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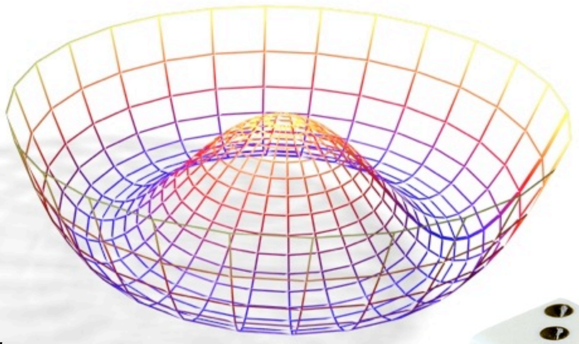
Practical Statistics for Particle Physics



Kyle Cranmer,
New York University

Lecture 2

Outline

Lecture 1: Building a probability model
- preliminaries, the marked Poisson process
- incorporating systematics via nuisance parameters
- constraint terms
- examples of different “narratives” / search strategies

Lecture 2: Hypothesis testing
- simple models, Neyman-Pearson lemma, and likelihood ratio
- composite models and the profile likelihood ratio
- review of ingredients for a hypothesis test

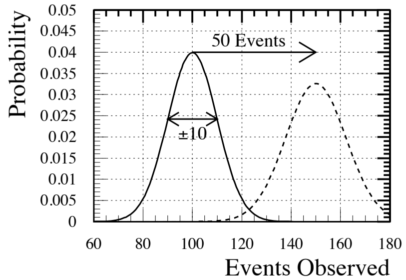
Lecture 3: Limits & Confidence Intervals
- the meaning of confidence intervals as inverted hypothesis tests
- asymptotic properties of likelihood ratios
- Bayesian approach

Hypothesis Testing

Hypothesis testing

One of the most common uses of statistics in particle physics is Hypothesis Testing (e.g. for discovery of a new particle)

- assume one has pdf for data under two hypotheses:
  - Null-Hypothesis, H_0: eg. background-only
  - Alternate-Hypothesis H_1: eg. signal-plus-background
- one makes a measurement and then needs to decide whether to **reject** or **accept** H_0



Hypothesis testing

Before we can make much progress with statistics, we need to decide what it is that we want to do.

- first let us define a few terms:
  - Rate of Type I error α
  - Rate of Type II β
  - Power = $1 - \beta$

		Actual condition	
		Guilty	Not guilty
Decision	Verdict of 'guilty'	True Positive	False Positive (i.e. guilt reported unfairly) **Type I error**
	Verdict of 'not guilty'	False Negative (i.e. guilt not detected) **Type II error**	True Negative

Treat the two hypotheses asymmetrically

- the Null is special.
  - Fix rate of Type I error, call it "the size of the test"

Now one can state "a well-defined goal"

- Maximize power for a fixed rate of Type I error

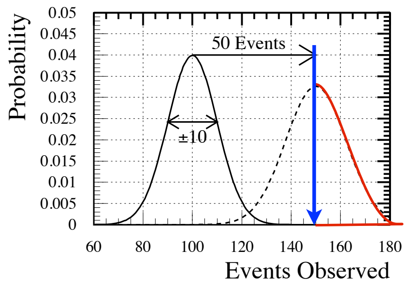
Hypothesis testing

The idea of a "5σ" discovery criteria for particle physics is really a conventional way to specify the size of the test

- usually 5σ corresponds to $\alpha = 2.87 \cdot 10^{-7}$
  - eg. a very small chance we reject the standard model

In the simple case of number counting it is obvious what region is sensitive to the presence of a new signal

- but in higher dimensions it is not so easy



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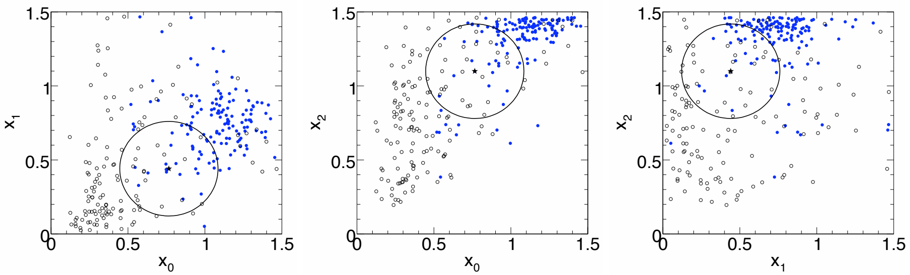

