

# Statistics for Particle Physics

## Lecture 4: Setting limits

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- 1 Upper Limits
  - Frequentist Confidence
  - Confidence Belts
  - Coverage
  - Bayesian Intervals
  - Feldman-Cousins
  - $CL_S$
- 2 Conclusions

# Frequentist Confidence

What is the probability that it will rain tomorrow?

There is only one tomorrow.

It will either rain or not rain.

The probability  $N_{rain}/N_{tomorrows}$  is either 0 or 1.

$P_{rain}$  is "unscientific" [von Mises]



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Suppose the forecast says it will rain.

Studies show this forecast is correct 90% of the time

The statement 'It will rain tomorrow' has a 90% probability of being true.

We can say 'It will rain tomorrow' with 90% confidence.

(Note how this depends on the ensemble used.)

We state  $X$  with confidence  $P$  if  $X$  is a member of an ensemble of statements of which at least  $P$  are true.

Note that 'at least'. 2 reasons

- 1 Higher confidences embrace lower ones. If  $X$  at 95% then  $X$  at 90%
- 2 Caters for composite hypotheses



# What frequentists can say about the Higgs mass

or any other measurement

$M_H$  has been measured with a technique that will give a value within 0.24 GeV of the true value 68% of the time

If we say the true value lies within  $\pm\sigma$  we will be correct 68% of the time

We say:  $124.85 < M_H < 125.33 \text{ GeV}$  with 68% confidence.

The statement is either true or false (time will tell) but belongs to a collection of statements of which (at least) 68% are true.

# Confidence Regions

also known as Confidence Intervals

Interval  $[x_-, x_+]$  such that

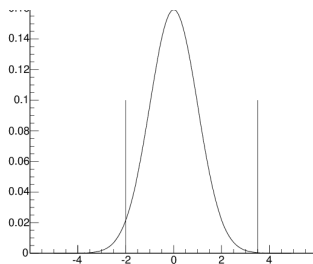
$$\int_{x_-}^{x_+} P(x) dx = CL$$

Choice over probability content  $CL$

(68%, 90%, 95%, 99%...)

Choice over strategy

- 1 Symmetric:  $\hat{x} - x_- = x_+ - \hat{x}$
- 2 Shortest: Interval that minimises  $x_+ - x_-$
- 3 Central:  $\int_{-\infty}^{x_-} P(x) dx = \int_{x_+}^{\infty} P(x) dx = \frac{1}{2}(1 - CL)$
- 4 Upper Limit:  $x_- = -\infty$ ,  $\int_{x_+}^{\infty} P(x) dx = 1 - CL$
- 5 Lower Limit:  $x_+ = \infty$ ,  $\int_{-\infty}^{x_-} P(x) dx = 1 - CL$



For the Gaussian (or any symmetric pdf) 1-3 are the same

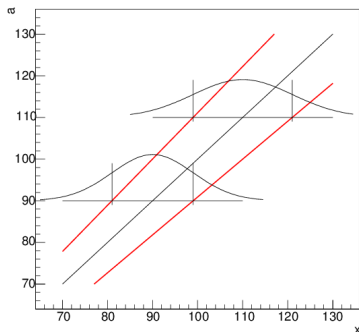
# Confidence Belts

Measured  $x = 100$  from Gaussian measurement  $\sigma = 10$ , say  $[90,110]$  is 68% central confidence region

Bit more complicated:  $x = 100$  from Gaussian measurement  $\sigma = 0.1x$  (10% measurement)

90 gives  $90 \pm 9$  but 110 gives  $110 \pm 11$ . 90 and 110 not equidistant.

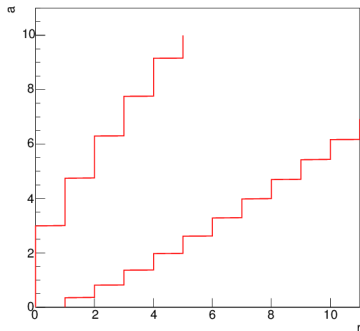
Confidence Belts are constructed horizontally and read vertically



- 1 For each  $a$ , construct desired confidence interval (here 68% central)
- 2 The result  $(x, a)$  lies inside the belt, with 68% confidence.
- 3 Measure  $x$
- 4 The result  $(x, a)$  lies inside the belt, with 68% confidence.
- 5 Read off  $a_+$  and  $a_-$ : 111.1, 90.9



# Confidence Belts for the Poisson Distribution



Horizontal axis is discrete

For central 90% confidence  
require for each  $a$  the largest

$r_{lo}$  and smallest  $r_{hi}$  for which

$$\sum_{r=0}^{r_{lo}-1} e^{-a} \frac{a^r}{r!} \leq 0.05$$

$$\sum_{r=r_{hi}+1}^{\infty} e^{-a} \frac{a^r}{r!} \leq 0.05$$

For the second, easier to  
calculate

$$\sum_{r=0}^{r_{hi}} e^{-a} \frac{a^r}{r!} \geq 0.95$$

Whatever the value of  $a$ , the probability of the result falling in the belt is 90% **or more**. Proceed as for Gaussian...

