## Statistical Methods for Particle Physics Lecture 1: introduction & statistical tests

www.pp.rhul.ac.uk/~cowan/stat\_trisep.html



Lectures on Statistics TRISEP School 27, 28 June 2016



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#### Outline

Lecture 1: Introduction and review of fundamentals Review of probability Parameter estimation, maximum likelihood Statistical tests for discovery and limits

#### Lecture 2: Multivariate methods

Neyman-Pearson lemma Fisher discriminant, neural networks Boosted decision trees

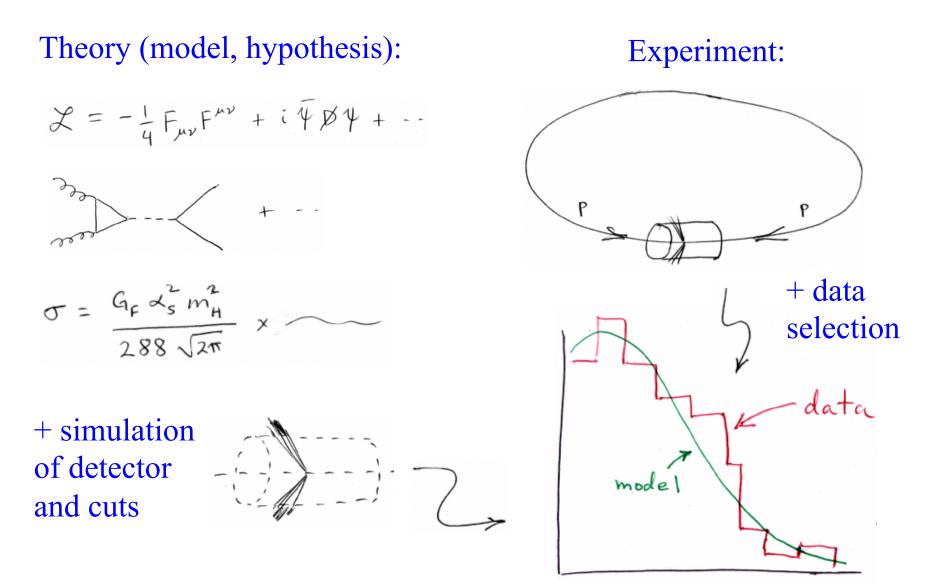
#### Lecture 3: Further topics

Nuisance parameters (Bayesian and frequentist) Experimental sensitivity Revisiting limits

#### 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) K.A. Olive et al. (Particle Data Group), *Review of Particle Physics*, Chin. Phys. C, 38, 090001 (2014); see also pdg.lbl.gov sections on probability, statistics, Monte Carlo

#### Theory ↔ Statistics ↔ Experiment



#### Quick review of probablility

Frequentist (*A* = outcome of repeatable observation):

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

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 <  $\alpha_{\rm s}$  < 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 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 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!)

#### Distribution, likelihood, model

Suppose the outcome of a measurement is *x*. (e.g., a number of events, a histogram, or some larger set of numbers).

The probability density (or mass) function or 'distribution' of x, which may depend on parameters  $\theta$ , is:

 $P(x|\theta)$  (Independent variable is x;  $\theta$  is a constant.)

If we evaluate  $P(x|\theta)$  with given data and regard it as a function of the parameter(s), then this is the likelihood:

 $L(\theta) = P(x|\theta)$  (Data x fixed; treat L as function of  $\theta$ .)

We will use the term 'model' to refer to the full function  $P(x|\theta)$  that contains the dependence both on *x* and  $\theta$ .

Quick review of 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:  $\vec{x} = (x_1, \ldots, x_n)$ 

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

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

Sometimes we say 'estimator' for the function of  $x_1, ..., x_n$ ; 'estimate' for the value of the estimator with a particular data set.

#### Maximum likelihood

The most important frequentist method for constructing estimators is to take the value of the parameter(s) that maximize the likelihood:  $\hat{\theta} = \operatorname{argmax} L(x|\theta)$ 

The resulting 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:

Under conditions usually satisfied in practice, bias of ML estimators is zero in the large sample limit, and the variance is as small as possible for unbiased estimators.