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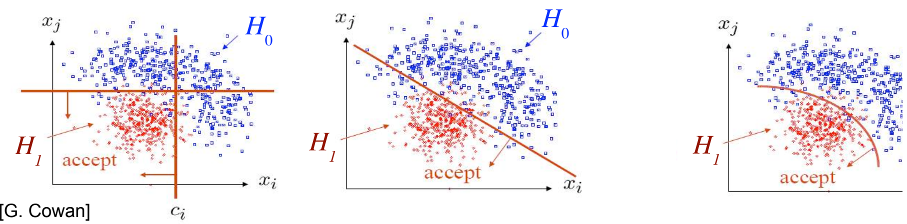


[G. Cowan]

The Neyman-Pearson Lemma

In 1928-1938 Neyman & Pearson developed a theory in which one must consider competing Hypotheses:

- the Null Hypothesis H_0 (background only)
- the Alternate Hypothesis H_1 (signal-plus-background)

Given some probability that we wrongly reject the Null Hypothesis

$$\alpha = P(x \notin W | H_0)$$

(Convention: if data falls in W then we accept H_0)

Find the region W such that we minimize the probability of wrongly accepting the H_0 (when H_1 is true)

$$\beta = P(x \in W | H_1)$$

The Neyman-Pearson Lemma

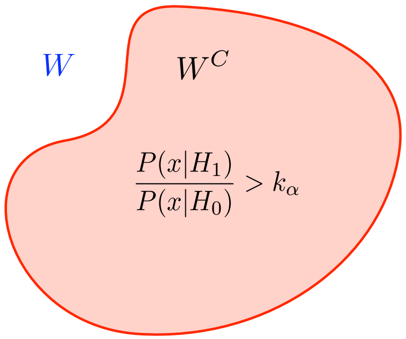
The region W that minimizes the probability of wrongly accepting H_0 is just a contour of the Likelihood Ratio

$$\frac{P(x|H_1)}{P(x|H_0)} > k_\alpha$$

Any other region of the same size will have less power

The likelihood ratio is an example of a **Test Statistic**, eg. a real-valued function that summarizes the data in a way relevant to the hypotheses that are being tested

A short proof of Neyman-Pearson



Consider the contour of the likelihood ratio that has size a given size (eg. probability under H_0 is 1-α)

A short proof of Neyman-Pearson

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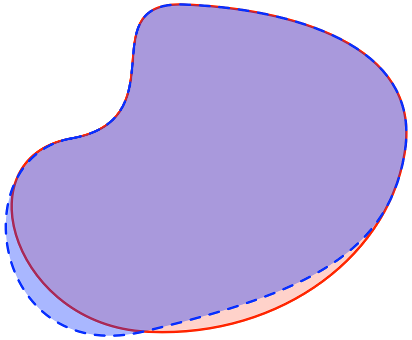

Now consider a variation on the contour that has the same size

A short proof of Neyman-Pearson

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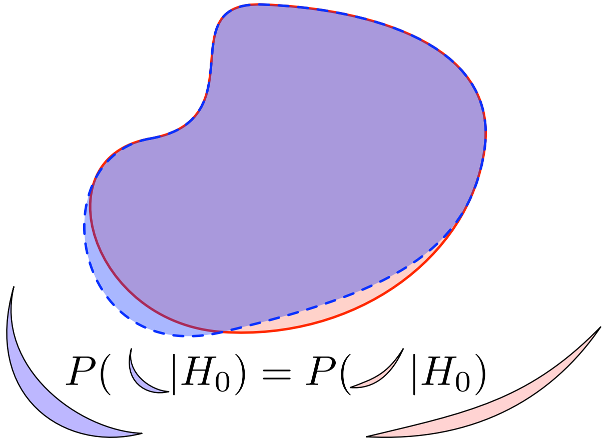

Now consider a variation on the contour that has the same size (eg. same probability under H_0)

