Statistics for Particle Physicists

Lecture 3: Hypothesis Tests, Confidence Intervals

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Outline

Lecture 1: Introduction, probability,

Lecture 2: Parameter estimation

→ Lecture 3: Hypothesis tests and confidence intervals

(some exercises here).

Lecture 4: Systematic uncertainties and further examples

Frequentist hypothesis tests

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

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

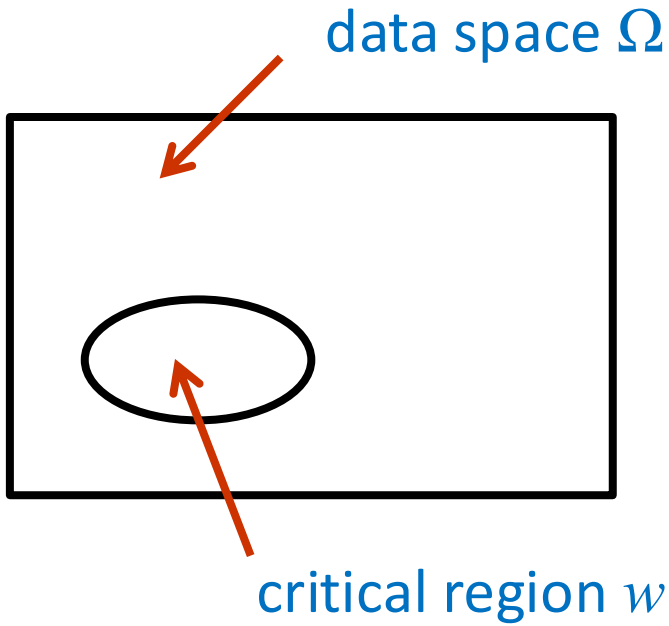
A test of H_0 is defined by specifying a critical region w of the data space such that there is no more than some (small) probability α, assuming H_0 is correct, to observe the data there, i.e.,

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

Need inequality if data are discrete.

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

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

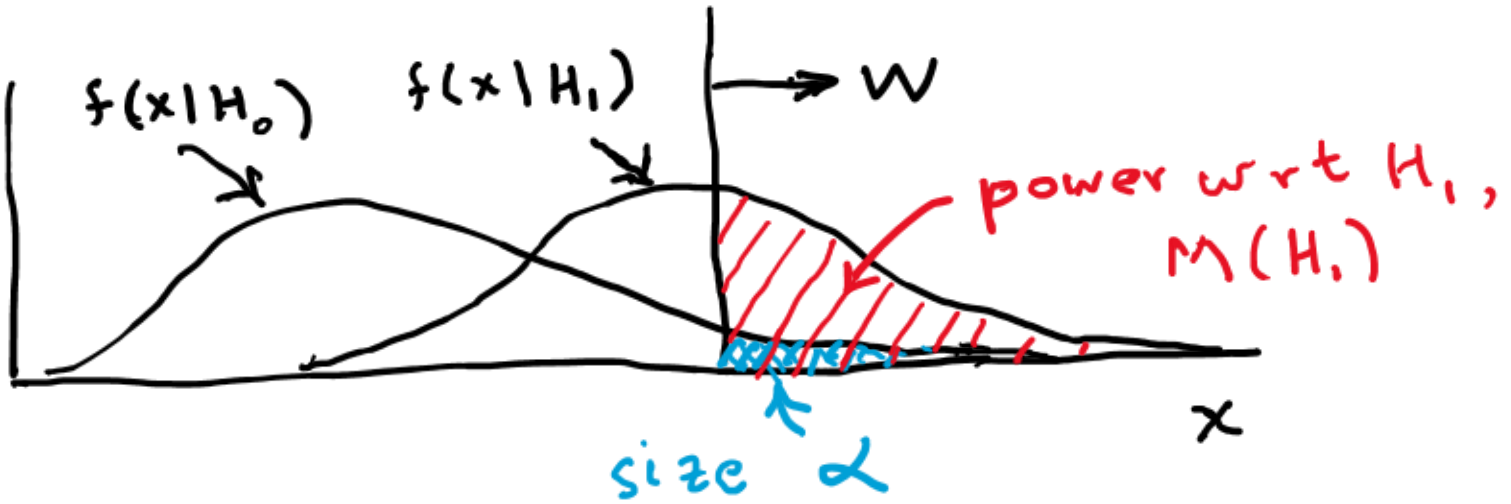


Definition of a test (2)

