

Statistical Methods for Particle Physics

Lecture 3: systematic uncertainties / further topics



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Outline

Lecture 1: Introduction and review of fundamentals

Probability, random variables, pdfs

Parameter estimation, maximum likelihood

Statistical tests for discovery and limits

Lecture 2: Multivariate methods

Neyman-Pearson lemma

Fisher discriminant, neural networks

Boosted decision trees

→ Lecture 3: Systematic uncertainties and further topics

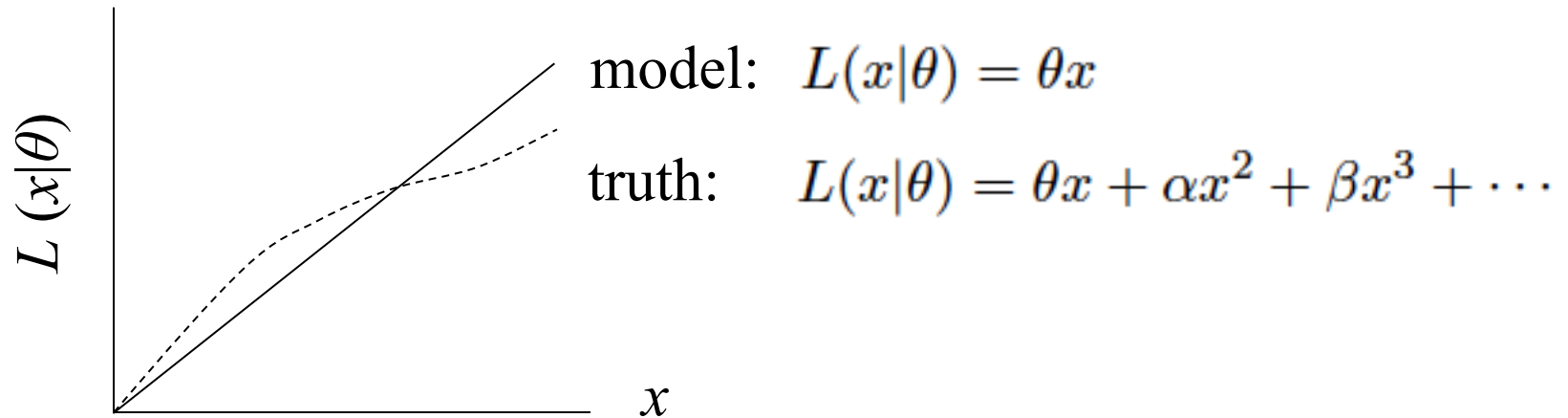
Nuisance parameters (Bayesian and frequentist)

Experimental sensitivity

The look-elsewhere effect

Systematic uncertainties and nuisance parameters

In general our model of the data is not perfect:



Can improve model by including additional adjustable parameters.

$$L(x|\theta) \rightarrow L(x|\theta, \nu)$$

Nuisance parameter \leftrightarrow systematic uncertainty. Some point in the parameter space of the enlarged model should be “true”.

Presence of nuisance parameter decreases sensitivity of analysis to the parameter of interest (e.g., increases variance of estimate).

Example: fitting a straight line

Data: (x_i, y_i, σ_i) , $i = 1, \dots, n$.

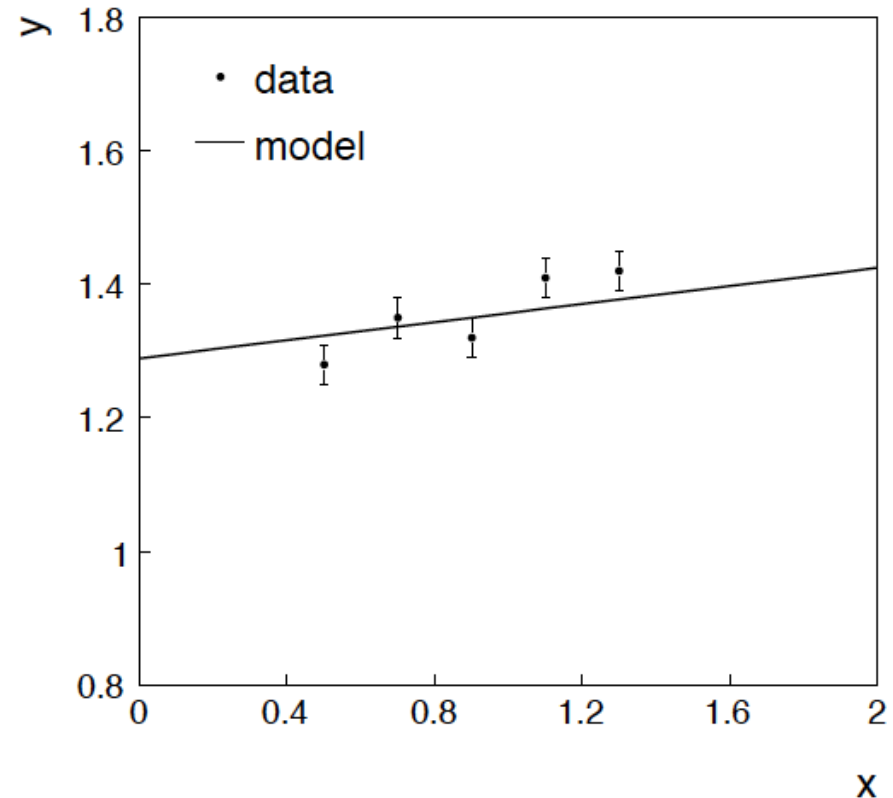
Model: y_i independent and all follow $y_i \sim \text{Gauss}(\mu(x_i), \sigma_i)$

$$\mu(x; \theta_0, \theta_1) = \theta_0 + \theta_1 x,$$

assume x_i and σ_i known.

Goal: estimate θ_0

Here suppose we don't care about θ_1 (example of a “nuisance parameter”)



Maximum likelihood fit with Gaussian data

In this example, the y_i are assumed independent, so the likelihood function is a product of Gaussians:

$$L(\theta_0, \theta_1) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi}\sigma_i} \exp \left[-\frac{1}{2} \frac{(y_i - \mu(x_i; \theta_0, \theta_1))^2}{\sigma_i^2} \right],$$

Maximizing the likelihood is here equivalent to minimizing

$$\chi^2(\theta_0, \theta_1) = -2 \ln L(\theta_0, \theta_1) + \text{const} = \sum_{i=1}^n \frac{(y_i - \mu(x_i; \theta_0, \theta_1))^2}{\sigma_i^2}.$$

i.e., for Gaussian data, ML same as Method of Least Squares (LS)

θ_1 known a priori

$$L(\theta_0) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi}\sigma_i} \exp \left[-\frac{1}{2} \frac{(y_i - \mu(x_i; \theta_0, \theta_1))^2}{\sigma_i^2} \right].$$

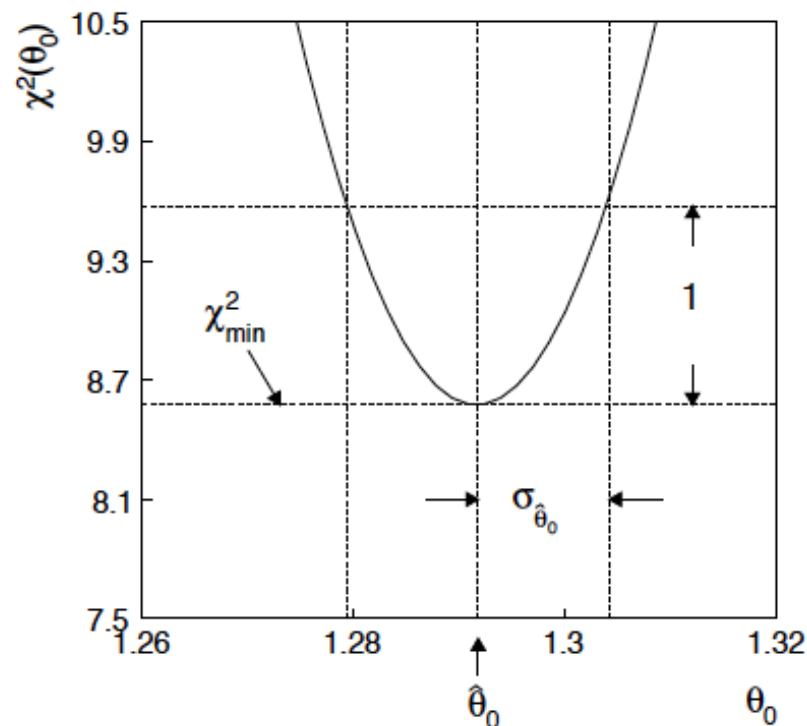
$$\chi^2(\theta_0) = -2 \ln L(\theta_0) + \text{const} = \sum_{i=1}^n \frac{(y_i - \mu(x_i; \theta_0, \theta_1))^2}{\sigma_i^2}.$$

For Gaussian y_i , ML same as LS

Minimize $\chi^2 \rightarrow$ estimator $\hat{\theta}_0$.

Come up one unit from χ_{\min}^2

to find $\sigma_{\hat{\theta}_0}$.



ML (or LS) fit of θ_0 and θ_1

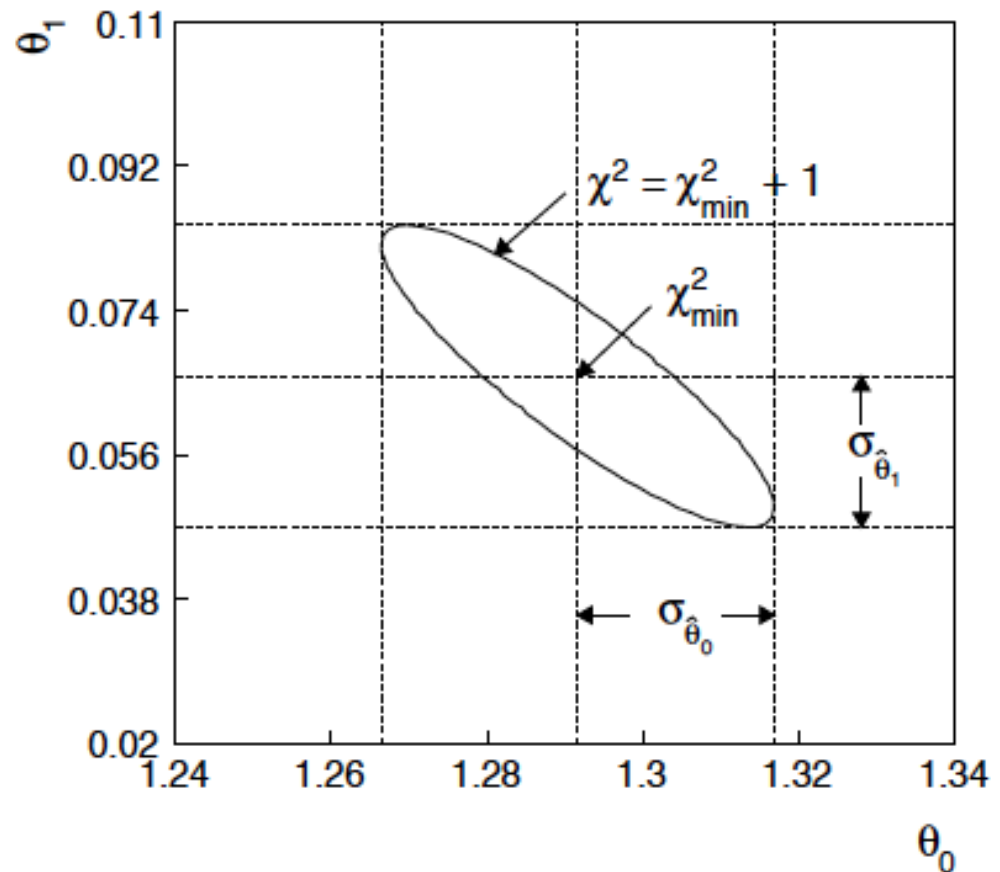
$$\chi^2(\theta_0, \theta_1) = -2 \ln L(\theta_0, \theta_1) + \text{const} = \sum_{i=1}^n \frac{(y_i - \mu(x_i; \theta_0, \theta_1))^2}{\sigma_i^2} .$$

Standard deviations from
tangent lines to contour

$$\chi^2 = \chi_{\min}^2 + 1 .$$

Correlation between

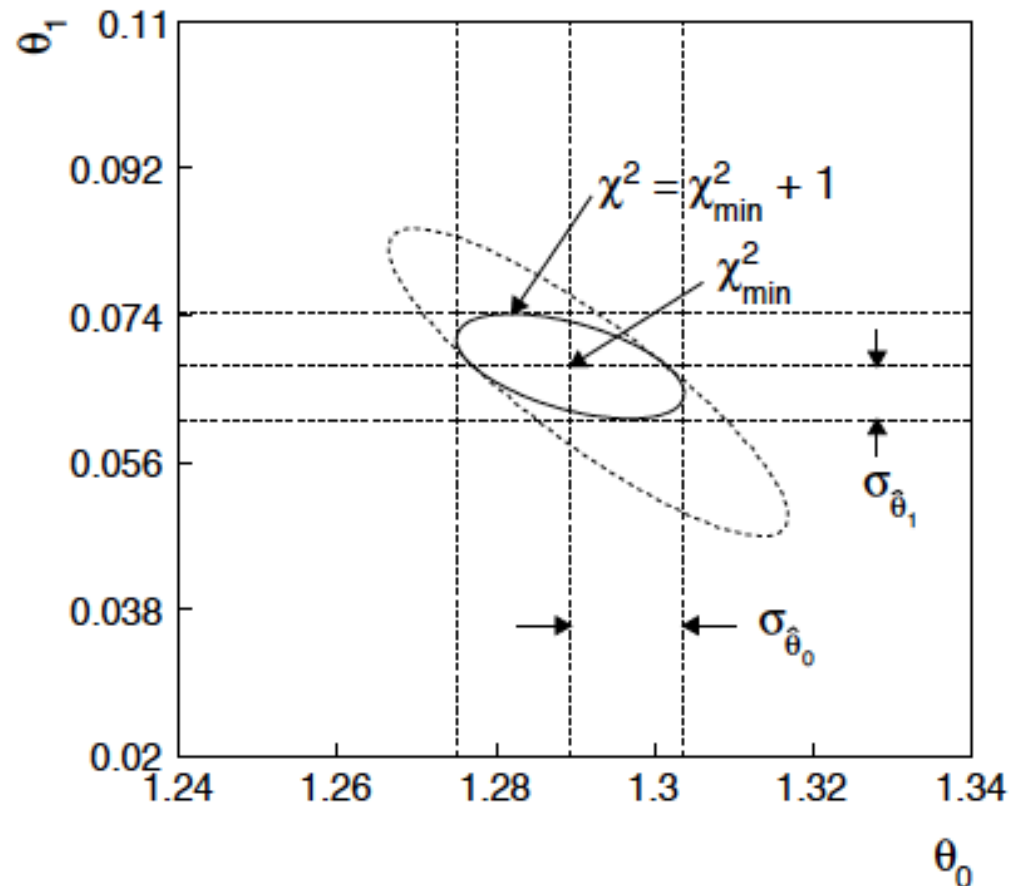
$\hat{\theta}_0$, $\hat{\theta}_1$ causes errors
to increase.



