Collie:
COnfidence Level LImit Evaluator
V00.03.16

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Outline

- ✗ Functional aspects of Collie
  - What is being calculated?
  - What do you need to calculate something?
  - What's going on behind the scenes?
- ✗ Operational aspects of collie
  - Creating CollieIO files
  - Calculations available in Collie
- ✗ Voiding your warranty
  - Abuse of the input assumptions
  - What should cross checks should be made?

Content Warning

This tutorial covers a large range of concepts. Ideally this would be done in 2-3 separate presentations. If it feels a bit dense to you, you're not alone.

Many “advanced topics” are not included in this tutorial. The scope of this presentation is based on the numerous questions I've received from users.

Functional Aspects of Collie

Collie

- ✗ Collie is a software suite designed to generate semi-Frequentist confidence levels which are used to calculate a range of products

- ✗ The products available via Collie

  p-Values for TEST or NULL hypothesis. Or confidence level (CL) depending on which book you read.

  Cross section limit ratio: Signal scaling factor required to exclude at X% CL

  Luminosity limit ratio: Lumi scaling factor required to exclude a model at X% CL

  3-Sigma evidence: Lumi scaling factor required to observe a model at 3-Sigma

  Cross section measurement: In the case of an excess in data, cross section scan or floating cross section measurements

- ✗ The confidence level calculations available in Collie

  CLfast: Fast, diagnostic tool ignoring systematics *(!!not useful for real results!!)*

  CLsyst: Standard Gaussian smearing treatment for systematics

  CLfit: Single binned-likelihood fit, maximized over systematics

  CLfit2: Double binned-likelihood fit, maximized over systematics

Some Definitions

- ✗ Compound hypotheses vs Simple hypotheses

  Simple: The model probability distribution (PDF) is fully specified (eg, Gaussian with μ=3, σ=1.2)

  Compound: Indicates an underspecified PDF (eg, Gaussian with μ=3)

  Operationally speaking: Your hypothesis has uncertainties (nuisance parameters) which impact the predictions and you must account for this.

- ✗ Nuisance parameter

  A parameter intrinsic to your MC model, but which is not the model parameter you're trying to test. Can be a systematic uncertainty or a theoretical parameter.

  Example: Luminosity is known to about 6%. This means the ***TRUE*** signal and/or background rates could be above or below what you predict in your Monte Carlo.

  Operationally speaking: To test outcomes of your compound model, you must tranform to a simple hypothesis by assigning the nuisance parameter a pre-specified PDF (ie, a prior)

The General Problem

- ✗ If possible, use data to distinguish two hypotheses:
  - ✗ **H0** ⇨ null hypothesis: background-only model, eg Standard Model
  - ✗ **H1** ⇨ a test hypothesis: presence of a new particle, coupling, etc.

H0 is a compound hypothesis, with some set of nuisance parameters

H1 has the same form, but add model params and extra nuisance params

Simple Example: **H0** describes the Standard Model background expectation for the result of an analysis. Nuisance parameters can be luminosity, acceptance, Standard Model cross section, etc...

H1 is the same as **H0**, but add a new physics signal. The model can be parametrized by mass / cross section / etc, and extra nuisance parameters come from signal acceptance, model parameters, etc...

Complicating Factors

- ✗ The hypotheses, **H1** & **H0**, are often subdivided according to final states with unique signatures
  - Orthogonal (*usually*) search channels defined to maximize acceptance, isolate high S/B regions, etc.
- ✗ The null hypothesis, **H0**, is the sum of several contributing Standard Model processes
  - Nuisance parameters are generally correlated amongst backgrounds (and signals!), but not always
- ✗ Discriminant distributions for expected and observed events are binned into histograms
  - Discriminating variable can be an observable (eg, angular distribution) or multi-variable function (Neural Nets, likelihood ratios, etc).
  - Nuisance parameters can affect rates, shapes, or both. Many are asymmetric and are not necessarily Gaussian.

The Semi-Frequentist Method

- ✗ A few words on the “As-Frequentist-as-possible” treatment

  Standard algorithm in all Collie calculation classes

- ✗ Given hypotheses, **H1** & **H0**, we must simulate outcomes of repeated experiments

  Assume data is drawn randomly from a Poisson parent distribution

  ⇒ Generate pseudo-data via random Poisson with mean value from expected backgrounds (**H0**) or signal-plus-background (**H1**)

  Systematics are a tricky Frequentist problem, so use a Bayesian model

  ⇒ Model uncertainties on nuisance parameters as Gaussian-distributed, sample randomly for each pseudo-experiment

  ⇒ Vary nominal background prediction according to smeared values of nuisance parameters, change mean of random Poisson each time

  Generate ~20k pseudo-experiments for **H1** & **H0**. This algorithm defines basis of CLfast & CLsyst calculations.

The Statistical Test

- ✗ Collie utilizes a negative Poisson log-likelihood ratio (LLR) test statistic to evaluate statistical significance (*test statistic = ordering rule*)
  - Used to order data outcomes relative to each other in hypothesis significance

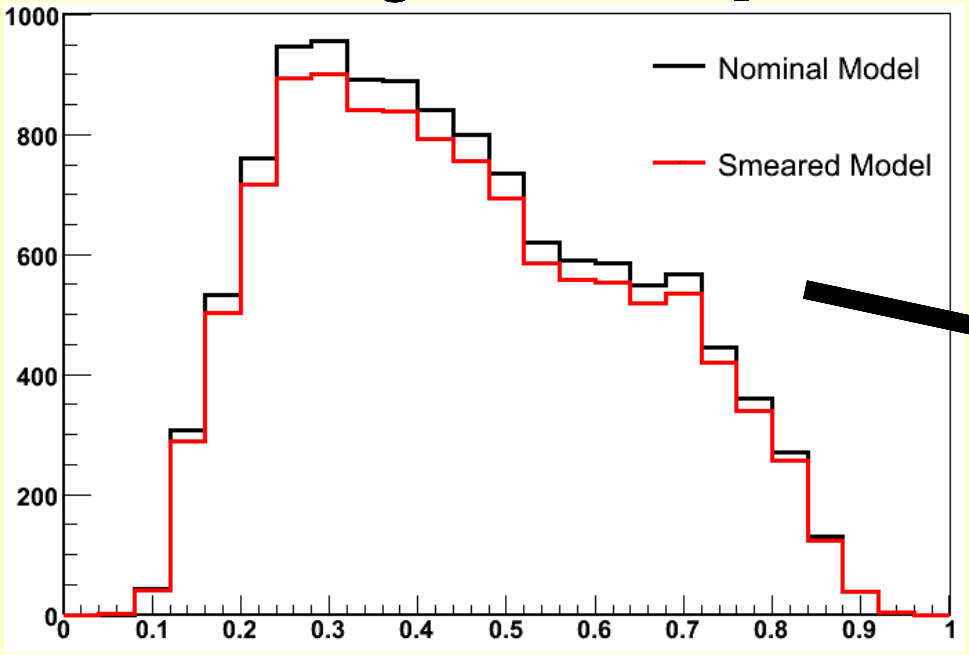
$$Q(\vec{s},\vec{b},\vec{d}) = \prod_{i=0}^{N_C}\prod_{j=0}^{N_{bins}} \frac{(s+b)_{ij}^{d_{ij}} e^{-(s+b)_{ij}}}{d_{ij}!} / \frac{b_{ij}^{d_{ij}} e^{-b_{ij}}}{d_{ij}!}$$

$$LLR(\vec{s},\vec{b},\vec{d}) = -2\mathrm{Log}(Q) = \sum_{i=0}^{N_C}\sum_{j=0}^{N_{bins}} s_{ij} - d_{ij}\ln\left(1+\frac{s_{ij}}{b_{ij}}\right)$$

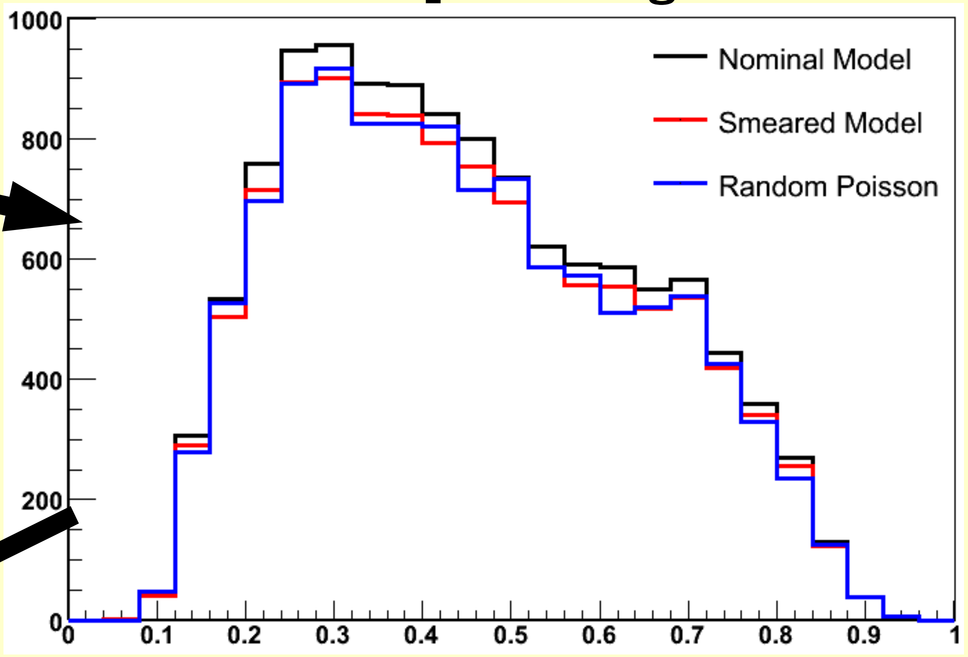
- ✗ LLR is linear in channels and bins: channel addition is natural formulation
- ✗ Implicitly imports info on the shapes of the parent distributions
- ✗ LLR value is evaluated *for each set of pseudo-data*, generating distributions for **H1** and **H0** hypotheses
  - Each outcome is ordered according to the LLR value
  - The frequency of relative outcomes defines confidence levels

Same Thing in Pictures

Start by randomly smearing nominal model according to nuisance parameters



Generate pseudo-data via random Poisson trials per histogram bin



Using pseudo-data from random Poisson trials, evaluate LLR value and insert into histogram.

This process is repeated many times (O(10k) for both **H0** and **H1**. The observed LLR value is also evaluated.

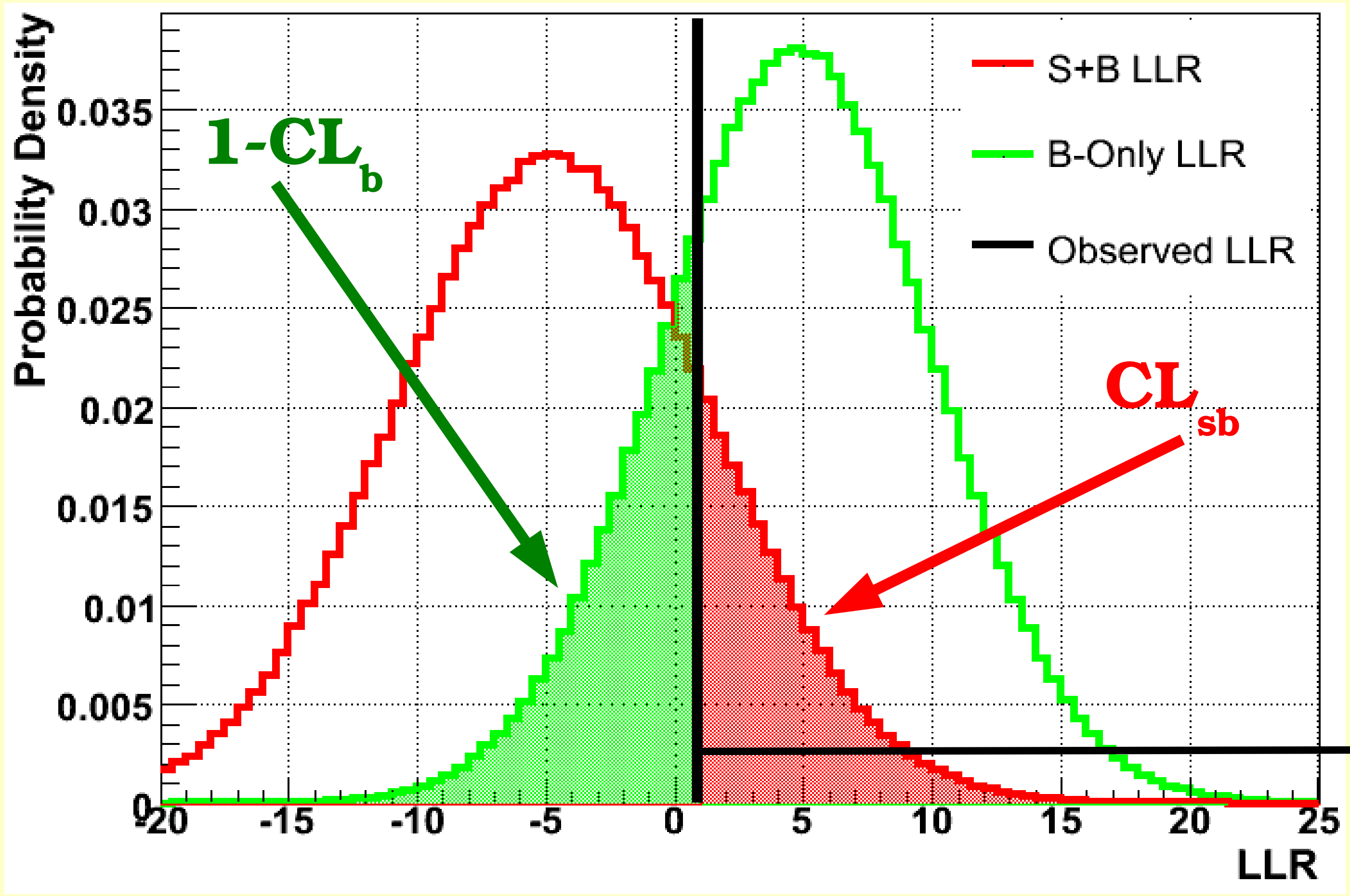
Example LLR Distributions

- ✗ Confidence levels are defined based on infinite integral of LLR distributions

