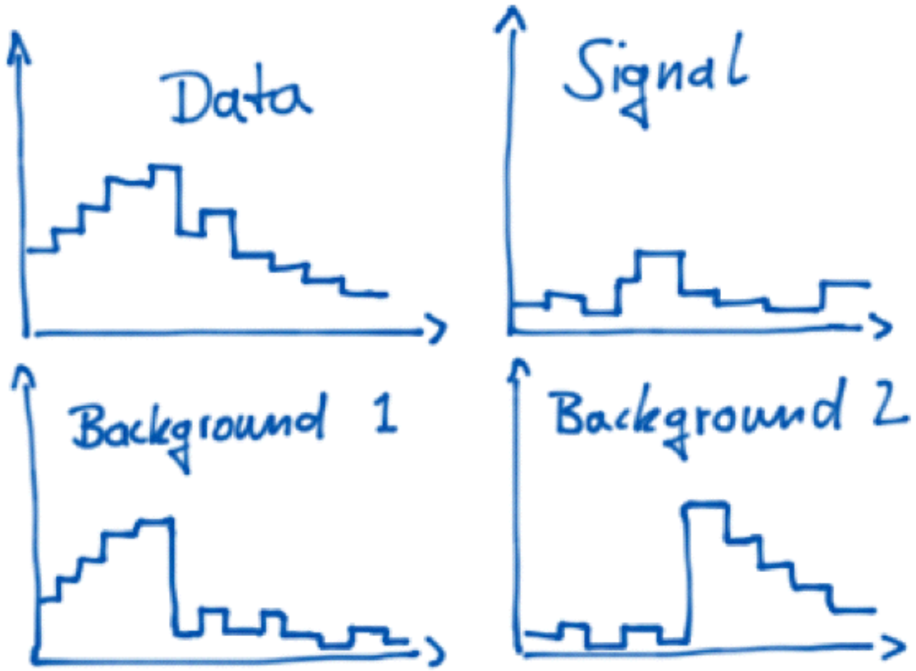
http://cdsweb.cern.ch/record/1456844.

