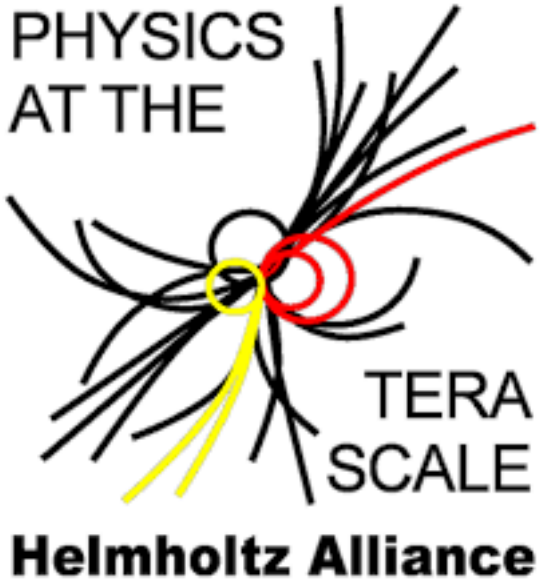
Statistics for Particle Physics
Lecture 1: Hypothesis Testing



Terascale Statistics School
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Outline

Lectures/tutorials from me:

→	1)	Monday 16:00	Hypothesis testing
	2)	Tuesday 9:00	Frequentist parameter estimation
		Tuesday 11:00	
	3)	Tuesday 14:00	Confidence limits
		Tuesday 16:00	
	4)	Wednesday 9:00	Bayesian parameter estimation
	5)	Wednesday 14:00	Errors on errors

More resources in the University of London course:

https://www.pp.rhul.ac.uk/~cowan/stat_course.html

Hypothesis, likelihood

Suppose the entire result of an experiment (set of measurements) is a collection of numbers $\boldsymbol{x}$.

A (simple) hypothesis is a rule that assigns a probability to each possible data outcome:

$$P(\mathbf{x}|H) \quad = \quad \text{the likelihood of } H$$

Often we deal with a family of hypotheses labeled by one or more undetermined parameters (a composite hypothesis):

$$P(\mathbf{x}|\boldsymbol{\theta}) = L(\boldsymbol{\theta}) \qquad = \quad \text{the "likelihood function"}$$

Note:

1) For the likelihood we treat the data $\boldsymbol{x}$ as fixed.
2) The likelihood function $L(\boldsymbol{\theta})$ is not a pdf for $\boldsymbol{\theta}$.

Frequentist hypothesis tests

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

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

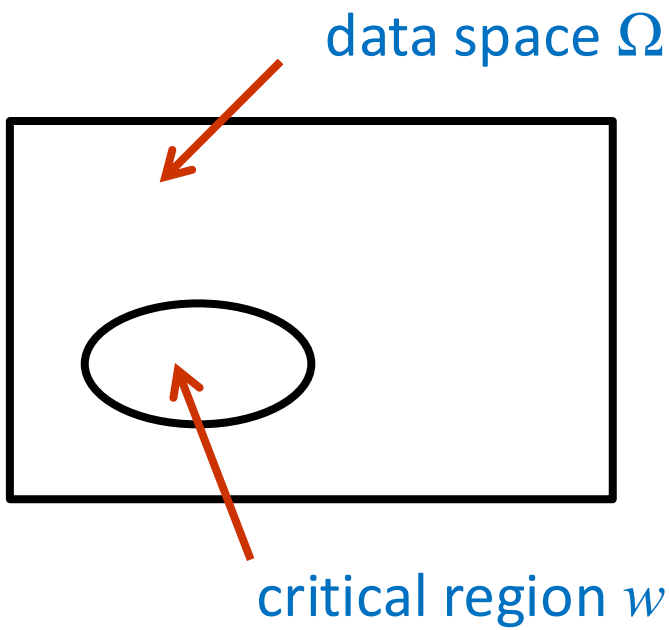
A test of H_0 is defined by specifying a critical region w of the data space such that there is no more than some (small) probability α, assuming H_0 is correct, to observe the data there, i.e.,

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

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.

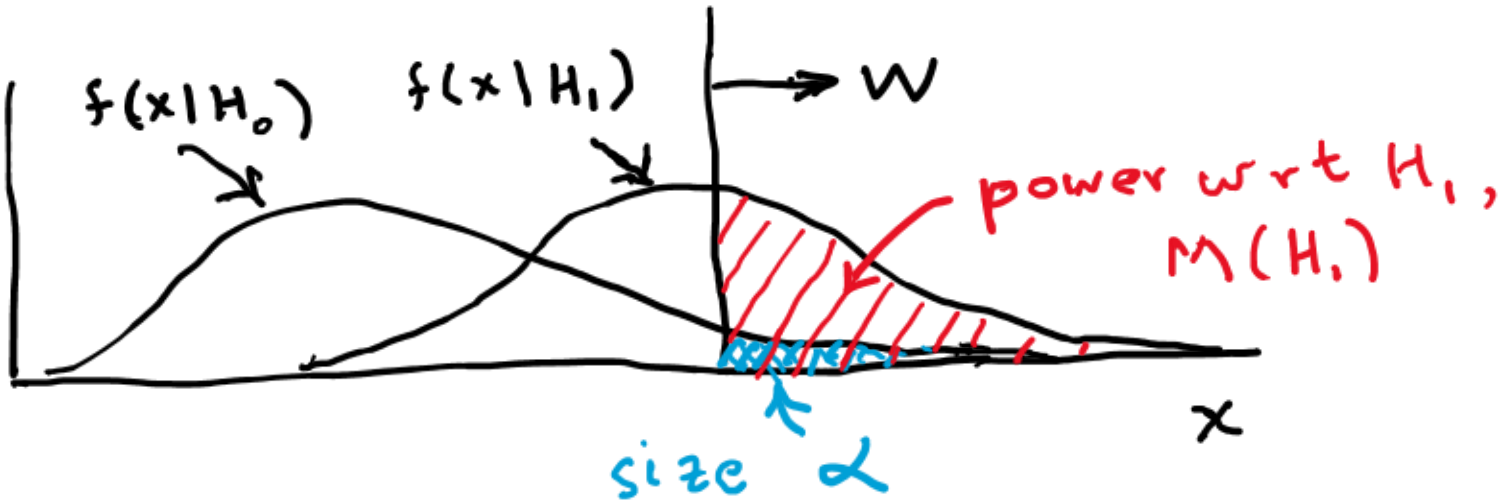


Definition of a test (2)

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.