  Think of this as the "Prior Predictive Ensemble" of outcomes

  CL_b = fraction of **H0** pseudo-experiments less signal-like than data

  CL_{sb} = fraction of **H1** pseudo-experiments less signal-like than data



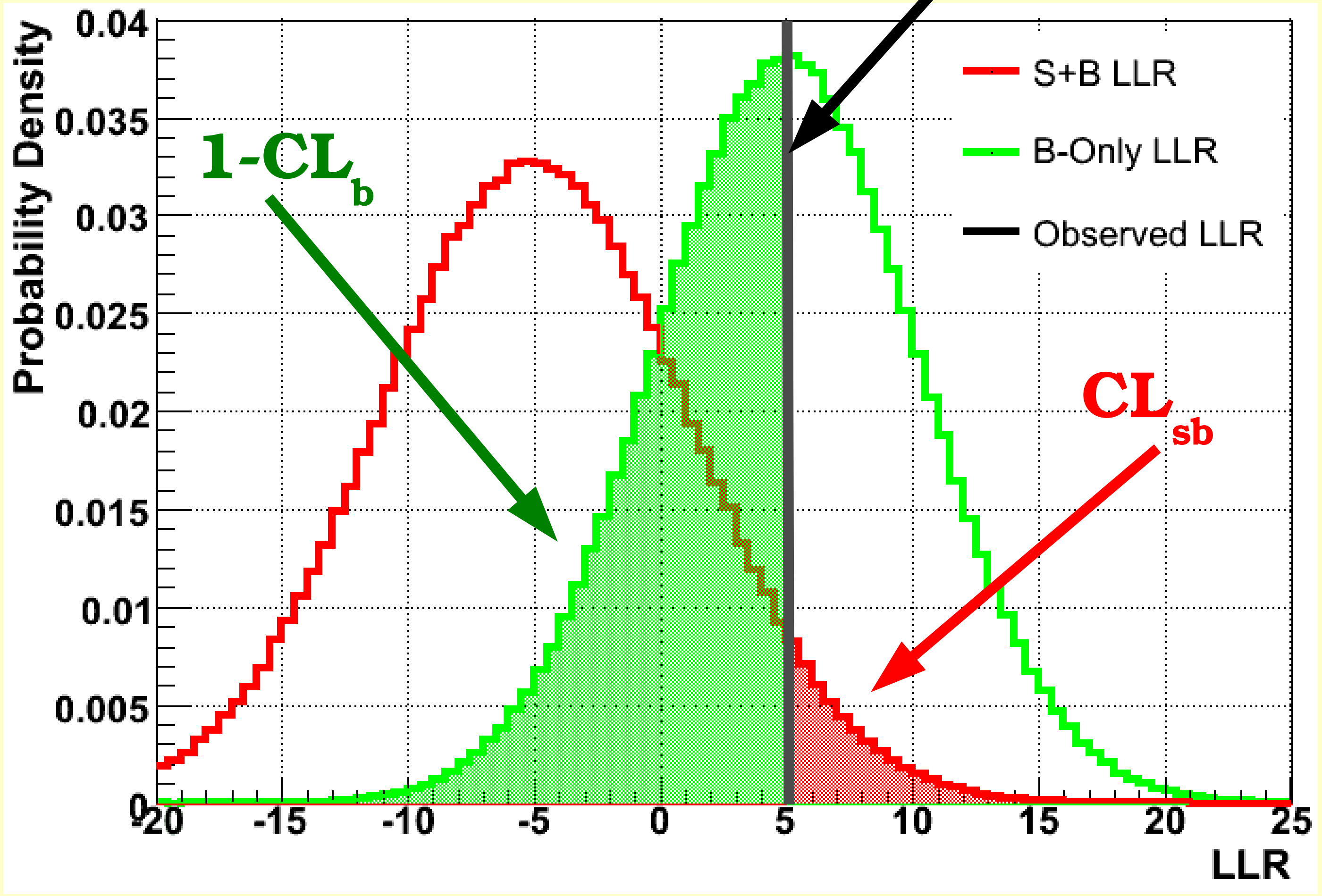
Integrate LLR distributions in bkgd-like direction

Example LLR Distributions

✗ Expected limits assume data = median expected background outcome

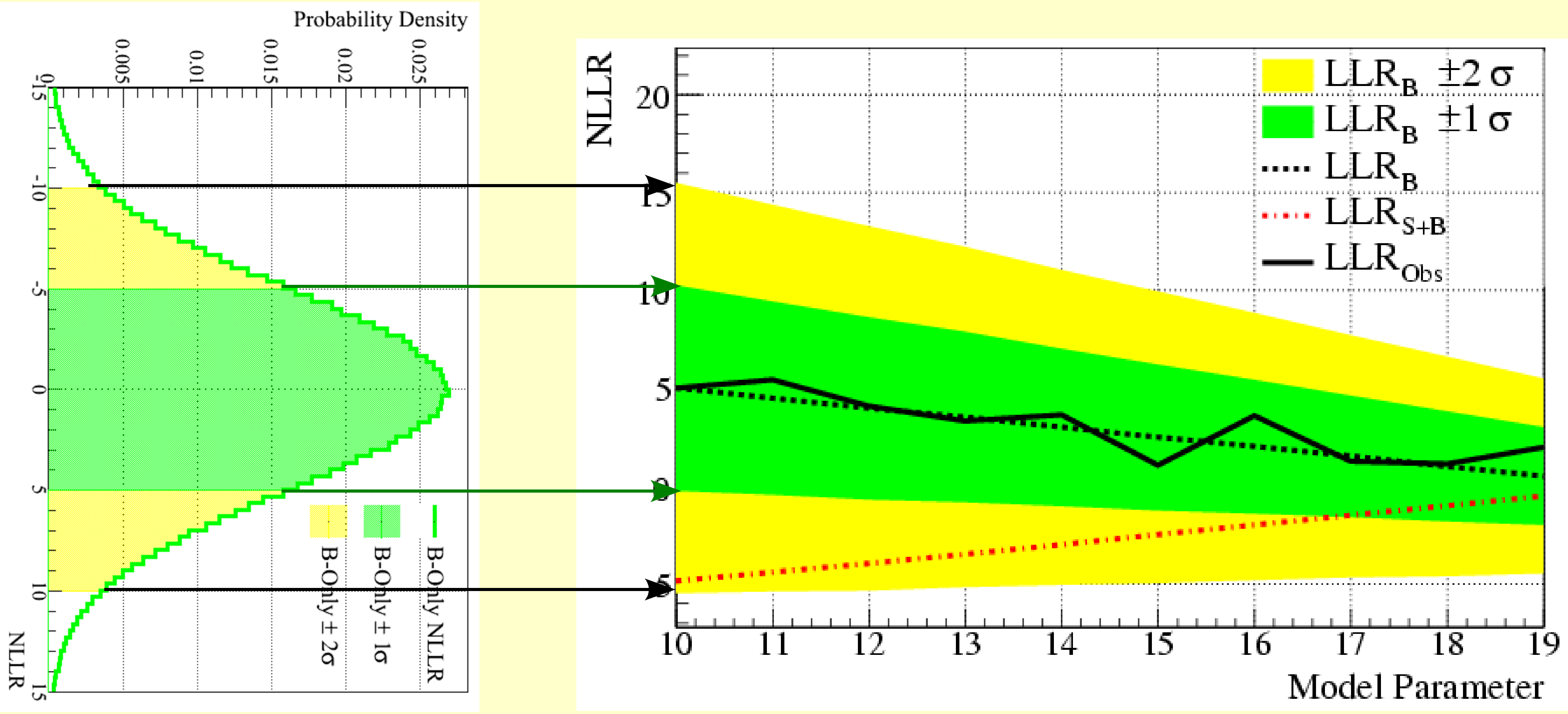
CL_b = 50% if background is well-modeled

"Expected" Data = Median Bkgd Outcome



Connecting with Standard LLR Plots

- ✗ We commonly plot LLR values as a function of a model variable, eg Higgs mass
  - *Thes are just "overhead" views of LLR distributions at each Higgs mass*



Confidence Levels

✗ Now that we've introduced Confidence Levels, let's give definitions

Confidence interval: a range of values of a model parameter

Confidence level: the fraction of outcomes predicted to fall outside the specified confidence interval

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Statistically Speaking:

$$\mathrm{PROB}_{x;\phi,\theta}\ (\ u(x) < \phi < v(x)\ ) = 1\text{-}\alpha \quad \text{for all } \phi,\theta$$

x = test statistic, ϕ = parameter of interest (eg, xsec), θ = nuisance parameters

$1\text{-}\alpha$ = confidence level, $u(x)$ = lower limit, $v(x)$ = upper limit

---

For example: Luminosity = 1000 ± 60 1/pb quoted at 1-sigma

±60 1/pb defines the confidence interval

1-sigma defines a confidence level of 68%

68% of possible true luminosity values lie within $940 < L < 1060$ 1/pb

The CLs Statistic

- ✗ Given our confidence levels for our two hypotheses: $\mathbf{CL_{sb}}$ and $\mathbf{CL_b}$

  We want to describe confidence intervals relative to specific outcomes

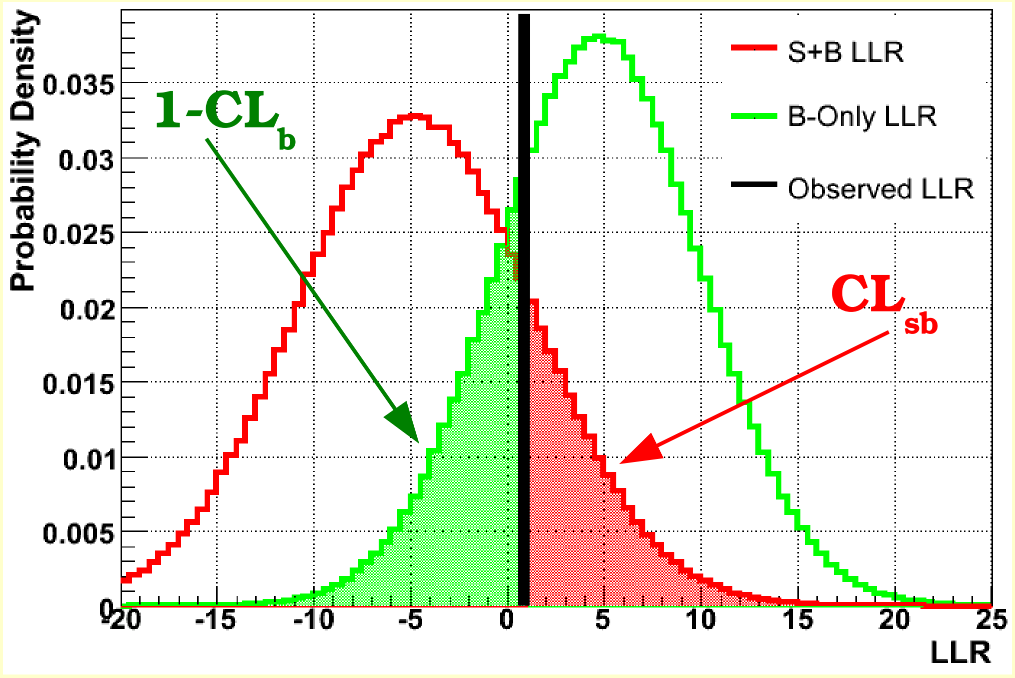
  1) Observed limits defined relative to observed data value
  2) Expected limits defined relative to median background prediction

  A strict Frequentist definition would use $\mathbf{CL_{sb}}$ to define confidence interval

- ✗ The CLs prescription introduces an inherit dependence on the background model description

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

New interval defined for 1-CLs = 1-α



The CLs Statistic

✗ Given our confidence levels for our two hypotheses: **CL$_{sb}$** and **CL$_{b}$**

We want to describe confidence intervals relative to specific outcomes

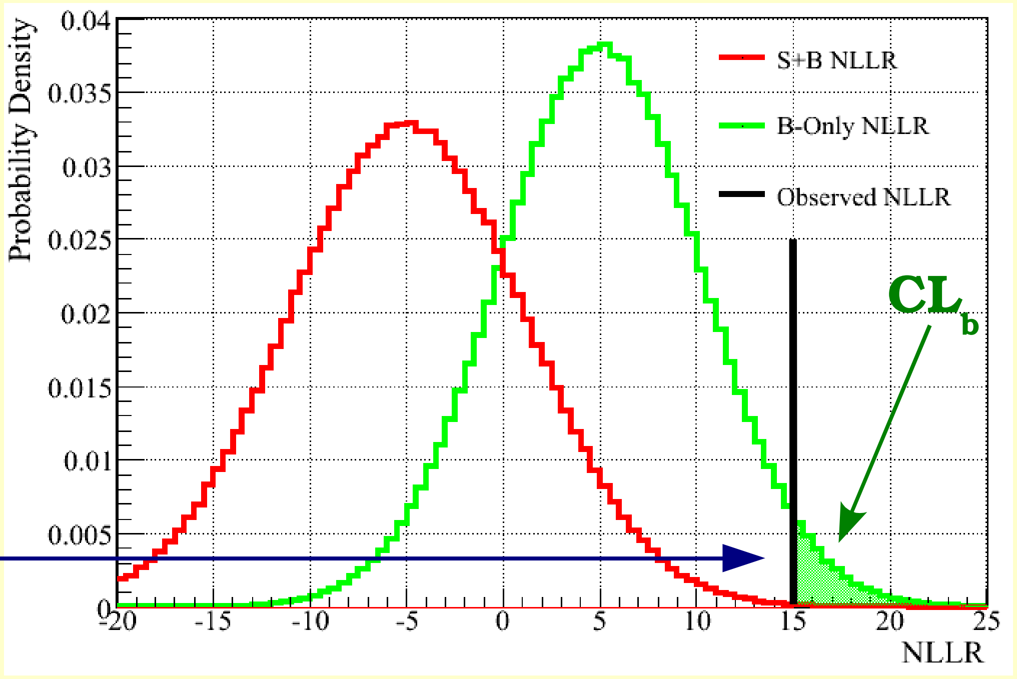
1) Observed limits defined relative to observed data value
2) Expected limits defined relative to median background prediction

A strict Frequentist definition would use **CL$_{sb}$** to define confidence interval

✗ The CLs prescription introduces an inherit dependence on the background model description

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

New interval defined for 1-CLs = 1-α
Provides essential protection against poor background modeling.