Model Building with HistFactory

- Tool to build models from input histograms

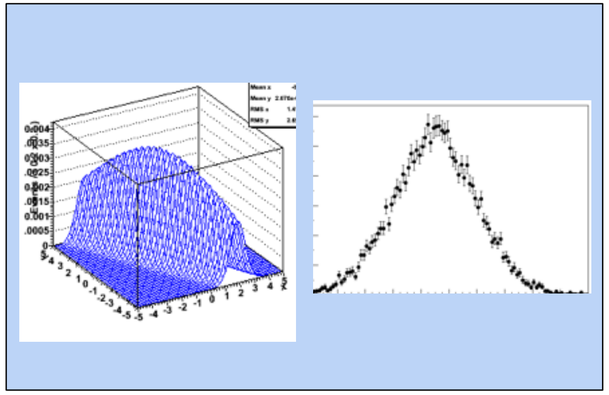


RooFit
Workspace

RooFit/RooStats at LHC (Higgs

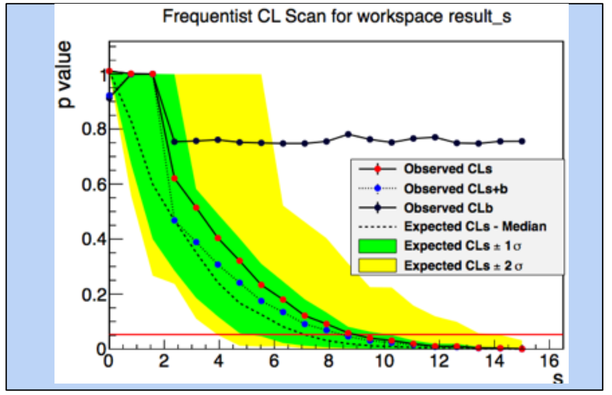
Class RooWorkspace

Simplify packaging and sharing of models



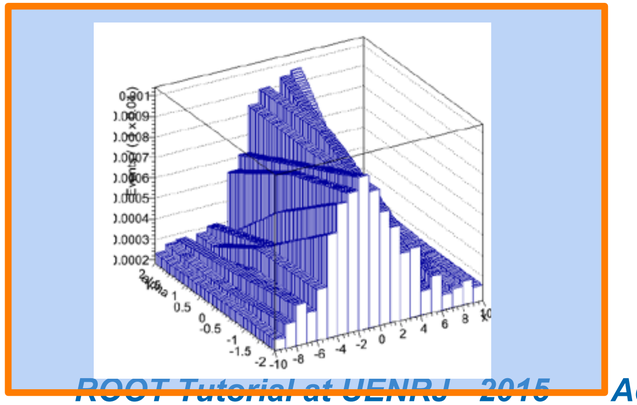
RooStats toolkit

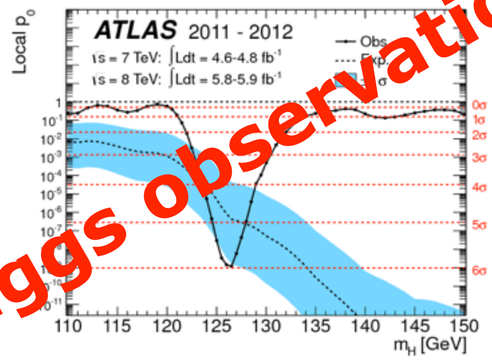
Statistical tests based on likelihoods from RooFit models



HistFactory package

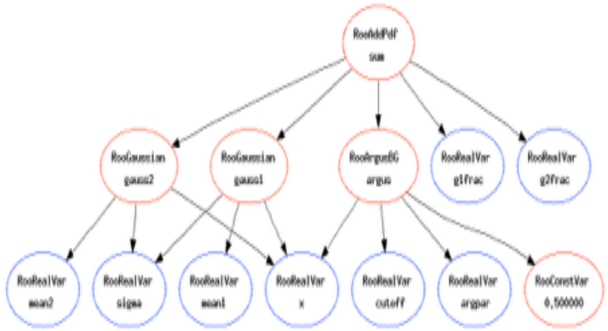
Constructing models from Monte Carlo templates



