

Statistical Methods for Particle Physics

<https://indico.mitp.uni-mainz.de/event/118/>



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Outline

Lecture 1:

Quick review of probability

Parameter estimation, maximum likelihood

Statistical tests for discovery and limits

Lecture 2:

Nuisance parameters and systematic uncertainties

Tests from profile likelihood ratio

More parameter estimation, Bayesian methods

Experimental sensitivity

Some statistics books, papers, etc.

G. Cowan, *Statistical Data Analysis*, Clarendon, Oxford, 1998

R.J. Barlow, *Statistics: A Guide to the Use of Statistical Methods in the Physical Sciences*, Wiley, 1989

Ilya Narsky and Frank C. Porter, *Statistical Analysis Techniques in Particle Physics*, Wiley, 2014.

L. Lyons, *Statistics for Nuclear and Particle Physics*, CUP, 1986

F. James., *Statistical and Computational Methods in Experimental Physics*, 2nd ed., World Scientific, 2006

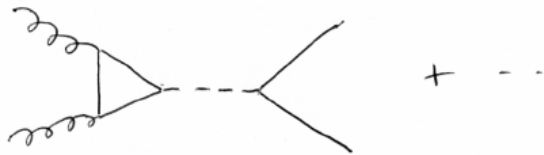
S. Brandt, *Statistical and Computational Methods in Data Analysis*, Springer, New York, 1998 (with program library on CD)

C. Patrignani et al. (Particle Data Group), *Review of Particle Physics*, Chin. Phys. C, 40, 100001 (2016); see also pdg.lbl.gov sections on probability, statistics, Monte Carlo

Theory \leftrightarrow Statistics \leftrightarrow Experiment

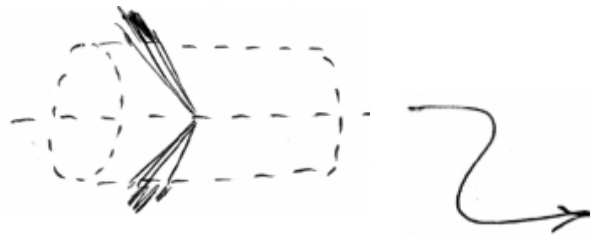
Theory (model, hypothesis):

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\Psi} \not{D} \Psi + \dots$$

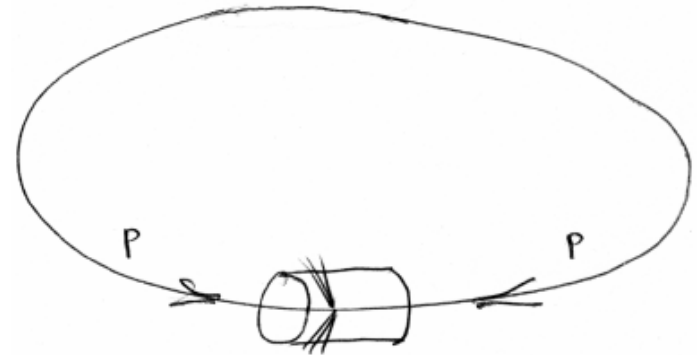


$$\sigma = \frac{G_F \alpha_S^2 m_H^2}{288 \sqrt{2}\pi} \times \text{wavy line}$$

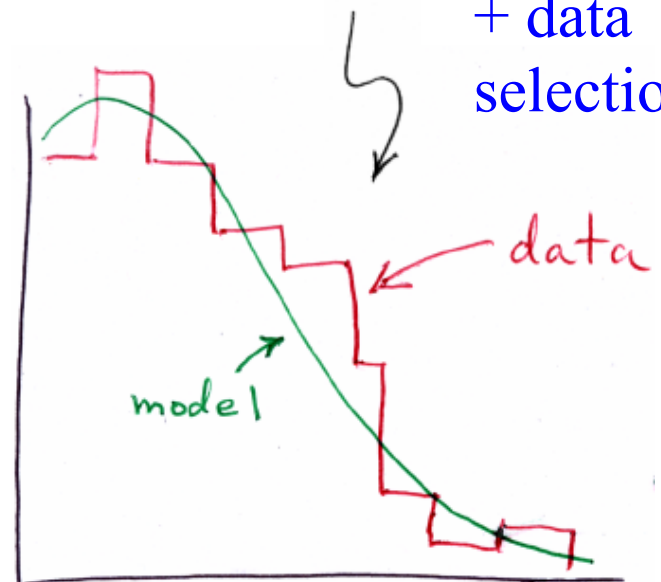
+ simulation
of detector
and cuts



Experiment:



+ data
selection



Quick review of probability

Frequentist (A = outcome of repeatable observation):

$$P(A) = \lim_{n \rightarrow \infty} \frac{\text{outcome is } A}{n}$$

Subjective (A = hypothesis):

$P(A)$ = degree of belief that A is true

Conditional probability:

$$P(A|B) = \frac{P(A \cap B)}{P(B)}$$

Bayes' theorem:

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)} = \frac{P(B|A)P(A)}{\sum_i P(B|A_i)P(A_i)}$$

Frequentist Statistics – general philosophy

In frequentist statistics, probabilities are associated only with the data, i.e., outcomes of repeatable observations (shorthand: \vec{x}).

Probability = limiting frequency

Probabilities such as

P (Higgs boson exists),

$P(0.117 < \alpha_s < 0.121)$,

etc. are either 0 or 1, but we don't know which.

The tools of frequentist statistics tell us what to expect, under the assumption of certain probabilities, about hypothetical repeated observations.

A hypothesis is preferred if the data are found in a region of high predicted probability (i.e., where an alternative hypothesis predicts lower probability).

Bayesian Statistics – general philosophy

In Bayesian statistics, use subjective probability for hypotheses:

probability of the data assuming hypothesis H (the likelihood)

prior probability, i.e., before seeing the data

$$P(H|\vec{x}) = \frac{P(\vec{x}|H)\pi(H)}{\int P(\vec{x}|H)\pi(H) dH}$$

posterior probability, i.e., after seeing the data

normalization involves sum over all possible hypotheses

Bayes' theorem has an “if-then” character: **If** your prior probabilities were $\pi(H)$, **then** it says how these probabilities should change in the light of the data.

No general prescription for priors (subjective!)

The likelihood function

Suppose the entire result of an experiment (set of measurements) is a collection of numbers \mathbf{x} , and suppose the joint pdf for the data \mathbf{x} is a function that depends on a set of parameters θ :

$$P(\mathbf{x}|\theta)$$

Now evaluate this function with the data obtained and regard it as a function of the parameter(s). This is the **likelihood function**:

$$L(\theta) = P(\mathbf{x}|\theta)$$

(\mathbf{x} constant)

The likelihood function for i.i.d.*. data

* i.i.d. = independent and identically distributed

Consider n independent observations of x : x_1, \dots, x_n , where x follows $f(x; \theta)$. The joint pdf for the whole data sample is:

$$f(x_1, \dots, x_n; \theta) = \prod_{i=1}^n f(x_i; \theta)$$

In this case the likelihood function is

$$L(\vec{\theta}) = \prod_{i=1}^n f(x_i; \vec{\theta}) \quad (x_i \text{ constant})$$

Frequentist parameter estimation

Suppose we have a pdf characterized by one or more parameters:

$$f(x; \theta) = \frac{1}{\theta} e^{-x/\theta}$$

random variable parameter

Suppose we have a **sample** of observed values: $\vec{x} = (x_1, \dots, x_n)$

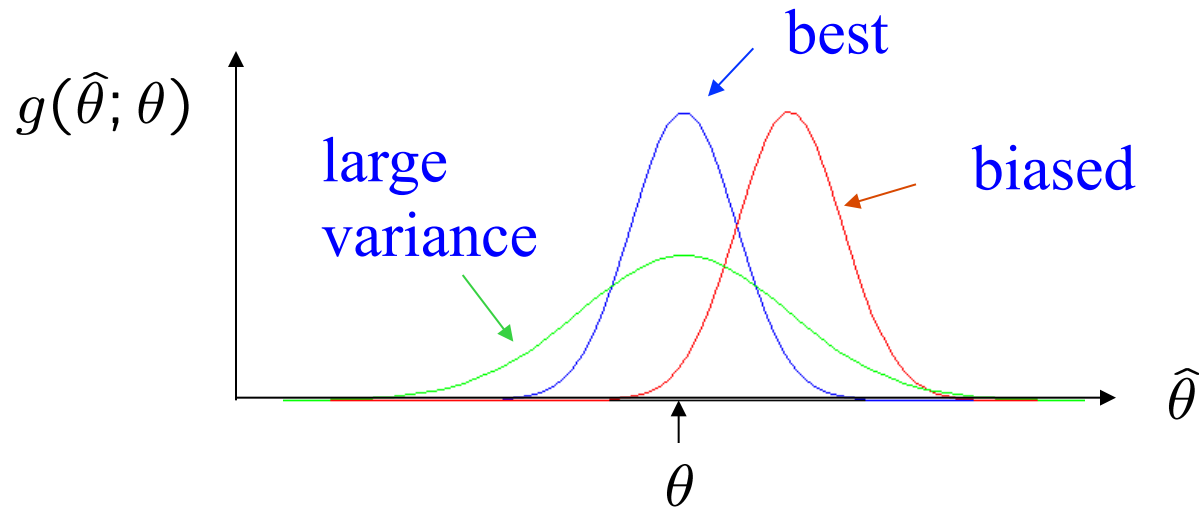
We want to find some function of the data to **estimate** the parameter(s):

$$\hat{\theta}(\vec{x}) \quad \leftarrow \text{estimator written with a hat}$$

Sometimes we say ‘estimator’ for the function of x_1, \dots, x_n ;
‘estimate’ for the value of the estimator with a particular data set.

Properties of estimators

Estimators are functions of the data and thus characterized by a sampling distribution with a given (co)variance:

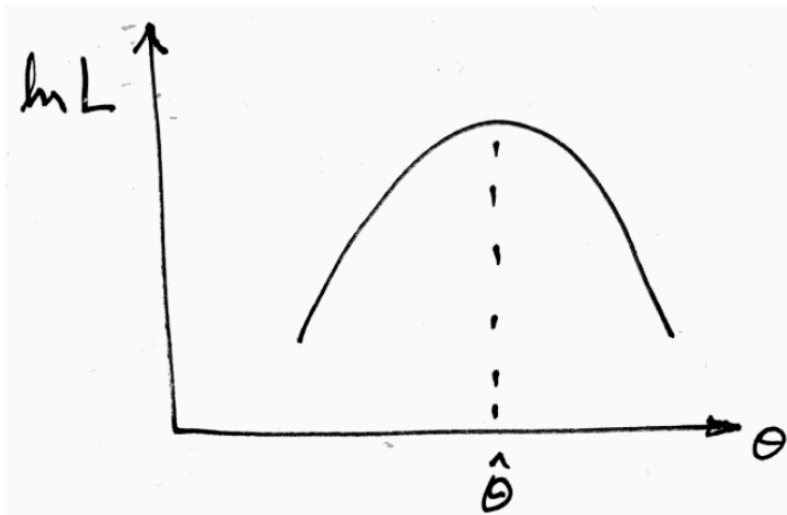


In general they may have a nonzero bias: $b = E[\hat{\theta}] - \theta$

Want small variance and small bias, but in general cannot optimize with respect to both; some trade-off necessary.

Maximum Likelihood (ML) estimators

The most important frequentist method for constructing estimators is to take the value of the parameter(s) that maximize the likelihood (or equivalently the log-likelihood):



$$\hat{\theta} = \operatorname{argmax}_{\theta} L(x|\theta)$$

In some cases we can find the ML estimator as a closed-form function of the data; more often it is found numerically.

ML example: parameter of exponential pdf

Consider exponential pdf, $f(t; \tau) = \frac{1}{\tau} e^{-t/\tau}$

and suppose we have i.i.d. data, t_1, \dots, t_n

The likelihood function is $L(\tau) = \prod_{i=1}^n \frac{1}{\tau} e^{-t_i/\tau}$

The value of τ for which $L(\tau)$ is maximum also gives the maximum value of its logarithm (the log-likelihood function):

$$\ln L(\tau) = \sum_{i=1}^n \ln f(t_i; \tau) = \sum_{i=1}^n \left(\ln \frac{1}{\tau} - \frac{t_i}{\tau} \right)$$

ML example: parameter of exponential pdf (2)

Find its maximum by setting $\frac{\partial \ln L(\tau)}{\partial \tau} = 0$,

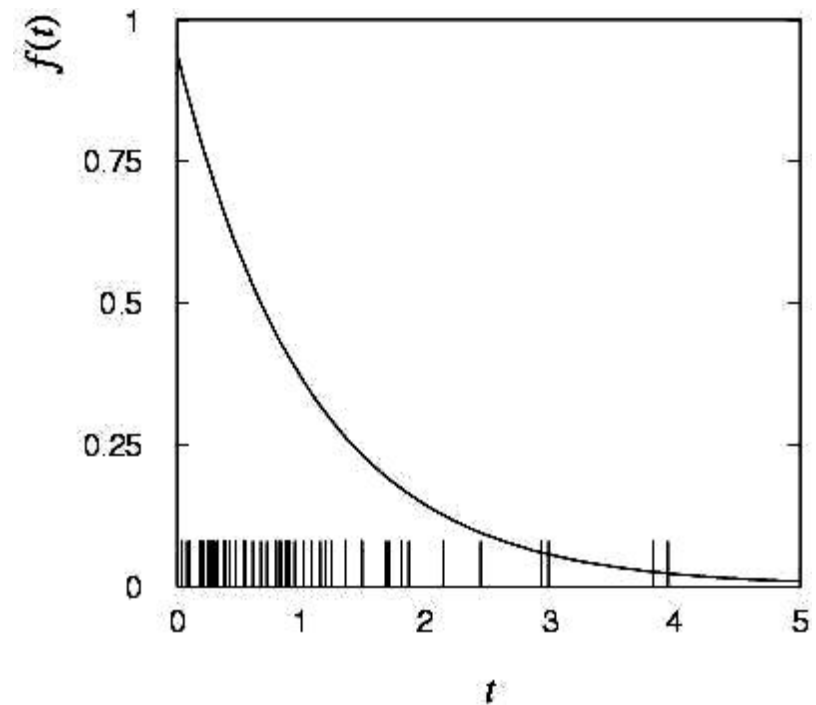
$$\rightarrow \hat{\tau} = \frac{1}{n} \sum_{i=1}^n t_i$$

Monte Carlo test:

generate 50 values
using $\tau = 1$:

We find the ML estimate:

$$\hat{\tau} = 1.062$$



ML example: parameter of exponential pdf (3)

For the exponential distribution one has for mean, variance:

$$E[t] = \int_0^{\infty} t \frac{1}{\tau} e^{-t/\tau} dt = \tau$$

$$V[t] = \int_0^{\infty} (t - \tau)^2 \frac{1}{\tau} e^{-t/\tau} dt = \tau^2$$

For the ML estimator $\hat{\tau} = \frac{1}{n} \sum_{i=1}^n t_i$ we therefore find

$$E[\hat{\tau}] = E \left[\frac{1}{n} \sum_{i=1}^n t_i \right] = \frac{1}{n} \sum_{i=1}^n E[t_i] = \tau \quad \longrightarrow \quad b = E[\hat{\tau}] - \tau = 0$$

$$V[\hat{\tau}] = V \left[\frac{1}{n} \sum_{i=1}^n t_i \right] = \frac{1}{n^2} \sum_{i=1}^n V[t_i] = \frac{\tau^2}{n} \quad \longrightarrow \quad \sigma_{\hat{\tau}} = \frac{\tau}{\sqrt{n}}$$

Variance of estimators: Monte Carlo method

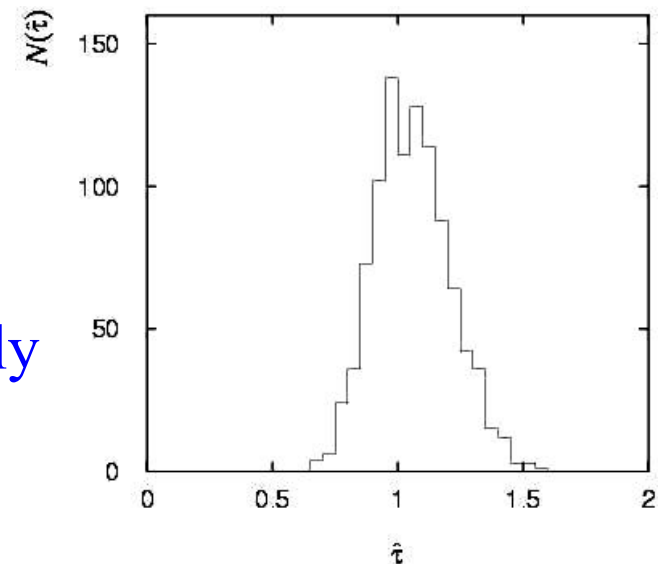
Having estimated our parameter we now need to report its ‘statistical error’, i.e., how widely distributed would estimates be if we were to repeat the entire measurement many times.

One way to do this would be to simulate the entire experiment many times with a Monte Carlo program (use ML estimate for MC).

For exponential example, from sample variance of estimates we find:

$$\hat{\sigma}_{\hat{\tau}} = 0.151$$

Note distribution of estimates is roughly Gaussian – (almost) always true for ML in large sample limit.



Variance of estimators from information inequality

The **information inequality** (RCF) sets a lower bound on the variance of any estimator (not only ML):

$$V[\hat{\theta}] \geq \left(1 + \frac{\partial b}{\partial \theta}\right)^2 \bigg/ E \left[-\frac{\partial^2 \ln L}{\partial \theta^2} \right]$$

← Minimum Variance Bound (MVB)
($b = E[\hat{\theta}] - \theta$)

Often the bias b is small, and equality either holds exactly or is a good approximation (e.g. large data sample limit). Then,

$$V[\hat{\theta}] \approx -1 \bigg/ E \left[\frac{\partial^2 \ln L}{\partial \theta^2} \right]$$

Estimate this using the 2nd derivative of $\ln L$ at its maximum:

$$\hat{V}[\hat{\theta}] = - \left(\frac{\partial^2 \ln L}{\partial \theta^2} \right)^{-1} \bigg|_{\theta=\hat{\theta}}$$

Variance of estimators: graphical method

Expand $\ln L(\theta)$ about its maximum:

$$\ln L(\theta) = \ln L(\hat{\theta}) + \left[\frac{\partial \ln L}{\partial \theta} \right]_{\theta=\hat{\theta}} (\theta - \hat{\theta}) + \frac{1}{2!} \left[\frac{\partial^2 \ln L}{\partial \theta^2} \right]_{\theta=\hat{\theta}} (\theta - \hat{\theta})^2 + \dots$$

First term is $\ln L_{\max}$, second term is zero, for third term use information inequality (assume equality):

$$\ln L(\theta) \approx \ln L_{\max} - \frac{(\theta - \hat{\theta})^2}{2\widehat{\sigma}_{\hat{\theta}}^2}$$

$$\text{i.e., } \ln L(\hat{\theta} \pm \hat{\sigma}_{\hat{\theta}}) \approx \ln L_{\max} - \frac{1}{2}$$

→ to get $\hat{\sigma}_{\hat{\theta}}$, change θ away from $\hat{\theta}$ until $\ln L$ decreases by 1/2.