A Higgs Search Example

- ✗ We begin by defining our confidence level requirement: CL = 95%
  - Given the SM Higgs cross section, very likely 1-CLs < 95%
  - Thus, slowly increase signal rate until 1-CLs = 95%

  We thus define:

  u(t) < SM Xsec < v(t) @ 95% CL

  u(t) = 0, v(t) = cross section satisfying 1-CLs

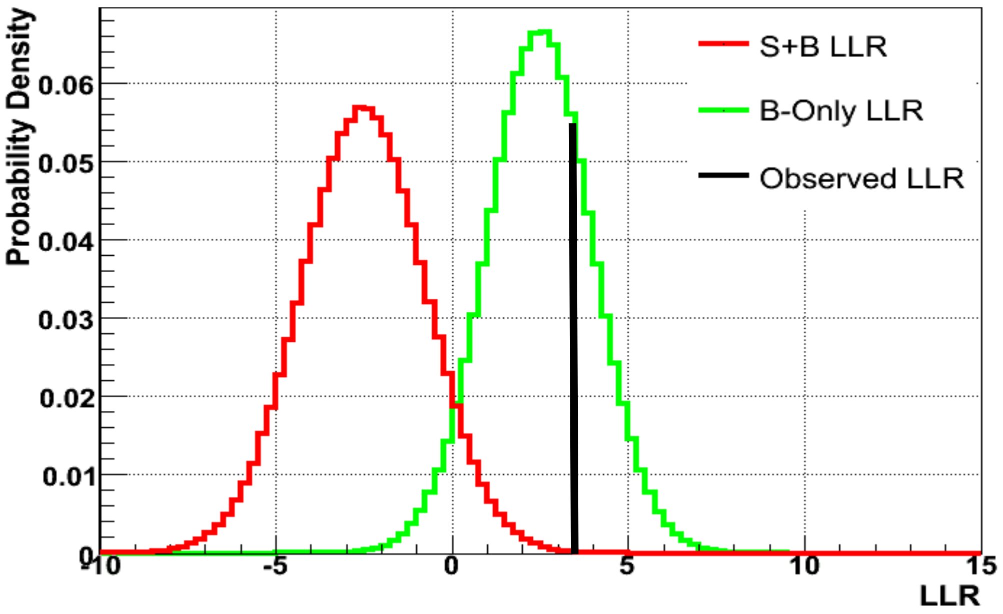
- ✗ In general, this method *overcovers*: CLsb < 5%
  - This is deemed acceptable based on our uncertain background model

- ✗ Because the lower limit=0, we use infinite integrals to define CL values
  - Thus, these CL values can be interpreted as p-Values

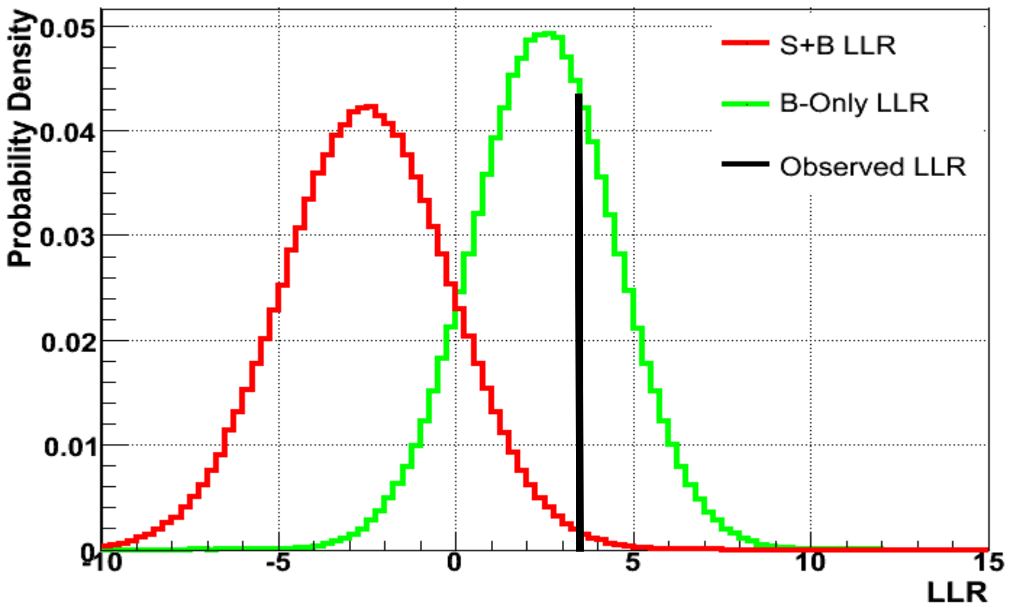
Marginalization

- ✗ Marginalization: broadening of nominal PDF via incorporation of systematics
- ✗ Compare "baseline" LLR (no systematics) to marginalized LLR distributions
  - No systematics: width of LLR dist given by Poisson uncertainty of samples
  - With systematics: width is proportional to quadrature sum of Poisson uncertainty and systematics uncertainty $\sigma^2_{tot} \propto \sigma^2_{Poisson} + \sigma^2_{systematics}$
  - Mean & observed LLR values remain the same, widths increase
  - Background CL increases and the ability to distinguish **H1** & **H0** decreases

Baseline LLR Distributions: CLfast



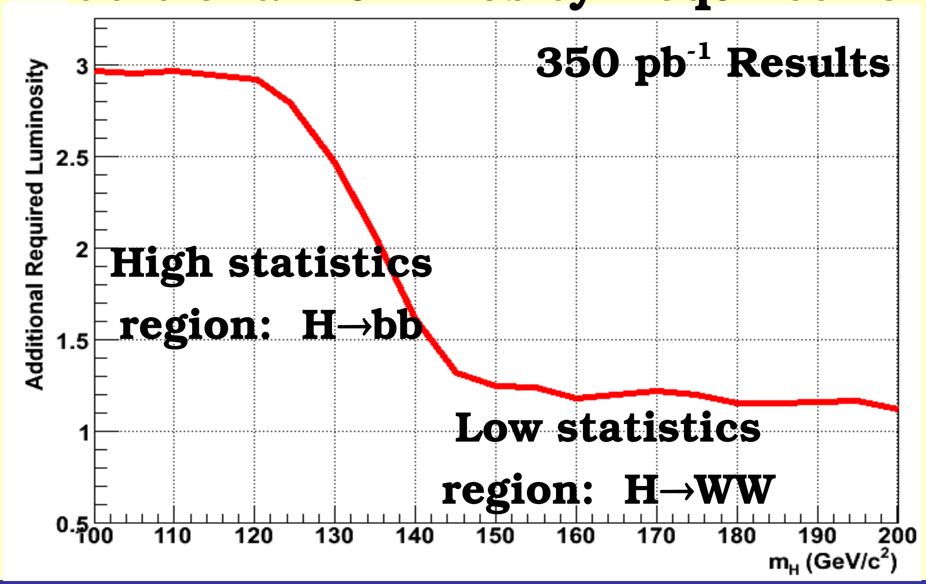
Marginalized LLR Distributions: CLsyst

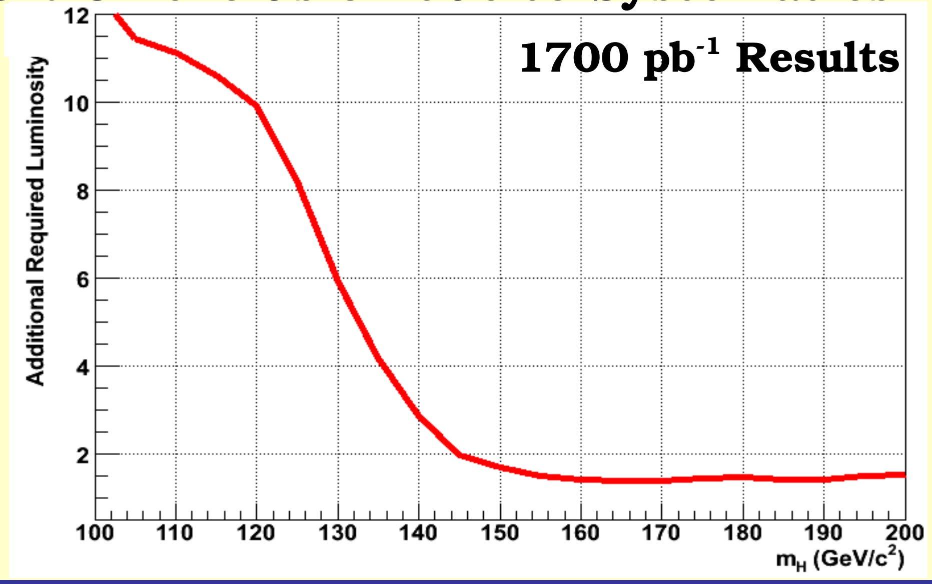


Impact of Systematics

- ✗ Impact of systematics on limit depends on the statistics of the channel
  - Low statistics ⇒ Statistical uncertainty generally **large** WRT systematics
  - High statistics ⇒ Statistical uncertainty generally **small** WRT systematics
  - **Statistics limited** vs **systematics limited** analyses
- ✗ Can visualize by looking at ratio of limits with and without systematics
  - Convert to effective luminosity lost due to impact of systematics
- ✗ Painful, somewhat unavoidable, but we should be able to lessen this

Additional Luminosity Required for 95% CL exclusion due to Systematics





The Profile Likelihood

- ✗ To counteract the degrading effects of uncertainties on nuisance parameters, we begin by defining the Profile Likelihood
  - Likelihood becomes a function of signal, bkgd, data, and nuisance parameters
  - Maximizing the Profile Likelihood to a set of data points defines our "best fit" for that data in a given hypothesis

$$Q=\frac{L(x|\theta_{R1},\hat{\theta}_S)}{L(x|\theta_{R0},\hat{\hat{\theta}}_S)}$$

$\longleftarrow$ Two independent likelihood maximizations are performed over nuisance parameters parameters, one for each pseudoexperiment

$\theta_{R1}\ \theta_{R0}$: Physics parameters in ***H1*** and ***H0***, respectively

$\hat{\theta}_S$: Nuisance parameters which maximize L for ***H1***

$\hat{\hat{\theta}}_S$: Nuisance parameters which maximize L for ***H0***

The Profile Likelihood

✗ Must define the best fit of our MC model to data

Assume prediction of N events per bin is a function of nuisance parameters

$$\hat{B}_i \rightarrow B_i \prod_{k=0}^{N_{syst}} (1+\sigma_i^k S_k)$$

B_i = nominally predicted bin content

σ_i^k = fractional uncertainty

S_k = N sigma deviation from nominal

Assume data is Poisson distributed, derive constraint via statistical power of data shape and systematic priors

$$L = \prod_{i=0}^{N_{bins}} \frac{P(\hat{B}_i)}{P(D_i)} \times \prod_{k=0}^{N_{syst}} \frac{G(\hat{\sigma}_k)}{G(\sigma_k^0)}$$

P(X) = Poisson PDF for X events

G(Y) = Gaussian PDF for systematic Y

Minimize Chi2 by varying S_k values

can "float" nuisance parameters by removing S^2 constraint

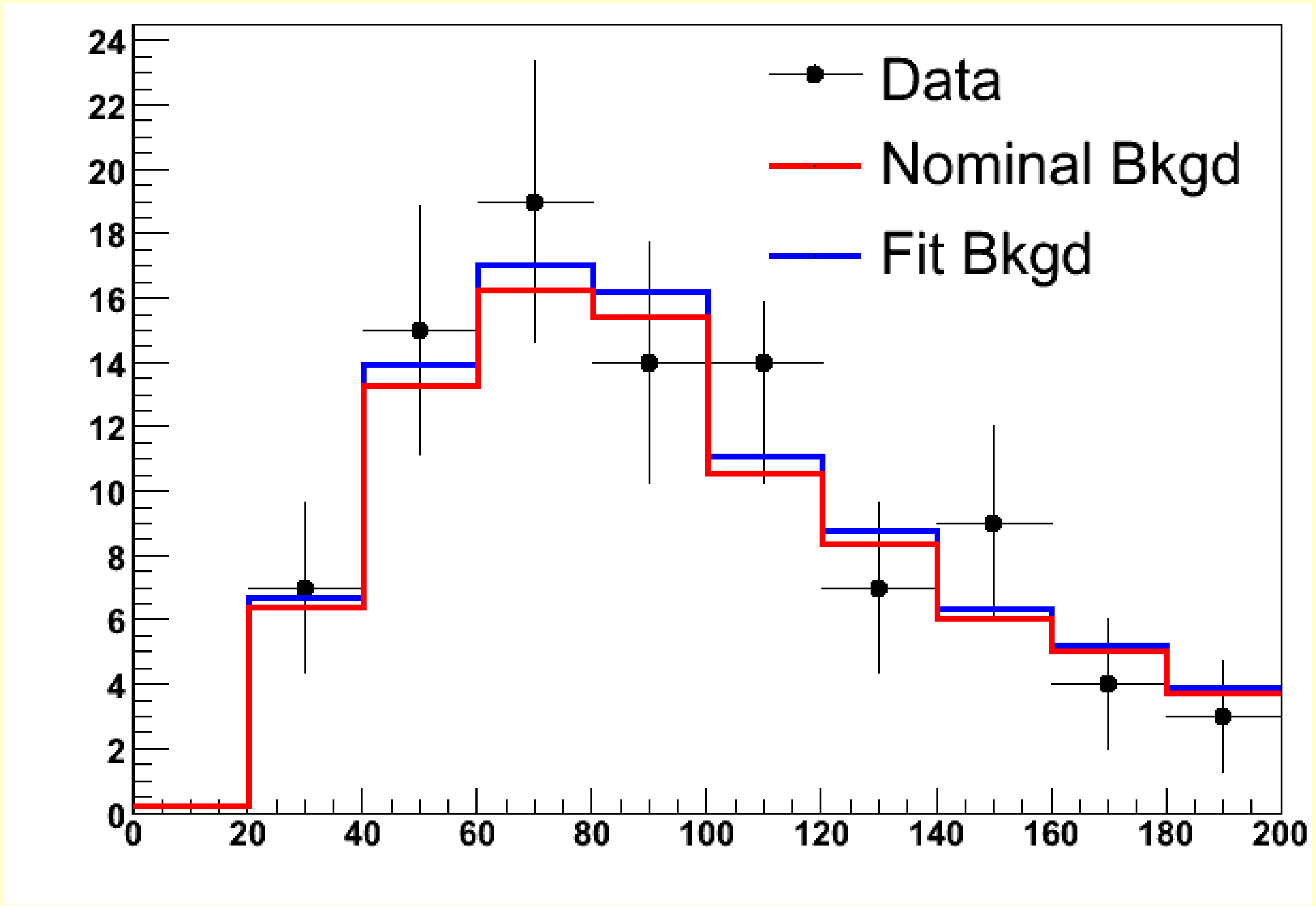
$$\chi^2 = -2\ln L = 2\sum_{i=0}^{N_{bins}} (\hat{B}_i - D_i) - D_i \ln\left(\frac{\hat{B}_i}{D_i}\right) + \sum_{k=0}^{N_{syst}} S_k^2$$