If we have a measurement $t_1 \sim \text{Gauss}(\theta_1, \sigma_{t_1})$

$$\chi^2(\theta_0, \theta_1) = \sum_{i=1}^n \frac{(y_i - \mu(x_i; \theta_0, \theta_1))^2}{\sigma_i^2} + \frac{(\theta_1 - t_1)^2}{\sigma_{t_1}^2}.$$

The information on θ_1
improves accuracy of $\hat{\theta}_0$.



Bayesian method

We need to associate prior probabilities with θ_0 and θ_1 , e.g.,

$$\begin{aligned}\pi(\theta_0, \theta_1) &= \pi_0(\theta_0) \pi_1(\theta_1) && \text{'non-informative', in any} \\ \pi_0(\theta_0) &= \text{const.} && \text{case much broader than } L(\theta_0) \\ \pi_1(\theta_1) &= \frac{1}{\sqrt{2\pi}\sigma_{t_1}} e^{-(\theta_1 - t_1)^2 / 2\sigma_{t_1}^2} && \leftarrow \text{based on previous} \\ &&& \text{measurement}\end{aligned}$$

Putting this into Bayes' theorem gives:

$$p(\theta_0, \theta_1 | \vec{y}) \propto \prod_{i=1}^n \frac{1}{\sqrt{2\pi}\sigma_i} e^{-(y_i - \mu(x_i; \theta_0, \theta_1))^2 / 2\sigma_i^2} \pi_0 \frac{1}{\sqrt{2\pi}\sigma_{t_1}} e^{-(\theta_1 - t_1)^2 / 2\sigma_{t_1}^2}$$

posterior \propto likelihood \times prior

Bayesian method (continued)

We then integrate (marginalize) $p(\theta_0, \theta_1 | x)$ to find $p(\theta_0 | x)$:

$$p(\theta_0 | x) = \int p(\theta_0, \theta_1 | x) d\theta_1 .$$

In this example we can do the integral (rare). We find

$$p(\theta_0 | x) = \frac{1}{\sqrt{2\pi}\sigma_{\theta_0}} e^{-(\theta_0 - \hat{\theta}_0)^2 / 2\sigma_{\theta_0}^2} \quad \text{with}$$

$$\hat{\theta}_0 = \text{same as ML estimator}$$

$$\sigma_{\theta_0} = \sigma_{\hat{\theta}_0} \text{ (same as before)}$$

Usually need numerical methods (e.g. Markov Chain Monte Carlo) to do integral.

Digression: marginalization with MCMC

Bayesian computations involve integrals like

$$p(\theta_0|x) = \int p(\theta_0, \theta_1|x) d\theta_1 .$$

often high dimensionality and impossible in closed form,
also impossible with ‘normal’ acceptance-rejection Monte Carlo.

Markov Chain Monte Carlo (MCMC) has revolutionized
Bayesian computation.




MCMC (e.g., Metropolis-Hastings algorithm) generates
correlated sequence of random numbers:

cannot use for many applications, e.g., detector MC;
effective stat. error greater than if all values independent .

Basic idea: sample multidimensional $\vec{\theta}$,
look, e.g., only at distribution of parameters of interest.

MCMC basics: Metropolis-Hastings algorithm

Goal: given an n -dimensional pdf $p(\vec{\theta})$,
generate a sequence of points $\vec{\theta}_1, \vec{\theta}_2, \vec{\theta}_3, \dots$

- 1) Start at some point $\vec{\theta}_0$
- 2) Generate $\vec{\theta} \sim q(\vec{\theta}; \vec{\theta}_0)$  Proposal density $q(\vec{\theta}; \vec{\theta}_0)$
e.g. Gaussian centred
about $\vec{\theta}_0$
- 3) Form Hastings test ratio $\alpha = \min \left[1, \frac{p(\vec{\theta})q(\vec{\theta}_0; \vec{\theta})}{p(\vec{\theta}_0)q(\vec{\theta}; \vec{\theta}_0)} \right]$
- 4) Generate $u \sim \text{Uniform}[0, 1]$
- 5) If $u \leq \alpha$, $\vec{\theta}_1 = \vec{\theta}$,  ← move to proposed point
else $\vec{\theta}_1 = \vec{\theta}_0$  ← old point repeated
- 6) Iterate

Metropolis-Hastings (continued)

This rule produces a *correlated* sequence of points (note how each new point depends on the previous one).

For our purposes this correlation is not fatal, but statistical errors larger than if points were independent.

The proposal density can be (almost) anything, but choose so as to minimize autocorrelation. Often take proposal density symmetric: $q(\vec{\theta}; \vec{\theta}_0) = q(\vec{\theta}_0; \vec{\theta})$

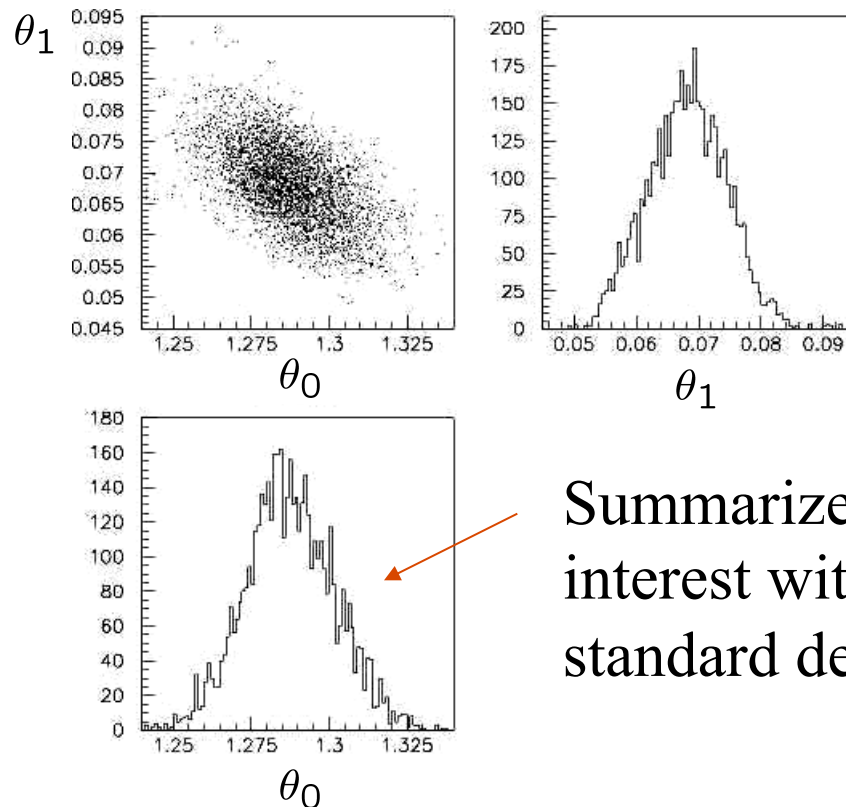
Test ratio is (*Metropolis-Hastings*): $\alpha = \min \left[1, \frac{p(\vec{\theta})}{p(\vec{\theta}_0)} \right]$

I.e. if the proposed step is to a point of higher $p(\vec{\theta})$, take it; if not, only take the step with probability $p(\vec{\theta})/p(\vec{\theta}_0)$.

If proposed step rejected, hop in place.

Example: posterior pdf from MCMC

Sample the posterior pdf from previous example with MCMC:



Summarize pdf of parameter of interest with, e.g., mean, median, standard deviation, etc.

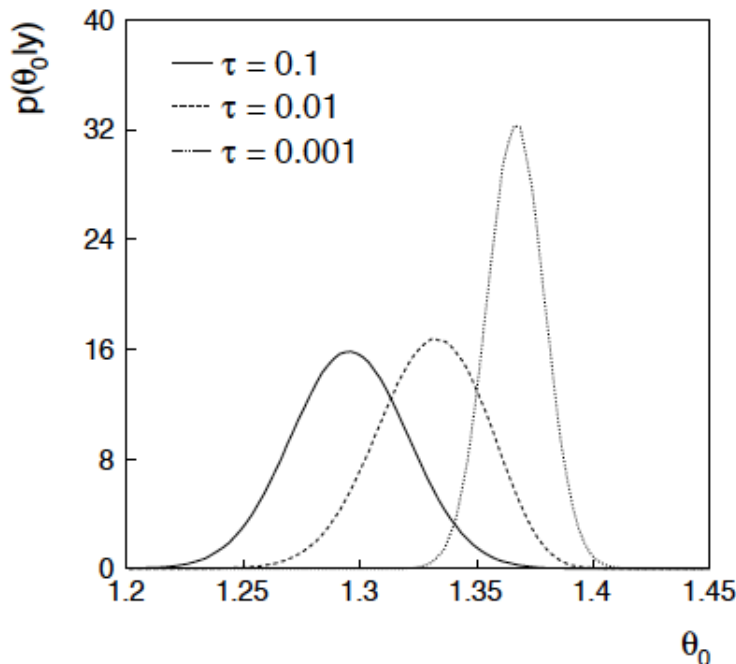
Although numerical values of answer here same as in frequentist case, interpretation is different (sometimes unimportant?)

Bayesian method with alternative priors

Suppose we don't have a previous measurement of θ_1 but rather, e.g., a theorist says it should be positive and not too much greater than 0.1 "or so", i.e., something like

$$\pi_1(\theta_1) = \frac{1}{\tau} e^{-\theta_1/\tau}, \quad \theta_1 \geq 0, \quad \tau = 0.1 .$$

From this we obtain (numerically) the posterior pdf for θ_0 :



This summarizes all knowledge about θ_0 .

Look also at result from variety of priors.

Large sample distribution of the profile likelihood ratio (Wilks' theorem, cont.)


Suppose problem has likelihood $L(\boldsymbol{\theta}, \boldsymbol{\nu})$, with

$$\boldsymbol{\theta} = (\theta_1, \dots, \theta_N) \quad \leftarrow \text{parameters of interest}$$

$$\boldsymbol{\nu} = (\nu_1, \dots, \nu_M) \quad \leftarrow \text{nuisance parameters}$$

Want to test point in $\boldsymbol{\theta}$ -space. Define **profile likelihood ratio**:

$$\lambda(\boldsymbol{\theta}) = \frac{L(\boldsymbol{\theta}, \hat{\boldsymbol{\nu}}(\boldsymbol{\theta}))}{L(\hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\nu}})}, \quad \text{where } \hat{\boldsymbol{\nu}}(\boldsymbol{\theta}) = \underset{\boldsymbol{\nu}}{\operatorname{argmax}} L(\boldsymbol{\theta}, \boldsymbol{\nu})$$

 “profiled” values of $\boldsymbol{\nu}$

and define $q_\theta = -2 \ln \lambda(\boldsymbol{\theta})$.

Wilks' theorem says that distribution $f(q_\theta | \boldsymbol{\theta}, \boldsymbol{\nu})$ approaches the chi-square pdf for N degrees of freedom for large sample (and regularity conditions), **independent of the nuisance parameters $\boldsymbol{\nu}$** .

p -values in cases with nuisance parameters

Suppose we have a statistic q_θ that we use to test a hypothesized value of a parameter θ , such that the p -value of θ is

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

Fundamentally we want to reject θ only if $p_\theta < \alpha$ for all ν .

→ “exact” confidence interval

Recall that for statistics based on the profile likelihood ratio, the distribution $f(q_\theta | \theta, \nu)$ becomes independent of the nuisance parameters in the large-sample limit.

But in general for finite data samples this is not true; one may be unable to reject some θ values if all values of ν must be considered, even those strongly disfavoured by the data (resulting interval for θ “overcovers”).

Profile construction (“hybrid resampling”)

K. Cranmer, PHYSTAT-LHC Workshop on Statistical Issues for LHC Physics, 2008.
oai:cds.cern.ch:1021125, cdsweb.cern.ch/record/1099969.

Approximate procedure is to reject θ if $p_\theta \leq \alpha$ where the p -value is computed assuming the profiled values of the nuisance parameters:

$$\hat{\hat{v}}(\theta)$$

“double hat” notation means value of parameter that maximizes likelihood for the given θ .

The resulting confidence interval will have the correct coverage for the points $(\theta, \hat{\hat{v}}(\theta))$.

Elsewhere it may under- or overcover, but this is usually as good as we can do (check with MC if crucial or small sample problem).