Example of variance by graphical method

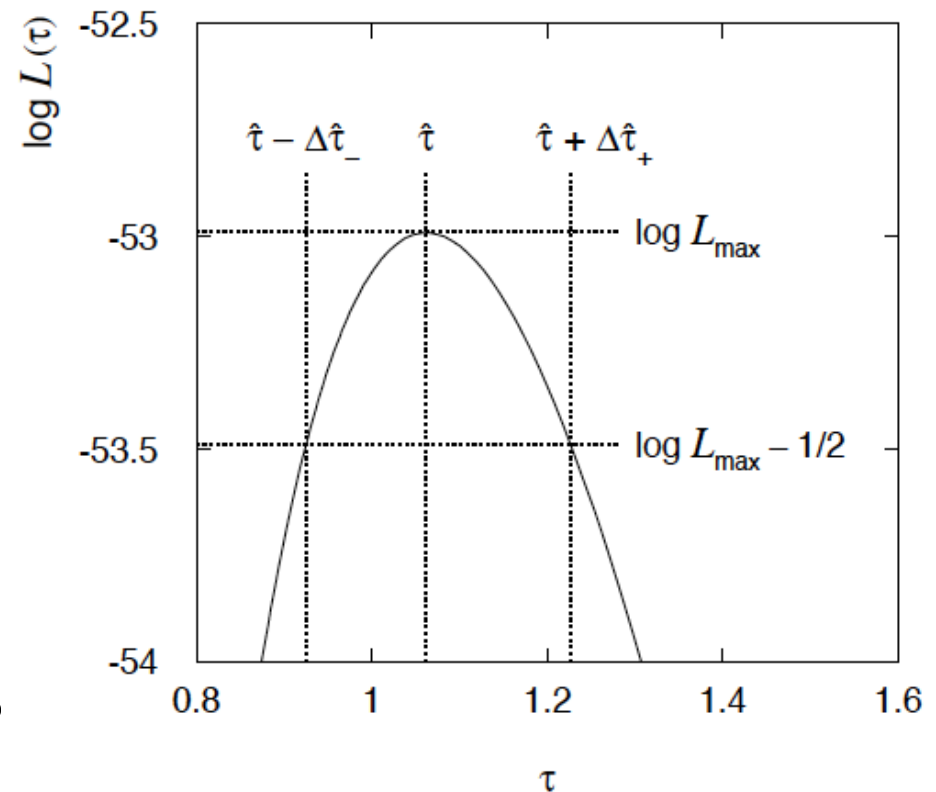
ML example with exponential:

$$\hat{\tau} = 1.062$$

$$\Delta\hat{\tau}_- = 0.137$$

$$\Delta\hat{\tau}_+ = 0.165$$

$$\hat{\sigma}_{\hat{\tau}} \approx \Delta\hat{\tau}_- \approx \Delta\hat{\tau}_+ \approx 0.15$$



Not quite parabolic $\ln L$ since finite sample size ($n = 50$).

Information inequality for N parameters

Suppose we have estimated N parameters $\vec{\theta} = (\theta_1, \dots, \theta_N)$.

The (inverse) minimum variance bound is given by the Fisher information matrix:

$$I_{ij} = E \left[-\frac{\partial^2 \ln L}{\partial \theta_i \partial \theta_j} \right] = -n \int f(x; \vec{\theta}) \frac{\partial^2 \ln f(x; \vec{\theta})}{\partial \theta_i \partial \theta_j} dx$$

The information inequality then states that $V - I^{-1}$ is a positive semi-definite matrix, where $V_{ij} = \text{cov}[\hat{\theta}_i, \hat{\theta}_j]$. Therefore

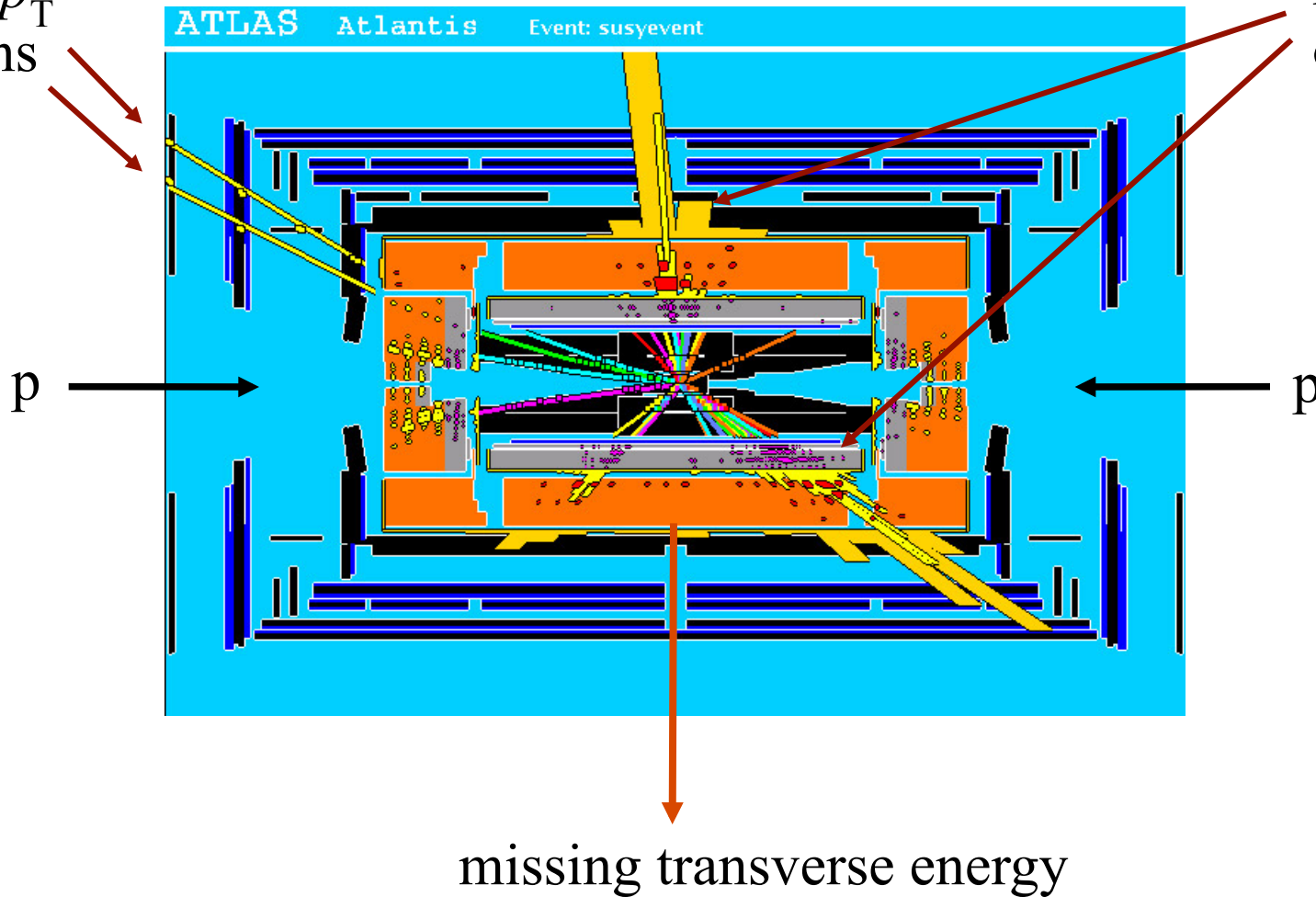
$$V[\hat{\theta}_i] \geq (I^{-1})_{ii}$$

Often use I^{-1} as an approximation for covariance matrix, estimate using e.g. matrix of 2nd derivatives at maximum of L .

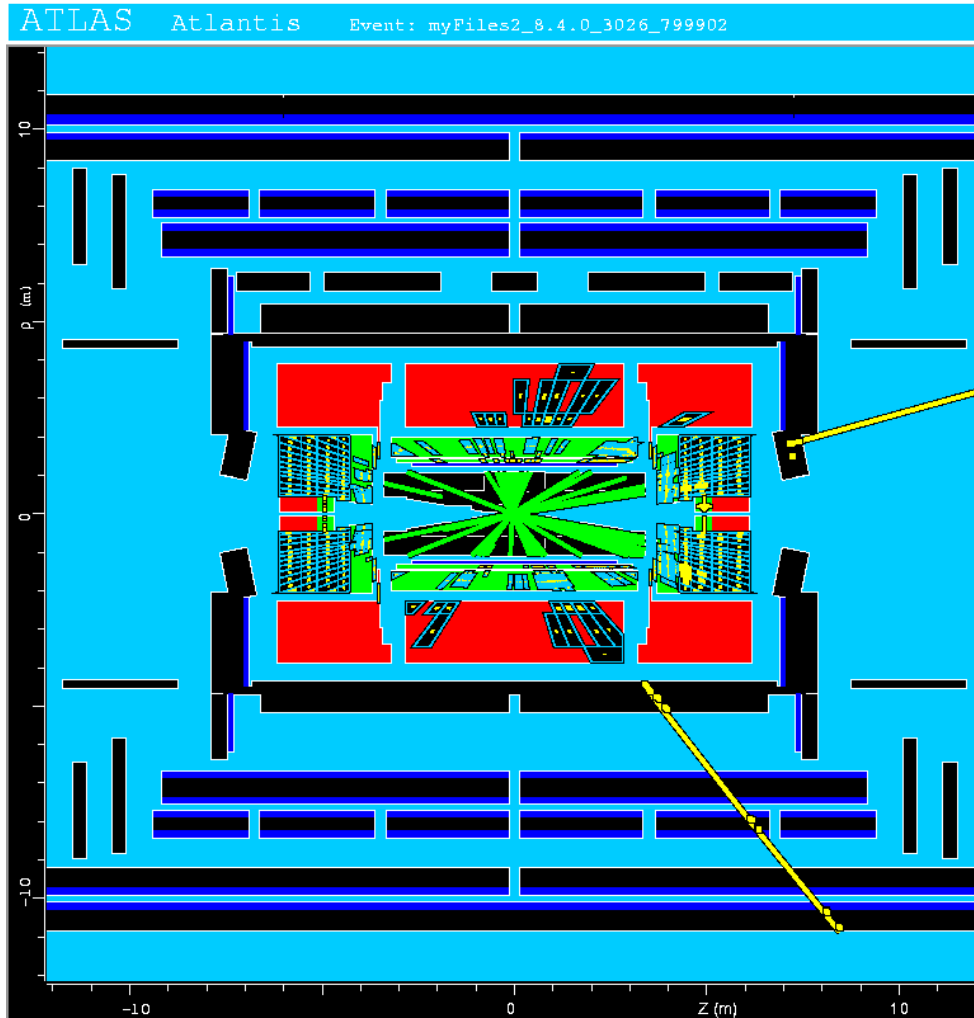
Prelude to statistical tests: A simulated SUSY event

high p_T
muons

high p_T jets
of hadrons



Background events



This event from Standard Model $t\bar{t}$ production also has high p_T jets and muons, and some missing transverse energy.

→ can easily mimic a SUSY event.

Frequentist statistical tests

Suppose a measurement produces data \mathbf{x} ; consider a hypothesis H_0 we want to test and alternative H_1

H_0, H_1 specify probability for \mathbf{x} : $P(\mathbf{x}|H_0), P(\mathbf{x}|H_1)$

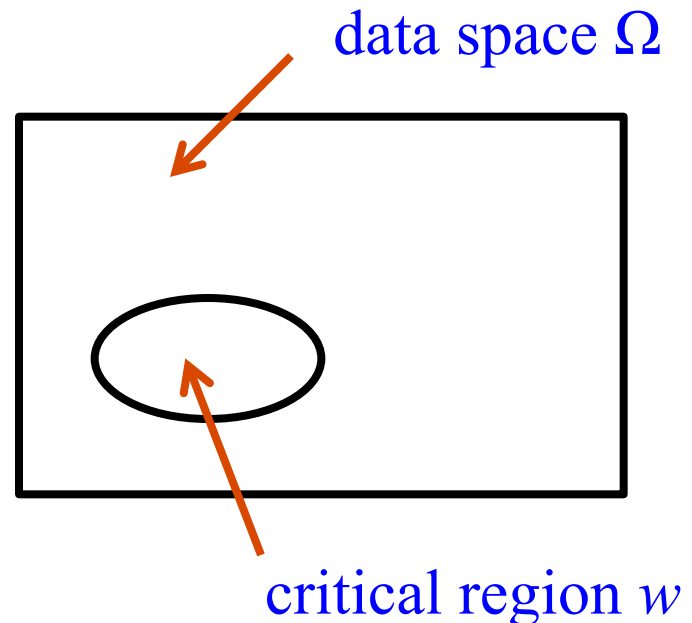
A test of H_0 is defined by specifying a **critical region** w of the data space such that there is no more than some (small) probability α , assuming H_0 is correct, to observe the data there, i.e.,

$$P(\mathbf{x} \in w | H_0) \leq \alpha$$

Need inequality if data are discrete.

α is called the **size** or **significance level** of the test.

If \mathbf{x} is observed in the critical region, reject H_0 .

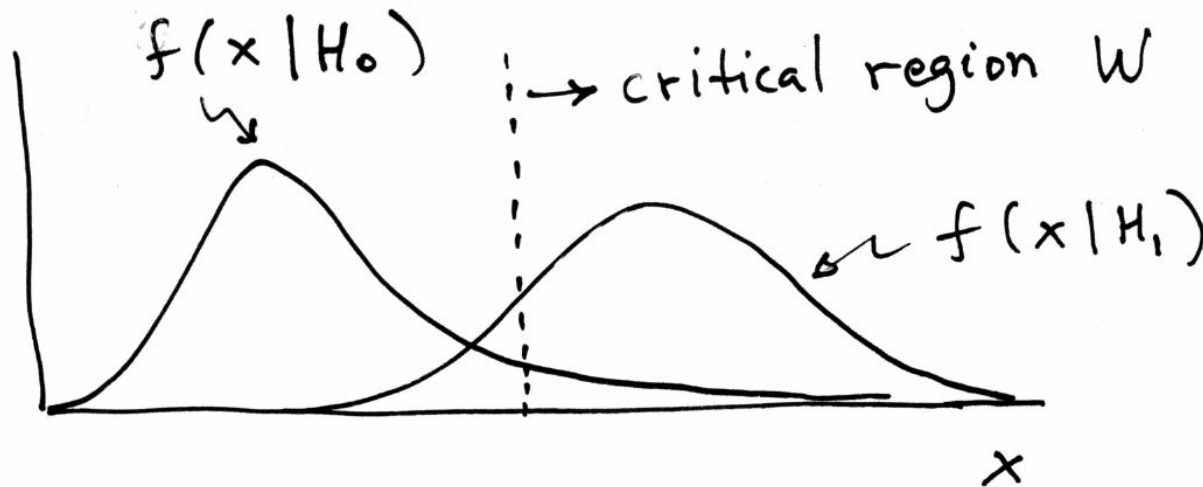


Definition of a test (2)

But in general there are an infinite number of possible critical regions that give the same significance level α .

So the choice of the critical region for a test of H_0 needs to take into account the alternative hypothesis H_1 .

Roughly speaking, place the critical region where there is a low probability to be found if H_0 is true, but high if H_1 is true:



Classification viewed as a statistical test

Probability to reject H_0 if true (type I error): $\alpha = \int_W f(\mathbf{x}|H_0)d\mathbf{x}$

α = size of test, significance level, false discovery rate

Probability to accept H_0 if H_1 true (type II error) $\beta = \int_{\bar{W}} f(\mathbf{x}|H_1)d\mathbf{x}$

$1 - \beta$ = power of test with respect to H_1

Equivalently if e.g. H_0 = background, H_1 = signal, use efficiencies:

$$\varepsilon_b = \int_W f(\mathbf{x}|H_0) = \alpha$$

$$\varepsilon_s = \int_W f(\mathbf{x}|H_1) = 1 - \beta = \text{power}$$

Purity / misclassification rate

Consider the probability that an event of signal (s) type classified correctly (i.e., the event selection purity),

Use Bayes' theorem:

Here W is signal region

$$P(s|\mathbf{x} \in W) = \frac{P(\mathbf{x} \in W|s)P(s)}{P(\mathbf{x} \in W|s)P(s) + P(\mathbf{x} \in W|b)P(b)}$$

posterior probability = signal purity
= 1 – signal misclassification rate

Note purity depends on the prior probability for an event to be signal or background as well as on s/b efficiencies.

Physics context of a statistical test

Event Selection: data = individual event; goal is to classify

Example: separation of different particle types (electron vs muon) or known event types (ttbar vs QCD multijet).

E.g. test H_0 : event is background vs. H_1 : event is signal.

Use selected events for further study.

Search for New Physics: data = a sample of events. Test null hypothesis

H_0 : all events correspond to Standard Model (background only),

against the alternative

H_1 : events include a type whose existence is not yet established (signal plus background)

Many subtle issues here, mainly related to the high standard of proof required to establish presence of a new phenomenon. The optimal statistical test for a search is closely related to that used for event selection.

Statistical tests for event selection

Suppose the result of a measurement for an individual event is a collection of numbers $\vec{x} = (x_1, \dots, x_n)$

x_1 = number of muons,

x_2 = mean p_T of jets,

x_3 = missing energy, ...

\vec{x} follows some n -dimensional joint pdf, which depends on the type of event produced, i.e., was it

$$pp \rightarrow t\bar{t}, \quad pp \rightarrow \tilde{g}\tilde{g}, \dots$$

For each reaction we consider we will have a **hypothesis** for the pdf of \mathbf{x} , e.g., $p(\mathbf{x}|\mathbf{b})$, $p(\mathbf{x}|\mathbf{s})$

E.g. here call H_0 the **background** hypothesis (the event type we want to reject); H_1 is **signal** hypothesis (the type we want).

Selecting events

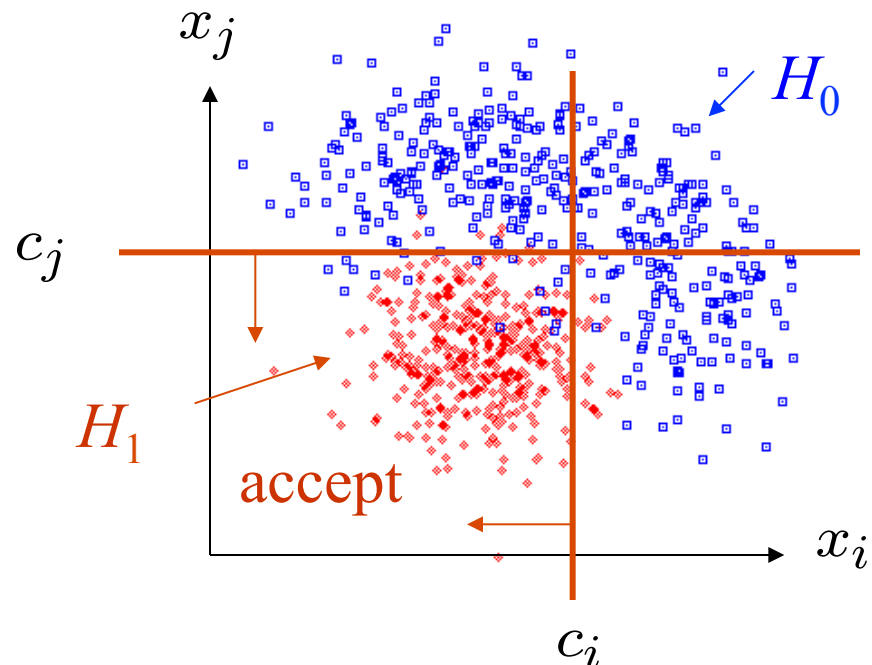
Suppose we have a data sample with two kinds of events, corresponding to hypotheses H_0 and H_1 and we want to select those of type H_1 .

Each event is a point in \vec{x} space. What ‘decision boundary’ should we use to accept/reject events as belonging to event types H_0 or H_1 ?