# Coverage

The probability, given  $a$ , that the statement ' $a_{lo} \leq a \leq a_{hi}$ ' will be true  
May exceed the quoted confidence level ('overcover') but should never be less ('undercover')

Example: suppose  $a = 3.5$  and we want a 90% central limit

There is a probability  $e^{-3.5} = 3\%$  of getting 0 events, leading to  $a_{hi} = 3.0$ , which is wrong

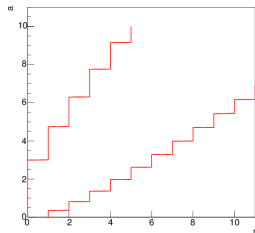
There is a probability  $3.5e^{-3.5} = 11\%$  of getting 1 event, leading to  $a_{hi} = 4.7$ , which is right

...

There is a probability  $3.5^7 e^{-3.5} / 7! = 4\%$  of getting 7 events, leading to  $a_{lo} = 3.3$ , which is right

There is a probability  $3.5^8 e^{-3.5} / 8! = 2\%$  of getting 8 events, leading to  $a_{lo} = 4.0$ , which is wrong

Total 'right' probability 94%. - 4% overcoverage



# Upper Limits

Why all this matters

Many analyses are 'searches for...' ... most of these are unsuccessful

But you have to say something! Not just 'We looked but didn't see anything.'

Use upper limit confidence region as way of reporting: 'We see nothing, so  $a \leq a_{hi}$  at some confidence level.'

## Example

*Simple use case :  $P(0; 2.996) = 0.05$  and  $2.996 \sim 3$ . So if you see 0 events, you can say with 95% confidence that the true value is less than 3.0*

*Use this to calculate limit on branching fraction, cross section, or whatever you're measuring*

# Bayesian 'credible intervals'

Bayesian has no problems saying 'It will probably rain tomorrow' or 'The probability that  $124.85 < M_H < 125.33\text{GeV}$  is 68%'

Downside is that another Bayesian can say 'It will probably not rain tomorrow' and 'The probability that  $124.85 < M_H < 125.33\text{GeV}$  is 86%' with equal validity.

Bayesian has prior (or posterior) belief pdf  $P(a)$  and defines region  $R$  such that  $\int_R P(a) da = 90\%$  (or whatever)

Same ambiguity as to choice of content (68%, 90%, 95%...) and strategy (central, symmetric, upper limit...). So Bayesian credible intervals look a lot like frequentist confidence intervals. But...

# Two happy coincidences

## Gaussian Limits

Bayesian credible intervals on Gaussians, with a flat prior, are the same as Frequentist confidence intervals

F quotes 68% or 95% or ... confidence intervals.

B quotes 68% or 95% or ... credible intervals.

They are numerically the same

## Poisson upper limits

The Frequentist Poisson upper limit is given by  $\sum_{r=0}^{r=r_{data}} e^{-a_{hi}} a_{hi}^r / r!$

The Bayesian Poisson flat prior upper limit is given by

$$\int_0^{a_{hi}} e^{-a} a^{r_{data}} / r_{data}! da$$

Integration by parts gives a series - same as the Frequentist limit

Bayesian will also say : 'I see zero events - the probability is 95% the true value 3.0 or less.'

This is a coincidence - does not apply for lower limits

# Limits in the presence of background

When it gets tricky

Typically background  $N_B$  and efficiency  $\eta$ , and want  $N_S = \frac{N_D - N_B}{\eta}$   
(Any uncertainties in  $\eta$  and  $N_B$  handled by profiling or marginalising)  
Actual number of background events Poisson in  $N_B$ .

## Straightfoward case

See 12 events, expected background 3.4,  $\eta = 1$ :  $N_S = 8.6$   
though error is  $\sqrt{12}$  not  $\sqrt{8.6}$

## Hard case

But suppose you see 4 events. or 3 events. Or zero events...  
Can you say  $N_S = 0.6$ ? or  $-0.4$ ? Or  $-3.4$ ???

We will look at 4 methods of getting out of this fix

## Example

See 3 events with expected background 3.40. What is the 95% limit on  $N_S$ ?

