Introduction to statistics / statistical tools & the HistFitter framework

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+ many other people

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ATLAS EXPERIMENT
http://atlas.ch

HistFitter

Overview

- Introduction to statistics (short)
- Introduction to statistical analysis (RooFit, RooStats, HistFactory)
- HistFitter overview
  - Introduction & strategy
- HistFitter tutorial
  - Running a fit & visualization
  - Calculating limits

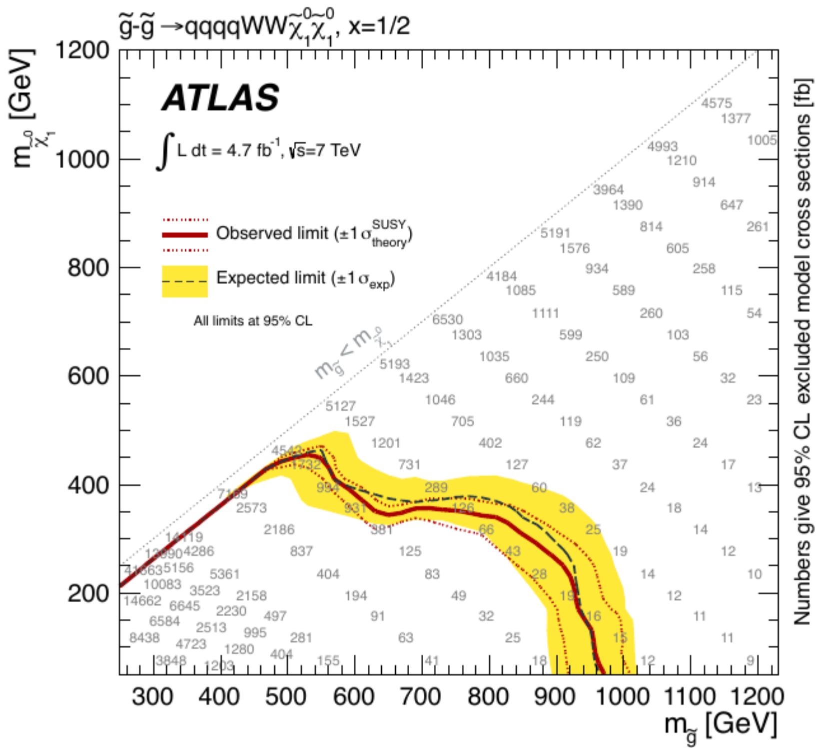
Introduction to HEP statistics

Largely borrowed from lectures/slides by W. Verkerke

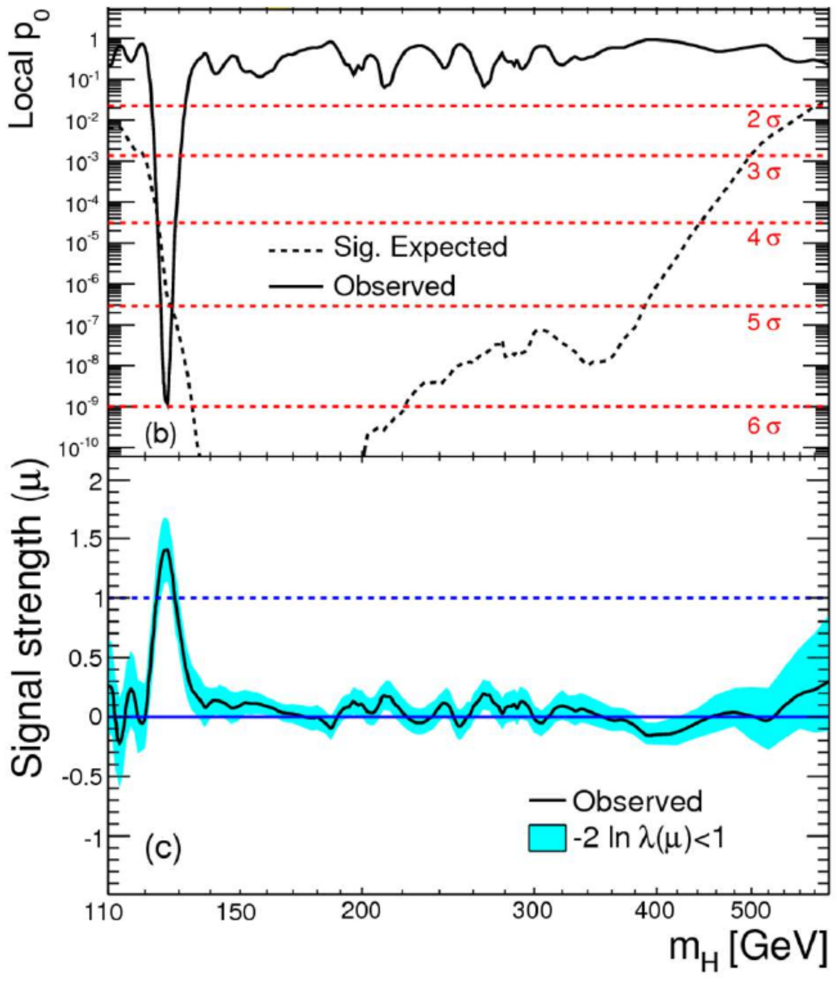
…some more advanced examples

Basic questions

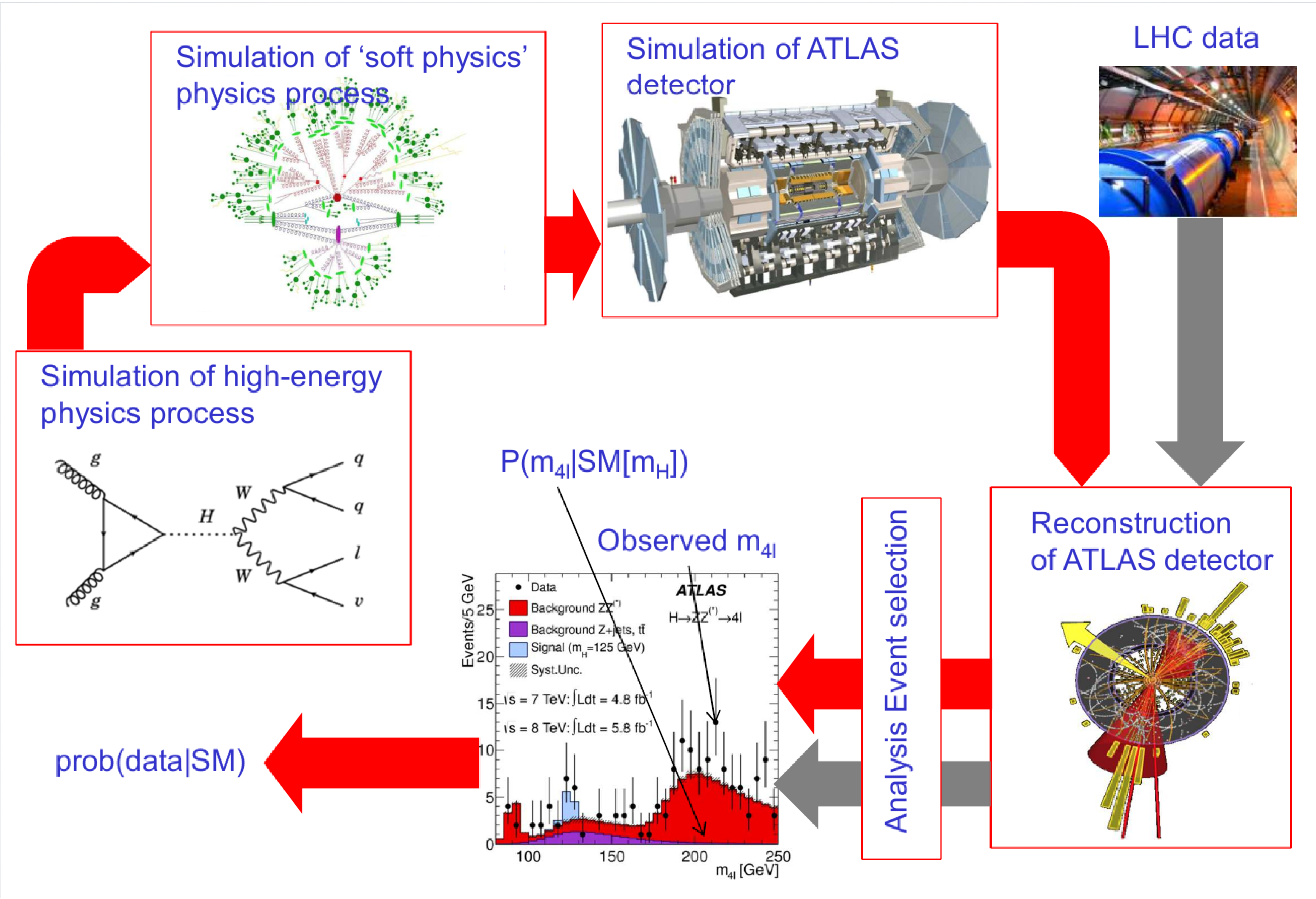
- Physics questions we want to answer...
  - Is the Higgs boson a SM Higgs boson?
  - What is its production cross section and couplings?
  - Is there any SUSY in ATLAS data?
    - If not, what models do not agree with data?
- Enormous efforts in many channels, millions of plots with signal/backgrounds expectations, with systematics and observed data
- How do you conclude on these questions?
- Statistical tests construct probabilistic statements/models on P(theory|data) or P(data|theory)
  - Likelihood fits
  - Systematics/uncertainties
  - Hypothesis testing
  - Setting limits ...
- <u>Result:</u> decisions based on these tests



As a layman I would now say, I think we have it



HEP workflow



Simulation of high-energy physics process

Simulation of ‘soft physics’ physics process

Simulation of ATLAS detector

LHC data

Reconstruction of ATLAS detector

Analysis Event selection

Observed m_{4l}

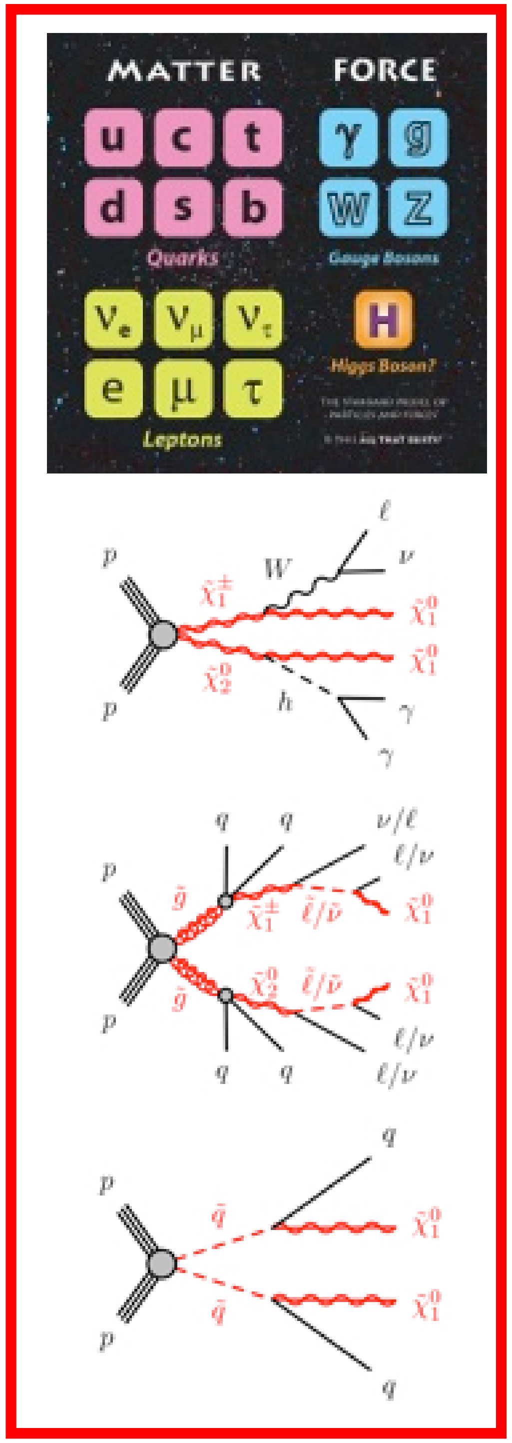
$P(m_{4l}|SM[m_H])$

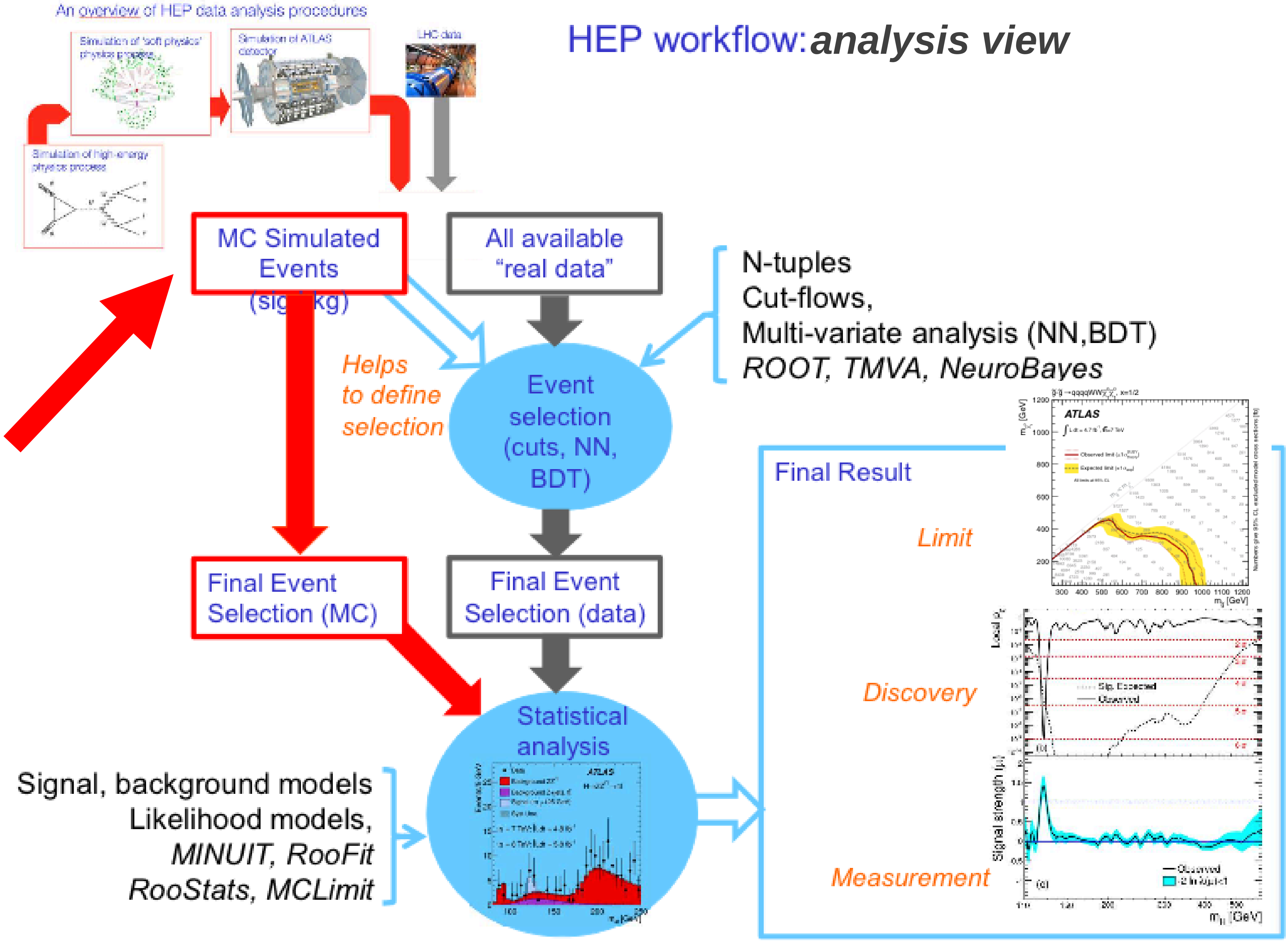
prob(data|SM)

W. Verkerke

Federica may have introduced some aspects here to you.

HEP data analysis





HEP workflow: *analysis view*

MC Simulated Events (sig, bkg)

All available “real data”

Helps to define selection

Event selection (cuts, NN, BDT)

N-tuples
Cut-flows,
Multi-variate analysis (NN,BDT)
ROOT, TMVA, NeuroBayes

Final Event Selection (MC)

Final Event Selection (data)

Statistical analysis

Signal, background models
Likelihood models,
MINUIT, RooFit
RooStats, MCLimit

Final Result

W. Verkerke

- HEP Data Analysis is (should be) for a large part the reduction of a physics theory(s) to a statistical model
- Statistical/probability model: Given a measurement ***x*** (eg N events), what is the probability to observe each possible ***x***, under the hypothesis that the physics theory is true?

Simple statistical example

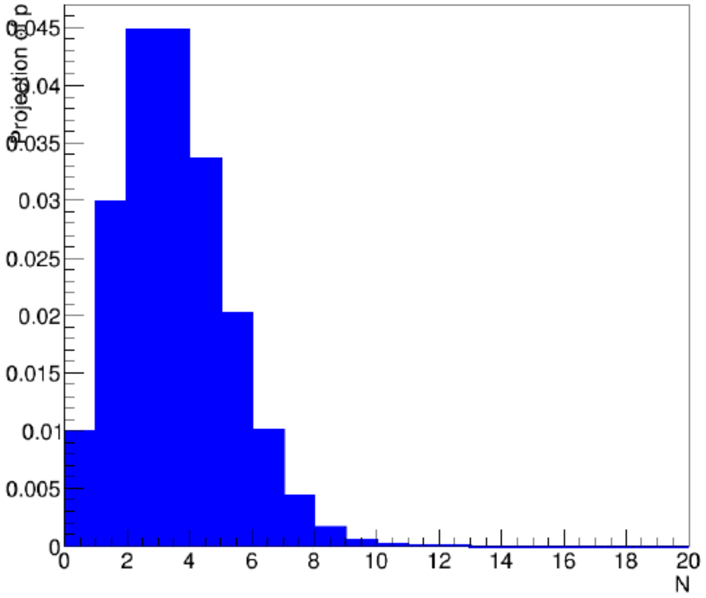
- Central concept in statistics is the ‘probability model’ : assigns a probability to each possible experimental outcome

- Example: a HEP counting experiment
  - Count number of events in your signal region (SR) in your data (specific lumi): Poisson distribution
  - Given the *expected(MC)* event count, the probability model is fully specified

$$P(N|\mu)=\frac{\mu^N e^{-\mu}}{N!}$$

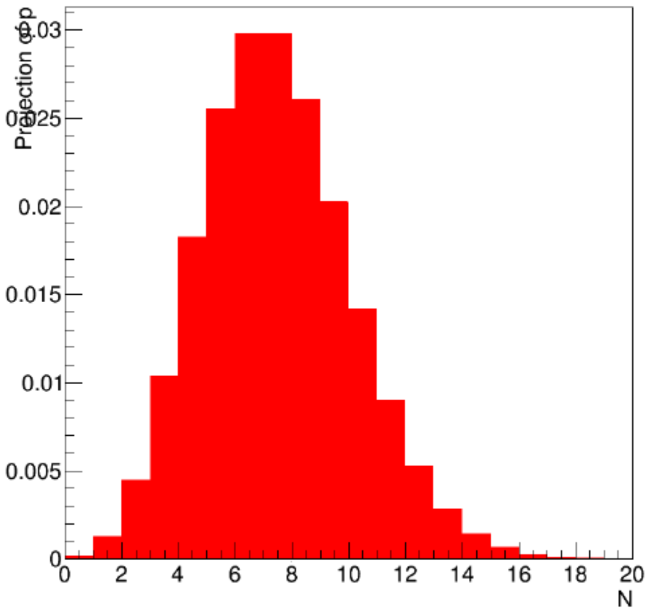
PROBABILITY

μ=3 (“bkg only”)

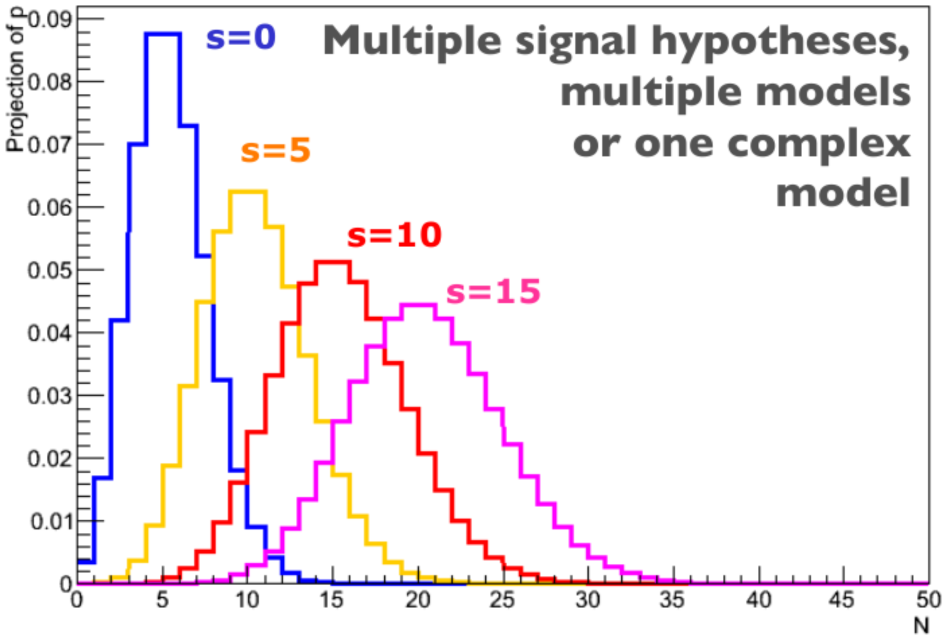


Poisson(N| b)

μ=7 (“bkg+signal”)



Poisson(N| s + b)



Multiple signal hypotheses, multiple models or one complex model

Poisson(N| s + b)