Perhaps select events with ‘cuts’:

$$x_i < c_i$$

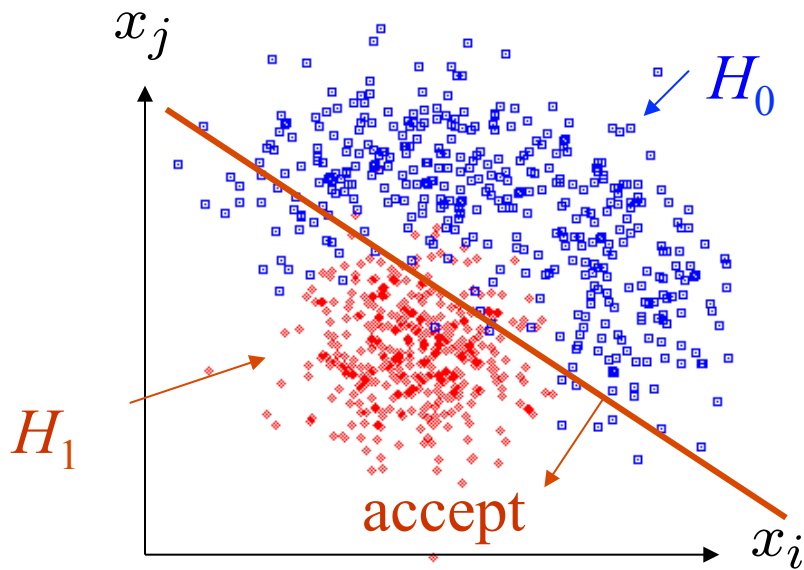
$$x_j < c_j$$



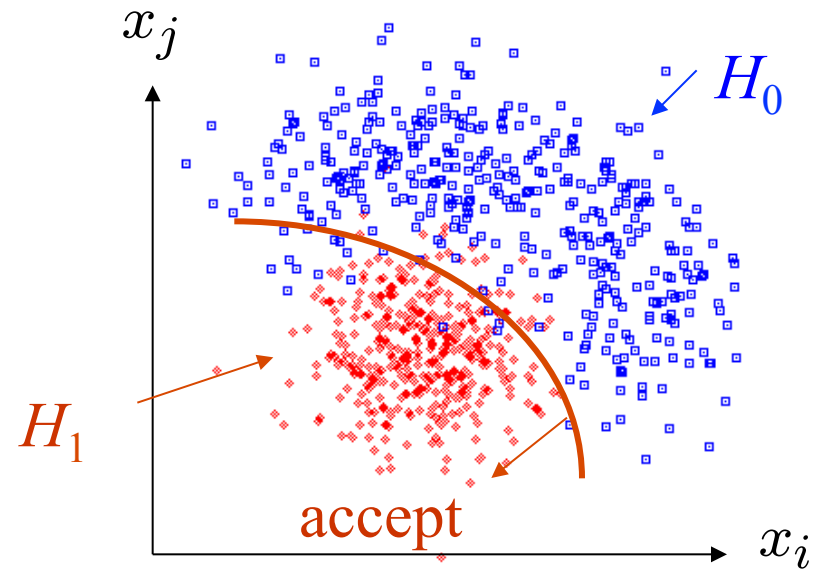
Other ways to select events

Or maybe use some other sort of decision boundary:

linear



or nonlinear



How can we do this in an ‘optimal’ way?

Test statistics

The boundary of the critical region for an n -dimensional data space $\mathbf{x} = (x_1, \dots, x_n)$ can be defined by an equation of the form

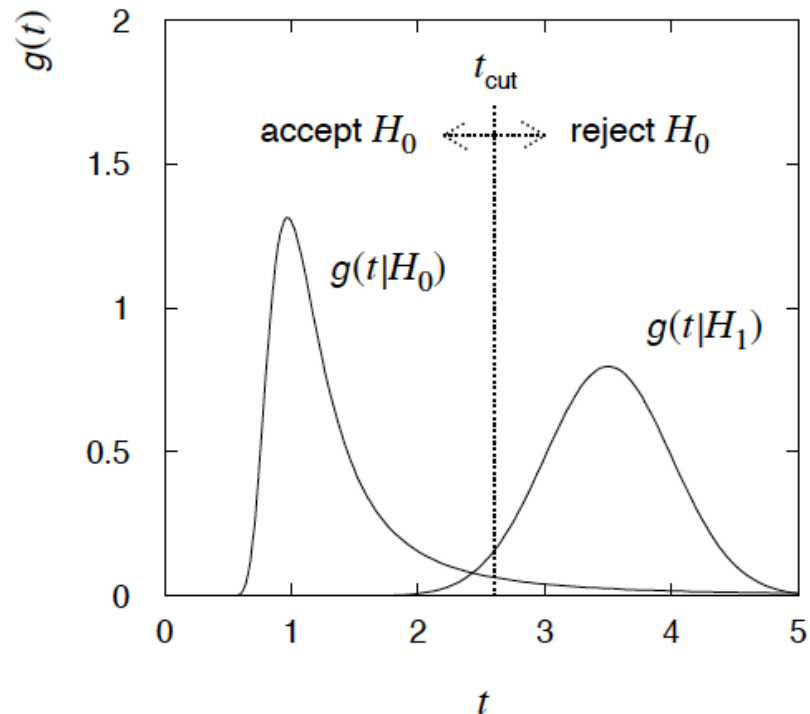
$$t(x_1, \dots, x_n) = t_{\text{cut}}$$

where $t(x_1, \dots, x_n)$ is a scalar **test statistic**.

We can work out the pdfs $g(t|H_0)$, $g(t|H_1)$, \dots

Decision boundary is now a single ‘cut’ on t , defining the critical region.

So for an n -dimensional problem we have a corresponding 1-d problem.



Test statistic based on likelihood ratio

How can we choose a test's critical region in an 'optimal way'?

Neyman-Pearson lemma states:

To get the highest power for a given significance level in a test of H_0 , (background) versus H_1 , (signal) the critical region should have

$$\frac{f(\mathbf{x}|H_1)}{f(\mathbf{x}|H_0)} > c$$

inside the region, and $\leq c$ outside, where c is a constant chosen to give a test of the desired size.

Equivalently, optimal scalar test statistic is

$$t(\mathbf{x}) = \frac{f(\mathbf{x}|H_1)}{f(\mathbf{x}|H_0)}$$

N.B. any monotonic function of this is leads to the same test.

Neyman-Pearson doesn't usually help

We usually don't have explicit formulae for the pdfs $f(\mathbf{x}|s)$, $f(\mathbf{x}|b)$, so for a given \mathbf{x} we can't evaluate the likelihood ratio

$$t(\mathbf{x}) = \frac{f(\mathbf{x}|s)}{f(\mathbf{x}|b)}$$

Instead we may have Monte Carlo models for signal and background processes, so we can produce simulated data:

generate $\mathbf{x} \sim f(\mathbf{x}|s)$ \rightarrow $\mathbf{x}_1, \dots, \mathbf{x}_N$

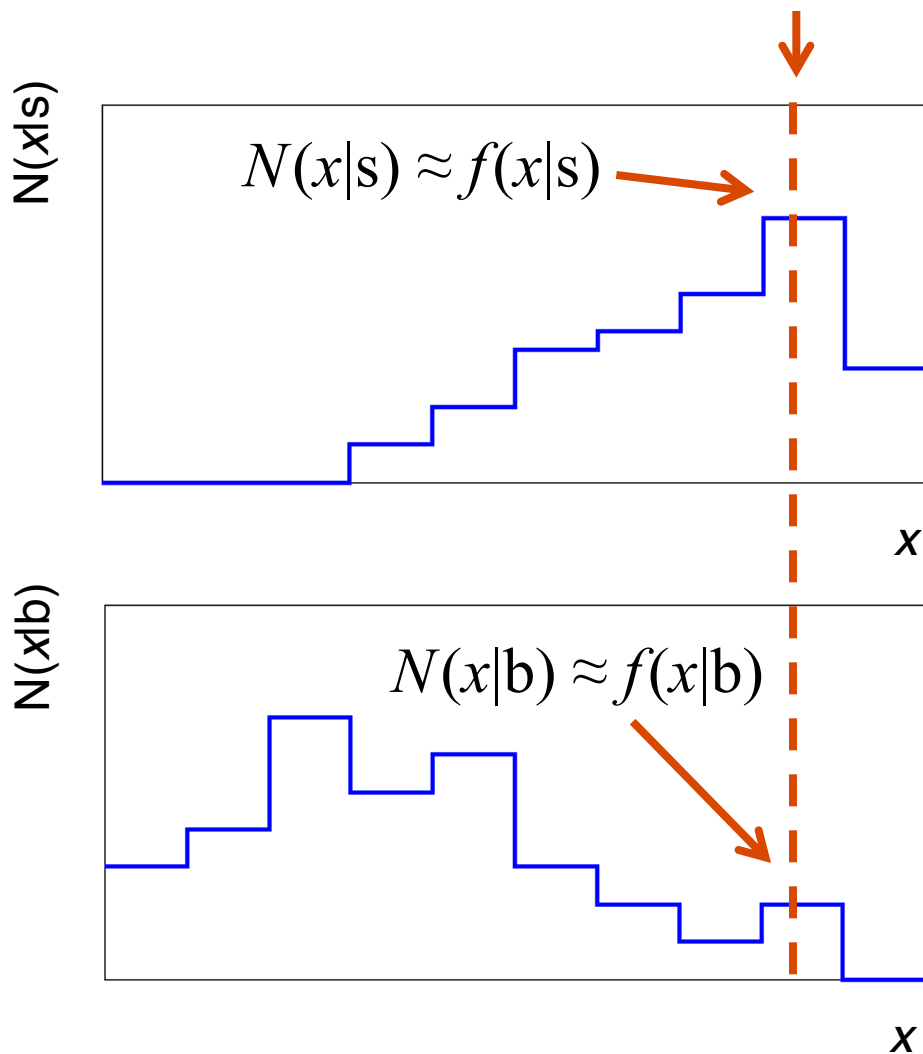
generate $\mathbf{x} \sim f(\mathbf{x}|b)$ \rightarrow $\mathbf{x}_1, \dots, \mathbf{x}_N$

This gives samples of “training data” with events of known type.

Can be expensive (1 fully simulated LHC event \sim 1 CPU minute).

Approximate LR from histograms

Want $t(x) = f(x|s)/f(x|b)$ for x here



One possibility is to generate MC data and construct histograms for both signal and background.

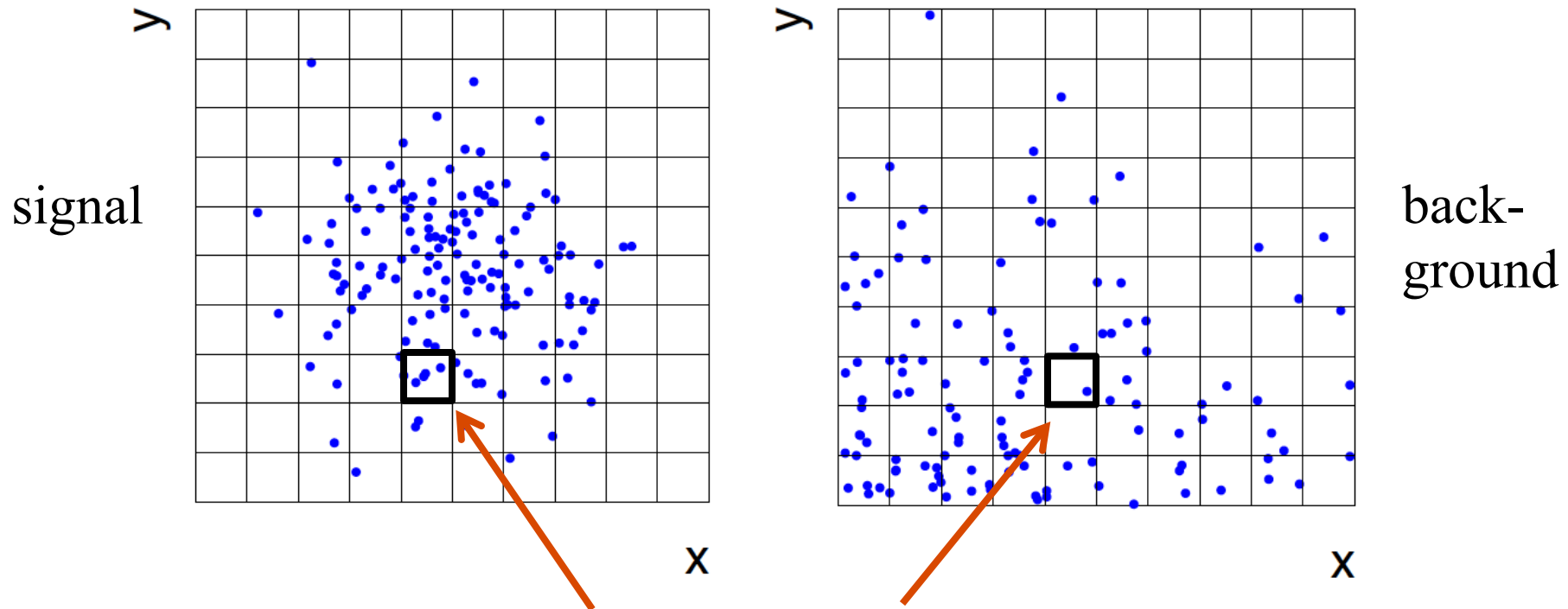
Use (normalized) histogram values to approximate LR:

$$t(x) \approx \frac{N(x|s)}{N(x|b)}$$

Can work well for single variable.

Approximate LR from 2D-histograms

Suppose problem has 2 variables. Try using 2-D histograms:



Approximate pdfs using $N(x,y|s)$, $N(x,y|b)$ in corresponding cells.

But if we want M bins for each variable, then in n -dimensions we have M^n cells; can't generate enough training data to populate.

→ Histogram method usually not usable for $n > 1$ dimension.

Strategies for multivariate analysis

Neyman-Pearson lemma gives optimal answer, but cannot be used directly, because we usually don't have $f(\mathbf{x}|\mathbf{s})$, $f(\mathbf{x}|\mathbf{b})$.

Histogram method with M bins for n variables requires that we estimate M^n parameters (the values of the pdfs in each cell), so this is rarely practical.

A compromise solution is to assume a certain functional form for the test statistic $t(\mathbf{x})$ with fewer parameters; determine them (using MC) to give best separation between signal and background.

Alternatively, try to estimate the probability densities $f(\mathbf{x}|\mathbf{s})$ and $f(\mathbf{x}|\mathbf{b})$ (with something better than histograms) and use the estimated pdfs to construct an approximate likelihood ratio.

Multivariate methods

Many new (and some old) methods esp. from Machine Learning:

Fisher discriminant

(Deep) neural networks

Kernel density methods

Support Vector Machines

Decision trees

 Boosting

 Bagging

This is a large topic -- see e.g. lectures

http://www.pp.rhul.ac.uk/~cowan/stat/stat_2.pdf (from around p 38)

and references therein.

Testing significance / goodness-of-fit

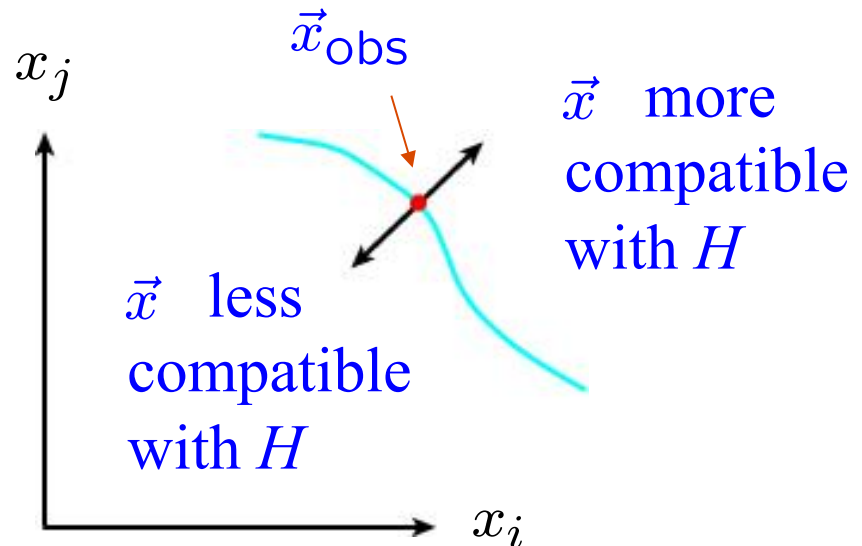
Suppose hypothesis H predicts pdf $f(\vec{x}|H)$ for a set of observations $\vec{x} = (x_1, \dots, x_n)$.

We observe a single point in this space: \vec{x}_{obs}

What can we say about the validity of H in light of the data?

Decide what part of the data space represents less compatibility with H than does the point \vec{x}_{obs} .

This region therefore has greater compatibility with some alternative H' .



p-values

Express ‘goodness-of-fit’ by giving the *p*-value for *H*:

p = probability, under assumption of *H*, to observe data with equal or lesser compatibility with *H* relative to the data we got.



This is not the probability that *H* is true!

In frequentist statistics we don’t talk about $P(H)$ (unless *H* represents a repeatable observation). In Bayesian statistics we do; use Bayes’ theorem to obtain

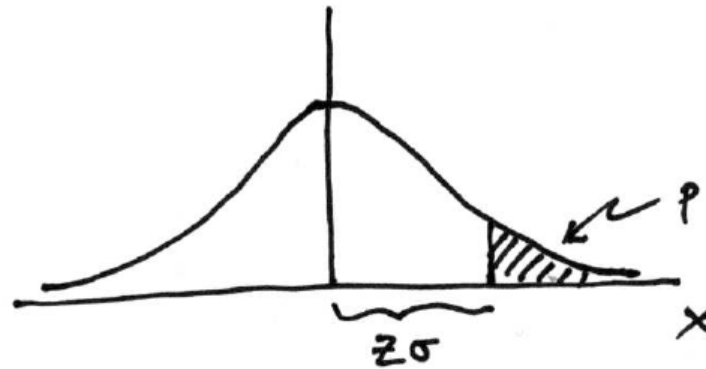
$$P(H|\vec{x}) = \frac{P(\vec{x}|H)\pi(H)}{\int P(\vec{x}|H)\pi(H) dH}$$

where $\pi(H)$ is the prior probability for *H*.

For now stick with the frequentist approach; result is *p*-value, regrettably easy to misinterpret as $P(H)$.

Significance from p -value

Often define significance Z as the number of standard deviations that a Gaussian variable would fluctuate in one direction to give the same p -value.



$$p = \int_Z^{\infty} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} dx = 1 - \Phi(Z) \quad \mathbf{1 - TMath::Freq}$$

$$Z = \Phi^{-1}(1 - p) \quad \mathbf{TMath::NormQuantile}$$

Test statistics and p -values

Consider a parameter μ proportional to rate of signal process.

Often define a function of the data (test statistic) q_μ that reflects level of agreement between the data and the hypothesized value μ .

Usually define q_μ so that higher values increasingly incompatibility with the data (more compatible with a relevant alternative).

We can define critical region of test of μ by $q_\mu \geq \text{const.}$, or equivalently define the p -value of μ as:

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

observed value of q_μ

pdf of q_μ assuming μ

Equivalent formulation of test: reject μ if $p_\mu < \alpha$.

Confidence interval from inversion of a test

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 confidence interval will by construction contain the true value of μ with probability of at least $1 - \alpha$.

The interval will cover the true value of μ with probability $\geq 1 - \alpha$.

Equivalently, the parameter values in the confidence interval have p -values of at least α .