A short proof of Neyman-Pearson

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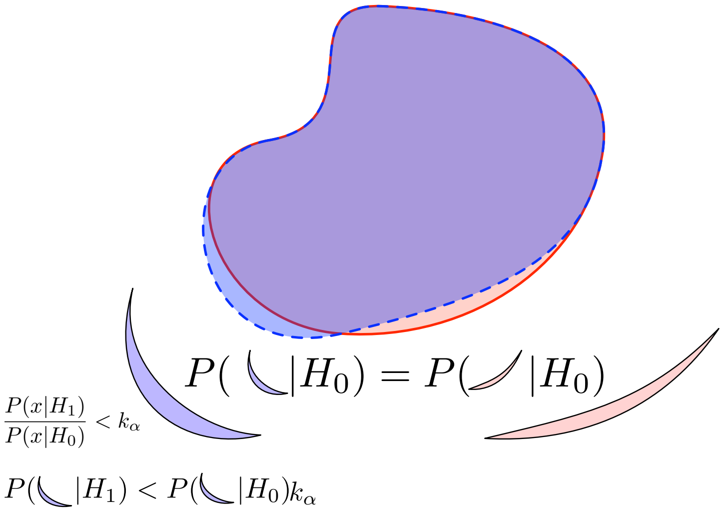

Because the new area is outside the contour of the likelihood ratio, we have an inequality

A short proof of Neyman-Pearson

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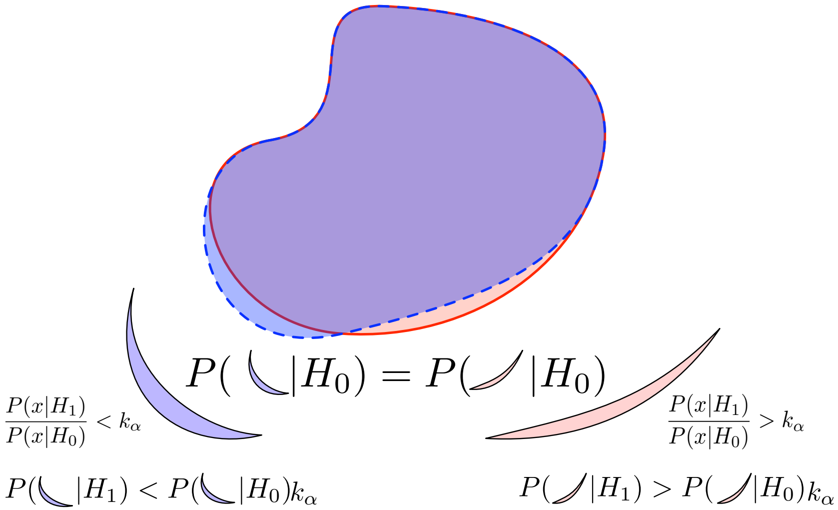
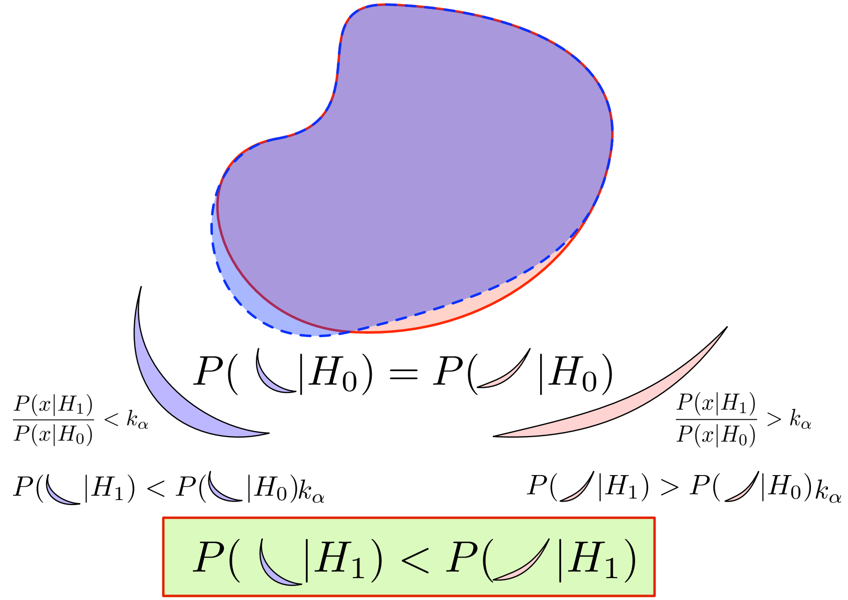


And for the region we lost, we also have an inequality

Together they give...