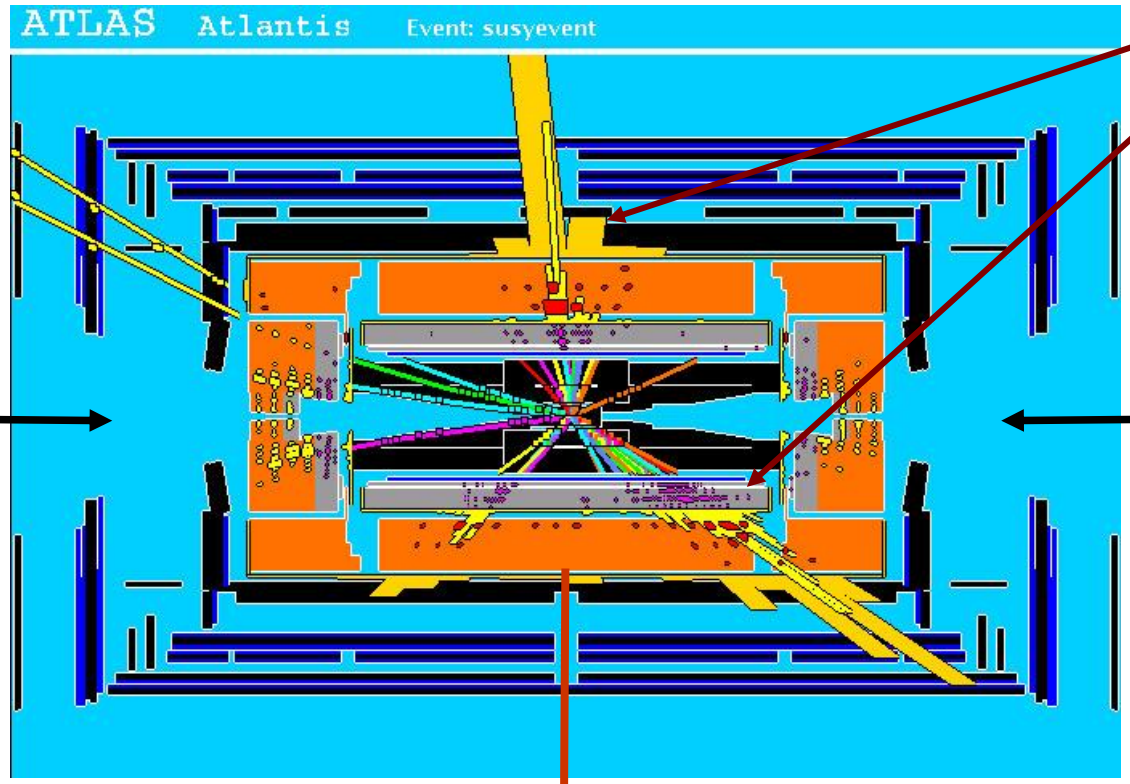
Select events for which where H_0 is rejected as "candidate events of type s". Equivalent Particle Physics terminology:

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

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

Particle Physics context for a hypothesis test

A simulated SUSY event ("signal"):



high p_T muons

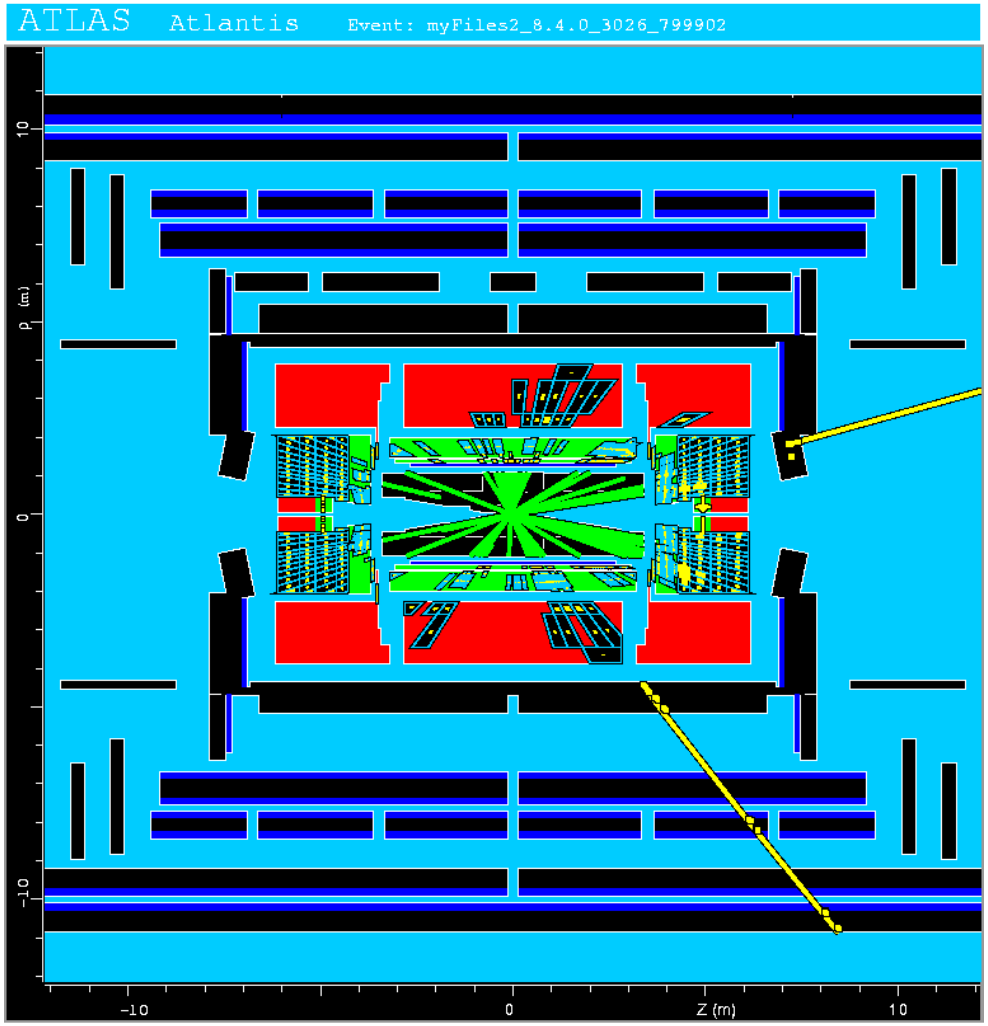
high p_T jets of hadrons

p

p

missing transverse energy

Background events



This event from Standard Model ttbar production also has high p_{T} jets and muons, and some missing transverse energy.

→ can easily mimic a signal event.

Classification of proton-proton collisions

Proton-proton collisions can be considered to come in two classes:

signal (the kind of event we're looking for, $y = 1$)
background (the kind that mimics signal, $y = 0$)

For each collision (event), we measure a collection of features:

x_1 = energy of muon
x_2 = angle between jets
x_3 = total jet energy
x_4 = missing transverse energy
x_5 = invariant mass of muon pair
x_6 = ...

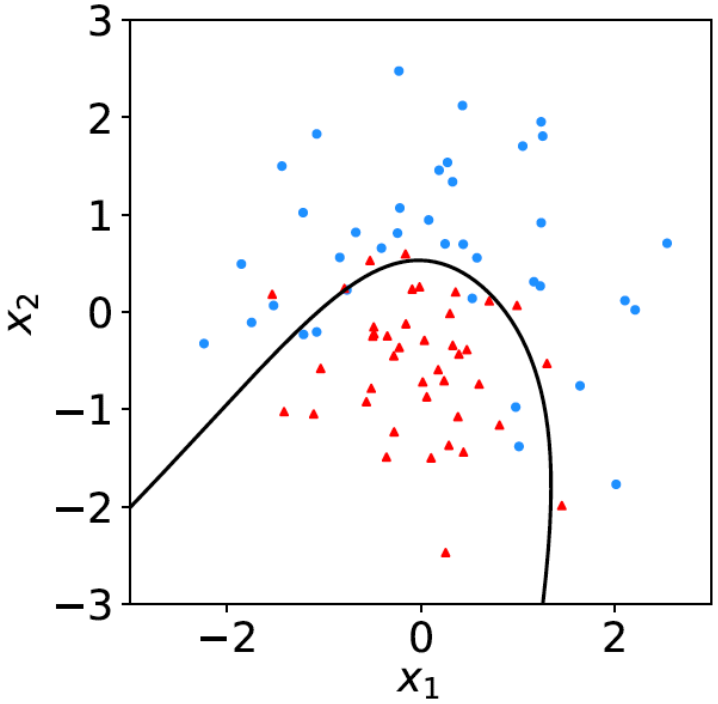
The real events don't come with true class labels, but computer-simulated events do. So we can have a set of simulated events that consist of a feature vector $\boldsymbol{x}$ and true class label y (0 for background, 1 for signal):

$$(\boldsymbol{x}, y)_1, (\boldsymbol{x}, y)_2, \ldots, (\boldsymbol{x}, y)_N$$

The simulated events are called "training data".

