

Statistics for Particle Physicists

Lecture 3: Hypothesis Tests, Confidence Intervals



Summer Student Lectures
CERN
9 – 12 July 2024

<https://indico.cern.ch/event/1347523/timetable/>



Glen Cowan
Physics Department
Royal Holloway, University of London
g.cowan@rhul.ac.uk
www.pp.rhul.ac.uk/~cowan

Outline

Lecture 1: Introduction, probability,

Lecture 2: Parameter estimation

→ Lecture 3: Hypothesis tests and confidence intervals
(some exercises [here](#)).

Lecture 4: Introduction to Machine Learning

Frequentist hypothesis 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 $\mathbf{x}$: $P(\mathbf{x}|H_0), P(\mathbf{x}|H_1)$

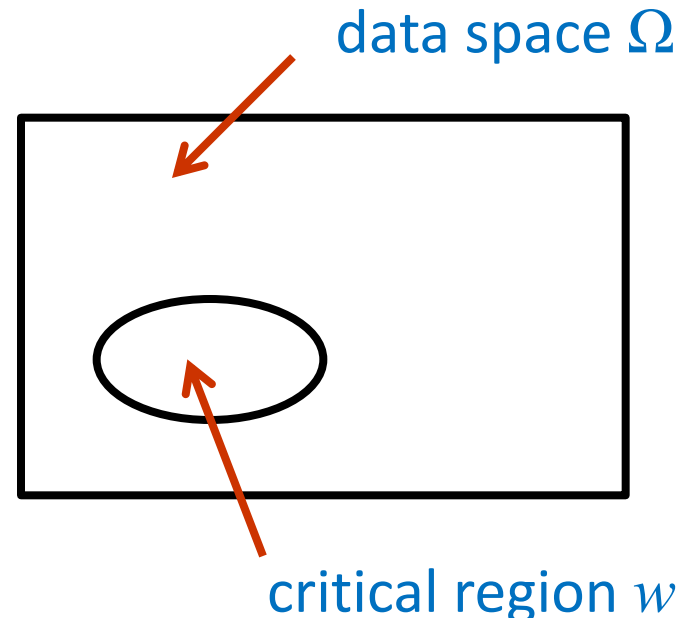
A test of H_0 is defined by specifying a critical region w of the data space such that there is no more than some (small) probability α , assuming H_0 is correct, to observe the data there, i.e.,

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

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 .

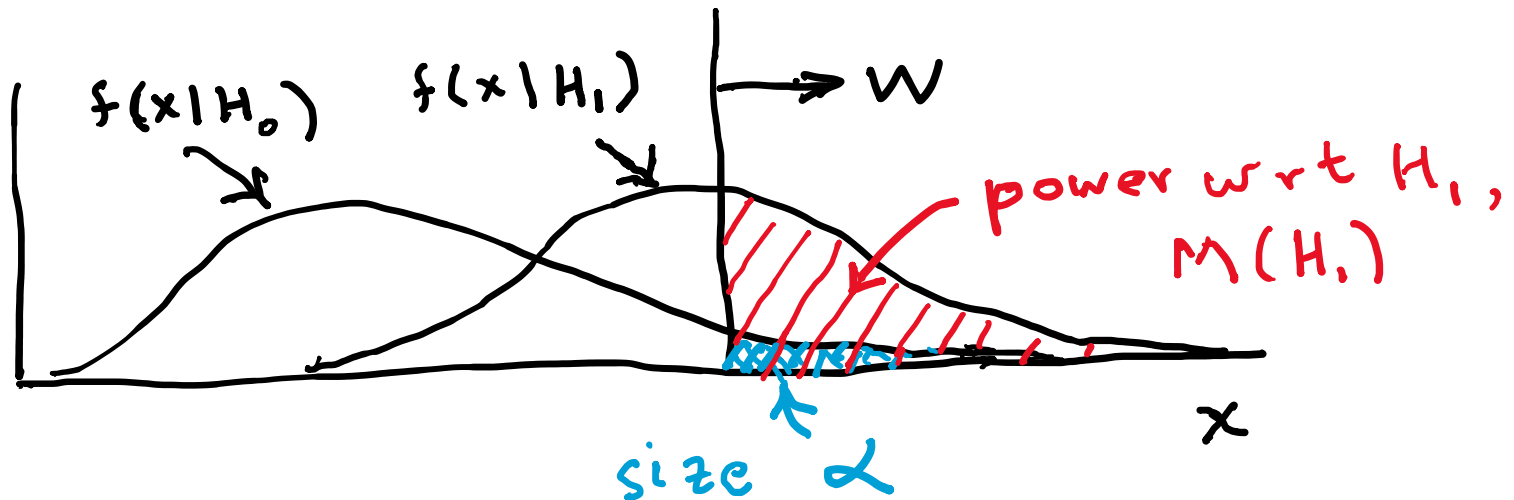


Definition of a test (2)

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

Use the alternative hypothesis H_1 to motivate where to place the critical region.