A short proof of Neyman-Pearson

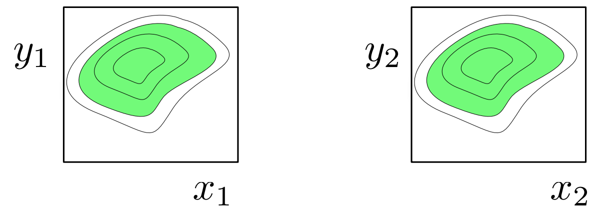


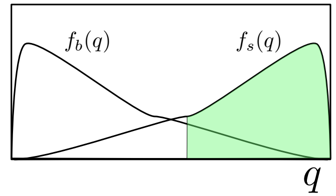
The new region region has less power.

2 discriminating variables

Often one uses the output of a neural network or multivariate algorithm in place of a true likelihood ratio.

- That's fine, but what do you do with it?
- If you have a fixed cut for all events, this is what you are doing:





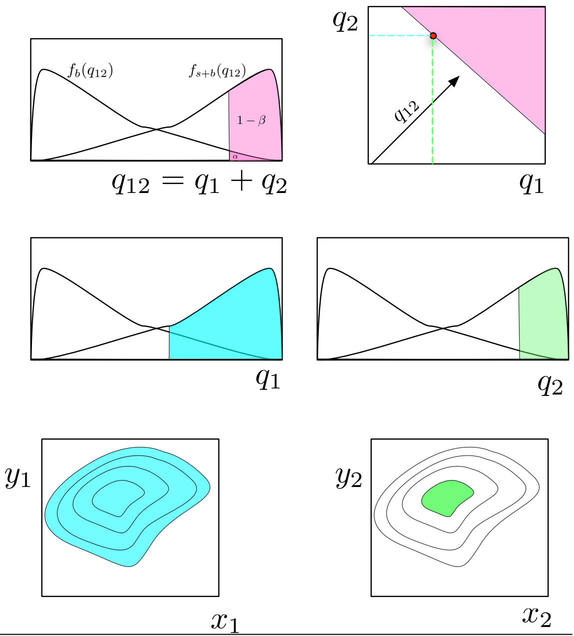
$$q = \ln Q = -s + \ln\left(1 + \frac{s f_s(x,y)}{b f_b(x,y)}\right)$$

Experiments vs. Events

Ideally, you want to cut on the likelihood ratio for your experiment

- equivalent to a sum of log likelihood ratios

Easy to see that includes experiments where one event had a high LR and the other one was relatively small

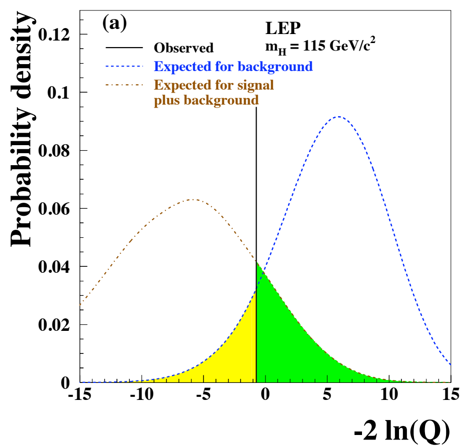


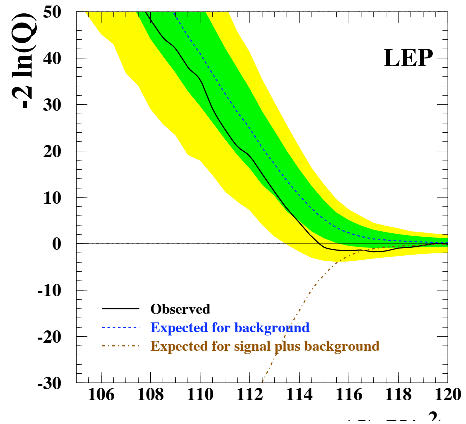
LEP Higgs

A simple likelihood ratio with no free parameters

$$Q = \frac{L(x|H_1)}{L(x|H_0)} = \frac{\prod_i^{N_{chan}} Pois(n_i|s_i+b_i) \prod_j^{n_i} \frac{s_i f_s(x_{ij}) + b_i f_b(x_{ij})}{s_i+b_i}}{\prod_i^{N_{chan}} Pois(n_i|b_i) \prod_j^{n_i} f_b(x_{ij})}$$