Distributions of the features

If we consider only two features $\boldsymbol{x} = (x_1, x_2)$, we can display the results in a scatter plot (red: $y = 0$, blue: $y = 1$).



For real events, the dots are black (true type is not known).

For each real event test the hypothesis that it is background.

(Related to this: test that a sample of events is *all* background.)

The test's critical region is defined by a "decision boundary" – without knowing the event type, we can classify them by seeing where their measured features lie relative to the boundary.

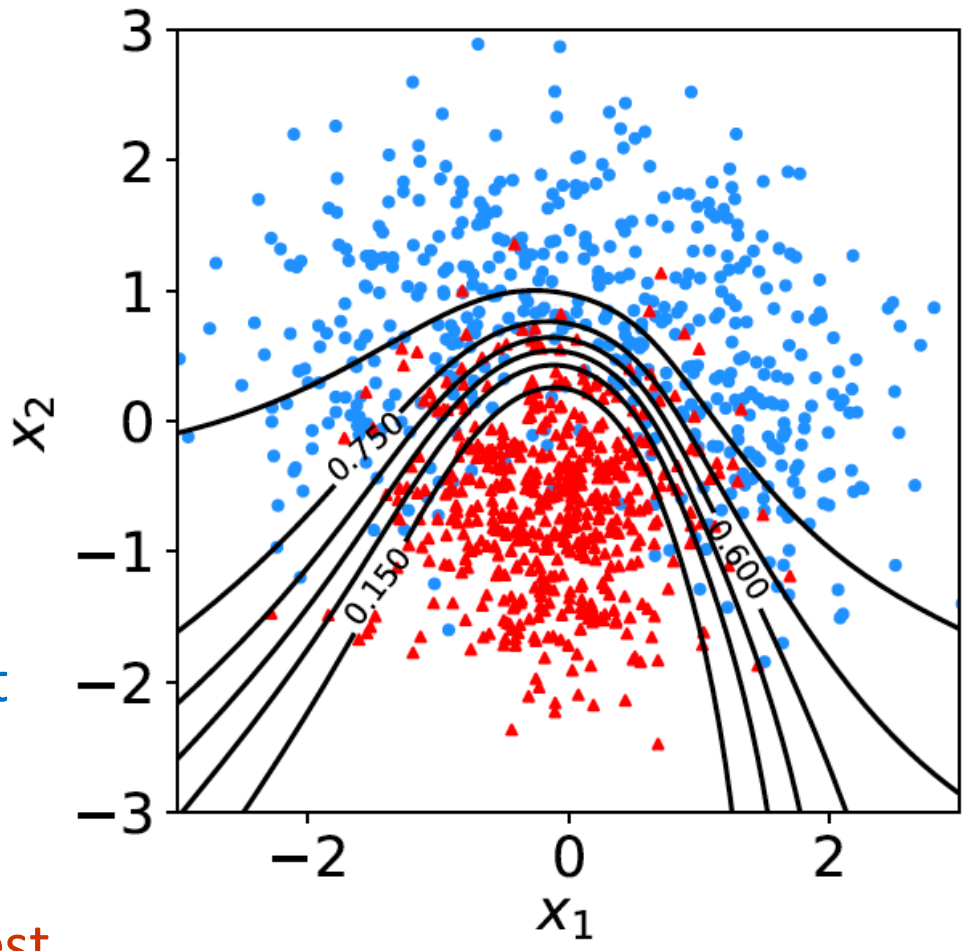
Decision function, test statistic

A surface in an n-dimensional space can be described by

$$t(x_1, \ldots, x_n) = t_c$$

scalar function

constant

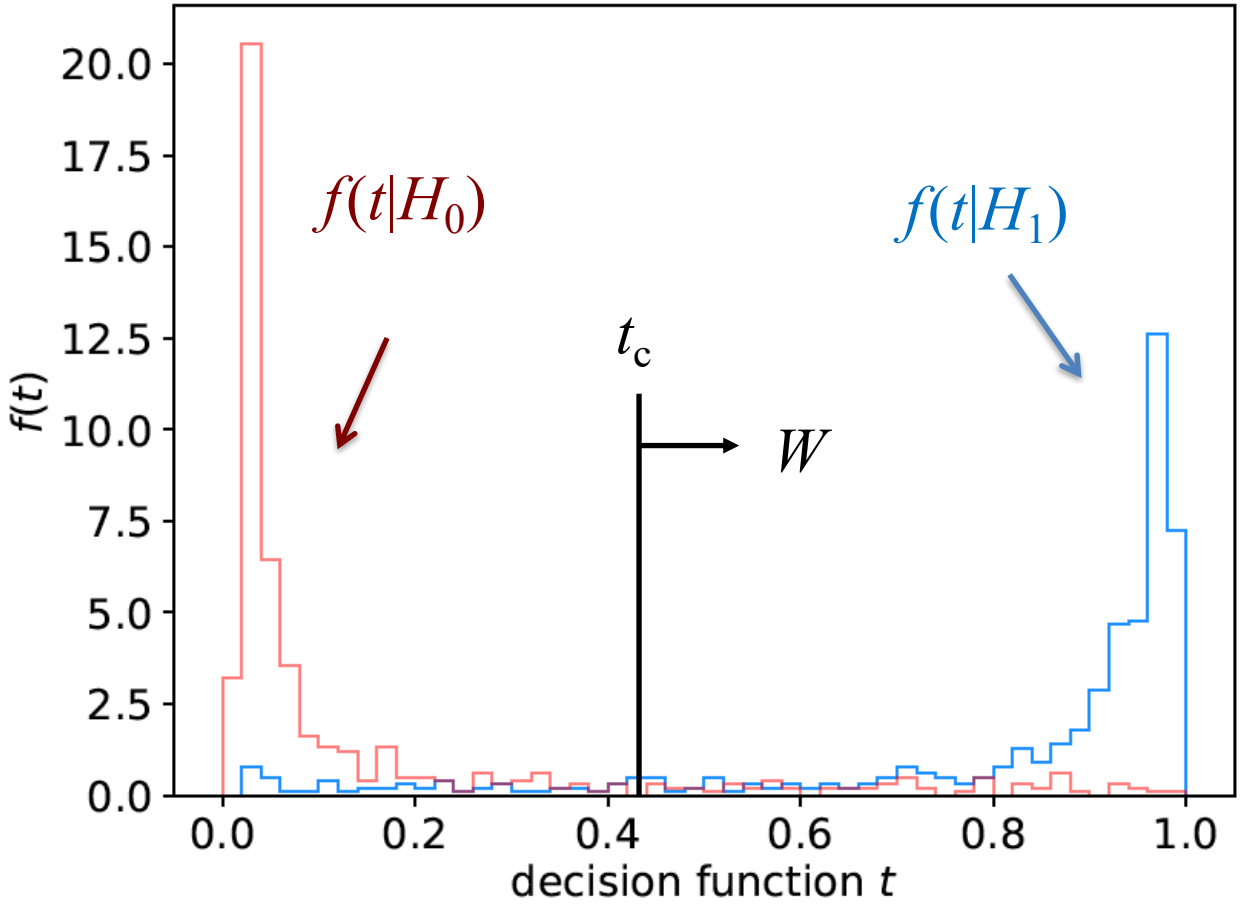


Different values of the constant t_c result in a family of surfaces.