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 $$\varepsilon_{\mathrm{b}} = \int_W f(\mathbf{x}|H_0)\, d\mathbf{x} = \alpha$$

signal efficiency $$\varepsilon_{\mathrm{s}} = \int_W f(\mathbf{x}|H_1)\, d\mathbf{x} = 1 - \beta = \mathrm{power}$$

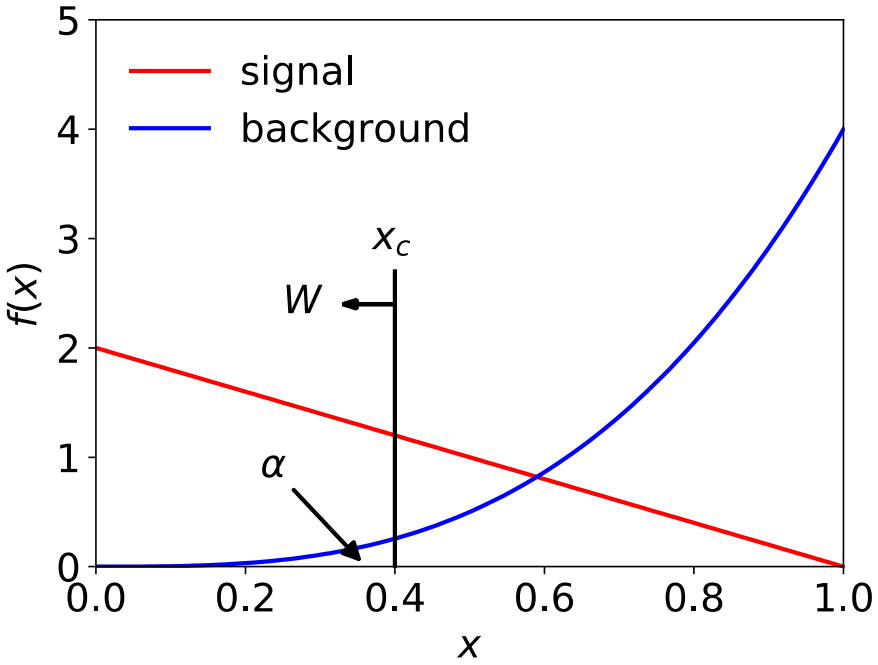
Example of a test for classification

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

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

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

with $0 \le x \le 1$.



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: $W = \{x : x \le x_c\}$, 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:

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

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

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

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:

$$\pi_{\mathrm{s}} = 0.001$$
$$\pi_{\mathrm{b}} = 0.999$$

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

$$P(\mathrm{s}|x \leq x_{\mathrm{c}}) = \frac{P(x \leq x_{\mathrm{c}}|\mathrm{s})\pi_{\mathrm{s}}}{P(x \leq x_{\mathrm{c}}|\mathrm{s})\pi_{\mathrm{s}} + P(x \leq x_{\mathrm{c}}|\mathrm{b})\pi_{\mathrm{b}}}$$