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



Classification viewed as a statistical test

Suppose events come in two possible types:

s (signal) and b (background)

For each event, test hypothesis that it is background, i.e., $H_0 = b$.

Carry out test on many events, each is either of type s or b, i.e., here the hypothesis is the “true class label”, which varies randomly from event to event, so we can assign to it a frequentist probability.

Select events for which where H_0 is rejected as “candidate events of type s”. Equivalent Particle Physics terminology:

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

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

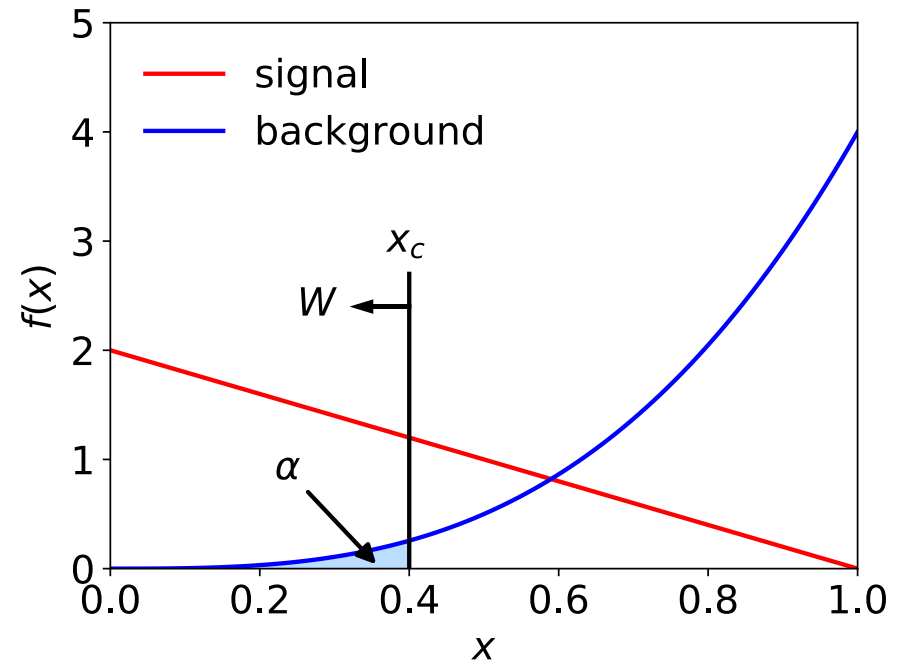
Example of a test for classification

Suppose we can measure for each event a quantity x , where

$$f(x|s) = 2(1 - x)$$

$$f(x|b) = 4x^3$$

with $0 \leq x \leq 1$.



For each event in a mixture of signal (s) and background (b) test

H_0 : event is of type b

using a critical region W of the form: $W = \{x : x \leq x_c\}$, where x_c is a constant that we choose to give a test with the desired size α .

Classification example (2)

Suppose we want $\alpha = 10^{-4}$. Require:

$$\alpha = P(x \leq x_c | b) = \int_0^{x_c} f(x|b) dx = \left. \frac{4x^4}{4} \right|_0^{x_c} = x_c^4$$

and therefore $x_c = \alpha^{1/4} = 0.1$

For this test (i.e. this critical region W), the power with respect to the signal hypothesis (s) is

$$M = P(x \leq x_c | s) = \int_0^{x_c} f(x|s) dx = 2x_c - x_c^2 = 0.19$$

Note: the optimal size and power is a separate question that will depend on goals of the subsequent analysis.

Classification example (3)

Suppose that the prior probabilities for an event to be of type s or b are:

$$\pi_s = 0.001$$

$$\pi_b = 0.999$$

The “purity” of the selected signal sample (events where b hypothesis rejected) is found using Bayes’ theorem:

$$\begin{aligned} P(s|x \leq x_c) &= \frac{P(x \leq x_c|s)\pi_s}{P(x \leq x_c|s)\pi_s + P(x \leq x_c|b)\pi_b} \\ &= 0.655 \end{aligned}$$