Problem is reduced to finding the best decision function or test statistic $t(\boldsymbol{x})$.

Distribution of $t(\boldsymbol{x})$

By forming a test statistic $t(\boldsymbol{x})$, the boundary of the critical region in the n-dimensional $\boldsymbol{x}$-space is determined by a single single value t_c.

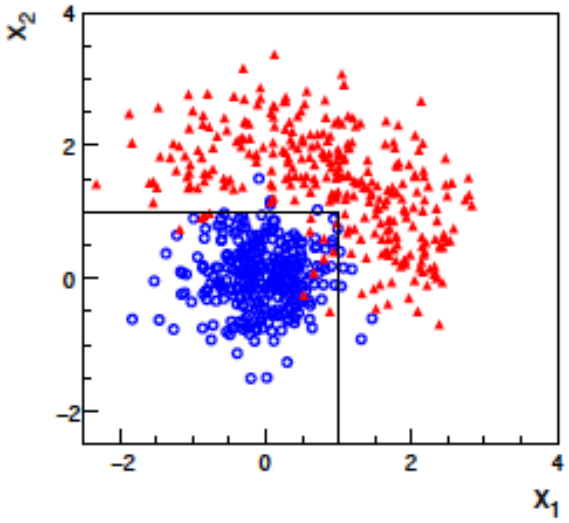


Types of decision boundaries

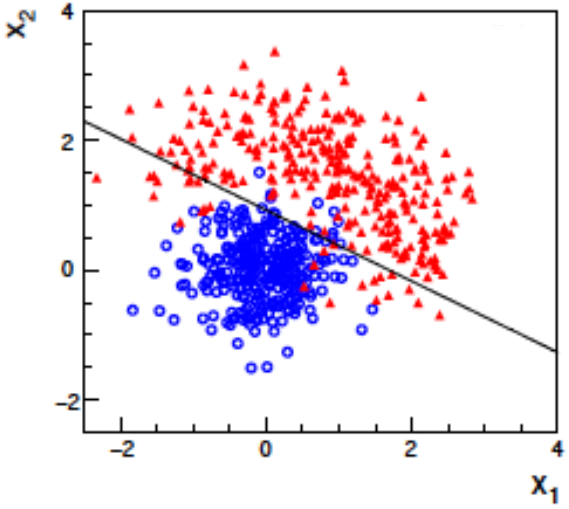
So what is the optimal boundary for the critical region, i.e., what is the optimal test statistic $t(\boldsymbol{x})$?

First find best $t(\boldsymbol{x})$, later address issue of optimal size of test.

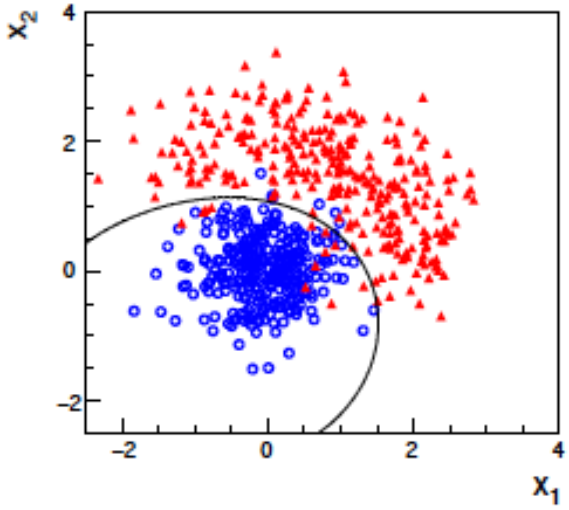
Remember $\boldsymbol{x}$-space can have many dimensions.



"cuts"



linear



non-linear

Test statistic based on likelihood ratio

How can we choose a test's critical region in an 'optimal way', in particular if the data space is multidimensional?

Neyman-Pearson lemma states:

For a test of H_0 of size α, to get the highest power with respect to the alternative H_1 we need for all $\boldsymbol{x}$ in the critical region W

"likelihood ratio (LR)" →

$$\frac{P(\mathbf{x}|H_1)}{P(\mathbf{x}|H_0)} \geq c_\alpha$$

inside W and $\leq c_\alpha$ outside, where c_α is a constant chosen to give a test of the desired size.

Equivalently, optimal scalar test statistic is

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

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 $f(\boldsymbol{x}|\mathrm{s}), f(\boldsymbol{x}|\mathrm{b})$, so for a given $\boldsymbol{x}$ 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 $\boldsymbol{x} \sim f(\boldsymbol{x}|\mathrm{s}) \quad \rightarrow \quad \boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$

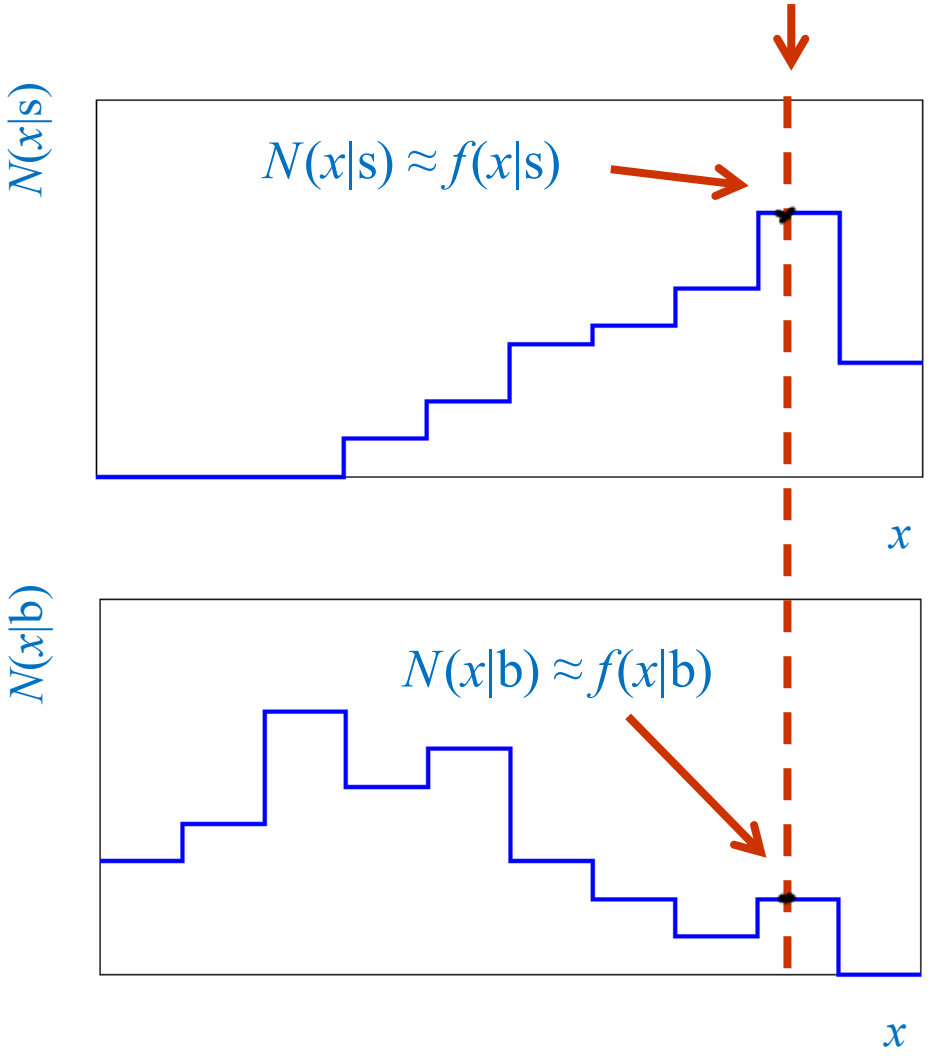
generate $\boldsymbol{x} \sim f(\boldsymbol{x}|\mathrm{b}) \quad \rightarrow \quad \boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$

This gives samples of "training data" with events of known type.

