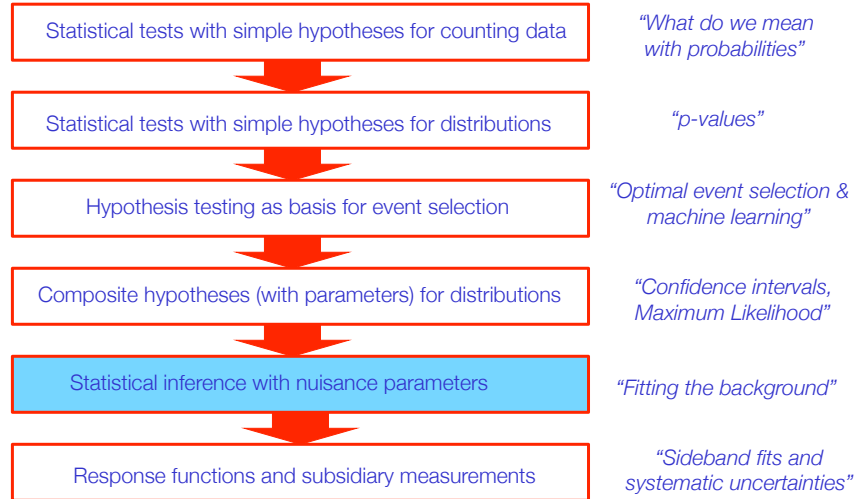


Next subject...

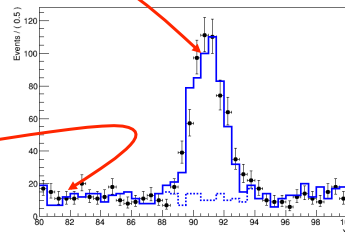
- Start with basics, gradually build up to complexity of



So far we've only considered the *ideal* experiment

- The “only thing” you need to do (as an experimental physicist) is to formulate the likelihood function for your measurement
- For an ideal experiment, where signal and background are assumed to have perfectly known properties, this is trivial

$$L(\vec{N} | \mu) = \prod_{bins} Poisson(N_i | \mu \cdot \tilde{s}_i + \tilde{b}_i)$$



- So far only considered a single parameter in the likelihood: the physics *parameter of interest*, usually denoted as μ

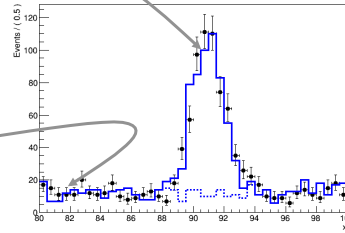
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The imperfect experiment

- In realistic measurements many effect that we don't control exactly influence measurements of parameter of interest
- How do you model these uncertainties in the likelihood?

$$L(\vec{N} | \mu) =$$

$$\prod_{bins} Poisson(N_i | \mu \cdot \tilde{s}_i + \tilde{b}_i)$$



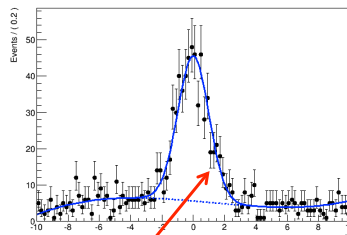
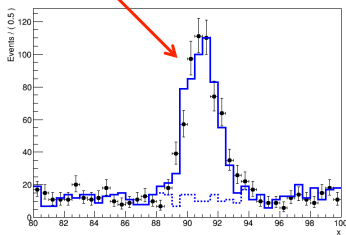
Signal and background predictions are affected by (systematic) uncertainties

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Adding parameters to the model

- We can describe uncertainties in our model by adding new parameters of which the value is uncertain

$$L(\vec{N} | \mu) = \prod_{bins} Poisson(N_i | \mu \cdot \tilde{s}_i + \tilde{b}_i)$$



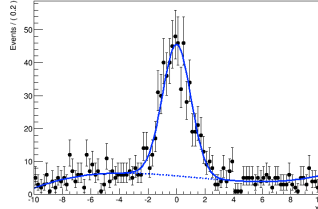
$$L(x | f, m, \sigma, a_0, a_1, a_2) = fG(x, m, \sigma) + (1 - f)Poly(x, a_0, a_1, a_2)$$

- These additional model parameters are not 'of interest', but we need them to model uncertainties → 'Nuisance parameters'

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What are the nuisance parameters of your *physics model*?

- *Empirical modeling of uncertainties*, e.g. polynomial for background, Gaussian for signal, is easy to do, but may lead to hard questions



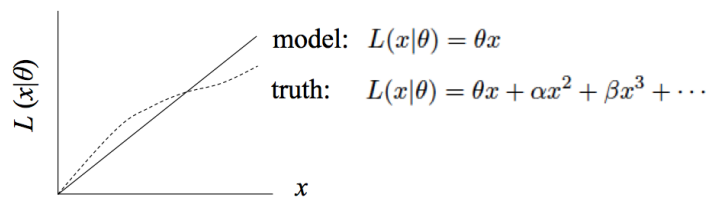
$$L(x|f, m, \sigma, a_0, a_1, a_2) = fG(x, m, \sigma) + (1-f)Poly(x, a_0, a_1, a_2)$$

- **Is your model correct?** (Is true signal distr. captured by a Gaussian?)
- **Is your model flexible enough?** (4th order polynomial, or better 6th?)
- **How do model parameters connect to known detector/theory uncertainties in your distribution?**
 - what conceptual uncertainty do your parameters represent?

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The statisticians view on nuisance parameters

- In general, our model of the data is not perfect



- Can improve modeling by including additional adjustable parameters
- Goal: **some point in the parameter space of the enlarged model should be "true"**
- Presence of nuisance parameters decreases the sensitivity of the analysis of the parameter(s) of interest

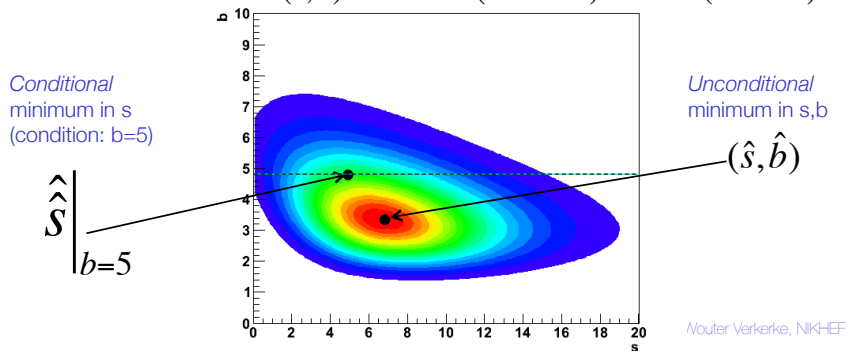
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Treatment of nuisance parameters in parameter estimation

- In POI parameter estimation, the effect of NPs incorporated through *unconditional minimization*
 - I.e. minimize Likelihood w.r.t all parameter simultaneously.
- Simple example with 2-bin Poisson counting experiment

$$L(s) = \text{Poisson}(10 | s + 5)$$

$$L(s, b) = \text{Poisson}(10 | s + b) \text{Poisson}(10 | 3 \cdot b)$$



Treatment of nuisance parameters in variance estimation

- Maximum likelihood estimator of parameter variance is based on 2nd derivative of Likelihood
 - For multi-parameter problems this 2nd derivative is generalized by the **Hessian Matrix** of partial second derivatives

$$\hat{\sigma}(p)^2 = \hat{V}(p) = \left(\frac{d^2 \ln L}{d^2 p} \right)^{-1} \Rightarrow \hat{\sigma}(p_i)^2 = \hat{V}(p_{ii}) = (H^{-1})_{ii}$$

$$H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \dots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \dots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \dots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

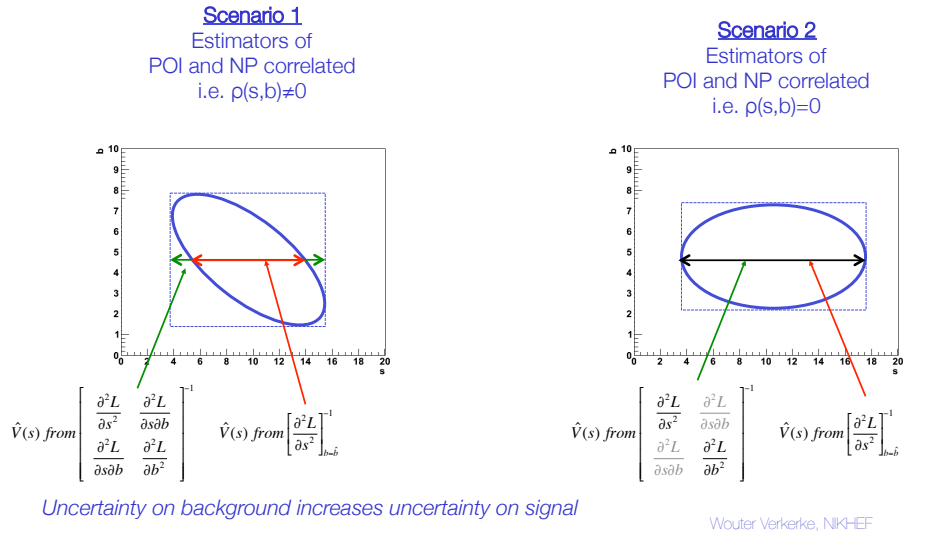
- For multi-parameter likelihoods estimate of **covariance** V_{ij} of pair of 2 parameters in addition to variance of individual parameters
 - Usually re-expressed in terms dimensionless correlation coefficients ρ

$$V_{ij} = \rho_{ij} \sqrt{V_{ii} V_{jj}}$$

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Treatment of nuisance parameters in variance estimation

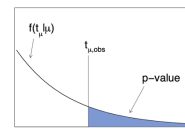
- Effect of NPs on variance estimates visualized



Treatment of NPs in hypothesis testing and conf. intervals

- We've covered frequentist hypothesis testing and interval calculation using likelihood ratios based on a likelihood with a single parameter (of interest) $L(\mu)$
 - Result is p-value on hypothesis with given μ value, or
 - Result is a confidence interval $[\mu_-, \mu_+]$ with values of μ for which p-value is at or above a certain level (the confidence level)
- How do you do this with a likelihood $L(\mu, \theta)$ where θ is a nuisance parameter?
 - With a test statistics q_μ , we calculate p-value for hypothesis θ as

$$p_\mu = \int_{q_{\mu, obs}}^{\infty} f(q_\mu | \mu, \theta) dq_\mu$$



- But what values of θ do we use for $f(q_\mu | \mu, \theta)$?
Fundamentally, we want to reject μ only if $p < \alpha$ for all θ
→ Exact confidence interval

Hypothesis testing & conf. intervals with nuisance parameters

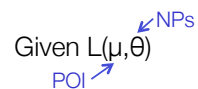
- The goal is that the parameter of interest should be covered at the stated confidence **for every value of the nuisance parameter**
- if there is **any value** of the nuisance parameter which makes the data consistent with the parameter of interest, that value of the POI should be considered:
 - e.g. don't claim discovery if any background scenario is compatible with data
- But: technically very challenging and significant problems with over-coverage
 - Example: **how broadly should 'any background scenario' be defined?** Should we include background scenarios that are clearly incompatible with the observed data?