$$= 0.655$$

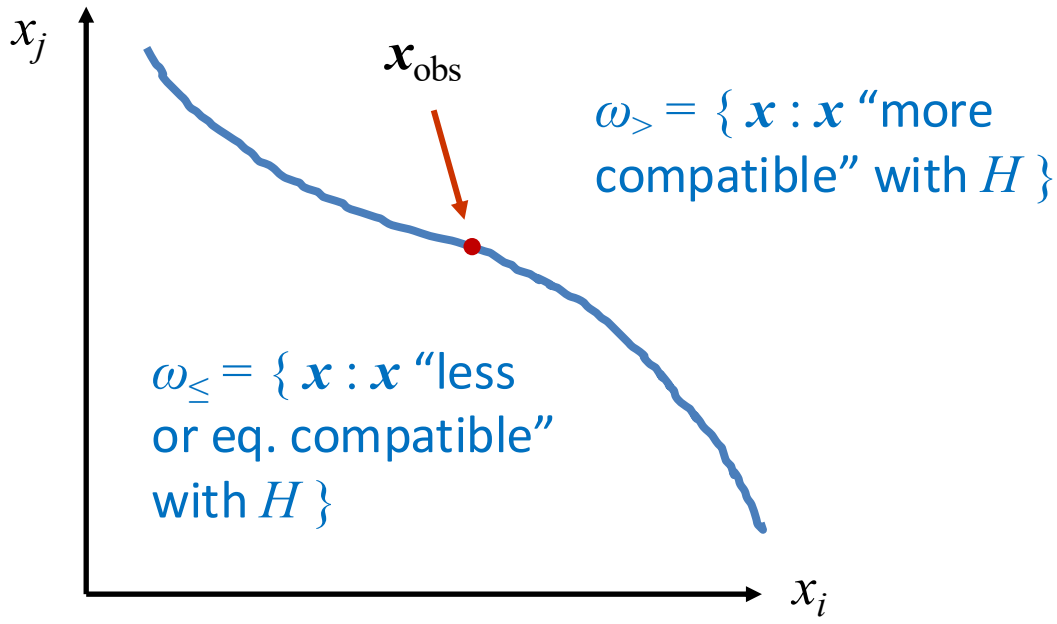
Testing significance / goodness-of-fit

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

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

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 $\boldsymbol{x}_{\text{obs}}$. (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

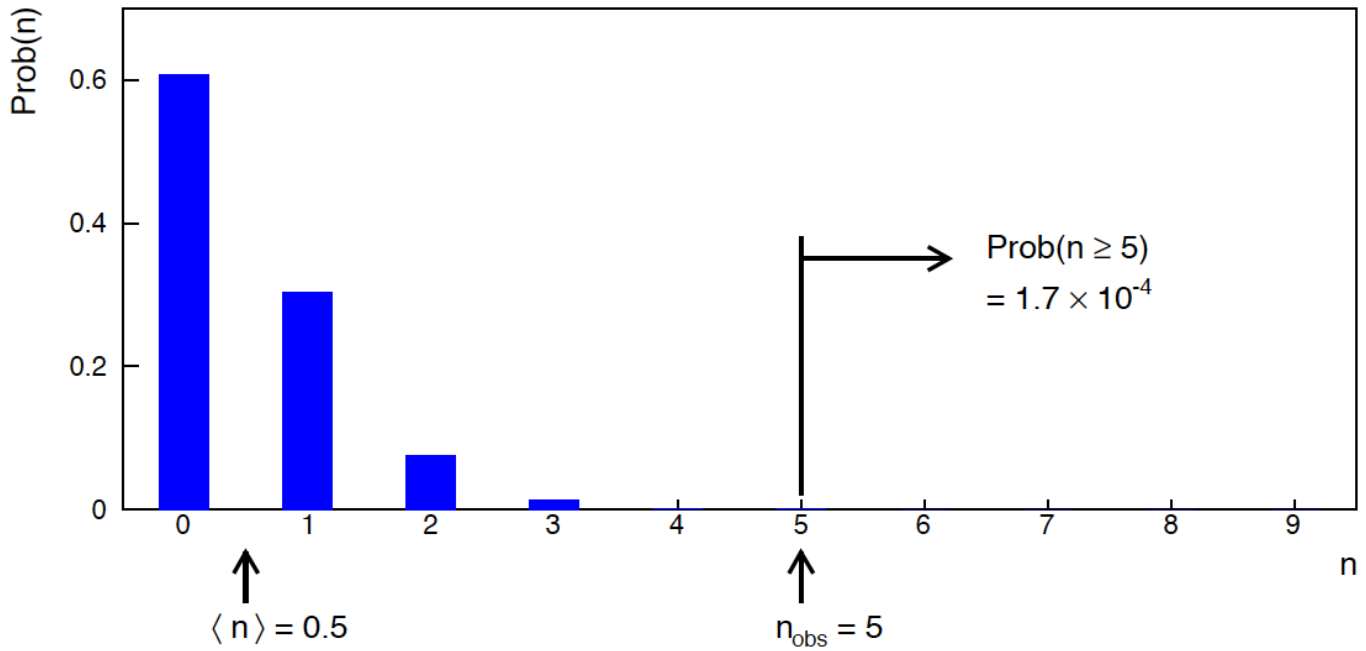
Suppose $b = 0.5$ (known), and we observe $n_{\text{obs}} = 5$.