To find edge of interval (the “limit”), set $p_\mu = \alpha$ and solve for μ .

The Poisson counting experiment

Suppose we do a counting experiment and observe n events.

Events could be from *signal* process or from *background* – we only count the total number.

Poisson model:

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

s = mean (i.e., expected) # of signal events

b = mean # of background events

Goal is to make inference about s , e.g.,

test $s = 0$ (rejecting $H_0 \approx$ “discovery of signal process”)

test all non-zero s (values not rejected = confidence interval)

In both cases need to ask what is relevant alternative hypothesis.

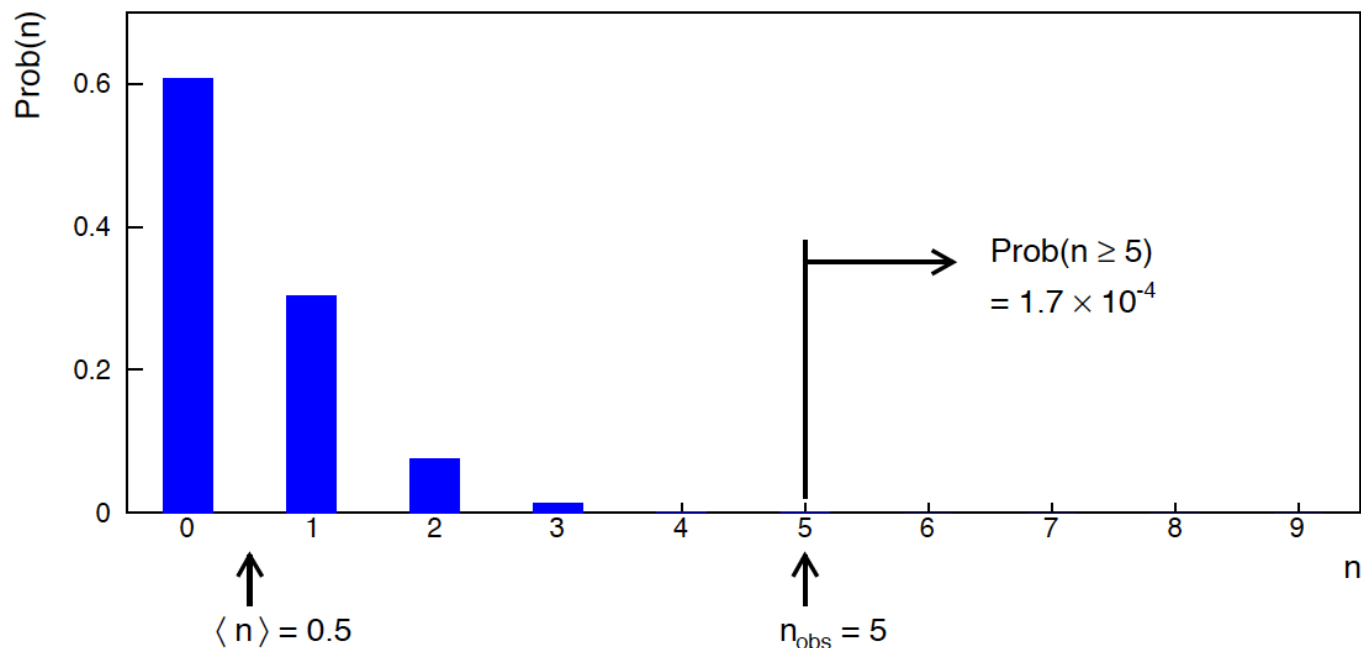
Poisson counting experiment: discovery p -value

Suppose $b = 0.5$ (known), and we observe $n_{\text{obs}} = 5$.

Should we claim evidence for a new discovery?

Take n itself as the test statistic, p -value for hypothesis $s = 0$ is

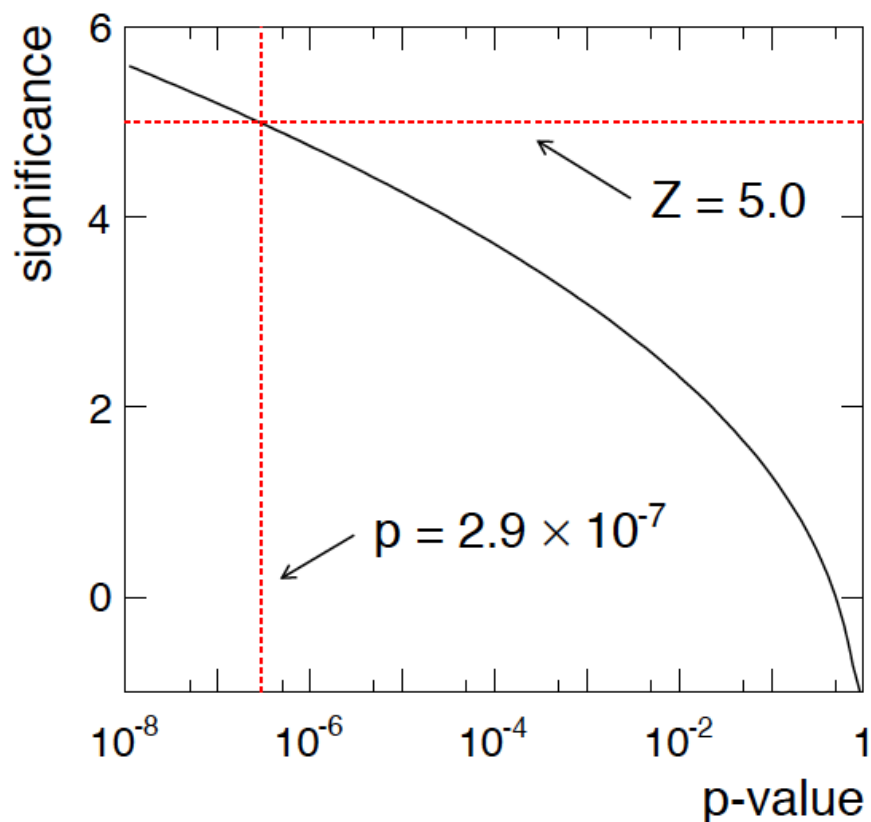
$$\begin{aligned} p\text{-value} &= P(n \geq 5; b = 0.5, s = 0) \\ &= 1.7 \times 10^{-4} \neq P(s = 0)! \end{aligned}$$



Poisson counting experiment: discovery significance

Equivalent significance for $p = 1.7 \times 10^{-4}$: $Z = \Phi^{-1}(1 - p) = 3.6$

Often claim discovery if $Z > 5$ ($p < 2.9 \times 10^{-7}$, i.e., a “5-sigma effect”)



In fact this tradition should be revisited: p -value intended to quantify probability of a signal-like fluctuation assuming background only; not intended to cover, e.g., hidden systematics, plausibility signal model, compatibility of data with signal, “look-elsewhere effect” (~multiple testing), etc.

Frequentist upper limit on Poisson parameter

Consider again the case of observing $n \sim \text{Poisson}(s + b)$.

Suppose $b = 4.5$, $n_{\text{obs}} = 5$. Find upper limit on s at 95% CL.

Relevant alternative is $s = 0$ (critical region at low n)

p -value of hypothesized s is $P(n \leq n_{\text{obs}}; s, b)$

Upper limit s_{up} at $\text{CL} = 1 - \alpha$ found by solving $p_s = \alpha$ for s :

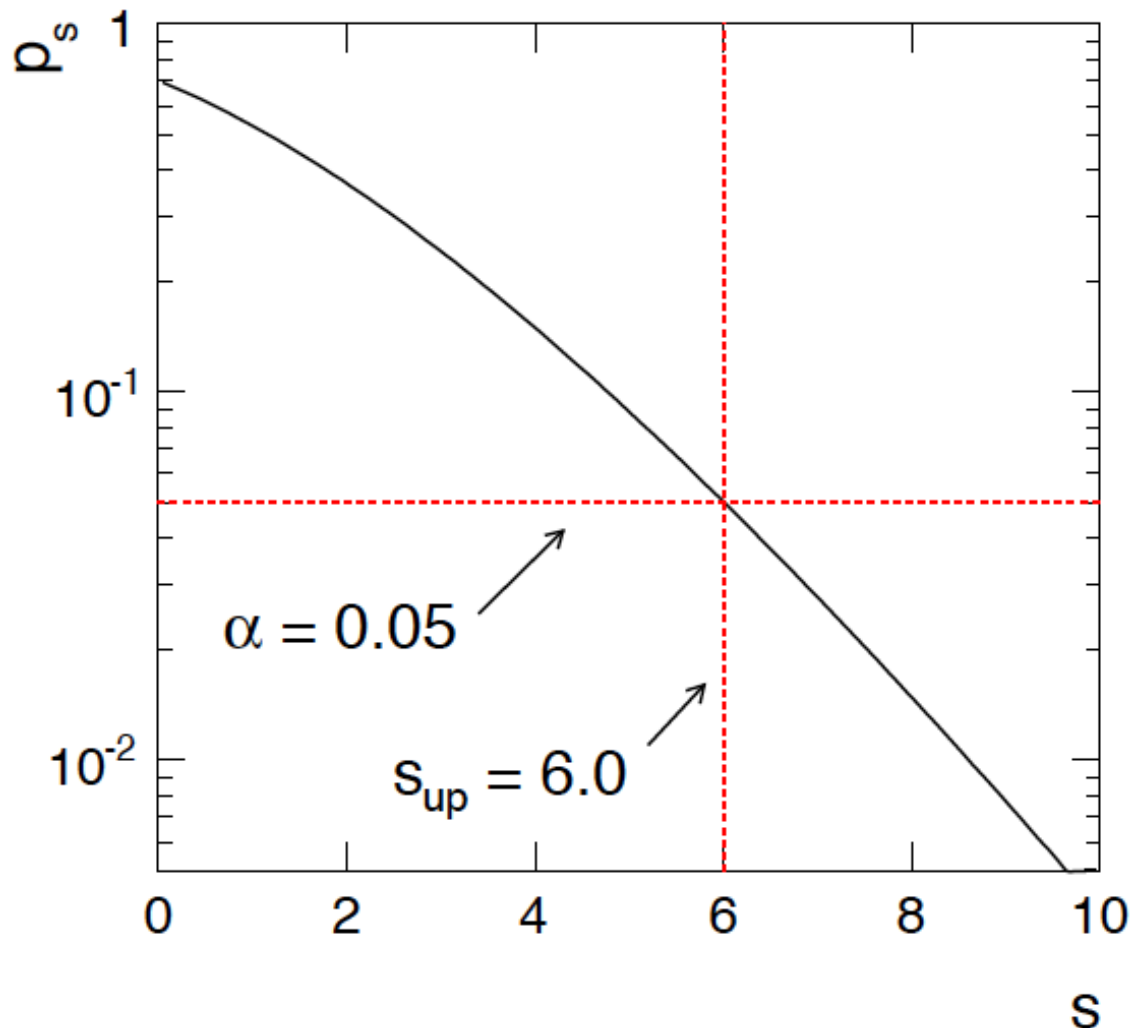
$$\alpha = P(n \leq n_{\text{obs}}; s_{\text{up}}, b) = \sum_{n=0}^{n_{\text{obs}}} \frac{(s_{\text{up}} + b)^n}{n!} e^{-(s_{\text{up}} + b)}$$

$$s_{\text{up}} = \frac{1}{2} F_{\chi^2}^{-1}(1 - \alpha; 2(n_{\text{obs}} + 1)) - b$$

$$= \frac{1}{2} F_{\chi^2}^{-1}(0.95; 2(5 + 1)) - 4.5 = 6.0$$

Frequentist upper limit on Poisson parameter

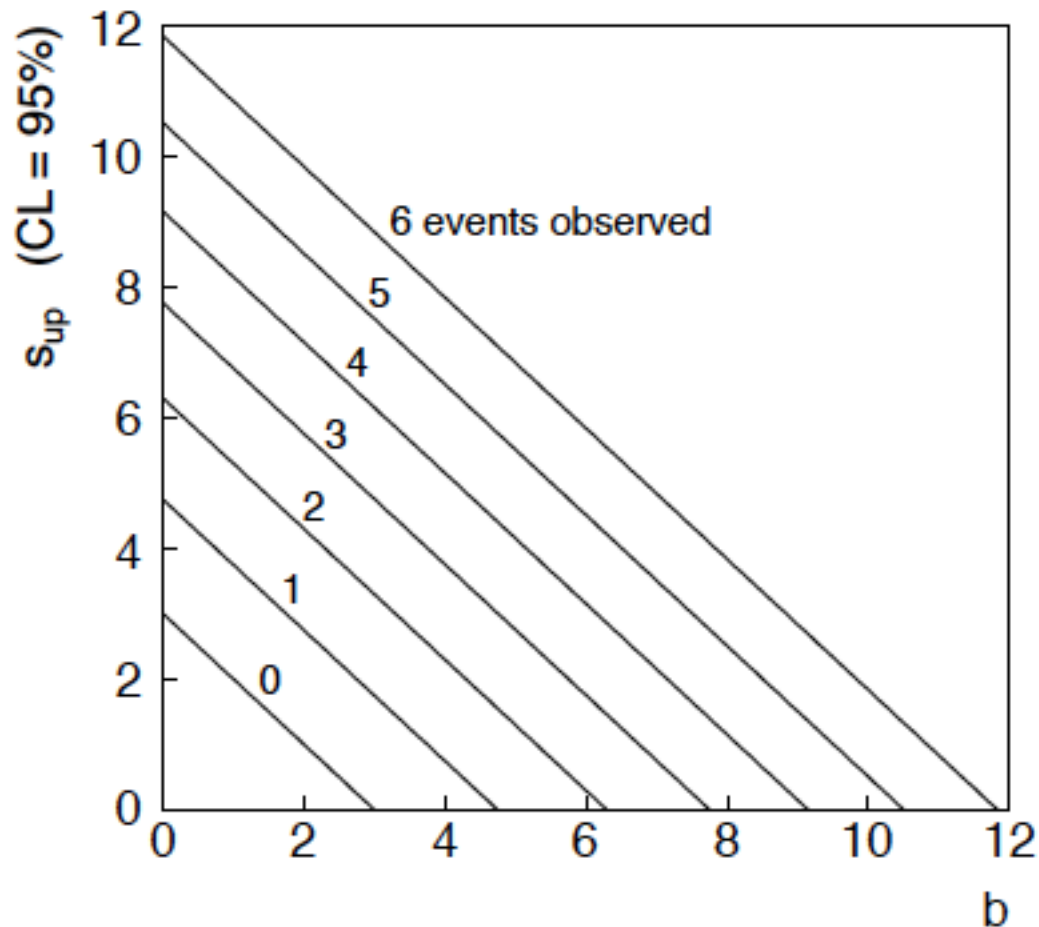
Upper limit s_{up} at $\text{CL} = 1 - \alpha$ found from $p_s = \alpha$.



$n_{\text{obs}} = 5,$
 $b = 4.5$

$n \sim \text{Poisson}(s+b)$: frequentist upper limit on s

For low fluctuation of n formula can give negative result for s_{up} ; i.e. confidence interval is empty.



Limits near a physical boundary

Suppose e.g. $b = 2.5$ and we observe $n = 0$.

If we choose $CL = 0.9$, we find from the formula for s_{up}

$$s_{\text{up}} = -0.197 \quad (CL = 0.90)$$

Physicist:

We already knew $s \geq 0$ before we started; can't use negative upper limit to report result of expensive experiment!

Statistician:

The interval is designed to cover the true value only 90% of the time — this was clearly not one of those times.

Not uncommon dilemma when testing parameter values for which one has very little experimental sensitivity, e.g., very small s .

Expected limit for $s = 0$

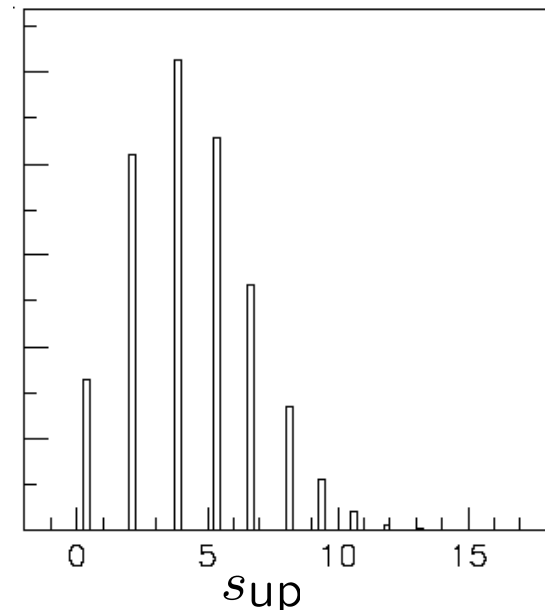
Physicist: I should have used $CL = 0.95$ — then $s_{\text{up}} = 0.496$

Even better: for $CL = 0.917923$ we get $s_{\text{up}} = 10^{-4}$!

Reality check: with $b = 2.5$, typical Poisson fluctuation in n is at least $\sqrt{2.5} = 1.6$. How can the limit be so low?

Look at the mean limit for the no-signal hypothesis ($s = 0$) (sensitivity).

Distribution of 95% CL limits with $b = 2.5$, $s = 0$.
Mean upper limit = 4.44



The Bayesian approach to limits

In Bayesian statistics need to start with ‘prior pdf’ $\pi(\theta)$, this reflects degree of belief about θ before doing the experiment.

Bayes’ theorem tells how our beliefs should be updated in light of the data x :

$$p(\theta|x) = \frac{L(x|\theta)\pi(\theta)}{\int L(x|\theta')\pi(\theta') d\theta'} \propto L(x|\theta)\pi(\theta)$$

Integrate posterior pdf $p(\theta|x)$ to give interval with any desired probability content.

For e.g. $n \sim \text{Poisson}(s+b)$, 95% CL upper limit on s from

$$0.95 = \int_{-\infty}^{s_{\text{sup}}} p(s|n) ds$$

Bayesian prior for Poisson parameter

Include knowledge that $s \geq 0$ by setting prior $\pi(s) = 0$ for $s < 0$.

Could try to reflect ‘prior ignorance’ with e.g.

$$\pi(s) = \begin{cases} 1 & s \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

Not normalized but this is OK as long as $L(s)$ dies off for large s .

Not invariant under change of parameter — if we had used instead a flat prior for, say, the mass of the Higgs boson, this would imply a non-flat prior for the expected number of Higgs events.

Doesn’t really reflect a reasonable degree of belief, but often used as a point of reference;

or viewed as a recipe for producing an interval whose frequentist properties can be studied (coverage will depend on true s).