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The profile likelihood construction as compromise

- For LHC the following prescription is used:

Given $L(\mu, \theta)$



perform hypothesis test for each value of μ (the POI),

using values of nuisance parameter(s) θ that best fit the data under the hypothesis μ

- Introduce the following notation

$\hat{\theta}(\mu)$ M.L. estimate of θ for a given value of μ
(i.e. a conditional ML estimate)

- The resulting confidence interval will have exact coverage for the points $(\mu, \hat{\theta}(\mu))$
 - Elsewhere it may overcover or undercover (but this can be checked)

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The profile likelihood ratio

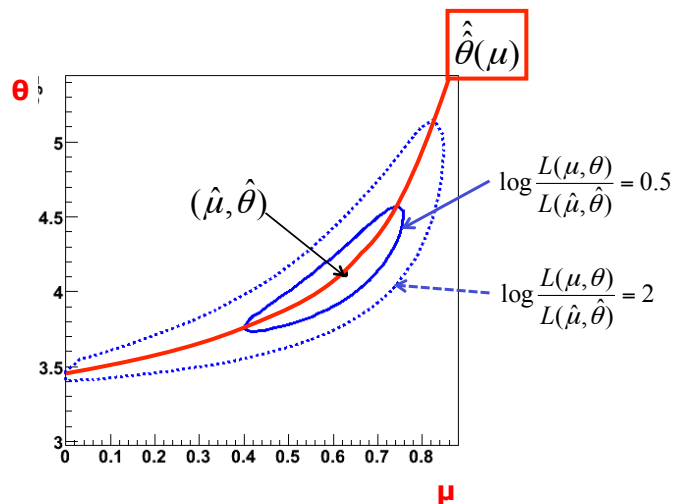
- With this prescription we can construct the **profile likelihood ratio** as test statistic

$$\begin{array}{ccc}
 \text{Likelihood for given } \mu & & \text{Maximum Likelihood for given } \mu \\
 \lambda(\mu) = \frac{L(\mu)}{L(\hat{\mu})} & \xrightarrow{\text{green arrow}} & \lambda(\mu) = \frac{L(\mu, \hat{\theta}(\mu))}{L(\hat{\mu}, \hat{\theta})} \\
 \text{Maximum Likelihood} & & \text{Maximum Likelihood}
 \end{array}$$

- NB: value profile likelihood ratio does *not* depend on θ

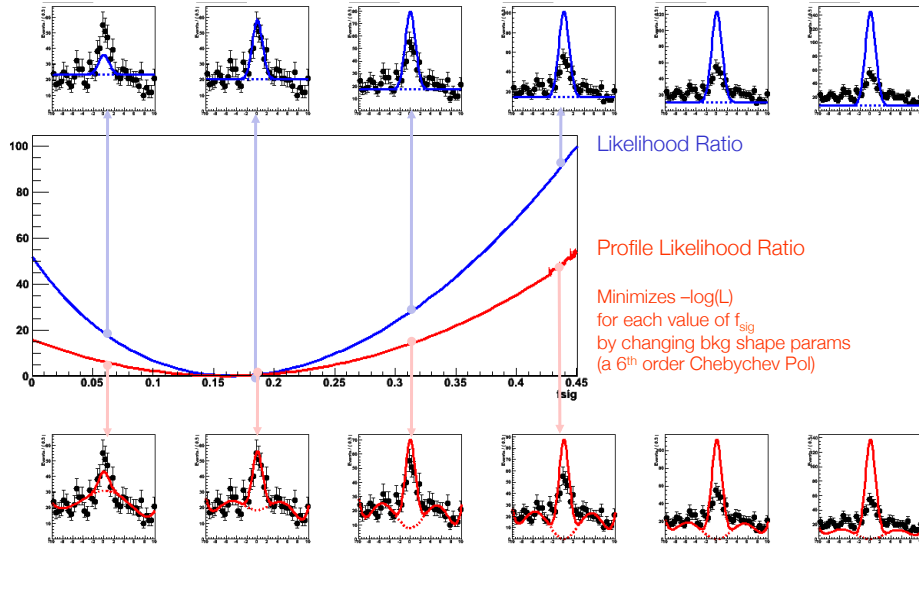
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Profiling illustration with one nuisance parameter

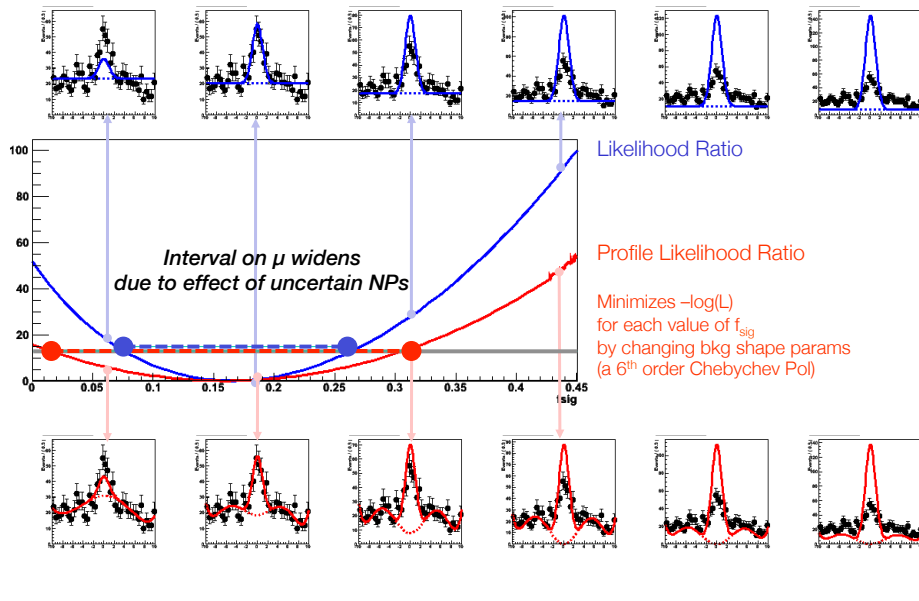


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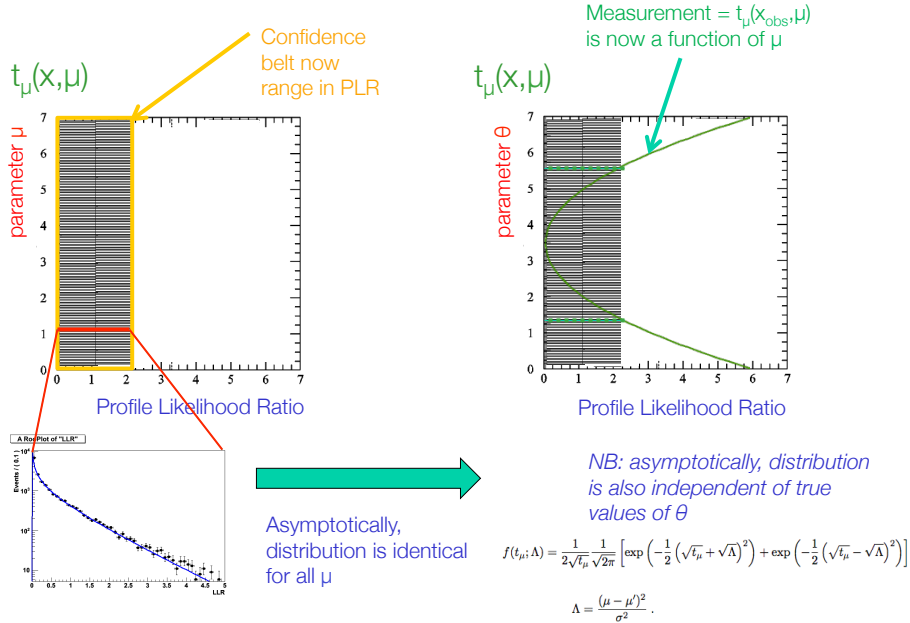
Profile scan of a Gaussian plus Polynomial probability model



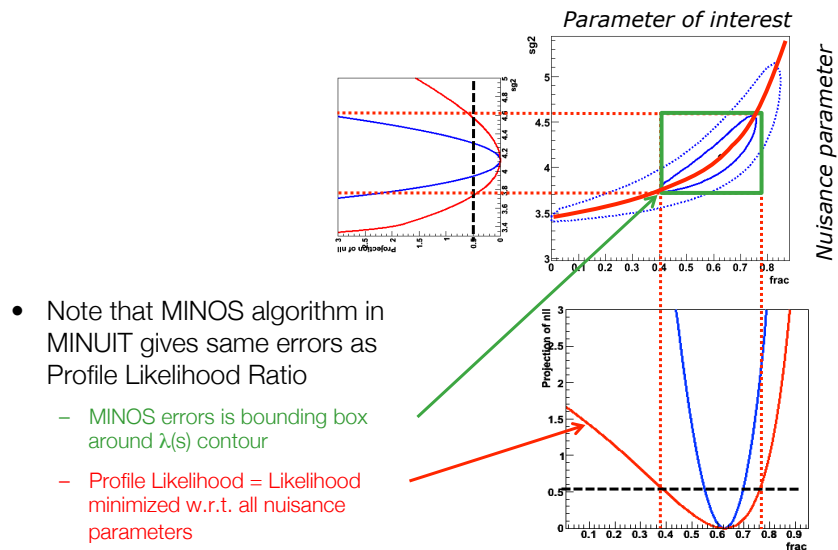
Profile scan of a Gaussian plus Polynomial probability model