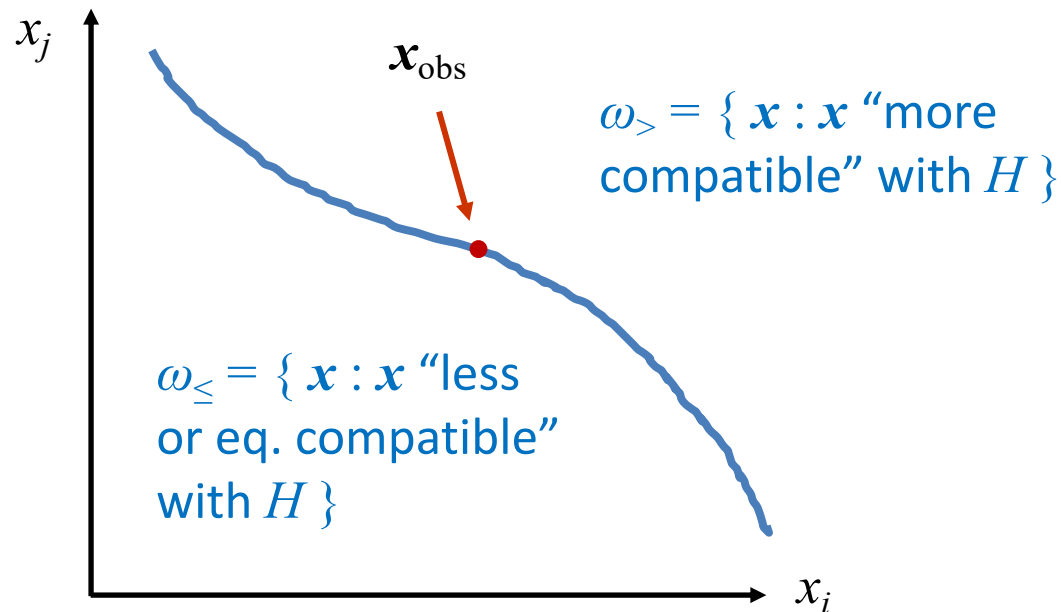
Testing significance / goodness-of-fit

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

We observe a single point in this space: $\mathbf{x}_{\text{obs}}$.

How can we quantify the level of compatibility between the data and the predictions of H ?

Decide what part of the data space represents equal or less compatibility with H than does the point $\mathbf{x}_{\text{obs}}$. (Not unique!)



p -values

Express level of compatibility between data and hypothesis (sometimes ‘goodness-of-fit’) by giving the p -value for H :

$$p = P(\mathbf{x} \in \omega_{\leq}(\mathbf{x}_{\text{obs}}) | H)$$

- = probability, under assumption of H , to observe data with equal or lesser compatibility with H relative to the data we got.
- = probability, under assumption of H , to observe data as discrepant with H as the data we got or more so.

Basic idea: if there is only a very small probability to find data with even worse (or equal) compatibility, then H is “disfavoured by the data”.

If the p -value is below a user-defined threshold α (e.g. 0.05) then H is rejected (equivalent to hypothesis test of size α as seen earlier).



p -value of H is not $P(H)$

The p -value of H is not the probability that H is true!

In frequentist statistics we don't talk about $P(H)$ (unless H represents a repeatable observation).

If we do define $P(H)$, e.g., in Bayesian statistics as a degree of belief, then we need to 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 $P(H)$.

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.

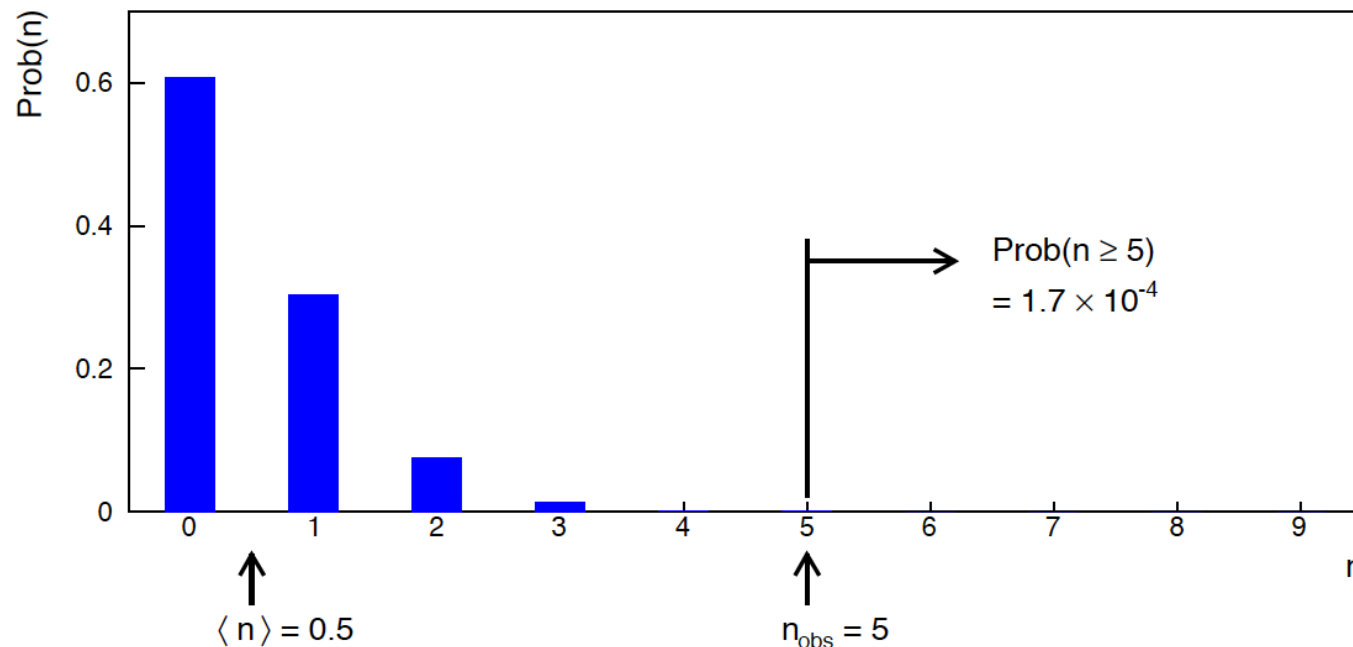
Poisson counting experiment: discovery p -value