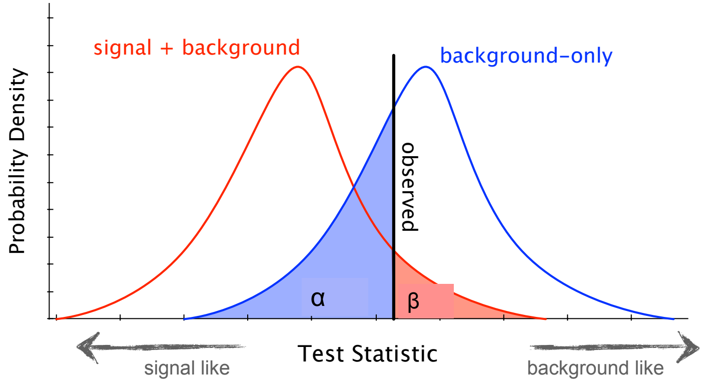
$$q = \ln Q = -s_{tot} + \sum_i^{N_{chan}} \sum_j^{n_i} \ln\left(1 + \frac{s_i f_s(x_{ij})}{b_i f_b(x_{ij})}\right)$$





The Test Statistic and its distribution

Consider this schematic diagram



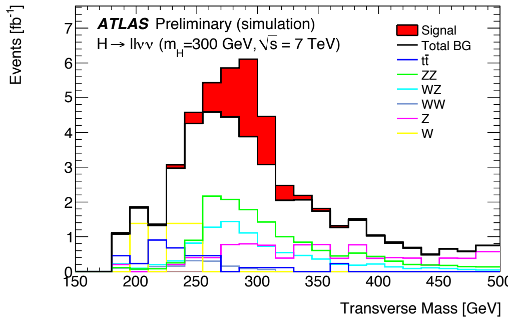
The "**test statistic**" is a single number that quantifies the entire experiment, it could just be number of events observed, but often its more sophisticated, like a likelihood ratio. What test statistic do we choose?

And how do we build the **distribution**? Usually "toy Monte Carlo", but what about the uncertainties... what do we do with the nuisance parameters?

The Marked Poisson model

Recall our marked Poisson model

- **observables**: n events each with some value of discriminating variable m
- **auxiliary measurements:** a_i
- **parameters:** $\boldsymbol{\alpha}$



$$P(\mathbf{m},\mathbf{a}|\boldsymbol{\alpha}) = \mathrm{Pois}(n|s(\boldsymbol{\alpha})+b(\boldsymbol{\alpha}))\prod_j^n \frac{s(\boldsymbol{\alpha})f_s(m_j|\boldsymbol{\alpha})+b(\boldsymbol{\alpha})f_b(m_j|\boldsymbol{\alpha})}{s(\boldsymbol{\alpha})+b(\boldsymbol{\alpha})} \times \prod_{i\in\mathrm{syst}} G(a_i|\alpha_i,\sigma_i)$$

Useful to separate parameters into $\boldsymbol{\alpha}=(\boldsymbol{\mu},\boldsymbol{\nu})$

- **parameters of interest** $\boldsymbol{\mu}$: cross sections, masses, coupling constants, ...
- **nuisance parameters** $\boldsymbol{\nu}$: reconstruction efficiencies, energy scales, ...
  - note: not all of the nuisance parameters need to have constraint terms

Our number counting example

From our general model

$$P(\mathbf{m},\mathbf{a}|\boldsymbol{\alpha}) = \mathrm{Pois}(n|s(\boldsymbol{\alpha})+b(\boldsymbol{\alpha}))\prod_j^n \frac{s(\boldsymbol{\alpha})f_s(m_j|\boldsymbol{\alpha})+b(\boldsymbol{\alpha})f_b(m_j|\boldsymbol{\alpha})}{s(\boldsymbol{\alpha})+b(\boldsymbol{\alpha})} \times \prod_{i\in\mathrm{syst}} G(a_i|\alpha_i,\sigma_i)$$