- Suppose we measure N = 7 events (Nobs), then can calculate the probability
- P(Nobs|hypothesis) is called **LIKELIHOOD** **- L(Nobs|b), L(Nobs|s+b), L(observed data|theory)**

p(Nobs|b) = 2.2% **p(Nobs|s+b) = 14.9%**

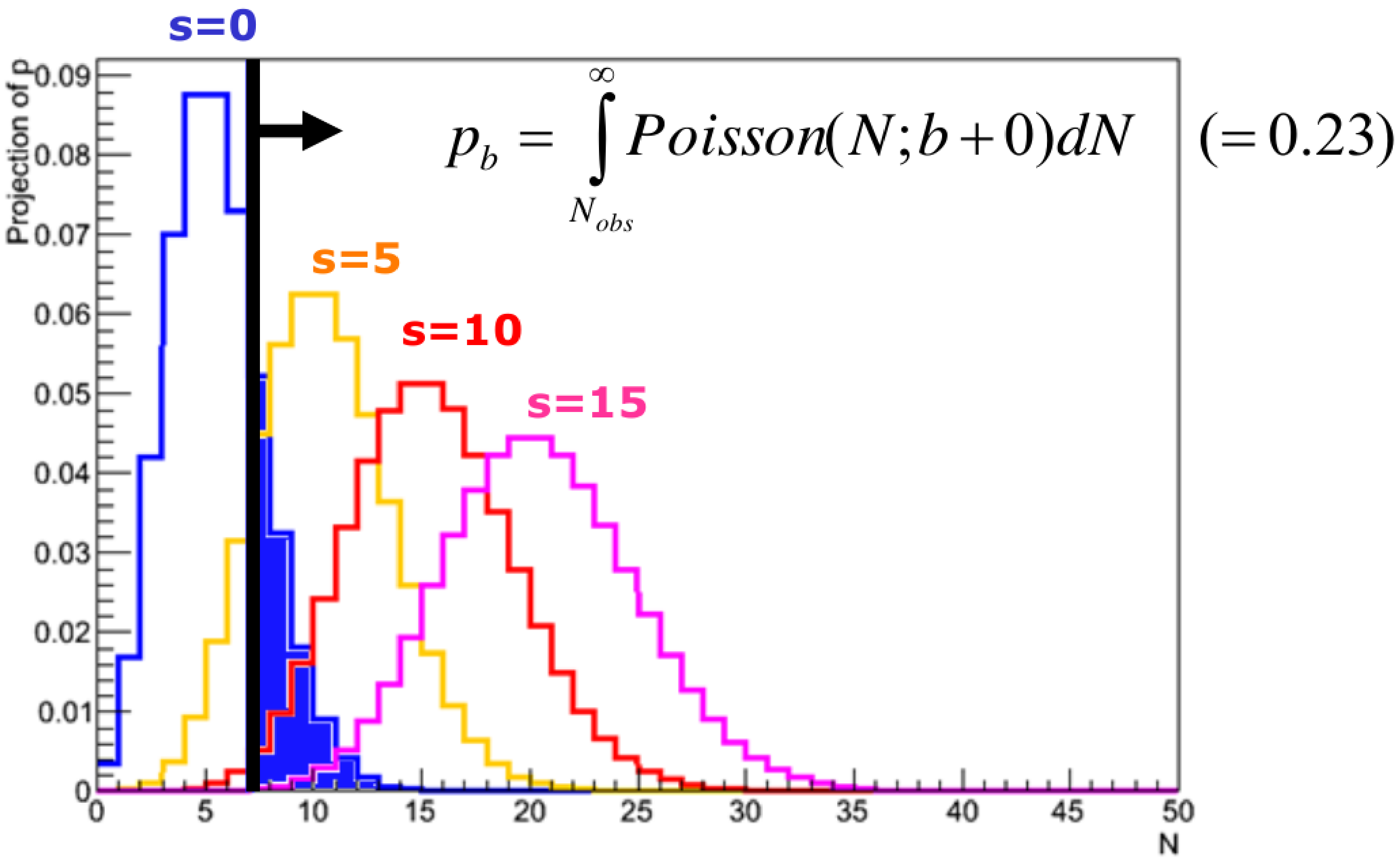
  - Data is more likely under s+b hypothesis than bkg-only

W. Verkerke

p-value

- **P-VALUE:** probability to obtain observed data, or more extreme, given the hypothesis in future repeated identical experiments

- For our example from previous page:
  - For the bkg-only hypothesis: $\mathbf{p_b}$ = Fraction of future measurements with N=Nobs (or larger) if s=0



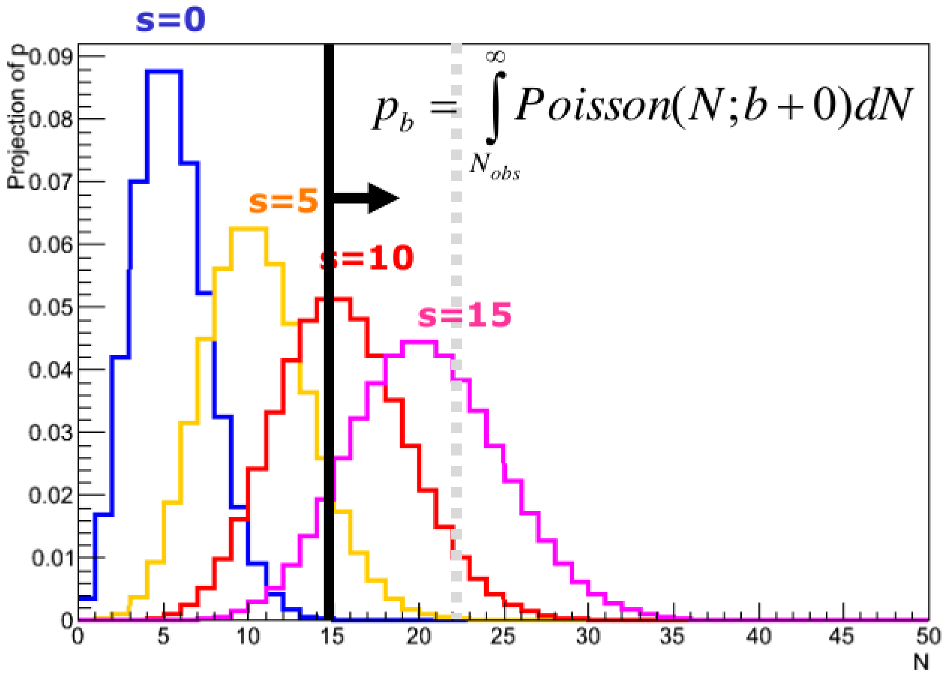
$$p_b = \int_{N_{obs}}^{\infty} Poisson(N; b+0)\,dN \quad (=0.23)$$

- Frequentist p-values (apologies to Bayesians) -- see links later

Excess over background

- **p_b** or p-values of background hypothesis is used to quantify ‘discovery’
- ‘discovery’ = excess of events over background expectation

- One more example:
  - Nobs=15 for same model, what is **p_b**?



$$p_b = \int_{N_{obs}}^{\infty} Poisson(N; b+0)dN$$

$$(= 0.00022)$$

- Results customarily expressed as odds of a Gaussian fluctuation with equal p-value: **significance, Zn, z-value**

- Nobs = 15 → Zn = 3.5σ

- Nobs = 22 → **Zn = 5σ**
  or **p_b < 2.87 ×10^{-7}**

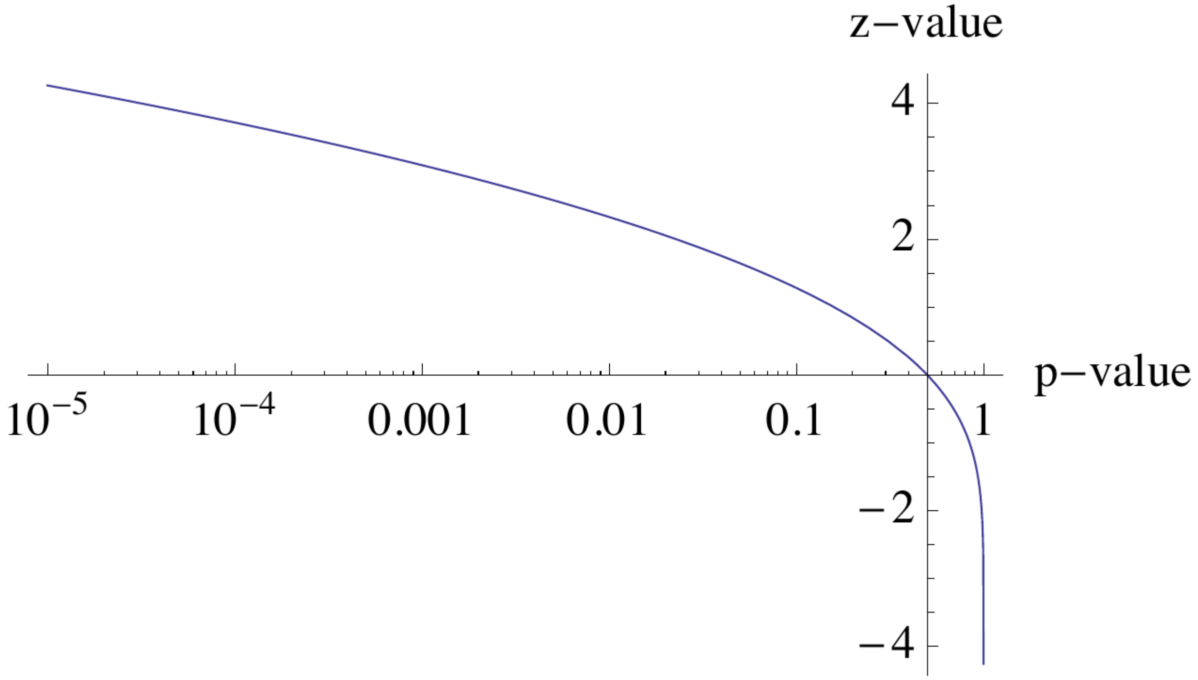


Fig. 1. Relationship between p-value and z-value.

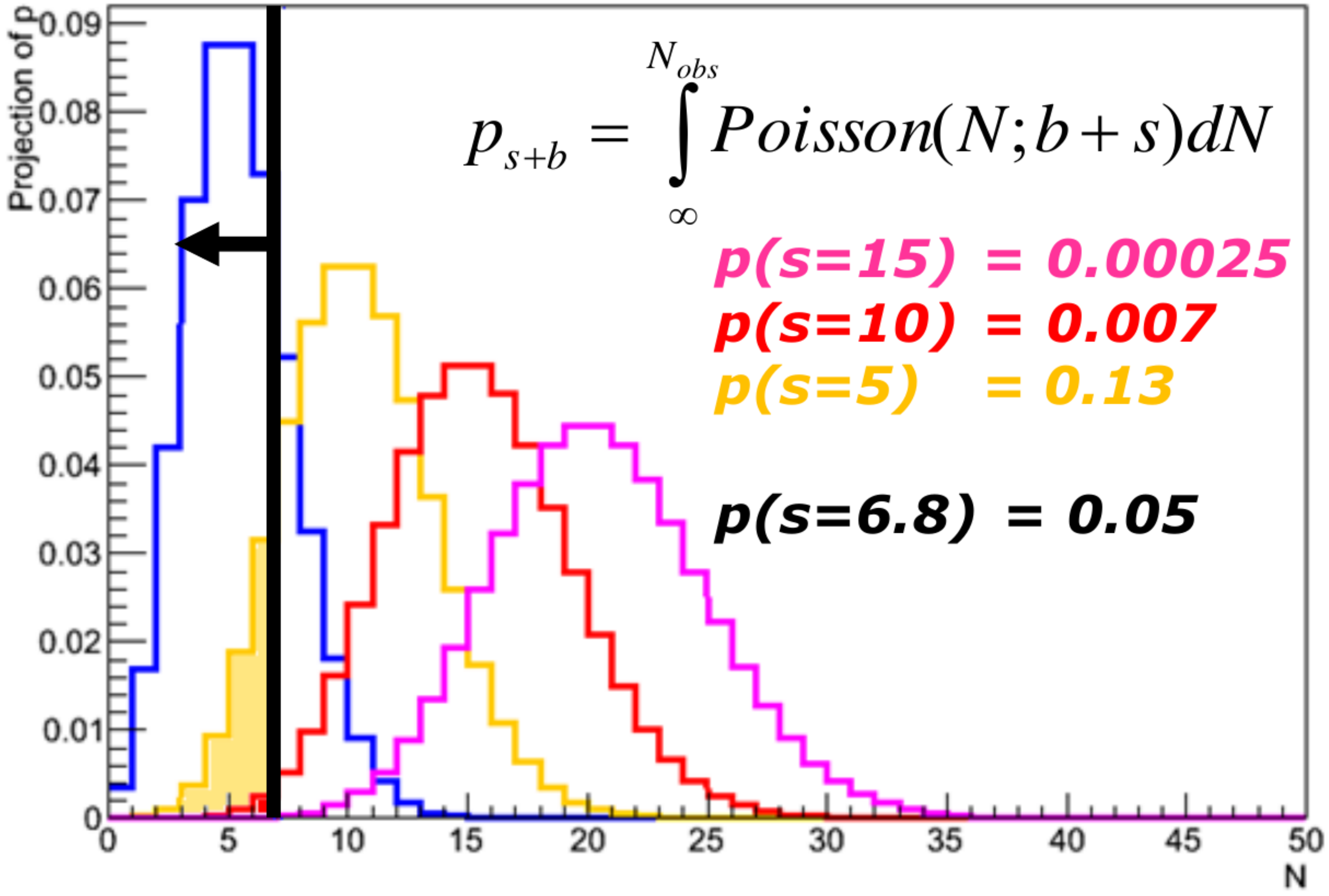
z-value =

`sqrt(2.) * TMath :: ErfInverse(1. - 2. * pvalue)`

$$p\text{-value} = \int_{z\text{-value}}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} dx,$$

Upper limits

- Can also define p-value for s+b hypothesis $\mathbf{p_{s+b}}$
  - Note convention change: integration range in $\mathbf{p_{s+b}}$ is flipped



- Convention: express result as value (upper limit) of **s** for which $\mathbf{p_{s+b}} = 5\%$

  or excluded at 95% confidence level (95% C.L.)
- Our example:
  - s>6.8 is excluded at 95% C.L.

Modified Upper limits : CLs

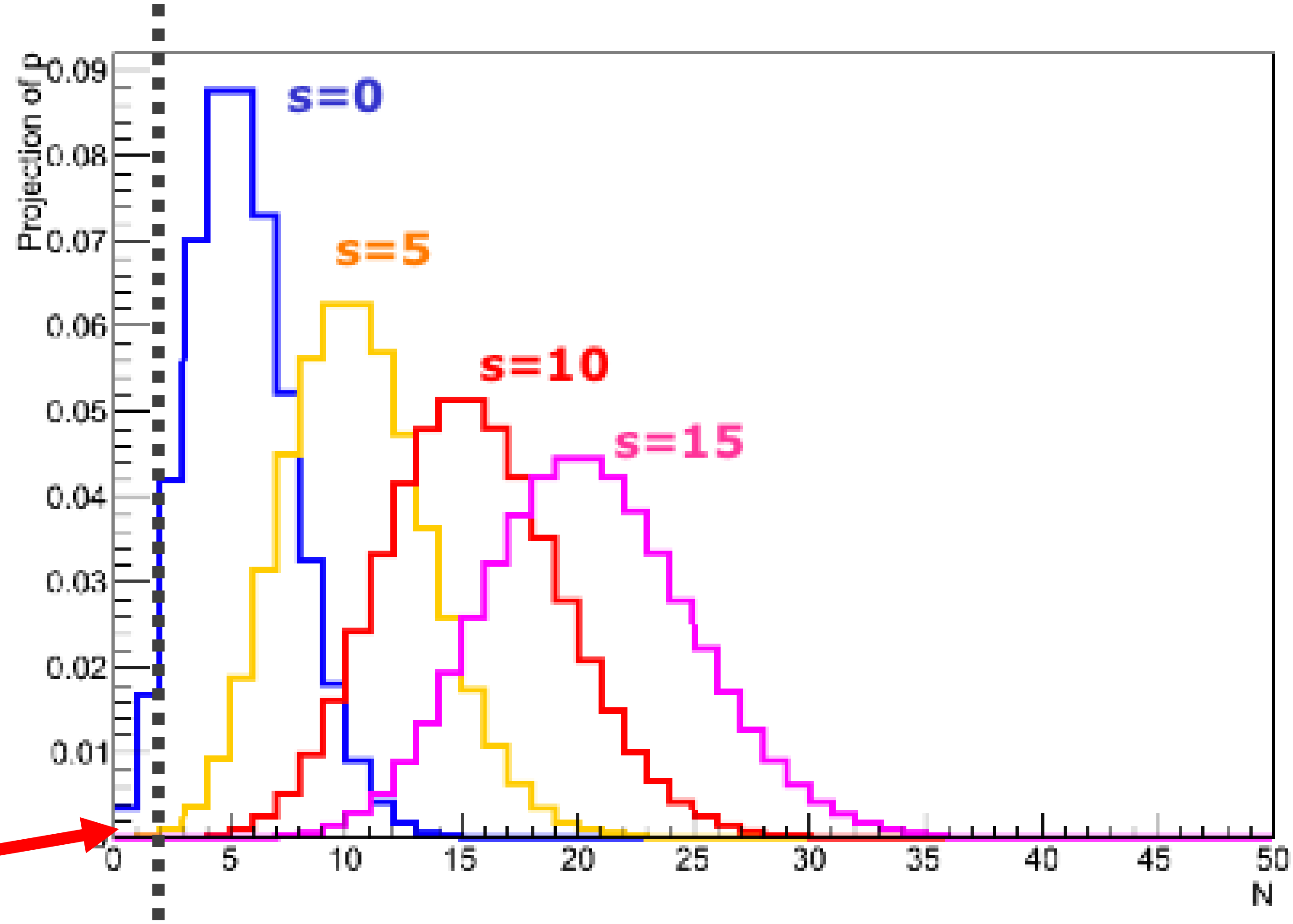
- Interpretation of $\mathbf{p_{s+b}}$ in terms of inference on signal only is problematic
  - Since $\mathbf{p_{s+b}}$ quantifies consistency with data of signal + background
  - Problem apparent when observed data has downward fluctuation wrt background expectation

- Example: Nobs = 2 → $\mathbf{p_{s+b}(s=0) = 0.04}$
  - **s≥0 excluded at 95% C.L. ???**

- Modified approach to protect against such inference on signal (LHC convention):
  - Instead of requiring $\mathbf{p_{s+b}} = 5\%$,

    require

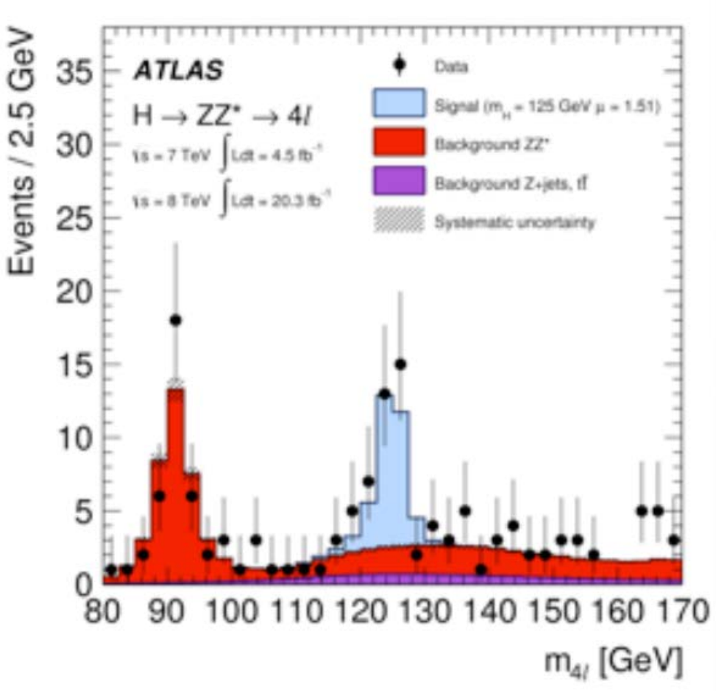
$$\mathrm{CL}_s \equiv \frac{p_{s+b}}{\boxed{1-p_b}} = 5\%$$

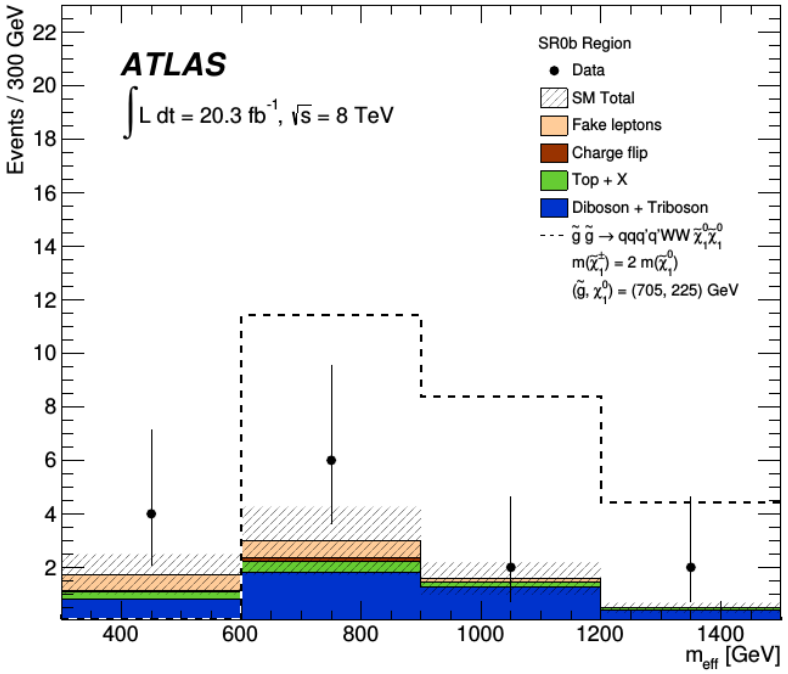


- Example: Nobs = 2 → **s>3.4 excluded at 95% CLs**
- For large Nobs effect on limit is small as $\mathbf{p_b} \to 0$
- https://twiki.cern.ch/twiki/pub/AtlasProtected/StatisticsTools/CLsInfo.pdf

More complex examples

- Typical analysis is not a simple counting experiment
  - Many intrinsic uncertainties on signal and bkg
  - Result is a distribution, not a single number
    - SUSY searches: discovery is cut&count, but many exclusion limits are shape-fits/multi-bin





- Any result can be converted into a single number by constructing a ***test statistic***
  - A test statistic compresses all signal-to-background discrimination power into one number
  - Most powerful discriminators are ***Likelihood Ratios*** *(Neyman-Pearson lemma)*
  - q_μ is a common test statistic (LHC convention)

$$q_\mu = -2\ln\frac{L(data\,|\,\mu)}{L(data\,|\,\hat{\mu})}$$

Likelihood ratio test statistic

- **Signal strength μ** = signal rate / nominal signal rate (also know as μ_{SIG})
  - Bkg-only hypothesis: **μ** = 0
  - Bkg + signal hypo: **μ** = 1
  - Bkg + 2 X signal hypo: **μ** = 2
- Likelihood with nominal signal strength (**μ** = 1)