Prototype search analysis

Search for signal in a region of phase space; result is histogram of some variable x giving numbers:

$$\mathbf{n} = (n_1, \dots, n_N)$$

Assume the n_i are Poisson distributed with expectation values

$$E[n_i] = \mu s_i + b_i$$

strength parameter

where

$$s_i = s_{\text{tot}} \int_{\text{bin } i} f_s(x; \boldsymbol{\theta}_s) dx, \quad b_i = b_{\text{tot}} \int_{\text{bin } i} f_b(x; \boldsymbol{\theta}_b) dx.$$

signal

background

Prototype analysis (II)

Often also have a subsidiary measurement that constrains some of the background and/or shape parameters:

$$\mathbf{m} = (m_1, \dots, m_M)$$

Assume the m_i are Poisson distributed with expectation values

$$E[m_i] = u_i(\boldsymbol{\theta})$$

↑ nuisance parameters ($\boldsymbol{\theta}_s, \boldsymbol{\theta}_b, b_{\text{tot}}$)

Likelihood function is

$$L(\mu, \boldsymbol{\theta}) = \prod_{j=1}^N \frac{(\mu s_j + b_j)^{n_j}}{n_j!} e^{-(\mu s_j + b_j)} \prod_{k=1}^M \frac{u_k^{m_k}}{m_k!} e^{-u_k}$$

The profile likelihood ratio

Base significance test on the profile likelihood ratio:

$$\lambda(\mu) = \frac{L(\mu, \hat{\boldsymbol{\theta}})}{L(\hat{\mu}, \hat{\boldsymbol{\theta}})}$$

maximizes L for Specified μ

maximize L

The likelihood ratio of point hypotheses gives optimum test (Neyman-Pearson lemma).

The profile LR should be near-optimal in present analysis with variable μ and nuisance parameters $\boldsymbol{\theta}$.

Test statistic for discovery

Try to reject background-only ($\mu = 0$) hypothesis using

$$q_0 = \begin{cases} -2 \ln \lambda(0) & \hat{\mu} \geq 0 \\ 0 & \hat{\mu} < 0 \end{cases}$$

Here data in critical region (high q_0) only when estimated signal strength $\hat{\mu}$ is positive.

Could also want two-sided critical region, e.g., if presence of signal process could lead to suppression (and/or enhancement) in number of events.

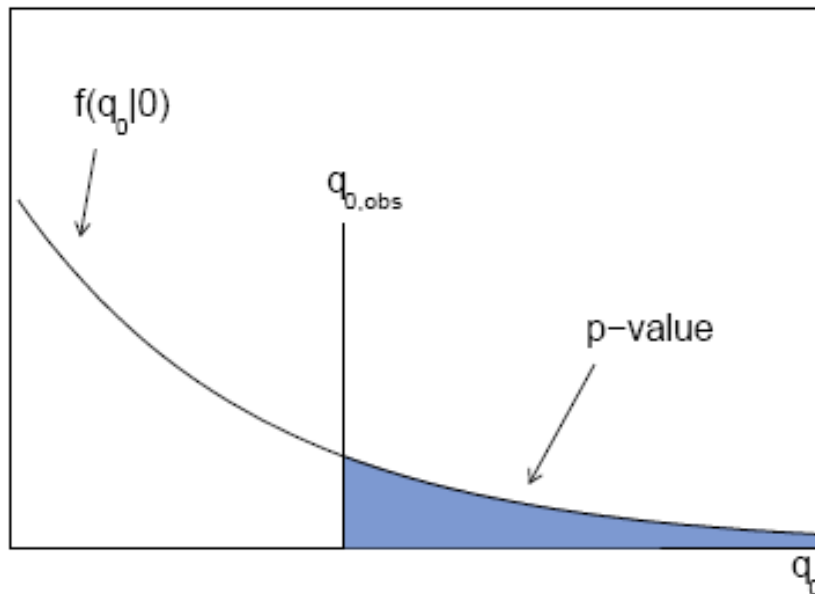
Note that even if physical models have $\mu \geq 0$, we allow $\hat{\mu}$ to be negative. In large sample limit its distribution becomes Gaussian, and this will allow us to write down simple expressions for distributions of our test statistics.

p -value for discovery

Large q_0 means increasing incompatibility between the data and hypothesis, therefore p -value for an observed $q_{0,\text{obs}}$ is

$$p_0 = \int_{q_{0,\text{obs}}}^{\infty} f(q_0|0) dq_0$$

will get formula for this later

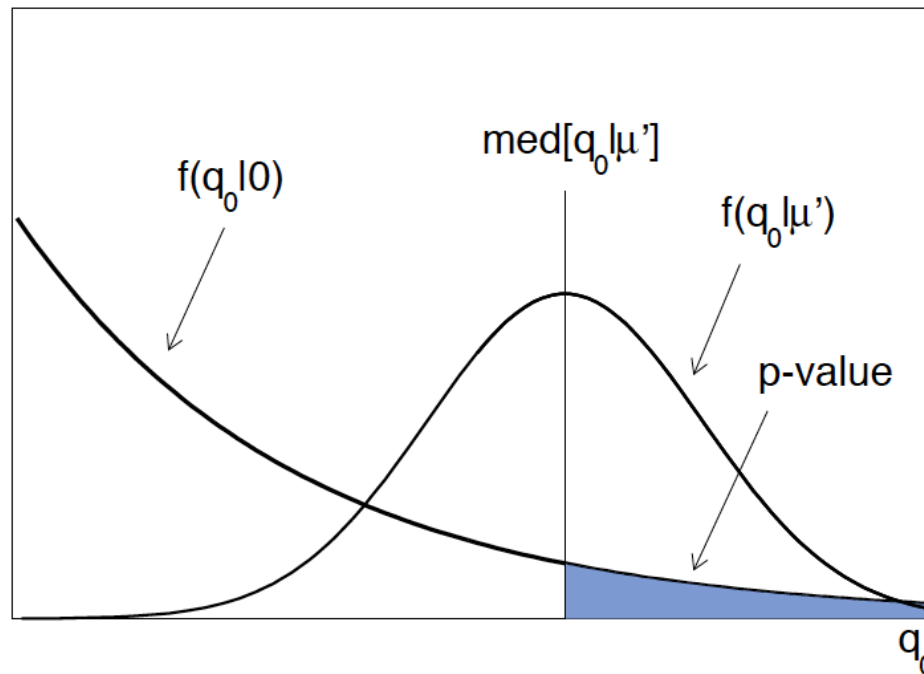


From p -value get equivalent significance,

$$Z = \Phi^{-1}(1 - p)$$

Expected (or median) significance / sensitivity

When planning the experiment, we want to quantify how sensitive we are to a potential discovery, e.g., by given median significance assuming some nonzero strength parameter μ' .



So for p -value, need $f(q_0|0)$, for sensitivity, will need $f(q_0|\mu')$,

Distribution of q_0 in large-sample limit

Assuming approximations valid in the large sample (asymptotic) limit, we can write down the full distribution of q_0 as

$$f(q_0|\mu') = \left(1 - \Phi\left(\frac{\mu'}{\sigma}\right)\right) \delta(q_0) + \frac{1}{2} \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{q_0}} \exp\left[-\frac{1}{2} \left(\sqrt{q_0} - \frac{\mu'}{\sigma}\right)^2\right]$$

The special case $\mu' = 0$ is a “half chi-square” distribution:

$$f(q_0|0) = \frac{1}{2} \delta(q_0) + \frac{1}{2} \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{q_0}} e^{-q_0/2}$$

In large sample limit, $f(q_0|0)$ independent of nuisance parameters; $f(q_0|\mu')$ depends on nuisance parameters through σ .

Cumulative distribution of q_0 , significance

From the pdf, the cumulative distribution of q_0 is found to be

$$F(q_0|\mu') = \Phi\left(\sqrt{q_0} - \frac{\mu'}{\sigma}\right)$$

The special case $\mu' = 0$ is

$$F(q_0|0) = \Phi(\sqrt{q_0})$$

The p -value of the $\mu = 0$ hypothesis is

$$p_0 = 1 - F(q_0|0)$$

Therefore the discovery significance Z is simply

$$Z = \Phi^{-1}(1 - p_0) = \sqrt{q_0}$$

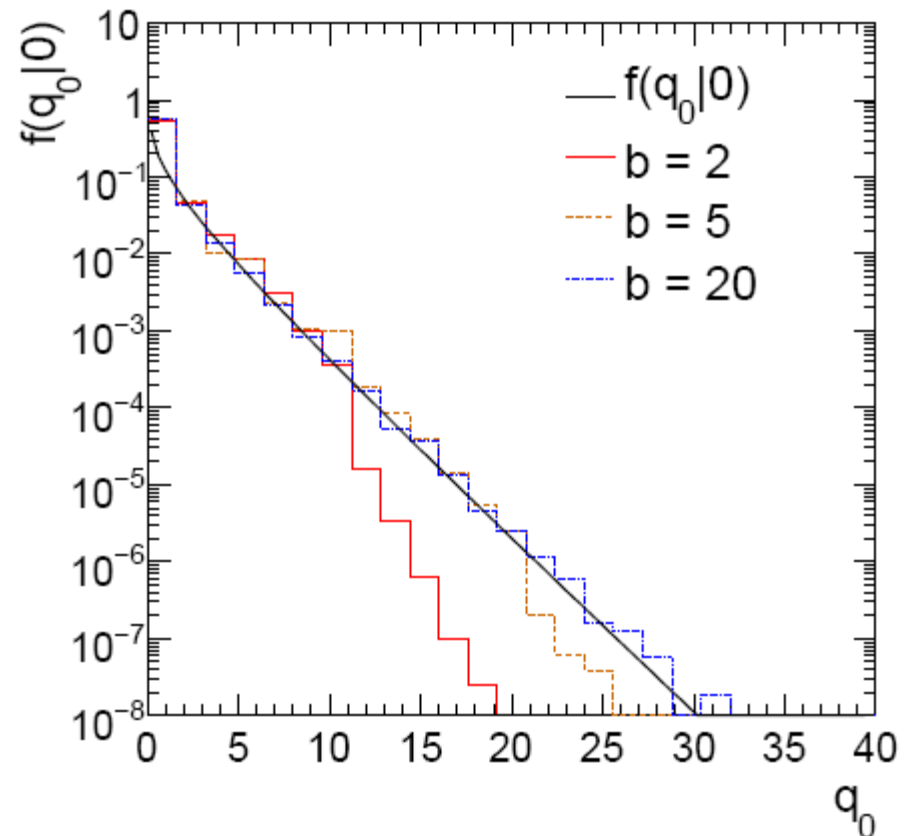
Monte Carlo test of asymptotic formula

$$n \sim \text{Poisson}(\mu s + b)$$

$$m \sim \text{Poisson}(\tau b)$$

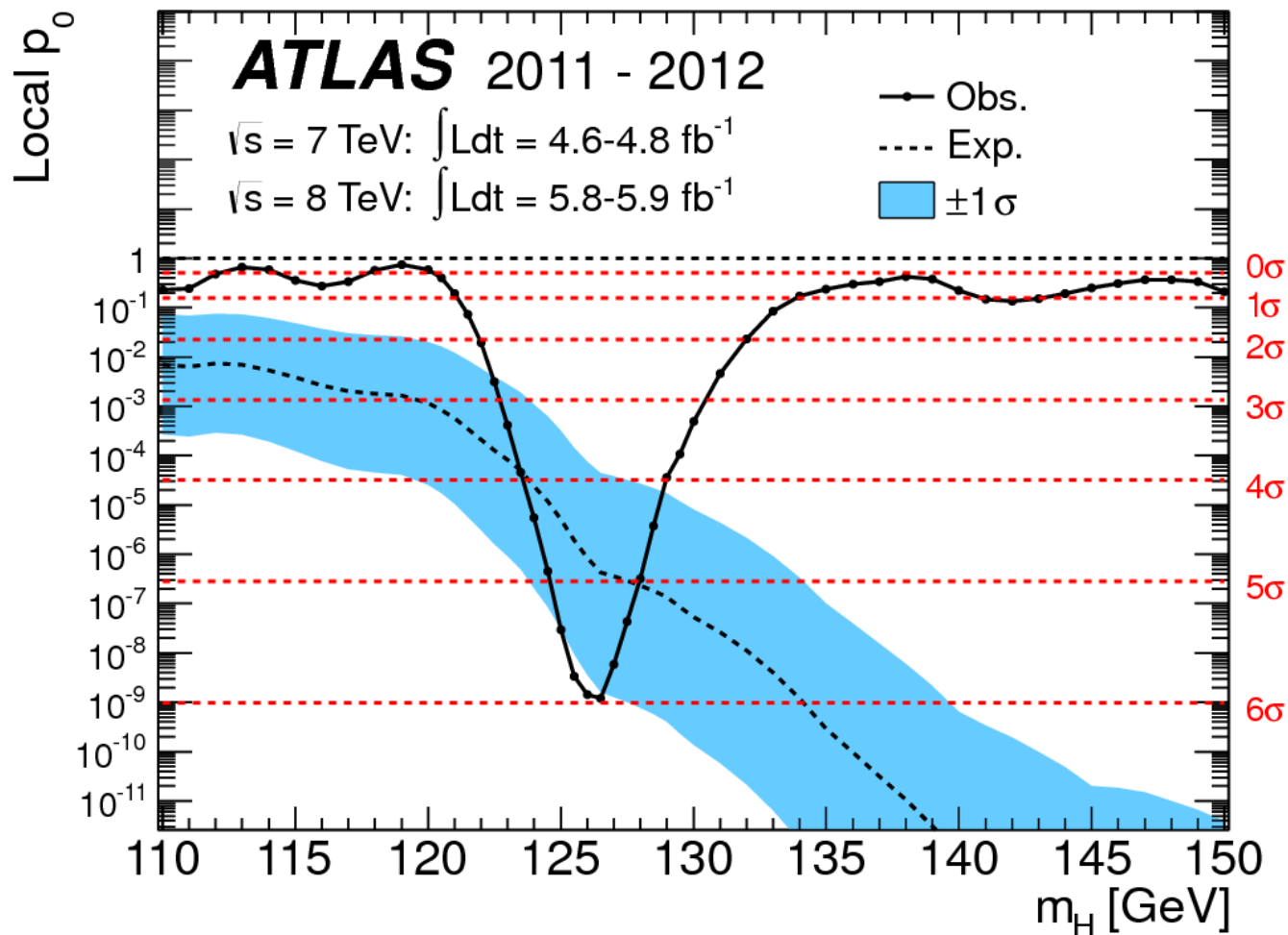
Here take $\tau = 1$.