- Use these to construct a statistic that is as close as possible to the optimal likelihood ratio (→ Machine Learning).

Approximate LR from histograms

Want $t(x) = f(x|\mathrm{s})/f(x|\mathrm{b})$ 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:

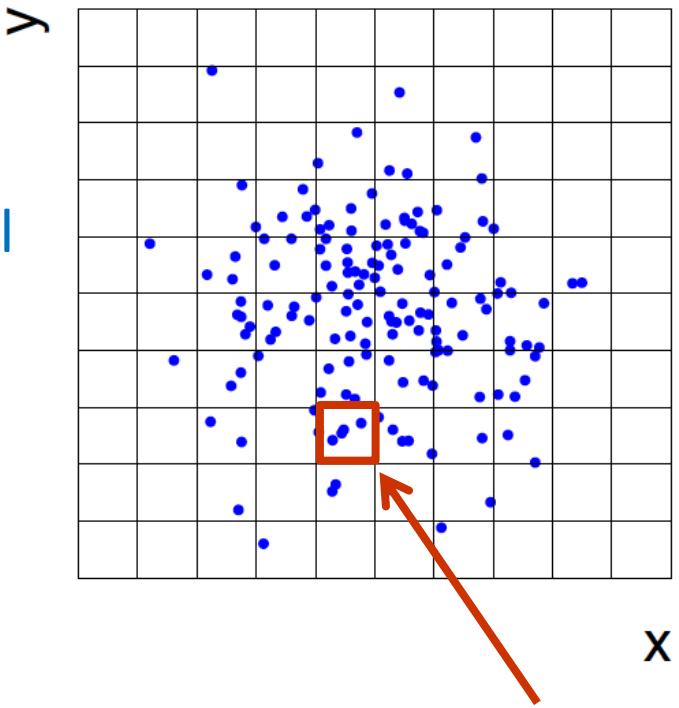
$$t(x) \approx \frac{N(x|s)}{N(x|b)}$$

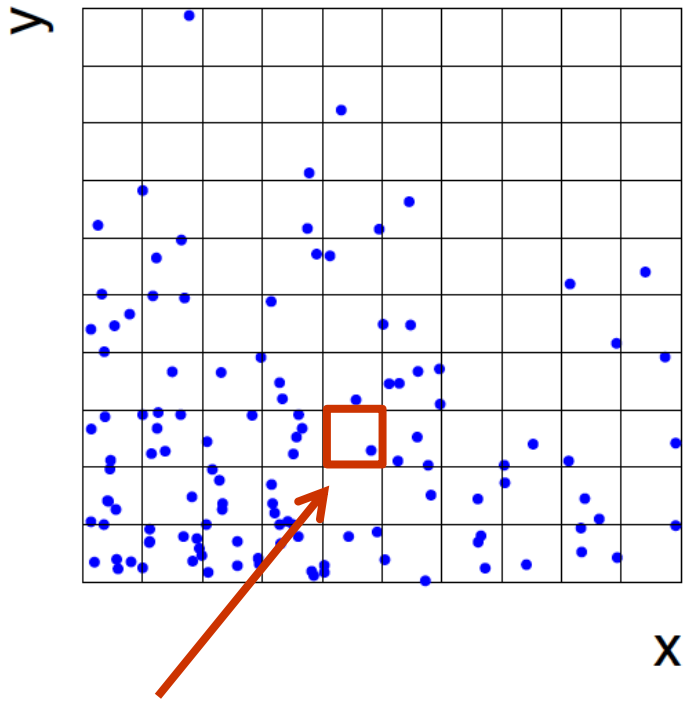
Can work well for single variable.

Approximate LR from 2D-histograms

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

signal





back-ground

Approximate pdfs using $N(x,y|\mathrm{s})$, $N(x,y|\mathrm{b})$ 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 $f(\boldsymbol{x}|\mathrm{s}), f(\boldsymbol{x}|\mathrm{b})$.

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 $t(\boldsymbol{x})$ with fewer parameters; determine them (using MC) to give best separation between signal and background.

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

Multivariate methods (Machine Learning)

Many new (and some old) methods:

- Fisher discriminant
- (Deep) Neural Networks
- Kernel density methods
- Support Vector Machines
- Decision trees
  - Boosting
  - Bagging