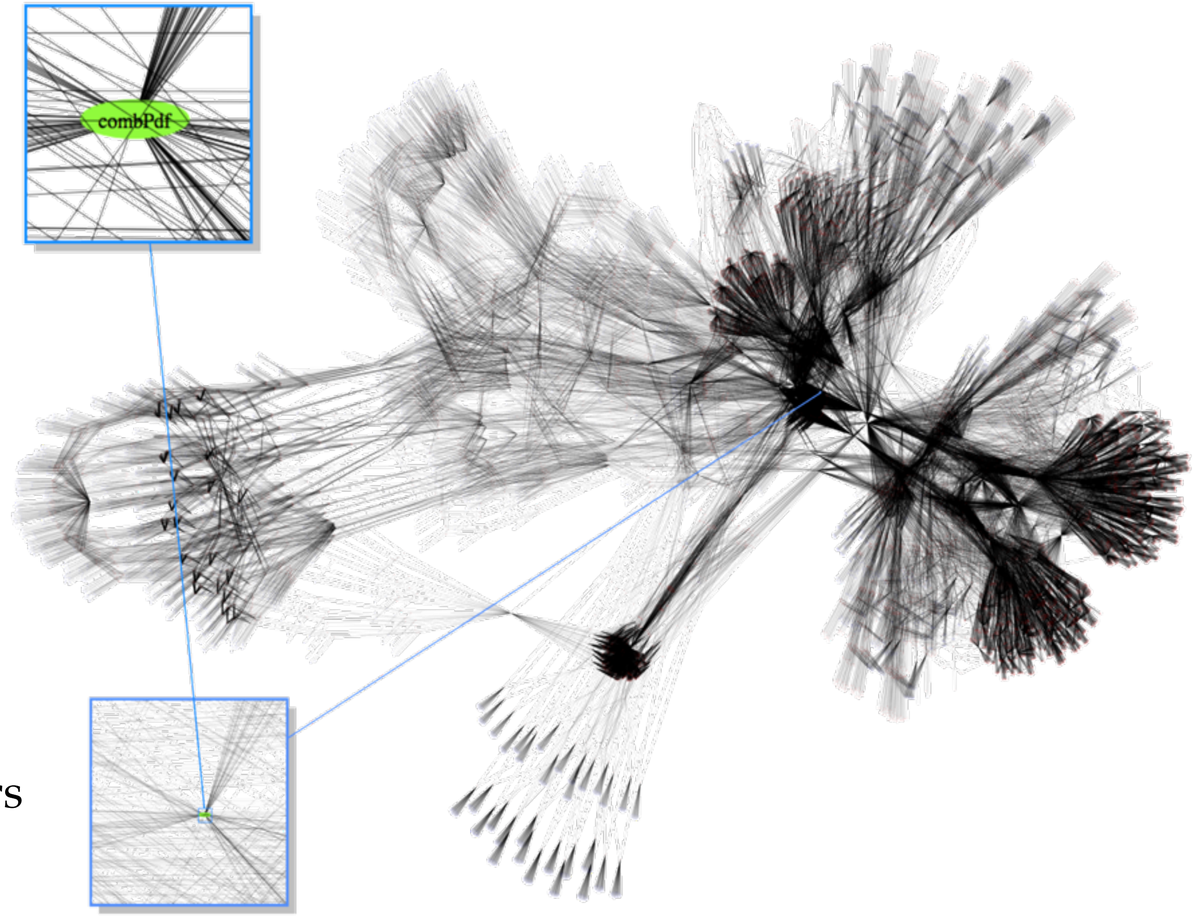


Higgs observation

How well does it scale?



Graph of the full ATLAS Higgs combination model

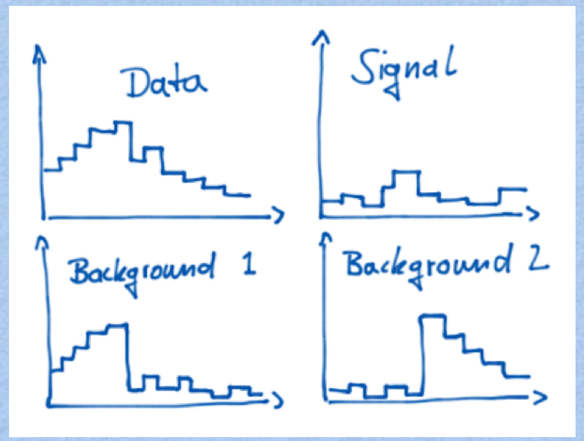


Model has ~23.000 function objects, ~1600 parameters

Reading/writing of full model takes ~4 seconds

ROOT file with workspace is ~6 Mb

HistFactory



*see also HistFactory doc (*https://cdsweb.cern.ch/record/1456844/files/CERN-OPEN-2012-016.pdf*)*

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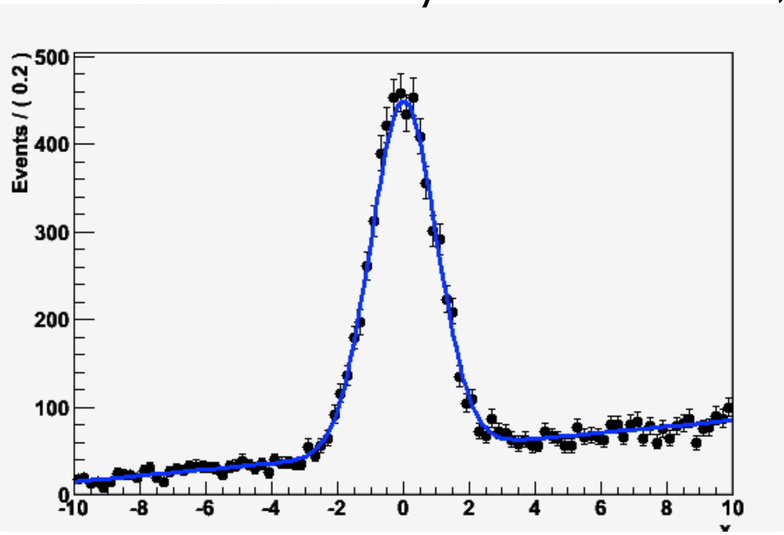