PLR Confidence interval vs MINOS



Link between MINOS errors and profile likelihood



- Note that MINOS algorithm in MINUIT gives same errors as Profile Likelihood Ratio
 - MINOS errors is bounding box around $\lambda(s)$ contour
 - Profile Likelihood = Likelihood minimized w.r.t. all nuisance parameters

NB: Similar to graphical interpretation of variance estimators, but those always assume an elliptical contour from a perfectly parabolic likelihood

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Summary on NPs in confidence intervals

- Exact confidence intervals are difficult with nuisance parameters
 - Interval should cover for any value of nuisance parameters
 - Technically difficult and significant over-coverage common
- LHC solution Profile Likelihood ratio → Guaranteed coverage at *measured* values of nuisance parameters only
 - Technically replace likelihood ratio with profile likelihood ratio
 - Computationally more intensive (need to minimize likelihood w.r.t all nuisance parameters for each evaluation of the test statistic), but still very tractable
- Asymptotically confidence intervals constructed with profile likelihood ratio test statistics correspond to (MINOS) likelihood ratio intervals
 - As distribution of profile likelihood becomes asymptotically independent of θ , coverage for all values of θ restored

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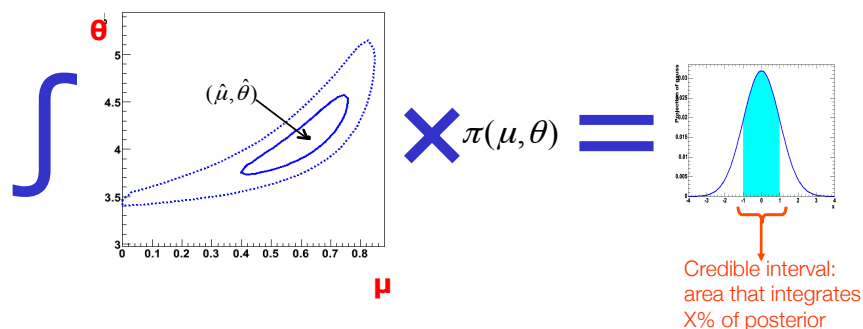
Dealing with nuisance parameters in Bayesian intervals

- Elimination of nuisance parameters in Bayesian interval: **Integrate over the full subspace of all nuisance parameters;**

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

$$P(\mu | x) \propto \int (L(x | \mu, \vec{\theta}) \pi(\mu) \pi(\vec{\theta})) d\vec{\theta}$$

- You are left with posterior pdf for μ



Computational aspects of dealing with nuisance parameters

- Dealing with many nuisance parameters is computationally intensive in both Bayesian and (LHC) Frequentist approach
- Profile Likelihood approach
 - Computational challenge = **Minimization** of likelihood w.r.t. all nuisance parameters for every point in the profile likelihood curve
 - Minimization can be a difficult problem, e.g. if there are strong correlations, or multiple minima
- Bayesian approach
 - Computational challenge = **Integration** of posterior density of all nuisance parameters
 - Requires sampling of very potentially very large space.
 - Markov Chain MC and importance sampling techniques can help, but still very CPU consuming

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Other procedures that have been tried*

- Hybrid Frequentist-Bayesian approach ('Cousins-Highland / Z_N ')
 - Integrate likelihood over nuisance parameters

$$L_m(\mu) = \int \left(L(\mu, \vec{\theta}) \pi(\vec{\theta}) \right) d\vec{\theta}$$

- Then treat integrated L_m as test statistic \rightarrow obtain p-value from its distribution
- In practice integral is performed using MC integration, so often described as a 'sampling method'

$$L_m(\mu) = \frac{1}{N} \sum_{MC} L(\mu, \vec{\theta}_i) \pi(\vec{\theta}_i)$$

- Method has been shown to have bad coverage

- Ad-hoc sampling methods of various types.
 - Usually amount to either MC integration or fancy error propagation

Note that sampling the conditional estimator $\hat{\mu} \Big|_{\theta}$ over sample of θ values obtained from $\pi(\theta)$ is just glorified error propagation!

* But are known to have problems

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How much do answers differ between methods?

A Prototype Problem

What is significance Z of an observation $x = 178$ events in a signal like region, if my expected background $b = 100$ with a 10% uncertainty?

- if you use the ATLAS TDR formula $Z_5 = 5.5$
- if you use Cousins-Highland $Z_N = 5.0$

The question seems simple enough, but it is not actually well-posed

- what do I mean by 10% background uncertainty?

Typically, we consider an auxiliary measurement y used to estimate background (Type I systematic)

- eg: a sideband counting experiment where background in sideband is a factor τ bigger than in signal region

$$L_P(x, y | \mu, b) = \text{Pois}(x | \mu + b) \cdot \text{Pois}(y | \tau b)$$

Kyle Cranmer (BNL)

PhyStat 2007, CERN, June 26, 2007

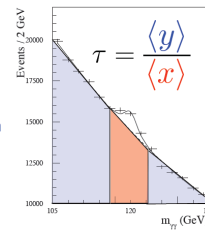
These slide discuss a 'prototype' likelihood that statisticians like:

$$\text{Poisson}(N_{\text{sig}} | s+b) \cdot \text{Poisson}(N_{\text{ctrl}} | \tau \cdot b)$$

NB: This is one of the very few problems with nuisance parameters with can be exactly calculation

Example Sideband Measurement

Sideband measurement used to extrapolate / interpolate the background rate in signal-like region



For now ignore uncertainty in extrapolation.

$$L_P(x, y | \mu, b) = \text{Pois}(x | \mu + b) \cdot \text{Pois}(y | \tau b)$$

Kyle Cranmer (BNL)

PhyStat 2007, CERN, June 26, 2007

Recent comparisons results from PhyStat 2007

Comparison of Methods for Prototype Problem

In my contribution to PhyStat2005, I considered this problem and compared the coverage for several methods

- See Linnemann's PhyStat03 paper

Major results:

- Cousins-Highland result (Z_N) badly under-covers (only 4.2σ !)
 - rate of Type I error is 110 times higher than stated!
 - much less luminosity required

Profile Likelihood Ratio (MINUIT/MINOS) works great out to 5σ !

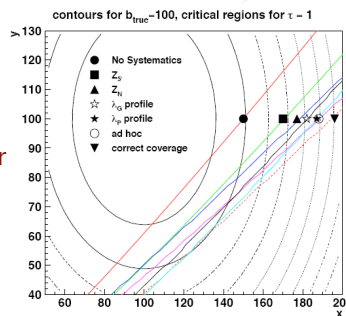


Figure 7. A comparison of the various methods critical boundary $x_{crit}(y)$ (see text). The concentric ovals represent contours of L_G from Eq. 15.

Method	$L_G (Z\sigma)$	$L_P (Z\sigma)$	$x_{crit}(y=100)$
No Syst	3.0	3.1	150
Z_5	4.1	4.1	171
Z_N (Sec. 4.1)	4.2	4.2	178
ad hoc	4.6	4.7	188
$Z_{\tau} = Z_{B_5}$	4.9	5.0	185
profile λ_P	5.0	5.0	185
profile λ_G	4.7	4.7	~ 182

Exact solution

Kyle Cranmer (BNL)

Statistics Forum, May 11, 2007

15

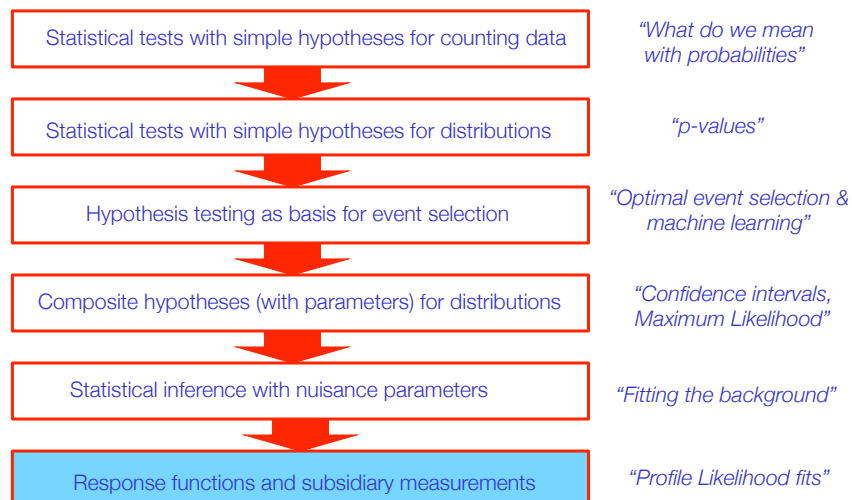
Summary of statistical treatment of nuisance parameters

- Each statistical method has an associated technique to propagate the effect of uncertain NPs on the estimate of the POI
 - Parameter estimation → Joint unconditional estimation
 - Variance estimation → Replace d^2L/dp^2 with Hessian matrix
 - Hypothesis tests & confidence intervals → Use profile likelihood ratio
 - Bayesian credible intervals → Integration ('Marginalization')
- Be sure to use the right procedure with the right method
 - Anytime you integrate a Likelihood you are a Bayesian
 - If you are minimizing the likelihood you are usually a Frequentist
 - If you sample something chances are you performing either a (Bayesian) Monte Carlo integral, or are doing glorified error propagation
- Answers can differ substantially between methods!
 - This is not always a problem, but can also be a consequence of a difference in the problem statement

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Overview

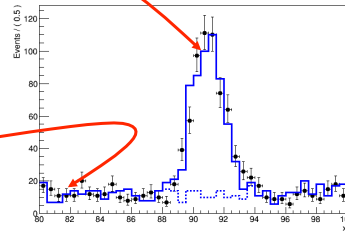
- Start with basics, gradually build up to complexity of



The *ideal* experiment

- The “only thing” you need to do (as an experimental physicist) is to formulate the likelihood function for your measurement
- For an ideal experiment, where signal and background are assumed to have perfectly known properties, this is trivial

$$L(\vec{N} | \mu) = \prod_{bins} Poisson(N_i | \mu \cdot \tilde{s}_i + \tilde{b}_i)$$



- Only a single* parameter in the likelihood: the physics *parameter of interest*, usually denoted as μ

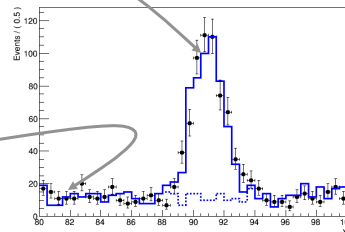
*Unless there are of course multiple POIs...