Should we claim evidence for a new discovery?

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

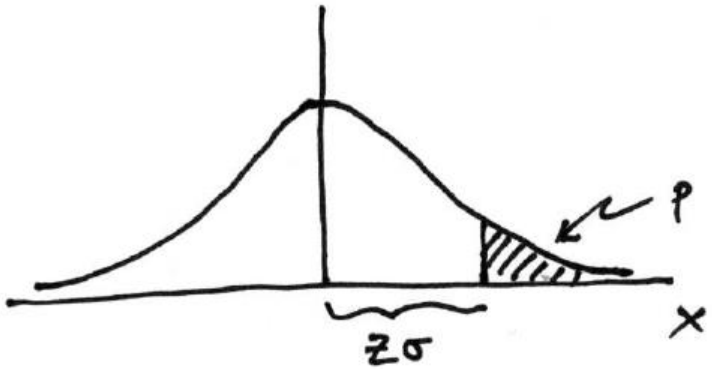
$$p\text{-value} = P(n \geq 5; b = 0.5, s = 0)$$

$$= 1.7 \times 10^{-4} \neq P(s = 0)!$$



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.



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

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

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

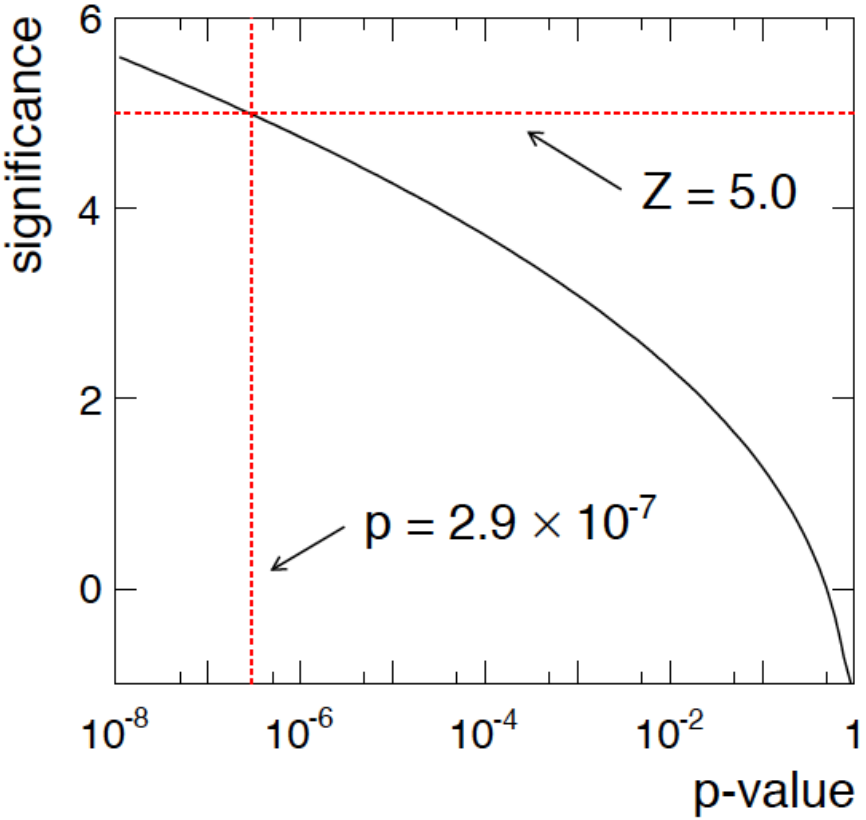
```
in python (scipy.stats):
p = 1 - norm.cdf(Z) = norm.sf(Z)
Z = norm.ppf(1-p)
```