Bayesian interval with flat prior for s

Solve to find limit s_{up} :

$$s_{\text{up}} = \frac{1}{2} F_{\chi^2}^{-1} [p, 2(n+1)] - b$$

where

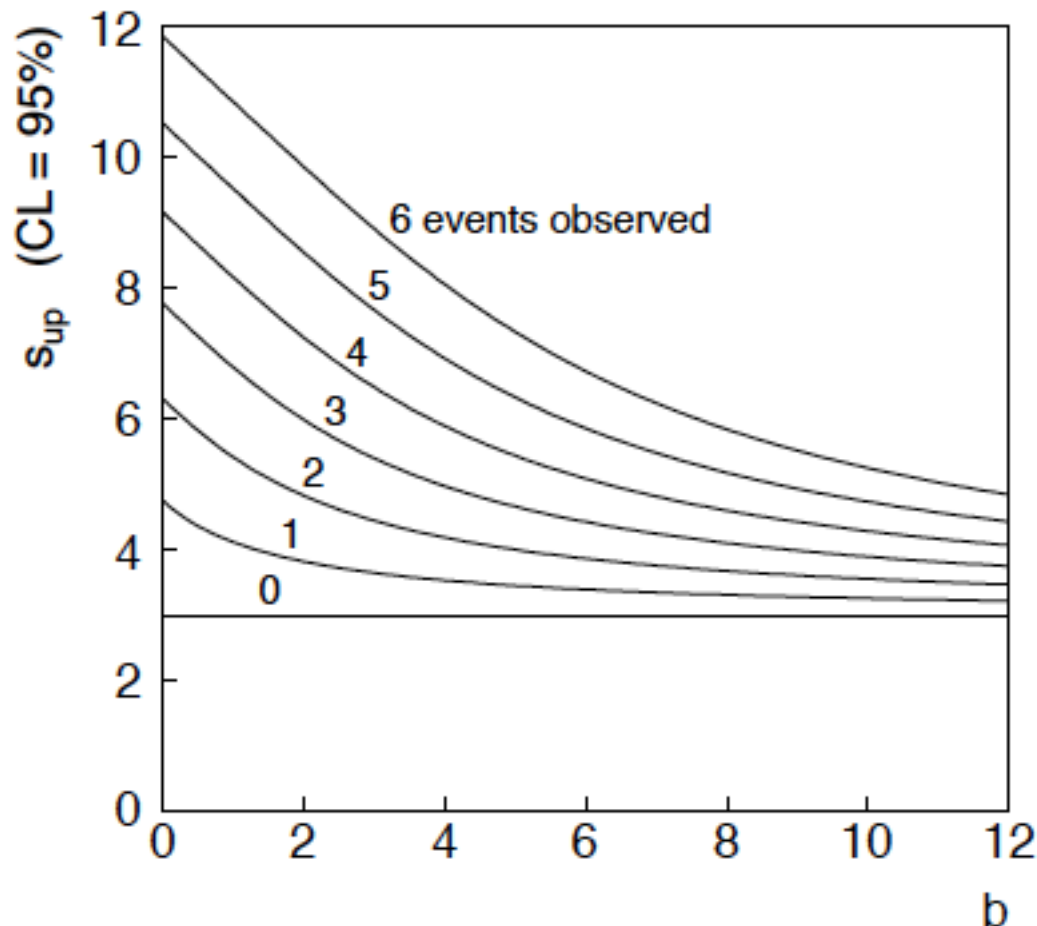
$$p = 1 - \alpha \left(1 - F_{\chi^2} [2b, 2(n+1)] \right)$$

For special case $b = 0$, Bayesian upper limit with flat prior numerically same as one-sided frequentist case ('coincidence').

Bayesian interval with flat prior for s

For $b > 0$ Bayesian limit is everywhere greater than the (one sided) frequentist upper limit.

Never goes negative. Doesn't depend on b if $n = 0$.



Approximate confidence intervals/regions from the likelihood function

Suppose we test parameter value(s) $\theta = (\theta_1, \dots, \theta_n)$ using the ratio

$$\lambda(\theta) = \frac{L(\theta)}{L(\hat{\theta})} \quad 0 \leq \lambda(\theta) \leq 1$$

Lower $\lambda(\theta)$ means worse agreement between data and hypothesized θ . Equivalently, usually define

$$t_\theta = -2 \ln \lambda(\theta)$$

so higher t_θ means worse agreement between θ and the data.

p -value of θ therefore

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

need pdf

Confidence region from Wilks' theorem

Wilks' theorem says (in large-sample limit and providing certain conditions hold...)

$$f(t_{\theta}|\theta) \sim \chi_n^2$$

chi-square dist. with # d.o.f. =
of components in $\theta = (\theta_1, \dots, \theta_n)$.

Assuming this holds, the p -value is

$$p_{\theta} = 1 - F_{\chi_n^2}(t_{\theta}) \quad \text{where} \quad F_{\chi_n^2}(t_{\theta}) \equiv \int_0^{t_{\theta}} f_{\chi_n^2}(t'_{\theta}) dt'_{\theta}$$

To find boundary of confidence region set $p_{\theta} = \alpha$ and solve for t_{θ} :

$$t_{\theta} = F_{\chi_n^2}^{-1}(1 - \alpha) = -2 \ln \frac{L(\theta)}{L(\hat{\theta})}$$

Confidence region from Wilks' theorem (cont.)

i.e., boundary of confidence region in θ space is where

$$\ln L(\theta) = \ln L(\hat{\theta}) - \frac{1}{2} F_{\chi_n^2}^{-1}(1 - \alpha)$$

For example, for $1 - \alpha = 68.3\%$ and $n = 1$ parameter,

$$F_{\chi_1^2}^{-1}(0.683) = 1$$

and so the 68.3% confidence level interval is determined by

$$\ln L(\theta) = \ln L(\hat{\theta}) - \frac{1}{2}$$

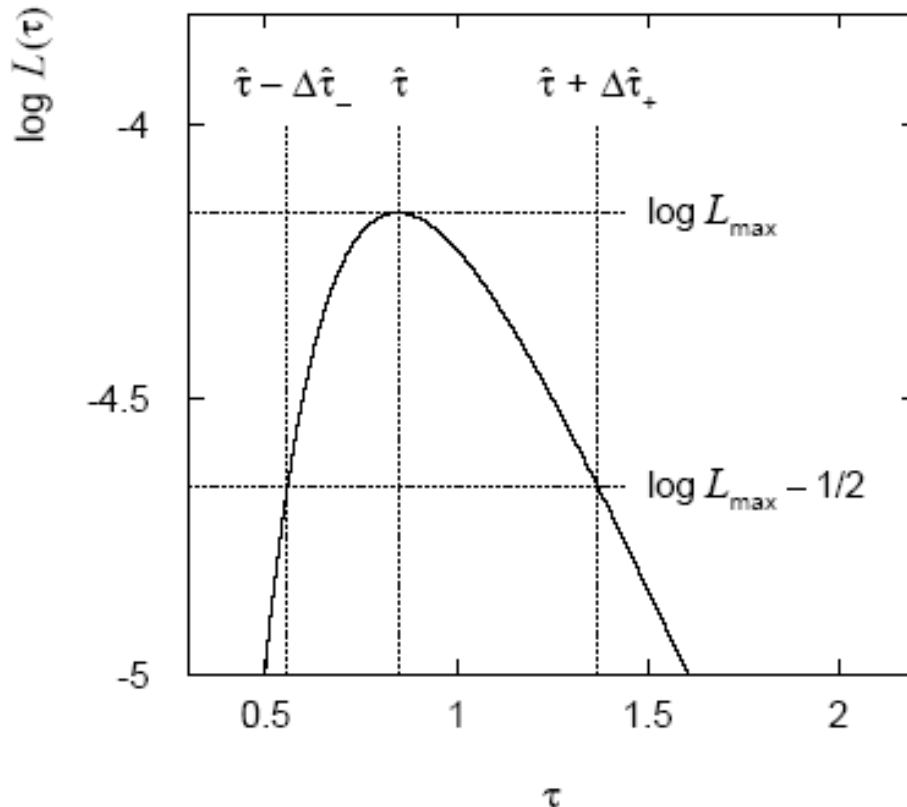
Same as recipe for finding the estimator's standard deviation, i.e.,

$[\hat{\theta} - \sigma_{\hat{\theta}}, \hat{\theta} + \sigma_{\hat{\theta}}]$ is a 68.3% CL confidence interval.

Example of interval from $\ln L$

For $n = 1$ parameter, $CL = 0.683$, $Q_\alpha = 1$.

Exponential example, now with only 5 events:



Parameter estimate and approximate 68.3% CL confidence interval:

$$\hat{\tau} = 0.85^{+0.52}_{-0.30}$$

Multiparameter case

For increasing number of parameters, $CL = 1 - \alpha$ decreases for confidence region determined by a given

$$Q_\alpha = F_{\chi_n^2}^{-1}(1 - \alpha)$$

Q_α	$1 - \alpha$				
	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
1.0	0.683	0.393	0.199	0.090	0.037
2.0	0.843	0.632	0.428	0.264	0.151
4.0	0.954	0.865	0.739	0.594	0.451
9.0	0.997	0.989	0.971	0.939	0.891

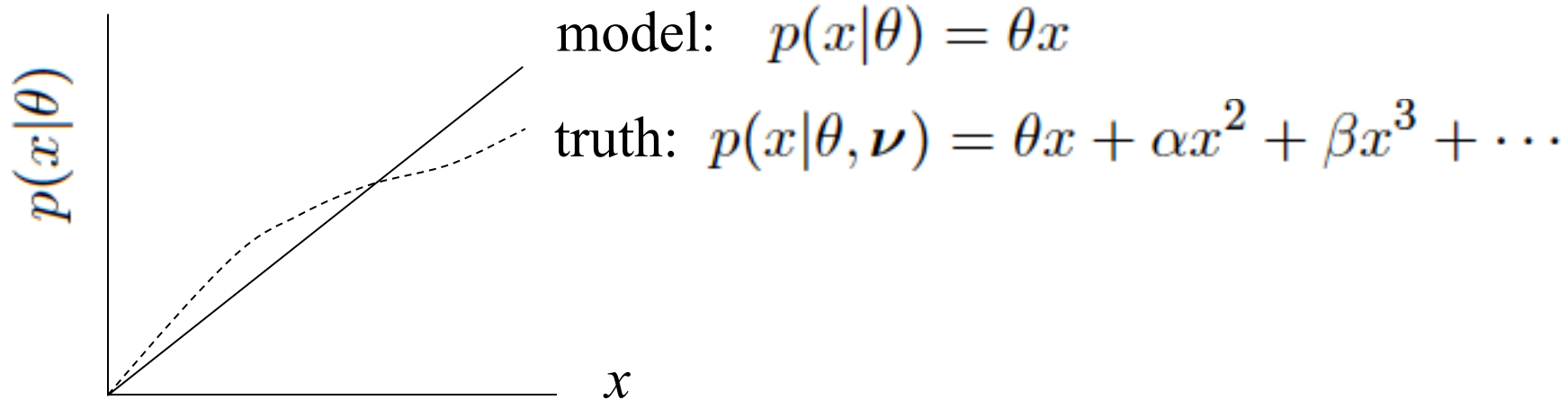
Multiparameter case (cont.)

Equivalently, Q_α increases with n for a given $\text{CL} = 1 - \alpha$.

$1 - \alpha$	\bar{Q}_α				
	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
0.683	1.00	2.30	3.53	4.72	5.89
0.90	2.71	4.61	6.25	7.78	9.24
0.95	3.84	5.99	7.82	9.49	11.1
0.99	6.63	9.21	11.3	13.3	15.1

Systematic uncertainties and nuisance parameters

In general our model of the data is not perfect:



Can improve model by including additional adjustable parameters.

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

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).

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

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

But what values of ν to use for $f(q_\theta | \theta, \nu)$?

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

→ “exact” confidence interval

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 (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 value of the nuisance parameter that best fits the data for the specified θ :

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

“double hat” notation means profiled value, i.e., 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).

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 $\boldsymbol{\nu}$

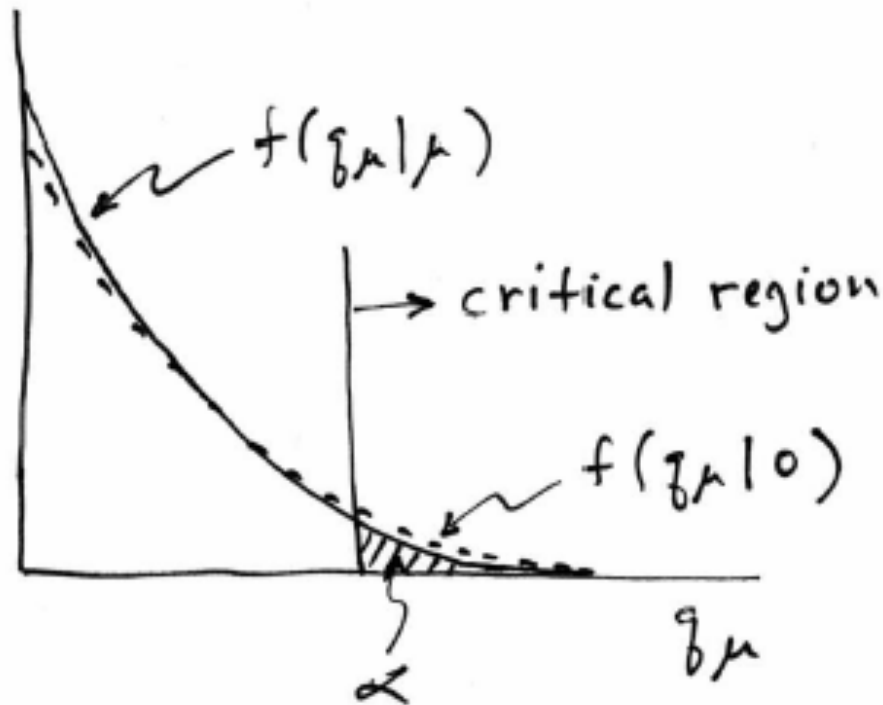
and define $q_\theta = -2 \ln \lambda(\boldsymbol{\theta})$.

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 $\boldsymbol{\nu}$** .

Low sensitivity to μ

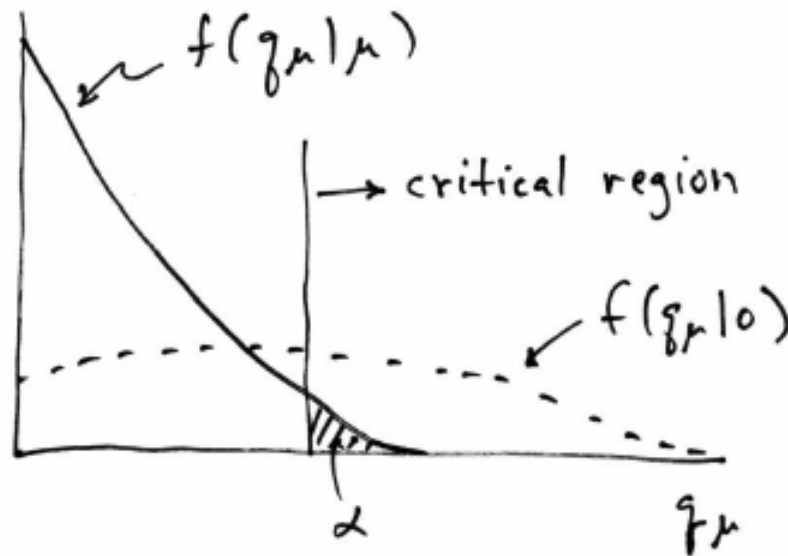
It can be that the effect of a given hypothesized μ is very small relative to the background-only ($\mu = 0$) prediction.

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:

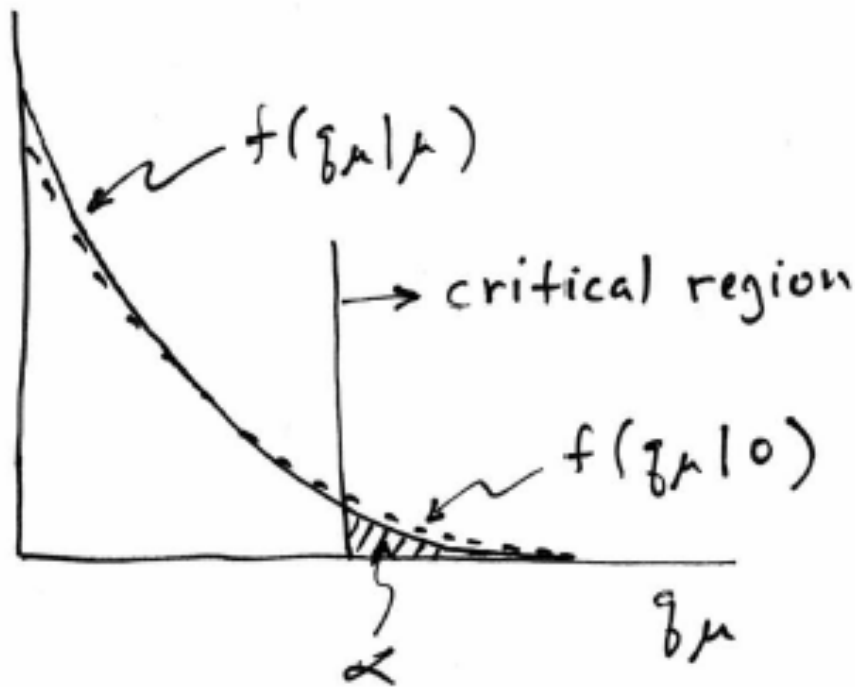


That is, the power (probability to reject μ if $\mu = 0$) is substantially higher than α . Use this power as a measure of the sensitivity.

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

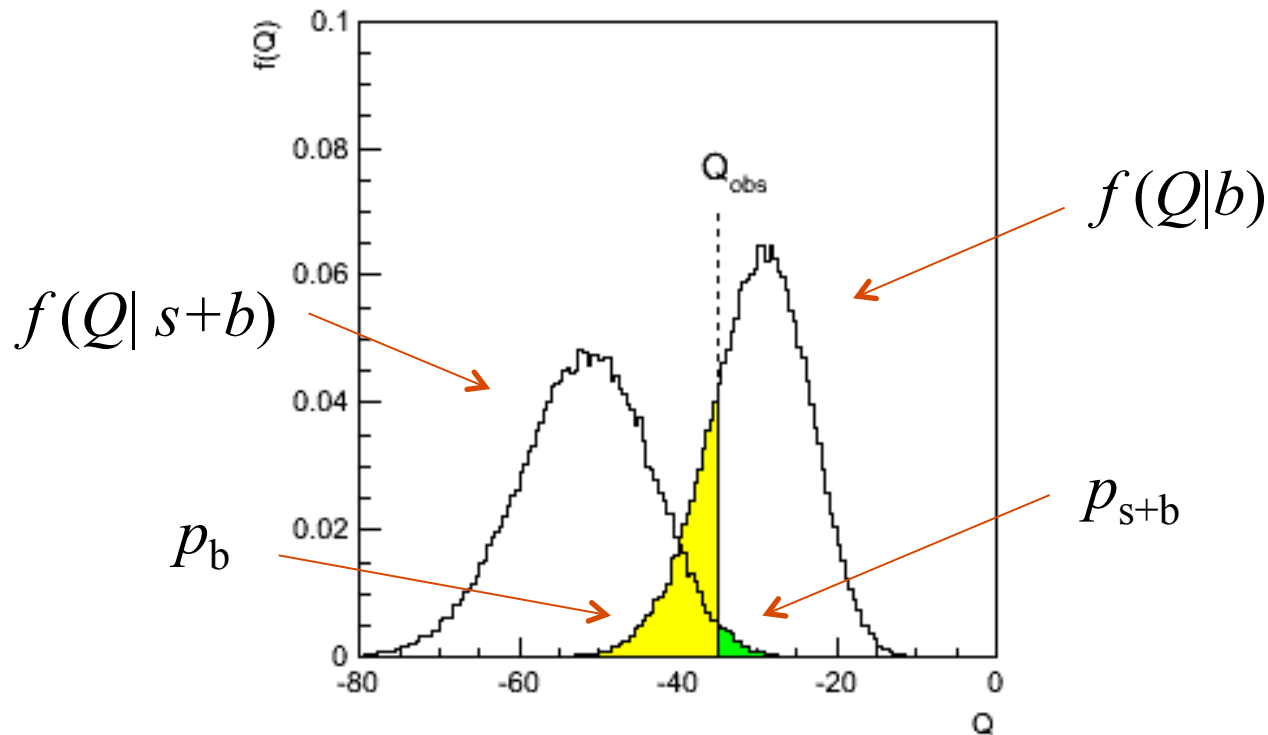
T. Junk, Nucl. Instrum. Methods Phys. Res., Sec. A **434**, 435 (1999); A.L. Read, J. Phys. G **28**, 2693 (2002).