# Method 1: Pure frequentist

$N_D - N_B$  is an unbiased estimator of  $N_S$  and its properties are known  
Quote the result. Even if it is non-physical

## Argument for doing so

This is needed for balance: if there is really no signal, approx. half of the experiments will give positive values and half negative. If the negative results don't publish, but the positive ones do, people will be fooled.

If  $N_D < N_B$ , we know that the background has fluctuated downwards. But this cannot be incorporated into the formalism

Upper limit from 3 is 7.75, as  $\sum_0^3 e^{-7.75} 7.75^r / r! = 0.05$

95% upper limit on  $N_S = 7.75 - 3.40 = 4.35$

What if  $N_B$  were 8.0? Then publish  $-0.25$ ! For a 95% confidence limit one accepts that 5% of the results can be wrong. This (unlikely) case is clearly one of them. So what?

## Method 2: Go Bayesian

Assign a uniform prior to  $N_S$ , for  $N_S > 0$ , zero for  $N_S < 0$ .

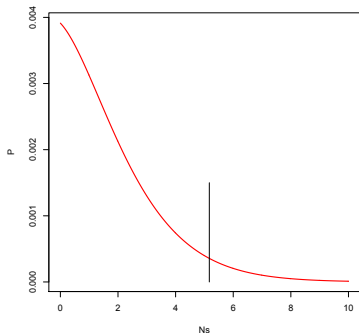
The posterior is then just the likelihood,

$$P(N_S | N_D, N_B) = e^{-(N_S + N_B)} \frac{(N_S + N_B)^{N_D}}{N_D!}$$

Required Limit from integrating  $\int_0^{N_{hi}} P(N_S) dN_S = 0.95$

$$P(N_S) \propto e^{-(N_s + 3.40)} \frac{(N_s + 3.4)^3}{3!}$$

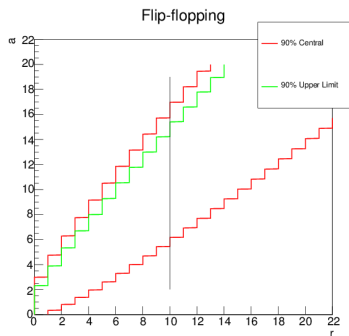
Limit is 5.17





# Method 3: Feldman-Cousins 1: Motivation

## The Unified Approach



In principle, can use 90% central or 90% upper limit, and the probability of the result lying in the band is at least 90%.

In practice, you would quote an upper limit if you get a low result, but if you get a high result you would quote a central limit. **Flip-flopping**. Break shown here for  $r = 10$

Confidence belt is the green one for  $r < 10$  and the red one for  $r \geq 10$ . Probability of lying in the band no longer 90%. Undercoverage. Method breaks down if used in this way

## Method 3: Feldman-Cousins 2: Method

Plot  $r \equiv N_D$  horizontally as before, but  $N_S$  vertically. So different  $N_B \rightarrow$  different plot. Probability values  $P(r; N_S) = e^{-(N_S+N_B)} \frac{(N_S+N_B)^r}{r!}$

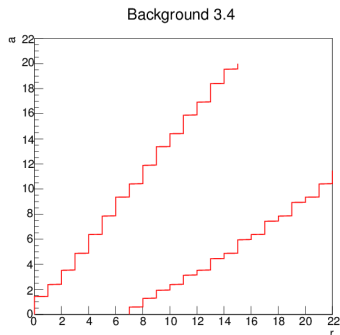
For any  $N_S$  have to define region  $R$  such that  $\sum_{r \in R} P(r; N_S) \geq 90\%$ .

First suggestion: rank  $r$  by probability and take them in order (would give shortest interval)

Drawback: outcomes with  $r \ll N_B$  will have small probabilities and all  $N_S$  will get excluded. But such events happen - want to say something constructive, not just 'This was unlikely'

Better suggestion: For each  $r$ , compare  $P(r; N_S)$  with the largest possible value obtained by varying  $N_S$ . This is either at  $N_S = r - N_B$  (if  $r \geq N_B$ ) or 0 (if  $r \leq N_B$ ) Rank on the ratio

# Method 3: Feldman-Cousins 3: Example



Flip-flopping incorporated! Coverage is correct.  
For  $r = 3$  get limit 4.86

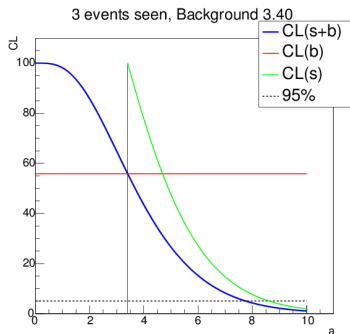
There are two arguments raised against the method

It deprives the physicist of the choice of whether to publish an upper limit or a range. Could be embarrassing if you look for something weird and are 'forced' to publish a non-zero result. *But isn't this the point?*

If two experiments with different  $N_B$  get the same small  $N_D$ , the one with the higher  $N_B$  will quote a smaller limit on  $N_S$ . The worse experiment gets the better result!