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The *imperfect* experiment

- In realistic measurements many effect that we don't control exactly influence measurements of parameter of interest
- How do you model these uncertainties in the likelihood?

$$L(\vec{N} | \mu) = \prod_{bins} Poisson(N_i | \mu \cdot \tilde{s}_i + \tilde{b}_i)$$



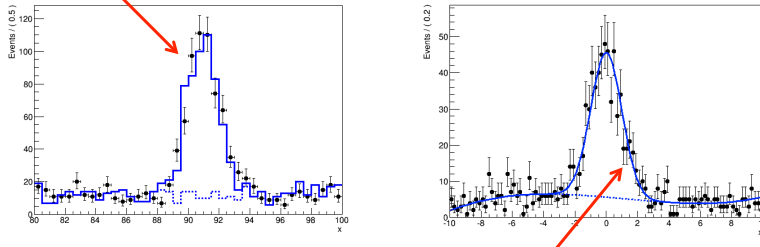
Signal and background predictions are affected by (systematic) uncertainties

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Adding parameters to the model

- But parametric form of detector and theory systematic uncertainties is often, at first sight, elusive

$$L(\vec{N} | \mu) = \prod_{bins} Poisson(N_i | \mu \cdot \tilde{s}_i + \tilde{b}_i)$$

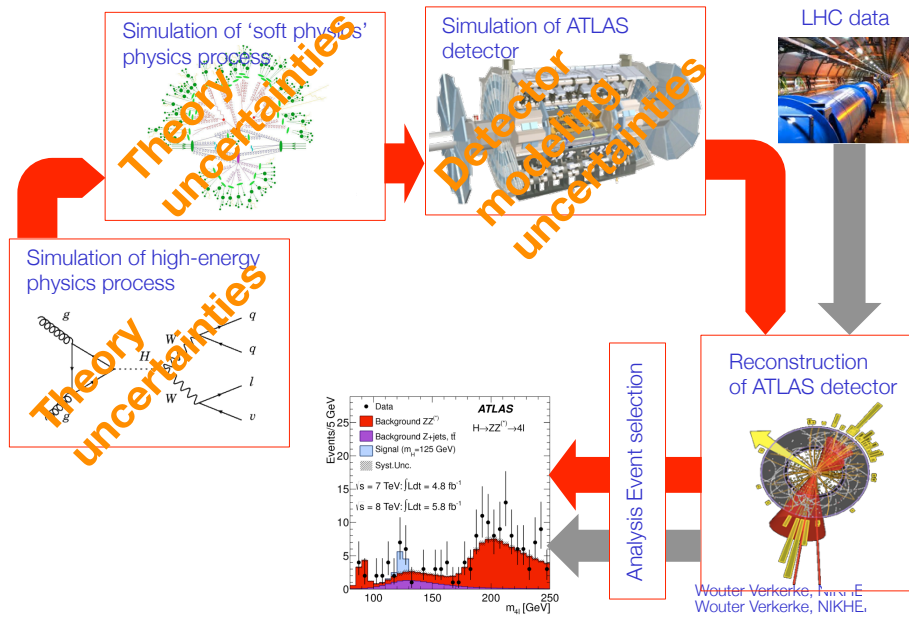


$$L(x | f, m, \sigma, a_0, a_1, a_2) = fG(x, m, \sigma) + (1-f)Poly(x, a_0, a_1, a_2)$$

- Ad-hoc parameterizations (like above) do not necessarily capture all uncertain degrees of freedom, provide no meaningful insight in effect of known systematic uncertainties on the analysis.

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The simulation workflow and origin of uncertainties



Typical systematic uncertainties in HEP

- **Detector-simulation related**
 - “The Jet Energy scale uncertainty is 5%”
 - “The b-tagging efficiency uncertainty is 20% for jets with $p_T < 40$ ”
- **Physics/Theory related**
 - The top cross-section uncertainty is 8%
 - “Vary the factorization scale by a factor 0.5 and 2.0 and consider the difference the systematic uncertainty”
 - “Evaluate the effect of using Herwig and Pythia and consider the difference the systematic uncertainty”
- **MC simulation statistical uncertainty**
 - Effect of (bin-by-bin) statistical uncertainties in MC samples

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What can you do with *systematic* uncertainties

- As most of the typical systematic prescriptions **have no immediately apparent parametric formulation in your likelihood**, common approach is ‘vary setting, rerun analysis, observe the difference’
- This common ‘naïve’ approach to assess effect of systematic uncertainties amounts to simple error propagation
- Error propagation procedure in a nutshell
 - Make nominal measurement (using your favorite statistical inference procedure)
 - Change setting in detector simulation or theory (e.g. shift Jet Calibration scale by ‘1 sigma’ up and down) Redo measurement procedure for each shift
 - Consider propagated effect of shifted setting the systematic uncertainty

$$\mu = \underbrace{\mu_{nom} \pm \sigma_{stat}}_{\text{From statistical analysis}} \pm \underbrace{(\mu_{syst}^{up} - \mu_{syst}^{down}) / 2}_{\text{Systematic uncertainty from error propagation}} \pm \dots$$

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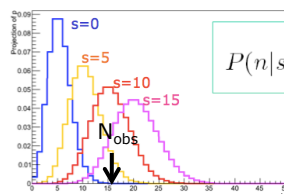
Pros and cons of the 'naïve' approach

- **Pros**
 - It's easy to do
 - It results in a seemingly easy-to-interpret table of systematics
- **Cons**
 - Uncorrelated source of systematic uncertainty can have correlated effect on measurement → **Completely ignored**
 - Magnitude of stated systematic uncertainty may be incompatible with measurement result → **Completely ignored**
 - **You lost the connection with fundamental statistical techniques** (i.e. evaluation of systematic uncertainties is completely detached from statistical procedure used to estimate physics quantity of interest) → **No prescription to make confidence intervals, Bayesian posteriors etc in this way**
 - No calibrated probabilistic statements possible (95% C.L.)
- 'Profiling' → Incorporate a description of systematic uncertainties in the likelihood function that is used in statistical procedures

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Everything starts with the likelihood

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



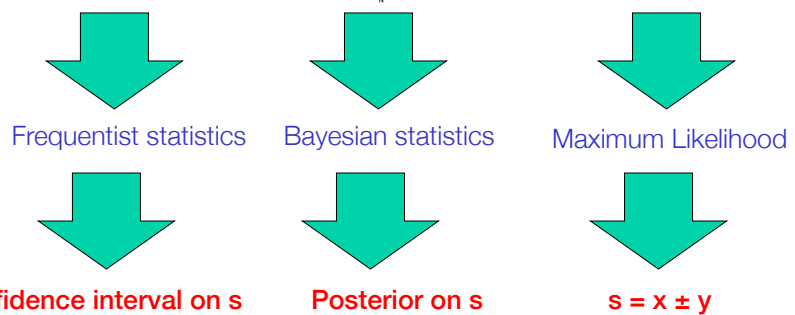
$$P(n|s+b) = \frac{(s+b)^n}{n!} e^{-(s+b)}$$

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)



Confidence interval on s

Posterior on s

s = x ± y

Everything starts with the likelihood

Frequentist statistics

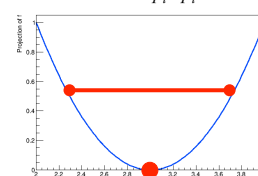
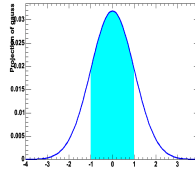
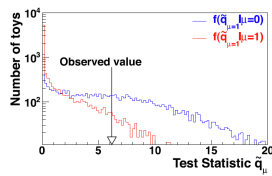
Bayesian statistics

Maximum Likelihood

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

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

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



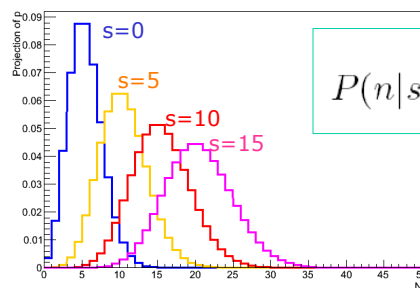
Confidence interval
or p-value

Posterior on s
or Bayes factor

$s = x \pm y$
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Introducing uncertainties – a non-systematic example

- The original model (with fixed b)



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

- Now consider b to be uncertain

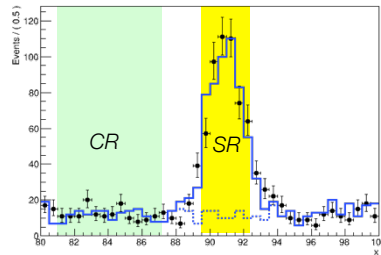
$$L(N|s) \rightarrow L(N|s,b)$$

- The experimental data contains insufficient to constrain both s and $b \rightarrow$ Need to add an additional measurement to constrain b

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The sideband measurement

- Suppose your data in reality looks like this →



Can estimate level of background in the 'signal region' from event count in a 'control region' elsewhere in phase space

$$L_{SR}(s, b) = \text{Poisson}(N_{SR} | s + b)$$

NB: Define parameter 'b' to represent the amount of bkg in the SR.

$$L_{CR}(b) = \text{Poisson}(N_{CR} | \tilde{\tau} \cdot b)$$

Scale factor τ accounts for difference in size between SR and CR

"Background uncertainty constrained from the data"

- Full likelihood of the measurement ('simultaneous fit')

$$L_{full}(s, b) = \text{Poisson}(N_{SR} | s + b) \cdot \text{Poisson}(N_{CR} | \tilde{\tau} \cdot b)$$

Generalizing the concept of the sideband measurement

- Background uncertainty from sideband clearly not a 'systematic uncertainty'

$$L_{full}(s, b) = \text{Poisson}(N_{SR} | s + b) \cdot \text{Poisson}(N_{CR} | \tilde{\tau} \cdot b)$$

- Now consider scenario where b is not measured from a sideband, but is taken from MC simulation **with an 8% cross-section 'systematic' uncertainty**

'Measured background rate by MC simulation'

$$L_{full}(s, b) = \text{Poisson}(N_{SR} | s + b) \cdot \text{Gauss}(\tilde{b} | b, 0.08)$$

'Subsidiary measurement' of background rate

- We can model this in the same way, because the cross-section uncertainty is also (ultimately) the result of a measurement*

Generalize: 'sideband' → 'subsidiary measurement'

What is a systematic uncertainty?