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

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

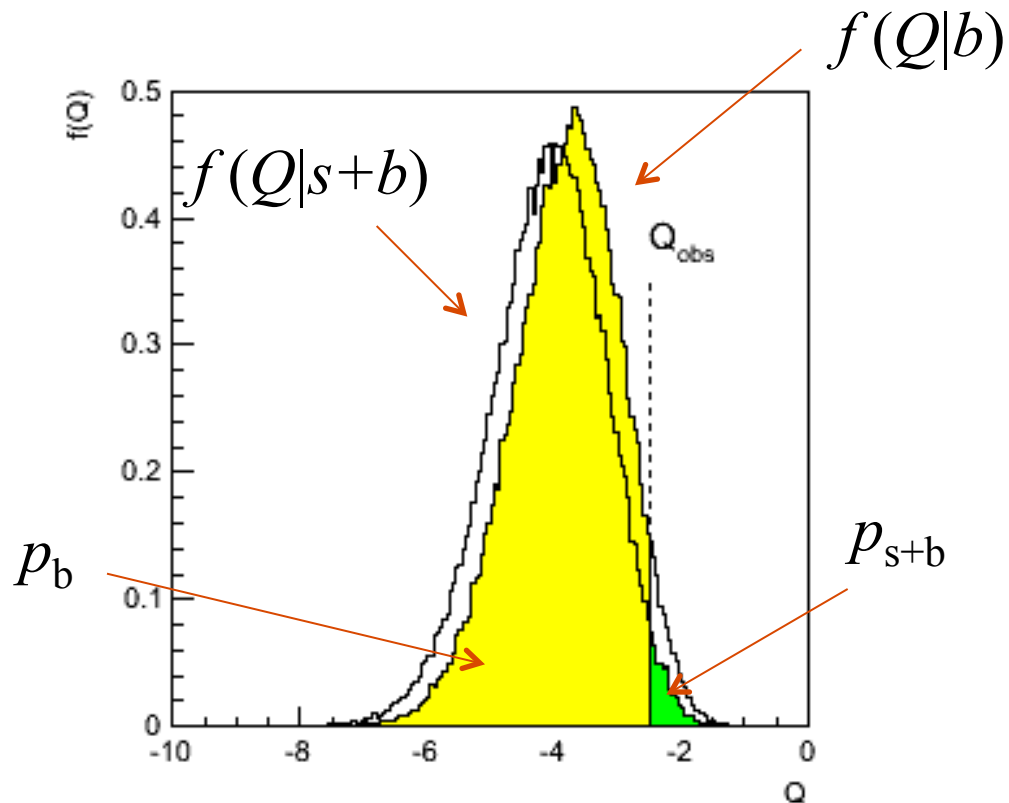
The CL_s procedure

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.,

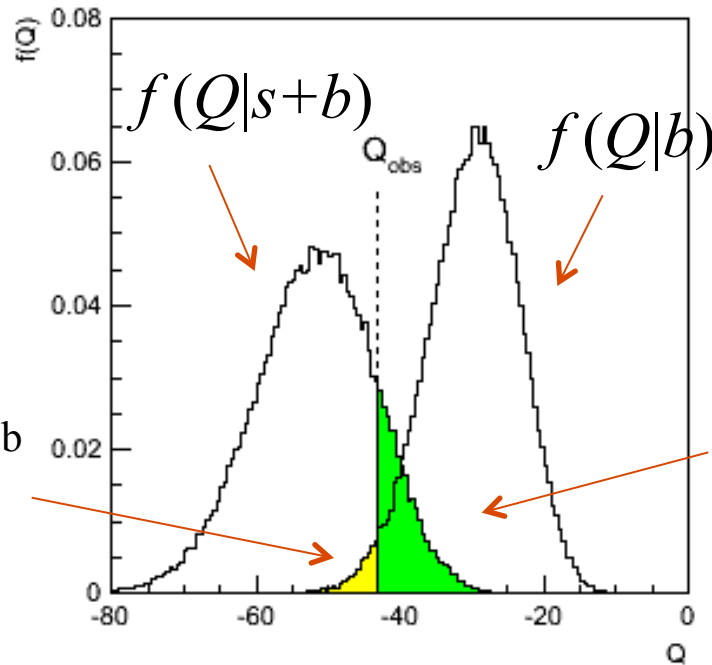
Define:

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

Reject $s+b$ hypothesis if:

$$CL_s \leq \alpha$$

$$1 - CL_b = p_b$$



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

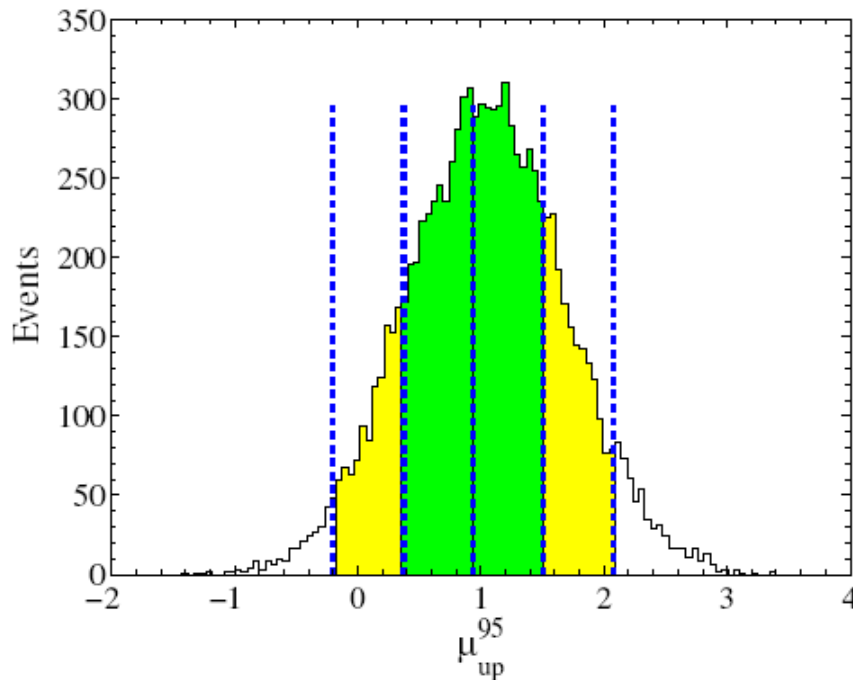
Increases “effective” p -value when the two distributions become close (prevents exclusion if sensitivity is low).

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.

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:

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

maximizes L for specified μ

maximize L

Define critical region of test of μ by the region of data space that gives the lowest values of $\lambda(\mu)$.

Important advantage of profile LR is that its distribution becomes **independent of nuisance parameters** in large sample limit.

Test statistic for discovery

Suppose relevant alternative to background-only ($\mu = 0$) is $\mu \geq 0$.

So take critical region for test of $\mu = 0$ corresponding to high q_0 and $\hat{\mu} > 0$ (data characteristic for $\mu \geq 0$).

That is, to test background-only hypothesis define statistic

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

i.e. here only large (positive) observed signal strength is evidence against the background-only hypothesis.

Note that even though here physically $\mu \geq 0$, 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.

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:

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

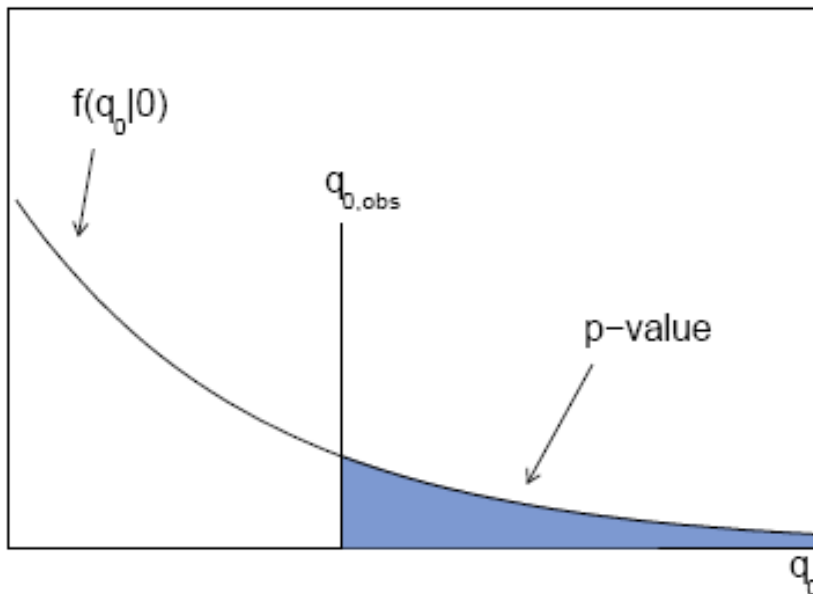
In large sample limit, $f(q_0|0)$ independent of nuisance parameters; $f(q_0|\mu')$ depends on nuisance parameters through σ .

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

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

use e.g. asymptotic formula



From *p*-value get equivalent significance,

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

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

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

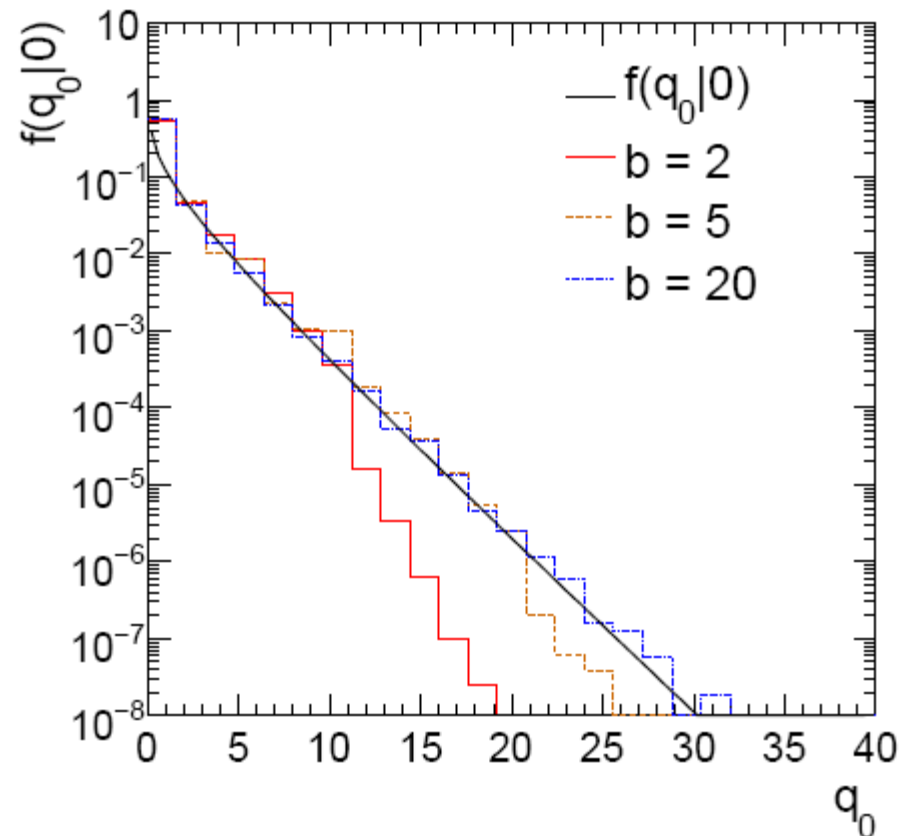
$$m \sim \text{Poisson}(\tau b)$$

μ = param. of interest

b = nuisance parameter

Here take s known, $\tau = 1$.

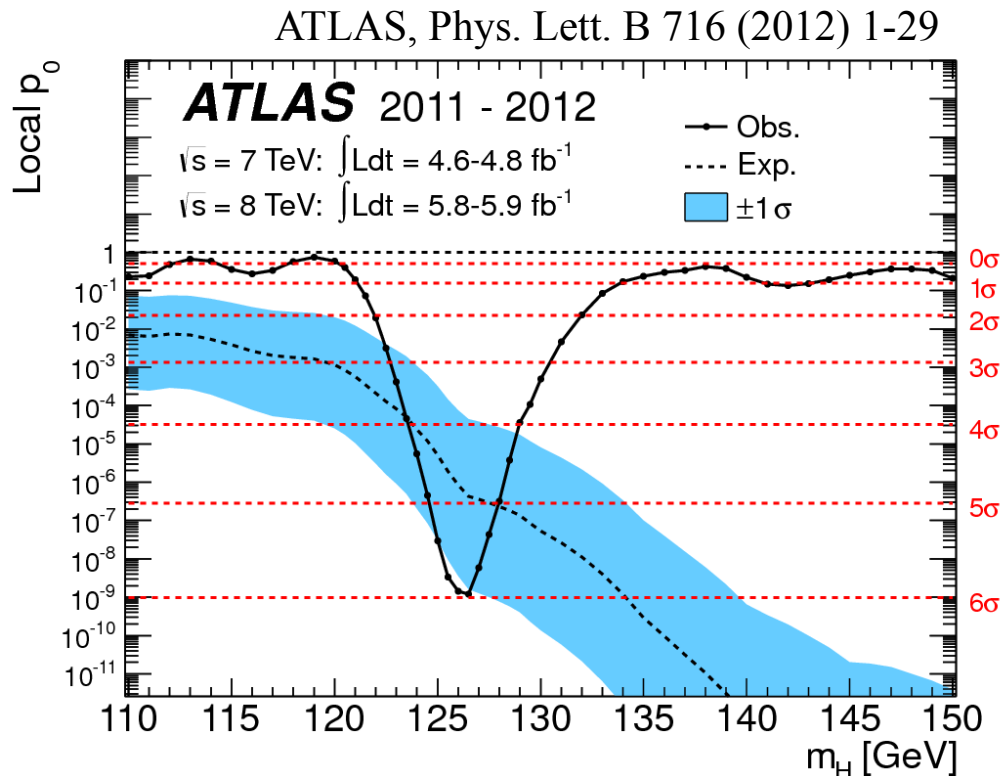
Asymptotic formula is good approximation to 5σ level ($q_0 = 25$) already for $b \sim 20$.



How to read the p_0 plot

The “local” p_0 means the p -value of the background-only hypothesis obtained from the test of $\mu = 0$ at each individual m_H , without any correction for the Look-Elsewhere Effect.

The “Expected” (dashed) curve gives the median p_0 under assumption of the SM Higgs ($\mu = 1$) at each m_H .



The blue band gives the width of the distribution ($\pm 1\sigma$) of significances under assumption of the SM Higgs.

Test statistic for upper limits

For purposes of setting an upper limit on μ 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

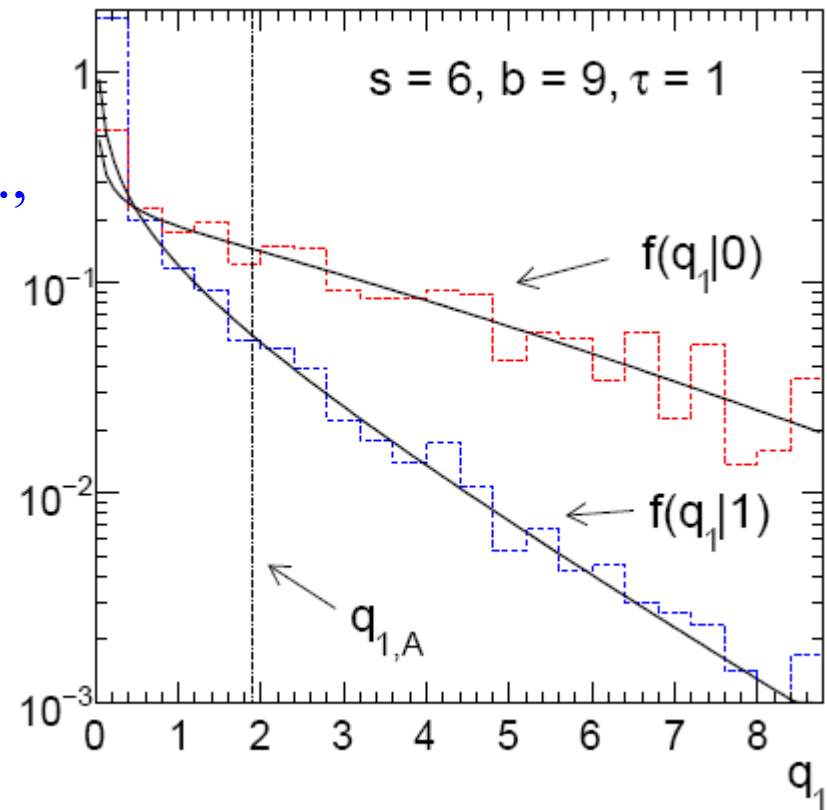
Consider again $n \sim \text{Poisson}(\mu s + b)$, $m \sim \text{Poisson}(\tau b)$
 Use q_μ to find p -value of hypothesized μ values.

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 $s = 6$, $b = 9$.

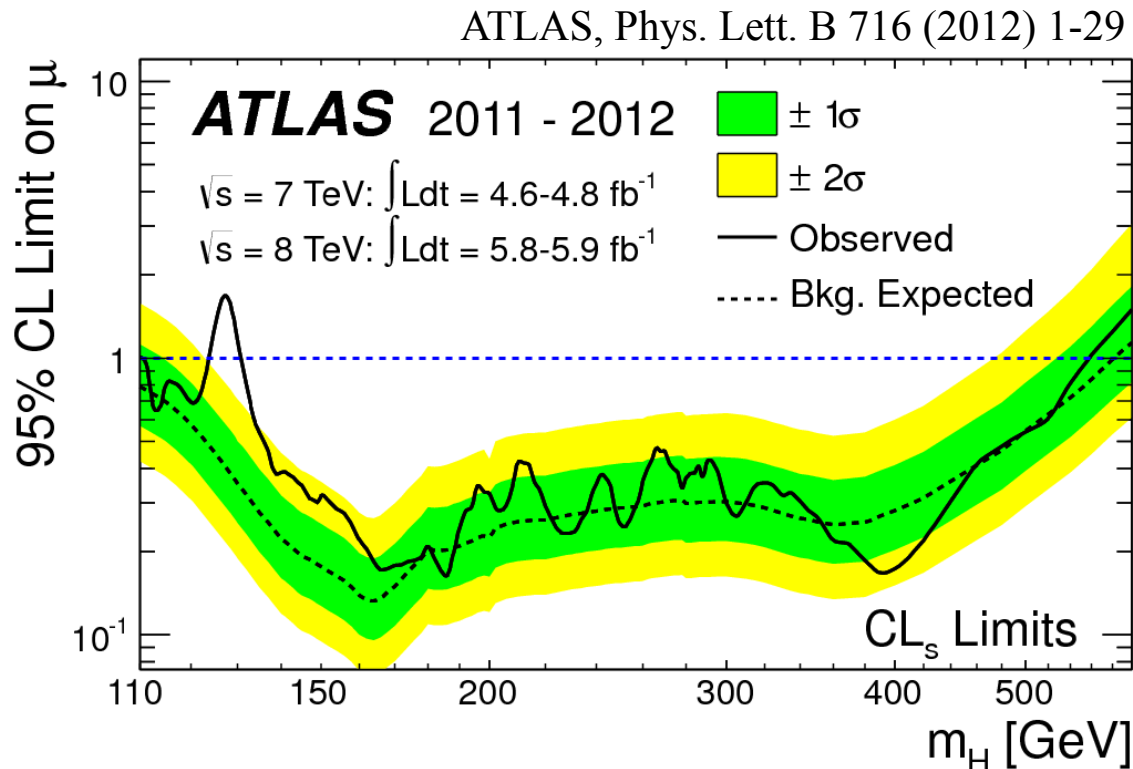


How to read the green and yellow limit plots

For every value of m_H , find the 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.