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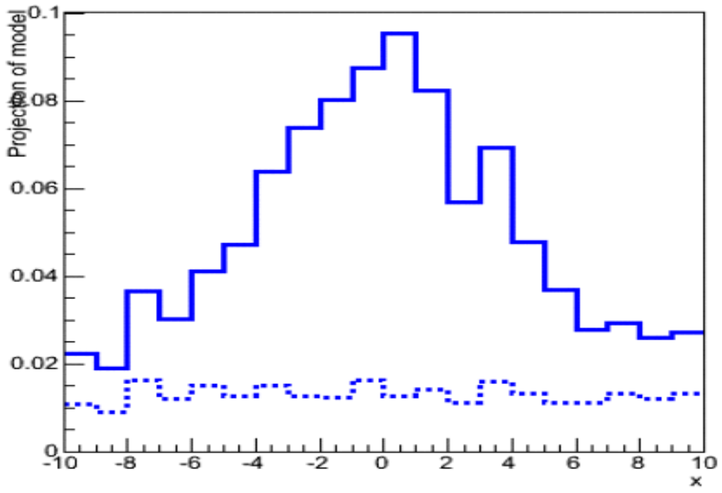

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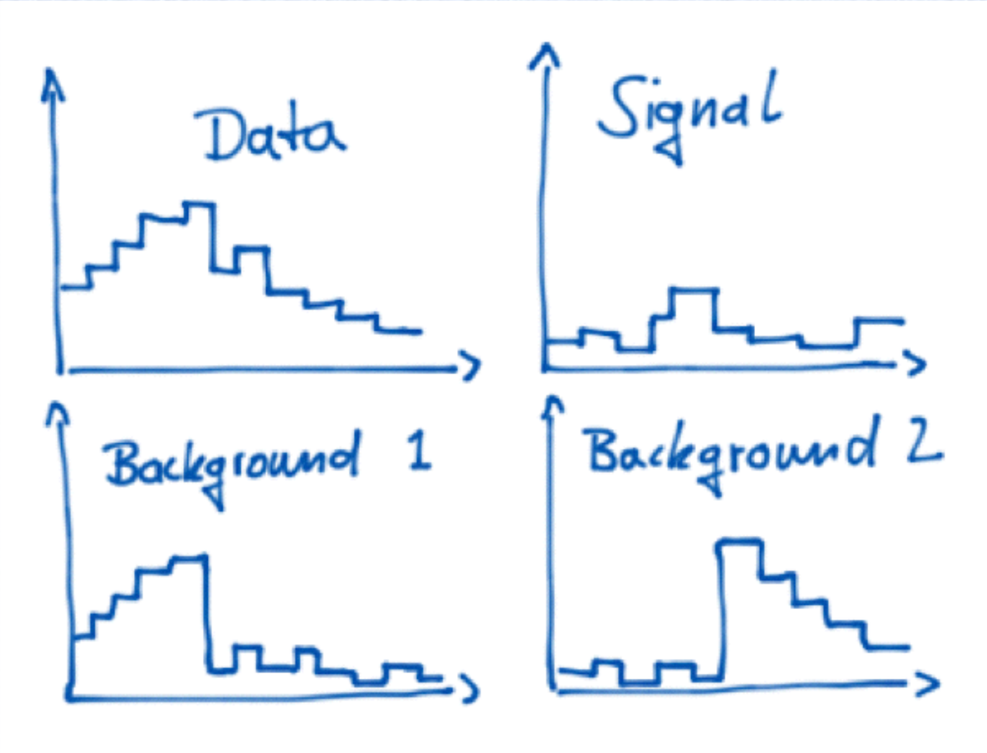


RooFit
Workspace

HistFactory concept

- Measurement
  - used to give global description of the model
  - can contain one or several channels
- Channel
  - disjoints selected regions of events
- Sample
  - set of process contributions to a channel

HistFactory

- Generalization of number counting models

$$\mathcal{P}(n_b|\mu) = \mathrm{Pois}(n_{\mathrm{tot}}|\mu S + B) \left[\prod_{b \in \mathrm{bins}} \frac{\mu \nu_b^{\mathrm{sig}} + \nu_b^{\mathrm{bkg}}}{\mu S + B} \right]$$

where n_b is the data histogram

in general HistFactory produces model of this form

$$\mathcal{P}(n_c, x_e, a_p \mid \phi_p, \alpha_p, \gamma_b) = \prod_{c \in \mathrm{channels}} \left[\mathrm{Pois}(n_c|\nu_c) \prod_{e=1}^{n_c} f_c(x_e|\boldsymbol{\alpha}) \right] \cdot G(L_0|\lambda, \Delta_L) \cdot \prod_{p \in \mathbb{S}+\boldsymbol{\Gamma}} f_p(a_p|\alpha_p)$$