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

Should we claim evidence for a new discovery?

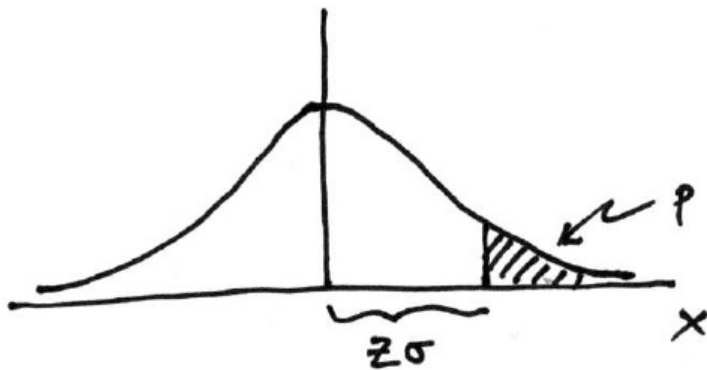
Give p -value for hypothesis $s = 0$:

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



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.



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

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

in ROOT:

```
p = 1 - TMath::Freq(Z)
Z = TMath::NormQuantile(1-p)
```

in python (scipy.stats):

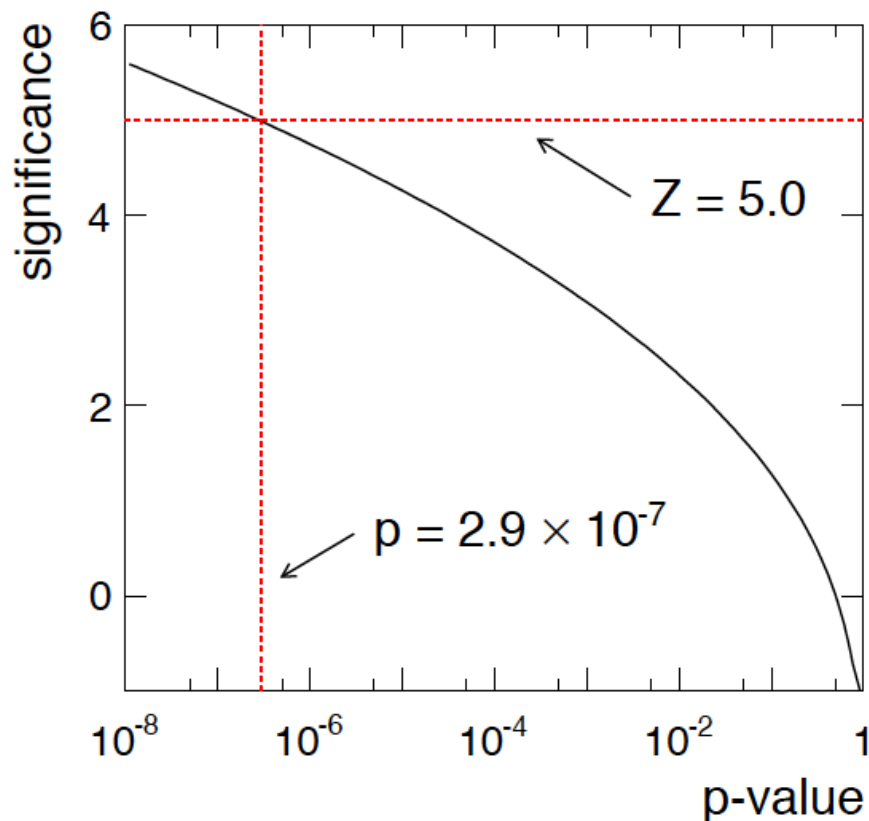
```
p = 1 - norm.cdf(Z) = norm.sf(Z)
Z = norm.ppf(1-p)
```

Result Z is a “number of sigmas”. Note this does not mean that the original data was Gaussian distributed.