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" (~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 $\boldsymbol{\theta} = (\theta_1, \ldots \theta_M)$ *use* same idea – result is a confidence "region" with boundary determined by $p_{\boldsymbol{\theta}} = \alpha$.

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 $P(\boldsymbol{x}|H,\theta)$.

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

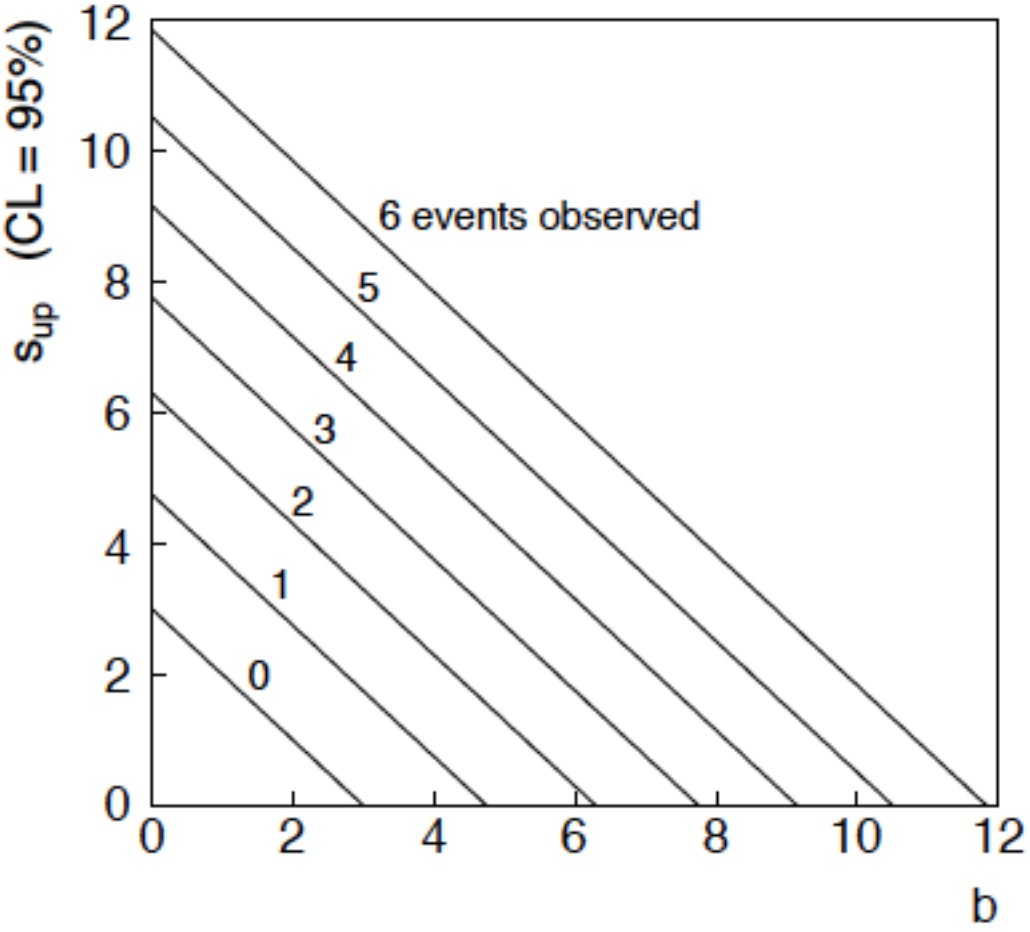
$$\alpha = P(n \leq n_{\text{obs}}; s_{\text{up}}, b) = \sum_{n=0}^{n_{\text{obs}}} \frac{(s_{\text{up}} + b)^n}{n!} e^{-(s_{\text{up}}+b)}$$