'likelihood assuming nominal signal strength'

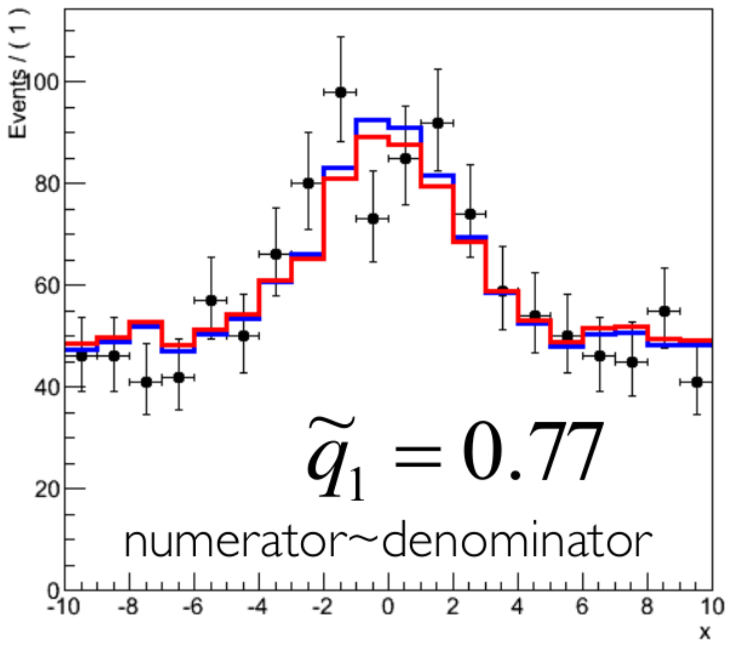
$$q_1 = -2\ln\frac{L(data\,|\,\mu=1)}{L(data\,|\,\hat{\mu})}$$

$\hat{\mu}$ is best fit value of μ

'likelihood of best fit'

- **Example:** simple s + b model with no uncertainties

*On signal-like data q1 is **small***



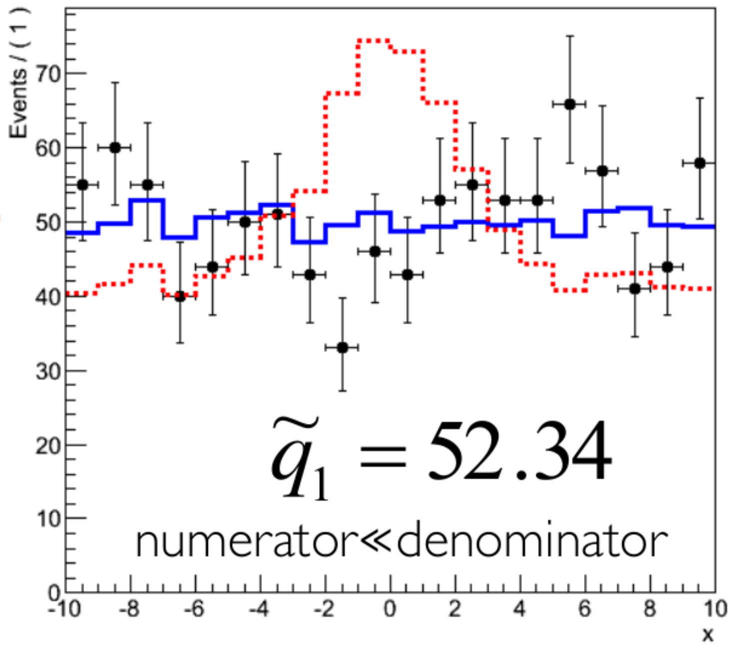
$$\tilde{q}_1 = 0.77$$

numerator~denominator

signal(μ=1)**+bkg**

best fit

*On background-like data q1 is **large***



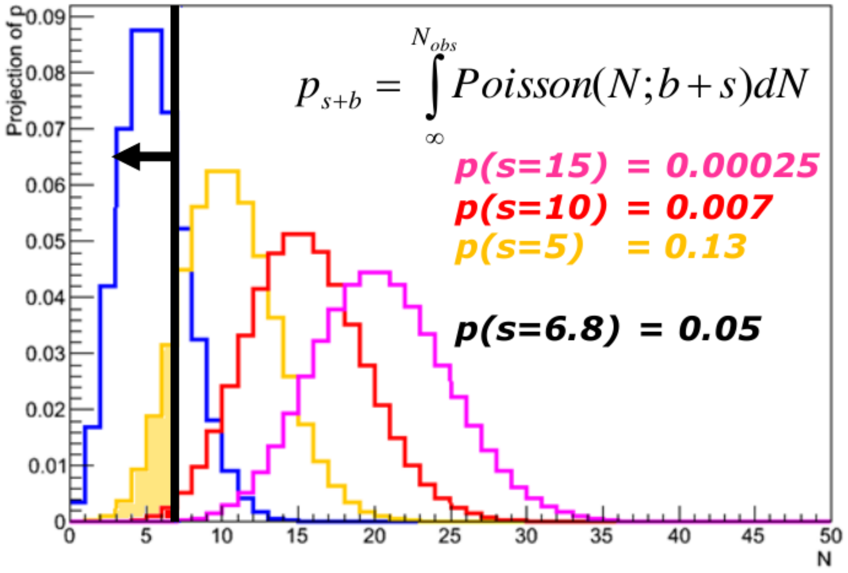
$$\tilde{q}_1 = 52.34$$

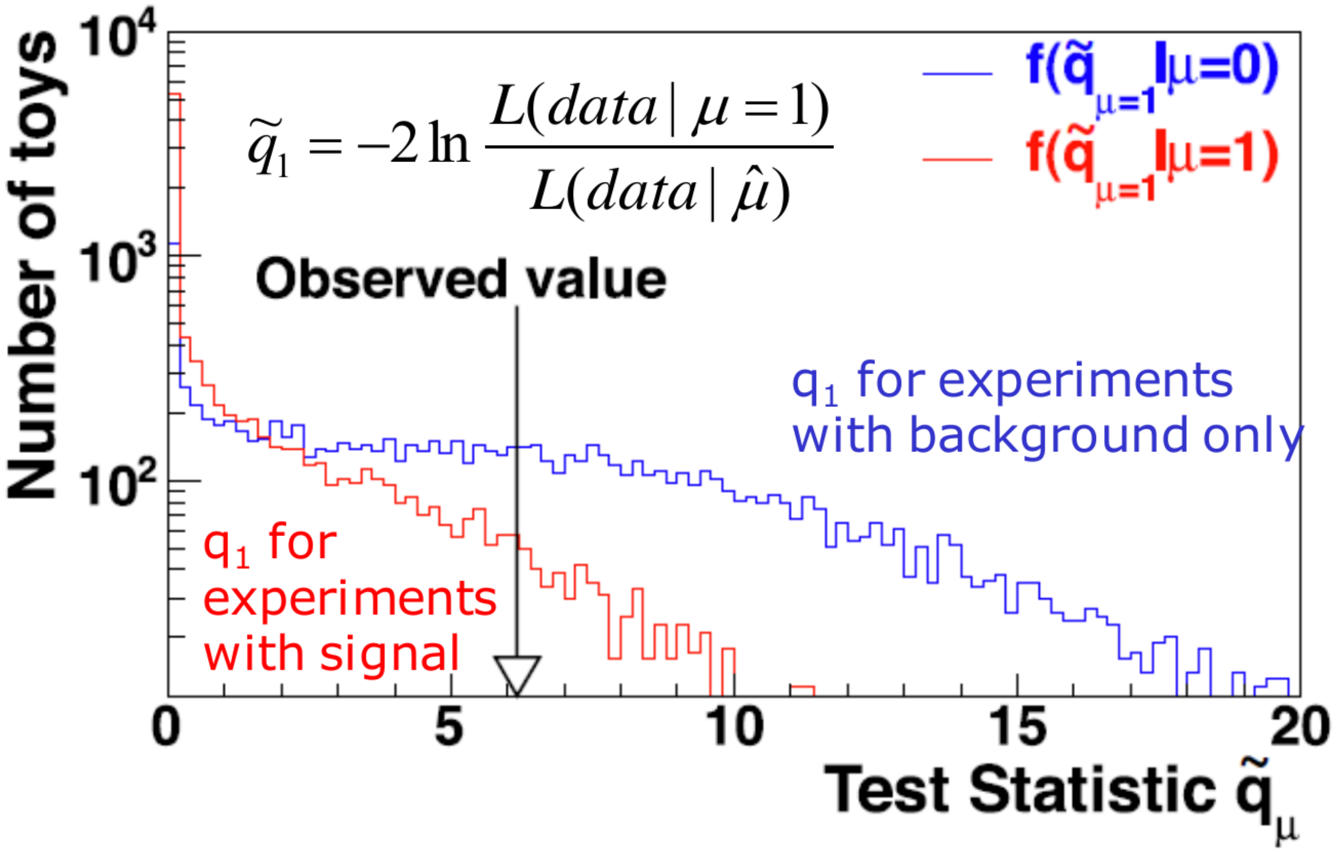
numerator≪denominator

Distribution of test statistic

- Value of q_1 on data is now the *measurement*
- Distribution of q_1 is **not** calculable → But can be obtained from pseudo-experiments (toys)
  - Generate a large number of pseudo-experiments with a given value of **μ**, calculate q_1 for each, plot distribution

Note analogy to Poisson counting example





- From q_{obs} and these test statistic distributions, f(q_μ), can then set limits or calculate discovery significance similar to what was shown for Poisson example

- Typically CPU-intensive to run many toy-experiments → approximate with **asymptotic formulae**, aka **asimov data** (only works in cases when Nobs≳10, see links for details)

Systematic uncertainties

- Typically HEP models will have uncertainties: experimental (JES,trigger eff.) or theoretical (Q,σ)

$$L(data\,|\,\mu) \rightarrow L(data\,|\,\mu,\vec{\theta}) \qquad L(data\,|\,\mu,\theta) = Poisson(N_i\,|\,\mu\cdot s_i(\theta)+b_i(\theta))\cdot p(\tilde{\theta},\theta)$$

- Models w/ uncertainties, described by additional parameters θ that describe effect of uncert.
- Likelihood includes *auxiliary measurement* terms that constrain the nuisance parameters θ
  - Auxiliary measurement given by performance group (jet perf.) or theory variations (renorm. scale up/down)

- Likewise uncertainties quantified by nuisance parameters are incorporated into test statistic using **Profile Likelihood Ratio**

$$q_\mu = -2\ln\frac{L(data\,|\,\mu)}{L(data\,|\,\hat{\mu})} \longrightarrow \tilde{q}_\mu = -2\ln\frac{L(data\,|\,\mu,\hat{\hat{\theta}}_\mu)}{L(data\,|\,\hat{\mu},\hat{\theta})}$$

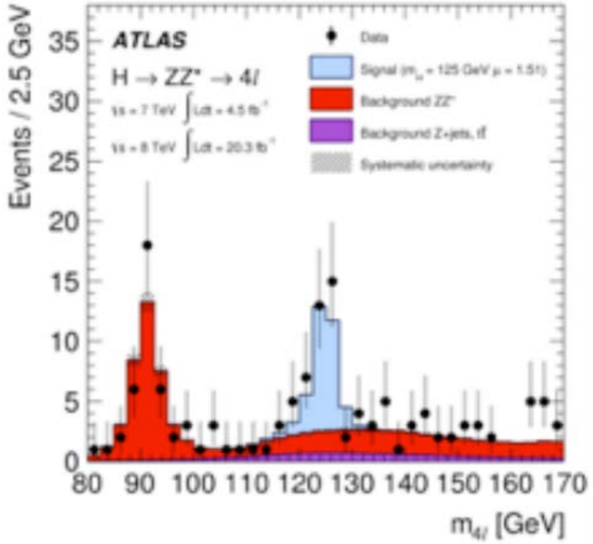
‘likelihood of best fit for a **given fixed value of μ’**

‘likelihood of best fit’

(with a constraint $0 \leq \hat{\mu} \leq \mu$)

Overview for a search

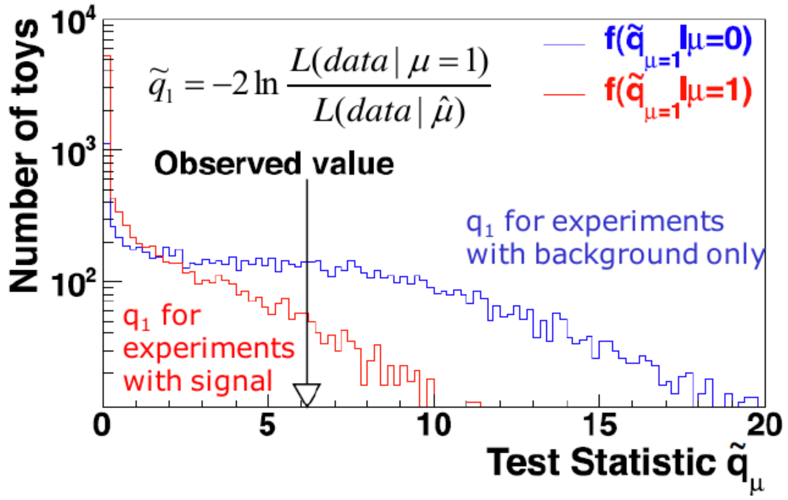
- Take Higgs search as example, and put it all together



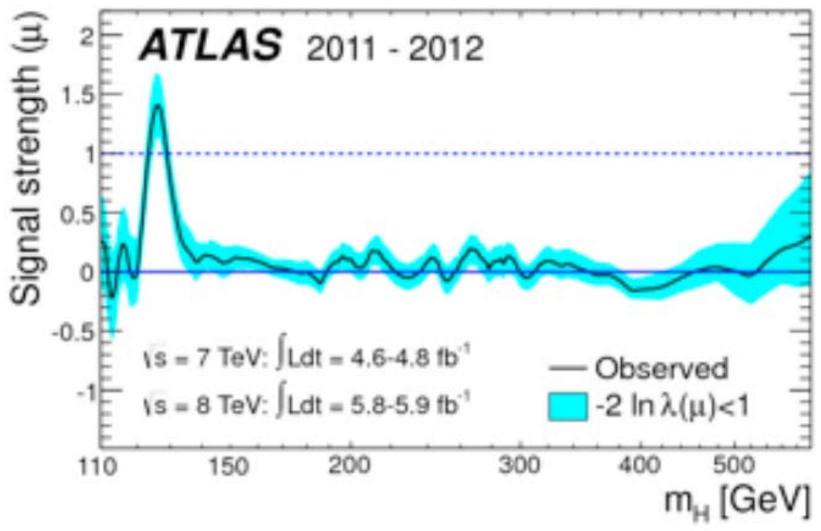
- Result from data is a distribution (eg m(4l))
- Model signal and background by PDF (probability density function) for a given Higgs mass hypothesis

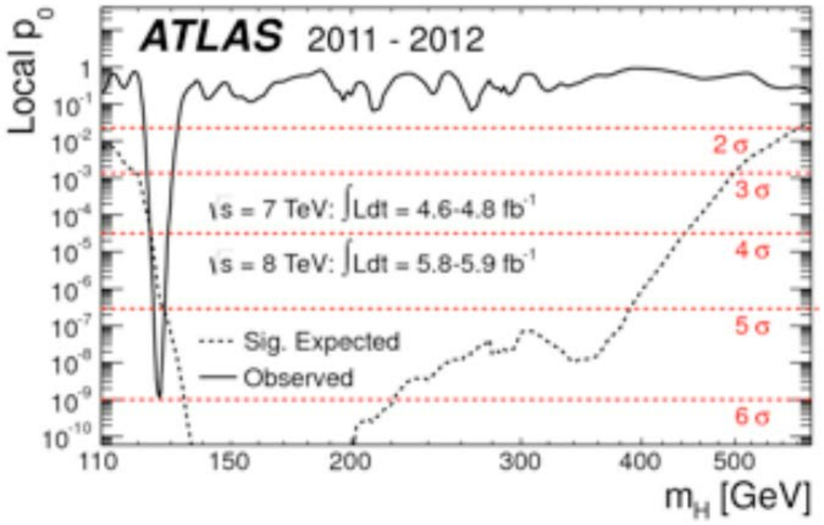
- Construct likelihood(s) by joining data and model(s)
- Construct test statistic ***q*****μ** from likelihoods

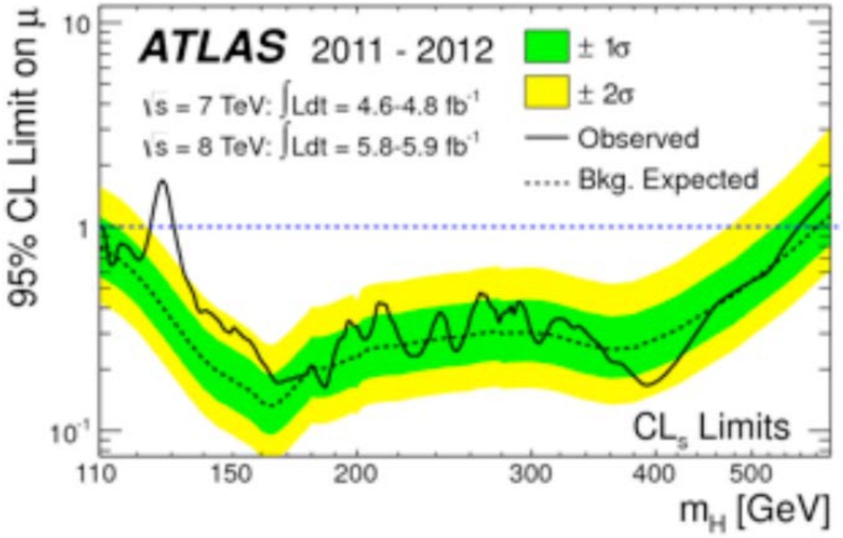
$$\tilde{q}_\mu(m_H) = -2\ln\frac{L(data\,|\,\mu, m_H\hat{\hat{\theta}}_\mu)}{L(data\,|\,\hat{\mu}, m_H\hat{\theta})}$$



- Obtain expected distributions of ***q*****μ**
- Determine discovery **p₀** and signal exclusion limit
- Repeat for each assumed m**H**





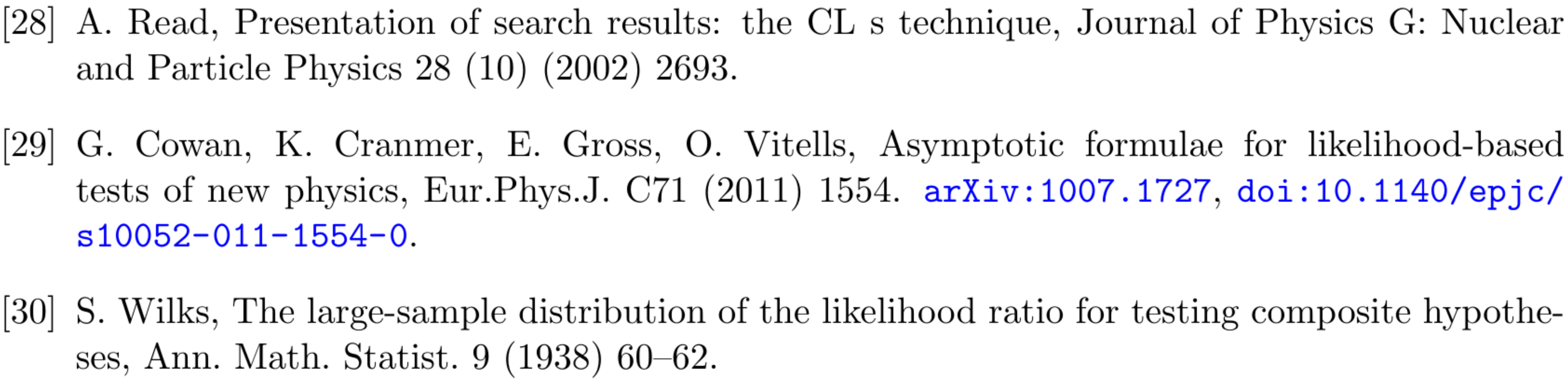


Links

- Statistics lectures (CERN school, 2014, W. Verkerke):
  - Part-1: https://indico.cern.ch/event/287744/contribution/7/material/slides/0.pdf
  - Part-2: https://indico.cern.ch/event/287744/contribution/11/material/slides/1.pdf
  - Part-3: https://indico.cern.ch/event/287744/contribution/14/material/slides/0.pdf

- Plotting the Differences Between Data and Expectation, G. Choudalakis, D. Casadei http://arxiv.org/abs/1111.2062

- CLs: https://twiki.cern.ch/twiki/pub/AtlasProtected/StatisticsTools/CLsInfo.pdf



[28] A. Read, Presentation of search results: the CL s technique, Journal of Physics G: Nuclear and Particle Physics 28 (10) (2002) 2693.

[29] G. Cowan, K. Cranmer, E. Gross, O. Vitells, Asymptotic formulae for likelihood-based tests of new physics, Eur.Phys.J. C71 (2011) 1554. arXiv:1007.1727, doi:10.1140/epjc/s10052-011-1554-0.

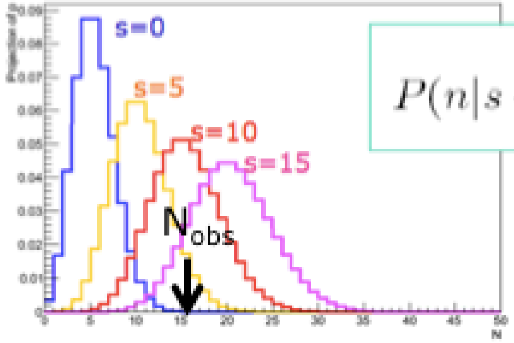
[30] S. Wilks, The large-sample distribution of the likelihood ratio for testing composite hypotheses, Ann. Math. Statist. 9 (1938) 60–62.

Introduction to statistics tools

Largely borrowed from lectures/slides by W. Verkerke

LIKELIHOOD, LIKELIHOOD, LIKELIHOOD...