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” ($\sim$ multiple testing), etc.

Confidence intervals by inverting a test

In addition to a 'point estimate' of a parameter we should report an interval reflecting its statistical uncertainty.

Confidence intervals for a parameter θ can be found by defining a test of the hypothesized value θ (do this for all θ):

Specify values of the data that are 'disfavoured' by θ (critical region) such that $P(\text{data in critical region} | \theta) \leq \alpha$ for a prespecified α , e.g., 0.05 or 0.1.

If data observed in the critical region, reject the value θ .

Now invert the test to define a confidence interval as:

set of θ values that are not rejected in a test of size α (confidence level CL is $1 - \alpha$).

Relation between confidence interval and p -value

Equivalently we can consider a significance test for each hypothesized value of θ , resulting in a p -value, p_θ .

If $p_\theta \leq \alpha$, then we reject θ .

The confidence interval at $CL = 1 - \alpha$ consists of those values of θ that are not rejected.

E.g. an upper limit on θ is the greatest value for which $p_\theta > \alpha$.

In practice find by setting $p_\theta = \alpha$ and solve for θ .

For a multidimensional parameter space $\theta = (\theta_1, \dots, \theta_M)$ use same idea – result is a confidence “region” with boundary determined by $p_\theta = \alpha$.

Coverage probability of confidence interval

If the true value of θ is rejected, then it's not in the confidence interval. The probability for this is by construction (equality for continuous data):

$$P(\text{reject } \theta | \theta) \leq \alpha = \text{type-I error rate}$$

Therefore, the probability for the interval to contain or “cover” θ is

$$P(\text{conf. interval “covers” } \theta | \theta) \geq 1 - \alpha$$

This assumes that the set of θ values considered includes the true value, i.e., it assumes the composite hypothesis $P(x|H, \theta)$.

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 from

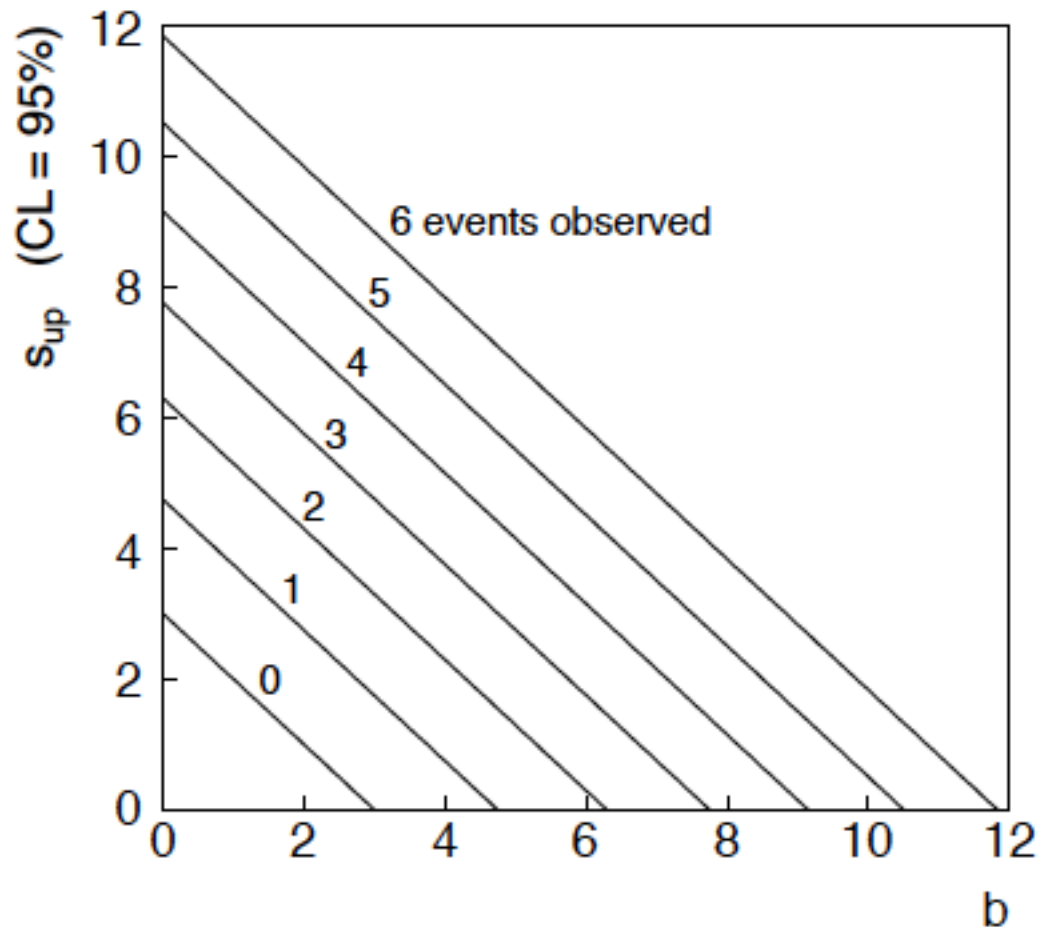
$$\alpha = P(n \leq n_{\text{obs}}; s_{\text{up}}, b) = \sum_{n=0}^{n_{\text{obs}}} \frac{(s_{\text{up}} + b)^n}{n!} e^{-(s_{\text{up}} + b)}$$