ML estimator may not in some cases be regarded as the optimal trade-off between these criteria (cf. regularized unfolding).

$$V_{ij} = \operatorname{cov}[\hat{\theta}_i, \hat{\theta}_j]$$

$$b = E[\hat{\theta}] - \theta$$

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,  $t_1, \ldots, t_n$ 

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

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

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

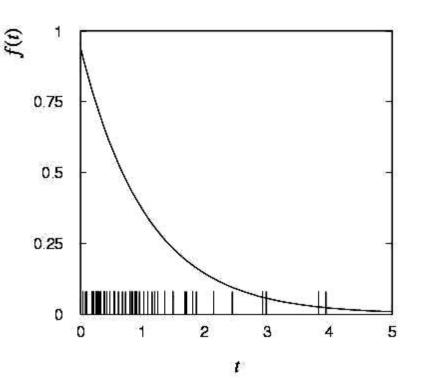
# ML example: parameter of exponential pdf (2) Find its maximum by setting $\frac{\partial \ln L(\tau)}{\partial \tau} = 0$ ,

Monte Carlo test: generate 50 values using  $\tau = 1$ :

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

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

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

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

Variance of estimators from information inequality

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

$$V[\hat{\theta}] \ge \left(1 + \frac{\partial b}{\partial \theta}\right)^2 / E\left[-\frac{\partial^2 \ln L}{\partial \theta^2}\right] \qquad \text{Bound (MVB)} \\ (b = E[\hat{\theta}] - \theta)$$

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

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

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

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

Variance of estimators: graphical method Expand  $\ln L(\theta)$  about its maximum:

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

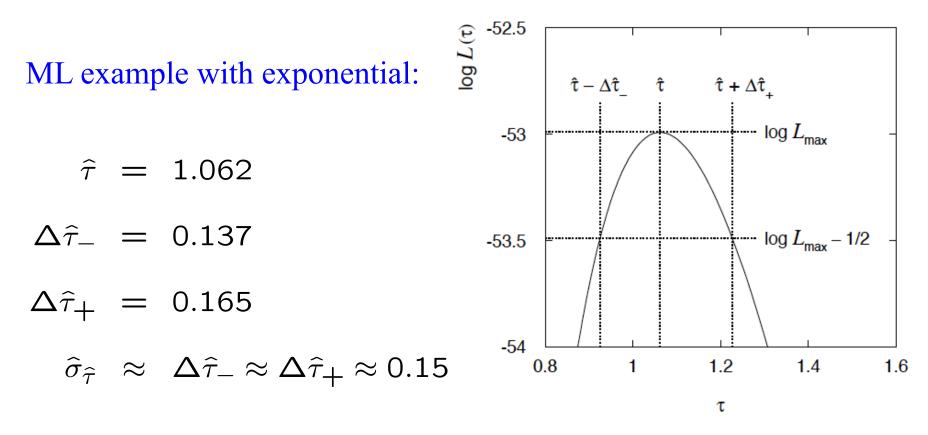
First term is  $\ln L_{max}$ , second term is zero, for third term use information inequality (assume equality):

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

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

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

#### Example of variance by graphical method



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

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

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

#### Frequentist statistical tests

Consider a hypothesis  $H_0$  and alternative  $H_1$ .

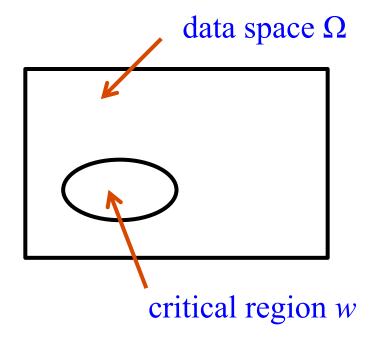
A test of  $H_0$  is defined by specifying a critical region *w* of the data space such that there is no more than some (small) probability  $\alpha$ , assuming  $H_0$  is correct, to observe the data there, i.e.,

$$P(x \in w \mid H_0) \le \alpha$$

Need inequality if data are discrete.

 $\alpha$  is called the size or significance level of the test.

If x is observed in the critical region, reject  $H_0$ .