Asymptotic formula is good approximation to 5σ level ($q_0 = 25$) already for $b \sim 20$.



Example of a p -value

ATLAS, Phys. Lett. B 716 (2012) 1-29



Back to Poisson counting experiment

$n \sim \text{Poisson}(s+b)$, where

s = expected number of events from signal,

b = expected number of background events.

To test for discovery of signal compute p -value of $s = 0$ hypothesis,

$$p = P(n \geq n_{\text{obs}} | b) = \sum_{n=n_{\text{obs}}}^{\infty} \frac{b^n}{n!} e^{-b} = 1 - F_{\chi^2}(2b; 2n_{\text{obs}})$$

Usually convert to equivalent significance: $Z = \Phi^{-1}(1 - p)$
where Φ is the standard Gaussian cumulative distribution, e.g.,
 $Z > 5$ (a 5 sigma effect) means $p < 2.9 \times 10^{-7}$.

To characterize sensitivity to discovery, give expected (mean or median) Z under assumption of a given s .

s/\sqrt{b} for expected discovery significance

For large $s + b$, $n \rightarrow x \sim \text{Gaussian}(\mu, \sigma)$, $\mu = s + b$, $\sigma = \sqrt{s + b}$.

For observed value x_{obs} , p -value of $s = 0$ is $\text{Prob}(x > x_{\text{obs}} | s = 0)$,:

$$p_0 = 1 - \Phi\left(\frac{x_{\text{obs}} - b}{\sqrt{b}}\right)$$

Significance for rejecting $s = 0$ is therefore

$$Z_0 = \Phi^{-1}(1 - p_0) = \frac{x_{\text{obs}} - b}{\sqrt{b}}$$

Expected (median) significance assuming signal rate s is

$$\text{median}[Z_0 | s + b] = \frac{s}{\sqrt{b}}$$

Better approximation for significance

Poisson likelihood for parameter s is

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

For now
no nuisance
params.

To test for discovery use profile likelihood ratio:

$$q_0 = \begin{cases} -2 \ln \lambda(0) & \hat{s} \geq 0, \\ 0 & \hat{s} < 0. \end{cases} \quad \lambda(s) = \frac{L(s, \hat{\theta}(s))}{L(\hat{s}, \hat{\theta})}$$

So the likelihood ratio statistic for testing $s = 0$ is

$$q_0 = -2 \ln \frac{L(0)}{L(\hat{s})} = 2 \left(n \ln \frac{n}{b} + b - n \right) \quad \text{for } n > b, \quad 0 \text{ otherwise}$$

Approximate Poisson significance (continued)

For sufficiently large $s + b$, (use Wilks' theorem),

$$Z = \sqrt{2 \left(n \ln \frac{n}{b} + b - n \right)} \quad \text{for } n > b \text{ and } Z = 0 \text{ otherwise.}$$

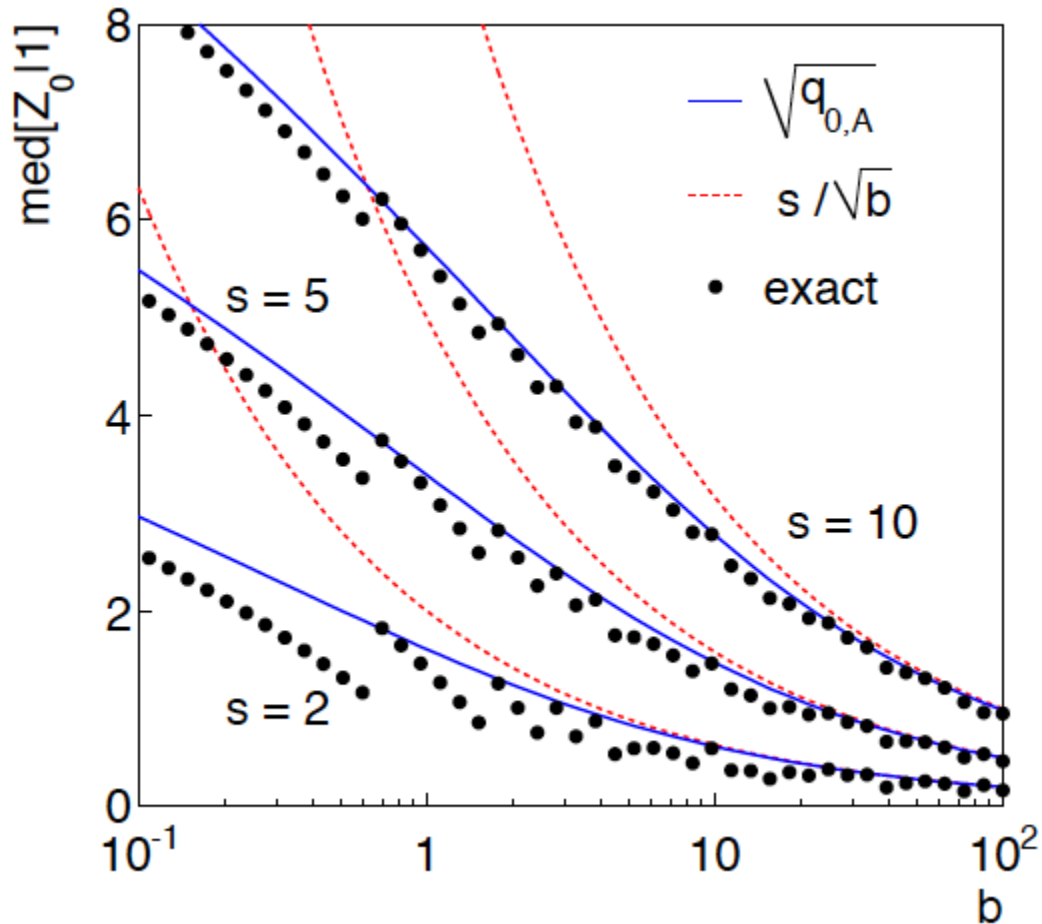
To find $\text{median}[Z|s]$, let $n \rightarrow s + b$ (i.e., the Asimov data set):

$$Z_A = \sqrt{2 \left((s + b) \ln \left(1 + \frac{s}{b} \right) - s \right)}$$

This reduces to s/\sqrt{b} for $s \ll b$.

$n \sim \text{Poisson}(s+b)$, median significance,
assuming s , of the hypothesis $s = 0$

CCGV, EPJC 71 (2011) 1554, arXiv:1007.1727



“Exact” values from MC,
jumps due to discrete data.

Asimov $\sqrt{q_{0,A}}$ good approx.
for broad range of s, b .

s/\sqrt{b} only good for $s \ll b$.

Extending s/\sqrt{b} to case where b uncertain

The intuitive explanation of s/\sqrt{b} is that it compares the signal, s , to the standard deviation of n assuming no signal, \sqrt{b} .

Now suppose the value of b is uncertain, characterized by a standard deviation σ_b .

A reasonable guess is to replace \sqrt{b} by the quadratic sum of \sqrt{b} and σ_b , i.e.,

$$\text{med}[Z|s] = \frac{s}{\sqrt{b + \sigma_b^2}}$$

This has been used to optimize some analyses e.g. where σ_b cannot be neglected.

Adding a control measurement for b

(The “on/off” problem: Cranmer 2005; Cousins, Linnemann, and Tucker 2008; Li and Ma 1983,...)

Measure two Poisson distributed values:

$n \sim \text{Poisson}(s+b)$ (primary or “search” measurement)

$m \sim \text{Poisson}(\tau b)$ (control measurement, τ known)

The likelihood function is

$$L(s, b) = \frac{(s+b)^n}{n!} e^{-(s+b)} \frac{(\tau b)^m}{m!} e^{-\tau b}$$

Use this to construct profile likelihood ratio (b is nuisance parameter):

$$\lambda(0) = \frac{L(0, \hat{b}(0))}{L(\hat{s}, \hat{b})}$$

Ingredients for profile likelihood ratio

To construct profile likelihood ratio from this need estimators:

$$\hat{s} = n - m/\tau ,$$

$$\hat{b} = m/\tau ,$$

$$\hat{b}(s) = \frac{n + m - (1 + \tau)s + \sqrt{(n + m - (1 + \tau)s)^2 + 4(1 + \tau)sm}}{2(1 + \tau)} .$$

and in particular to test for discovery ($s = 0$),

$$\hat{b}(0) = \frac{n + m}{1 + \tau}$$

Asymptotic significance

Use profile likelihood ratio for q_0 , and then from this get discovery significance using asymptotic approximation (Wilks' theorem):

$$Z = \sqrt{q_0} \\ = \left[-2 \left(n \ln \left[\frac{n+m}{(1+\tau)n} \right] + m \ln \left[\frac{\tau(n+m)}{(1+\tau)m} \right] \right) \right]^{1/2}$$

for $n > \hat{b}$ and $Z = 0$ otherwise.

Essentially same as in:

Robert D. Cousins, James T. Linnemann and Jordan Tucker, NIM A 595 (2008) 480–501; arXiv:physics/0702156.

Tipei Li and Yuqian Ma, Astrophysical Journal 272 (1983) 317–324.

Asimov approximation for median significance

To get median discovery significance, replace n , m by their expectation values assuming background-plus-signal model:

$$n \rightarrow s + b$$

$$m \rightarrow \tau b$$

$$Z_A = \left[-2 \left((s + b) \ln \left[\frac{s + (1 + \tau)b}{(1 + \tau)(s + b)} \right] + \tau b \ln \left[1 + \frac{s}{(1 + \tau)b} \right] \right) \right]^{1/2}$$

Or use the variance of $\hat{b} = m/\tau$, $V[\hat{b}] \equiv \sigma_b^2 = \frac{b}{\tau}$, to eliminate τ :

$$Z_A = \left[2 \left((s + b) \ln \left[\frac{(s + b)(b + \sigma_b^2)}{b^2 + (s + b)\sigma_b^2} \right] - \frac{b^2}{\sigma_b^2} \ln \left[1 + \frac{\sigma_b^2 s}{b(b + \sigma_b^2)} \right] \right) \right]^{1/2}$$

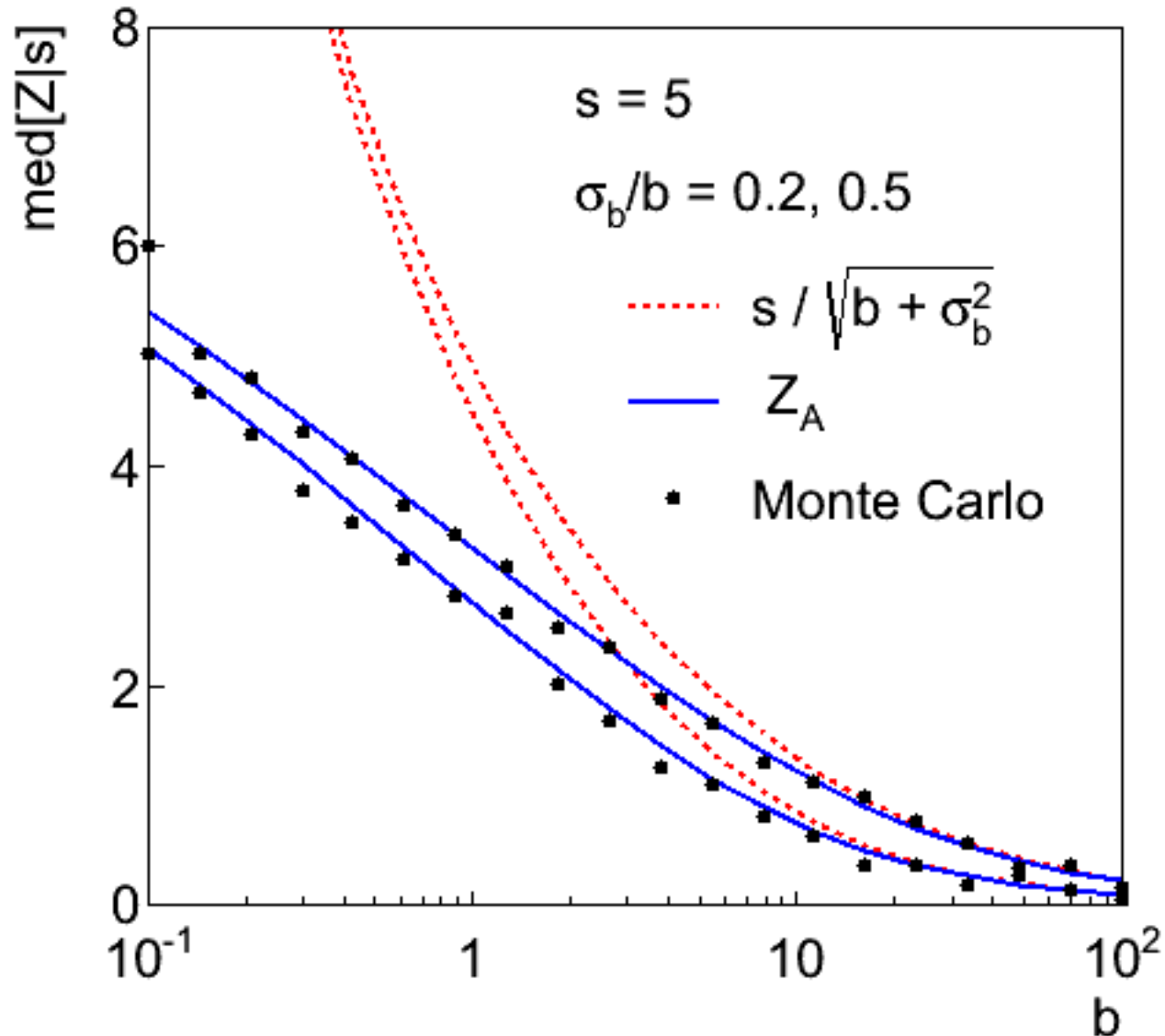
Limiting cases

Expanding the Asimov formula in powers of s/b and σ_b^2/b ($= 1/\tau$) gives

$$Z_A = \frac{s}{\sqrt{b + \sigma_b^2}} \left(1 + \mathcal{O}(s/b) + \mathcal{O}(\sigma_b^2/b) \right)$$

So this “intuitive” formula can be justified as a limiting case of the significance from the profile likelihood ratio test evaluated with the Asimov data set.