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

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

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

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



Approximate confidence intervals/regions from the likelihood function

Suppose we test parameter value(s) $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_n)$ using the ratio

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

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

$$t_{\boldsymbol{\theta}} = -2 \ln \lambda(\boldsymbol{\theta})$$

so higher $t_{\boldsymbol{\theta}}$ means worse agreement between $\boldsymbol{\theta}$ and the data.

p-value of $\boldsymbol{\theta}$ therefore $\qquad p_{\boldsymbol{\theta}} = \int_{t_{\boldsymbol{\theta},\mathrm{obs}}}^{\infty} f(t_{\boldsymbol{\theta}}|\boldsymbol{\theta})\, dt_{\boldsymbol{\theta}}$

need pdf

Confidence region from Wilks' theorem

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

$$f(t_{\boldsymbol{\theta}}|\boldsymbol{\theta}) \sim \chi^2_n$$

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

Assuming this holds, the p-value is

$$p_{\boldsymbol{\theta}} = 1 - F_{\chi^2_n}(t_{\boldsymbol{\theta}})$$ ← set equal to α

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

$$t_{\boldsymbol{\theta}} = F^{-1}_{\chi^2_n}(1 - \alpha)$$

Recall also

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

Confidence region from Wilks' theorem (cont.)

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

$$\ln L(\boldsymbol{\theta}) = \ln L(\hat{\boldsymbol{\theta}}) - \tfrac{1}{2} F^{-1}_{\chi^2_n}(1-\alpha)$$

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

$$F^{-1}_{\chi^2_1}(0.683) = 1$$

and so the 68.3% confidence level interval is determined by

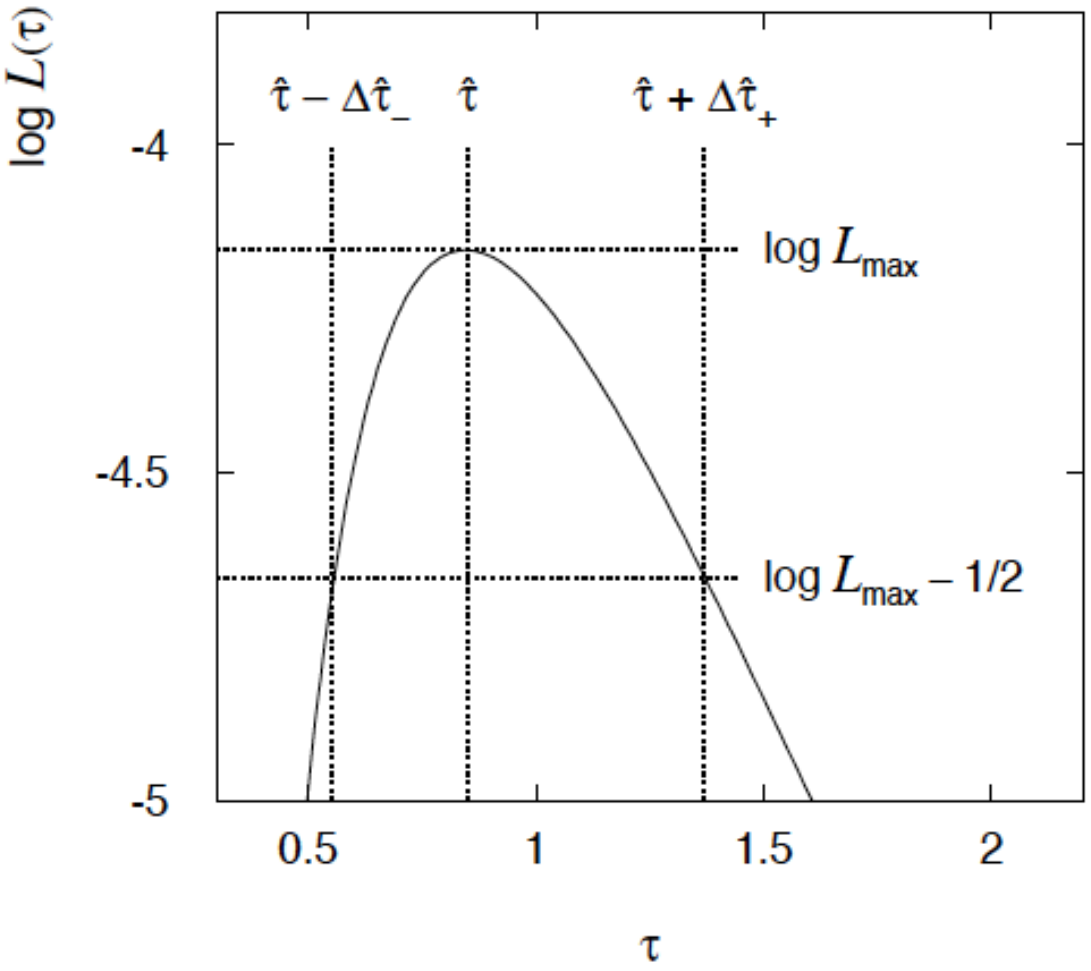
$$\ln L(\theta) = \ln L(\hat{\theta}) - \frac{1}{2}$$