p.d.f — luminosity constraint — parameter constraint

$$f_c(x_e|\phi_p, \alpha_p, \gamma_b) = \frac{\nu_{cb_e}}{\nu_c}$$

expected events/bin

$$\nu_c = \sum_{b \in \mathrm{bins\ of\ channel}\ c} \nu_{cb}$$

HistFactory Model

$$\mathcal{P}(n_{cb}, a_p \mid \phi_p, \alpha_p, \gamma_b) = \prod_{c \in \text{channels}} \prod_{b \in \text{bins}} \text{Pois}(n_{cb}|\nu_{cb}) \cdot G(L_0|\lambda, \Delta_L) \cdot \prod_{p \in \mathbb{S}+\boldsymbol{\Gamma}} P_p(a_p|\alpha_p)$$

expected number of events in a bin

luminosity constraint

parameter constraint

$$\nu_{cb}(\phi_p, \alpha_p, \gamma_b) = \lambda_{cs}\, \gamma_{cb}\, \phi_{cs}(\boldsymbol{\alpha})\, \eta_{cs}(\boldsymbol{\alpha})\, \sigma_{csb}(\boldsymbol{\alpha})$$

λ_{cs}	luminosity parameter for each sample of a channel
γ_{cb_e}	bin by bin scale factor (statistical + systematics)
$\phi_{cs} = \prod_{p \in \mathbb{N}_c} \phi_p$	product of unconstrained normalisation. Depend on P.O.I. (e.g. signal rate)
$\eta_{cs}(\boldsymbol{\alpha})$	normalisation uncertainty for each sample of a channel
σ_{csb_e}	nominal bin content and its uncertainty (from input histograms)

HistFactory Capabilities

- HistFactory can include:
  - multiple channels and samples
  - unconstrained normalisation for any sample
  - parametrize variation in normalization due to systematic effects
  - bin by bin statistical uncertainty (overall for all samples)
  - parametrize systematic variation of a single bin

	Constrained	Unconstrained
Normalization Variation	`OverallSys` (η_{cs})	`NormFactor` (ϕ_p)
Coherent Shape Variation	`HistoSys` σ_{csb}	–
Bin-by-bin variation	`ShapeSys` & `StatError` γ_{cb}	`ShapeFactor` γ_{csb}

HistFactory Capabilities (2)

- In addition the HistFactory can
  - can combine multiple channels
  - produce a RooFit workspace which can be used in RooStats
    - can be used to combine several measurements
- Configuration can be done in XML or directly in C++ or Python

How To Create a Model

- Simple counting model

$$\text{Poisson}(\, n_{obs} \mid \mu + b)\, \text{Gaussian}(\, b \mid b_0, \sigma_b)$$

```
// create first input histograms
int nobs = 3; double b = 1; double errb = 0.2;

// observed histogram
TH1D * hobs = new TH1D("hobs","hobs",1,0,1);
hobs->SetBinContent(1,nobs);

//signal histogram (assume expected one is 1)
TH1D * hs = new TH1D("hs","signal  histo",1,0,1);
hs->SetBinContent(1,1);


TH1D * hb = new TH1D("hb","bkg  histo",1,0,1);
hb->SetBinContent(1,b);
```

How To Create a Model (2)

- Create HistFactory Measurement class

```
HistFactory::Measurement meas("CountingModel","CountingModel");
meas.SetPOI("mu");

meas.SetLumi(1.0);
meas.SetLumiRelErr(0.1);  // not relevant
// this does not make lumi varying
meas.AddConstantParam("Lumi");
```

- Create Channels and Sample

```
HistFactory::Channel channel("SignalRegion");
channel.SetData(hobs);

HistFactory::Sample signal("signal");
signal.AddNormFactor("mu",1,0,30);
//signal.AddOverallSys("sig_unc",0.9, 1.1);
signal.SetHisto(hs);
channel.AddSample(signal);

HistFactory::Sample backg("background");
backg.SetHisto(h1_b);
backg.AddOverallSys("b_unc",1.-errb, 1+errb);  // b uncertainty
channel.AddSample(backg);

meas.AddChannel(channel);
```

How To Create a Model (3)