Consider a simple number counting model with $s(\alpha)\rightarrow s$, $b(\alpha)\rightarrow b$, and replace the constraint $G(a|\alpha,\sigma)\rightarrow \mathrm{Pois}(n_{\rm off}|\tau b)$ with τ known.

$$P(n_{\rm on}, n_{\rm off}|s,b) = \mathrm{Pois}(n_{\rm on}|s+b)\,\mathrm{Pois}(n_{\rm off}|\tau b).$$

We could simply use n_{on} as our test statistic, but to calculate the p-value we need to know distribution of n_{on}.

$$p = \sum_{n_{\rm on}=n_{obs}}^{\infty} \mathrm{Pois}(n_{\rm on}|s+b) \times \underbrace{\mathrm{Pois}(n_{\rm off}|\tau b)}_{\rm constant}$$

Observations:

- The distribution of n_{on} explicitly depends on both s and b.
- The distribution of n_{off} is independent of s
- If τb is very different from n_{off}, then the data are not consistent with the model parameters. However, the p-value derived from n_{on} is not small.

With nuisance parameters: Hybrid Solutions

Goal of Bayesian-frequentist hybrid solutions is to provide a frequentist treatment of the main measurement, while eliminating nuisance parameters (deal with systematics) with an intuitive Bayesian technique.

$$P(n_{\rm on}|s) = \int db\, \mathrm{Pois}(n_{\rm on}|s+b)\,\pi(b), \qquad p = \sum_{n_{\rm on}=n_{obs}}^{\infty} P(n_{\rm on}|s)$$

Tracing back the origin of $\pi(b)$

- clearly state prior $\eta(b)$; identify control samples (sidebands) and use:

$$\pi(b) = P(b|n_{\rm off}) = \frac{P(n_{\rm off}|b)\eta(b)}{\int db P(n_{\rm off}|b)\eta(b)}.$$

In a purely Frequentist approach we must need a test statistic that depends on both n_{on} and n_{off} and we must consider both random (eg. when generating toy Monte Carlo)

$$P(n_{\rm on}, n_{\rm off}|s,b) = \mathrm{Pois}(n_{\rm on}|s+b)\,\mathrm{Pois}(n_{\rm off}|\tau b).$$

Does it matter?

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This on/off problem has been studied extensively.

- instead of arguing about the merits of various methods, just go and check their rate of Type I error
- Results indicated large discrepancy in “claimed” significance and “true” significance for various methods
- eg. 5σ is really ~4σ for some points

So, yes, it does matter.

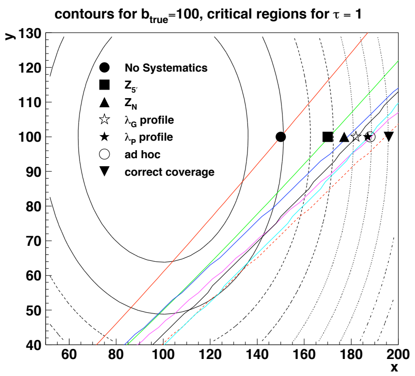

Figure 7. A comparison of the various methods critical bou ary $x_{crit}(y)$ (see text). The concentric ovals represent c tours of L_G from Eq. 15.

$$P(n_{\rm on}, n_{\rm off}|s,b) = {\rm Pois}(n_{\rm on}|s+b)\,{\rm Pois}(n_{\rm off}|\tau b).$$

http://www.physics.ox.ac.uk/phystat05/proceedings/files/Cranmer_LHCStatisticalChallenges.ps

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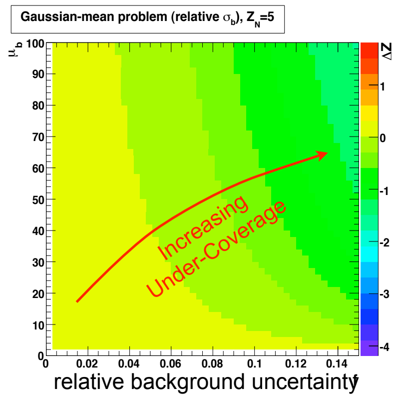