Example: fitting a straight line

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

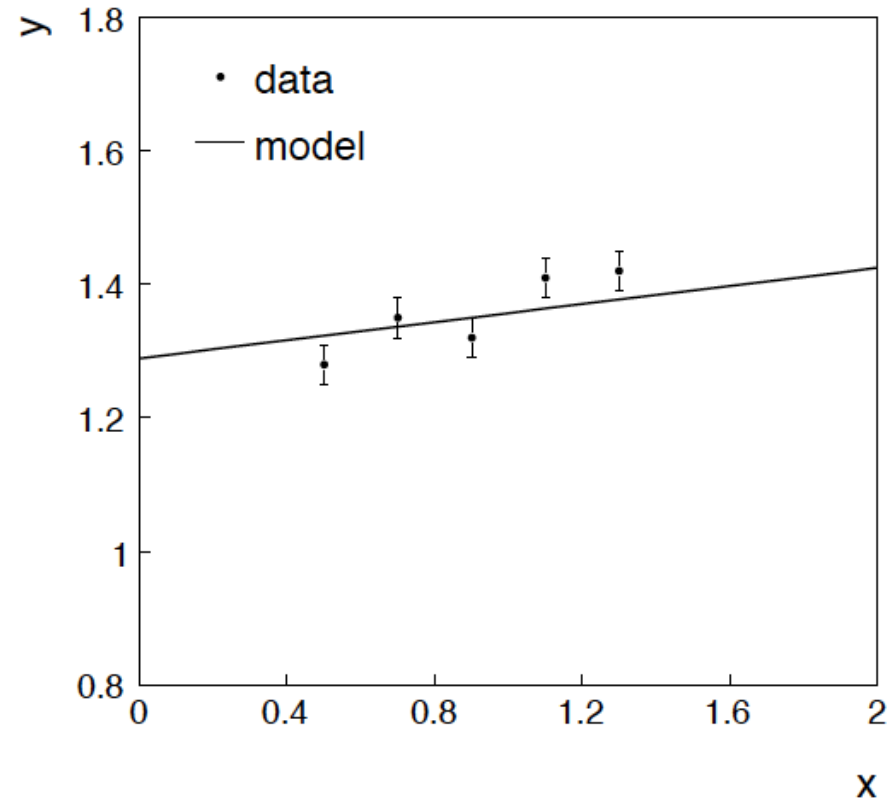
Model: y_i independent and all follow $y_i \sim \text{Gauss}(\mu(x_i), \sigma_i)$

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

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

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

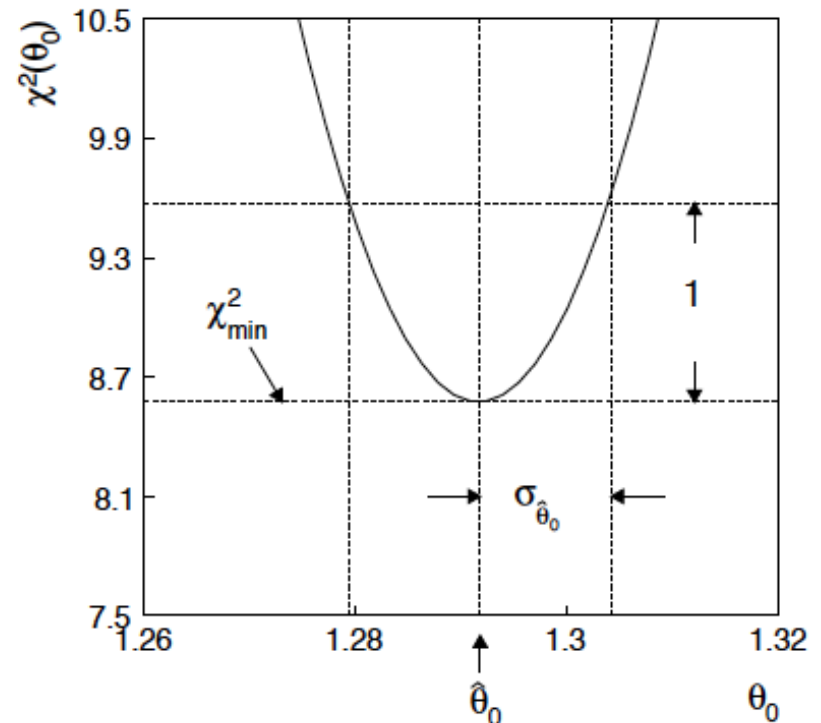
$$\chi^2(\theta_0) = -2 \ln L(\theta_0) + \text{const} = \sum_{i=1}^n \frac{(y_i - \mu(x_i; \theta_0, \theta_1))^2}{\sigma_i^2}.$$

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



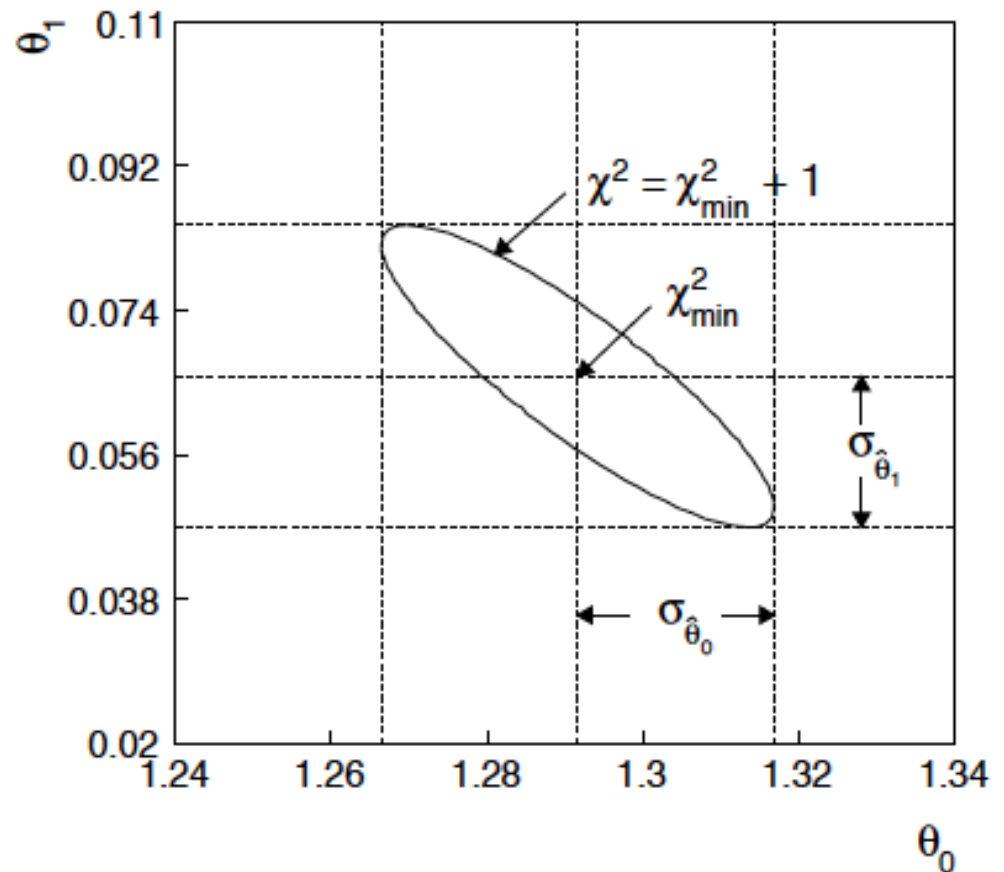
ML (or LS) fit of θ_0 and θ_1

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

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.

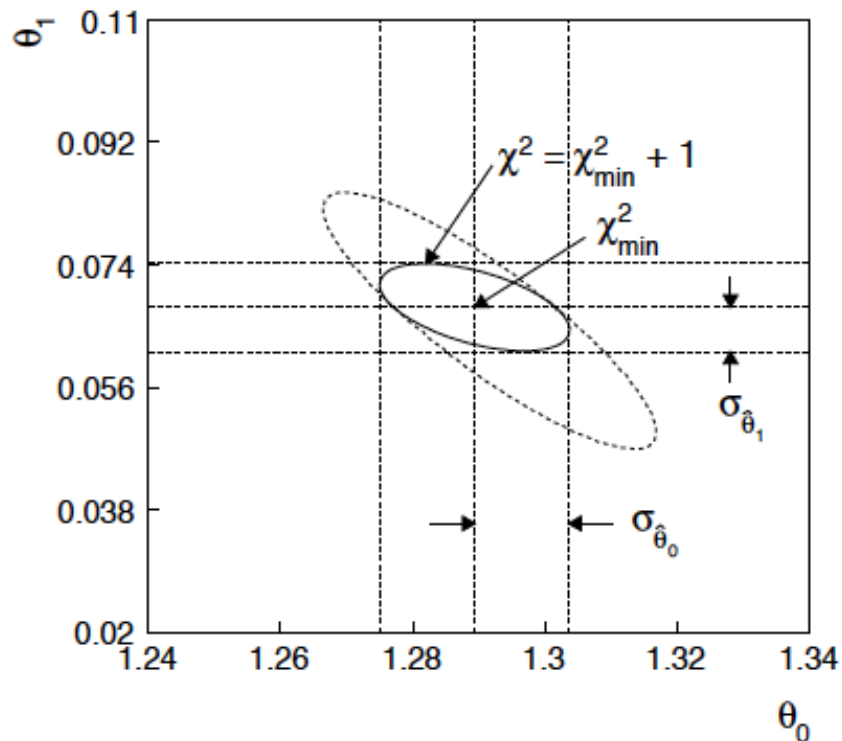


If we have a measurement $t_1 \sim \text{Gauss}(\theta_1, \sigma_{t_1})$

$$L(\theta_0, \theta_1) = \frac{1}{\sqrt{2\pi}\sigma_t} e^{-(t_1 - \theta_1)^2 / 2\sigma_{t_1}^2} \prod_{i=1}^n \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left[-\frac{1}{2} \frac{(y_i - \mu(x_i; \theta_0, \theta_1))^2}{\sigma_i^2}\right]$$

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

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



The Bayesian approach

In Bayesian statistics we can associate a probability with a hypothesis, e.g., a parameter value θ .

Interpret probability of θ as ‘degree of belief’ (subjective).

Need to start with ‘**prior pdf**’ $\pi(\theta)$, this reflects degree of belief about θ before doing the experiment.

Our experiment has data x , \rightarrow **likelihood function** $L(x|\theta)$.

Bayes’ theorem tells how our beliefs should be updated in light of the data x :

$$p(\theta|x) = \frac{L(x|\theta)\pi(\theta)}{\int L(x|\theta')\pi(\theta') d\theta'} \propto L(x|\theta)\pi(\theta)$$

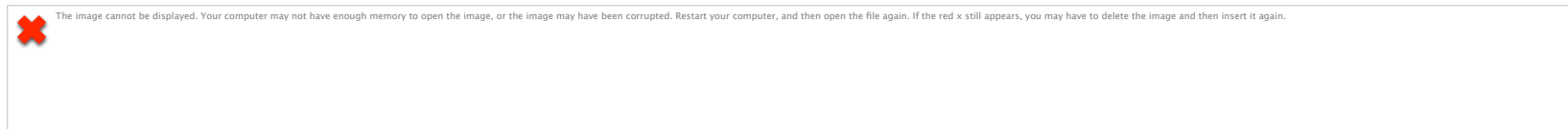
Posterior pdf $p(\theta|x)$ contains all our knowledge about θ .

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:



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: $q(\vec{\theta}; \vec{\theta}_0) = q(\vec{\theta}_0; \vec{\theta})$

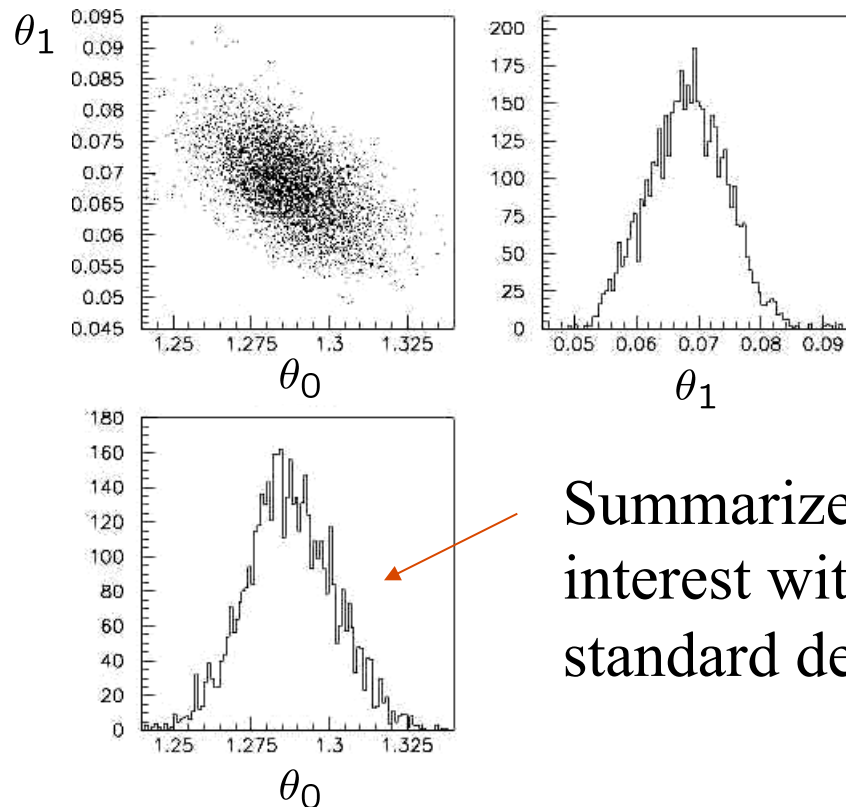
Test ratio is (*Metropolis-Hastings*): $\alpha = \min \left[1, \frac{p(\vec{\theta})}{p(\vec{\theta}_0)} \right]$

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.

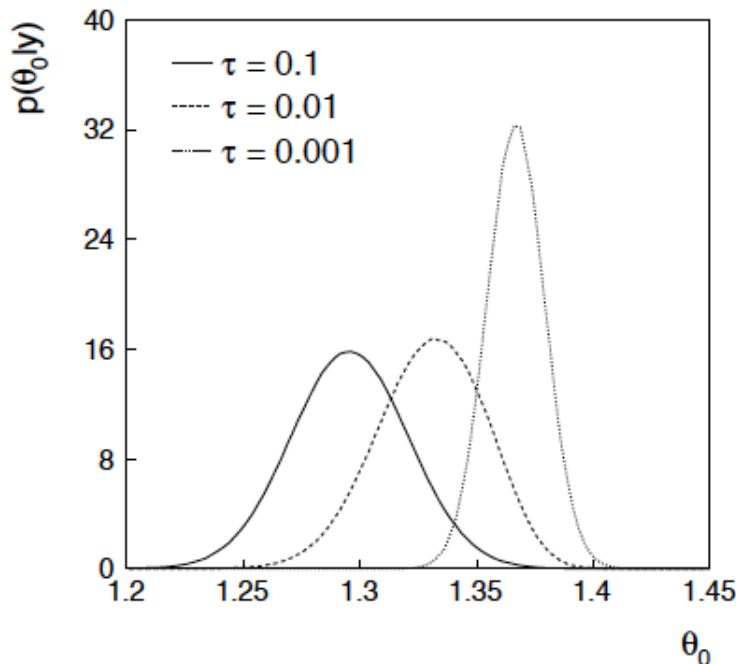
Although numerical values of answer here same as in frequentist case, interpretation is different (sometimes unimportant?)

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.

Expected discovery significance for counting experiment with background uncertainty

I. Discovery sensitivity for counting experiment with b known:

(a) $\frac{s}{\sqrt{b}}$

(b) Profile likelihood ratio test & Asimov: $\sqrt{2 \left((s + b) \ln \left(1 + \frac{s}{b} \right) - s \right)}$

II. Discovery sensitivity with uncertainty in b , σ_b :

(a) $\frac{s}{\sqrt{b + \sigma_b^2}}$

(b) Profile likelihood ratio test & Asimov:

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

Counting experiment with known background

Count a number of events $n \sim \text{Poisson}(s+b)$, 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),

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

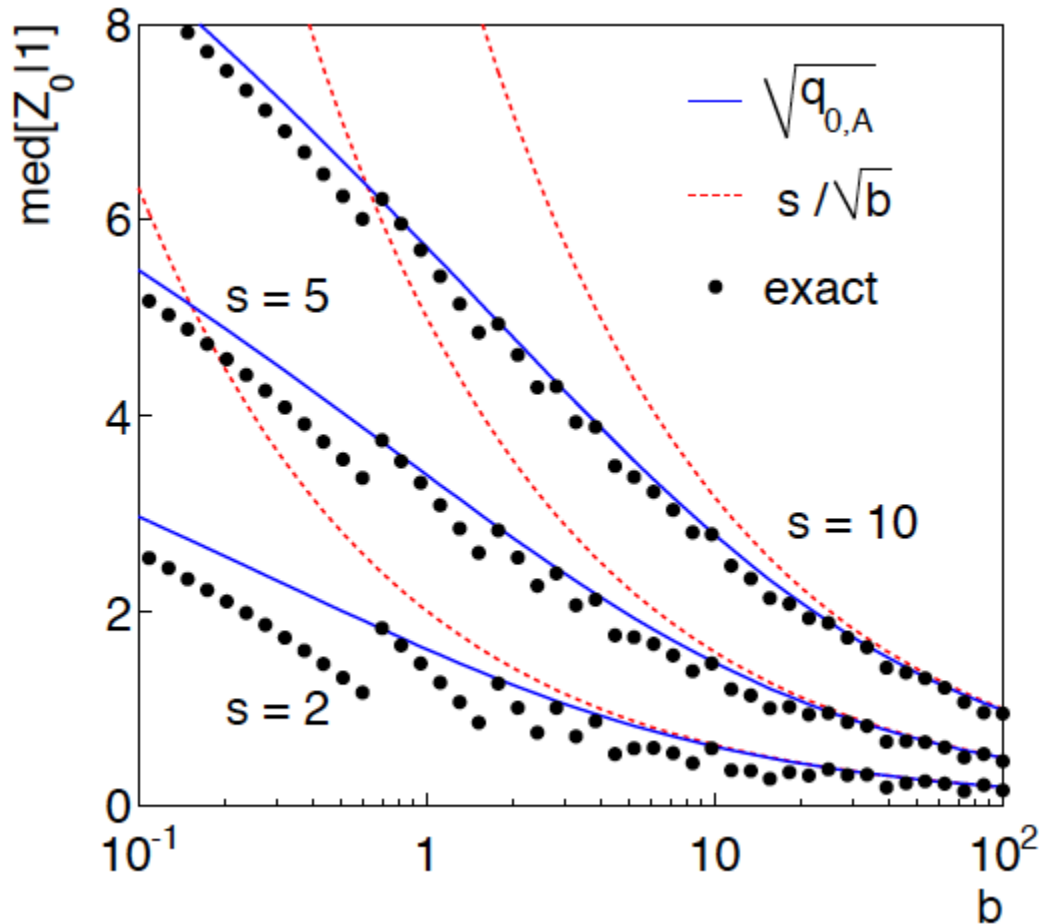
To find $\text{median}[Z|s]$, let $n \rightarrow s + b$ (i.e., the Asimov data set):

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

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.