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, 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

$$Q_\alpha = F^{-1}_{\chi^2_n}(1-\alpha)$$

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 $= 1 - \alpha$.

$1-\alpha$	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

Extra slides

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}

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

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 $s = 0$

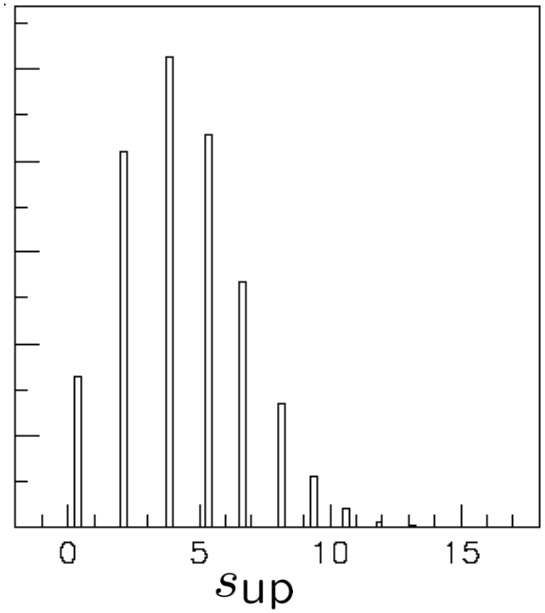
Physicist: I should have used CL = 0.95 — then $s_{\rm up} = 0.496$