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

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

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

For low fluctuation of n , formula can give negative result for s_{up} ; i.e. confidence interval is empty; all values of $s \geq 0$ have $p_s \leq \alpha$.



Limits near a boundary of the parameter space

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 $s = 0$

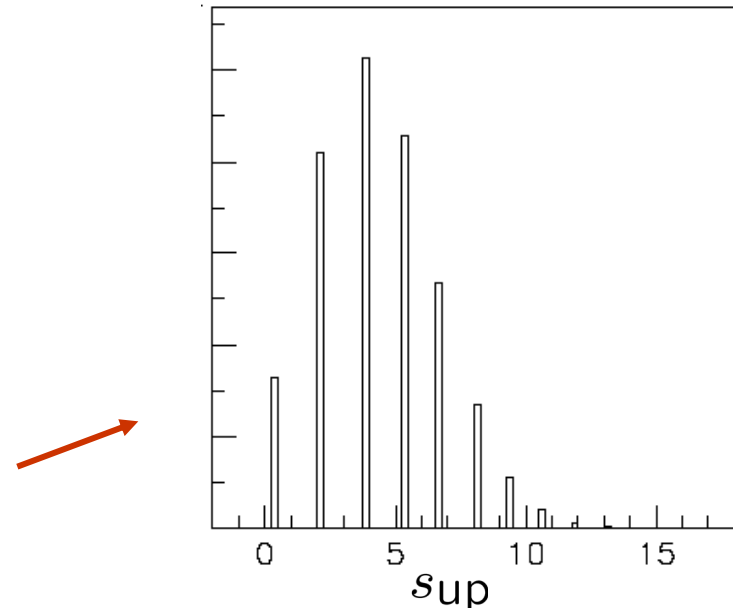
Physicist: I should have used $\text{CL} = 0.95$ — then $s_{\text{up}} = 0.496$

Even better: for $\text{CL} = 0.917923$ 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



Extra slides

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 provided 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

$$p_\theta = 1 - F_{\chi_n^2}(t_\theta) \quad \leftarrow \text{set equal to } \alpha$$

To find boundary of confidence region set $p_\theta = \alpha$ and solve for t_θ :

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

Recall also

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

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

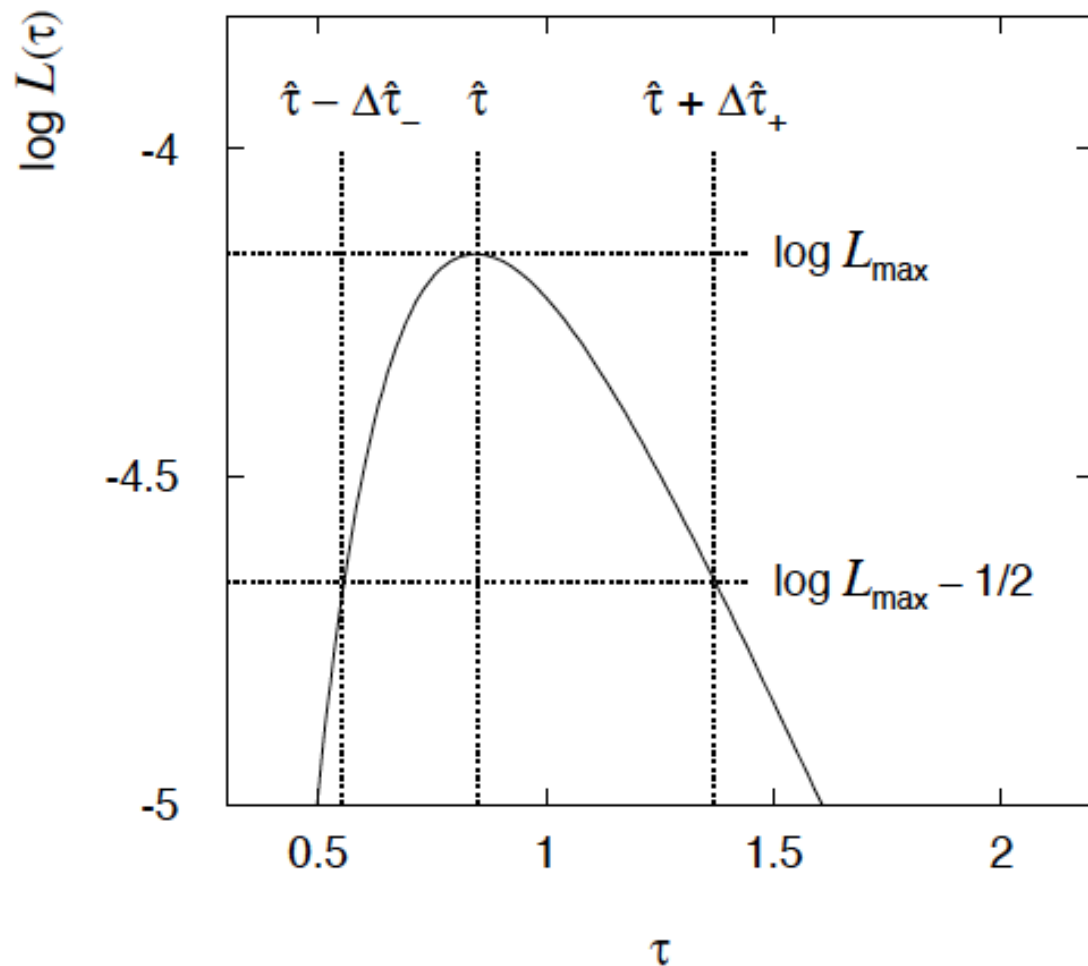
$$\ln L(\theta) = \ln L(\hat{\theta}) - \frac{1}{2}$$