The Profile Likelihood

- What's really happening?
  - Analyzer generates a background prediction based on MC, data (QCD), and best guesses for central values of nuisance parameters
    - *Many uncertainties on nuisance parameters are ~20-40%!*
  - Define “best fit to data” by minimizing our Poisson Chi2 over the central values of the nuisance parameters
    - *Each background source is varied independently according to uncertainties*
  - Uncertainties can (should!) be given as a function of final variable
    - *Correlations are important and rigorously maintained*
  - Penalty term for deviations from nominal prediction eliminates free fit to data
    - ⇒ constrains fit within errors of your best guess

$$\chi^2 = 2\sum_{i=0}^{N_{bins}} (B_i - D_i) - D_i \ln\left(\frac{B_i}{D_i}\right) + \sum_{k=0}^{N_{syst}} S_k^2$$

Profile LH Fitting Example



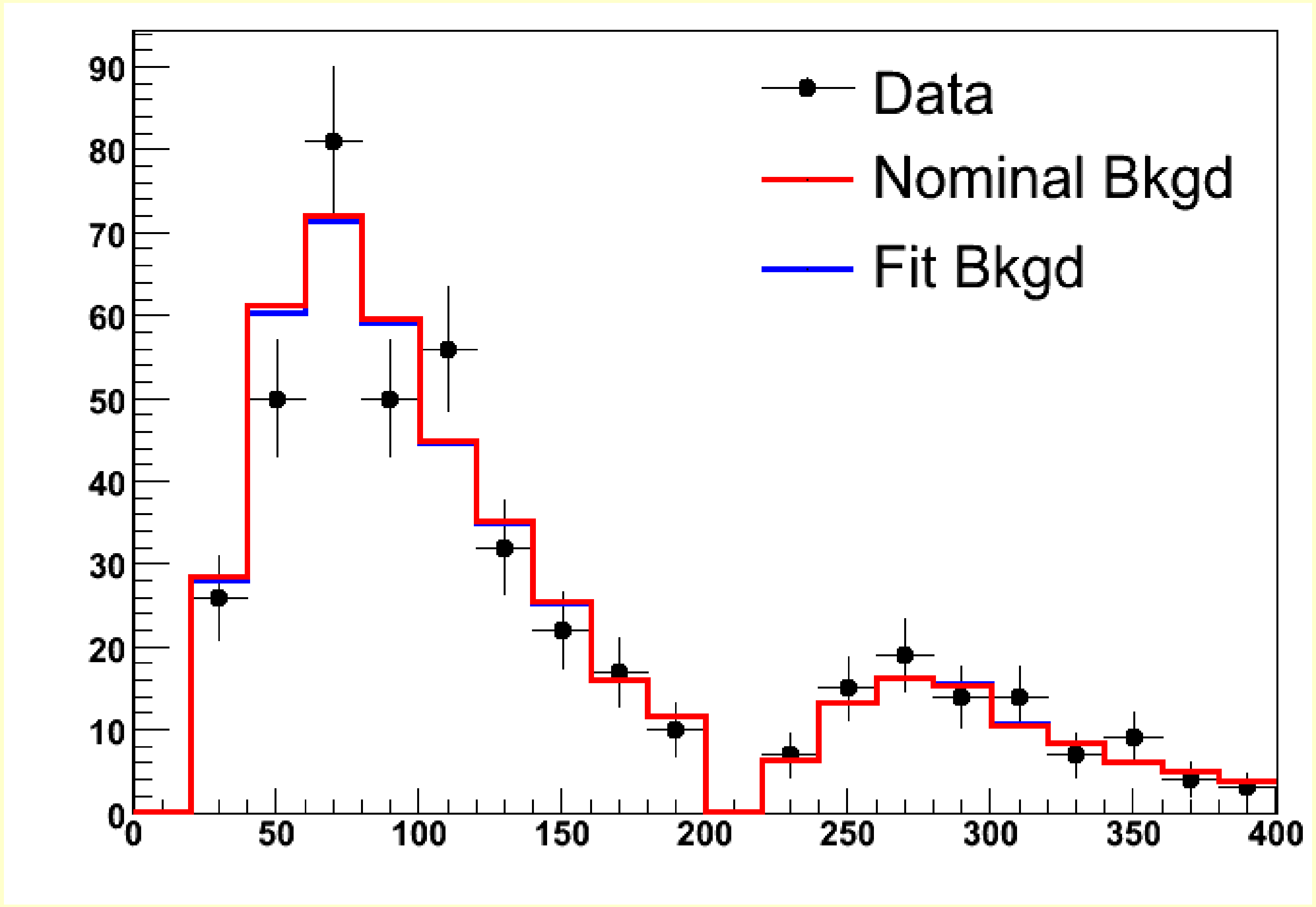
Prefit: Sig: 0.81, Bkgd: 85.2, Data: 92

Post-fit: Sig: 0.83, Bkgd: 89.3, Data: 92

Profile LH Fitting Example

✗ Add another channel to the fit

Increased statistics impacts fit via correlated nuisance parameters

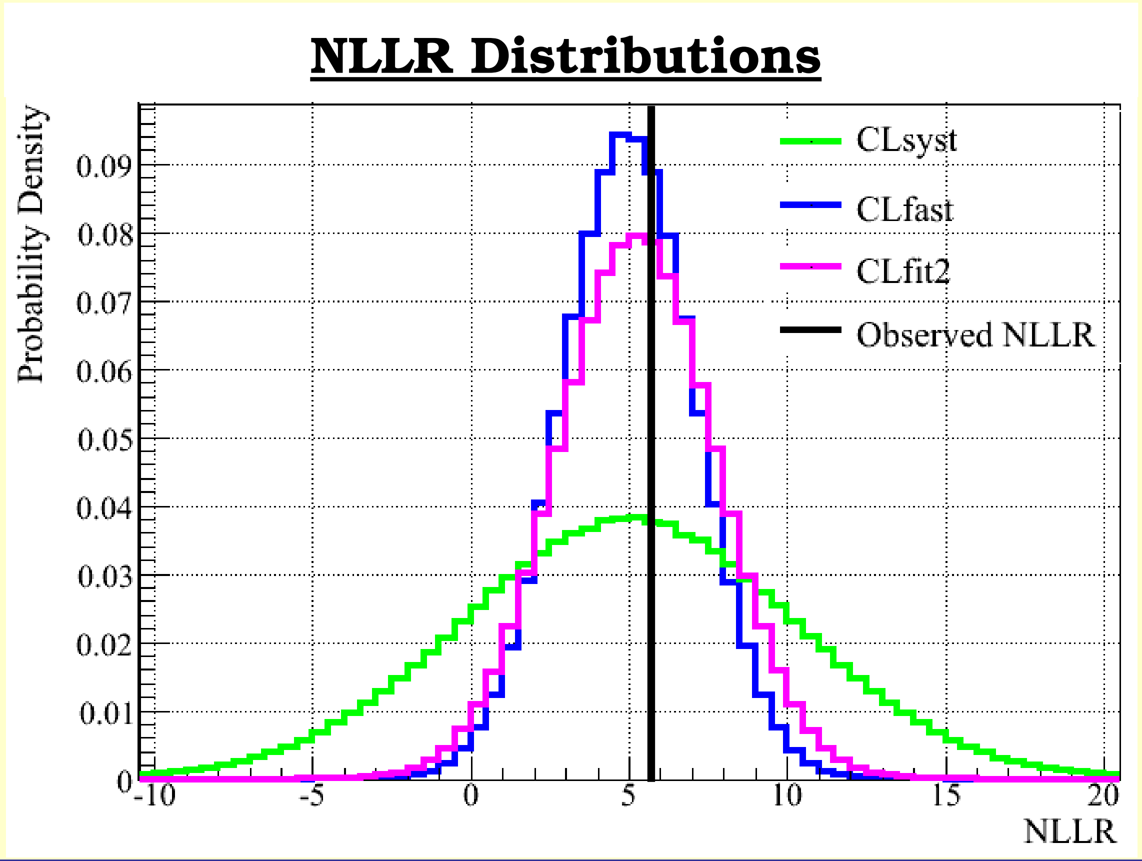


Prefit: Sig: 1.65, Bkgd: 440, Data: 436

Postfit: Sig: 1.65, Bkgd: 437, Data: 436

Profiling Example

- Comparing "baseline" (ie, no systematics) and smeared LLR distributions to those from the fitted profile-LH prescription
  - Fitted background CL moves closer to 50% (*better agreement with data*)
  - Separation of S+B and B-Only hypotheses roughly the same
  - Width of LLR distributions grows slightly, but less than CLsyst prescription



Applying to the Calculation

- ✗ Two general ways of implementing the fit:
  1) Fit each data distribution to a model (**H1** or **H0**), calculate LLR value after each fit

     CLfit *calculator class in Collie*

     Optionally remove regions with large S/B values to eliminate signal contamination

     Requires user input....beware....

  1) Perform two fits to each data distribution (**H1** & **H0**)

     CLfit2 *calculator class in Collie*

     Redefine LLR as Chi2 difference between fits

     This is the more robust application, and no user input

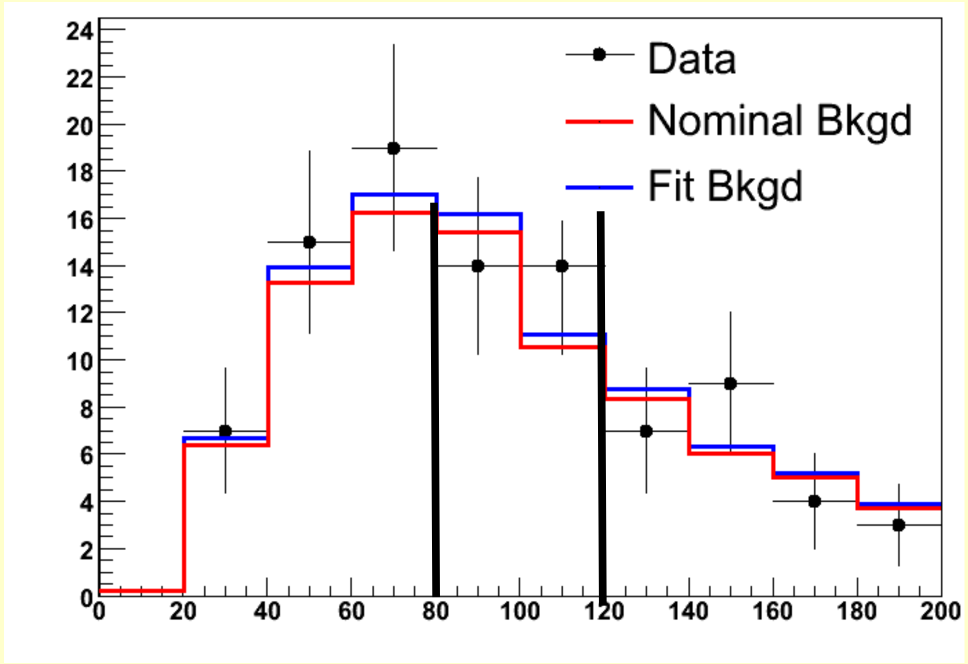
     More powerful, but it's 2x slower...