- **All** fundamental statistical procedures are based on the likelihood function as ‘description of the measurement’



$$P(n|s+b) = \frac{(s+b)^n}{n!} e^{-(s+b)}$$

NB: b is a constant in this example

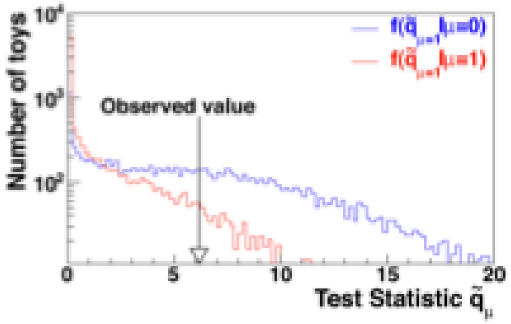
Definition: the Likelihood is P(observed data|theory)

e.g. L(15|s=0)

e.g. L(15|s=10)

Frequentist statistics

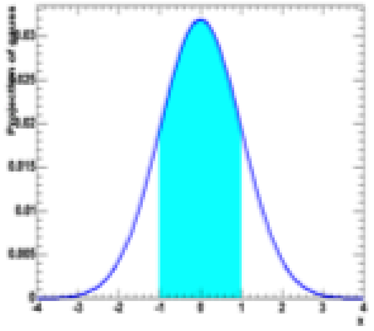
$$\lambda_\mu(\vec{N}_{obs}) = \frac{L(\vec{N}\,|\,\mu)}{L(\vec{N}\,|\,\hat{\mu})}$$



Confidence interval or p-value

Bayesian statistics

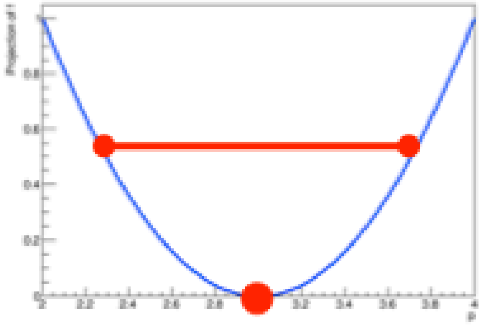
$$P(\mu) \propto L(x\,|\,\mu) \cdot \pi(\mu)$$



Posterior on s or Bayes factor

Maximum Likelihood

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



s = x ± y

Wouter Verkerke, NIKHEF

Modular software design

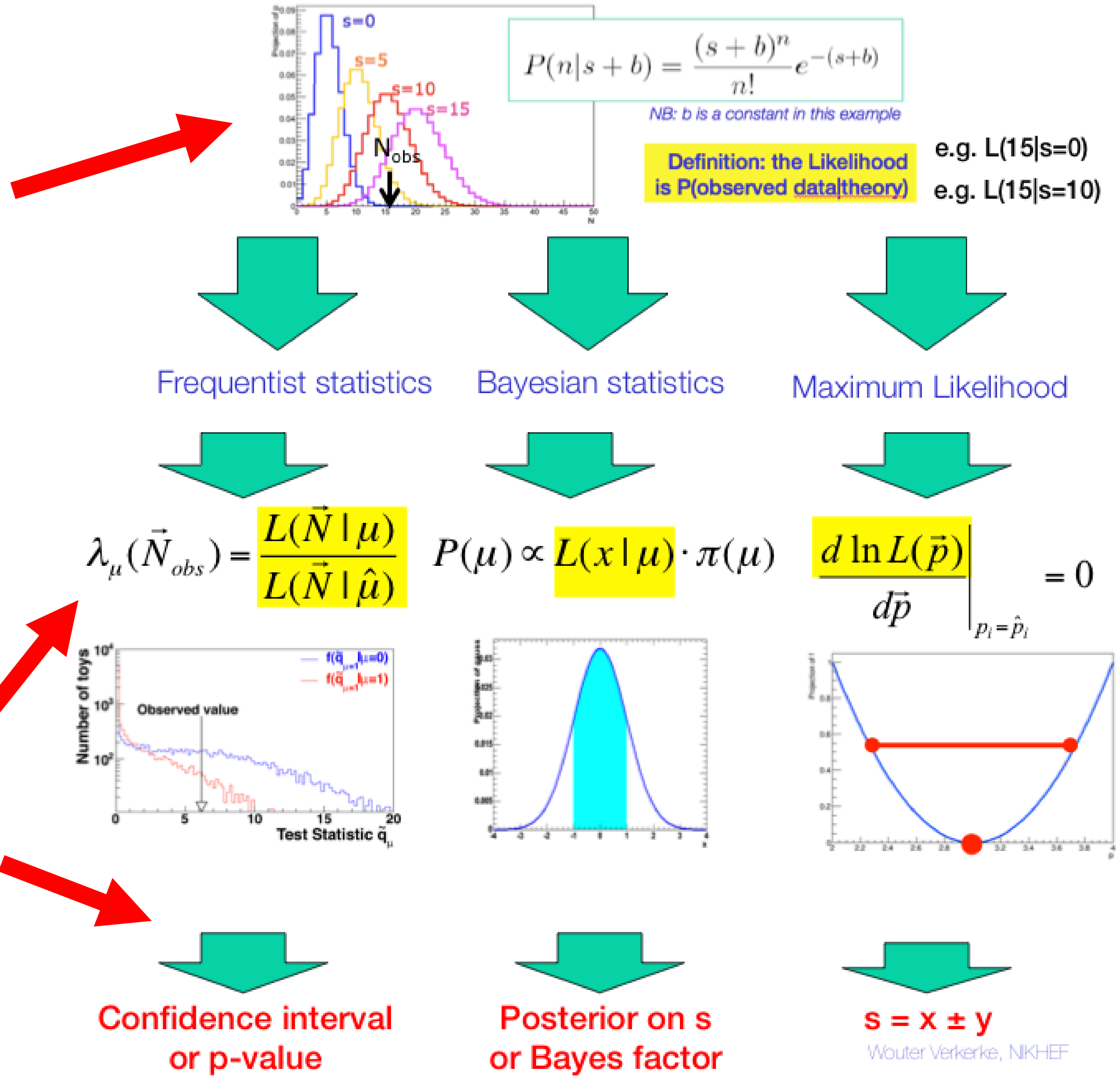
- **RooFit:** tool/language for building probability models: datasets, likelihoods, minimization, toy data, visualization

- **HistFactory:** tool to construct binned template models of arbitrary complexity using classes of physics concepts: channel/region, sample, uncertainties
  Builds a RooFit stat. model from HistFactory physics model

- **RooWorkspace:** persistent RooFit object to transport a likelihood, containing model/data. Completely factorizes process of building and using likelihood functions.

- **RooStats:** tool/suite to calculate intervals and perform hypothesis tests using a variety of statistical techniques; easy to use with RooWorkspace

- **All** fundamental statistical procedures are based on the likelihood function as 'description of the measurement'



$$P(n|s+b) = \frac{(s+b)^n}{n!}e^{-(s+b)}$$

NB: b is a constant in this example

Definition: the Likelihood is P(observed data|theory)

e.g. L(15|s=0)

e.g. L(15|s=10)

Frequentist statistics

Bayesian statistics

Maximum Likelihood

$$\lambda_\mu(\vec{N}_{obs}) = \frac{L(\vec{N}\,|\,\mu)}{L(\vec{N}\,|\,\hat{\mu})}$$

$$P(\mu) \propto L(x\,|\,\mu)\cdot\pi(\mu)$$

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

Confidence interval or p-value

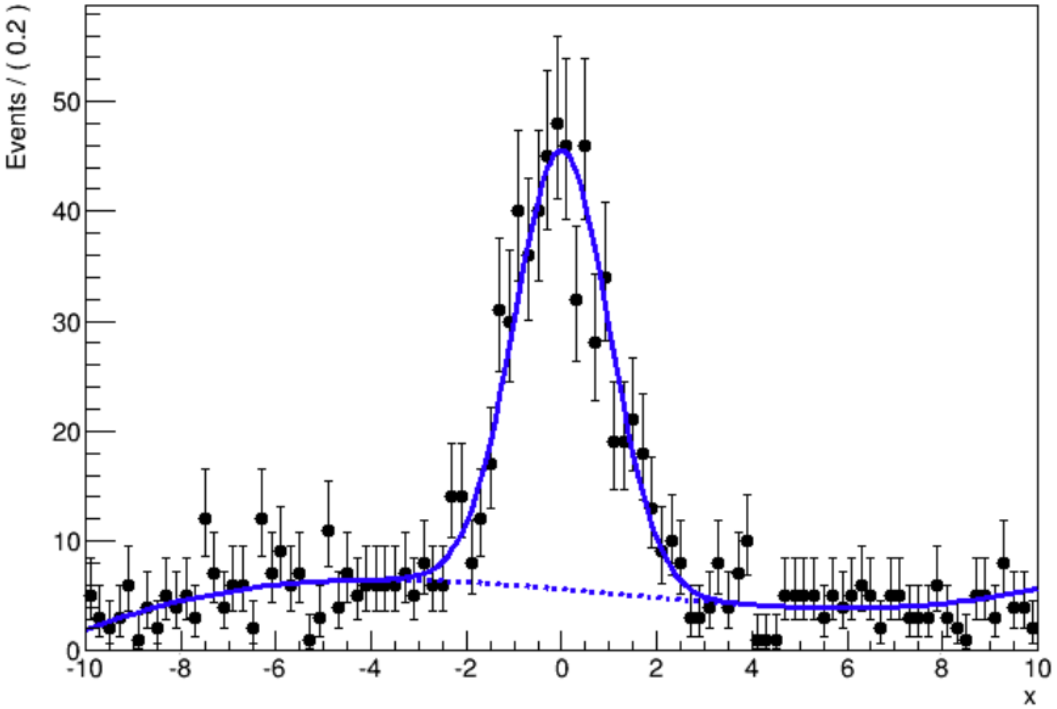
Posterior on s or Bayes factor

s = x ± y

Wouter Verkerke, NIKHEF

RooFit

- Focus: coding a probability density function PDF : how do you formulate a PDF in ROOT?

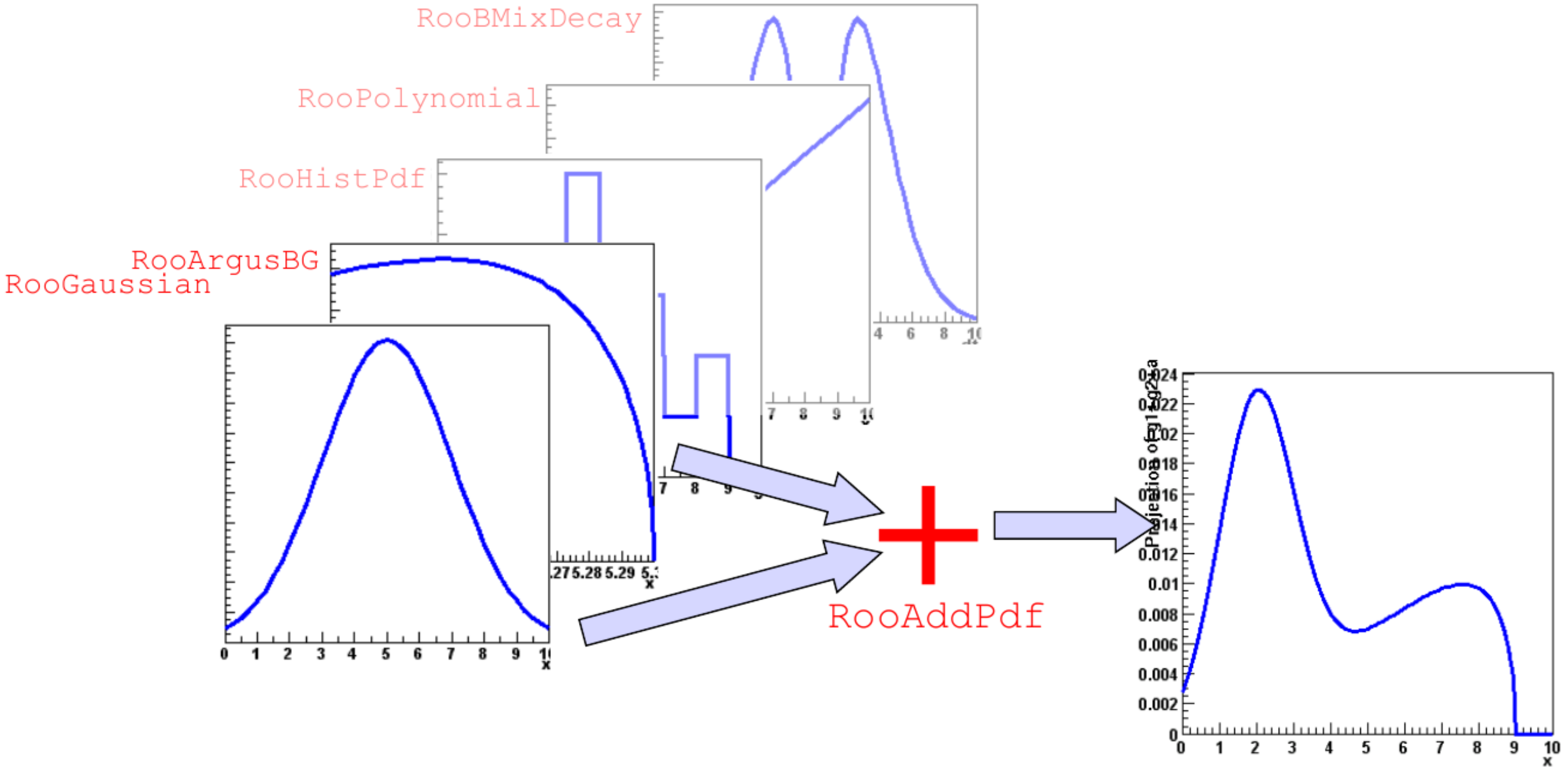


- Simple example: gauss (signal) + polynomial (bkg)
- Quickly becomes complicated: multidimensional, unbinned fits, non-trivial functions, non-analytic functions
- Core design philosophy:
  mathematical objects represented as C++ objects

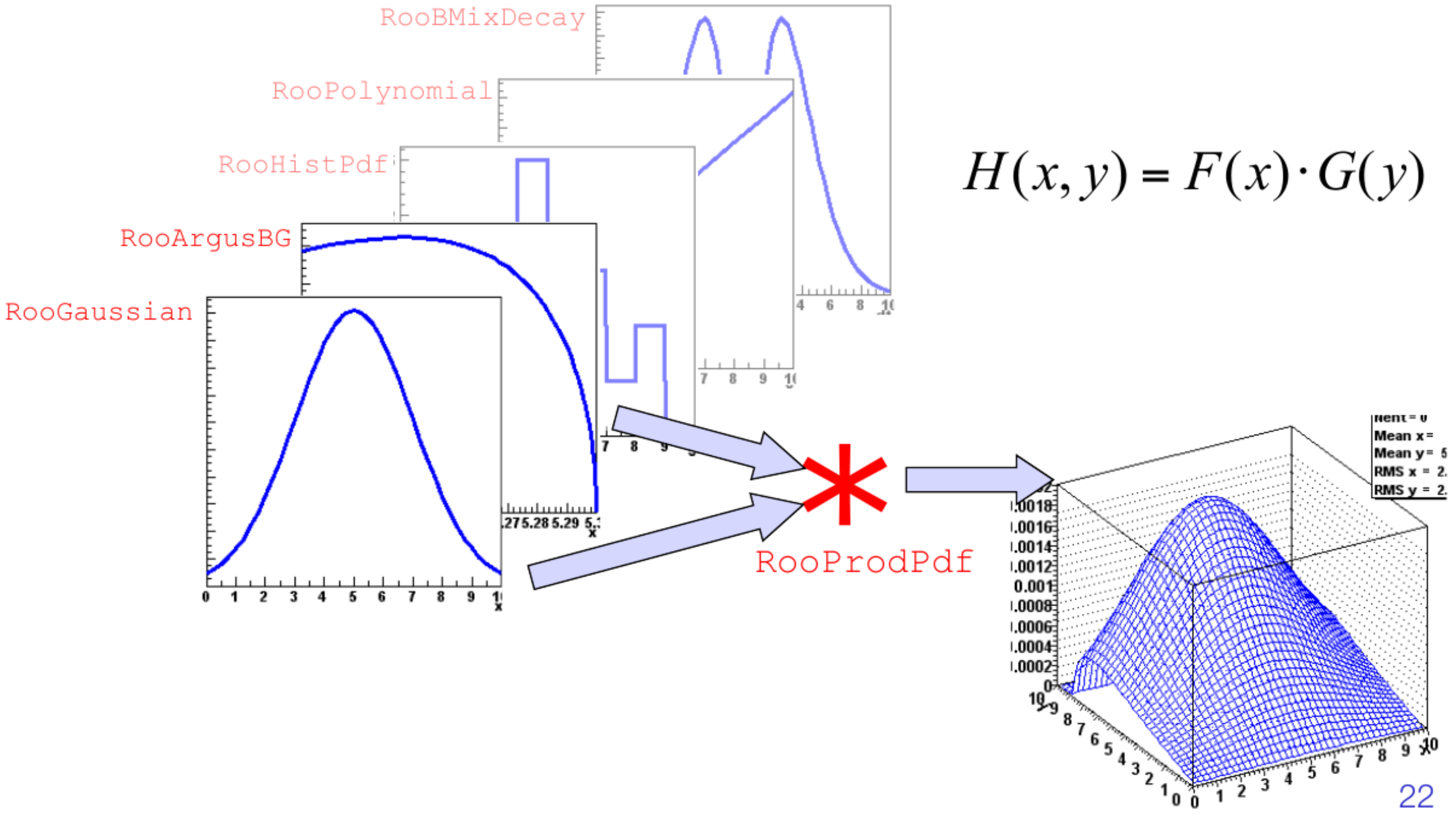
Mathematical concept		RooFit class
variable	x	`RooRealVar`
function	$f(x)$	`RooAbsReal`
PDF	$f(x)$	`RooAbsPdf`
space point	$\vec{x}$	`RooArgSet`
integral	$\int_{x_{\min}}^{x_{\max}} f(x)dx$	`RooRealIntegral`
list of space points		`RooAbsData`

RooFit - model building

- Easy to use standard components to build more complex/realistic models
- Addition



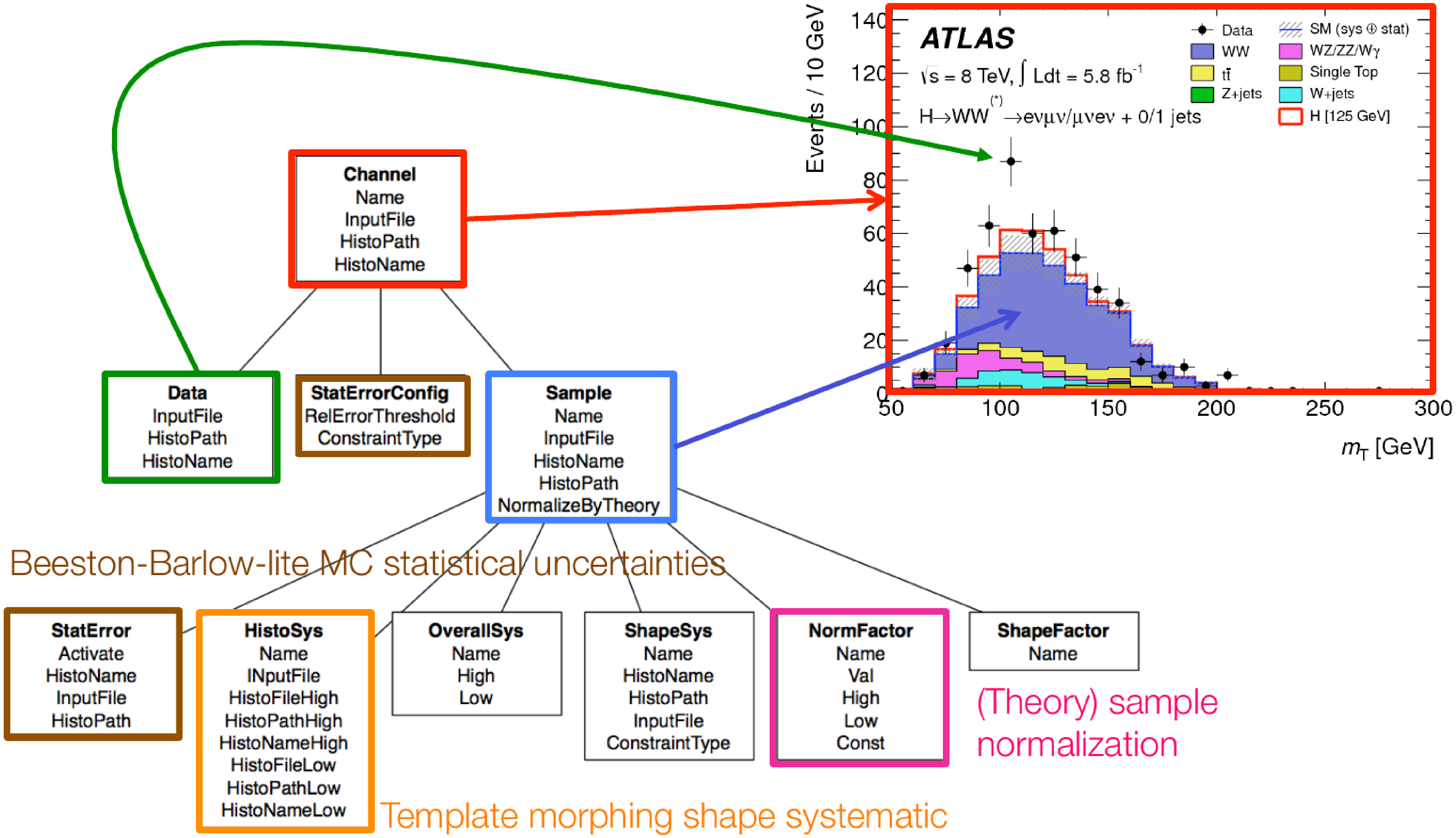
- Product (multi-dimensional)



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

HistFactory

- Structured building of complex models based on binned templates (histograms)
- Classes of physics concepts:
  - Channel = region of phase space
    - One or more channels are combined to form a measurement
  - Sample = physics process: either data-driven or described by Monte Carlo (MC) simulation
  - Systematics = intrinsic uncertainty on your model



Channel
Name
InputFile
HistoPath
HistoName

Data
InputFile
HistoPath
HistoName

StatErrorConfig
RelErrorThreshold
ConstraintType

Sample
Name
InputFile
HistoName
HistoPath
NormalizeByTheory

Beeston-Barlow-lite MC statistical uncertainties

StatError
Activate
HistoName
InputFile
HistoPath

HistoSys
Name
INputFile
HistoFileHigh
HistoPathHigh
HistoNameHigh
HistoFileLow
HistoPathLow
HistoNameLow