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 $\ln L(\theta)$

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



Our exponential example, now with only $n = 5$ events.

Can report ML estimate with approx. confidence interval from $\ln L_{\max} - 1/2$ as “asymmetric error bar”:

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

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 $CL = 1 - \alpha$.

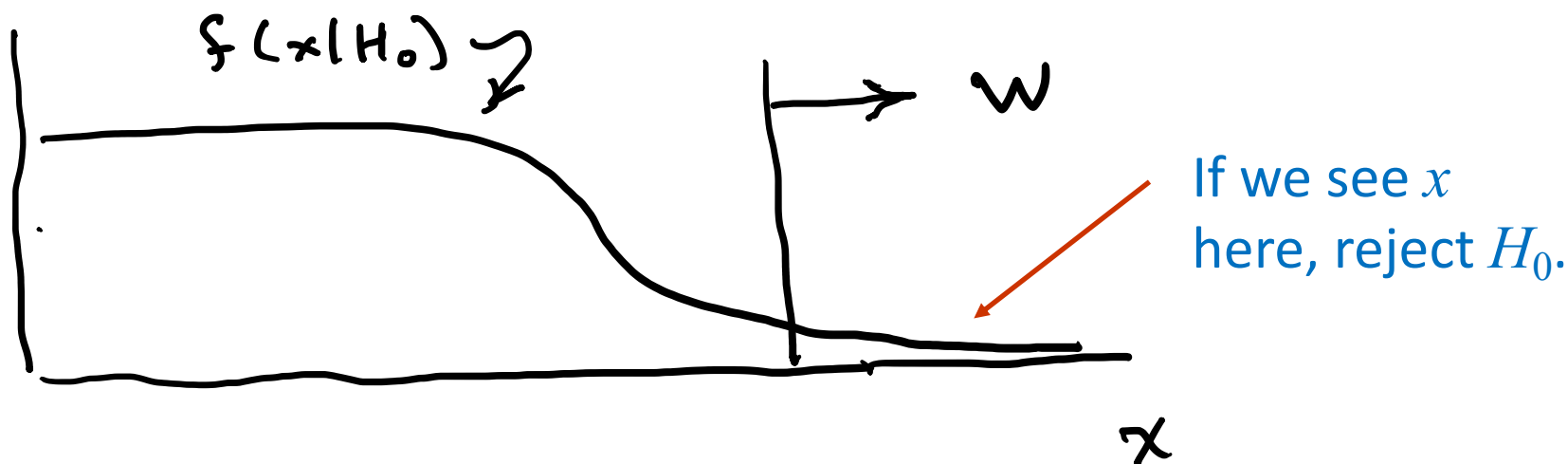
$1 - \alpha$	$\hat{Q}_\alpha$				
	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
0.683	1.00	2.30	3.53	4.72	5.89
0.90	2.71	4.61	6.25	7.78	9.24
0.95	3.84	5.99	7.82	9.49	11.1
0.99	6.63	9.21	11.3	13.3	15.1

Obvious where to put W ?

In the 1930s there were great debates as to the role of the alternative hypothesis.