Testing the formulae: $s = 5$



Using sensitivity to optimize a cut

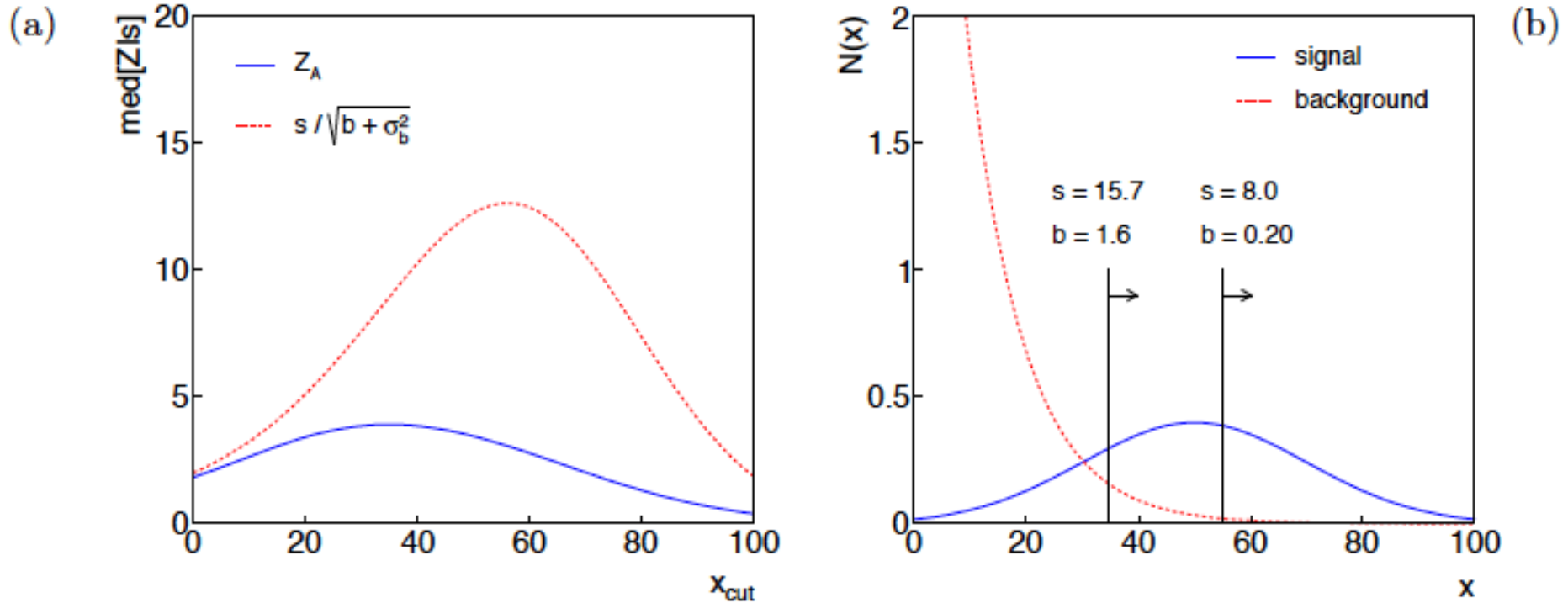


Figure 1: (a) The expected significance as a function of the cut value x_{cut} ; (b) the distributions of signal and background with the optimal cut value indicated.

Return to interval estimation

Suppose a model contains a parameter μ ; we want to know which values are consistent with the data and which are disfavoured.

Carry out a test of size α for all values of μ .

The values that are not rejected constitute a *confidence interval* for μ at confidence level $CL = 1 - \alpha$.

The probability that the true value of μ will be rejected is not greater than α , so by construction the confidence interval will contain the true value of μ with probability $\geq 1 - \alpha$.

The interval depends on the choice of the test (critical region).

If the test is formulated in terms of a p -value, p_μ , then the confidence interval represents those values of μ for which $p_\mu > \alpha$.

To find the end points of the interval, set $p_\mu = \alpha$ and solve for μ .

Test statistic for upper limits

cf. Cowan, Cranmer, Gross, Vitells, arXiv:1007.1727, EPJC 71 (2011) 1554.

For purposes of setting an upper limit on μ one can use

$$q_\mu = \begin{cases} -2 \ln \lambda(\mu) & \hat{\mu} \leq \mu \\ 0 & \hat{\mu} > \mu \end{cases} \quad \text{where} \quad \lambda(\mu) = \frac{L(\mu, \hat{\boldsymbol{\theta}})}{L(\hat{\mu}, \hat{\boldsymbol{\theta}})}$$

I.e. when setting an upper limit, an upwards fluctuation of the data is not taken to mean incompatibility with the hypothesized μ :

From observed q_μ find p -value:
$$p_\mu = \int_{q_{\mu, \text{obs}}}^{\infty} f(q_\mu | \mu) dq_\mu$$

Large sample approximation:

$$p_\mu = 1 - \Phi(\sqrt{q_\mu})$$

95% CL upper limit on μ is highest value for which p -value is not less than 0.05.

Monte Carlo test of asymptotic formulae

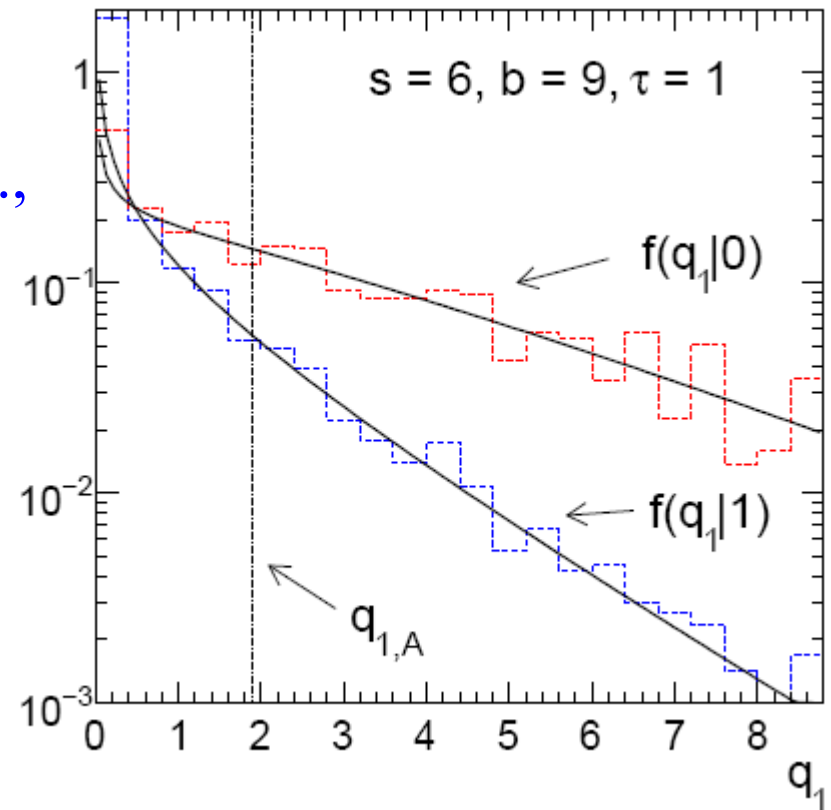
Consider again $n \sim \text{Poisson}(\mu s + b)$, $m \sim \text{Poisson}(\tau b)$
 Use q_μ to find p -value of hypothesized μ values.

E.g. $f(q_1|1)$ for p -value of $\mu = 1$.

Typically interested in 95% CL, i.e.,
 p -value threshold = 0.05, i.e.,
 $q_1 = 2.69$ or $Z_1 = \sqrt{q_1} = 1.64$.

Median[$q_1 | 0$] gives “exclusion sensitivity”.

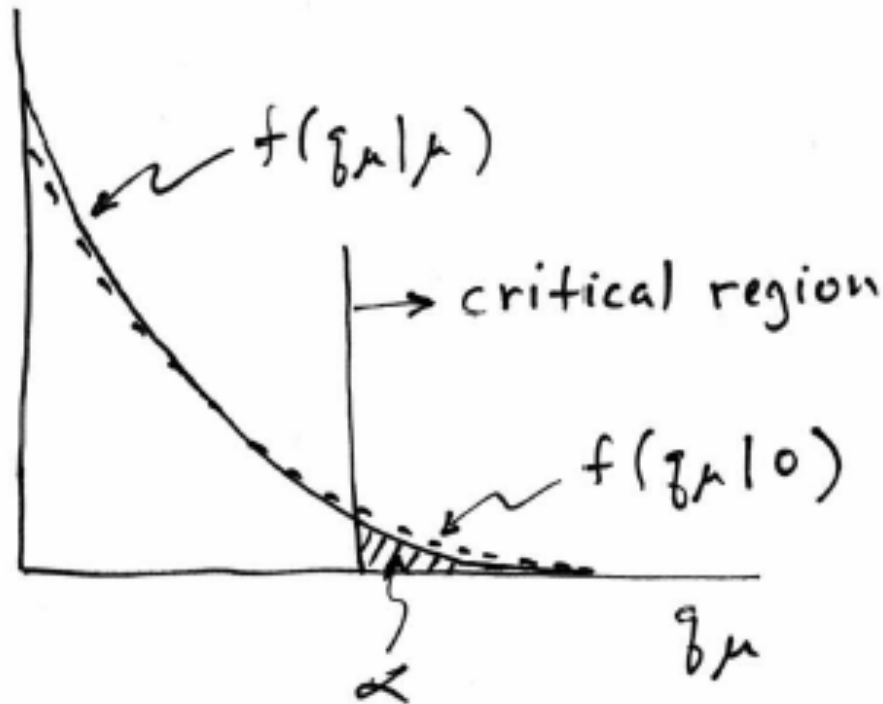
Here asymptotic formulae good
 for $s = 6$, $b = 9$.



Low sensitivity to μ

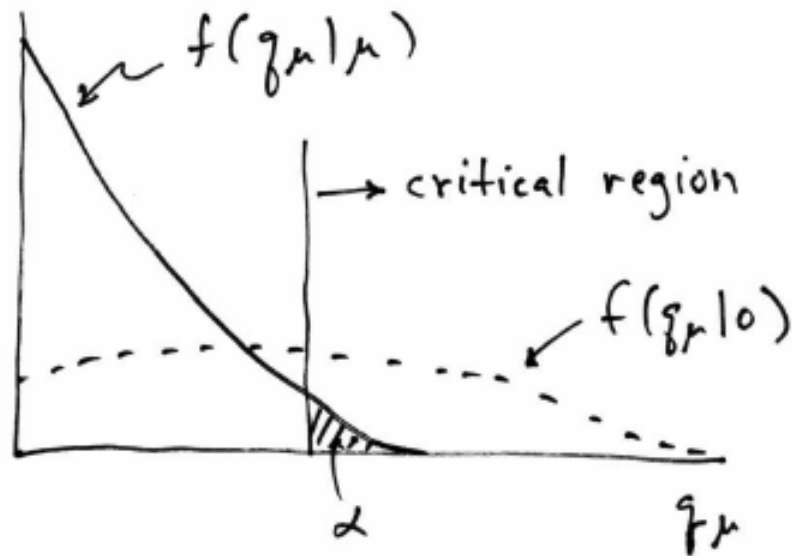
It can be that the effect of a given hypothesized μ is very small relative to the background-only ($\mu = 0$) prediction.

This means that the distributions $f(q_\mu|\mu)$ and $f(q_\mu|0)$ will be almost the same:



Having sufficient sensitivity

In contrast, having sensitivity to μ means that the distributions $f(q_\mu|\mu)$ and $f(q_\mu|0)$ are more separated:

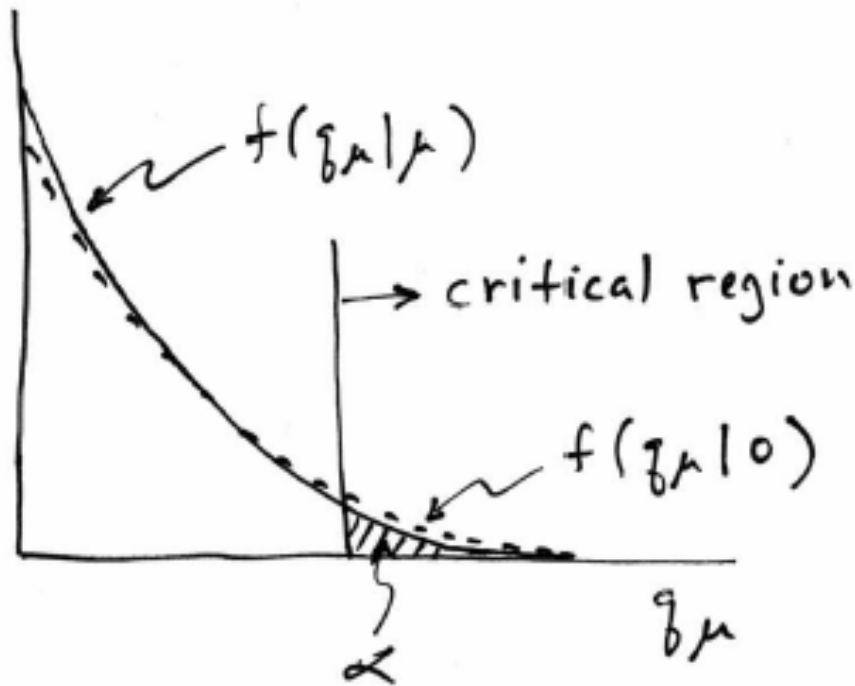


That is, the power (probability to reject μ if $\mu = 0$) is substantially higher than α . Use this power as a measure of the sensitivity.