As defined in slides 14-15

$$LLR_{new} = \chi^2_{min}(H1) - \chi^2_{min}(H0)$$

CLfit Bin Exclusion

- ✗ Optionally remove bins with large signal contribution from fit
  - Assuming you're fitting to **H0** hypothesis
  - Fit loses statistical power based on how many bins are removed
- ✗ Choice of window size is somewhat arbitrary, but needs care
  - Basic caveat: Exclude signals of the same size as the background fluctuation (can't probe smaller than that!)
  - Window must grow as signal grows, taken care of automatically (ie, during scaling procedure)



The User Interface to Collie

The Starting Point

- ✗ What do you need to get started?
  - A final variable capable of distinguishing signal from background.
  - A signal hypothesis in the form of some acceptable simulation.
  - A background hypothesis, ideally separated into major background components.
  - A data distribution.
  - Models for nuisance parameters.
- ✗ How should you package your inputs?
  - Collie can parametrize a model in 3-D (eg, mass, width, branching fraction)
  - Collie can utilize 1-D and 2-D final variables, input as histograms.
  - Collie assumes ALL of your input distributions are normalized to the expected number of events.
  - Nuisance parameters can be input in 3 separate ways:
    - ✗ Constant, ± 1-σ fractional uncertainties for each histogram bin (eg, Lumi)
    - ✗ Histograms of non-constant, ± 1-σ fractional uncertainties per bin (eg, JES)
    - ✗ Histogram resulting from varying the underlying nuisance parameter by ± 1-σ

A bit more detail

- ✗ Signal normalization

  If you normalize to expected numbers of events ($\mathbf{S=L\times\sigma^0\times\epsilon}$), limits are returned in units of the input signal cross section σ^0 : $\mathbf{R} = \sigma^{\mathrm{Limit}} / \sigma^0$

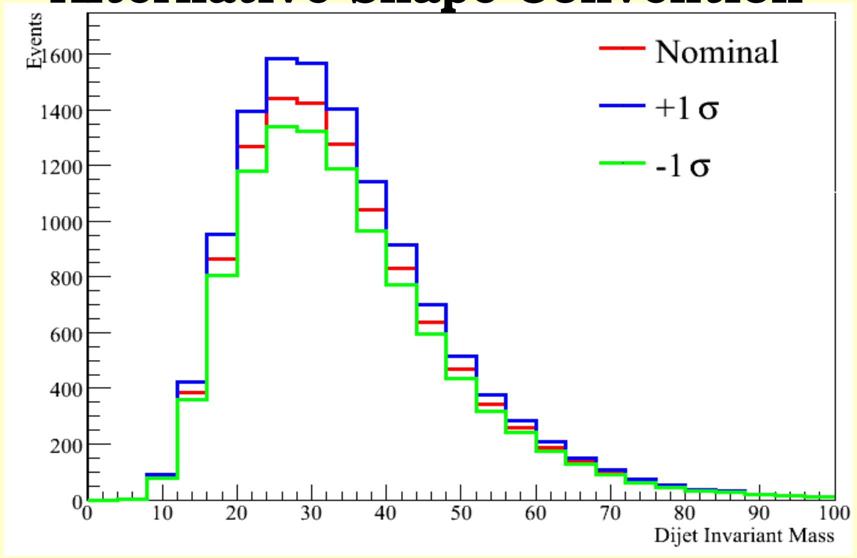
  If you normalize to efficiency times lumi ($\mathbf{S=L\times\epsilon}$), limits will be returned in of cross section

- ✗ Sign conventions for systematic uncertainties:

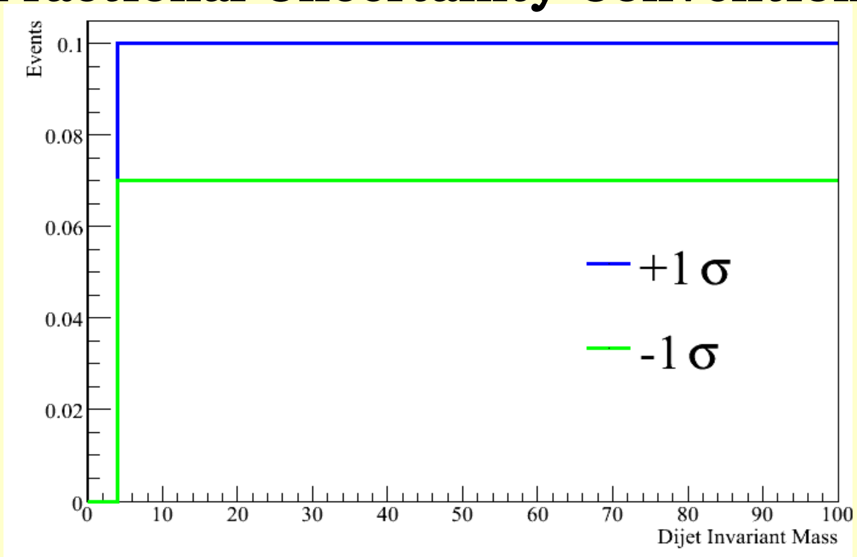
  For fractional uncertainties, there's ambiguity so we have to choose a convention. Ambiguity eliminated for alternative shapes.

  Example for an asymmetric flat uncertainty of +10%, -7%

Alternative Shape Convention



Fractional Uncertainty Convention



The Collie User Interface

- ✗ To be flexible, Collie is composed of two parts:

  File Creation: Interface classes designed to create formatted CollieIO files used in all Collie calculations.

  - Users input data, MC, and nuisance parameter distributions for all model parametrizations.
  - Internal "sanity checks" and closure tests are performed by Collie.
  - Resulting CollieIO files can be used, exchanged, or combined to generate a calculational product.

  Calculations: Classes which perform standardized calculations based on user input files.

  - Users provide formatted CollieIO files and design an executable for the calculation.
  - Calculations can be CPU intensive, so batch submission is recommended.

Getting/Building Collie

✗ Collie can be found in d0cvs

For a tagged version of Collie: `cvs co -r V00-03-16 collie`

For the most recent version of Collie: `cvs co -A collie`

untagged versions aren't guaranteed to be safe...

✗ Collie does not use the SRT gmake, but comes with its own makefile. To build collie:

```
1) cd collie

2) source setup_Collie.tcsh  (or use the bash version.  syntax depends
   on your shell, edit as needed)

3) make (ROOT may complain. Just ignore it. ROOT isn't a C++ authority!)
```

✗ A successful build will create the following files:

collie/lib/libCollieIO.so	collie/lib/libCollieLimit.so
collie/examples/collieIOmaker.exe	collie/examples/collieLimitCalc.exe
collie/examples/collieXsecCalc.exe	collie/examples/resultsFileCombiner.exe

Creating a CollieIO File

✗ The first step is creating an input file for calculations

Adapted from collie/examples/collieIOexample.cc

```
int main(int argc, char* argv[]) {

  //////////////////////////////////////////
  ///Create IO file with input parameters
  //////////////////////////////////////////
  CollieIOFile* cfile = new CollieIOFile();
  cfile->initFile("exampleCollieIOfile.root", "Test Channel");  //outputfile and channel name
  cfile->setInputHist(0.0,1.0,20); //Define your input histograms
  cfile->setCutoffs(0.0,1.0);   //Option to define physical cutoffs
  cfile->setRebin(1);           //Option to rebin histograms to a coarser binning
  cfile->setSmooth(false);        //Option to smooth histograms

  //Define backgrounds
  vector<string> bkgdNames;
  bkgdNames.push_back("Bkgd1");
  bkgdNames.push_back("Bkgd2");
  cfile->createChannel(bkgdNames);

  //Get your input histograms from somewhere (made up at random in the example)

  //or get them from a file:
  //  TFile infile("myInputFile.root");
  //  TH1D* data = (TH1D*)infile.Get("data");
  //  TH1D* signal = (TH1D*)infile.Get("signal");
  //  TH1D* bkgd1 = (TH1D*)infile.Get("bkgd1");
```

Creating a CollieIO File

✗ Continued from previous slide...

```
  //Backgrounds are passed in via vector
  vector<TH1D*> vbkgd;
  vbkgd.push_back(bkgd1);
  vbkgd.push_back(bkgd2);

  //Alpha parameters only matter when smoothing is utilized
  //  Input values don't matter if you're not smoothing.
  //  Don't smooth unless you know what you're doing.
  vector<double> valpha;

  //Each parameter point has a signal histo, data histo, and an array of backgrounds...
  //  Smoothing parameters are also passed in.
  cfile->createMassPoint(100, data, sig, -1, vbkgd,valpha);

  //Add systematics...either flat or by shape (ie, function of final variable)
  //   if by shape, must supply a histogram of the values in percent(%) fluctuations...
  //   Signal requires no index, but backgrounds must be specifically indexed (0->N bkgds)
  cfile->createFlatSigSystematic("Lumi",0.06,0.06,100);
  cfile->createShapeSigSystematic("SigShape",sigSystP,sigSystN,100);

  cfile->createFlatBkgdSystematic(0,"Lumi",0.06,0.06,100);
  cfile->createFlatBkgdSystematic(1,"Lumi",0.06,0.06,100);

  ///store channel
  cfile->storeFile();
}
```

Output of CollieIO Example

✗ Summarized result obtained after running collie/examples/collieIOmaker.exe

```
>>./collieIOmaker.exe

==>Created mass point 100
```

Report on I/O procedures, look for error warnings here

```
Mass: 100
     Data: 451
     Signal: 7.504
     Bkgd: Bkgd1, 150.00
     Bkgd: Bkgd2, 299.876
     Allbkgd: 449.88
```

Checksum integrals of input histograms. “Sanity check” that you get out what you put in

```
==>Saving inspection histos to
fv_exampleCollieIOfile.root
```

Output files:
fv_XY.root is a histogram file representing ***everything*** stored in the collieIO input file for your inspection. This is not your colleIO file!

```
==>Saving channel data to
exampleCollieIOfile.root....
```

XXX.root is your collieIO input file

CollieIO Systematics API

- ✗ There are six different methods for adding systematics at the CollieIO step, three each for signal and background:

  - Flat systematics: CollieIOFile::createFlatSigSystematic(...) and CollieIOFile::createFlatBkgdSystematic(...). Use this for things like luminosity where every bin gets the same uncertainty value.

  - User-Defined shape-dependent systematics: CollieIOFile::createSigSystematic(...) and CollieIOFile::createBkgdSystematic(...). Users may define any fractional uncertainty shape that they wish.

  - Shape-dependent systematics: CollieIOFile::createShapeSigSystematic(...) and CollieIOFile::createShapeBkgdSystematic(...). Users pass Collie alternative final variable shapes for systematic uncertainties (ie, the shapes you'd get for +/-1 sigma for a given systematic). There are many modification choices available for these methods, please read the instructions.

Please read the detailed usage instructions for each method in collie/io/include/CollieIOFile.hh

CollieIO Warnings and Errors

- ✗ Collie automatically checks for errors in the following areas:
  - Statistical uncertainties: Basic sanity checks, such as “Did you call TH1D::Sumw2()?”, “Are your statistical uncertainties larger than bin content?”, etc.
  - Systematic uncertainties: Do you have any systematics larger than ~50%? If so, you may consider a Log-Normal PDF. Otherwise, you may have the wrong systematics.
  - Systematic uncertainties: Are your shape systematics dominated by noise? If so, Collie will automatically flatten these.
  - Systematic uncertainties: Did you accidentally put the same shape systematic histogram in twice for both positive and negative fluctuations? This is a valid use case and Collie will interpret this as a symmetric fluctuation. But you'll still get a warning.
  - Histogram contents: Do you have underflow or overflow? Collie ignores under/overflow.
  - Histogram contents: Do you have bins with non-zero signal, non-zero data, and zero background? If so, you don't need Collie. You need to call a press conference or reconsider your background model. Collie will merge these bins to the nearest neighbor with highest S/B content.

Calculations Available in Collie

- ✗ Recall our definition of CLs

  Defends against false discovery when data<<bkgd (amongst others)

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

- ✗ The products available via Collie

  TEST (H1) or **NULL (H0)** Hypothesis p-Values:

  CL_{sb} or **CL_b** as defined on slides 11-16

  Cross Section Limit Calculator: Determines the factor by which the signal must be scaled to obtain **$1\text{-}CL_s \geq X$** (eg, 90%, 95%, etc)

  Luminosity Limit Calculator: Determines the factor by which the luminosity must be scaled to obtain **$1\text{-}CL_s \geq X$**

  3-Sigma Evidence Calculator: Determines the factor by which the luminosity must be scaled to obtain **$1\text{-}CL_b \geq X$**

  Cross Section Calculator: Scanned and floated signal size calculations available for signal-like excesses.

Example Limit Calculation

✗ Once you've created a CollieIO file, you can calculate something...

Adapted from collie/examples/exampleLimitCalculation.cc

```
void loadLimits(char* outfile, char* m) {

  //What mass point are we interested in
  int mass = atoi(m);

  //Open the CollieIOFile created in I/O example step...
  char options[1024]; bool ok = true;
  ////Specify the channel name given in the I/O step
  sprintf(options,"name='%s'","Test Channel");
  //Pass this information to the CollieLoader to extract the channel info
  CollieLoader loader;
  if (!loader.open("exampleCollieIOfile.root",options)) {
    std::cout << "Failed to open " << filename << " using " << options << "!\n";
    ok = false;
  }
  if(!ok) return;

  //Choose a systematics treatment...
  CLfast clcompute;  //The CLfast computation uses no systematics
  //  CLsyst clcompute;  //CLsyst applies all systematics via Gaussian distribution
  //  CLfit2 clcompute;  //profileLH fitting using two fits per pseudoexperiement
  //  CLfit clcompute;   //profileLH fitting using just one fit per pseudoexperiment

  // If you choose the CLfit option (faster than CLfit2), you must specify whether the fit will
  // include signal contributions.
  // clcompute.fitSignal(false);
  // clcompute.logSigExclusion(0.005);
```

Example Limit Calculation

- ✗ Continued from last slide...

```
 // This is the class for computing cross section limits
 CrossSectionLimit csLim;
 csLim.setup(&clcompute);        //Pass in the computer you chose
 csLim.setVerbose(false);
 csLim.setCLlevel(0.95);         //Set to 0.95 for 95% CL calculation (default = 0.95)
 csLim.setPrecision(0);          //0 is lowest(fastest), 4 is highest(slowest)
 csLim.calculateExpected(true);  //toggle on/off expected/observed limits
 csLim.calculateObserved(true);  //    to get speed things up if you wish

 //tell the container what point you're working on
 clresults.reset(v1[i],v2[i],v3[i]);

 //Extract the signal & background distributions associated with this point
 SigBkgdDist* sbd=loader.get(v1[i],v2[i],v3[i]);

 //calculate Confidence Levels
 clcompute.calculateCLs(*sbd,clresults,CLcompute::LEVEL_VERYFAST);
 //report your results for interested observers
 clresults.print();

 //Calculate a cross section limit...
 //These results are reported in the factor by which you must
 //multiply your nominal signal cross section to obtain a 95% CL
 //upper limit for this model... IE, multiply this factor by
 //your model xsec to get your limit in barns
 csLim.calculate(*sbd,clresults);

 //report your results for interested observers
 csLim.print();
}
```

Output of Limit Calculation

✗ Calculating limits for mH=105 from the example inputs

```
./collieLimitCalc.exe myOutput.root 100
```

Output stored in ROOT format in specified file, set mass point to -1 to get all in the input file

```
****************************************:
CLcompute Results:
      CLs_obs: 0.6462,  CLs_med: 0.7237
     CLsb_obs: 0.2235, CLsb_med: 0.1381
      CLb_obs: 0.6316,  CLb_med: 0.5168
     LLRobs: 0.5406, LLRb: 1.1609, LLRsb: -1.2352, lumifactor: 3.249
     LLRb_m2s: 5.1118, LLRb_m1s: 3.2550
     LLRb_p1s: -0.9013, LLRb_p2s: -3.1823
****************************************:
```

Report of non-scaled CL calculations

```
****************************************:
CrossSectionLimit calculator results::
==>CL level: 0.9500, N sigma: 0
==>Accuracy: 0.0010, Precision: 0
==>Scaling factor Exp: 1.900, Obs: 2.181
****************************************:
```

Report of limit calculation

```
 14.594 sec run time
```

Job timer

Combining Channels

✗ If you wish to combine two or more channels:

  Simply append appropriate distributions from the channels

✗ When combining channels, you must make sure that correlations amongst systematics are properly specified

  Collie will correlated all systematics whose names are identical. Eg, “lumi” and “lumi”, but not “Lumi” and “lumi”.

```
 CollieLoader loader;
 if (!loader.open(“collieIOfile1.root”,options)) {
   ok = false;
 }
 CollieLoader loader2;
 if (!loader2.open(“collieIOfile2.root”,options)) {
   ok = false;
 }
 if(!ok) return;

...Normal calculation setup...

 //Extract the signal & background distributions associated with this point
 SigBkgdDist* sbd1=loader1.get(v1[i],v2[i],v3[i]);
 SigBkgdDist* sbd2=loader2.get(v1[i],v2[i],v3[i]);

 //Append the two distributions
 sbd1->append(*sbd2);

  ...Continue with your calculations...
```

Combining Channels, ctd.