- Creating a RooWorkspace given the Measurement

```
RooWorkspace * w = HistFactory::MakeModelAndMeasurementFast(meas);
```

```
RooWorkspace(SignalRegion) SignalRegion workspace contents

variables
---------
(Lumi,alpha_b_unc,binWidth_obs_x_SignalRegion_0,binWidth_obs_x_SignalRegion_1,mu,nom_alpha_b_unc,nominalLumi,obs_x_SignalRegion,weightVar)

p.d.f.s
-------
RooRealSumPdf::SignalRegion_model[ binWidth_obs_x_SignalRegion_0 * L_x_signal_SignalRegion_overallSyst_x_Exp + binWidth_obs_x_SignalRegion_1 *
L_x_background_SignalRegion_overallSyst_x_Exp ] = 2/2
RooGaussian::alpha_b_uncConstraint[ x=alpha_b_unc mean=nom_alpha_b_unc sigma=1 ] = 1
RooGaussian::lumiConstraint[ x=Lumi mean=nominalLumi sigma=0.001 ] = 1
RooProdPdf::model_SignalRegion[ lumiConstraint * alpha_b_uncConstraint * SignalRegion_model(obs_x_SignalRegion) ] = 2

functions
--------
RooProduct::L_x_background_SignalRegion_overallSyst_x_Exp[ Lumi * background_SignalRegion_overallSyst_x_Exp ] = 1
RooProduct::L_x_signal_SignalRegion_overallSyst_x_Exp[ Lumi * signal_SignalRegion_overallSyst_x_Exp ] = 1
RooStats::HistFactory::FlexibleInterpVar::background_SignalRegion_epsilon[ paramList=(alpha_b_unc) ] = 1
RooHistFunc::background_SignalRegion_nominal[ depList=(obs_x_SignalRegion) ] = 1
RooProduct::background_SignalRegion_overallSyst_x_Exp[ background_SignalRegion_nominal * background_SignalRegion_epsilon ] = 1
RooHistFunc::signal_SignalRegion_nominal[ depList=(obs_x_SignalRegion) ] = 1
RooProduct::signal_SignalRegion_overallNorm_x_sigma_epsilon[ mu * signal_SignalRegion_epsilon ] = 1
RooProduct::signal_SignalRegion_overallSyst_x_Exp[ signal_SignalRegion_nominal * signal_SignalRegion_overallNorm_x_sigma_epsilon ] = 1
```

HistFactory Output

- makes a combined workspace with data

```
RooWorkspace(combined) combined contents

variables
---------
(channelCat,nom_alpha_b_unc,obs_x_SignalRegion,weightVar)

datasets
--------
RooDataSet::asimovData(obs_x_SignalRegion,weightVar,channelCat)
RooDataSet::obsData(channelCat,obs_x_SignalRegion)

named sets
----------
ModelConfig_GlobalObservables:(nom_alpha_b_unc)
ModelConfig_Observables:(obs_x_SignalRegion,weightVar,channelCat)
globalObservables:(nom_alpha_b_unc)
observables:(obs_x_SignalRegion,weightVar,channelCat)
```

- create also a ModelConfig

```
=== Using the following for ModelConfig ===
Observables:             RooArgSet:: = (obs_x_SignalRegion,weightVar,channelCat)
Parameters of Interest:  RooArgSet:: = (mu)
Nuisance Parameters:     RooArgSet:: = (alpha_b_unc)
Global Observables:      RooArgSet:: = (nom_alpha_b_unc)
PDF:                     RooSimultaneous::simPdf[ indexCat=channelCat SignalRegion=model_SignalRegion ] = 2
```