Follow-up work by Bob Cousins & Jordan Tucker, [physics/0702156]

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The Profile Likelihood Ratio

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Consider our general model with a single parameter of interest μ

- let μ=0 be no signal, μ=1 nominal signal

In the LEP approach the likelihood ratio is equivalent to:

$$Q_{\rm LEP} = \frac{P(\mathbf{m}|\mu=1,\nu)}{P(\mathbf{m}|\mu=0,\nu)}$$

- but this variable is sensitive to uncertainty on ν and makes no use of auxiliary measurements **a**

Alternatively, one can define **profile likelihood ratio**

$$\lambda(\mu) = \frac{P(\mathbf{m},\mathbf{a}|\mu,\hat{\hat{\nu}}(\mu;\mathbf{m},\mathbf{a})\,)}{P(\mathbf{m},\mathbf{a}|\hat{\mu},\hat{\nu})}$$

- where $\hat{\hat{\nu}}(\mu;\mathbf{m},\mathbf{a})$ is best fit with μ fixed (the constrained maximum likelihood estimator, depends on data)
- and $\hat{\nu}$ and $\hat{\mu}$ are best fit with both left floating (unconstrained)
- Tevatron used $Q_{\rm Tev} = \lambda(\mu=1)/\lambda(\mu=0)$ as generalization of $Q_{\rm LEP}$

An example

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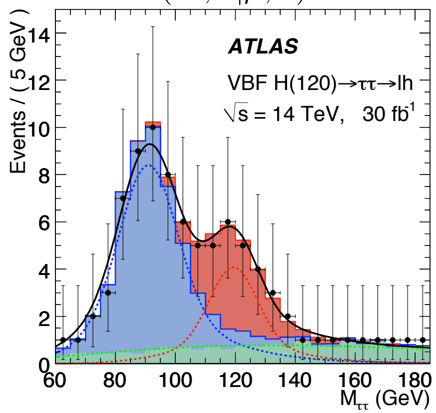
Essentially, you need to fit your model to the data twice:

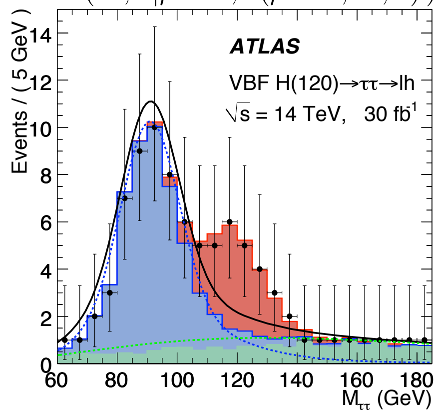
once with everything floating, and once with signal fixed to 0

$$\lambda(\mu=0) = \frac{P(\mathbf{m},\mathbf{a}|\mu=0,\hat{\hat{\nu}}(\mu=0;\mathbf{m},\mathbf{a})\,)}{P(\mathbf{m},\mathbf{a}|\hat{\mu},\hat{\nu})}$$

$$P(\mathbf{m},\mathbf{a}|\hat{\mu},\hat{\nu})$$



$$P(\mathbf{m},\mathbf{a}|\mu=0,\hat{\hat{\nu}}(\mu=0;\mathbf{m},\mathbf{a})\,)$$



Properties of the Profile Likelihood Ratio

After a close look at the profile likelihood ratio

$$\lambda(\mu) = \frac{P(\mathbf{m},\mathbf{a}|\mu,\hat{\hat{\nu}}(\mu;\mathbf{m},\mathbf{a}))}{P(\mathbf{m},\mathbf{a}|\hat{\mu},\hat{\nu})}$$

one can see the function is independent of true values of ν

- though its distribution might depend indirectly

Wilks's theorem states that under certain conditions the distribution of $-2\ln\lambda\ (\mu=\mu_0)$ given that the true value of μ is μ_0 converges to a chi-square distribution

- more on this tomorrow, but the important points are:
- "asymptotic distribution" is known and it is independent of ν
  - more complicated if parameters have boundaries (eg. $\mu \geq 0$)

Thus, we can calculate the p-value for the background-only hypothesis without having to generate Toy Monte Carlo!