- ✗ When combining channels, you must make sure that correlations amongst systematics are properly treated
  - Collie will correlated all systematics whose names are identical. Eg, “lumi” and “lumi”, but not “Lumi” and “lumi”.
- ✗ Users with many input channels may wish to used “condensed” IO files
  - Use the IO condenser program: examples/collieIOcondenser.cc
- ✗ Batch submission script:
  - collie/limit/macro/CollieBatch.perl
- ✗ Fitting macros (more on this later):
  - collie/limit/macro/fitResults.C
  - collie/limit/macro/fitXsec.C

Additional Tools

- ✗ Plotting macros for ROOT output of limit calculations:

  collie/limit/macro/plotCLb.C

  collie/limit/macro/plotFactor.C

  collie/limit/macro/plotCL.C

  collie/limit/macro/plotLLR.C

- ✗ Batch submission script:

  collie/limit/macro/CollieBatch.perl

- ✗ Fitting macros (more on this later):

  collie/limit/macro/fitResults.C

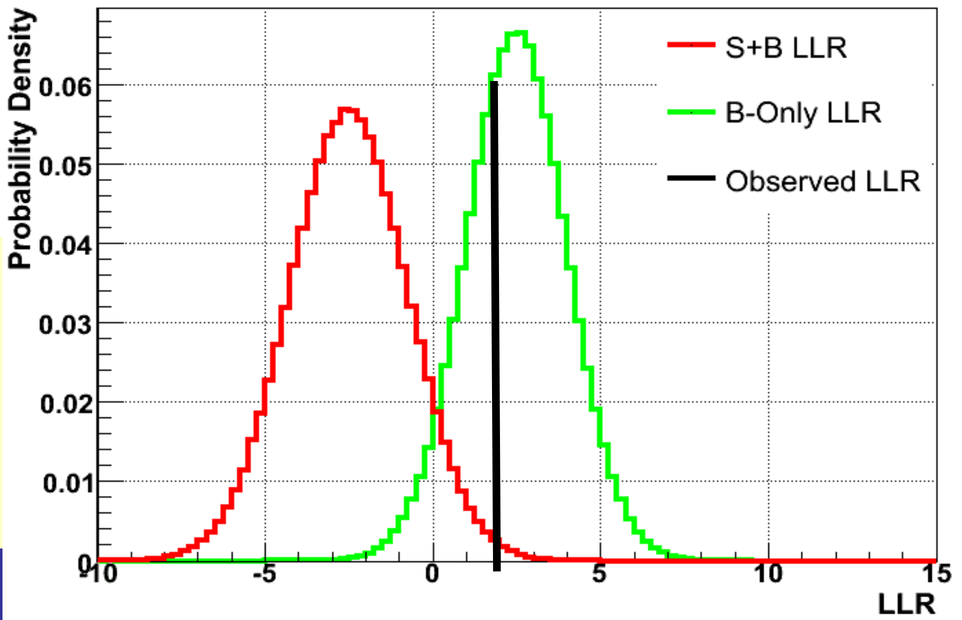
  collie/limit/macro/fitXsec.C

Viewing LLR Distributions

✗ You may wish to directly view your LLR distributions. Add the following lines to add histograms of LLR distributions to the output file.

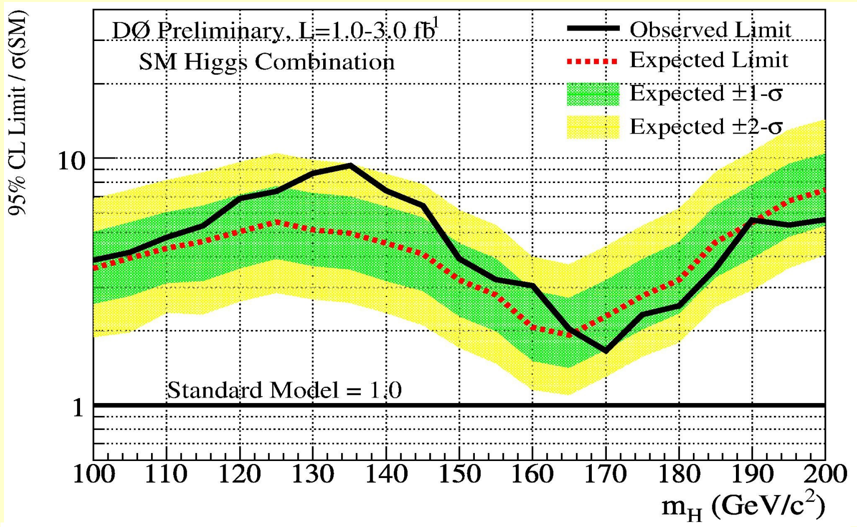
```
//calculate CLs...
clcompute.calculateCLs(*sbd,clresults,CLcompute::LEVEL_STANDARD);

//report your results for interested observers...
clresults.print();

//Add the following lines...
int bins = 5000; double min = -50; double max = 50;
TH1D* sigLLR = clcompute.getLLRdist_sb("LLR_SB",bins,min,max);
TH1D* bkgLLR = clcompute.getLLRdist_b("LLR_B",bins,min,max);
TH1D* LLRd = new TH1D("LLR_D","LLR_D",bins,min,max);
TH1D* LLRsigma1 = new TH1D("LLR_B_1sigmas","LLR_B_1sigmas",bins,min,max);
TH1D* LLRsigma2 = new TH1D("LLR_B_2sigmas","LLR_B_2sigmas",bins,min,max);

LLRd->Fill(clresults.llrobs);
LLRsigma2->Fill(clresults.llrb_m2s);
LLRsigma1->Fill(clresults.llrb_m1s);
LLRsigma1->Fill(clresults.llrb_p1s);
LLRsigma2->Fill(clresults.llrb_p2s);
```

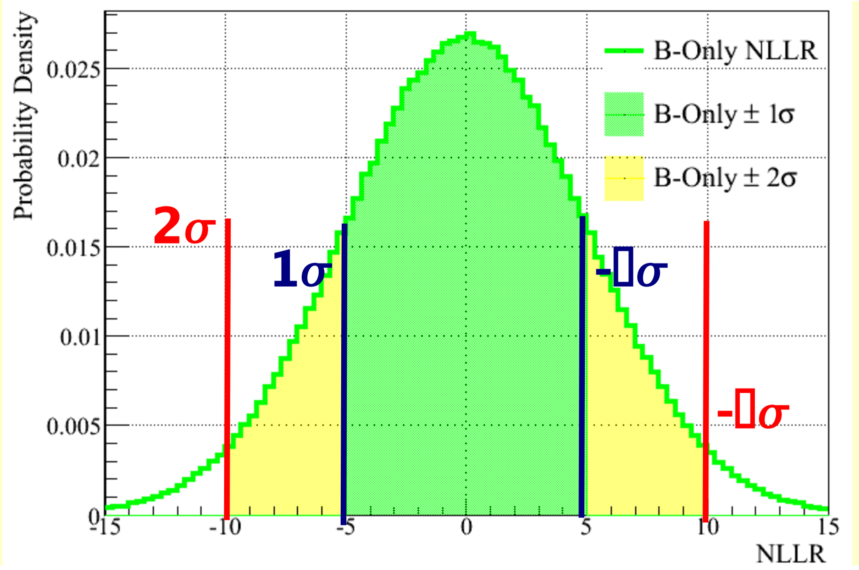
The above instructions provide non-scaled LLR distributions ⟶



Extracting ±1,2 Sigma Bands

- ✗ A pleasing limit presentation feature is the 1,2 sigma bands around the expected limit
  - A common misconception: "This is the error on the limit".
  - *There is no error on a limit unless you made a mistake! It's just a calculation.*
- ✗ The true interpretation is, "What limit would I get if the data disagreed with background to this degree?"
  - Determined by recalculating limits for 4 different outcomes
  - Bands enclose 68% and 95% of background outcomes, respectively.





```
// This is the class for computing cross section limits
CrossSectionLimit csLim;
csLim.setup(&clcompute);        //Pass in the computer you chose
csLim.setNSigma(2);             //Calculate +2 sigma
//csLim.setNSigma(-1);             //Calculate -2 sigma
```

Common Beginner Mistakes

- ✗ Problem: The CollieIO step doesn't report the correct histogram integrals!
  - Cause 1: Check that you specified the correct histogram parameters when you made the input files (see slide #24)
  - Cause 2: If you're using smoothing did not specify valid smoothing parameters (see next slide)

- ✗ Problem: The CollieIO step complains about my systematics histograms!
  - Cause 1: Collie will complain if you try to add a histogram that doesn't match the specified histogram parameters or is NULL.

- ✗ Problem: The calculation step complains when I load my input file!
  - Cause 1: Did you specify the correct channel name for the input file?
  - Cause 2: If you're appending two channels, do they have the same channel name?

Safety Net for Beginners

- ✗ The Collie Novice Flag
  - By default, Collie sets a flag defining the user as a novice
  - This flag will prevent you from using the following aspects:
    - Statistical Uncertainties, Smoothing, Interpolation, & Fitting
- ✗ No Statistical Uncertainties? Why??
  - By default, Collie assumes you either forgot, screwed up, or don't understand your statistical uncertainties.
  - By default, ROOT doesn't do a proper accounting of statistical uncertainties.
  - If you turn off the novice flag, Collie will test your statistical uncertainties for appropriateness. Check for warnings, but the ball's in your court....

Unsetting the Novice Flag

```
//Unsetting the novice flag in IO code
CollieIOFile* cfile = new CollieIOFile();
cfile->initFile("exampleCollieIOfile.root", "Test Channel");  //outputfile and channel name
cfile->setNoviceFlag(false);

//Unsetting the novice flag in calculation code
CLfast clcompute;  //The CLfast computation uses no systematics
clcompute.setNoviceFlag(false);

//Use of histogram statistical uncertainties can be enabled as follows:
clcompute->useHistoStats(true);
```

Potential Hazards in Collie

- ✗ Smoothing

  Collie contains an algorithm for histogram smoothing as an alternative to the sketchy one available in ROOT.

  ⇒ If you're using Collie's smoothing algorithm, I assume you know what you're doing. If you don't, contact me.

- ✗ Histogram binning

  Collie assumes you know what you're doing when you specify how many bins to use in your final variable.

  ⇒ Correct binning is intrinsically linked to the resolutions of observables and the statistics of your sample. **BINNING IS NOT AN OPTIMIZABLE VARIABLE FOR LIMIT CALCULATIONS!!**

- ✗ Data/MC agreement

  Collie assumes you've studied your backgrounds and you have reasonable agreement with data. Collie will happily calculate limits, etc for input channels that have no business trying to do so.

  ⇒ Perfect Data/MC agreement isn't mandatory, but you should double-check the output of the CollieIO step to ensure you agree with what is in the input file

Potential Hazards in Collie

✗ Systematic Uncertainties

If your systematics are larger than ~25-30%, you probably shouldn't be using the default Gaussian PDF for systematic uncertainties due to truncation issues

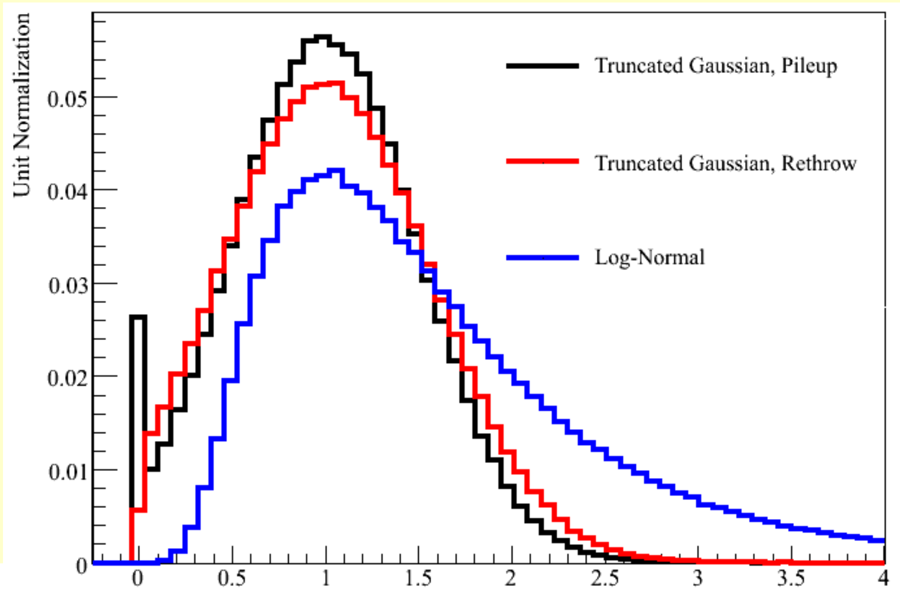
⇒ If you believe your event rate has a probability of 0 for 0 events, then switch to the log normal parametrization Specify this in the collieIO step: see below.