Spurious exclusion

Consider again the case of low sensitivity. By construction the probability to reject μ if μ is true is α (e.g., 5%).

And the probability to reject μ if $\mu = 0$ (the power) is only slightly greater than α .



This means that with probability of around $\alpha = 5\%$ (slightly higher), one excludes hypotheses to which one has essentially no sensitivity (e.g., $m_H = 1000$ TeV).

“Spurious exclusion”

Ways of addressing spurious exclusion

The problem of excluding parameter values to which one has no sensitivity known for a long time; see e.g.,

Virgil L. Highland, *Estimation of Upper Limits from Experimental Data*, July 1986, Revised February 1987, Temple University Report C00-3539-38.

In the 1990s this was re-examined for the LEP Higgs search by Alex Read and others

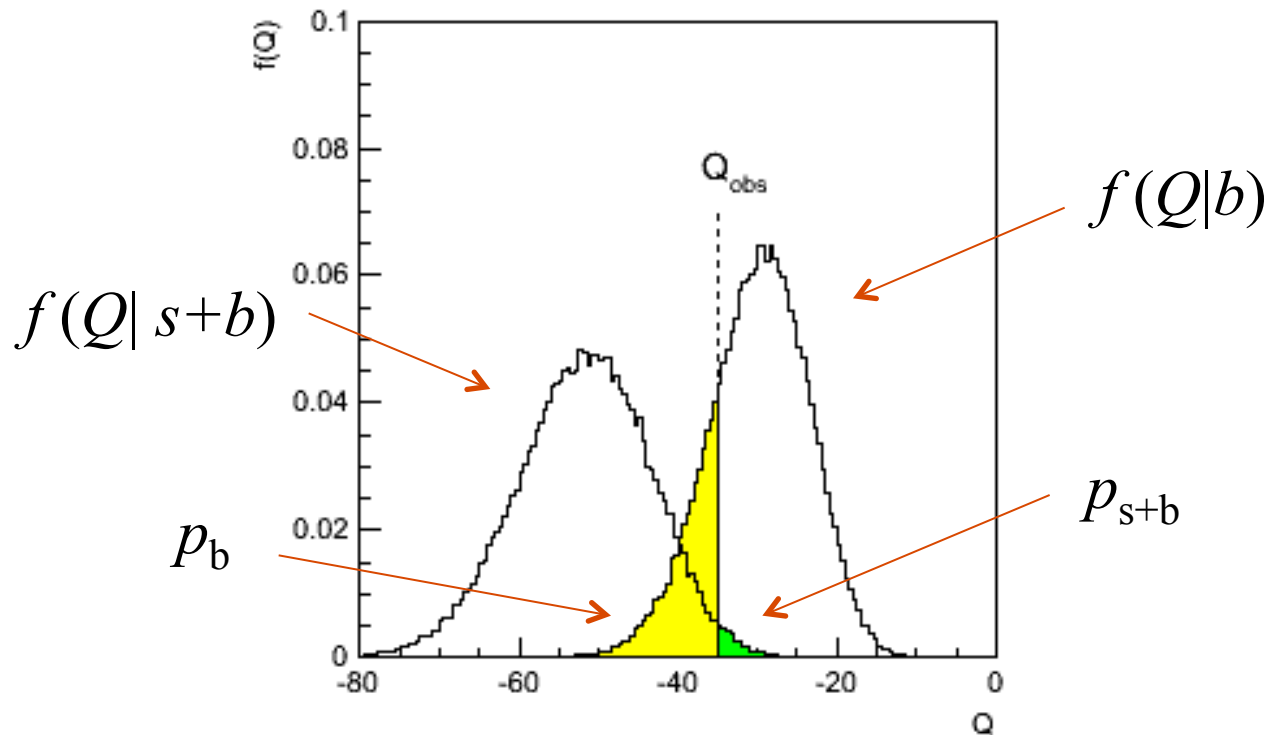
T. Junk, Nucl. Instrum. Methods Phys. Res., Sec. A **434**, 435 (1999); A.L. Read, J. Phys. G **28**, 2693 (2002).

and led to the “ CL_s ” procedure for upper limits.

Unified intervals also effectively reduce spurious exclusion by the particular choice of critical region.

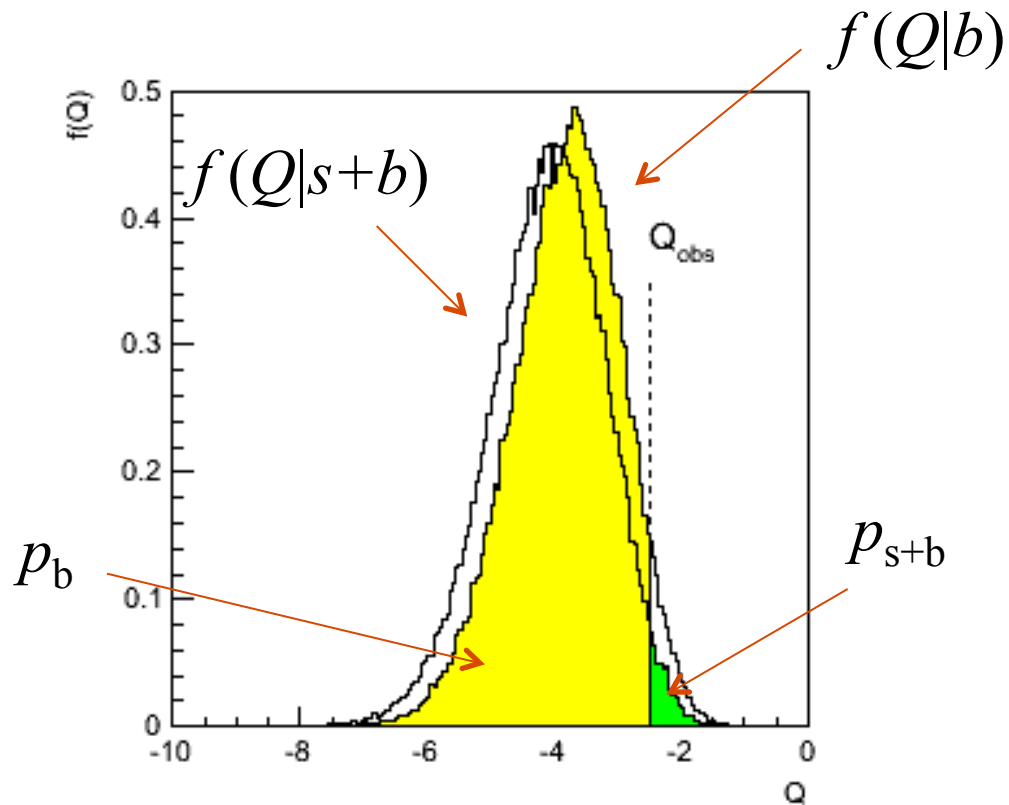
The CL_s procedure

In the usual formulation of CL_s , one tests both the $\mu = 0$ (b) and $\mu > 0$ ($\mu s+b$) hypotheses with the same statistic $Q = -2\ln L_{s+b}/L_b$:



The CL_s procedure (2)

As before, “low sensitivity” means the distributions of Q under b and $s+b$ are very close:



The CL_s procedure (3)

The CL_s solution (A. Read et al.) is to base the test not on the usual p -value (CL_{s+b}), but rather to divide this by CL_b (\sim one minus the p -value of the b -only hypothesis), i.e.,

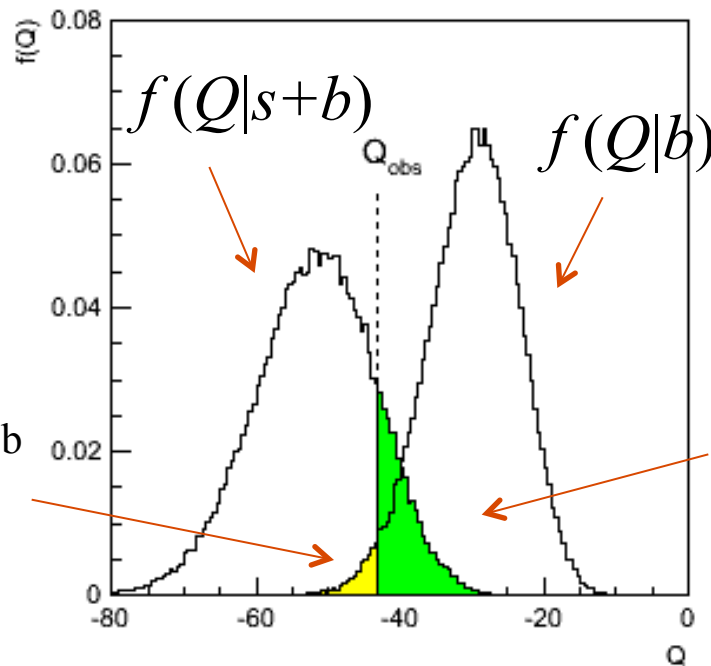
Define:

$$CL_s = \frac{CL_{s+b}}{CL_b} = \frac{p_{s+b}}{1 - p_b}$$

Reject $s+b$ hypothesis if:

$$CL_s \leq \alpha$$

$$1 - CL_b = p_b$$



$$CL_{s+b} = p_{s+b}$$

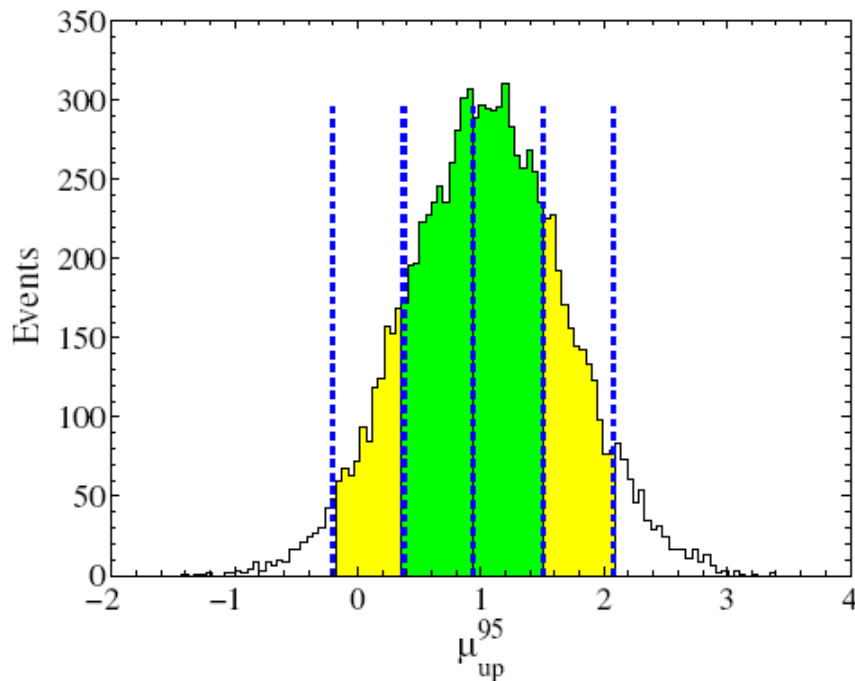
Reduces “effective” p -value when the two distributions become close (prevents exclusion if sensitivity is low).

Setting upper limits on $\mu = \sigma/\sigma_{\text{SM}}$

Carry out the CLs procedure for the parameter $\mu = \sigma/\sigma_{\text{SM}}$, resulting in an upper limit μ_{up} .

In, e.g., a Higgs search, this is done for each value of m_{H} .

At a given value of m_{H} , we have an observed value of μ_{up} , and we can also find the distribution $f(\mu_{\text{up}}|0)$:



$\pm 1\sigma$ (green) and $\pm 2\sigma$ (yellow) bands from toy MC;

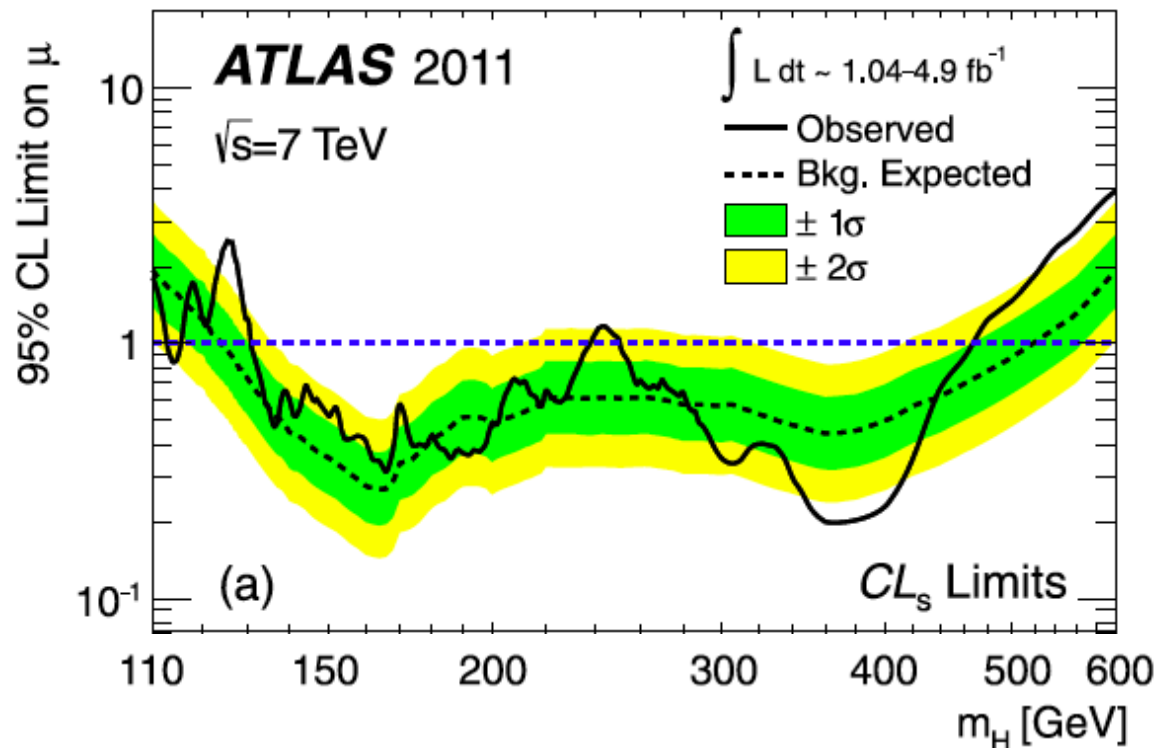
Vertical lines from asymptotic formulae.