Toy Monte Carlo

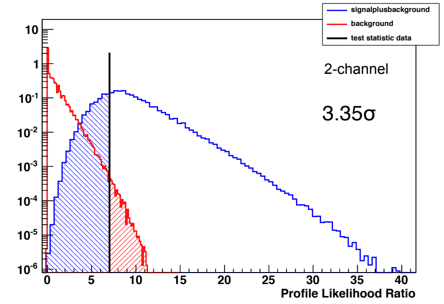
Explicitly build distribution by generating "toys" / pseudo experiments assuming a specific value of μ and ν.

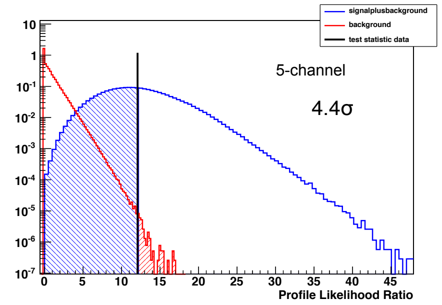
- randomize both main measurement **m** and auxiliary measurements **a**
- fit the model twice for the numerator and denominator of profile likelihood ratio
- evaluate $-2\ln\lambda(\mu)$ and add to histogram

Choice of μ is straight forward: typically $\mu=0$ and $\mu=1$, but choice of ν is less clear

- more on this tomorrow

This can be very time consuming. Plots below use millions of toy pseudo-experiments on a model with ~50 parameters.





What makes a statistical method

To describe a statistical method, you should clearly specify

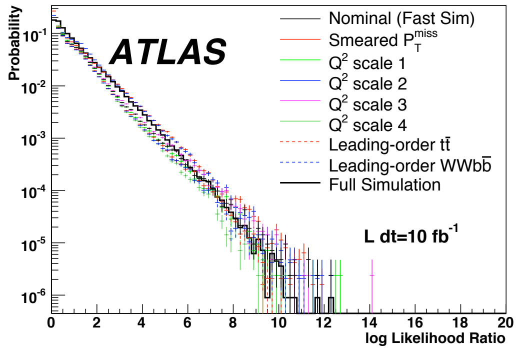
- choice of a test statistic
  - simple likelihood ratio (LEP) $Q_{LEP} = L_{s+b}(\mu=1)/L_b(\mu=0)$
  - ratio of profiled likelihoods (Tevatron) $Q_{TEV} = L_{s+b}(\mu=1,\hat{\hat{\nu}})/L_b(\mu=0,\hat{\hat{\nu}}')$
  - profile likelihood ratio (LHC) $\lambda(\mu) = L_{s+b}(\mu,\hat{\hat{\nu}})/L_{s+b}(\hat{\mu},\hat{\nu})$
- how you build the distribution of the test statistic
  - toy MC randomizing nuisance parameters according to $\pi(\nu)$
    - aka Bayes-frequentist hybrid, prior-predictive, Cousins-Highland
  - toy MC with nuisance parameters fixed (Neyman Construction)
  - assuming asymptotic distribution (Wilks and Wald, more tomorrow)
- what condition you use for limit or discovery
  - more on this tomorrow

Experimentalist Justification

So far this looks a bit like magic. How can you claim that you incorporated your systematic just by fitting the best value of your uncertain parameters and making a ratio?

It won't unless the the parametrization is sufficiently flexible.

So check by varying the settings of your simulation, and see if the profile likelihood ratio is still distributed as a chi-square



Here it is pretty stable, but it's not perfect (and this is a log plot, so it hides some pretty big discrepancies)

For the distribution to be independent of the nuisance parameters your parametrization must be sufficiently flexible.

A very important point

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If we keep pushing this point to the extreme, the physics problem goes beyond what we can handle practically

The p-values are usually predicated on the assumption that the **true distribution** is in the family of functions being considered

- eg. we have sufficiently flexible models of signal & background to incorporate all systematic effects
- but we don’t believe we simulate everything perfectly
- ..and when we parametrize our models usually we have further approximated our simulation.
  - nature -> simulation -> parametrization

At some point these approaches are limited by honest systematics uncertainties (not statistical ones). Statistics can only help us so much after this point. Now we must be physicists!