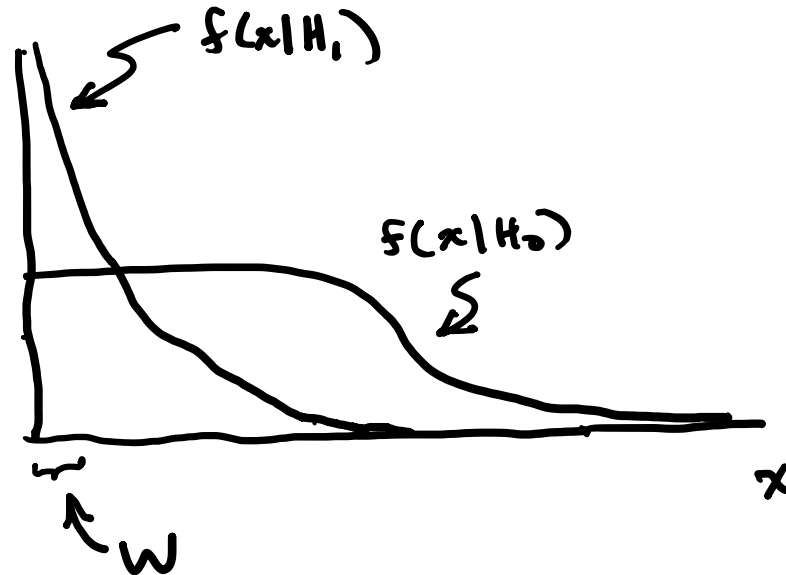
Fisher held that one could test a hypothesis H_0 without reference to an alternative.

Suppose, e.g., H_0 predicts that x (suppose positive) usually comes out low. High values of x are less characteristic of H_0 , so if a high value is observed, we should reject H_0 , i.e., we put W at high x :



Or not so obvious where to put W ?

But what if the only relevant alternative to H_0 is H_1 as below:



Here high x is more characteristic of H_0 and not like what we expect from H_1 . So better to put W at low x .

Neyman and Pearson argued that “less characteristic of H_0 ” is well defined only when taken to mean “more characteristic of some relevant alternative H_1 ”.

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:

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

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

$$P(x \in S - W \mid H_1) = \beta$$

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

$$\text{Power} = 1 - \beta$$

Distribution of the p -value

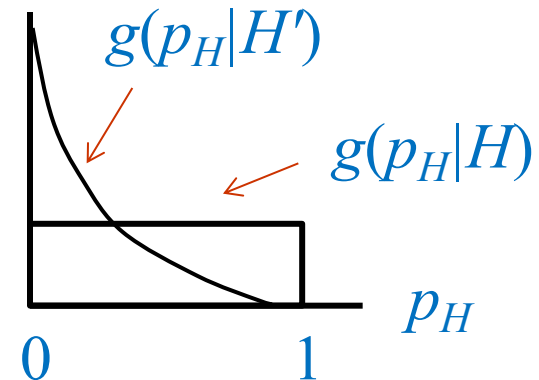
The p -value is a function of the data, and is thus itself a random variable with a given distribution. Suppose the p -value of H is found from a test statistic $t(\mathbf{x})$ as

$$p_H = \int_t^\infty f(t'|H) dt'$$

The pdf of p_H under assumption of H is

$$g(p_H|H) = \frac{f(t|H)}{|\partial p_H / \partial t|} = \frac{f(t|H)}{f(t|H)} = 1 \quad (0 \leq p_H \leq 1)$$

In general for continuous data, under assumption of H , $p_H \sim \text{Uniform}[0,1]$ and is concentrated toward zero for some (broad) class of alternatives.

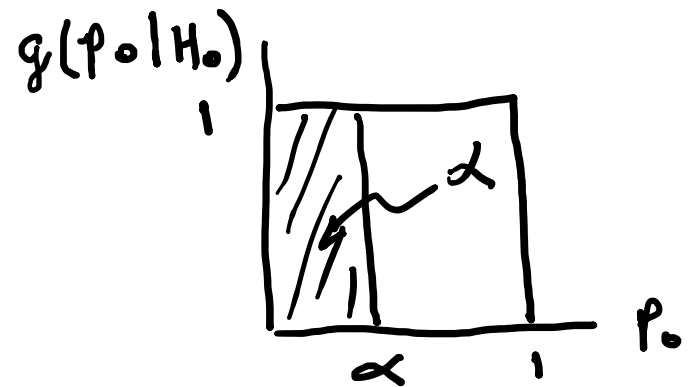


Using a p -value to define test of H_0

One can show that under assumption of a hypothesis H_0 , its p -value, p_0 , follows a uniform distribution in $[0,1]$.

So the probability to find p_0 less than a given α is

$$P(p_0 \leq \alpha | H_0) = \alpha$$



So we can define the critical region of a test of H_0 with size α as the set of data space where $p_0 \leq \alpha$.

Formally the p -value relates only to H_0 , but the resulting test will have a given power with respect to a given alternative H_1 .