How to read the green and yellow limit plots

For every value of m_H , find the CLs upper limit on μ .

Also for each m_H , determine the distribution of upper limits μ_{up} one would obtain under the hypothesis of $\mu = 0$.

The dashed curve is the median μ_{up} , and the green (yellow) bands give the $\pm 1\sigma$ (2σ) regions of this distribution.



ATLAS, Phys. Lett.
B 710 (2012) 49-66

Choice of test for limits (2)

In some cases $\mu = 0$ is no longer a relevant alternative and we want to try to exclude μ on the grounds that some other measure of incompatibility between it and the data exceeds some threshold.

If the measure of incompatibility is taken to be the likelihood ratio with respect to a two-sided alternative, then the critical region can contain both high and low data values.

→ unified intervals, G. Feldman, R. Cousins,
Phys. Rev. D 57, 3873–3889 (1998)

The Big Debate is whether to use one-sided or unified intervals in cases where small (or zero) values of the parameter are relevant alternatives. Professional statisticians have voiced support on both sides of the debate.

Unified (Feldman-Cousins) intervals

We can use directly

$$t_{\mu} = -2 \ln \lambda(\mu) \quad \text{where} \quad \lambda(\mu) = \frac{L(\mu, \hat{\boldsymbol{\theta}})}{L(\hat{\mu}, \hat{\boldsymbol{\theta}})}$$

as a test statistic for a hypothesized μ .

Large discrepancy between data and hypothesis can correspond either to the estimate for μ being observed high or low relative to μ .

This is essentially the statistic used for Feldman-Cousins intervals (here also treats nuisance parameters).

G. Feldman and R.D. Cousins, Phys. Rev. D 57 (1998) 3873.

Lower edge of interval can be at $\mu = 0$, depending on data.

Distribution of t_μ

Using Wald approximation, $f(t_\mu|\mu')$ is noncentral chi-square for one degree of freedom:

$$f(t_\mu|\mu') = \frac{1}{2\sqrt{t_\mu}} \frac{1}{\sqrt{2\pi}} \left[\exp\left(-\frac{1}{2}\left(\sqrt{t_\mu} + \frac{\mu - \mu'}{\sigma}\right)^2\right) + \exp\left(-\frac{1}{2}\left(\sqrt{t_\mu} - \frac{\mu - \mu'}{\sigma}\right)^2\right) \right]$$

Special case of $\mu = \mu'$ is chi-square for one d.o.f. (Wilks).

The p -value for an observed value of t_μ is

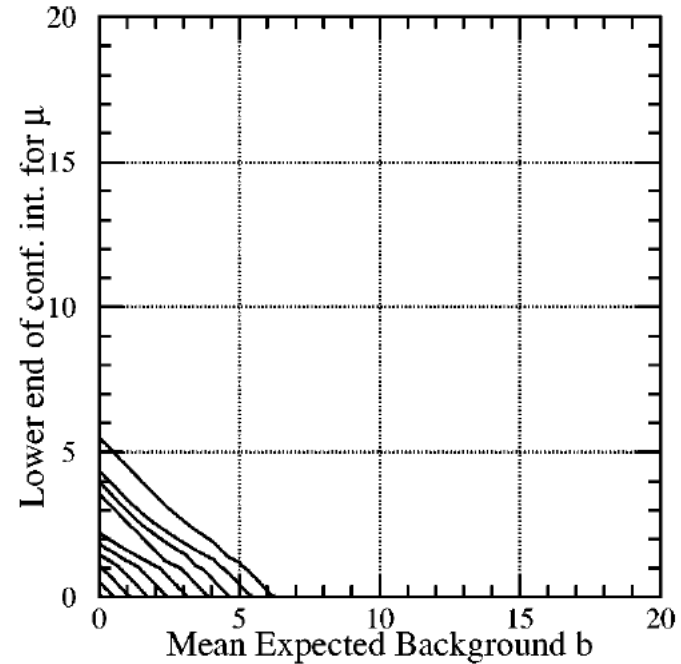
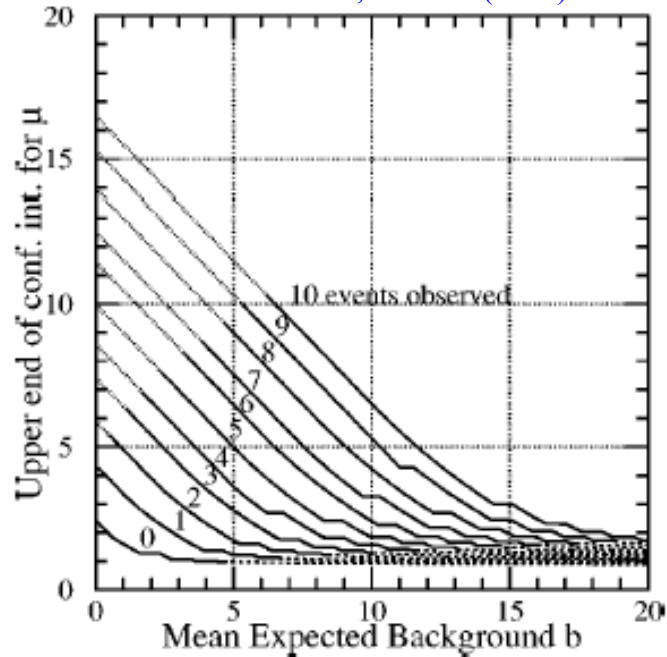
$$p_\mu = 1 - F(t_\mu|\mu) = 2(1 - \Phi(\sqrt{t_\mu}))$$

and the corresponding significance is

$$Z_\mu = \Phi^{-1}(1 - p_\mu) = \Phi^{-1}(2\Phi(\sqrt{t_\mu}) - 1)$$

Upper/lower edges of F-C interval for μ versus b for $n \sim \text{Poisson}(\mu+b)$

Feldman & Cousins, PRD 57 (1998) 3873



Lower edge may be at zero, depending on data.

For $n = 0$, upper edge has (weak) dependence on b .

Feldman-Cousins discussion

The initial motivation for Feldman-Cousins (unified) confidence intervals was to eliminate null intervals.

The F-C limits are based on a likelihood ratio for a test of μ with respect to the alternative consisting of all other allowed values of μ (not just, say, lower values).

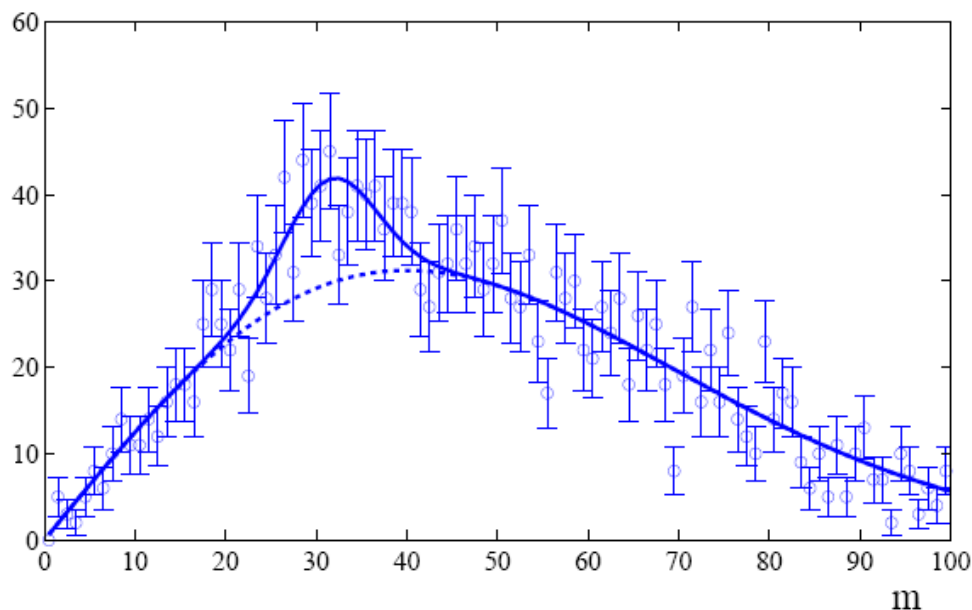
The interval's upper edge is higher than the limit from the one-sided test, and lower values of μ may be excluded as well. A substantial downward fluctuation in the data gives a low (but nonzero) limit.

This means that when a value of μ is excluded, it is because there is a probability α for the data to fluctuate either high or low in a manner corresponding to less compatibility as measured by the likelihood ratio.

The Look-Elsewhere Effect

Suppose a model for a mass distribution allows for a peak at a mass m with amplitude μ .

The data show a bump at a mass m_0 .



How consistent is this with the no-bump ($\mu = 0$) hypothesis?

Local p -value

First, suppose the mass m_0 of the peak was specified a priori.

Test consistency of bump with the no-signal ($\mu = 0$) hypothesis with e.g. likelihood ratio

$$t_{\text{fix}} = -2 \ln \frac{L(0, m_0)}{L(\hat{\mu}, m_0)}$$

where “fix” indicates that the mass of the peak is fixed to m_0 .

The resulting p -value

$$p_{\text{local}} = \int_{t_{\text{fix,obs}}}^{\infty} f(t_{\text{fix}}|0) dt_{\text{fix}}$$

gives the probability to find a value of t_{fix} at least as great as observed **at the specific mass m_0** and is called the **local p -value**.

Global p -value

But suppose we did not know where in the distribution to expect a peak.

What we want is the probability to find a peak at least as significant as the one observed **anywhere** in the distribution.

Include the mass as an adjustable parameter in the fit, test significance of peak using

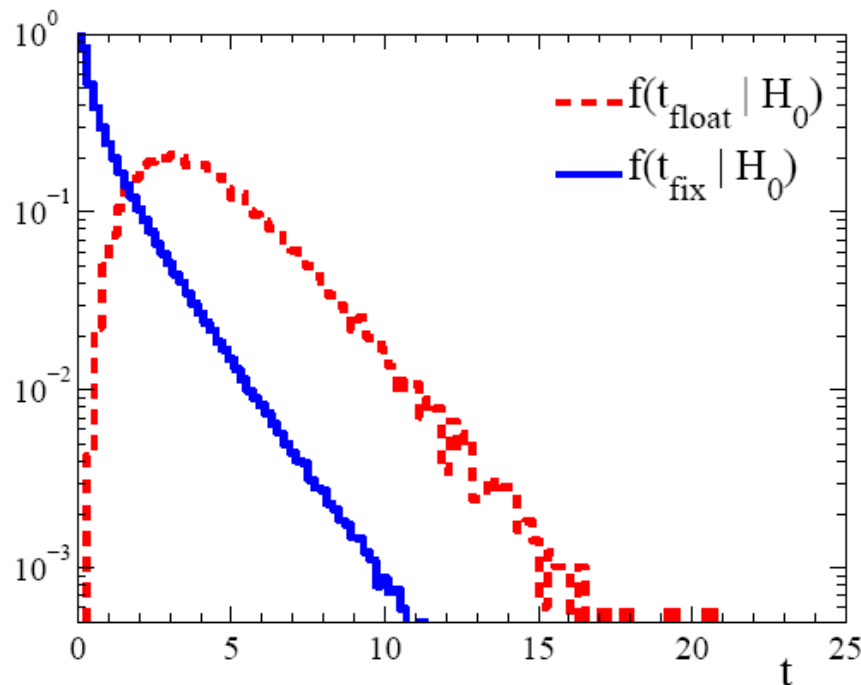
$$t_{\text{float}} = -2 \ln \frac{L(0)}{L(\hat{\mu}, \hat{m})} \quad (\text{Note } m \text{ does not appear in the } \mu = 0 \text{ model.})$$

$$p_{\text{global}} = \int_{t_{\text{float,obs}}}^{\infty} f(t_{\text{float}}|0) dt_{\text{float}}$$

Distributions of t_{fix} , t_{float}

For a sufficiently large data sample, $t_{\text{fix}} \sim \text{chi-square}$ for 1 degree of freedom (Wilks' theorem).

For t_{float} there are two adjustable parameters, μ and m , and naively Wilks theorem says $t_{\text{float}} \sim \text{chi-square}$ for 2 d.o.f.



In fact Wilks' theorem does not hold in the floating mass case because one of the parameters (m) is not defined in the $\mu = 0$ model.

So getting t_{float} distribution is more difficult.

Approximate correction for LEE

We would like to be able to relate the p -values for the fixed and floating mass analyses (at least approximately).

Gross and Vitells show the p -values are approximately related by

$$p_{\text{global}} \approx p_{\text{local}} + \langle N(c) \rangle$$

where $\langle N(c) \rangle$ is the mean number “upcrossings” of $t_{\text{fix}} = -2 \ln \lambda$ in the fit range based on a threshold

$$c = t_{\text{fix,obs}} = Z_{\text{local}}^2$$

and where $Z_{\text{local}} = \Phi^{-1}(1 - p_{\text{local}})$ is the local significance.

So we can either carry out the full floating-mass analysis (e.g. use MC to get p -value), or do fixed mass analysis and apply a correction factor (much faster than MC).