Profile likelihood with b uncertain

This is the well studied “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 :

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

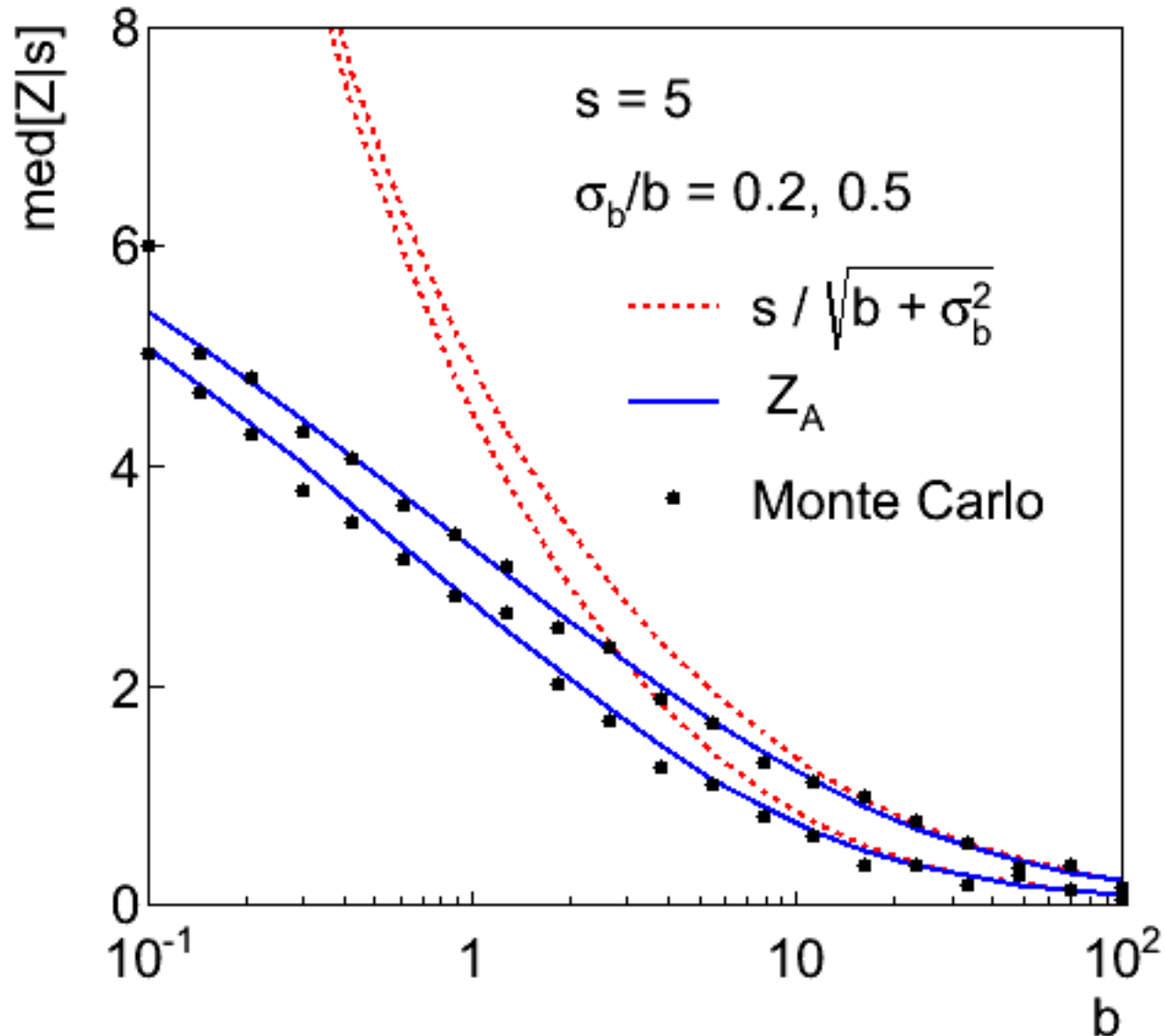
Limiting cases

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 the “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

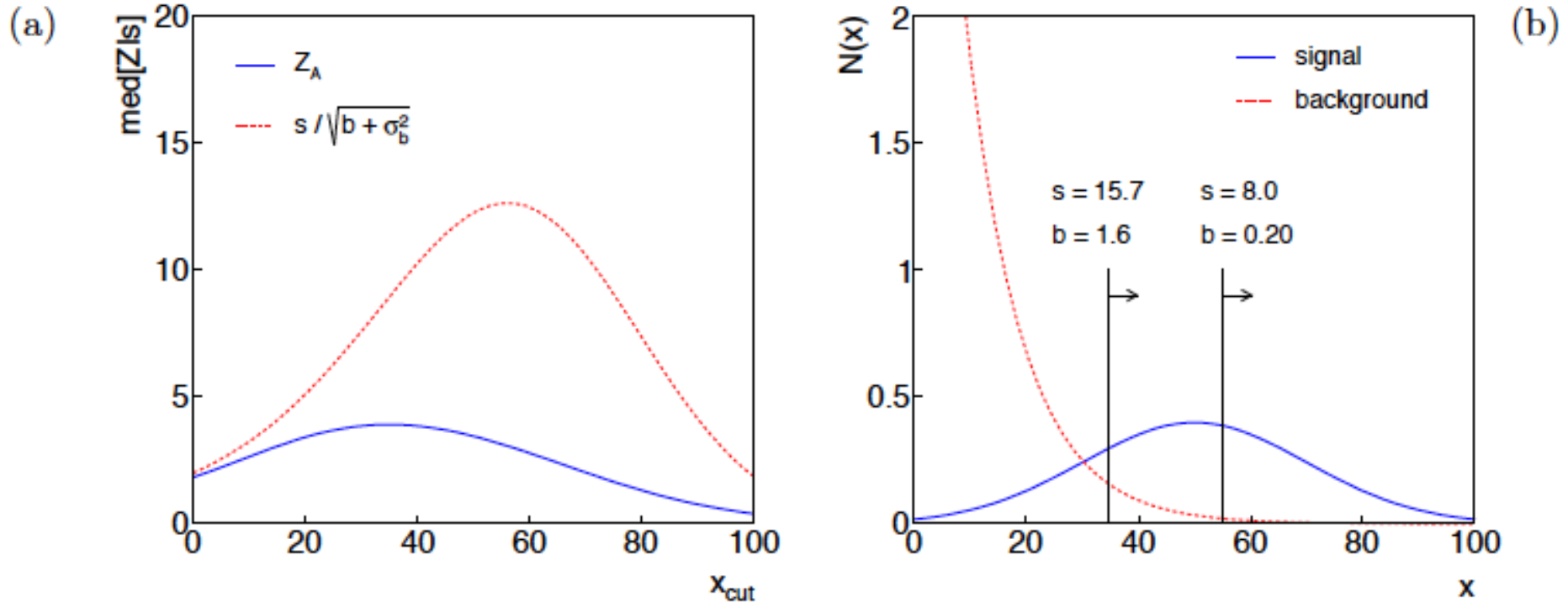


Figure 1: (a) The expected significance as a function of the cut value x_{cut} ; (b) the distributions of signal and background with the optimal cut value indicated.

Summary on discovery sensitivity

Simple formula for expected discovery significance based on profile likelihood ratio test and Asimov approximation:

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

For large b , all formulae OK.

For small b , s/\sqrt{b} and $s/\sqrt{(b+\sigma_b^2)}$ overestimate the significance.

Could be important in optimization of searches with low background.

Formula maybe also OK if model is not simple on/off experiment, e.g., several background control measurements (checking this).

Finally

Three lectures only enough for a brief introduction to:

Statistical tests for discovery and limits

Multivariate methods

Bayesian parameter estimation, MCMC

Experimental sensitivity

No time for many important topics

Properties of estimators (bias, variance)

Bayesian approach to discovery (Bayes factors)

The look-elsewhere effect, etc., etc.

Final thought: once the basic formalism is understood, most of the work focuses on writing down the likelihood, e.g., $P(x|q)$, and including in it enough parameters to adequately describe the data (true for both Bayesian and frequentist approaches).

Extra slides

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 .

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).

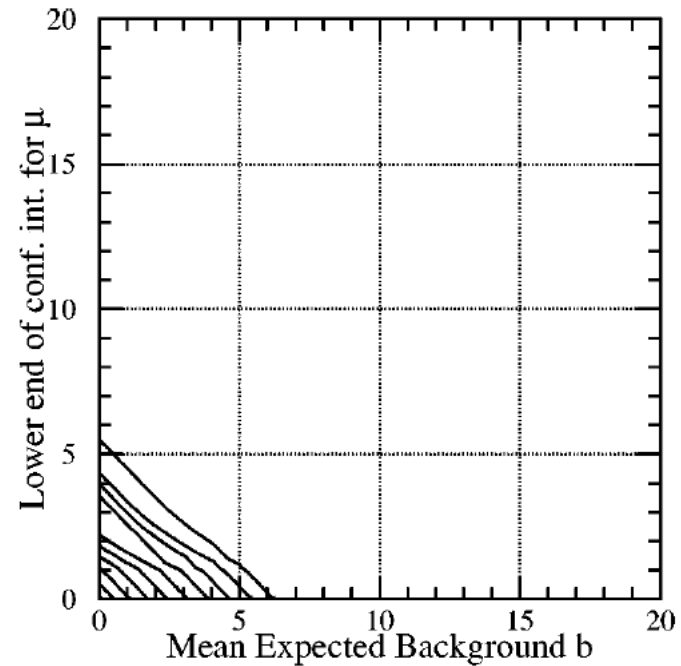
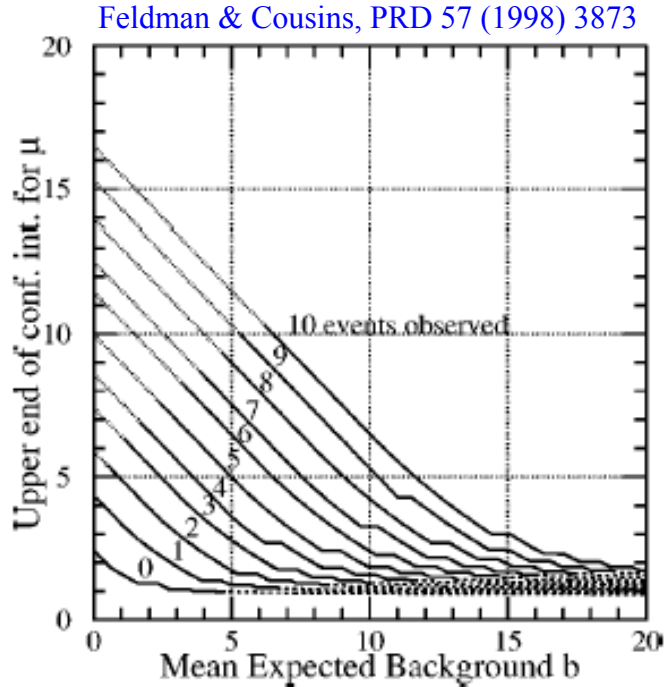
The p -value for an observed value of t_μ is

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

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



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).

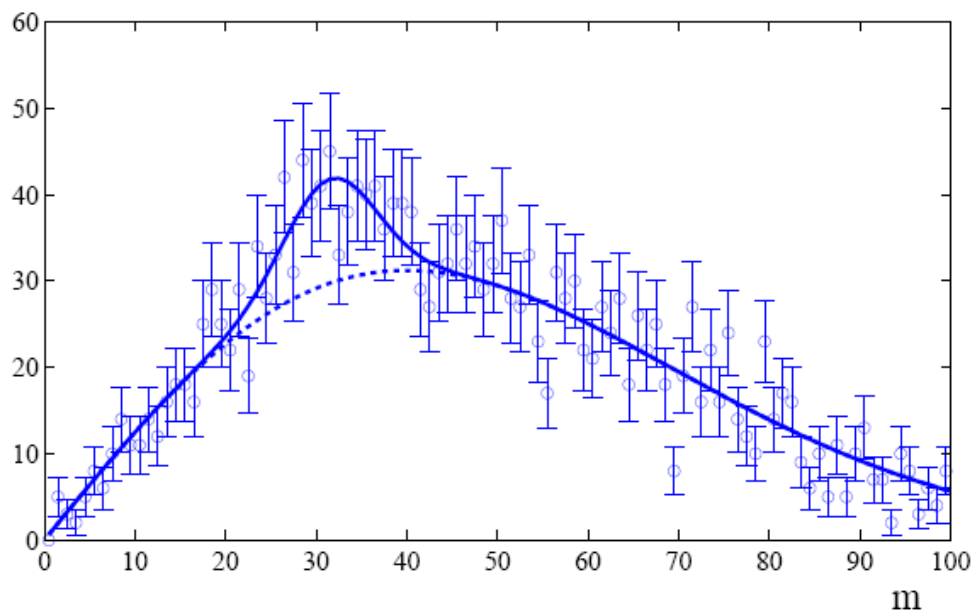
The interval's upper edge is higher than the limit from the one-sided test, and lower values of μ may be excluded as well. A substantial downward fluctuation in the data gives a low (but nonzero) limit.

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

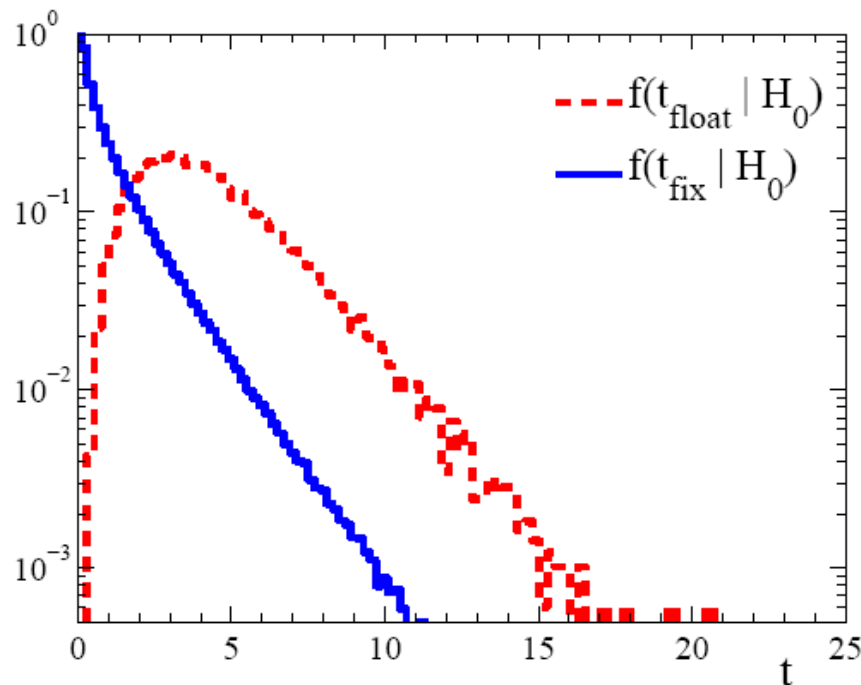
$$t_{\text{float}} = -2 \ln \frac{L(0)}{L(\hat{\mu}, \hat{m})} \quad (\text{Note } m \text{ does not appear in the } \mu = 0 \text{ model.})$$

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

Distributions of t_{fix} , t_{float}

For a sufficiently large data sample, $t_{\text{fix}} \sim$ 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 $t_{\text{float}} \sim$ 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).

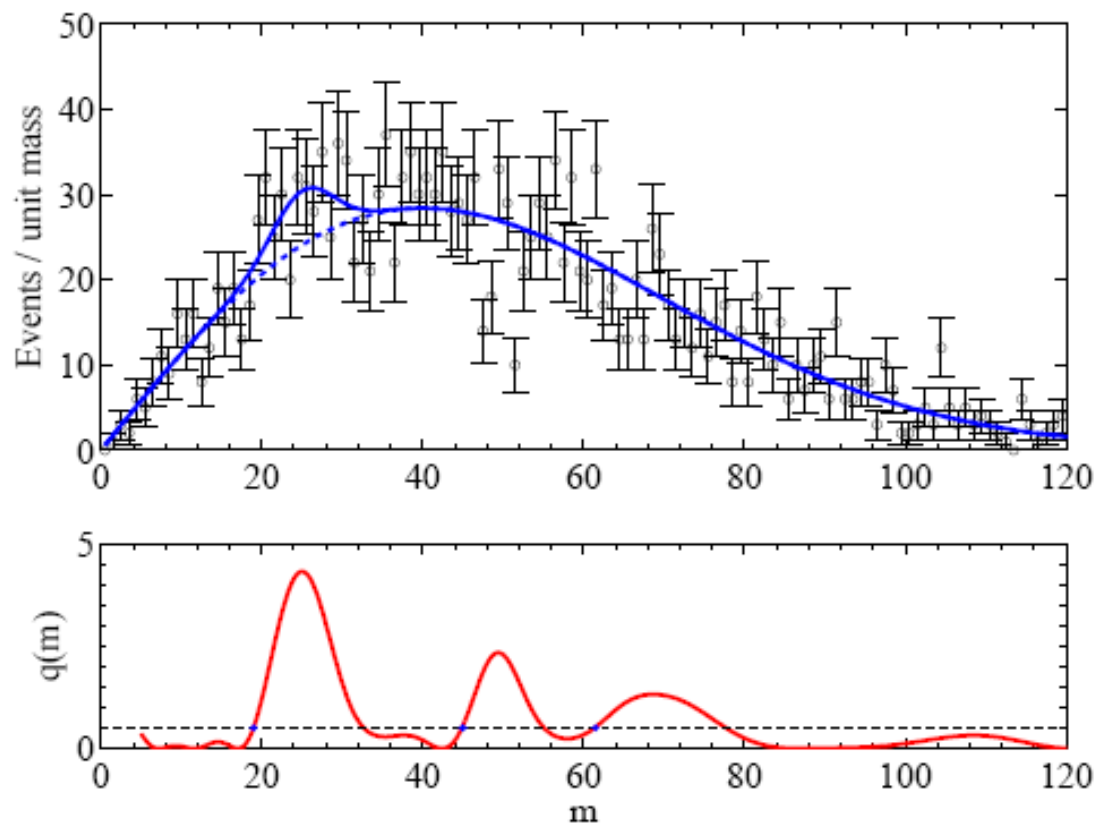
Upcrossings of $-2\ln L$

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.

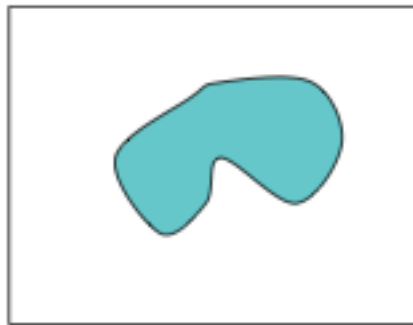


Multidimensional look-elsewhere effect

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

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

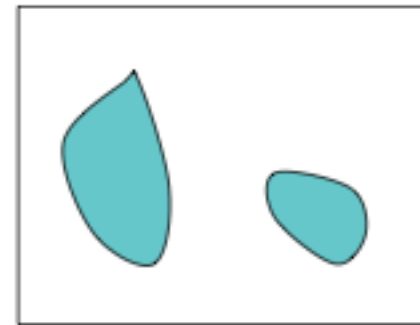
- Number of disconnected components minus number of 'holes'



$\varphi=1$



$\varphi=0$



$\varphi=2$

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 also problematic issue of testing many signal models (or parameter values) and thus excluding some for which one has little or no sensitivity.

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