More in the lectures by Stephen Jiggins

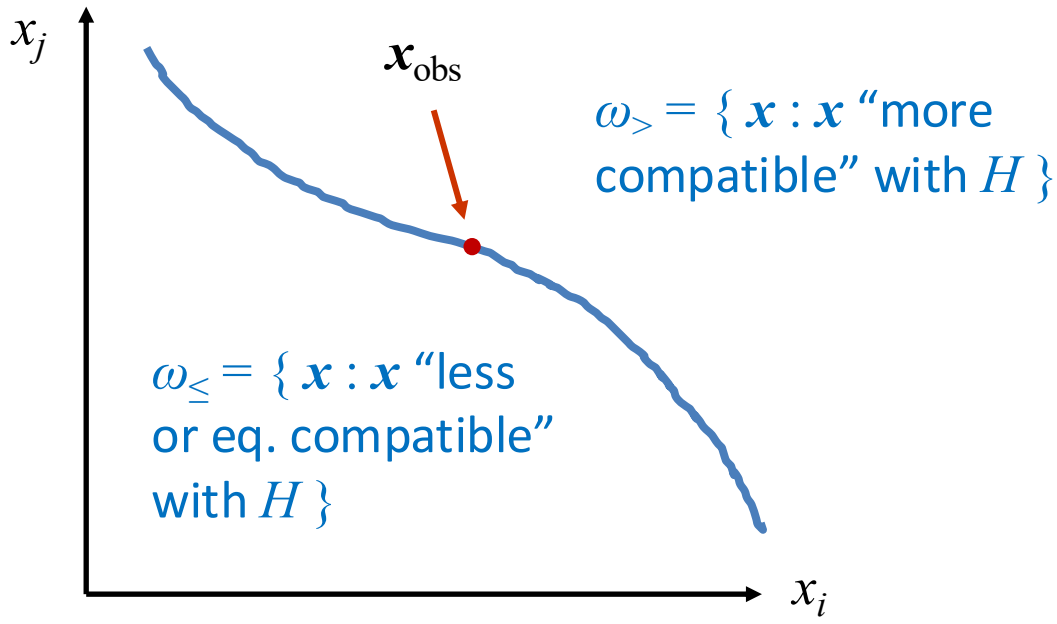
Testing significance / goodness-of-fit

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

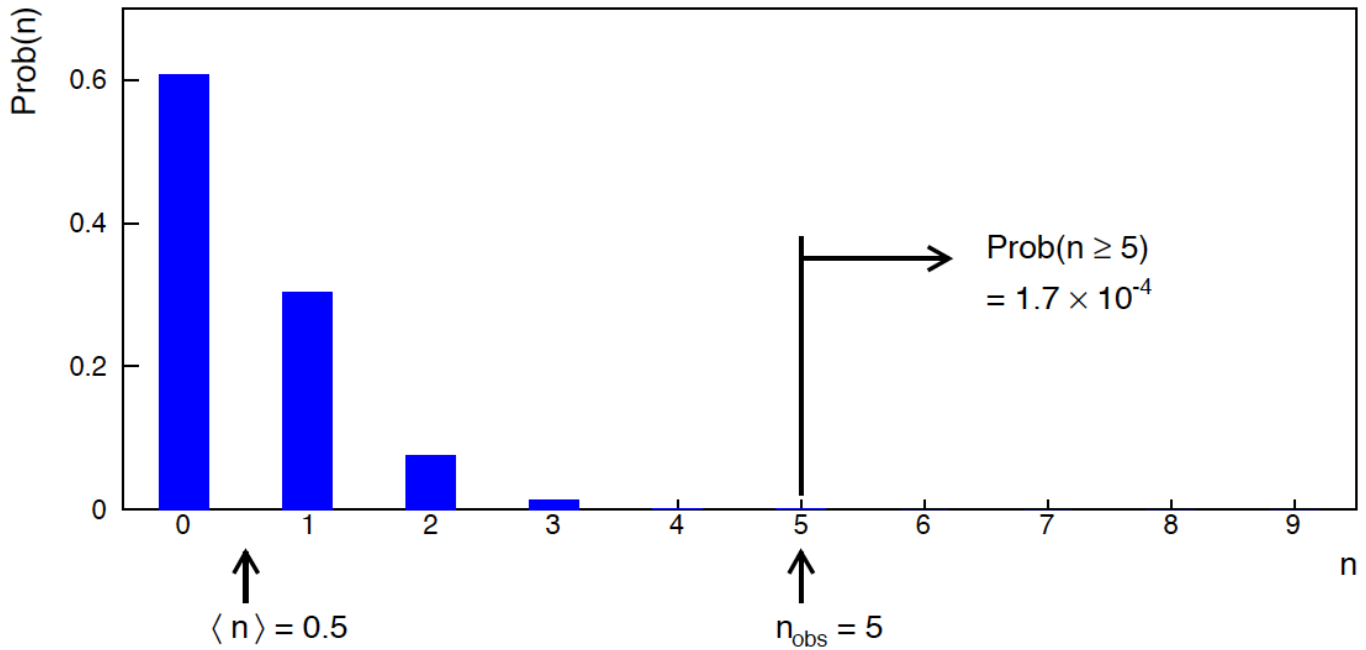
Suppose $b = 0.5$ (known), and we observe $n_{\text{obs}} = 5$.

Should we claim evidence for a new discovery?

Give p-value for hypothesis $s = 0$, suppose relevant alt. is $s > 0$.

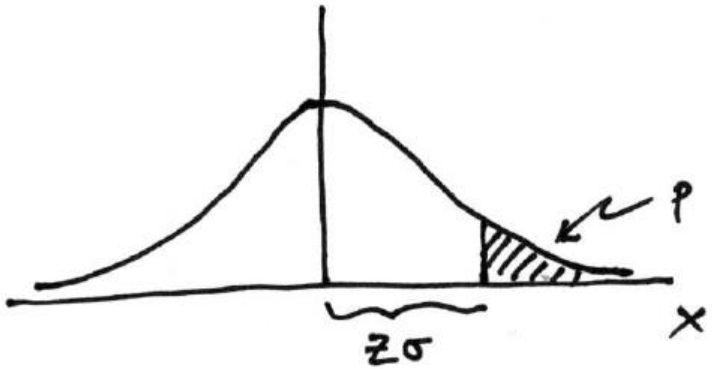
$$p\text{-value} = P(n \geq 5; b = 0.5, s = 0)$$

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



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.



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

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

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

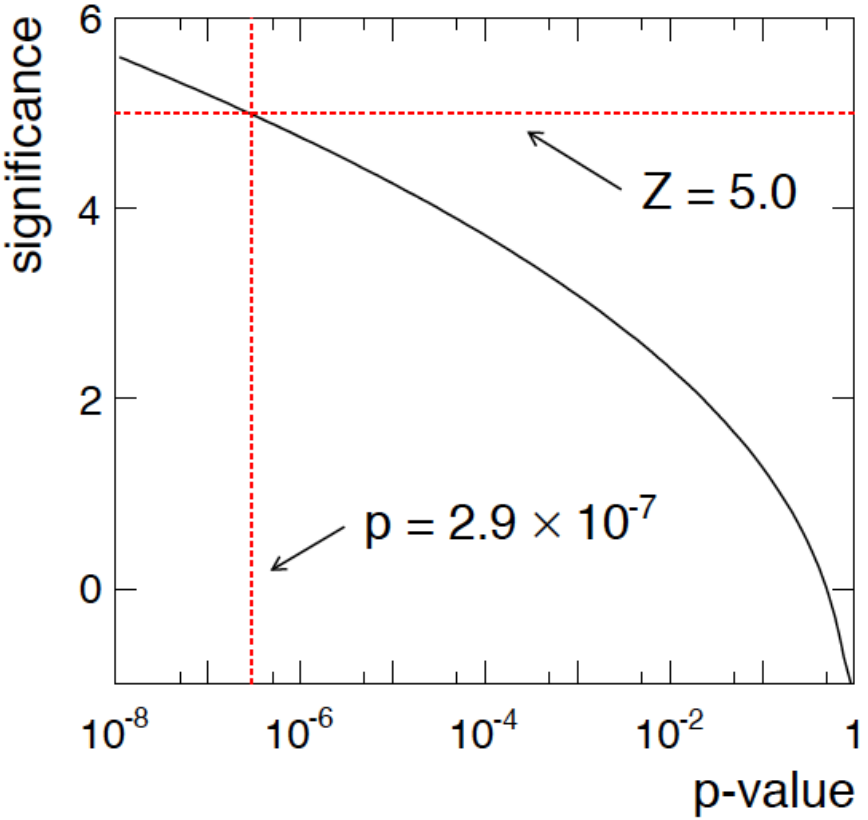
```
in python (scipy.stats):
p = 1 - norm.cdf(Z) = norm.sf(Z)
Z = norm.ppf(1-p)
```

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.

Extra slides

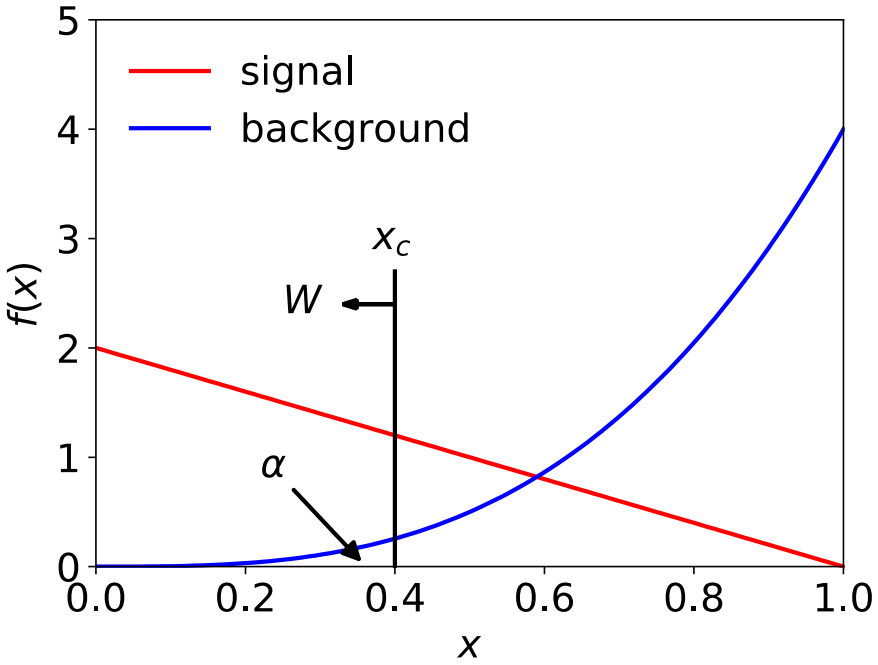
Example of a test for classification

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:

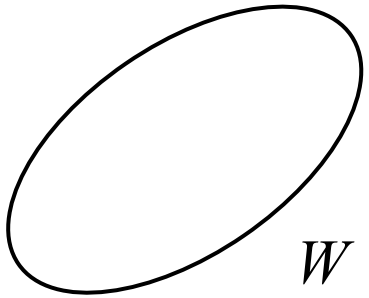
$$P(\mathrm{s}|x \leq x_{\mathrm{c}}) = \frac{P(x \leq x_{\mathrm{c}}|\mathrm{s})\pi_{\mathrm{s}}}{P(x \leq x_{\mathrm{c}}|\mathrm{s})\pi_{\mathrm{s}} + P(x \leq x_{\mathrm{c}}|\mathrm{b})\pi_{\mathrm{b}}}$$

$$= 0.655$$

Proof of Neyman-Pearson Lemma

Consider a critical region W and suppose the LR satisfies the criterion of the Neyman-Pearson lemma:

$$P(\boldsymbol{x}|H_1)/P(\boldsymbol{x}|H_0) \geq c_\alpha \quad \text{for all } \boldsymbol{x} \text{ in } W,$$
$$P(\boldsymbol{x}|H_1)/P(\boldsymbol{x}|H_0) \leq c_\alpha \quad \text{for all } \boldsymbol{x} \text{ not in } W.$$



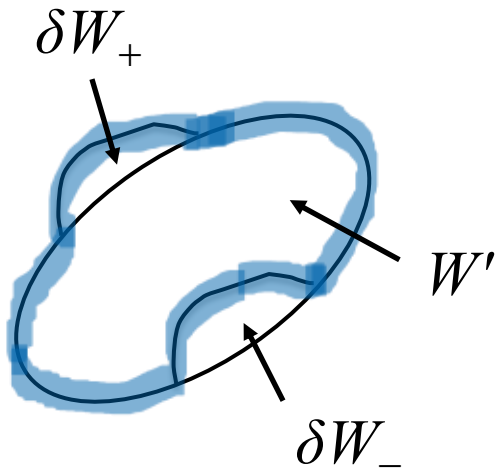
Try to change this into a different critical region W' retaining the same size α, i.e.,

$$P(\mathbf{x} \in W'|H_0) = P(\mathbf{x} \in W|H_0) = \alpha$$

To do so add a part δW_+, but to keep the size α, we need to remove a part δW_-, i.e.,

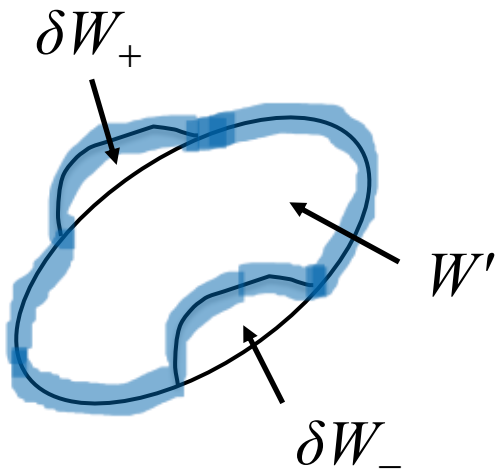
$$W \to W' = W + \delta W_+ - \delta W_-$$

$$P(\mathbf{x} \in \delta W_+|H_0) = P(\mathbf{x} \in \delta W_-|H_0)$$



Proof of Neyman-Pearson Lemma (2)

But we are supposing the LR is higher for all $\boldsymbol{x}$ in δW_- removed than for the $\boldsymbol{x}$ in δW_+ added, and therefore



$$P(\mathbf{x} \in \delta W_+ | H_1) \leq P(\mathbf{x} \in \delta W_+ | H_0) c_\alpha$$

$$P(\mathbf{x} \in \delta W_- | H_1) \geq P(\mathbf{x} \in \delta W_- | H_0) c_\alpha$$

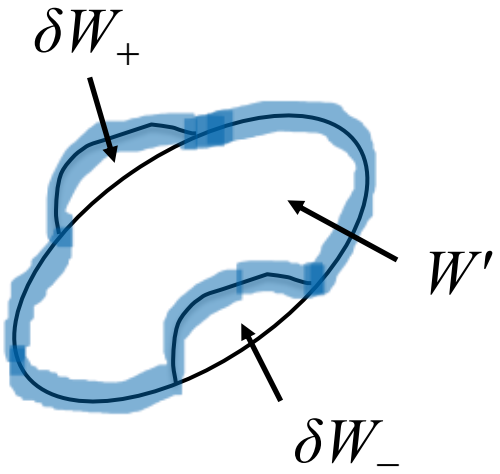
The right-hand sides are equal and therefore

$$P(\mathbf{x} \in \delta W_+ | H_1) \leq P(\mathbf{x} \in \delta W_- | H_1)$$

Proof of Neyman-Pearson Lemma (3)

We have

$$W \cup W' = W \cup \delta W_+ = W' \cup \delta W_-$$



Note W and δW_+ are disjoint, and W' and δW_- are disjoint, so by Kolmogorov's 3rd axiom,

$$P(\mathbf{x} \in W') + P(\mathbf{x} \in \delta W_-) = P(\mathbf{x} \in W) + P(\mathbf{x} \in \delta W_+)$$

Therefore

$$P(\mathbf{x} \in W'|H_1) = P(\mathbf{x} \in W|H_1) + P(\mathbf{x} \in \delta W_+|H_1) - P(\mathbf{x} \in \delta W_-|H_1)$$

≤ 0

Proof of Neyman-Pearson Lemma (4)

And therefore

$$P(\mathbf{x} \in W' | H_1) \leq P(\mathbf{x} \in W | H_1)$$

i.e. the deformed critical region W' cannot have higher power than the original one that satisfied the LR criterion of the Neyman-Pearson lemma.

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:

$n \sim$ Poisson(s+b) (primary or "search" measurement)

$m \sim$ Poisson(τb) (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):

$$\lambda(0) = \frac{L(0, \hat{\hat{b}}(0))}{L(\hat{s}, \hat{b})}$$

Ingredients for profile likelihood ratio

To construct profile likelihood ratio from this need estimators:

$$\hat{s} = n - m/\tau \,,$$

$$\hat{b} = m/\tau \,,$$

$$\hat{\hat{b}}(s) = \frac{n + m - (1+\tau)s + \sqrt{(n + m - (1+\tau)s)^2 + 4(1+\tau)sm}}{2(1+\tau)} \,.$$

and in particular to test for discovery ($s = 0$),

$$\hat{\hat{b}}(0) = \frac{n+m}{1+\tau}$$

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:

$$n \to s + b$$

$$m \to \tau b$$

$$Z_{\mathrm{A}} = \left[-2 \left((s+b) \ln \left[\frac{s + (1+\tau)b}{(1+\tau)(s+b)} \right] + \tau b \ln \left[1 + \frac{s}{(1+\tau)b} \right] \right) \right]^{1/2}$$