OverallSys
Name
High
Low

ShapeSys
Name
HistoName
HistoPath
InputFile
ConstraintType

NormFactor
Name
Val
High
Low
Const

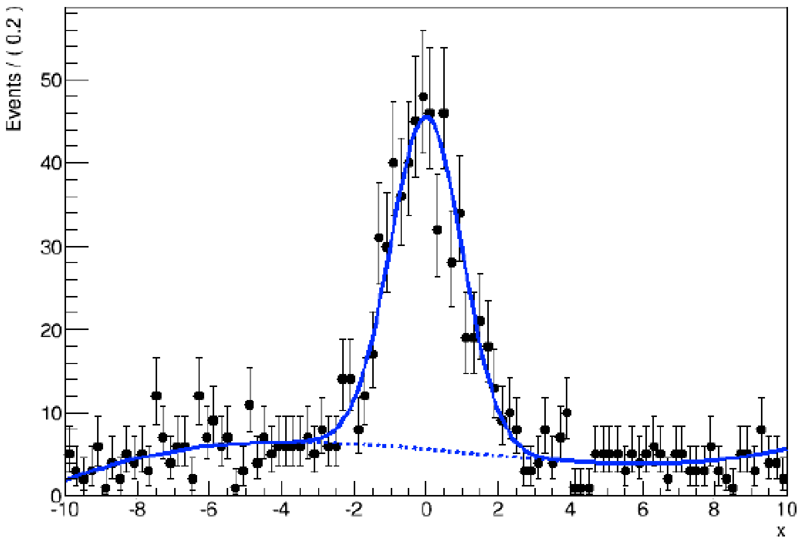
ShapeFactor
Name

(Theory) sample normalization

Template morphing shape systematic

Systematics : nuisance parameters

- Empirical modeling of your model is easy to do, but expect some hard questions
  - Gaussian for signal + polynomial for background



$$L(x \mid f, m, \sigma, a_0, a_1, a_2) = fG(x, m, \sigma) + (1-f)Poly(x, a_0, a_1, a_2)$$

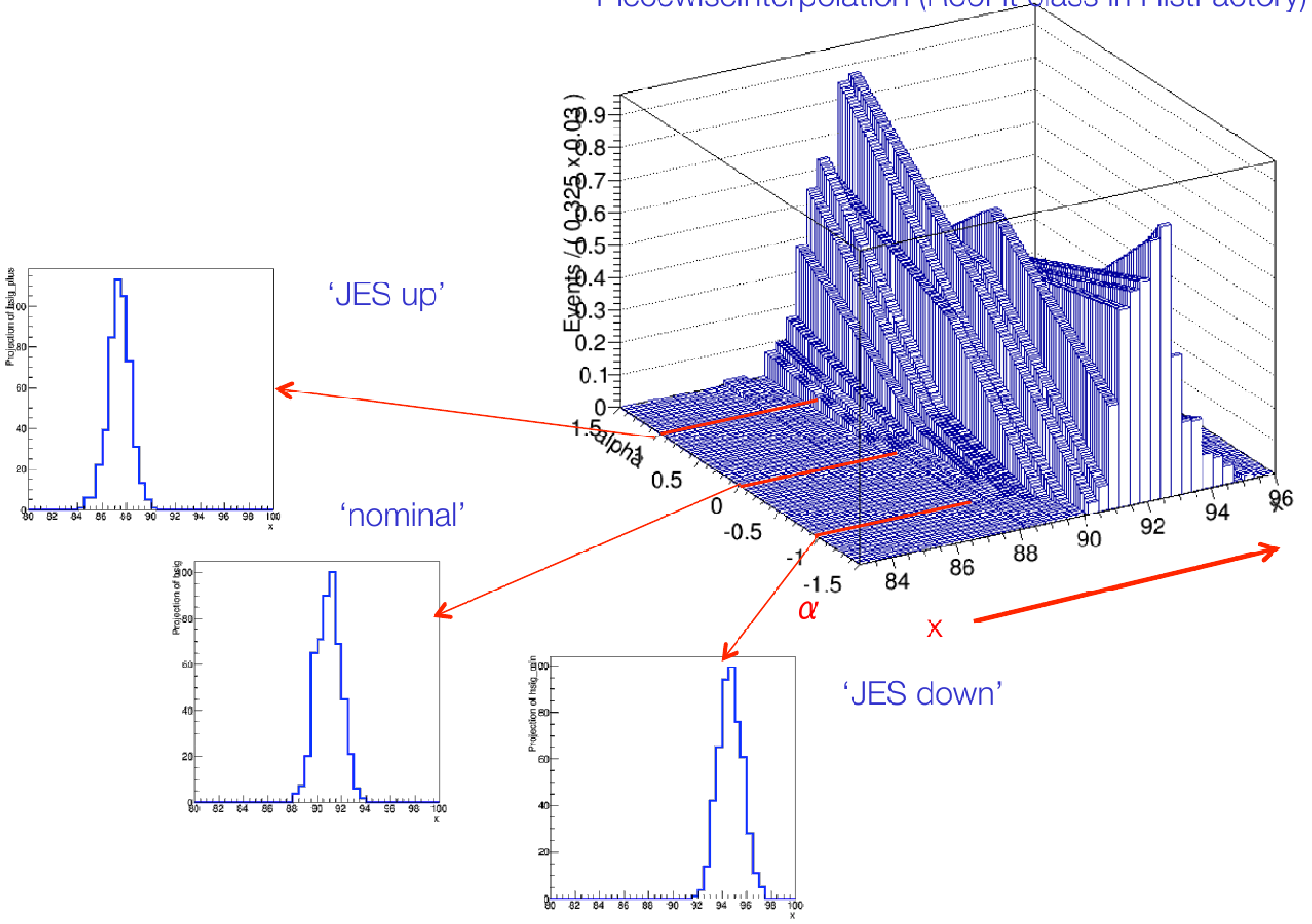
- Is your model correct?
  - Is the true signal distribution captured by a Gaussian?
- Is your model flexible enough?
  - Why use 4th order polynomial and not 6th order?
- How do your model parameters connect to known detector/theory uncertainties for your distribution?
  - What conceptual uncertainty does what parameter represent? And are all conceptual uncertainties represented?

Systematics modeling - interpolation

- A common solution is to introduce degrees of freedom in model that describe specific systematic/uncertainty!
- The +1/-1 σ variations sampled from MC simulation are compared to nominal MC response
    - (corrected/checked/double-checked to data by Perf. Groups)
- Interpolation, performed between **+1σ** ↔ **nominal** ↔ **-1σ** taken into the model as nuisance parameter

$$L(data\,|\,\mu,\theta) = Poisson(N_i\,|\,\mu\cdot s_i(\theta)+b_i(\theta))\cdot p(\tilde{\theta},\theta)$$

PiecewiseInterpolation (RooFit class in HistFactory)



'JES up'

'nominal'

'JES down'

RooWorkspace

- Complete description of likelihood persistable in a ROOT file
- Factorizes building and using likelihood functions
  - In setup, team member, place and time

- Construct RooFit model **`sum`** and persist to ROOT file

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

- Pass file to your colleague

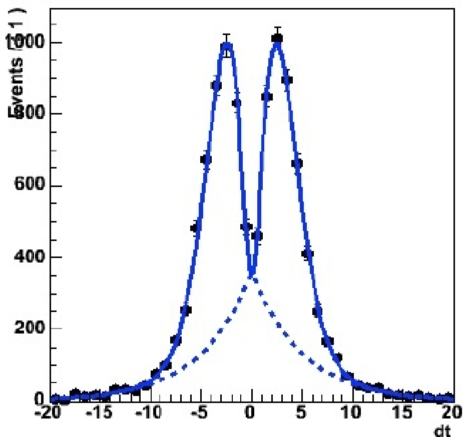
model.root

- Colleague resurrects likelihood, runs fit and produces plots

```
// Resurrect model and data
TFile f(“model.root”) ;
RooWorkspace* w = f.Get(“w”) ;
RooAbsPdf* model = w->pdf(“sum”) ;
RooAbsData* data = w->data(“xxx”) ;

// Use model and data
model->fitTo(*data) ;

RooPlot* frame =
         w->var(“dt”)->frame() ;
data->plotOn(frame) ;
model->plotOn(frame) ;
```

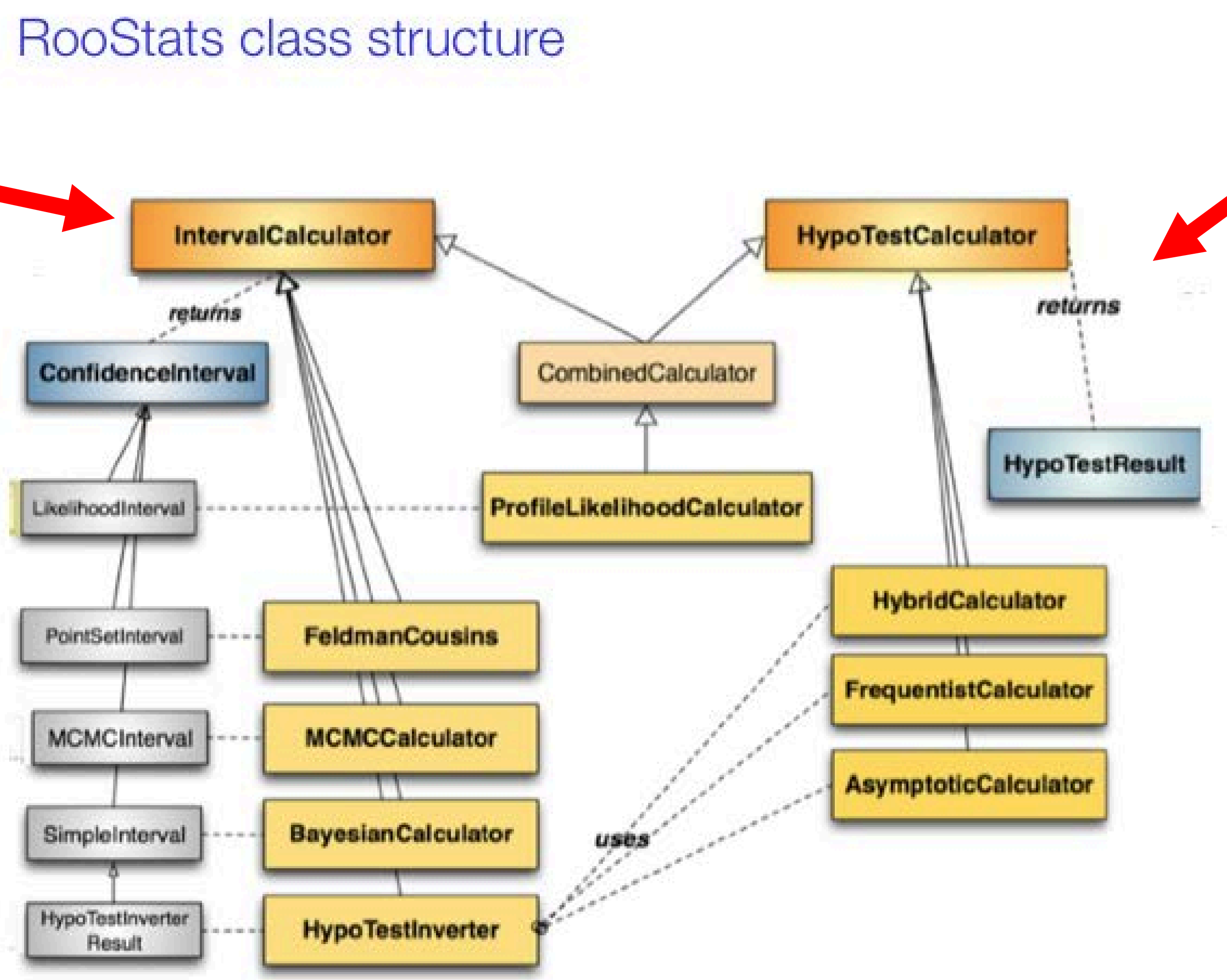


RooStats

- RooFit/HistFactory give tools to construct (complex) probability density functions
- RooWorkspace makes it possible to decouple statistical test tools from model contruction
- **RooStats** project/tools suite delivers a series of tools that can calculate intervals and perform hypothesis tests using a variety of statistical techniques
  - Frequentist/Bayesian/Likelihood-based methods (confidence/credible interval, hypothesis tests)

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

- Abstract interface for procedure to calculate a confidence interval
- Abstract interface for result: *s>6.8 is at 95% C.L.*


RooStats class structure

- Abstract interface for hypothesis tester to calculate a p-value
- Concrete result class: *<u>HypoTestResult</u>*
  $p_b = 0.023$
  $CL_S = 0.00513$

Overview

- **Step-0:** define signal/control/validation regions
  - Input TTrees (derived from xAOD), histograms, numbers
- **Step-1:** Construct PDF and the likelihood function

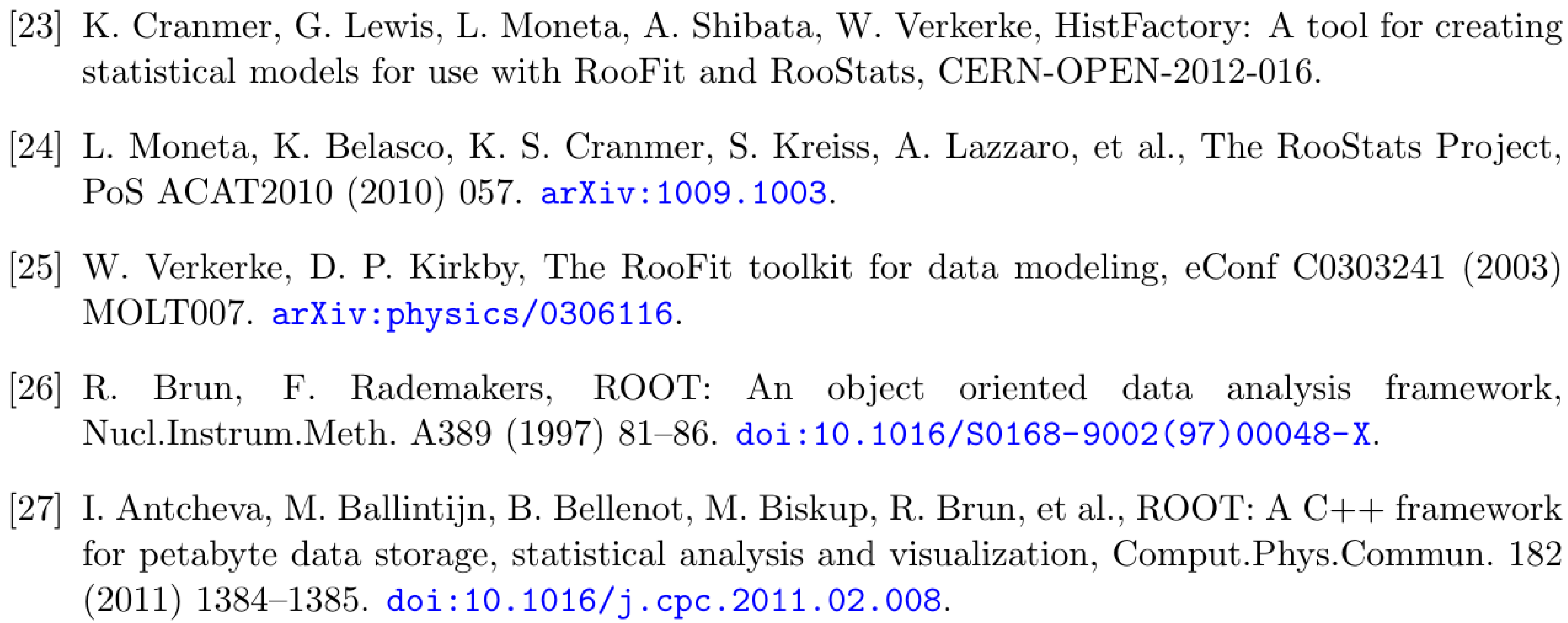
  RooFit or HistFactory + RooFit
  - Result from data is a distribution
  - Model signal and background by PDF (prob. density func.)
  - Construct likelihood(s) by joining data and model(s)
- ↓
- **RooWorkspace**
- ↓
- **Step-2:** Statistical tests on parameter of interest μ

  RooStats
  - Construct test statistic q_μ from likelihoods
  - Obtain expected distributions of q_μ for various μ values
  - Determine discovery p_0 and signal exclusion limit
- **Step-3:** Repeat for each model (assumed value m_H)

HistFitter
- adds steps-0 and 3
- allows full analysis chain from simple configuration file

Links

- RooFit overview (2004): http://www.nikhef.nl/~verkerke/talks/chep03/chep2003_v4.pdf
- ATLAS Statistics Forum page on Stat. Tools: https://twiki.cern.ch/twiki/bin/viewauth/AtlasProtected/StatisticsTools
- RooFit/RooStats at ACAT 2014: https://indico.cern.ch/event/258092/session/0/contribution/140/material/slides/1.pdf
- Higgs Combination procedure/explanation of CLs observed/expected and error bands: http://cds.cern.ch/record/1375842
- HistFactory documentation:
  https://cdsweb.cern.ch/record/1456844/
  https://twiki.cern.ch/twiki/bin/view/RooStats/HistFactory



[23] K. Cranmer, G. Lewis, L. Moneta, A. Shibata, W. Verkerke, HistFactory: A tool for creating statistical models for use with RooFit and RooStats, CERN-OPEN-2012-016.

[24] L. Moneta, K. Belasco, K. S. Cranmer, S. Kreiss, A. Lazzaro, et al., The RooStats Project, PoS ACAT2010 (2010) 057. arXiv:1009.1003.

[25] W. Verkerke, D. P. Kirkby, The RooFit toolkit for data modeling, eConf C0303241 (2003) MOLT007. arXiv:physics/0306116.

[26] R. Brun, F. Rademakers, ROOT: An object oriented data analysis framework, Nucl.Instrum.Meth. A389 (1997) 81–86. doi:10.1016/S0168-9002(97)00048-X.

[27] I. Antcheva, M. Ballintijn, B. Bellenot, M. Biskup, R. Brun, et al., ROOT: A C++ framework for petabyte data storage, statistical analysis and visualization, Comput.Phys.Commun. 182 (2011) 1384–1385. doi:10.1016/j.cpc.2011.02.008.

HistFitter introduction

Introduction

- **HistFitter** is a statistical tool/framework used in (almost) all SUSY WG analyses since 2012 for fitting, interpretation and presentation of fit results
  - Developed in SUSY strong production 1-lepton group, quickly adopted as recommended tool
  - Small core team: Max Baak, Geert-Jan Besjes, David Cote, Alex Koutsman, Jeanette Lorenz and Dan Short
  - Also used (more and more) in Higgs, Exotics and Top WGs

- **HistFitter** is:
  - built on top of RooFit/HistFactory and RooStats
  - consists of Python part for configuration and C++ part for CPU-intensive calculations

- Why HistFitter?
- **HistFitter** extends RooFit/HistFactory and RooStats in four key areas:
  - Programmable framework: performing complete analysis (steps 0-4) from a simple configuration file
  - Analysis strategy: common physics analysis strategy concepts, such as control/signal/validation regions, woven into the fabric of HistFitter design
  - Bookkeeping: can keep track of numerous data models, from histogram production until final statistical tests → handy when working with large collections of signal hypotheses (*signal grids*)
  - Presentation and interpretation: multiple methods are provided to determine statistical significance of signal hypotheses, and produce publication-quality tables and plot summarizing the fit results (*step 4*)

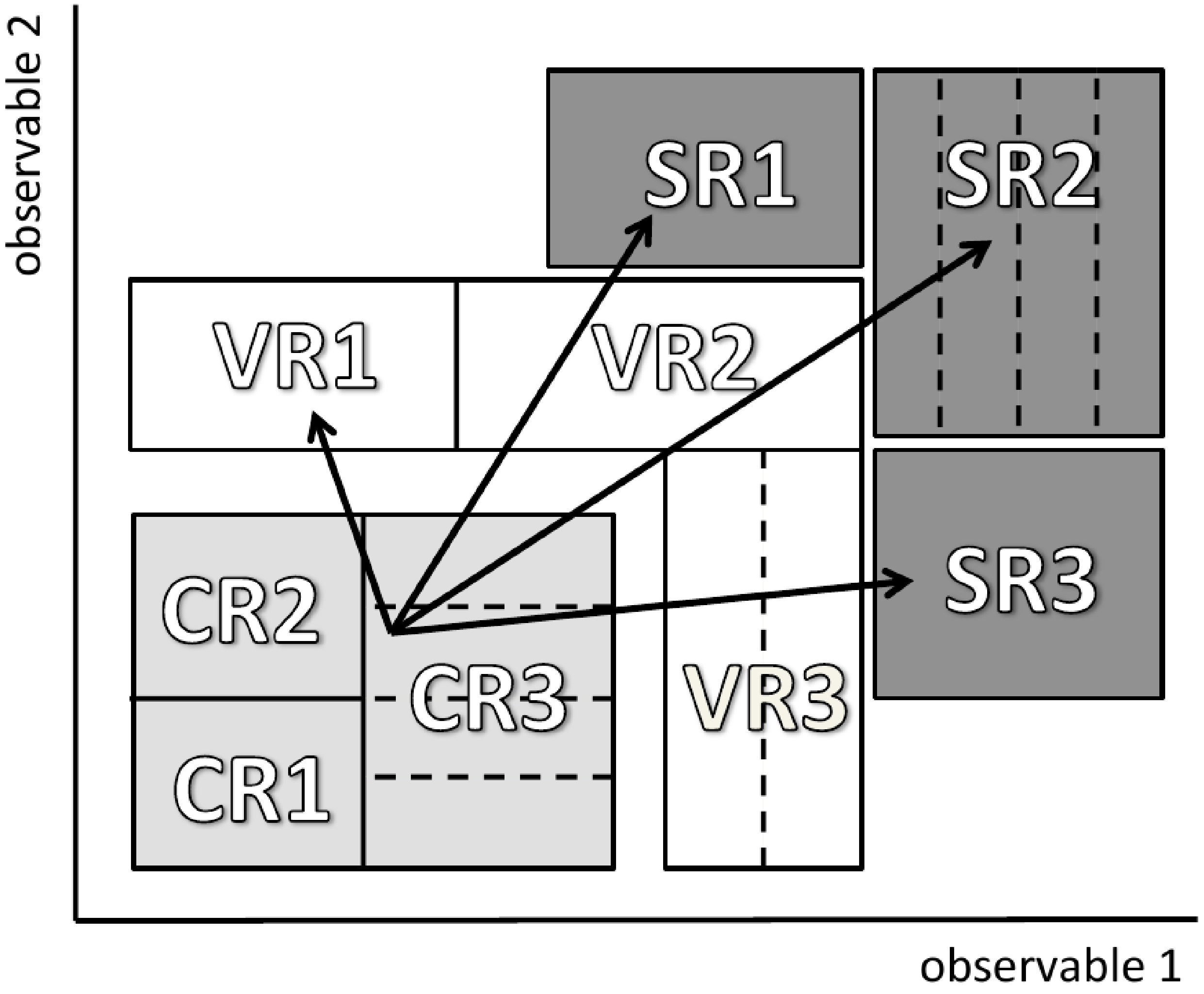
Data analysis strategy

- Particle physics analyze large data samples for measurements of discovery
- Data interpretation relies on using external - simulation, Monte Carlo (MC) - predictions for backgrounds and signal
- HistFitter configures and builds parametric models from these predictions