*But for an event with large background to get a small number of events is much less likely.*

## Method 4: $CL_s$



$CL_{s+b}$ : Probability of getting a result this small (or less) from  $s + b$  events. Same as strict frequentist.

$CL_b$ :  $CL_{s+b}$  for  $s = 0$  - no signal, just background

$$CL_s = \frac{CL_{s+b}}{CL_b}$$

Apply as if confidence level  $1 - CL_s$

Result larger than strict frequentist ('conservative') ('over-covers')

In our example 8.61 for  $s + b$ , 5.21 for  $s$

## Summary so far

Given 3 observed events, and an expected background of 3.4 events, what is the 95% upper limit on the 'true' number of events?

Answers:

Strict Frequentist	4.35
Bayesian (uniform prior)	5.17
Feldman-Cousins	4.86
$CL_s$	5.21

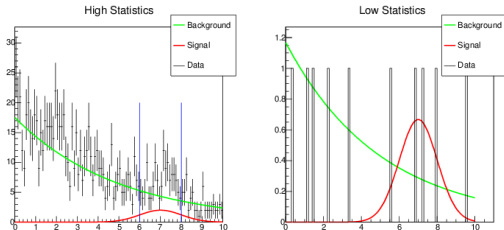
Take your pick!

All are correct. (Well, not wrong.)

### Golden Rule

Say what you are doing, and if possible give the raw numbers

# Extension: not just numbers



Simple counting not (usually) exploiting full information

Better: Likelihood

$$\ln L_{s+b} = \sum_i \ln N_s S(x_i) + N_b B(x_i) \quad \ln L_b = \sum_i \ln N_b B(x_i)$$

Look at  $L_{s+b}/L_b$ , or  $-2 \ln(L_{s+b}/L_b)$

Get confidence quantities from simulations/data

## Extension: From numbers to masses

Limits on Numbers-of-events/signal strength may translate to limits on Branching Ratios

$$BR = \frac{N_s}{N_{total}}$$

or limits on cross sections

$$\sigma = \frac{N_s}{\int \mathcal{L} dt}$$

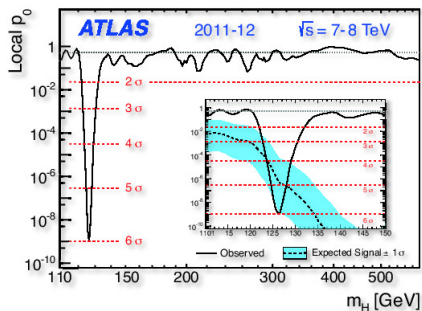
These may translate to limits on other parameters, depending on the theory

In some cases (e.g.  $M_H$ ) these parameters also affect detection efficiency, and may require changing strategy (hence different backgrounds)

Need to repeat analysis for all (of many)  $M_H$  values



# Significance plots



For each  $M_H$  (or whatever): find signal and plot  $CL_s$  (or whatever) significance of signal

Small values indicate: unlikely to get a signal this large just from background

Often also plot expected (from MC) significance assuming signal hypothesis is true. Better measure of 'good experiment'

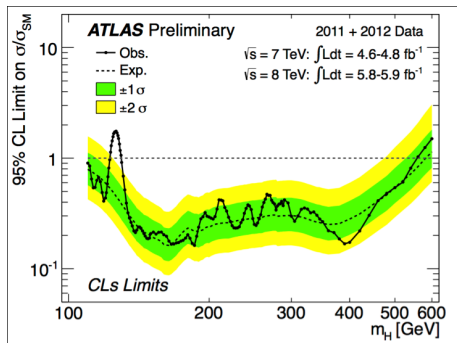
# Green-and-yellow plots

Basically same data, but fix  $CL$  at chosen value (here 95%)

At this value, find limit on signal strength and interpret as  $\sigma/\sigma_{SM}$

Again, plot actual data and expected (from MC) limit, with variations.

*If there is no signal, 68% of experiments should give results in the green band, 95% in the yellow band*



Statistics is a tool for doing physics.

A good physicist understands their tools.

Read books and conference proceedings, go to seminars, talk to people, experiment with the data, and **understand** what you are doing.

And you will succeed.

Have a great time!