⇒ *If you have at least 1 MC event in a bin, it's hard to motivate a non-zero probability for 0 evts*

✗ Systematic Uncertainties

How well do you believe your uncertainty anyway? Does 100% uncertain make sense?

⇒ A better solution might be to remove the PDF constraint, assign a sensible uncertainty, and let a poorly known systematic "float".



```
 //Specify Log Normal for a systematic
cfile->setLogNormalFlag("YourSystName", true, 100);

//remove the PDF constraint for a systematic
cfile->setBkgdFloatFlag(0, "systName", true,100);
```

Systematics: Fitting vs Pseudo-Experiments

- ✗ A common misconception:

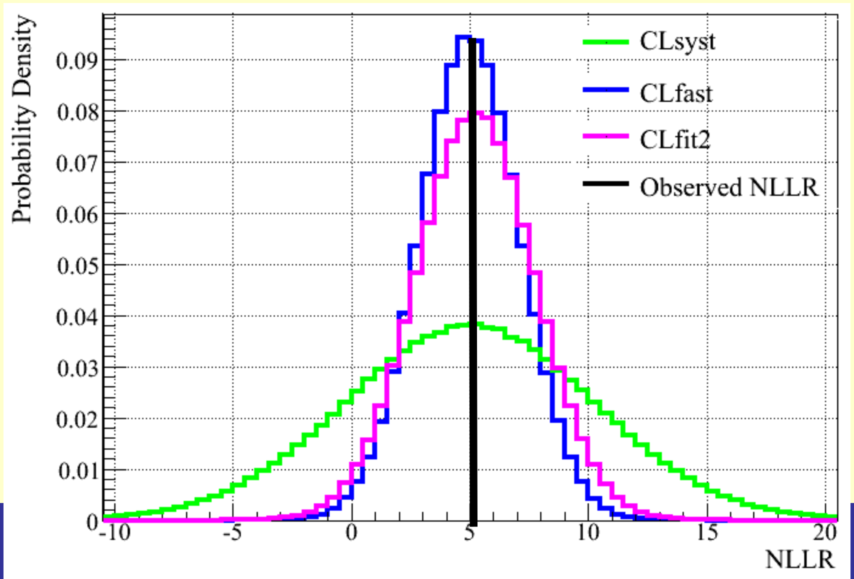
  "If I overestimate my uncertainties, it's OK because Collie will just find the true value for me."

- ✗ For a single fit to a single set of data or pseudo-data, this is true.

  MINUIT determines the covariance matrix by sampling the chi2 response functions in each eigenvector direction. This results in a per-fit estimate of uncertainty size.

- ✗ However, **all** of your pseudo-experiments are drawn from the systematic uncertainty priors that you've supplied.

  If you specify 100% uncertainty when you really mean 20%, your LLR distributions will be 5x wider than they should. Thus, your sensitivity is necessarily degraded.



Fit Quality Testing

An important issue for users to understand

Collie runs fixed algorithms designed for a broad range of HEP problems. In the case of fitting, Collie makes the implicit assumption that the user has constructed an appropriate fit model. Thus, it is the user's responsibility to generate and understand their backgrounds, systematics, and correlations.

Testing your Fit

- ✗ The Collie fitting test can be performed after CollieIO file creation
  - Just the additional lines to be added to the example calculations.
  - The fit test can be run at the same time as the calculation, but I recommend testing before calculating.

```
#include <FitTest.hh>

//Add before the masspoint loop
FitTest fitTest;
fitTest.setIterations(2000);   //Determines how many trials will be run in the test
fitTest.testPE(true);          //Toggles whether to test pseudo-experiments


//Add inside the masspoint loop
fitTest.runTest(sbd,sigLLRcut);   //Pass the SigBkgdDist you want to test.  Appending is OK.
                                  //The "sigLLRcut" is the same cutoff used by CLfit.  If
                                  //you're not using CLfit, then you can ignore this.
```

- ✗ The fit test creates an output file with information about your fit
  - Global information about the input channels
  - Response information from MINUIT about fit convergence
  - "Best fit" values for all your nuisance parameters when fit to data
  - Individual nuisance parameter response and pull functions

Testing your Fit

✗ Examine your fit test results using the macro

collie/limit/macro/fitResults.C

==>Detailed instructions are included inside the macro

```
>> root -l
root [0] .L fitResults.C
root [1] makePlots("fitTest.root")
Before fit=========>  Sig: 335.7244, Bkgd: 12051.4437, Data: 12437.0
After S+B fit=====>  Sig: 245.7548, Bkgd: 12187.0099, Data: 12437.0
After B-Only fit==>  Sig: 341.4754, Bkgd: 12427.3283, Data: 12437.0
Sideband data: 9171, Ignored data: 3266
Sideband bins: 27, Ignored bins: 23
```

✗ Basic report includes:

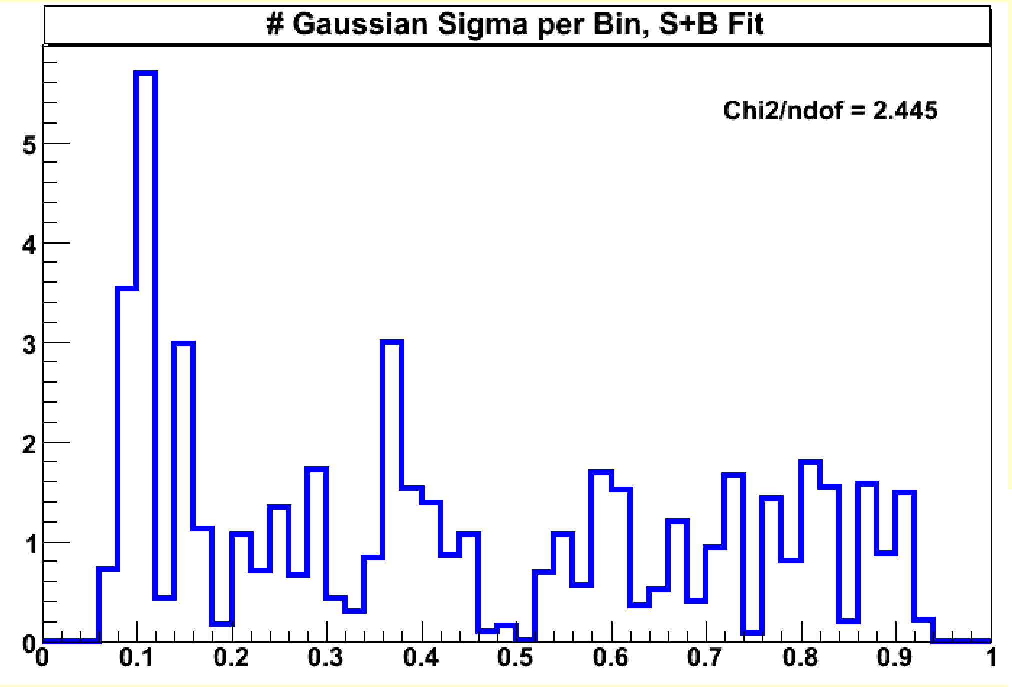
Sig, Bkgd, & Data integrals before and after fitting

Data integral that would be included/ignored in a CLfit (single-fit) calculation

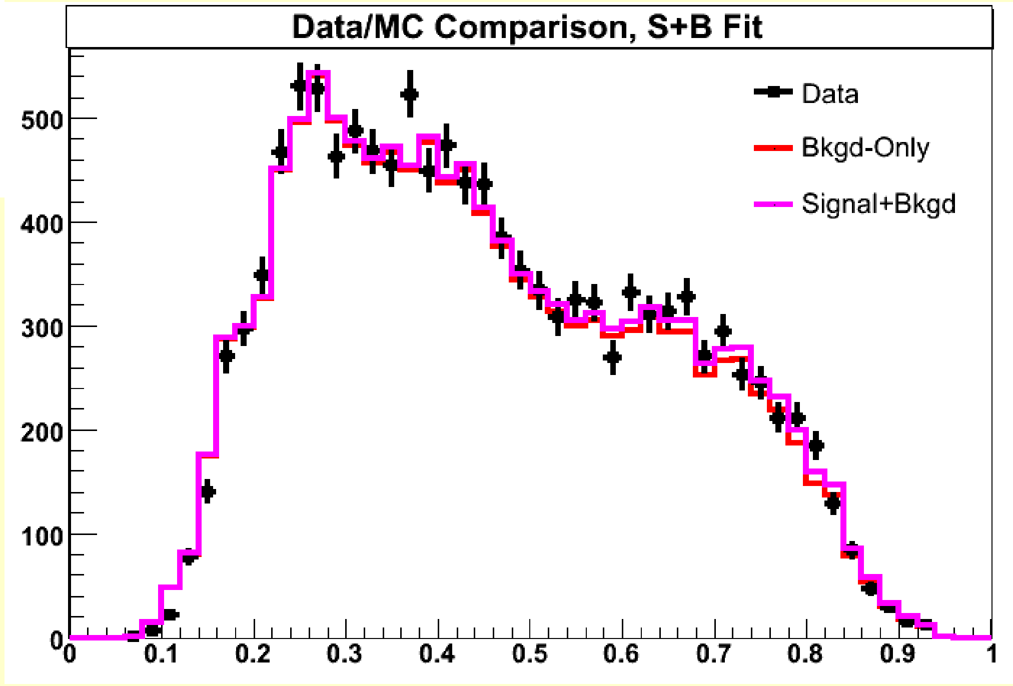
Bins that would be included/ignored in a CLfit (single-fit) calculation

Testing your Fit

✗ Input Distribution Diagnostics



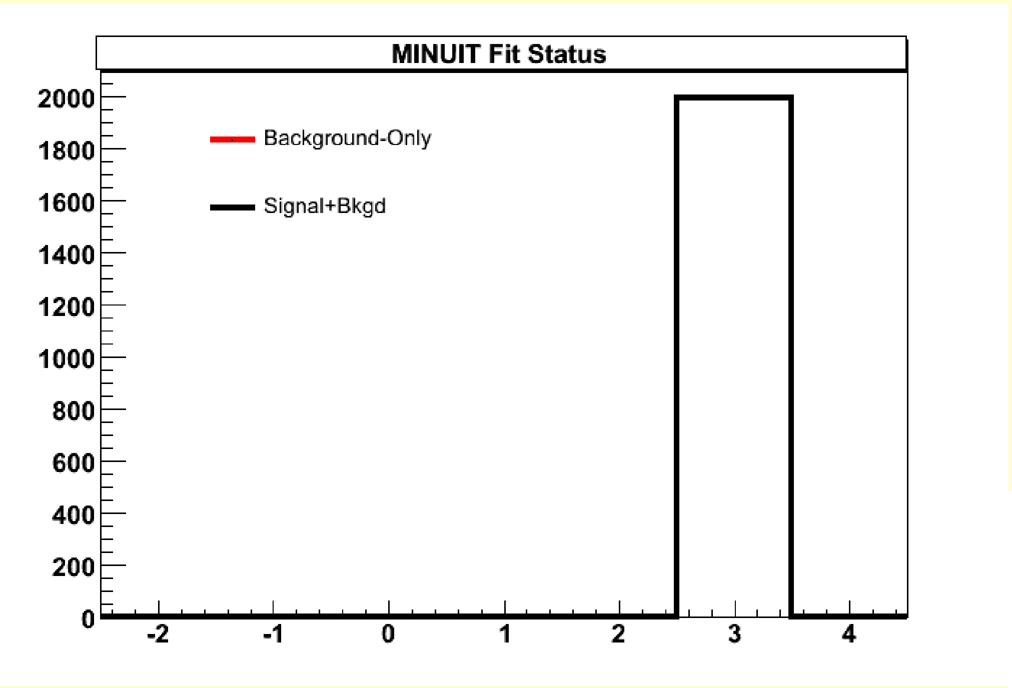
Comparison of input distributions: Background, Signal+Bkgd, & Data



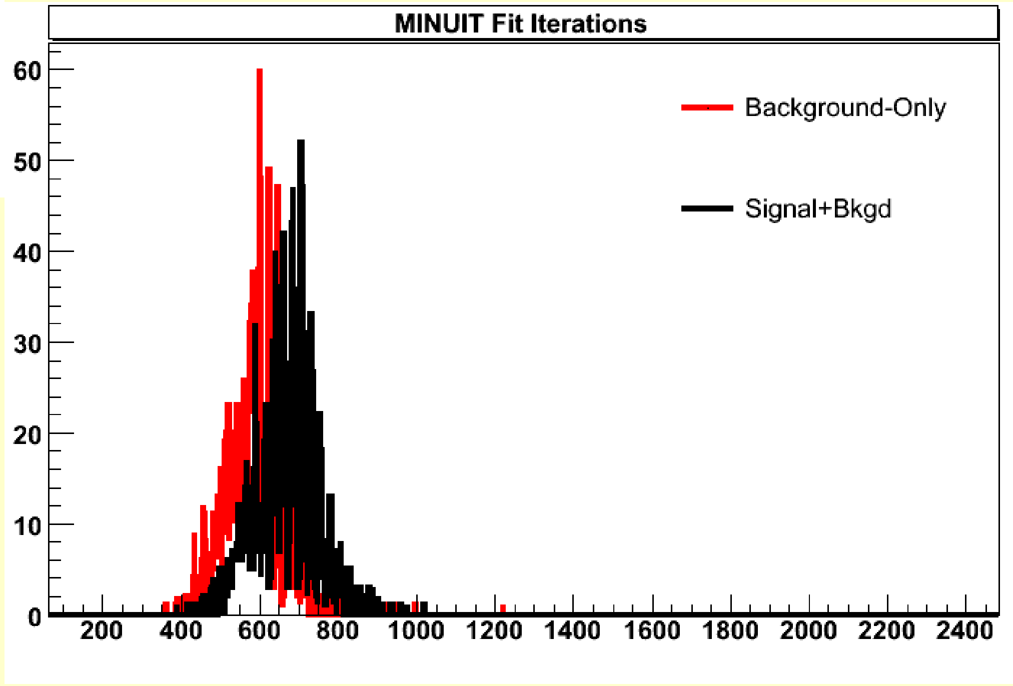
Report on # of Gaussian sigmas per bin compared to data. Available before and after fits.