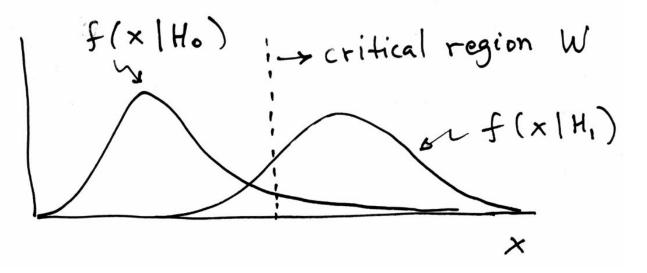


## Definition of a test (2)

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

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:



#### Type-I, Type-II errors

Rejecting the hypothesis  $H_0$  when it is true is a Type-I error. The maximum probability for this is the size of the test:

$$P(x \in W \mid H_0) \le \alpha$$

But we might also accept  $H_0$  when it is false, and an alternative  $H_1$  is true.

This is called a Type-II error, and occurs with probability

$$P(x \in \mathbf{S} - W | H_1) = \beta$$

One minus this is called the power of the test with respect to the alternative  $H_1$ :

Power = 
$$1 - \beta$$

#### *p*-values

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:  $\vec{x}_{ODS}$ 

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

Express level of compatibility 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!

Requires one to say what part of data space constitutes lesser compatibility with *H* than the observed data (implicitly this means that region gives better agreement with some alternative).

#### Test statistics and *p*-values

Consider a parameter  $\mu$  proportional to rate of signal process.

Often define a function of the data (test statistic)  $q_{\mu}$  that reflects level of agreement between the data and the hypothesized value  $\mu$ .

Usually define  $q_{\mu}$  so that higher values increasingly incompatibility with the data (more compatible with a relevant alternative).

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

 $p_{\mu} = \int_{q_{\mu,obs}}^{\infty} f(q_{\mu}|\mu) \, dq_{\mu}$ observed value of  $q_{\mu}$  pdf of  $q_{\mu}$  assuming  $\mu$ Equivalent formulation of test: reject  $\mu$  if  $p_{\mu} < \alpha$ .

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Confidence interval from inversion of a test

Carry out a test of size  $\alpha$  for all values of  $\mu$ .

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

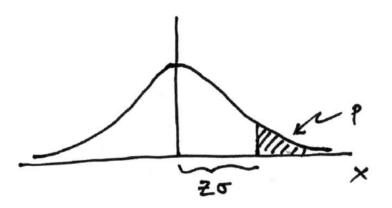
The confidence interval will by construction contain the true value of  $\mu$  with probability of at least  $1 - \alpha$ .

The interval will cover the true value of  $\mu$  with probability  $\geq 1 - \alpha$ . Equivalently, the parameter values in the confidence interval have *p*-values of at least  $\alpha$ .

To find edge of interval (the "limit"), set  $p_{\mu} = \alpha$  and solve for  $\mu$ .

#### 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.



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

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

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.,

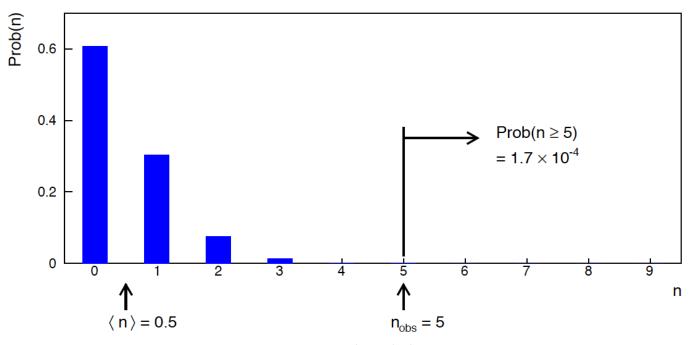
test s = 0 (rejecting  $H_0 \approx$  "discovery of signal process")

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

In both cases need to ask what is relevant alternative hypothesis. G. Cowan TRISEP 2016 / Statistics Lecture 1 Poisson counting experiment: discovery *p*-value Suppose b = 0.5 (known), and we observe  $n_{obs} = 5$ . Should we claim evidence for a new discovery?