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

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

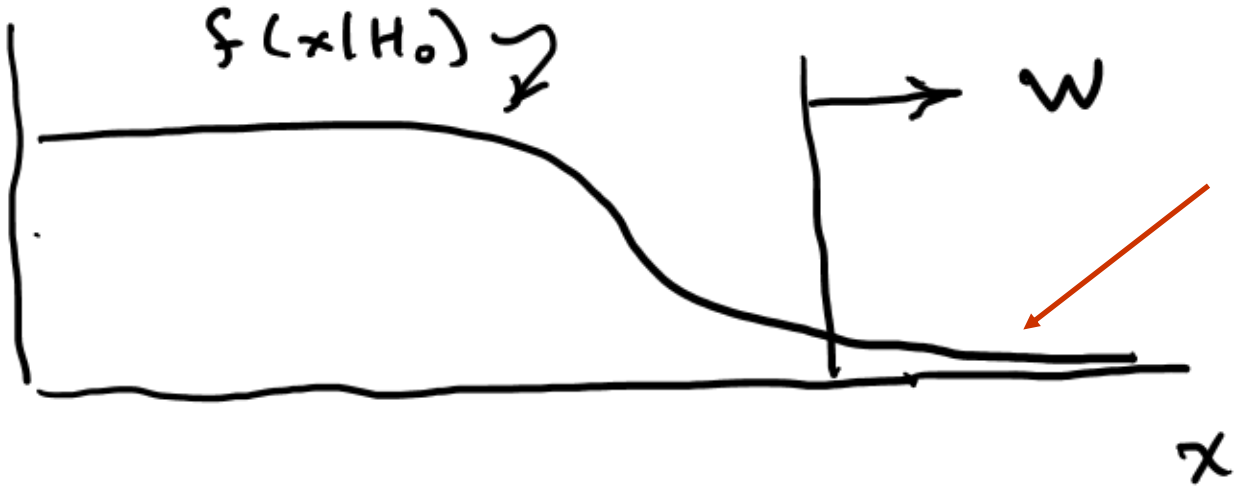


Obvious where to put W?

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.

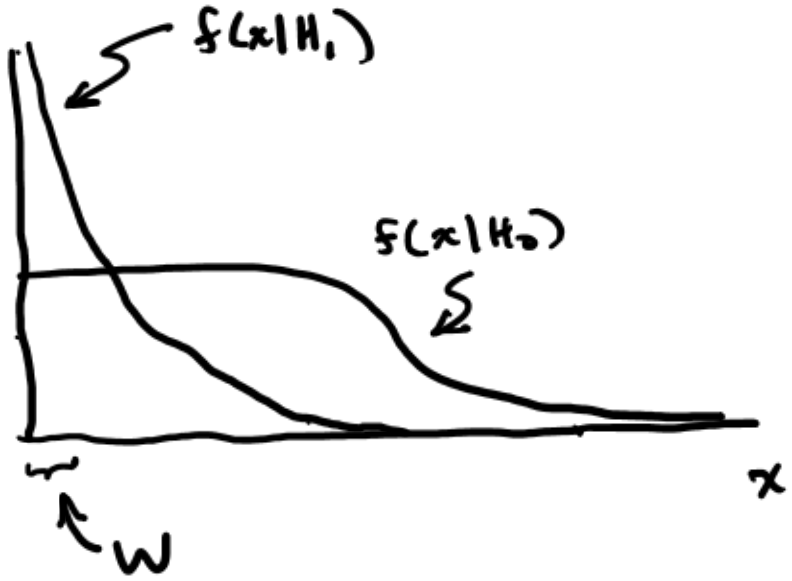
Suppose, e.g., H_0 predicts that x (suppose positive) usually comes out low. High values of x are less characteristic of H_0, so if a high value is observed, we should reject H_0, i.e., we put W at high x:



If we see x here, reject H_0.

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

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

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

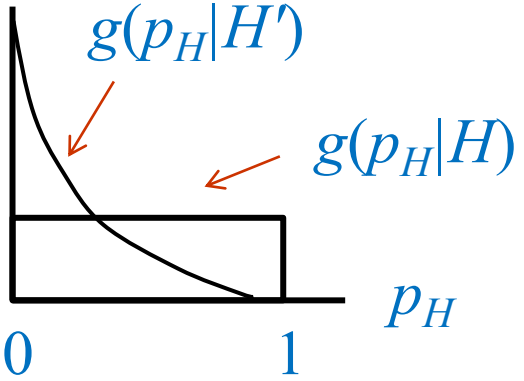
The p-value is a function of the data, and is thus itself a random variable with a given distribution. Suppose the p-value of H is found from a test statistic $t(\boldsymbol{x})$ as

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

The pdf of p_H under assumption of H is

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

In general for continuous data, under assumption of H, $p_H \sim$ 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.