Testing your Fit

✗ MINUIT Diagnostics



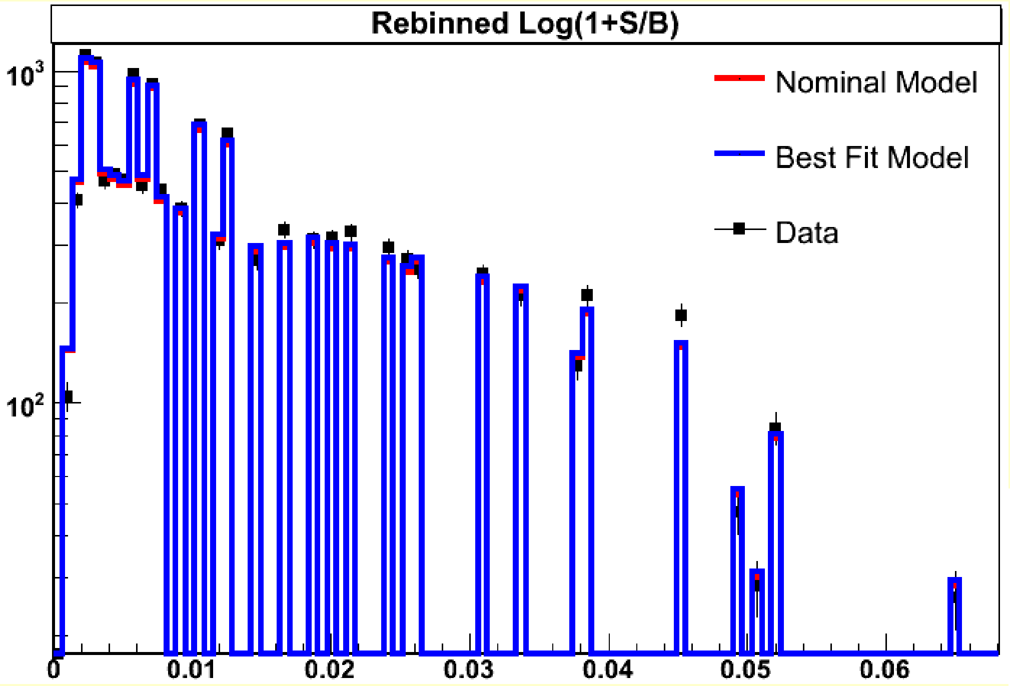
Number of MINUIT iterations required for convergence. S+B fit should take a bit more.



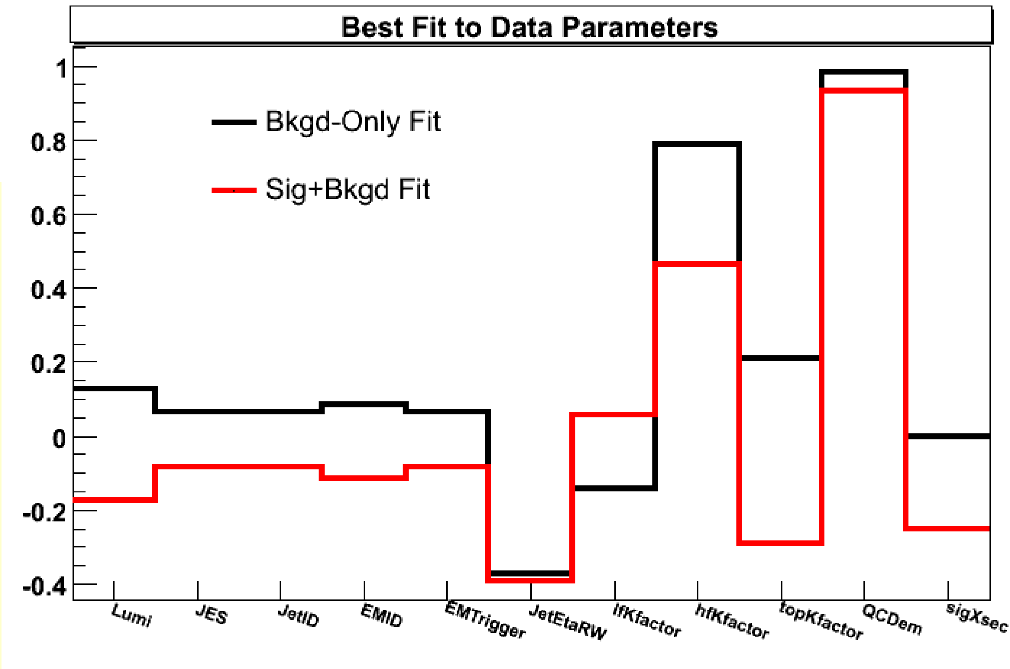
MINUIT fit status. Anything other than 3 is bad news....

Testing your Fit

✗ Fit diagnostics



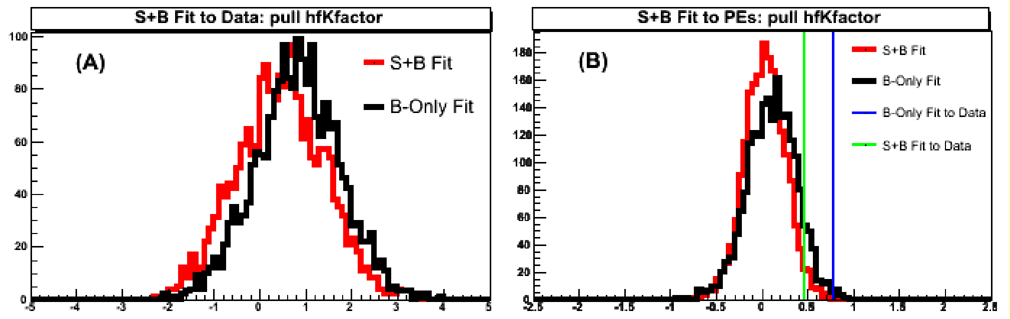
Best fit central values for nuisance parameters. Reported in units of N-sigma.

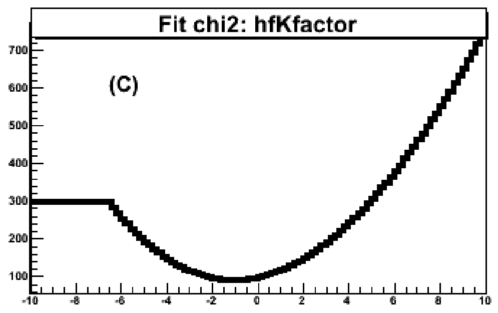


Histogram of Log(1+S/B) for data, nominal background, best fit background, and data.

Testing your Fit

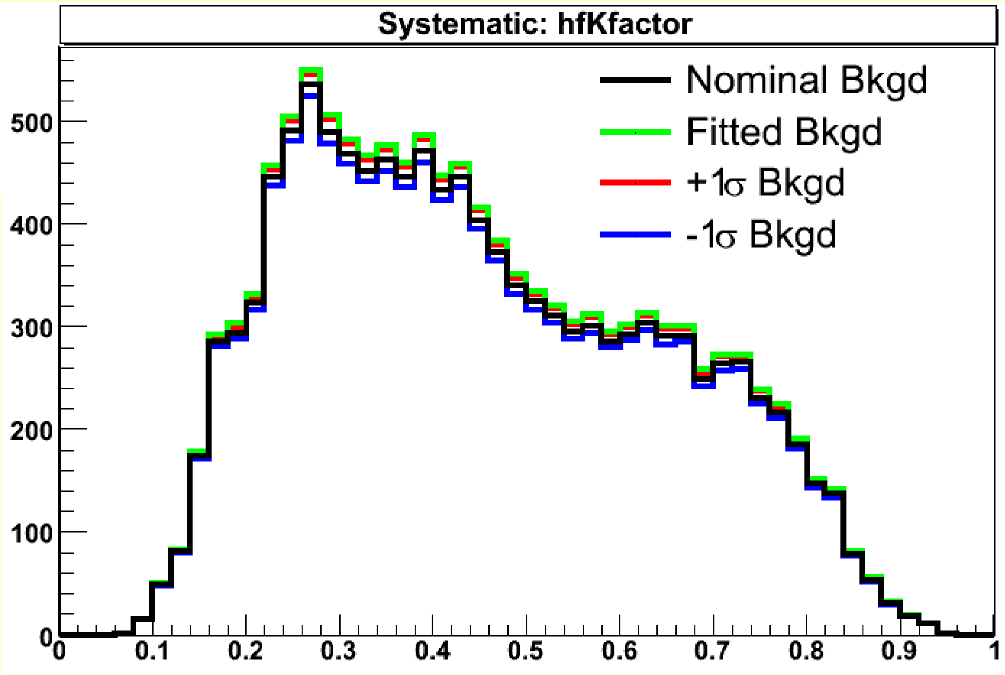
✗ Per-systematic diagnostics





(A) Smeared Fit to Data
Mean: 0.830
Width: 0.909
(B) Fit to PseudoData
Mean: 0.116
Width: 0.260
(C) χ^2 Response Function
Minimum: -1.00
RMS: 0.398

Comparison of nominal, best fit, and +/- 1 sigma fluctuations.

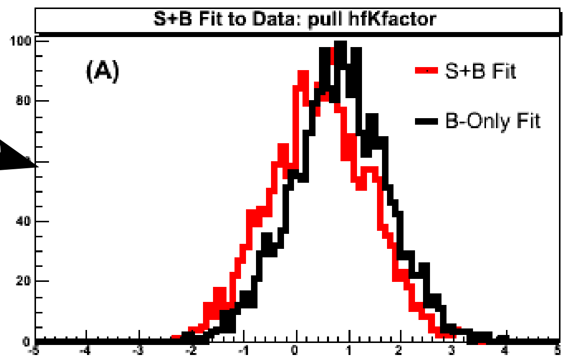


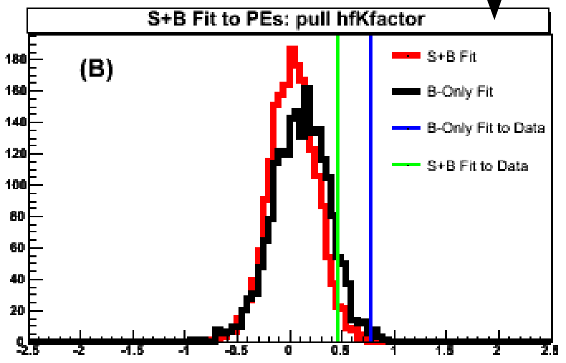
Pull functions for smeared MC fits to data (A), nominal MC fits to pseudo-experiments (B), 1-D floating Chi2 response function (C), and associated statistics.

Testing your Fit

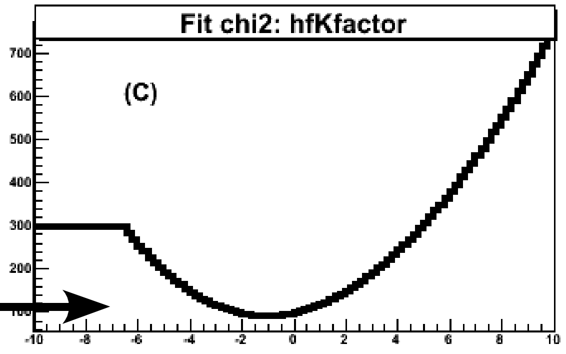
Pull function for fits to data: An N-dimensional systematic test. By injecting unit Gaussian (or log-normal) distributions, this plot shows the resulting distribution of systematic values after fitting to data. 1sigma in and 1sigma out means no constraint in data. Widths less than 1.0 indicate a data-driven constraint on the systematic.

Pull function for fits to pseudo-data: An N-dimensional systematic test. Nominal MC is fit to pseudo-experiments. This plot indicates how much each systematic is being moved to accommodate the range of pseudo-experiment outcomes. Vary narrow pulls usually correspond to a flat chi2 response (see below).





The chi2 response function: while holding all other systematics fixed, vary this parameter from -N sigma to +N sigma. Curvature provides info on how much of this change your data will accommodate. Location of minimum provides info on relative data/MC agreement.



(A) Smeared Fit to Data

Mean: 0.830

Width: 0.909

(B) Fit to PseudoData

Mean: 0.116

Width: 0.260

(C) χ^2 Response Function

Minimum: -1.00

RMS: 0.398

Tips & Tricks

- ✗ Speeding things up:
  1) You can calculate expected and observed limits in separate jobs. Recombine output files with collie/examples/resultsFileCombiner.exe:

  ./resultsFileCombiner.exe newFile.root listOfExpFiles.txt listOfObsFiles.txt

  2) When fitting, MINUIT's Fortran code needs to output messages (fort.99 file). You can speed up I/O by creating a symbolic link to /dev/null: **ln -s /dev/null fort.99**
  3) Collie's search algorithm starts at a signal rate of 0.75. If your limit will be far from this, you can speed up the search by seeding with a value close to what you might expect

```
// This is the class for computing cross section limits
CrossSectionLimit csLim;
csLim.setup(&clcompute);          //Pass in the computer you chose
csLim.setSearchSeed(10);          //Speed things up if your limit will be closer to 10 than 1
```

- ✗ Use baby steps to understand how your inputs behave with fitting:
  1) Start with CLfast: check limits and LLR plots. Do things look OK?
  2) Next try CLsyst: check limits and LLR plots. Still OK?
  3) RUN A FIT TEST!! Do things look sensible?
  4) Run with CLfit2: check limits and LLR plots for compatibility with (1) & (2)

Wrap Up

- ✗ Collie is a software package for the statistical treatment for a system of N compound analysis channels with implicit correlations amongst uncertainties on nuisance parameters
  - Documented via DZero note (#4975 & #5309) *...not complete...*
  - Available within DZero CVS
  - *Examples available within the package*
- ✗ Statistics EB review of Collie will hopefully be done very, very soon

- ✗ Users are encouraged to get started using Collie
  - Try to not use as a "black box". Knowing what to expect will help eliminate mistakes.
  - Expect EBs to want to see sensible results from Collie's fitting tests!
  - Feedback and questions are very welcome.