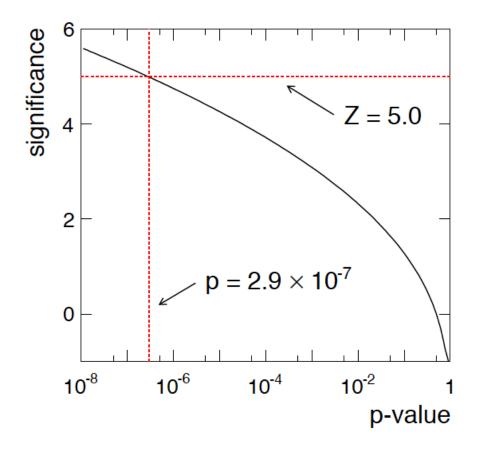
Take *n* itself as the test statistic, *p*-value for hypothesis s = 0 is

$$p$$
-value =  $P(n \ge 5; b = 0.5, s = 0)$   
=  $1.7 \times 10^{-4} \ne P(s = 0)!$ 



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## 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 signallike 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( $n \le n_{\text{obs}}; s, b$ )

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

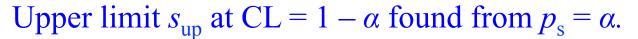
$$\alpha = P(n \le n_{\text{obs}}; s_{\text{up}}, b) = \sum_{n=0}^{n_{\text{obs}}} \frac{(s_{\text{up}} + b)^n}{n!} e^{-(s_{\text{up}} + b)}$$

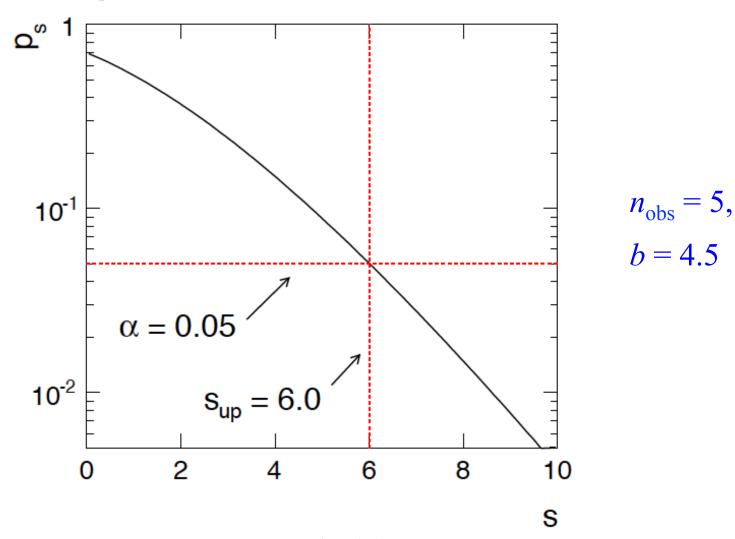
$$s_{\rm up} = \frac{1}{2} F_{\chi^2}^{-1} (1 - \alpha; 2(n_{\rm obs} + 1)) - b$$

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

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#### Frequentist upper limit on Poisson parameter

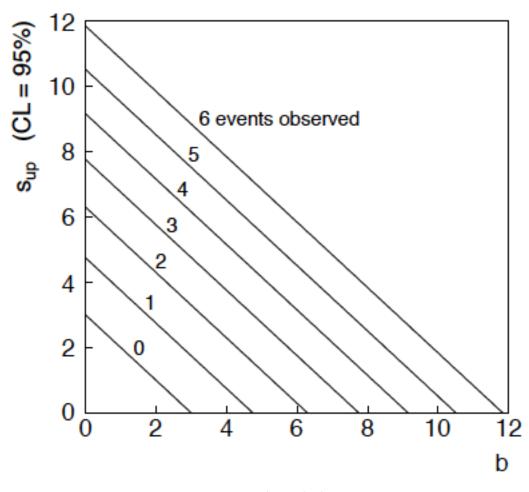




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# $n \sim \text{Poisson}(s+b)$ : frequentist upper limit on *s* For low fluctuation of *n* formula can give negative result for $s_{up}$ ; i.e. confidence interval is empty.