- Typically one defines several phase space regions to study a specific phenomenon

- Definition depends on the purpose:
  - **Signal region:** signal-rich region (SR)
  - **Control region:** background-rich region (CR), fit simulated backgrounds to data
  - **Validation region:** validation of extrapolation (VR)

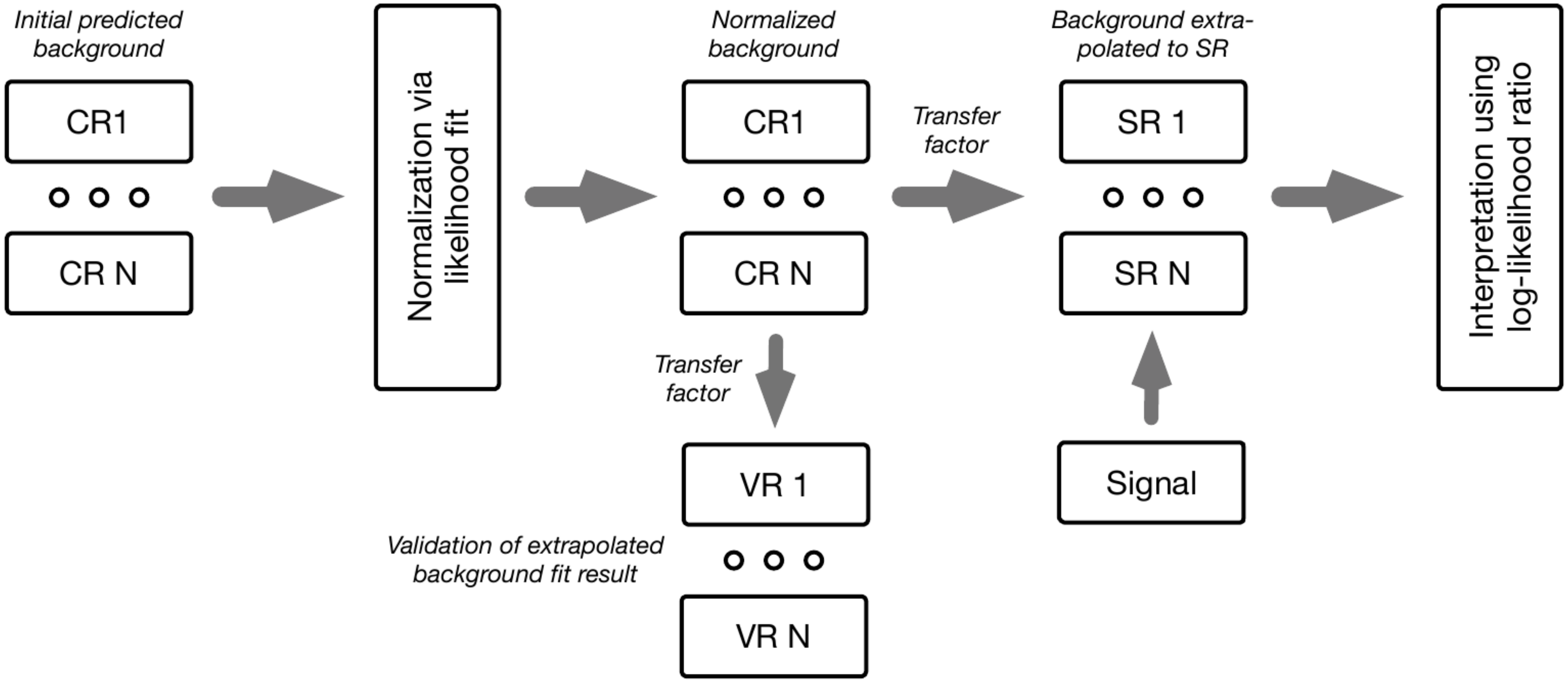
- Concepts of CR/SR/VR woven into the fabric of HistFitter



Analysis strategy flow

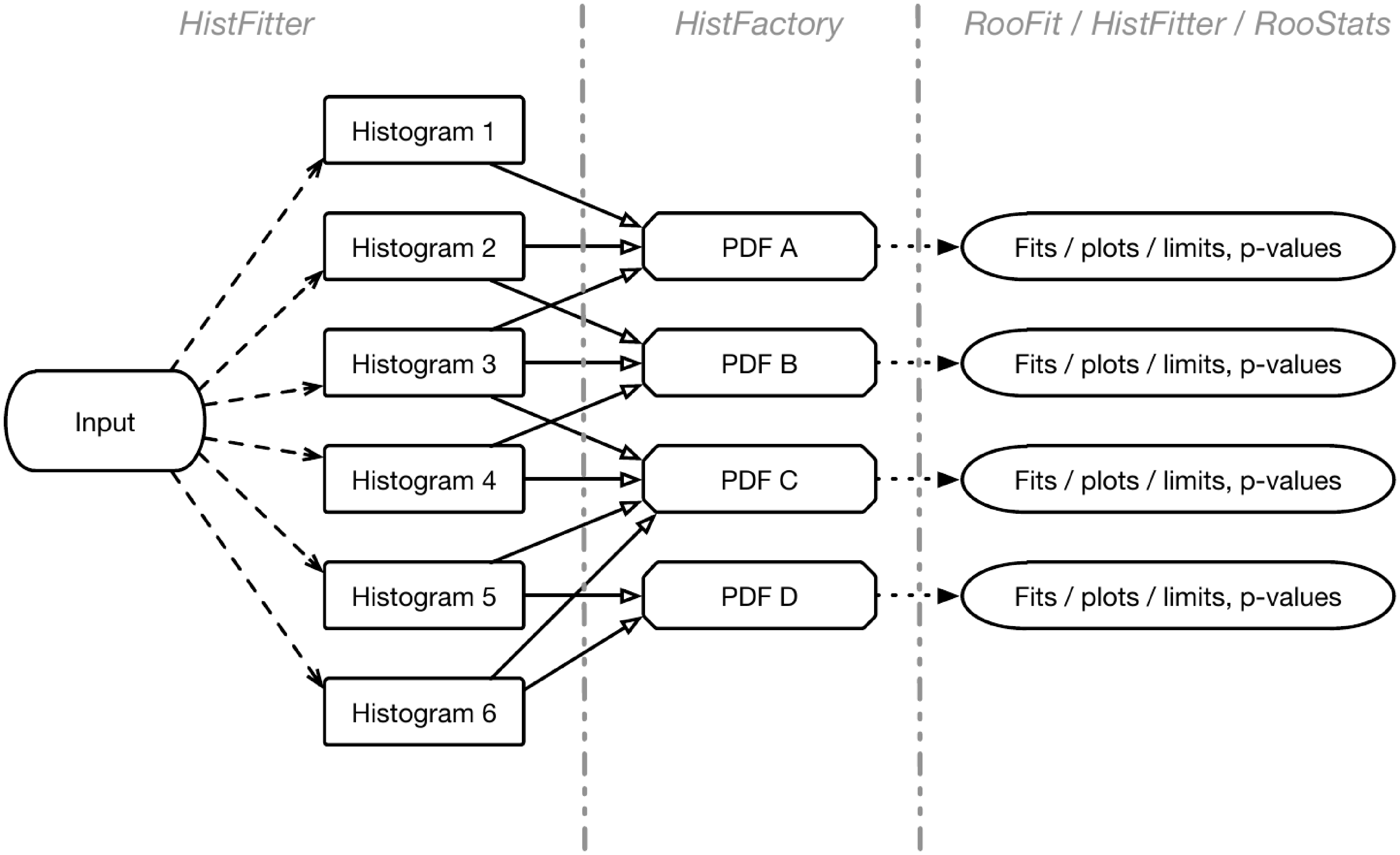
- Each CR/VR/SR modeled by a separate PDF, combined in a simultaneous fit
- Parameters shared in all regions → consistent background/signal prediction and systematics
  - Sharing user-defined

- Analysis flow:
  - Backgrounds normalized to data in a fit of control regions
  - Extrapolate to validation/signal regions using transfer factors (ratio of events between CR and SR/VR)
  - If good agreement in VR, unblind the SR
  - If no excess, add signal prediction and interpret/set limits



Processing sequence

- Based on user-defined configuration file, processing sequence of HistFitter split in three stages



step-0	**step-1**	**step-2/3**
Histogram production	PDF construction Workspace building	Analysis of models

Model construction

- Models constructed using HistFactory from input histograms
- General form of the constructed likelihood:

$$L(\boldsymbol{n}, \boldsymbol{\theta}^0 | \mu_{\mathrm{sig}}, \boldsymbol{b}, \boldsymbol{\theta}) \;=\; P_{\mathrm{SR}} \times P_{\mathrm{CR}} \times C_{\mathrm{syst}}$$

  - P = Poisson measurements of number of observed events in CR/SR (VR)
  - C = Constraint terms for systematic uncertainties, auxiliary measurements
  - Likelihood depends on number of observed events in all regions (n), predictions for various background processes (b), the nuisance parameter (θ) parametrizing the systematic uncertainties with their central value (θ^0) and signal strength (μ_{SIG})

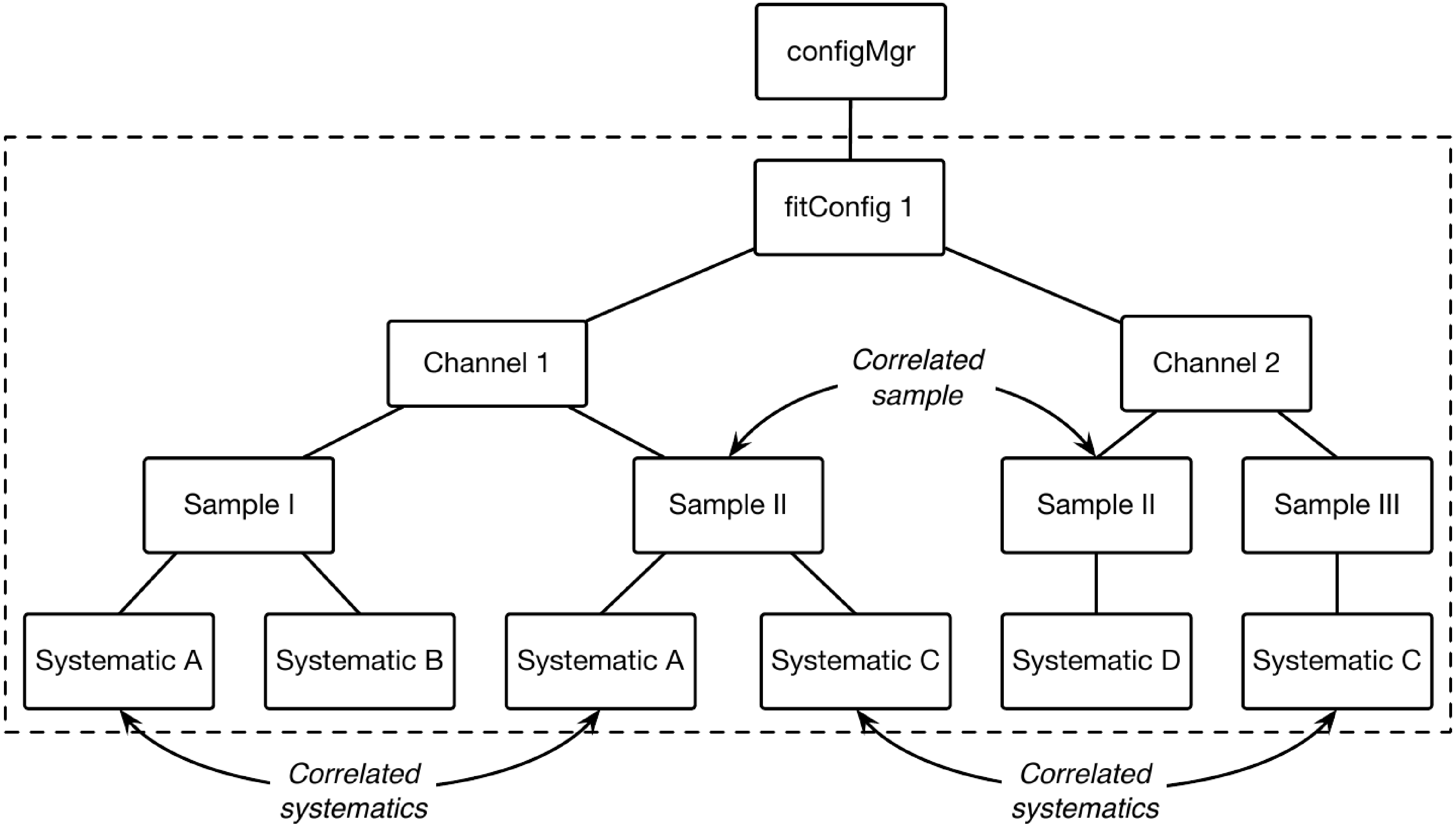
- Likelihood has multiple building blocks:
  - Control/validation/signal regions: called `channel` in HistFitter (HistFactory)
  - Signal and background processes: called `sample` in HistFitter (HistFactory)
  - Uncertainties: called `systematic` in HistFitter (HistFactory)
    - Including statistical/theory/experimental uncertainties

- HistFitter is designed to build and manipulate PDFs of nearly arbitrary complexity
- Bookkeeping/configuration machinery realized through a user-defined Python configuration file

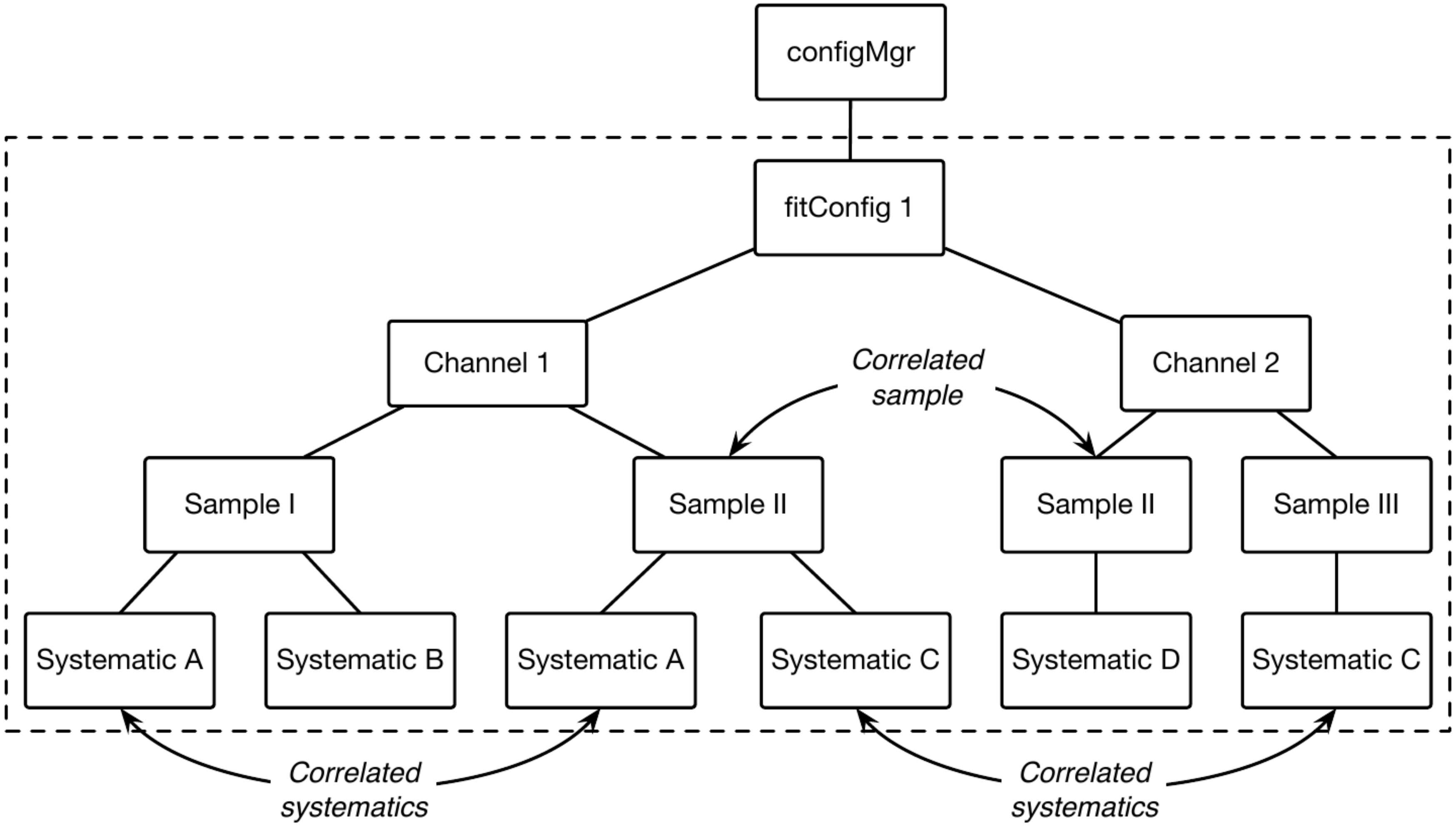
- Configuration manager (`configManager`) highest level (singleton) object in Python and C++
- Manages `fitConfig` objects that contain PDF and meta-data

Fit configuration

- `fitConfig` objects summarize `channels, samples and systematics` together with corresponding input histograms



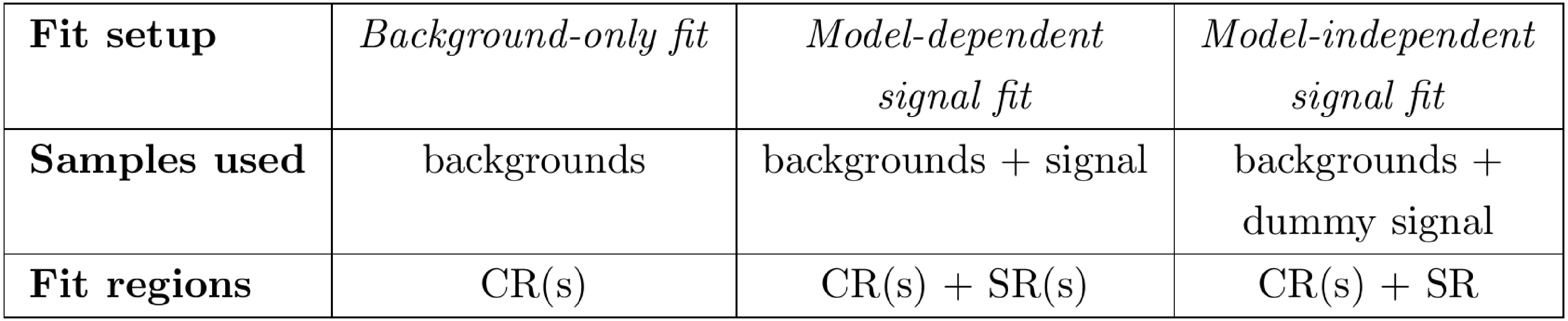
Fit configuration properties



- `fitConfig`: can be cloned/extended (see next slide)
- `channels:` either single-bin or multi-bin (shape), property as CR/VR/SR
- `samples:` input from TTree, TH1 or raw (hard-coded) floats, correlated between channels
- `systematics`: provided as ±1σ variation of nominal histogram; input from TTree, TH1 or raw floats; can be correlated between samples and/or channels; many types available extended from HistFactory base types (see later); trickle-down mechanism (see backup)

Common fit strategies

- **Background-only fit**: estimate background yields in validation/signal regions; including *only* CRs in the fit to data; no signal component included in fit configuration
- **Model-dependent signal fit**: set exclusion limit on a specific signal model; possible use of multi-binned (or multi-SR) shape fit for a robust signal estimation - aka ***exclusion fit***
- **Model-*in*dependent signal fit**: to obtain model-independent upper limits on number of BSM events beyond background prediction; only usable with one single-bin SR (otherwise not model-independent) - aka ***discovery fit***

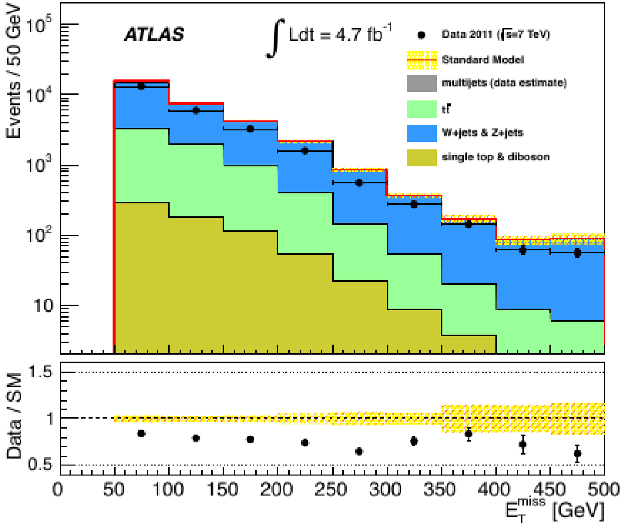


Fit setup	*Background-only fit*	*Model-dependent signal fit*	*Model-independent signal fit*
Samples used	backgrounds	backgrounds + signal	backgrounds + dummy signal
Fit regions	CR(s)	CR(s) + SR(s)	CR(s) + SR