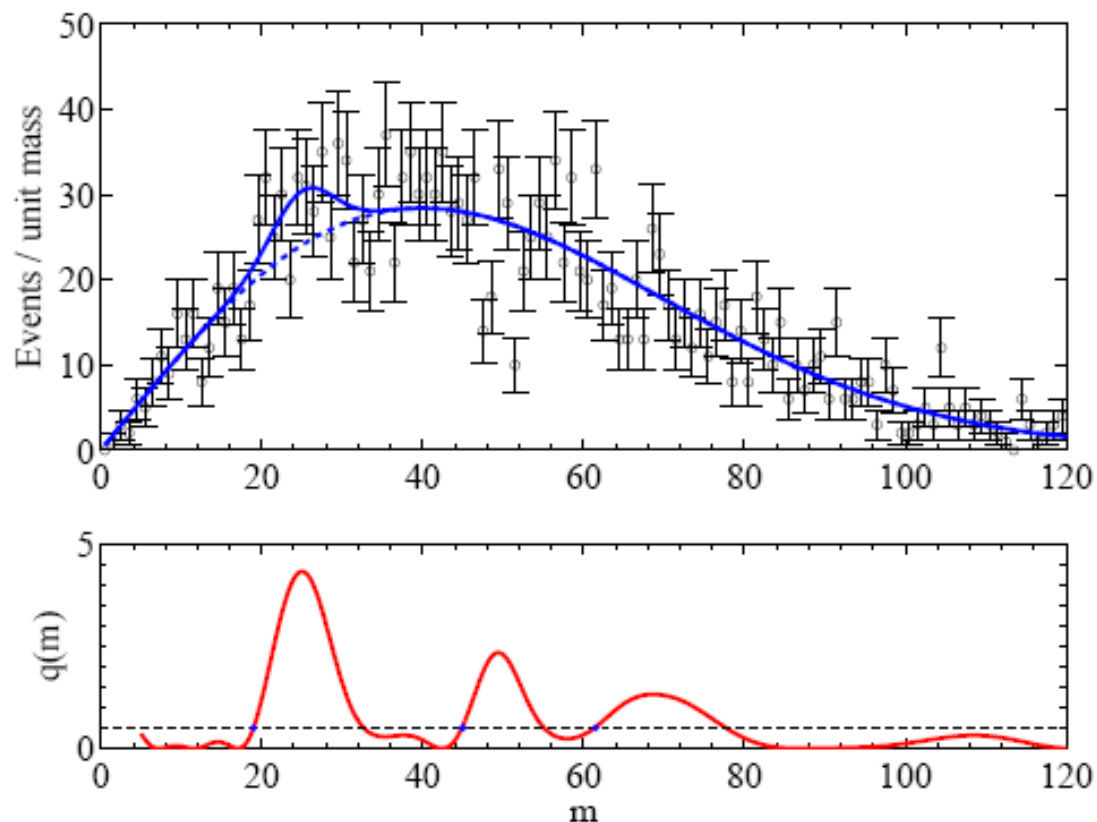
Upcrossings of $-2\ln L$

The Gross-Vitells formula for the trials factor requires $\langle N(c) \rangle$, the mean number “upcrossings” of $t_{\text{fix}} = -2\ln \lambda$ in the fit range based on a threshold $c = t_{\text{fix}} = Z_{\text{fix}}^2$.

$\langle N(c) \rangle$ can be estimated from MC (or the real data) using a much lower threshold c_0 :

$$\langle N(c) \rangle \approx \langle N(c_0) \rangle e^{-(c-c_0)/2}$$

In this way $\langle N(c) \rangle$ can be estimated without need of large MC samples, even if the the threshold c is quite high.

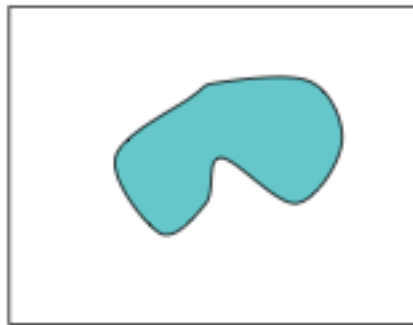


Multidimensional look-elsewhere effect

Generalization to multiple dimensions: number of upcrossings replaced by expectation of Euler characteristic:

$$E[\varphi(A_u)] = \sum_{d=0}^n \mathcal{N}_d \rho_d(u)$$

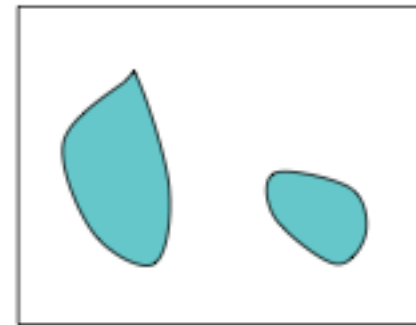
- Number of disconnected components minus number of 'holes'



$\varphi=1$



$\varphi=0$



$\varphi=2$

Applications: astrophysics (coordinates on sky), search for resonance of unknown mass and width, ...

Summary on Look-Elsewhere Effect

Remember the Look-Elsewhere Effect is when we test a single model (e.g., SM) with multiple observations, i.e., in multiple places.

Note there is no look-elsewhere effect when considering exclusion limits. There we test specific signal models (typically once) and say whether each is excluded.

With exclusion there is, however, the analogous issue of testing many signal models (or parameter values) and thus excluding some even in the absence of signal (“spurious exclusion”)

Approximate correction for LEE should be sufficient, and one should also report the uncorrected significance.

“There's no sense in being precise when you don't even know what you're talking about.” — John von Neumann

Why 5 sigma?

Common practice in HEP has been to claim a discovery if the p -value of the no-signal hypothesis is below 2.9×10^{-7} , corresponding to a significance $Z = \Phi^{-1}(1 - p) = 5$ (a 5σ effect).

There a number of reasons why one may want to require such a high threshold for discovery:

- The “cost” of announcing a false discovery is high.

- Unsure about systematics.

- Unsure about look-elsewhere effect.

- The implied signal may be a priori highly improbable (e.g., violation of Lorentz invariance).

Why 5 sigma (cont.)?

But the primary role of the p -value is to quantify the probability that the background-only model gives a statistical fluctuation as big as the one seen or bigger.

It is not intended as a means to protect against hidden systematics or the high standard required for a claim of an important discovery.

In the processes of establishing a discovery there comes a point where it is clear that the observation is not simply a fluctuation, but an “effect”, and the focus shifts to whether this is new physics or a systematic.

Providing LEE is dealt with, that threshold is probably closer to 3σ than 5σ .

Partial summary

Systematic uncertainties can be taken into account by including more (nuisance) parameters into the model.

Reduces sensitivity to the parameter of interest

Treatment of nuisance parameters:

Frequentist: profile

Bayesian: marginalize

Asymptotic formulae for profile likelihood ratio statistic

Independent of nuisance parameters for large sample

Experimental sensitivity

Discovery: expected (median) significance for test of background- only hypothesis assuming presence of signal.

Limits: expected limit on signal rate assuming no signal.


Other topics: CLs, Look-elsewhere effect, ...


Extra slides


Bayesian model selection (‘discovery’)


The probability of hypothesis H_0 relative to an alternative H_1 is often given by the posterior odds:

$$\frac{P(H_0|x)}{P(H_1|x)} = \frac{P(x|H_0)}{P(x|H_1)} \times \frac{\pi(H_0)}{\pi(H_1)}$$

no Higgs 

Higgs 

Bayes factor B_{01} 

prior odds 

The Bayes factor is regarded as measuring the weight of evidence of the data in support of H_0 over H_1 .

Interchangeably use $B_{10} = 1/B_{01}$

Assessing Bayes factors

One can use the Bayes factor much like a p -value (or Z value).

The Jeffreys scale, analogous to HEP's 5σ rule:

B_{10}	Evidence against H_0
1 to 3	Not worth more than a bare mention
3 to 20	Positive
20 to 150	Strong
> 150	Very strong

Kass and Raftery, *Bayes Factors*, J. Am Stat. Assoc 90 (1995) 773.

Rewriting the Bayes factor

Suppose we have models H_i , $i = 0, 1, \dots$,

each with a likelihood $p(x|H_i, \vec{\theta}_i)$

and a prior pdf for its internal parameters $\pi_i(\vec{\theta}_i)$

so that the full prior is $\pi(H_i, \vec{\theta}_i) = p_i \pi_i(\vec{\theta}_i)$

where $p_i = P(H_i)$ is the overall prior probability for H_i .

The Bayes factor comparing H_i and H_j can be written

$$B_{ij} = \frac{P(H_i|\vec{x})}{P(H_i)} \bigg/ \frac{P(H_j|\vec{x})}{P(H_j)}$$

Bayes factors independent of $P(H_i)$

For B_{ij} we need the posterior probabilities marginalized over all of the internal parameters of the models:

$$\begin{aligned} P(H_i|\vec{x}) &= \int P(H_i, \vec{\theta}_i|\vec{x}) d\vec{\theta}_i \\ &= \frac{\int L(\vec{x}|H_i, \vec{\theta}_i) p_i \pi_i(\vec{\theta}_i) d\vec{\theta}_i}{P(x)} \end{aligned}$$

Use Bayes theorem

So therefore the Bayes factor is

$$B_{ij} = \frac{\int L(\vec{x}|H_i, \vec{\theta}_i) \pi_i(\vec{\theta}_i) d\vec{\theta}_i}{\int L(\vec{x}|H_j, \vec{\theta}_j) \pi_j(\vec{\theta}_j) d\vec{\theta}_j}$$

Ratio of marginal likelihoods

The prior probabilities $p_i = P(H_i)$ cancel.

Numerical determination of Bayes factors

Both numerator and denominator of B_{ij} are of the form

$$m = \int L(\vec{x}|\vec{\theta})\pi(\vec{\theta}) d\vec{\theta} \quad \leftarrow \text{‘marginal likelihood’}$$

Various ways to compute these, e.g., using sampling of the posterior pdf (which we can do with MCMC).

Harmonic Mean (and improvements)

Importance sampling

Parallel tempering (\sim thermodynamic integration)

Nested Sampling (MultiNest), ...

Kass and Raftery, *Bayes Factors*, J. Am. Stat. Assoc. 90 (1995) 773-795.

Cong Han and Bradley Carlin, *Markov Chain Monte Carlo Methods for Computing Bayes Factors: A Comparative Review*, J. Am. Stat. Assoc. 96 (2001) 1122-1132.

Phil Gregory, *Bayesian Logical Data Analysis for the Physical Sciences*, Cambridge University Press, 2005.

Priors for Bayes factors

Note that for Bayes factors (unlike Bayesian limits), the prior cannot be improper. If it is, the posterior is only defined up to an arbitrary constant, and so the Bayes factor is ill defined

Possible exception allowed if both models contain *same* improper prior; but having same parameter name (or Greek letter) in both models does not fully justify this step.

If improper prior is made proper e.g. by a cut-off, the Bayes factor will retain a dependence on this cut-off.

In general for Bayes factors, all priors must reflect “meaningful” degrees of uncertainty about the parameters.

Harmonic mean estimator

E.g., consider only one model and write Bayes theorem as:

$$\frac{\pi(\boldsymbol{\theta})}{m} = \frac{p(\boldsymbol{\theta}|\mathbf{x})}{L(\mathbf{x}|\boldsymbol{\theta})}$$

$\pi(\boldsymbol{\theta})$ is normalized to unity so integrate both sides,

$$m^{-1} = \int \frac{1}{L(\mathbf{x}|\boldsymbol{\theta})} p(\boldsymbol{\theta}|\mathbf{x}) d\boldsymbol{\theta} = E_p[1/L]$$

posterior
expectation



Therefore sample $\boldsymbol{\theta}$ from the posterior via MCMC and estimate m with one over the average of $1/L$ (the harmonic mean of L).

M.A. Newton and A.E. Raftery, *Approximate Bayesian Inference by the Weighted Likelihood Bootstrap*, Journal of the Royal Statistical Society B 56 (1994) 3-48.

Improvements to harmonic mean estimator

The harmonic mean estimator is numerically very unstable; formally infinite variance (!). Gelfand & Dey propose variant:

Rearrange Bayes thm; multiply both sides by arbitrary pdf $f(\boldsymbol{\theta})$:

$$\frac{f(\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{x})}{L(\mathbf{x}|\boldsymbol{\theta})\pi(\boldsymbol{\theta})} = \frac{f(\boldsymbol{\theta})}{m}$$

Integrate over $\boldsymbol{\theta}$: $m^{-1} = \int \frac{f(\boldsymbol{\theta})}{L(\mathbf{x}|\boldsymbol{\theta})\pi(\boldsymbol{\theta})} p(\boldsymbol{\theta}|\mathbf{x}) = E_p \left[\frac{f(\boldsymbol{\theta})}{L(\mathbf{x}|\boldsymbol{\theta})\pi(\boldsymbol{\theta})} \right]$

Improved convergence if tails of $f(\boldsymbol{\theta})$ fall off faster than $L(\mathbf{x}|\boldsymbol{\theta})\pi(\boldsymbol{\theta})$

Note harmonic mean estimator is special case $f(\boldsymbol{\theta}) = \pi(\boldsymbol{\theta})$.

A.E. Gelfand and D.K. Dey, *Bayesian model choice: asymptotics and exact calculations*, Journal of the Royal Statistical Society B 56 (1994) 501-514.

Importance sampling

Need pdf $f(\boldsymbol{\theta})$ which we can evaluate at arbitrary $\boldsymbol{\theta}$ and also sample with MC.

The marginal likelihood can be written

$$m = \int \frac{L(\mathbf{x}|\boldsymbol{\theta})\pi(\boldsymbol{\theta})}{f(\boldsymbol{\theta})} f(\boldsymbol{\theta}) d\boldsymbol{\theta} = E_f \left[\frac{L(\mathbf{x}|\boldsymbol{\theta})\pi(\boldsymbol{\theta})}{f(\boldsymbol{\theta})} \right]$$

Best convergence when $f(\boldsymbol{\theta})$ approximates shape of $L(\mathbf{x}|\boldsymbol{\theta})\pi(\boldsymbol{\theta})$.

Use for $f(\boldsymbol{\theta})$ e.g. multivariate Gaussian with mean and covariance estimated from posterior (e.g. with MINUIT).