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#### Prototype search analysis

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

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

Assume the  $n_i$  are Poisson distributed with expectation values

$$E[n_i] = \mu s_i + b_i$$
  
strength parameter  
$$f_s(x; \boldsymbol{\theta}_s) \, dx \,, \quad b_i = b_{\text{tot}} \int f_b(x; \boldsymbol{\theta}_b) \, dx \,.$$

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:

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

Assume the  $m_i$  are Poisson distributed with expectation values

$$E[m_i] = u_i(\boldsymbol{\theta})$$
  
nuisance parameters ( $\boldsymbol{\theta}_{s}, \boldsymbol{\theta}_{b}, b_{tot}$ )

Likelihood function is

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

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## The profile likelihood ratio

Base significance test on the profile likelihood ratio:

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

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

That is, to test background-only hypothesis define statistic

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

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

Note that even though here physically  $\mu \ge 0$ , we allow 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. Cowan, Cranmer, Gross, Vitells, arXiv:1007.1727, EPJC 71 (2011) 1554

#### 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

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

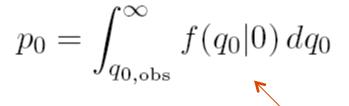
The special case  $\mu' = 0$  is a "half chi-square" distribution:

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

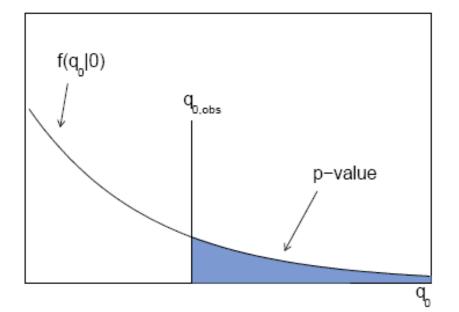
In large sample limit,  $f(q_0|0)$  independent of nuisance parameters;  $f(q_0|\mu')$  depends on nuisance parameters through  $\sigma$ .

#### *p*-value for discovery

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



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

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

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

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

Therefore the discovery significance Z is simply

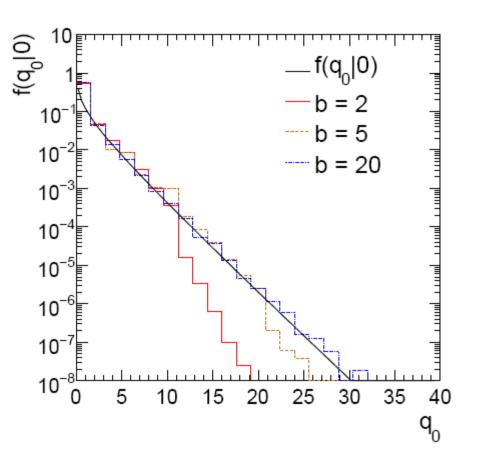
$$Z = \Phi^{-1}(1 - p_0) = \sqrt{q_0}$$

#### 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  $5\sigma$ level ( $q_0 = 25$ ) already for  $b \sim 20$ .



### Test statistic for upper limits

For purposes of setting an upper limit on  $\mu$  use

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

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

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

Large sample approximation:

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

95% CL upper limit on  $\mu$  is highest value for which *p*-value is not less than 0.05.

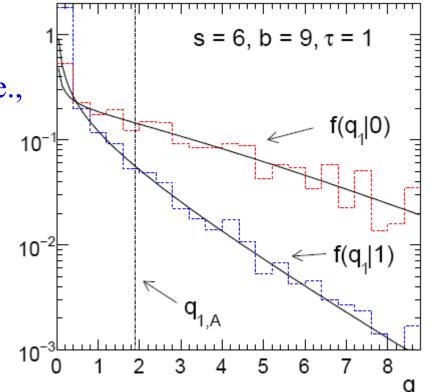
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#### Monte Carlo test of asymptotic formulae

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



## Finishing Lecture 1

So far we have introduced the basic ideas of:
Probability (frequentist, subjective)
Parameter estimation (maximum likelihood)
Statistical tests (reject *H* if data found in critical region)
Confidence intervals (region of parameter space not rejected by a test of each parameter value)

We saw tests based on the profile likelihood ratio statistic

Sampling distribution independent of nuisance parameters in large sample limit; simple formulae for p-value.

Formula for upper limit can give empty confidence interval if e.g. data fluctuate low relative to expected background. More on this later.