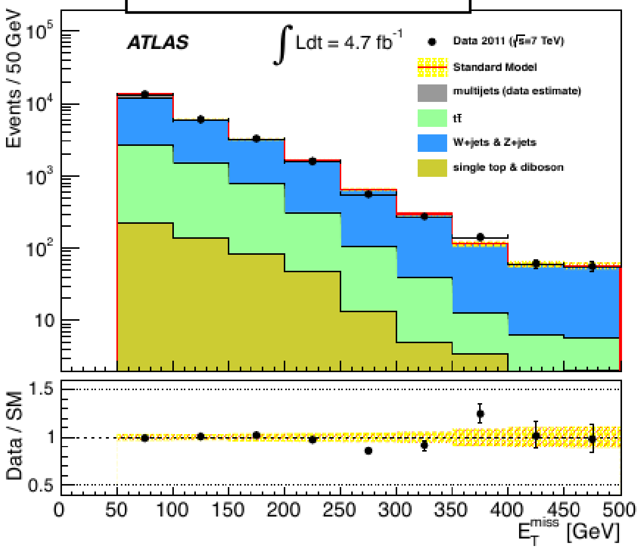
Presentation of results

- HistFitter includes a collection of tools (scripts/functions) to present/understand fit results

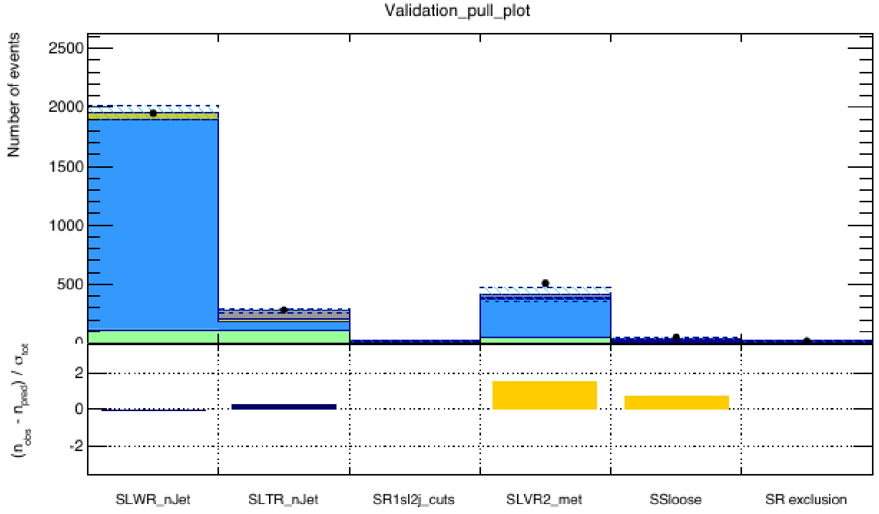
Before Fit



After Fit



After Fit VRs pull plot



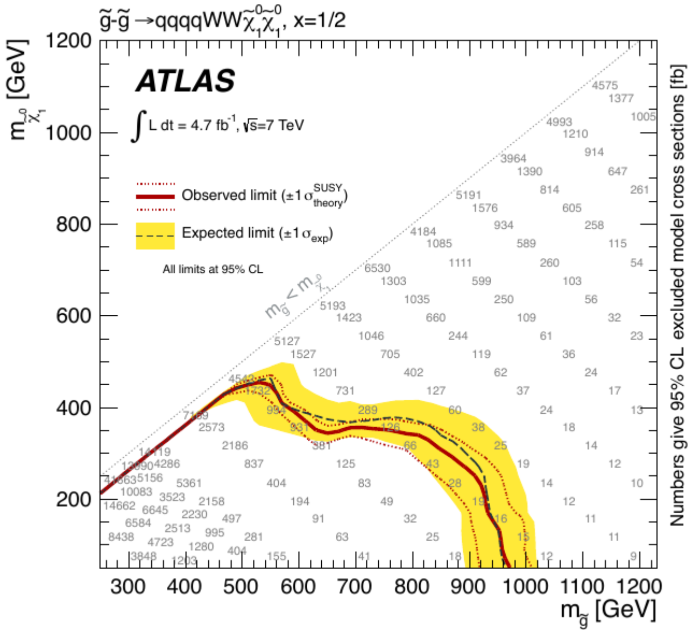
Yields Table

Signal Region	SR1	SR2
Observed events	16	19
Fitted bkg events	19.54 ± 3.93	20.47 ± 5.14
Fitted Top events	4.02 ± 0.96	4.32 ± 1.04
Fitted *V*+jets events	9.89 ± 1.86	10.47 ± 1.91
Fitted other background events	1.14 ± 0.15	1.19 ± 0.16
Fitted QCD events	4.49 ± 2.72	4.49 ± 4.24
MC exp. SM events	24.85	26.32
MC exp. Top events	8.42	9.11
MC exp. *V*+jets events	10.82	11.55
MC exp. other background events	1.13	1.17
Data-driven exp. QCD events	4.49	4.49

Systematics Table

Uncertainty of channel	SR1	SR2
Total background expectation	19.54	20.47
Total statistical ($\sqrt{N_{\rm exp}}$)	±4.42	±4.52
Total background systematic	±3.93 [20.14%]	±5.14 [25.09%]
QCD background	±2.66	±4.20
Statistical uncertainties	±2.54	±1.86
Jet Energy Scale	±1.15	±1.17
Top yield	±0.82	±0.88
Renormalization scale (Top)	±0.34	±0.39
V+jets yields	±0.28	±0.29
Renormalization scale (*V*+jets)	±0.14	±0.03

Exclusion contour with upper limits



Model-independent upper limits

Signal channel	$\langle\sigma_{\rm vis}\rangle^{95}_{\rm obs}$[fb]	$S^{95}_{\rm obs}$	$S^{95}_{\rm exp}$	$p(s=0)$
SR3b	0.19	3.9	$4.4^{+1.7}_{-0.6}$	0.50
SR0b	0.80	16.3	$8.9^{+3.6}_{-2.0}$	0.03

HistFitter & documentation

- HistFitter paper on arXiv: http://arxiv.org/abs/1410.1280
- HistFitter webpage with doxgen documentation: http://cern.ch/histfitter
- Tutorial (to be discussed next): https://twiki.cern.ch/twiki/bin/view/Main/HistFitterTutorialOutsideAtlas
- ACAT 2014 talk on HistFitter: https://indico.cern.ch/event/258092/session/8/contribution/39

HistFitter tutorial

Running HistFitter

- `HistFitter.py <options> <configuration_file>`

- **-t:** Create histograms in all regions used for all backgrounds, signal, data from TTrees
- **-w**: Build workspaces from histograms
- **-f:** Fit
- **-D**: various drawing options, to be discussed later
- **-L:** log level {VERBOSE,DEBUG,INFO,WARNING,ERROR,FATAL,ALWAYS}
- **-m PARAM**: run Minos for asymmetric error calculation
  - optionally give parameter names comma separated; for all parameters use ‘ALL’ or ‘all’
- **-l**: Calculate upper limit
- **-p**: Calculate the CLs value for a specific signal model (for exclusion)
- **-i**: interactive mode, keeps you in python command line, but shows plots on your screen

- To see all options run: `HistFitter.py --help`

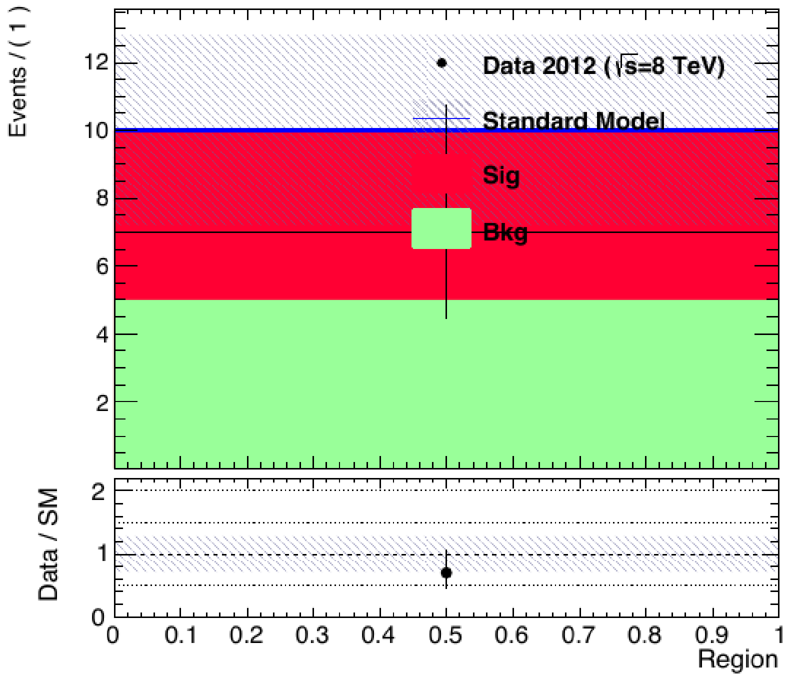
Simple example

- Simple example with one region with one bin:

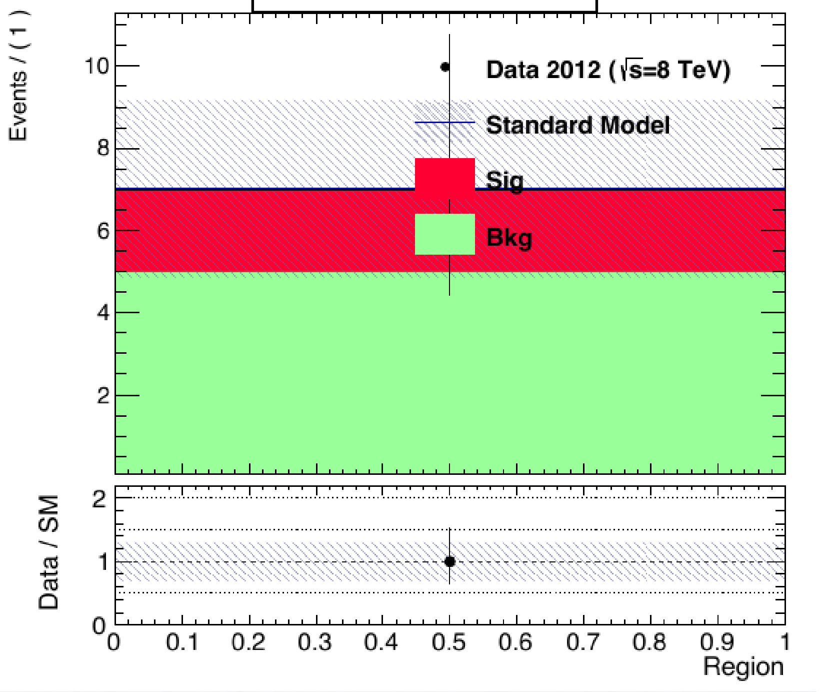
```
HistFitter.py -w -f -D "before,after,corrMatrix" -i
analysis/tutorial/MyUserAnalysis.py
```

- Creates the workspace
- Runs the fit
- Plots before/after fit regions and correlation matrix
- Keeps you in interactive mode

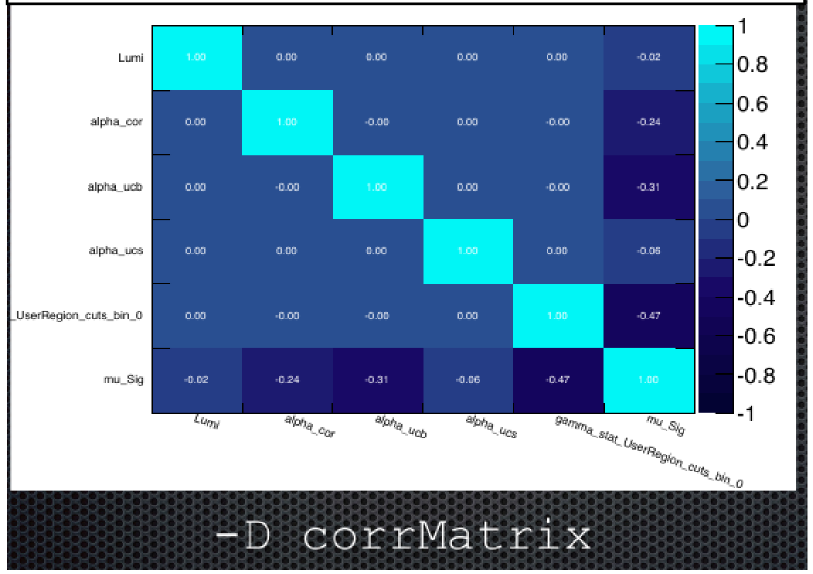
Before Fit



After Fit



correlations matrix



	Lumi	alpha_cor	alpha_ucb	alpha_ucs	gamma_stat_UserRegion_cuts_bin_0	mu_Sig
Lumi	1.00	0.00	0.00	0.00	0.00	-0.02
alpha_cor	0.00	1.00	-0.00	0.00	-0.00	-0.24
alpha_ucb	0.00	-0.00	1.00	0.00	-0.00	-0.31
alpha_ucs	0.00	0.00	0.00	1.00	0.00	-0.06
_UserRegion_cuts_bin_0	0.00	-0.00	-0.00	0.00	1.00	-0.47
mu_Sig	-0.02	-0.24	-0.31	-0.06	-0.47	1.00

`-D corrMatrix`

Config file explained - I

- Define a configManager and setup a `fitConfig` ana named SPlusB
- `from configManager import configMgr`
  `ana = configMgr.addFitConfig("SPlusB")`

- Add one channel/region to the `fitConfig`
- `chan = ana.addChannel("cuts",["UserRegion"],1,0.5,1.5)`

- One defines the region/channel in cutsDict (as one would in ROOT for TTree call)
- Here include all:
- `configMgr.cutsDict["UserRegion"] = "1."`

- Channels can also be binned (shape-fit)
- `chan = ana.addChannel("myObs", ["mySelection"], nBins, varLow, varHigh)`

Config file explained - II

- Define samples: bkgSample, sigSample and dataSample

-
  ```
  # Define samples
  bkgSample = Sample("Bkg",kGreen-9) # define a background sample with color KGreen-9 if plotting
  bkgSample.setStatConfig(True) #This sample gets statistical uncertainties
  bkgSample.buildHisto([nbkg],"UserRegion","cuts") #Build histograms from numbers defined by the user
  bkgSample.buildStatErrors([nbkgErr],"UserRegion","cuts")

  sigSample = Sample("Sig",kPink) #A signal sample with color kPink
  sigSample.setNormFactor("mu_Sig",1.,0.,100.) # This samples receives a normalization parameter
  sigSample.setStatConfig(True) #This sample gets statistical uncertainties
  sigSample.setNormByTheory() # and uncertainties due to the luminosity are added
  sigSample.buildHisto([nsig],"UserRegion","cuts")
  sigSample.buildStatErrors([nsigErr],"UserRegion","cuts")

  dataSample = Sample("Data",kBlack) #Data sample
  dataSample.setData()
  dataSample.buildHisto([ndata],"UserRegion","cuts")

  # add all samples to the fitconfig object and thus to all channels
  ana.addSamples([bkgSample,sigSample,dataSample])
  ```

Config file explained - III

- Add systematics to signal/background samples
- Correlating systematics happens by giving them the same name

```
# Set uncorrelated systematics for bkg and signal (1 +- relative uncertainties)
ucb = Systematic("ucb", configMgr.weights, 1.2,0.8, "user","userOverallSys")
ucs = Systematic("ucs", configMgr.weights, 1.1,0.9, "user","userOverallSys")
# correlated systematic between background and signal (1 +- relative uncertainties)
corb = Systematic("cor",configMgr.weights, [1.1],[0.9], "user","userHistoSys")
cors = Systematic("cor",configMgr.weights, [1.15],[0.85], "user","userHistoSys")

bkgSample.addSystematic(corb)
bkgSample.addSystematic(ucb)
sigSample.addSystematic(cors)
sigSample.addSystematic(ucs)
```

Table production

- **YieldsTable.py** produces customizable tables of yields before/after fit
- Example: `YieldsTable.py -s Top,WZ,BG,QCD -c SLWR_nJet,SLTR_nJet -w results/MyConfigExample/BkgOnly_combined_NormalMeasurement_model_afterFit.root -o MyYieldsTable.tex`

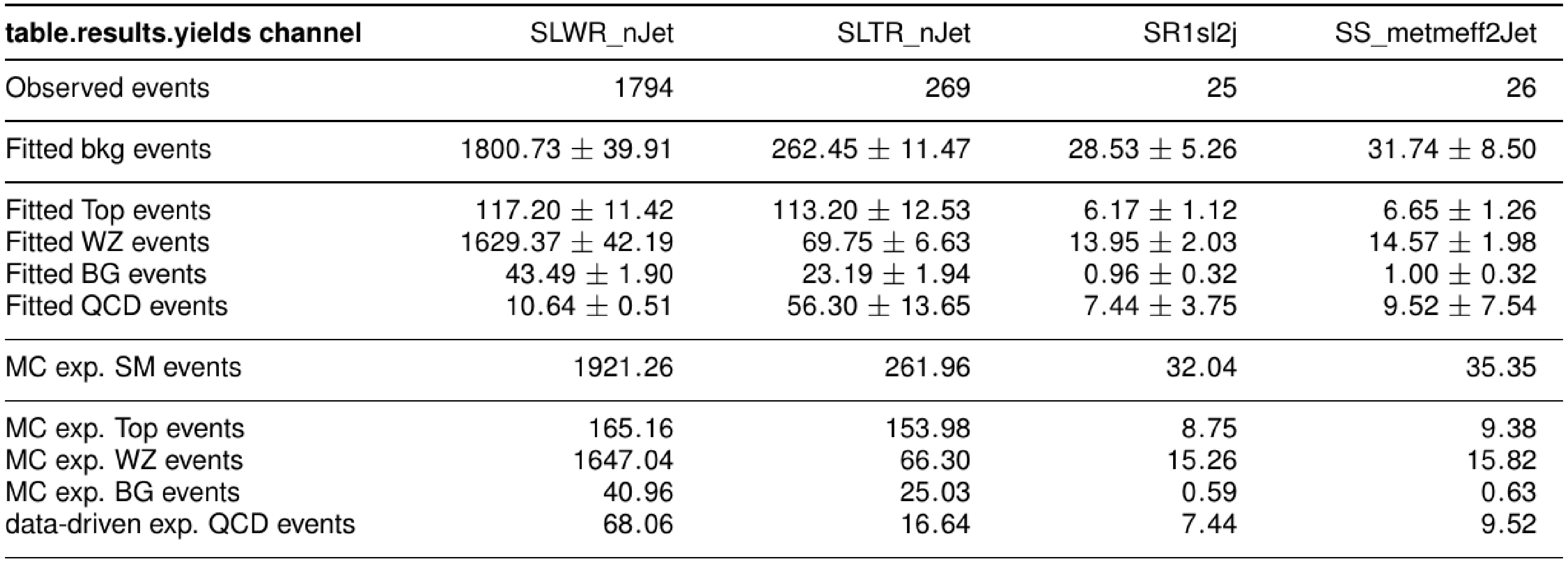
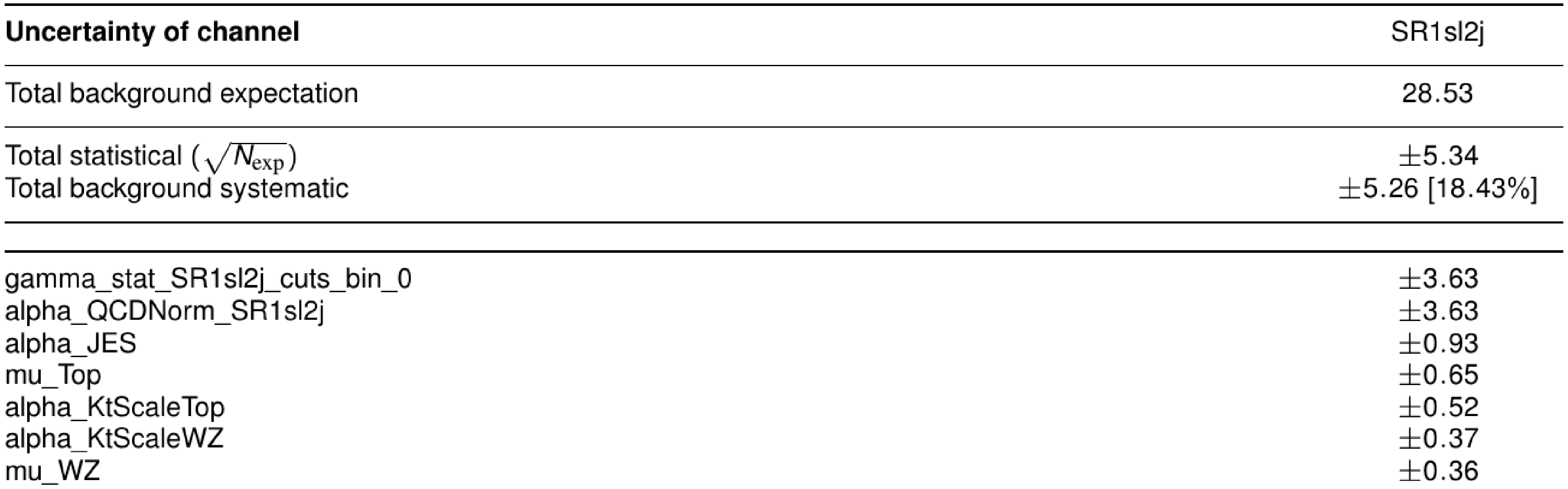


table.results.yields channel	SLWR_nJet	SLTR_nJet	SR1sl2j	SS_metmeff2Jet
Observed events	1794	269	25	26
Fitted bkg events	1800.73 ± 39.91	262.45 ± 11.47	28.53 ± 5.26	31.74 ± 8.50
Fitted Top events	117.20 ± 11.42	113.20 ± 12.53	6.17 ± 1.12	6.65 ± 1.26
Fitted WZ events	1629.37 ± 42.19	69.75 ± 6.63	13.95 ± 2.03	14.57 ± 1.98
Fitted BG events	43.49 ± 1.90	23.19 ± 1.94	0.96 ± 0.32	1.00 ± 0.32
Fitted QCD events	10.64 ± 0.51	56.30 ± 13.65	7.44 ± 3.75	9.52 ± 7.54
MC exp. SM events	1921.26	261.96	32.04	35.35
MC exp. Top events	165.16	153.98	8.75	9.38
MC exp. WZ events	1647.04	66.30	15.26	15.82
MC exp. BG events	40.96	25.03	0.59	0.63
data-driven exp. QCD events	68.06	16.64	7.44	9.52

- **SysTable.py** produces customizable tables of systematic breakdown per region (or sample)
- Example: `SysTable.py -w results/MyConfigExample/BkgOnly_combined_NormalMeasurement _model_afterFit.root -c SR1sl2j -o systable_SR1sl2j.tex`