- Concept & definitions of 'systematic uncertainties' originates from physics, not from fundamental statistical methodology.
 - E.g. Glen Cowans (excellent) 198pp book "statistical data analysis" does not discuss systematic uncertainties at all
- A common definition is
 - "Systematic uncertainties are all uncertainties that are not directly due to the statistics of the data"
- But the notion of 'the data' is a key source of ambiguity:
 - does it include control measurements?
 - does it include measurements that were used to perform basic (energy scale) calibrations?

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Typical systematic uncertainties in HEP

- **Detector-simulation related**
 - "The Jet Energy scale uncertainty is 5%"
 - "The b-tagging efficiency uncertainty is 20% for jets with $p_T < 40$ "

Subsidiary measurement is an actual measurement
→ conceptually similar to a 'sideband' fit
- **Physics/Theory related**
 - The top cross-section uncertainty is 8%
 - "Vary the factorization scale by a factor 0.5 and 2.0 and consider the difference the systematic uncertainty"
 - "Evaluate the effect of using Herwig and Pythia and consider the difference the systematic uncertainty"

Subsidiary measurement unclear, but origin of prescription may well be another measurement (if yes, like sideband, if no, what is source of info?)
- **MC simulation statistical uncertainty**
 - Effect of (bin-by-bin) statistical uncertainties in MC samples

Subsidiary measurement is a Poisson counting experiment (but now in MC events), otherwise conceptually identical to a 'sideband fit'

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Typical systematic uncertainties in HEP

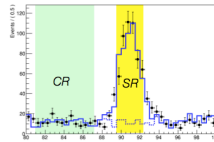
- **Detector-simulation related**
 - "The Jet Energy scale uncertainty is 5%"
 - "The b-tagging efficiency uncertainty is 20%"

Subsidiary measurement is an actual measurement → conceptually to a 'sideband fit'
- **Almost all systematic uncertainties are similar in nature to 'sidebands' measurements of some form or shape**
 - Can always model systematics like sidebands in the Likelihood
 - And even when they are not the (in)direct result of some measurement (certainty theory uncertainties) we can still model them in that form
- **MC simulation statistical uncertainty**
 - Effect of (bin-by-bin) statistical uncertainties in MC samples

Subsidiary measurement is a Poisson counting experiment (but now in MC events), otherwise conceptually identical to a 'sideband fit'

Modeling a detector calibration uncertainty

$$L_{full}(s, b) = \text{Poisson}(N_{SR} | s + b) \cdot \text{Gauss}(\tilde{b} | b, 0.08)$$



- **Now consider a detector uncertainty**, e.g. jet energy scale calibration, which can affect the analysis acceptance in a non-trivial way (unlike the cross-section example)

$$L(N, \tilde{\alpha} | s, \alpha) = \text{Poisson}(N | s + \tilde{b}(\alpha / \tilde{\alpha}) \cdot 2) \cdot \text{Gauss}(\tilde{\alpha} | \alpha, \sigma_{\alpha})$$

Signal rate (our parameter of interest) → $\tilde{b}(\alpha / \tilde{\alpha}) \cdot 2$
 Observed event count → N
 Nominal background expectation from MC (a constant), obtained with $a=\tilde{a}$ → s
 Response function for JES uncertainty (a 1% JES change results in a 2% acceptance change) → $\tilde{b}(\alpha / \tilde{\alpha}) \cdot 2$
 Nominal calibration → α
 Assumed calibration → $\tilde{\alpha}$
 Uncertainty on nominal calibration (here 5%) → σ_{α}
 "Subsidiary measurement" Encodes 'external knowledge' on JES calibration → $\tilde{\alpha}$

Modeling a detector calibration uncertainty

- Simplify expression by renormalizing “subsidiary measurement”

$$L(N | s, \alpha) = \text{Poisson}(N | s + \tilde{b}(1 + 0.1\alpha)) \cdot \text{Gauss}(0 | \alpha, 1)$$

\tilde{b} is highlighted in yellow in the original image.

Signal rate (our parameter of interest) points to $\tilde{b}(1 + 0.1\alpha)$.
Observed event count points to N .
Nominal background expectation from MC (a constant) points to \tilde{b} .
Response function for normalized JES parameter points to $(1 + 0.1\alpha)$.
[a unit change in α – a 5% JES change – still results in a 10% acceptance change] is associated with the response function.
Normalized subsidiary measurement points to $\text{Gauss}(0 | \alpha, 1)$.
The scale of parameter α is now chosen such that values ± 1 corresponds to the nominal uncertainty (in this example 5%) is associated with the Gaussian.

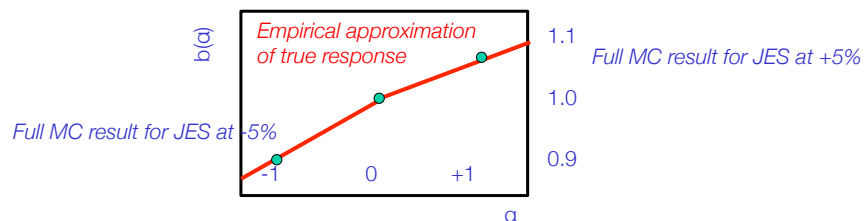
Gauss($\tilde{\alpha} | \alpha, \sigma_\alpha$)

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The response function as empirical model of full simulation

$$L(N, 0 | s, \alpha) = \text{Poisson}(N | s + \underbrace{b(\alpha)}_{\text{response function}}) \cdot \text{Gauss}(0 | \alpha, 1)$$

- Note that the response function is generally not linear, but can in principle *always be determined by your full simulation chain*
 - But you cannot run your full simulation chain for any arbitrary ‘systematic uncertainty variation’ → Too much time consuming
 - Typically, run full MC chain for nominal and $\pm 1\sigma$ variation of systematic uncertainty, and approximate response for other values of NP with interpolation
 - For example run at nominal JES and with JES shifted up and down by $\pm 5\%$



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What is a systematic uncertainty?

- It is an uncertainty in the Likelihood of your physics measurement that is characterized deterministically, up to a set of parameters, of which the true value is unknown.
- A fully specified systematic uncertainty defines
 - 1: A set of one or more parameters of which the true value is unknown,
 - 2: A response model that describes the effect of those parameters on the measurement (*sampled from full simulation, and interpolation*)
 - 3: A subsidiary measurement of the parameters that constrains the values the parameters can take (implies a specific distribution: Gaussian (*default, CLT*), Poisson (*low-stats counting*), or otherwise)

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Names and conventions – ‘profiling’ & ‘constraints’

- The full likelihood function of the form

$$L(N, 0 | s, \alpha) = \text{Poisson}(N | s + b(\alpha)) \cdot \text{Gauss}(0 | \alpha, 1)$$

is usually referred to by physicists as a ‘profile likelihood’, and systematics are said to be ‘profiled’ when incorporated this way

- Note: statisticians use the word profiling for something else
- Physicists often refer to the subsidiary measurement as a ‘constraint term’
 - This is correct in the sense that it constrains the parameter α , but this labeling commonly lead to mistaken statements (e.g. that it is a pdf for α)
 - But it is *not* a pdf in the NP

~~Gauss(α | 0, 1)~~

Gauss(0 | α , 1)
↑

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Names and conventions

- The ‘subsidiary measurement’ as simplified form of the ‘full calibration measurement’ also illustrates another important point
 - The full likelihood is simply a *joint likelihood of a physics measurement and a calibration measurement* where both terms are treated on equal footing in the statistical procedure
 - In a perfect world, not bound by technical modelling constraints you would use this likelihood

$$L(N, \bar{y} | s, \alpha) = \text{Poisson}(N | s + b(1 + 0.1\alpha)) \cdot L_{JES}(\bar{y} | \alpha, \vec{\theta})$$

where L_{JES} is the full calibration measurement as performed by the Jet calibration group, based on a dataset y , and which may have other parameters θ specific to the calibration measurement.

- Since we are bound by technical constrains, we substitute L_{JES} with simplified (Gaussian) form, but the statistical treatment and interpretation remains the same

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MC statistical uncertainties as systematic uncertainty

- Another example of modeling a systematic uncertainty: MC statistical uncertainty
- Follow same procedure again as before:
 - Define response function (this is trivial for MC statistics: it is the luminosity ratio of the MC sample and the data sample)
 - Define distribution for the ‘subsidiary measurement’ – This is a Poisson distribution – since MC simulation is also a Poisson process
 - Construct full likelihood (‘profile likelihood’)

$$L(N, N_{MC} | s, b) = \text{Poisson}(N | s + b) \cdot \text{Poisson}(N_{MC} | \tau \cdot b)$$

Constant factor $\tau = L(\text{MC})/L(\text{data})$

- Note uncanny similarity to full likelihood of a sideband measurement!

$$L(N, N_{cl} | s, b) = \text{Poisson}(N | s + b) \cdot \text{Poisson}(N_{cl} | \tau \cdot b)$$

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Modeling multiple systematic uncertainties

- Introduction of multiple systematic uncertainties presents no special issues
- Example JES uncertainty plus generator ISR uncertainty

$$L(N, 0 | s, \alpha_{JES}, \alpha_{ISR}) = P(N | s + b(1 + 0.1\alpha_{JES} + 0.05\alpha_{ISR})) \cdot G(0 | \alpha_{JES}, 1) \cdot G(0 | \alpha_{ISR}, 1)$$

Joint response function for both systematics
One subsidiary measurement for each source of uncertainty

- A brief note on correlations
 - Word “correlations” often used sloppily – **proper way is to think of correlations of parameter estimators**. Likelihood defines parameters $\alpha_{JES}, \alpha_{ISR}$. The (ML) estimates of these are denoted $\hat{\alpha}_{JES}, \hat{\alpha}_{ISR}$
 - The ML estimators of $\hat{\alpha}_{JES}, \hat{\alpha}_{ISR}$ using the Likelihood of the subsidiary measurements are uncorrelated (since the product factorize in this example)
 - The ML estimators of $\hat{\alpha}_{JES}, \hat{\alpha}_{ISR}$ using the full Likelihood may be correlated. This is due to physics modeling effects encoded in the joint response function