Or use the variance of $\hat{b} = m/\tau$, $V[\hat{b}] \equiv \sigma_b^2 = \dfrac{b}{\tau}$, to eliminate τ:

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

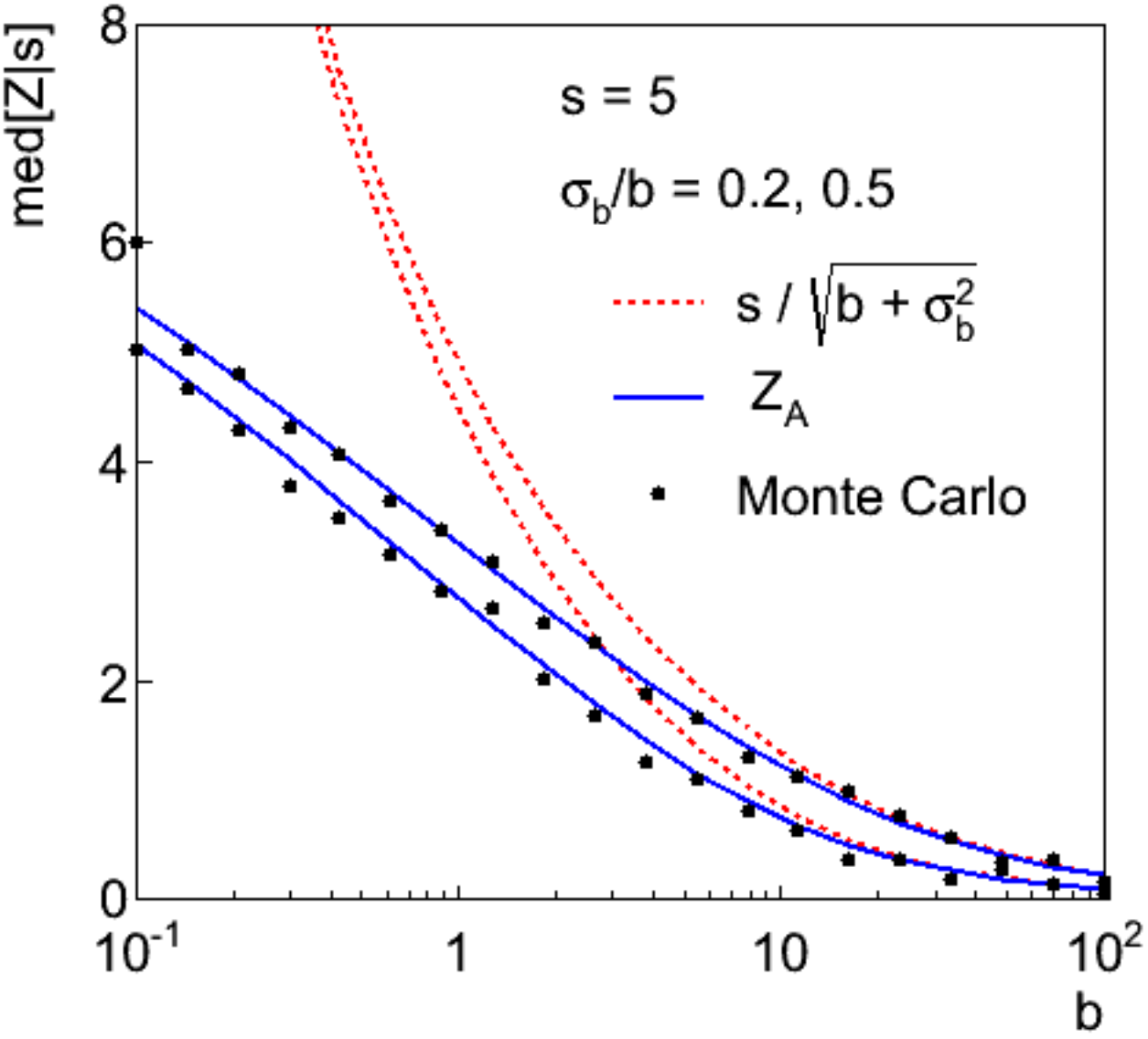
Limiting cases

Expanding the Asimov formula in powers of s/b and σ_b^2/b $(= 1/\tau)$ gives

$$Z_{\mathrm{A}} = \frac{s}{\sqrt{b + \sigma_b^2}} \left(1 + \mathcal{O}(s/b) + \mathcal{O}(\sigma_b^2/b)\right)$$

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

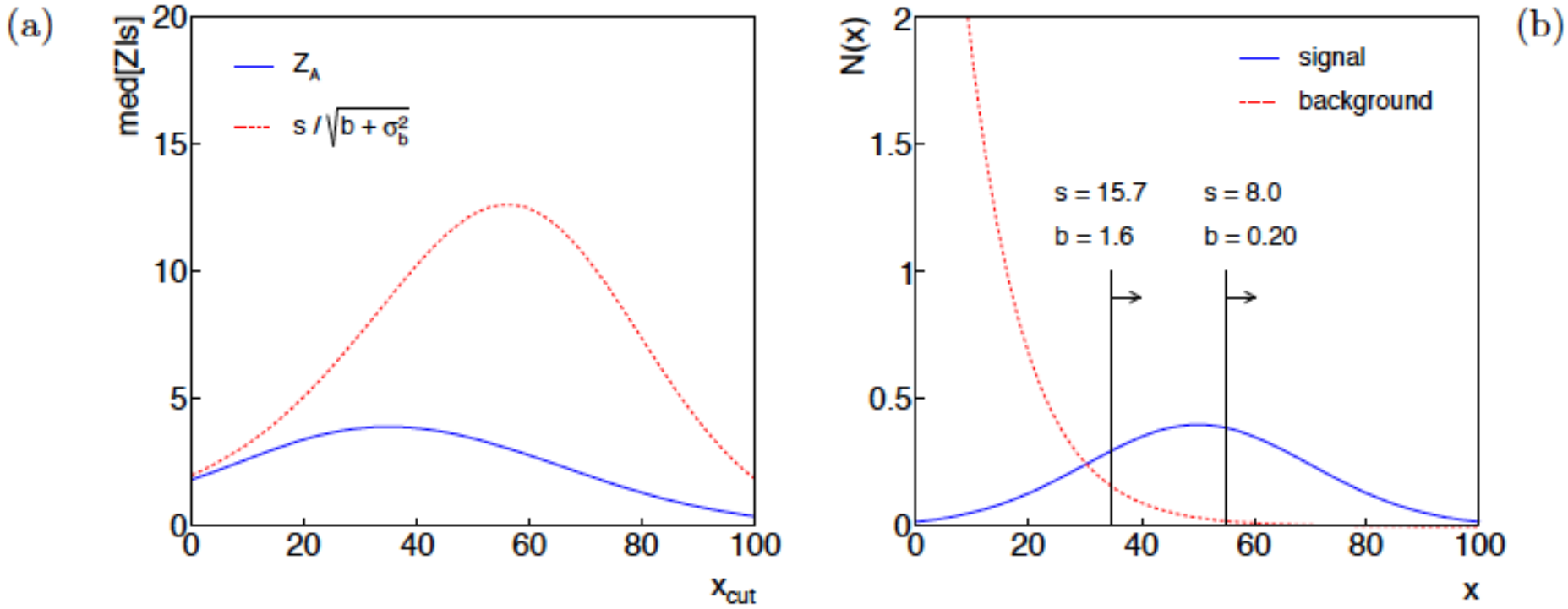


Figure 1: (a) The expected significance as a function of the cut value $x_{\rm cut}$; (b) the distributions of signal and background with the optimal cut value indicated.