Uncertainty of channel	SR1sl2j
Total background expectation	28.53
Total statistical ($\sqrt{N_{\mathrm{exp}}}$)	±5.34
Total background systematic	±5.26 [18.43%]
gamma_stat_SR1sl2j_cuts_bin_0	±3.63
alpha_QCDNorm_SR1sl2j	±3.63
alpha_JES	±0.93
mu_Top	±0.65
alpha_KtScaleTop	±0.52
alpha_KtScaleWZ	±0.37
mu_WZ	±0.36

Signal model hypothesis test

- Once you have unblinded your SR, one can calculate the CLs/p-value on specific signal models using the exclusion fit (aka model-dependent fit setup)
- As simple in HistFitter as calling:

```
HistFitter.py -p analysis/tutorial/MyUserAnalysis.py
```

- Will calculate:
  - CLs_observed = taking N observed events as data in all regions
  - CLs_expected = taking N expected events as data in all regions
  - CLs_expected ±1sigma experimental uncertainty = N expected as data, ±1sigma fit results
    - yellow band next slide
  - CLs_observed ±1sigma signal theory uncertainty = N observed as data, ±1sigma signal theory
    - need to set the name of the signal theory uncertainty systematic as `Systematic("SigXSec", ...)`
    - red-dotted lines next slide

- Setting calculator and test statistic type can be set in configManager (see backup):

```
## setting the parameters of the hypothesis test
#configMgr.nTOYs=5000
configMgr.calculatorType=2 # 2=asymptotic calculator, 0=frequentist calculator
configMgr.testStatType=3   # 3=one-sided profile likelihood test statistic (LHC default)
configMgr.nPoints=20       # number of values scanned of signal-strength for upper-limit 
determination of signal strength.
```

- Result of ‘-p’ stored in a ROOT file with ‘hypotest’ in the name:

```
results/MySimpleChannelAnalysis_fixSigXSecNominal_hypotest.root
```

Contour plot explained

- https://twiki.cern.ch/twiki/bin/view/AtlasProtected/SUSYLimitPlotting

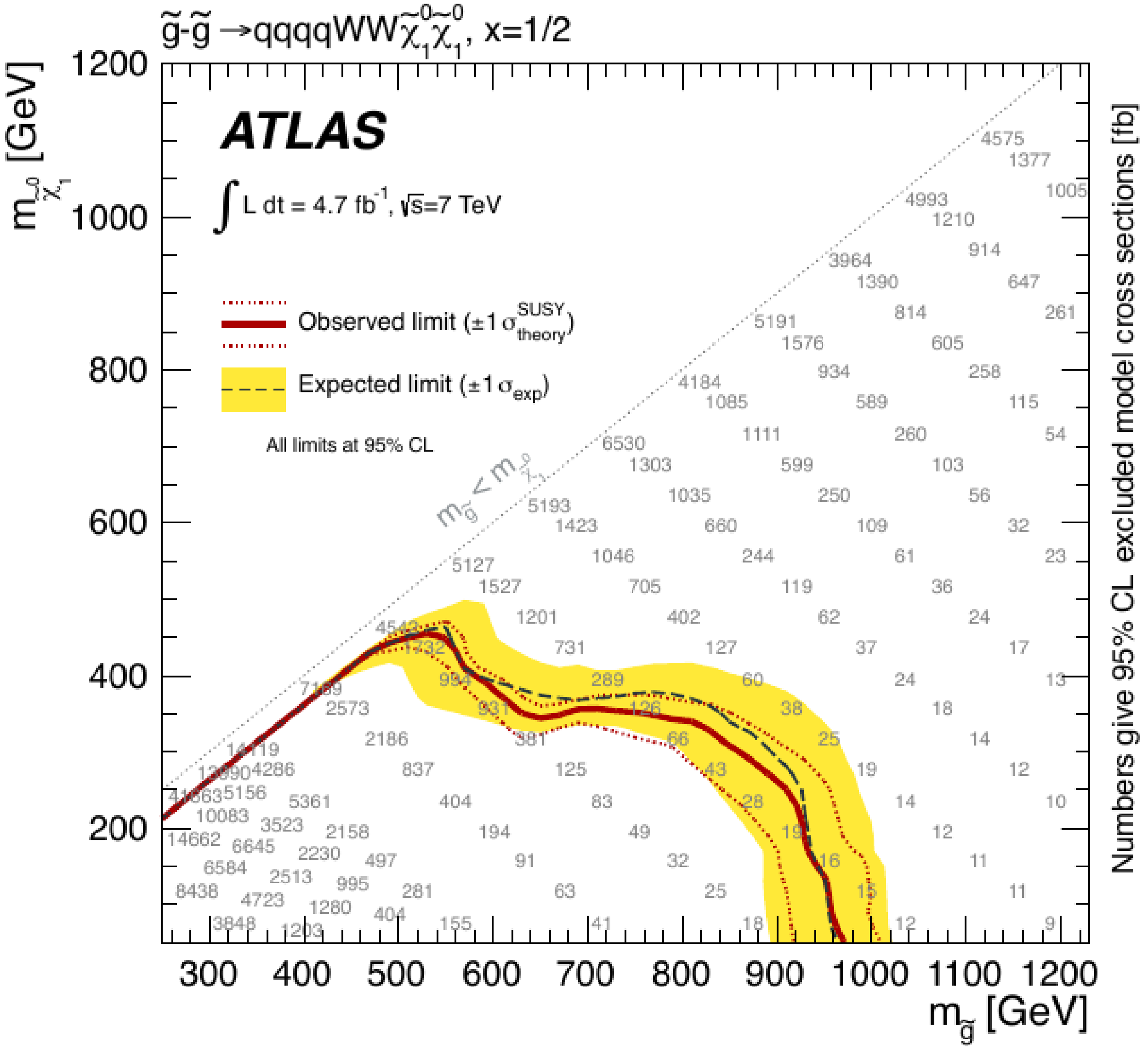
Description of limit lines

The model limits should be computed using the HistFitter package. We present the following limits:

1. **Observed limit** (thick solid dark-red line): all uncertainties are included in the fit as nuisance parameters, with the exception of the theoretical signal uncertainties (PDF, scales).
2. **Expected limit** (less thick long-dashed dark-blue line): all uncertainties are included in the fit as nuisance parameters, with the exception of the theoretical signal uncertainties (PDF, scales).

We present the following uncertainty bands:

- **±1σ lines around observed limit** (1) with style "thin dark-red dotted": re-run limit calculation (1) while increasing or decreasing the signal cross section by the theoretical signal uncertainties (PDF, scales).
- **±1σ band around expected limit** (2) with style "yellow band": the band contours are the ±1σ results of the fit (2).

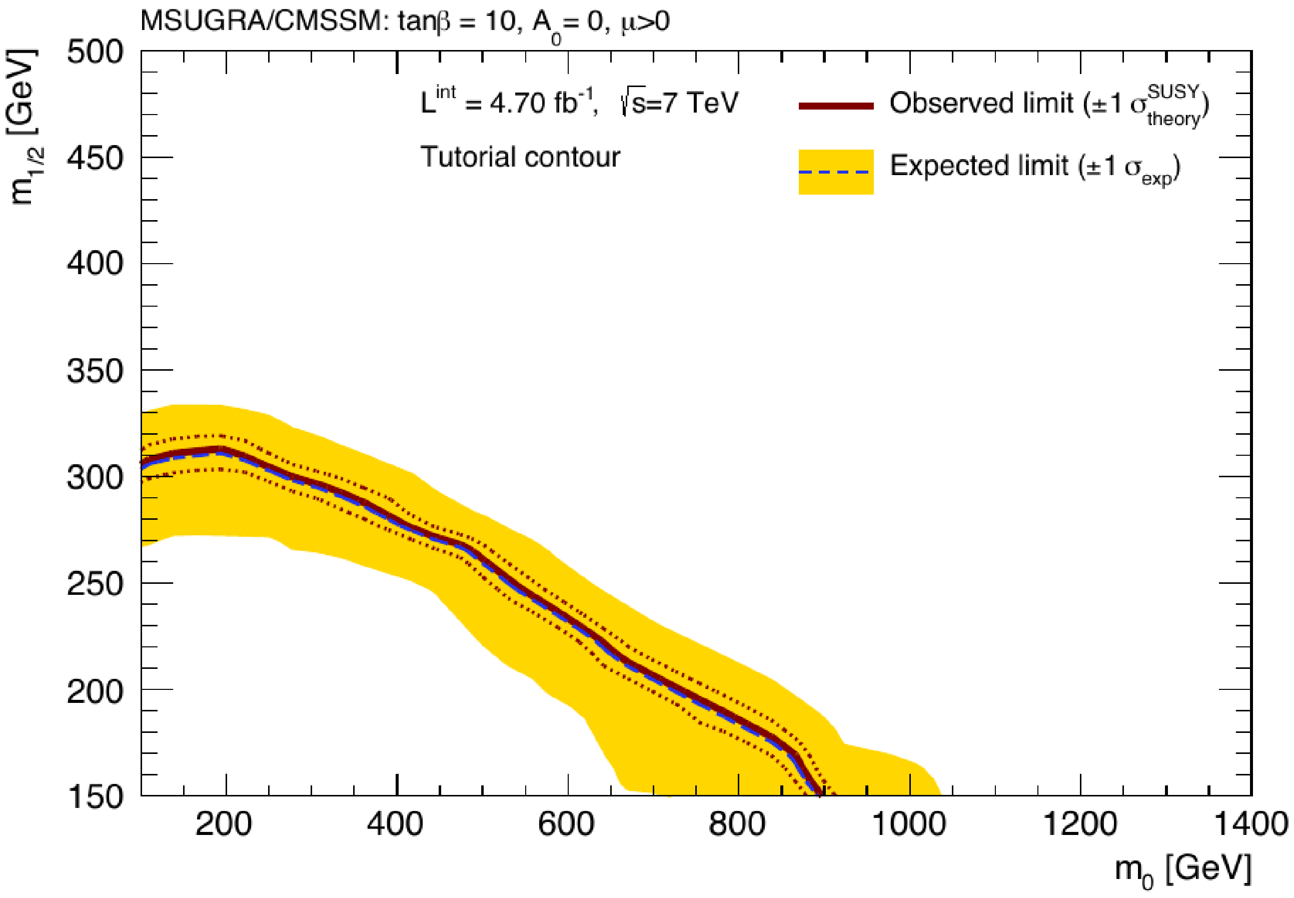


Contour plot production

- Typically a grid of signal model points with varying signal parameters (m_H or m_{gluino}) get processed to produce an exclusion contour
- Five steps to produce (Part 5 of tutorial):

1. run hypothesis tests over all grid points (results saved in multiple *hypotest* files)
2. merge all the output root files into one using `hadd` (if stored in a separate files)
3. transform this set of hypothesis tests into a plain-text file: `makelistfiles.C`
4. create TH2D(s) from the ascii data in this list file: `makecontourhists.C`
5. plot TH2D(s) to draw contour lines and cosmetics: `makecontourplots.C`

- at the requested CLs level, typically 95% CL, CLs<0.05

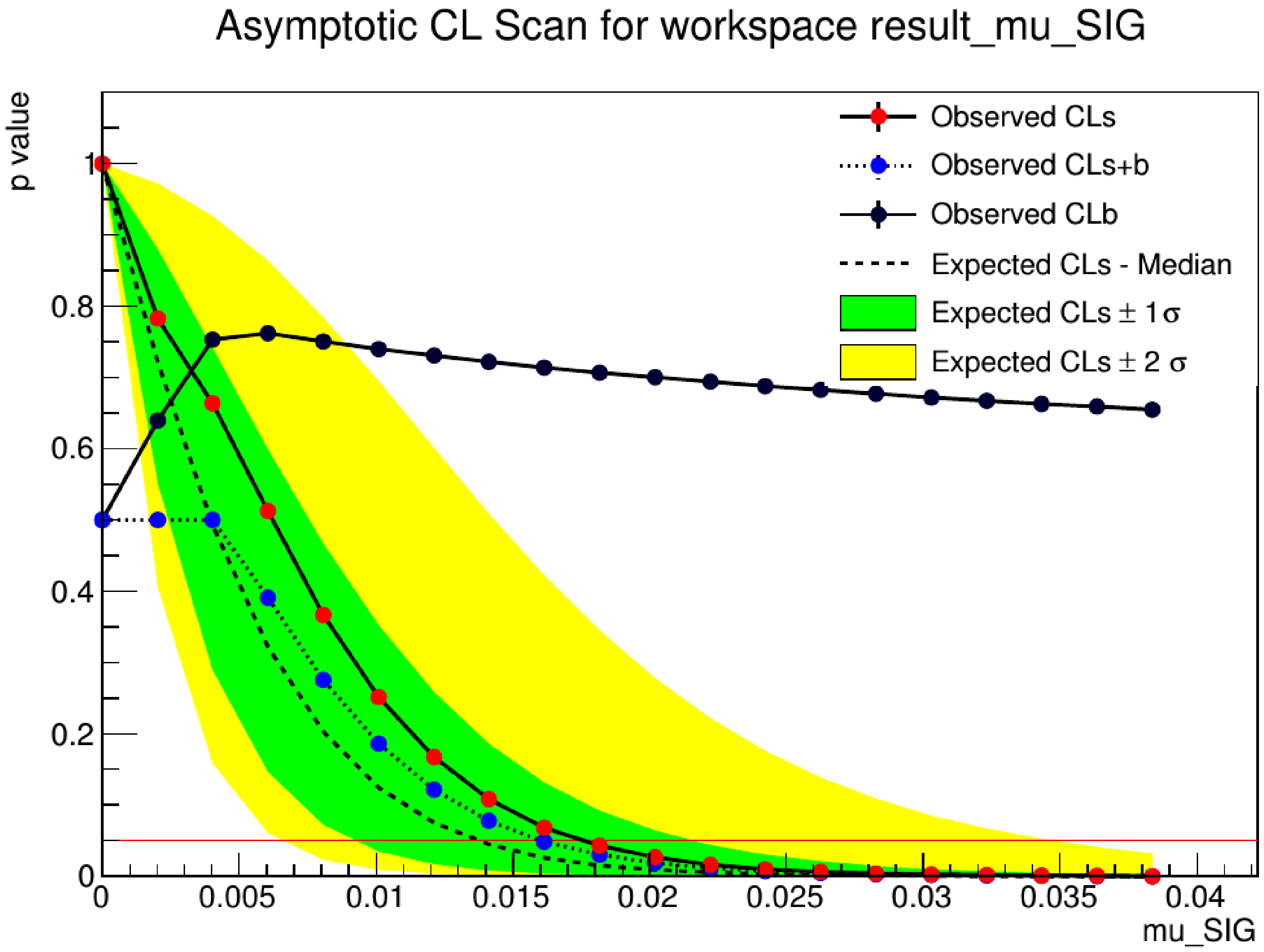


Signal strength upper limit

- Once you have unblinded your SR, one can set upper limits on specific signal models using the exclusion fit (aka model-dependent fit setup)
- As simple in HistFitter as calling:

```
HistFitter.py -l analysis/tutorial/MyUserAnalysis.py
```

  - Technicalities similar to ‘-p’



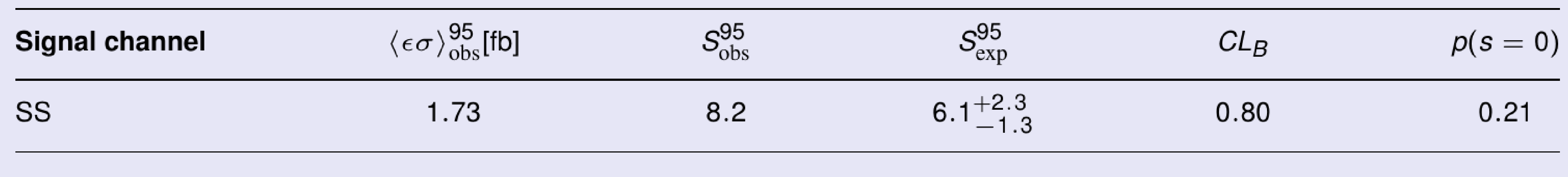
- Hypothesis test ***inversion***:
  - find the value of mu_SIG for which CLs below 0.05 (or other required value)
    - instead of calculating the p-value for the specific signal
  - run the hypothesis test for increasing values of signal strength mu_SIG
    - scan range determined automatically
    - upper limit on cross section = nominal cross section × upper limit on signal strength (grey numbers in contour plots, run for each signal grid point)

Model-independent upper limit

- Calculate the upper limit on the number of BSM physics events that we exclude in our SR
  - Typically used by theorists to check their favorite BSM model, that we have not looked at
- Requires the model-independent fit setup - aka discovery fit
  - ‘dummy signal’ = exactly one event in signal region (none in CRs)
  - upper limit on this ‘dummy signal’ = upper limit on BSM number of events
- Use the **UpperLimitTable.py** script:

```
UpperLimitTable.py -c SS -w
results/MyUpperLimitAnalysis_SS/SPlusB_combined_NormalMeasurement_model.root -
l 4.713 -n 1000
```

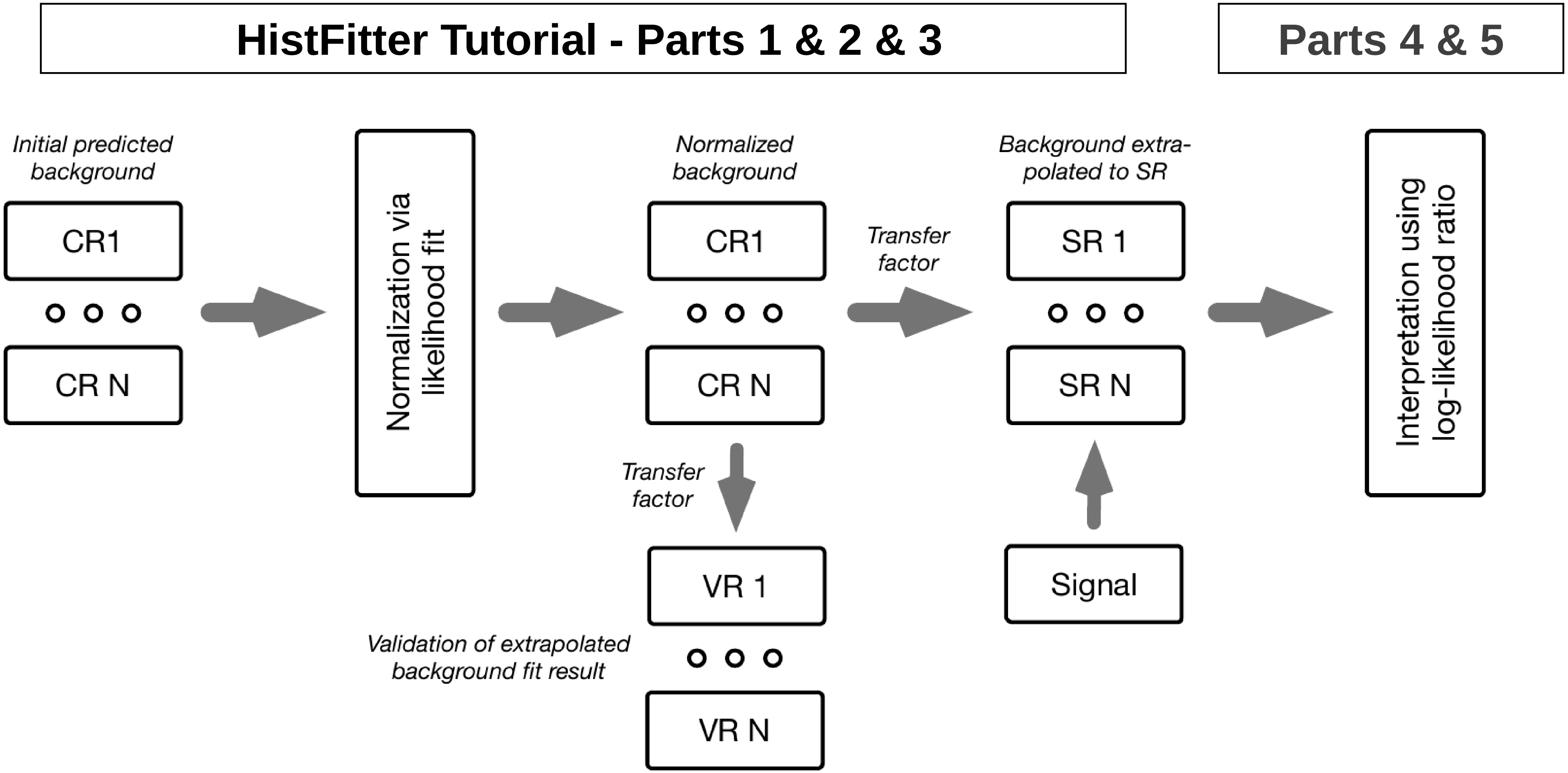
- Results in LaTeX table:



Signal channel	$\langle\epsilon\sigma\rangle^{95}_{\mathrm{obs}}$[fb]	S^{95}_{obs}	S^{95}_{exp}	CL_B	$p(s=0)$
SS	1.73	8.2	$6.1^{+2.3}_{-1.3}$	0.80	0.21

  - ⟨σvis⟩95_obs : 95% CL upper limits on the visible cross section obs
  - S95_obs :95% CL upper limits on the number of signal events obs
  - S95_exp : 95% CL upper limit on the number of signal events, given the expected number (and ±1σ excursions on the expectation) of background events
  - CLB: the confidence level observed for the background-only hypothesis
  - p(s = 0): discovery p-value - the probability, capped at 0.5, that a background-only experiment is more signal-like than the observed number of events in a signal region

HistFitter - tutorial



HistFitter Tutorial - Parts 1 & 2 & 3

Parts 4 & 5

Initial predicted background

CR1

CR N

Normalization via likelihood fit

Normalized background

CR1

CR N

Transfer factor

VR 1

VR N

Validation of extrapolated background fit result

Transfer factor

Background extrapolated to SR

SR 1

SR N

Signal

Interpretation using log-likelihood ratio

HistFitter tutorial start up

- A public version is available on the HistFitter webpage:
  http://histfitter.web.cern.ch/histfitter/Software/Install/index.html

  We use HistFitter-2.0.tar.gz for this tutorial.

- **Installation instructions:**
  - Untar the HistFitter package
  - Setup ROOT (if not already done) – use Root 5!
  - Go the HistFitter directory `cd HistFitter-2.0`
  - Run the HistFitter setup script `source setup.sh`
  - Go to the src/ directory and compile the C++ side of HistFitter `cd src && make`
  - Go back to the main HistFitter directory

  - **Input data here**:
    - Link the input data to your HistFitter directory as follows:
    - ln –s /project/etp3/jlorenz/shape_fit/samples/ samples