#### Extra slides

Large sample distribution of the profile likelihood ratio (Wilks' theorem, cont.) Suppose problem has likelihood  $L(\theta, \nu)$ , with

$$\theta = (\theta_1, \dots, \theta_N)$$
  $\leftarrow$  parameters of interest  
 $\nu = (\nu_1, \dots, \nu_M)$   $\leftarrow$  nuisance parameters

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

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

$$(10)$$
(profiled" values of  $\nu$ 

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

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

#### *p*-values in cases with nuisance parameters

Suppose we have a statistic  $q_{\theta}$  that we use to test a hypothesized value of a parameter  $\theta$ , such that the *p*-value of  $\theta$  is

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

Fundamentally we want to reject  $\theta$  only if  $p_{\theta} < \alpha$  for all v.

 $\rightarrow$  "exact" confidence interval

Recall that for statistics based on the profile likelihood ratio, the distribution  $f(q_{\theta}|\theta, v)$  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  $\theta$  values if all values of v must be considered, even those strongly disfavoured by the data (resulting interval for  $\theta$  "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  $\theta$  if  $p_{\theta} \le \alpha$  where the *p*-value is computed assuming the profiled values of the nuisance parameters:

$\hat{\hat{ u}}( heta)$	"double hat" notation means
	value of parameter that maximizes
	likelihood for the given $\theta$ .

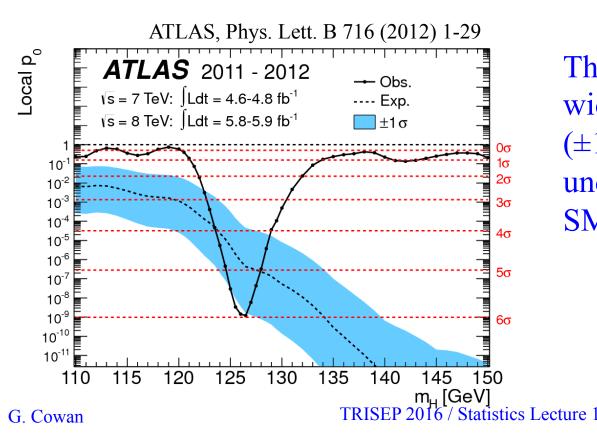
The resulting confidence interval will have the correct coverage for the points  $(\theta, \hat{v}(\theta))$ .

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).

#### 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  $m_{\rm H}$ , without any correct for the Look-Elsewhere Effect.

The "Expected" (dashed) curve gives the median  $p_0$  under assumption of the SM Higgs ( $\mu = 1$ ) at each  $m_{\rm H}$ .

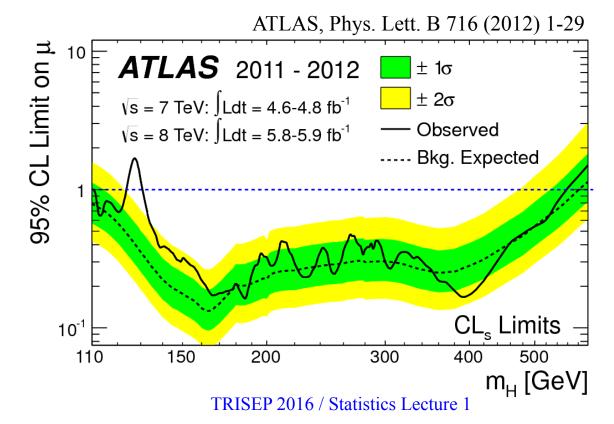


The blue band gives the width of the distribution  $(\pm 1\sigma)$  of significances under assumption of the SM Higgs.

How to read the green and yellow limit plots For every value of  $m_{\rm H}$ , find the upper limit on  $\mu$ .

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

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



#### How to read the "blue band"

On the plot of  $\hat{\mu}$  versus  $m_{\rm H}$ , the blue band is defined by

 $-2\ln\lambda(\mu) = -2\ln(L(\mu)/L(\hat{\mu})) < 1$  i.e.,  $\ln L(\mu) > \ln L(\hat{\mu}) - \frac{1}{2}$ 

i.e., it approximates the 1-sigma error band (68.3% CL conf. int.)