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Modeling systematic uncertainties in multiple channels

- Systematic effects that affect multiple measurements should be modeled coherently.
 - Example – Likelihood of two Poisson counting measurements

$$L(N_A, N_B | s, \alpha_{JES}) = P(N_A | s \cdot f_A + b_A(1 + 0.1\alpha_{JES})) \cdot P(N_B | s \cdot f_B + b_B(1 - 0.3\alpha_{JES})) \cdot G(0 | \alpha_{JES}, 1)$$

JES response function for channel A
JES response function for channel B
JES subsidiary measurement

- Effect of changing JES parameter α_{JES} coherently affects both measurement.
- Magnitude and sign effect does not need to be same, this is dictated by the physics of the measurement

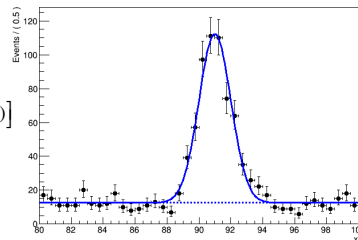
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Introducing response functions for shape uncertainties

- Modeling of systematic uncertainties in **Likelihoods describing distributions** follows the same procedure as for counting models

- Example: Likelihood modeling distribution in a di-lepton invariant mass. POI is the signal strength μ

$$L(\vec{m}_l | \mu) = \prod_i [\mu \cdot \text{Gauss}(m_l^{(i)}, 91, 1) + (1 - \mu) \cdot \text{Uniform}(m_l^{(i)})]$$



- Consider a lepton energy scale systematic uncertainty that affects this measurement

- The LES has been measured with a 1% precision
- The effect of LES on m_l has been determined to a 2% shift for 1% LES change

$$L(\vec{m}_l | \mu, \alpha_{LES}) = \prod_i [\underbrace{\mu \cdot \text{Gauss}(m_l^{(i)}, 91 \cdot (1 + 2\alpha_{LES}), 1)}_{\text{Response function}} + (1 - \mu) \cdot \underbrace{\text{Uniform}(m_l^{(i)})}_{\text{Subsidiary measurement}}] \cdot \underbrace{\text{Gauss}(0 | \alpha_{LES}, 1)}_{\text{Subsidiary measurement}}$$

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Response modeling for distributions

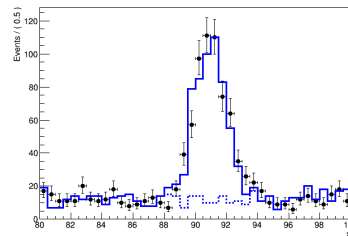
- For a change in the **rate**, response modeling of histogram-shaped distribution is straightforward: **simply scale entire distribution**

$$L(\vec{N} | \mu) = \prod_i \text{Poisson}(N_i | \mu \tilde{s}_i + \tilde{b}_i)$$

$$L(\vec{N} | \mu, \alpha) = \prod_i \text{Poisson}(N_i | \underbrace{\mu \tilde{s}_i \cdot (1 + 3.75\alpha)}_{\text{Response function for signal rate}} + \tilde{b}_i) \cdot \underbrace{\text{Gauss}(0 | \alpha, 1)}_{\text{Subsidiary measurement}}$$

Response function for signal rate Subsidiary measurement

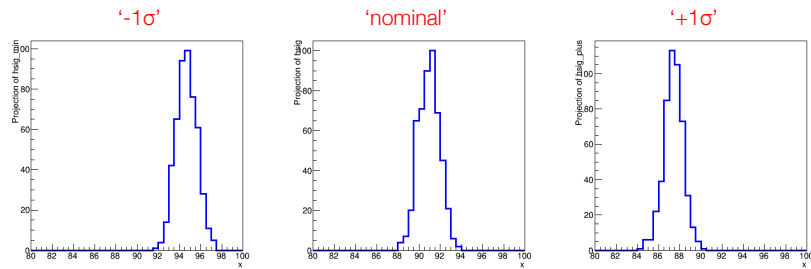
- But what about a systematic uncertainty that shifts the mean, or affects the distribution in another way?



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Modeling of shape systematics in the likelihood

- Effect of *any* systematic uncertainty that affects the shape of a distribution can in principle be obtained from MC simulation chain
 - Obtain histogram templates for distributions at '+1 σ ' and '-1 σ ' settings of systematic effect

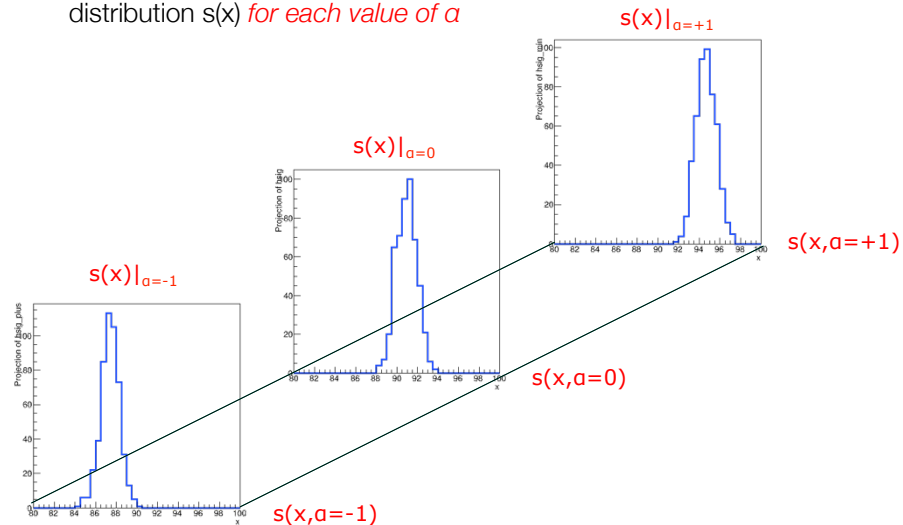


- Challenge: **construct an empirical response function based on the interpolation of the shapes of these three templates.**

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Need to interpolate between template models

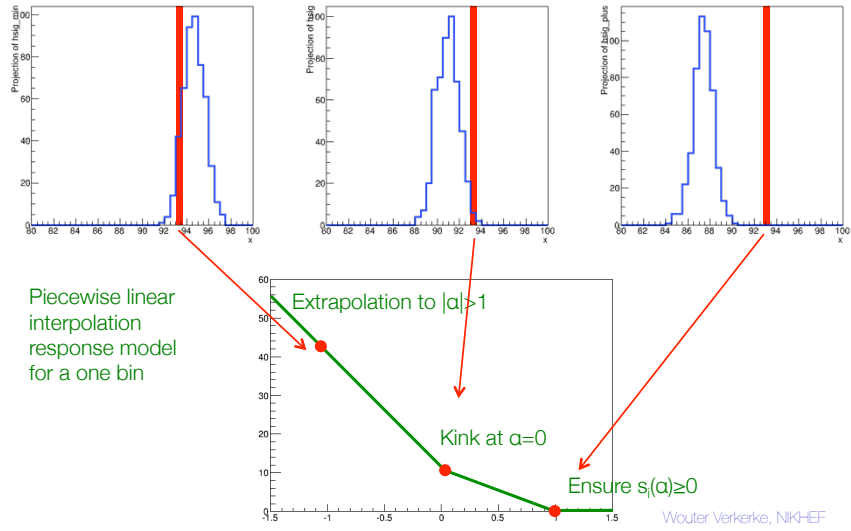
- Need to define 'morphing' algorithm to define distribution $s(x)$ *for each value of α*



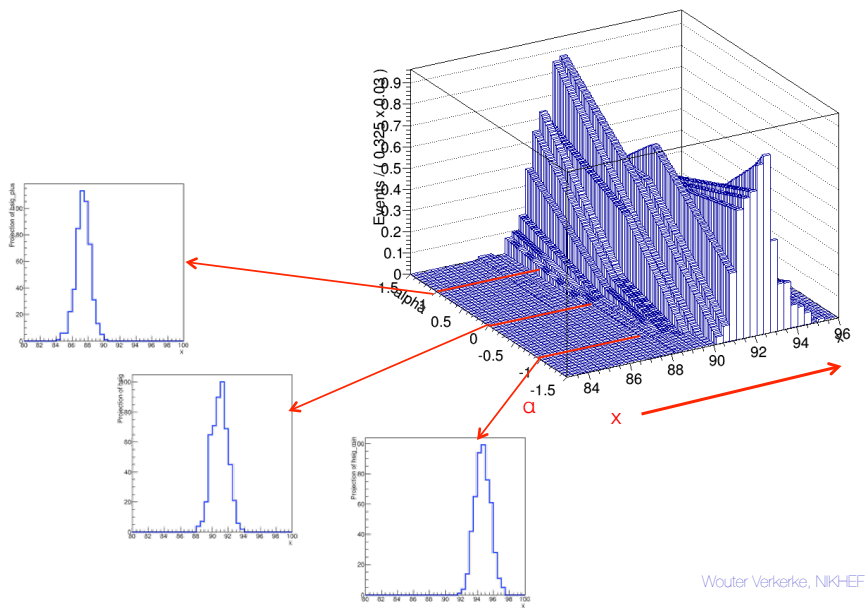
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Piecewise linear interpolation

- Simplest solution is piece-wise linear interpolation for each bin



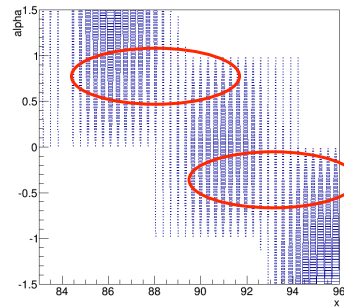
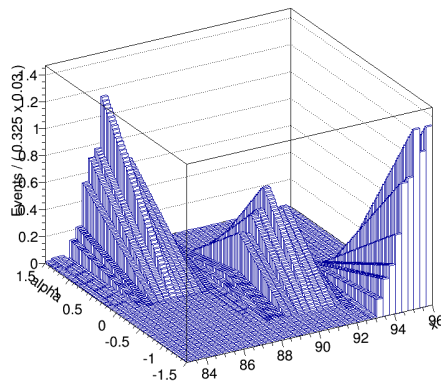
Visualization of bin-by-bin linear interpolation of distribution