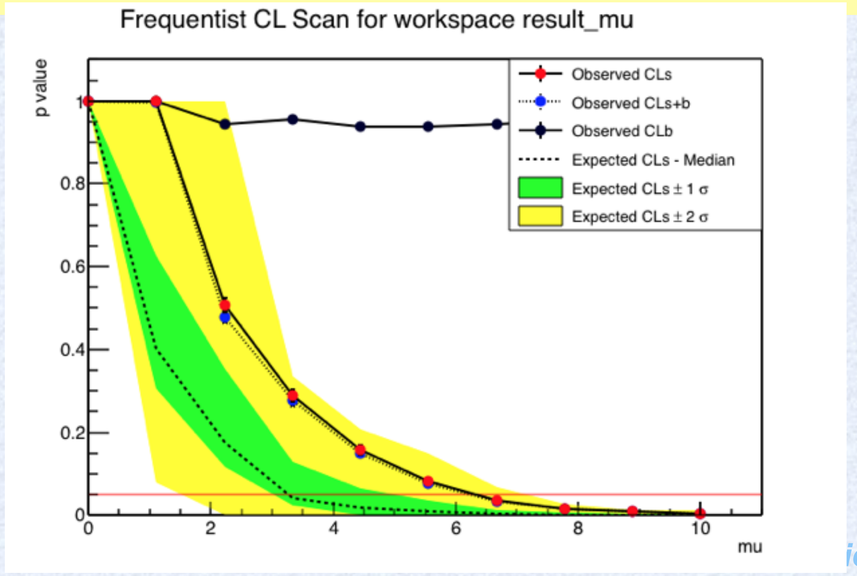
Using HistFactory Models

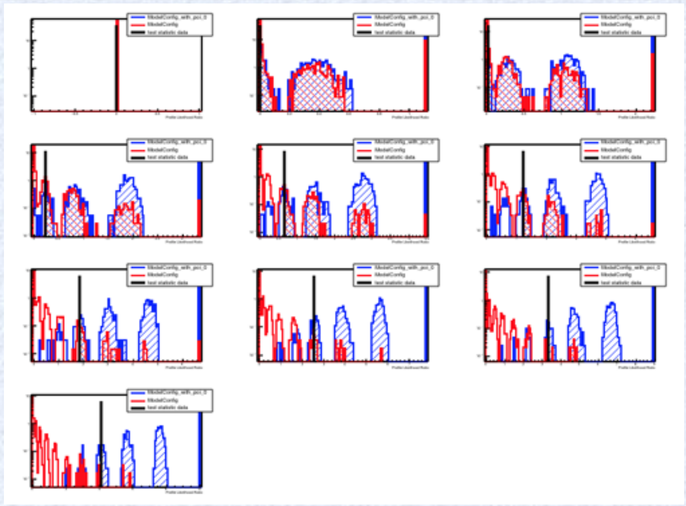
- Combined model saved in a ROOT file
- Model can be used directly in RooStats tools

```
root[] .L StandardHypoTestInvDemo.C
```

run for CLs (with frequentist calculator (type = 0) and one-side PL test statistics (type = 3) scan 10 points in [0,10]

```
root[] StandardHypoTestInvDemo("model.root","combined","ModelConfig","","obsData",0,3, true, 10, 0, 10)
```





Interpolation Options

HistFactory has different option for interpolating the systematic variations : η(α)

0) Linear
1) Exponential
2) Quadratic interp. linear extrapolation
4) Polynomial interpolation Exponential extrapolation (default)