Limitations of piece-wise linear interpolation

- Bin-by-bin interpolation looks spectacularly easy and simple, but be aware of its limitations
 - Same example, but with larger 'mean shift' between templates

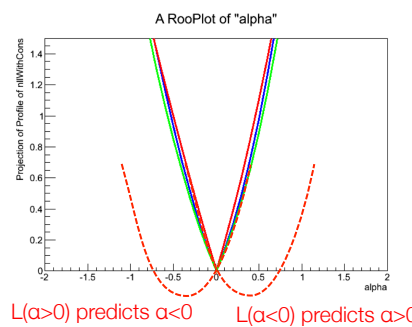
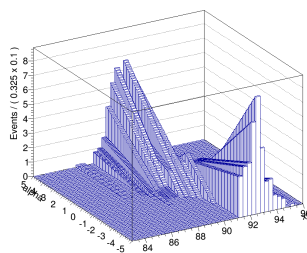
Note double peak structure around $|\alpha|=0.5$



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Non-linear interpolation options

- Piece-wise linear interpolation leads to kink in response functions that may result in pathological likelihood functions

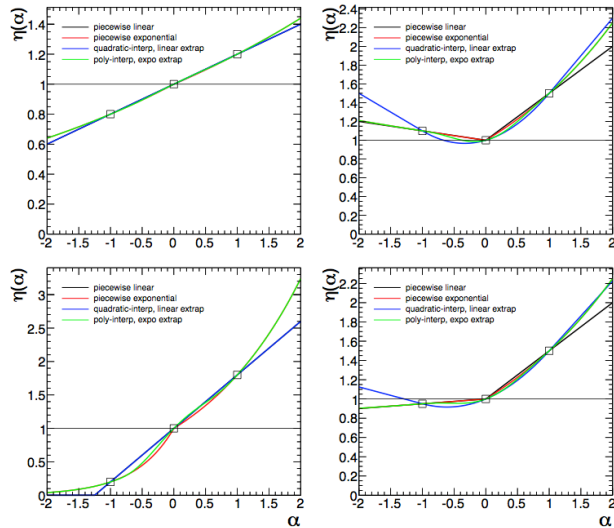


- A variety of other interpolation options exist that improve this
 - Parabolic interpolation/linear extrapolation (but causes shift of minimum)
 - Polynomial interpolation [orders 1,2,4,6]/linear extrapolation (order 1 term allows for asymmetric modeling of templates)

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Non-linear interpolation options

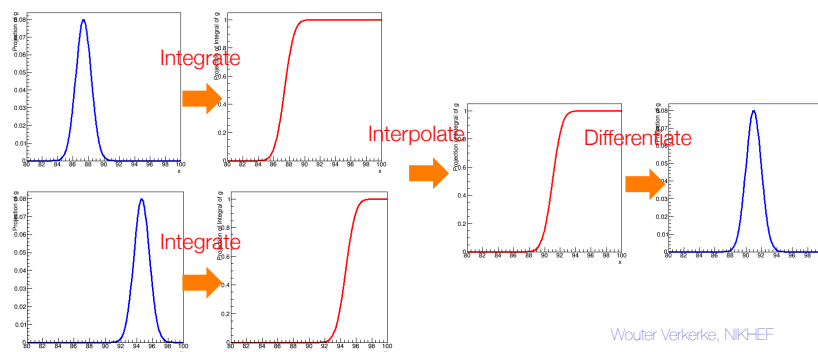
- Comparison of common interpolation options



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Other morphing strategies – ‘horizontal morphing’

- Other template morphing strategies exist that are less prone to unintended side effects
- A ‘horizontal morphing’ strategy was invented by Alex read.
 - Interpolates the cumulative distribution function instead of the distribution
 - Especially suitable for shifting distributions
 - Here shown on a continuous distribution, but also works on histograms
 - Drawback: computationally expensive, algorithm only worked out for 1 NP



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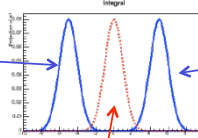
Yet another morphing strategy – ‘Moment morphing’

M. Baak & S. Gadatsch

- Given two template model $f_-(x)$ and $f_+(x)$ the strategy of moment morphing considers first two moment of template models (mean and variance)

$$\mu_- = \int x \cdot f_-(x) dx$$

$$V_- = \int (x - \mu_-)^2 \cdot f_-(x) dx$$



$$\mu_+ = \int x \cdot f_+(x) dx$$

$$V_+ = \int (x - \mu_+)^2 \cdot f_+(x) dx$$

- The goal of moment morphing is to construct an interpolated function that has linearly interpolated moments

$$\begin{aligned} \mu(\alpha) &= \alpha\mu_- + (1 - \alpha)\mu_+ \\ V(\alpha) &= \alpha V_- + (1 - \alpha)V_+ \end{aligned} \quad [1]$$

- It constructs this morphed function as combination of linearly transformed input models

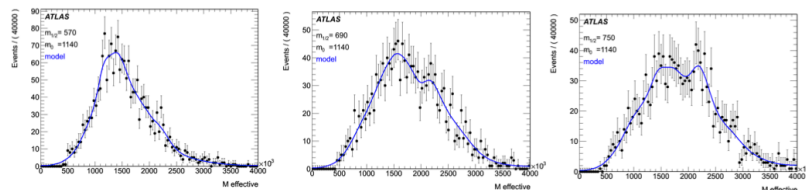
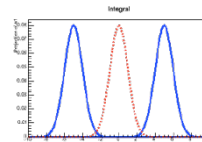
$$f(x, \alpha) \rightarrow \alpha f_-(ax + b) + (1 - \alpha) f_+(cx - d)$$

- Where constants a,b,c,d are chosen such so that $f(x, \alpha)$ satisfies conditions [1]

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Yet another morphing strategy – ‘Moment morphing’

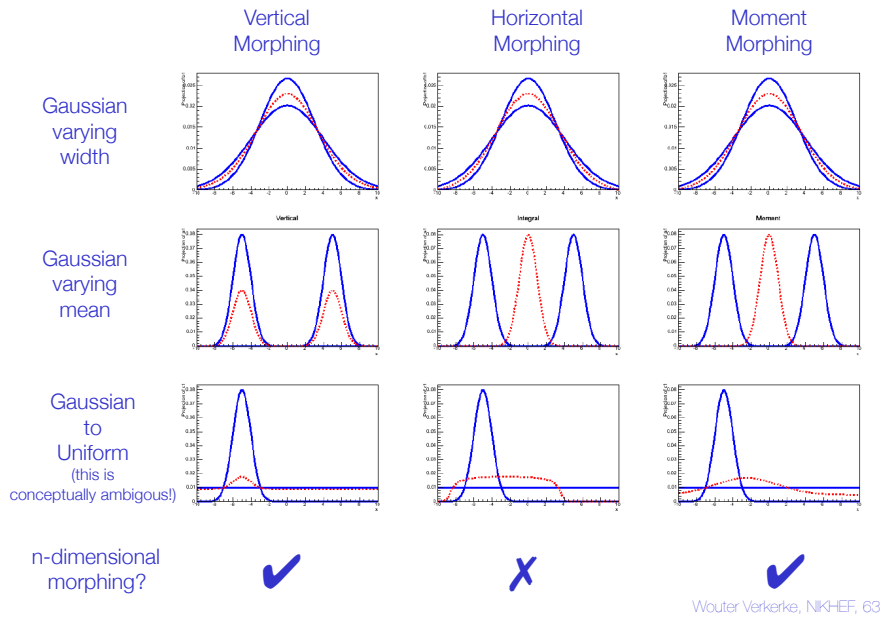
- For a Gaussian probability model with linearly changing mean and width, moment morphing of two Gaussian templates is the exact solution
- But also works well on ‘difficult’ distributions



- Good computational performance
 - Calculation of moments of templates is expensive, but just needs to be done once, otherwise very fast (just linear algebra)
$$f(x, \alpha) \rightarrow \alpha f_-(ax + b) + (1 - \alpha) f_+(cx - d)$$
- Multi-dimensional interpolation strategies exist

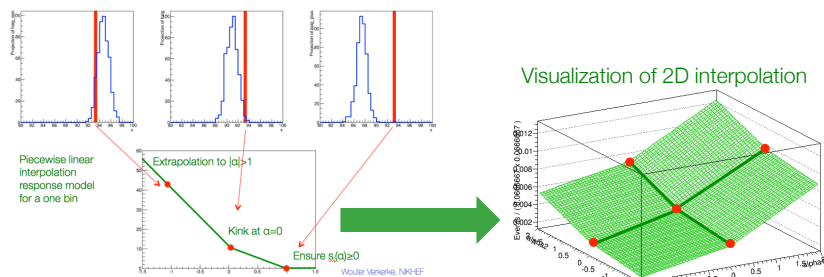
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There are other morphing algorithms to choose from



Piece-wise interpolation for >1 nuisance parameter

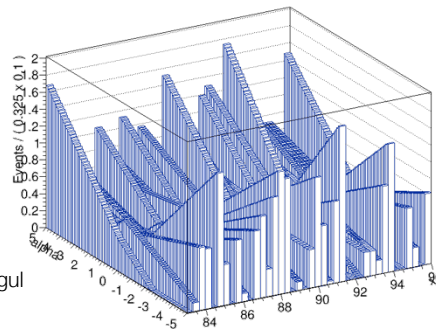
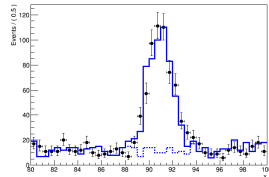
- Concept of piece-wise linear interpolation can be trivially extended to apply to morphing of >1 nuisance parameter.
 - Difficult to visualize effect on full distribution, but easy to understand concept at the individual bin level



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Shape, rate or no systematic?

- Be judicious with modeling of systematic with little or no significant change in shape (w.r.t MC template statistics)
 - Example morphing of a very subtle change in the background model
 - Is this a meaningful new degree of freedom in the likelihood model?

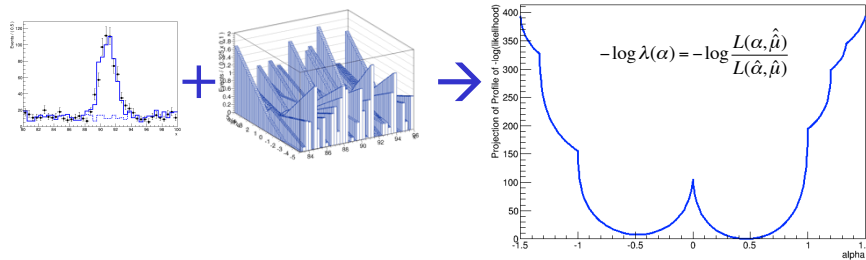


- A χ^2 or KS test between nominal and alternate template can help to decide if a shape uncertainty is meaningful
- Most systematic uncertainties affect both rate and shape, but can make independent decision on modeling rate (which less likely to affect fit stability)

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Fit stability due to insignificant shape systematics

- Shape of profile likelihood in NP clearly raises two points

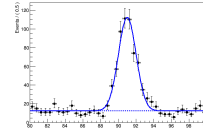


- 1) Numerical minimization process will be 'interesting'
- 2) MC statistical effects induce strongly defined minima that are fake
 - Because for this example all three templates were sampled from the same parent distribution (a uniform distribution)

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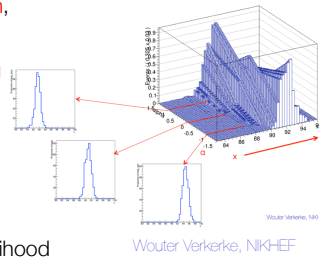
Recap on shape systematics & template morphing

- Implementation of shape systematic in likelihoods modeling distributions conceptually no different than rate systematics in counting experiments



$$L(\vec{m}_{ij} | \mu, \alpha_{LES}) = \prod_i \left[\mu \cdot \text{Gauss}(m_{ij}^{(i)}, 91 \cdot (1 + 2\alpha_{LES}, 1)) + (1 - \mu) \cdot \text{Uniform}(m_{ij}^{(i)}) \right] \cdot \text{Gauss}(0 | \alpha_{LES}, 1)$$

- For template modes obtained from MC simulation template provides a technical solution to implement response function
 - Simplest strategy piecewise linear interpolation, but only works well for small changes
 - Moment morphing better adapted to modeling of shifting distributions
 - Both algorithms extend to n-dimensional interpolation to model multiple systematic NPs in response function
 - Be judicious in modeling 'weak' systematics: MC systematic uncertainties will dominate likelihood



Modular software design

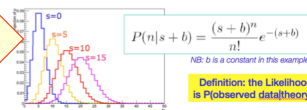
[RooFit/HistFactory](#)
Language for building probability models
 Comprises datasets, likelihoods, minimization, toy data generation, visualization and persistence

(RooFit Workspace)

[RooStats](#)
 Suite of statistical tests operating on RooFit probability models

Everything starts with the 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)



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RootFit core design philosophy

- Mathematical objects are represented as C++ objects

Mathematical concept	RootFit class
variable x	RootRealVar
function $f(x)$	RootAbsReal
PDF $f(x)$	RootAbsPdf
space point \vec{x}	RootArgSet
integral $\int_{x_{\min}}^{x_{\max}} f(x) dx$	RootRealIntegral
list of space points	RootAbsData

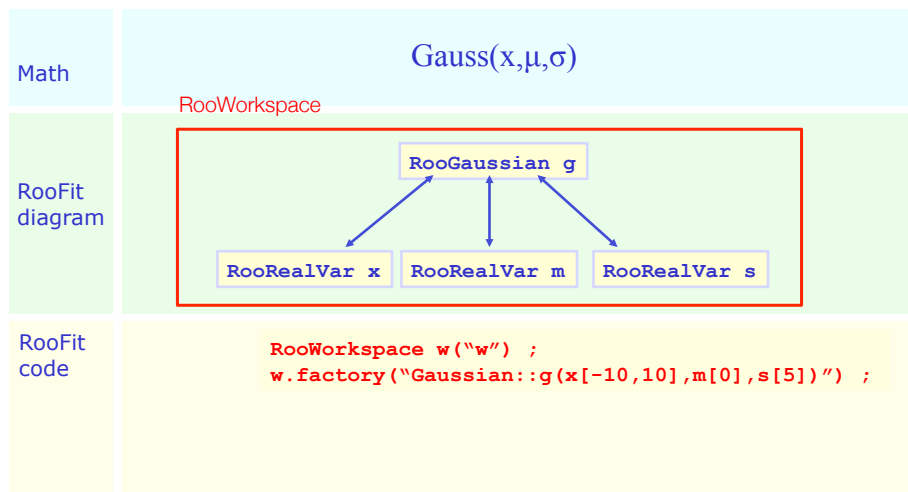
RootFit core design philosophy

- Instead of '`double Likelihood(double paramVec[])`', a flexible modular structure of 'programmed' functions

Math	Gauss(x, μ, σ)	
	RootWorkspace (keeps all parts together)	
RootFit diagram		
RootFit code	<pre>RootRealVar x("x","x",-10,10) ; RootRealVar m("m","y",0,-10,10) ; RootRealVar s("s","z",3,0.1,10) ; RootGaussian g("g","g",x,m,s) ; RootWorkspace w("w") ; w.import(g) ;</pre>	

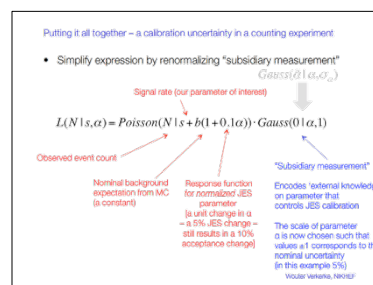
Roofit core design philosophy - Workspace

- Alternatively, a simple math-like 'factory language' can quickly populate a workspace with the same objects



Example 1: counting expt

- Will now demonstrate how to construct a model for a counting experiment with a systematic uncertainty



$$L(N | s, \alpha) = Poisson(N | s + b(1 + 0.1\alpha)) \cdot Gauss(0 | \alpha, 1)$$

```

// Subsidiary measurement of alpha
w.factory("Gaussian::subs(0,alpha[-5,5],1)") ;

// Response function mu(alpha)
w.factory("expr::mu('s+b(1+0.1*alpha)',s[20],b[20],alpha)") ;

// Main measurement
w.factory("Poisson::p(N[0,10000],mu)") ;

// Complete model Physics*Subsidiary
w.factory("PROD::model(p,subs)") ;
  
```

Example 2: unbinned L with syst.

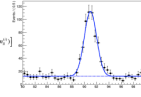
- Will now demonstrate how to code complete example of the unbinned profile likelihood of Section 5:

Introducing shape systematic uncertainties

- Modeling of systematic uncertainties in Likelihood describing distributions follows the same procedure as for counting models

- Example: Likelihood modeling distribution in a di-lepton invariant mass. POI is the signal strength μ

$$L(\mu, |s) = \prod_i [\mu \cdot \text{Gauss}(m_i^i; 91, (1+2\alpha_{LES}) \cdot 1) + (1-\mu) \cdot \text{Uniform}(m_i^i)] \cdot \text{Gauss}(0 | \alpha_{LES}, 1)$$



- Consider a lepton energy scale systematic uncertainty that affects this measurement

- The LES has been measured with a 1% precision

- The effect of LES on m_b has been determined to a 2% shift for 1% LES change

$$L(\mu, |s, \alpha_{LES}) = \prod_i [\mu \cdot \text{Gauss}(m_i^i; 91 \cdot (1 + 2\alpha_{LES}), 1) + (1-\mu) \cdot \text{Uniform}(m_i^i)] \cdot \text{Gauss}(0 | \alpha_{LES}, 1)$$

Response function Subsidiary measurement

Stuart Webber, NIKHEF

$$L(\vec{m}_\mu | \mu, \alpha_{LES}) = \prod_i [\mu \cdot \text{Gauss}(m_\mu^{(i)}; 91 \cdot (1 + 2\alpha_{LES}), 1) + (1-\mu) \cdot \text{Uniform}(m_\mu^{(i)})] \cdot \text{Gauss}(0 | \alpha_{LES}, 1)$$

```
// Subsidiary measurement of alpha
w.factory("Gaussian::subs(0,alpha[-5,5],1)");

// Response function m(alpha)
w.factory("expr::m_a(\"m*(1+2alpha)\",m[91,80,100],alpha)");

// Signal model
w.factory("Gaussian::sig(x[80,100],m_a,s[1])");

// Complete model Physics(signal plus background)*Subsidiary
w.factory("PROD::model(SUM(mu[0,1]*sig,Uniform::bkg(x)),subs)");
```

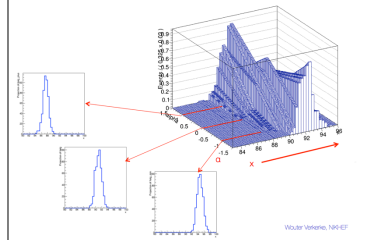
Example 3 : binned L with syst

- Example of template morphing systematic in a binned likelihood

$$s_i(\alpha, \dots) = \begin{cases} s_i^0 + \alpha \cdot (s_i^+ - s_i^0) & \forall \alpha > 0 \\ s_i^0 + \alpha \cdot (s_i^- - s_i^0) & \forall \alpha < 0 \end{cases}$$

$$L(\vec{N} | \alpha, \vec{s}^-, \vec{s}^0, \vec{s}^+) = \prod_{bins} P(N_i | s_i(\alpha, s_i^-, s_i^0, s_i^+)) \cdot G(0 | \alpha, 1)$$

Visualization of bin-by-bin linear interpolation of distribution



Walter Veronesi, NIKHEF

```
// Import template histograms in workspace
w.import(hs_0,hs_p,hs_m);

// Construct template models from histograms
w.factory("HistFunc::s_0(x[80,100],hs_0)");
w.factory("HistFunc::s_p(x,hs_p)");
w.factory("HistFunc::s_m(x,hs_m)");

// Construct morphing model
w.factory("PiecewiseInterpolation::sig(s_0,s_m,s_p,alpha[-5,5])");

// Construct full model
w.factory("PROD::model(ASUM(sig,bkg,f[0,1]),Gaussian(0,alpha,1))");
```