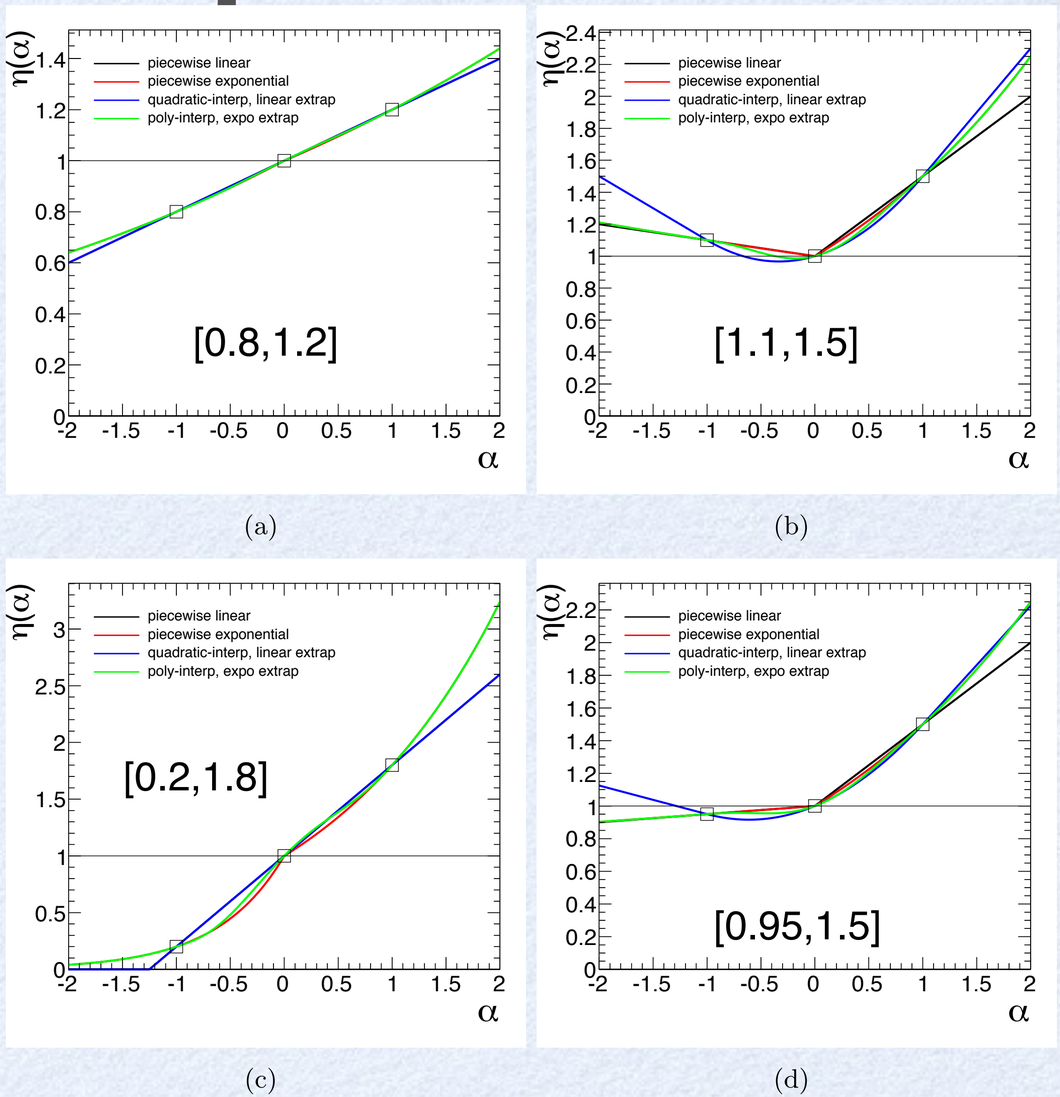


Figure 3: Comparison of the three interpolation options for different $\eta^{\pm}$. (a) $\eta^{-} = 0.8$, $\eta^{+} = 1.2$, (b) $\eta^{-} = 1.1$, $\eta^{+} = 1.5$, (c) $\eta^{-} = 0.2$, $\eta^{+} = 1.8$, and (d) $\eta^{-} = 0.95$, $\eta^{+} = 1.5$

Summary

- RooFit/RooStats allow you to perform advanced statistical data/analysis
  - LHC results (*e.g.* Higgs observation)
- Capable of using different tools and interpretations (Frequentist/ Bayesian) on the same model
- Generic tools capable to deal with large variety of models
  - based on histograms or un-binned data
  - multi-dimensional observations
- Provide tools to facilitate complex model building
  - HistFactory for histogram based analysis

Documentation

- RooStats TWiki: https://twiki.cern.ch/twiki/bin/view/RooStats/WebHome
- RooStats users guide (not really completed)
  - http://root.cern.ch/viewcvs/branches/dev/roostats/roofit/roostats/doc/usersguide/RooStats_UsersGuide.pdf
- For reference and citation: ACAT 2010 proceedings papers: http://arxiv.org/abs/1009.1003
- RooStats tutorial macros: http://root.cern.ch/root/html534/tutorials/roostats/index.html
- HistFactory document: https://cdsweb.cern.ch/record/1456844/files/CERN-OPEN-2012-016.pdf
- RooStats user support:
  - Request support via ROOT talk forum: http://root.cern.ch/phpBB2/viewforum.php?f=15 (questions on statistical concepts accepted)
  - contact me directly (email: Lorenzo.Moneta at cern.ch)
- Contacts for statistical questions:
  - ATLAS statistics forum:
    - TWiki: https://twiki.cern.ch/twiki/bin/view/AtlasProtected/StatisticsTools
  - CMS statistics committee:
    - TWiki: https://twiki.cern.ch/twiki/bin/view/CMS/StatisticsCommittee