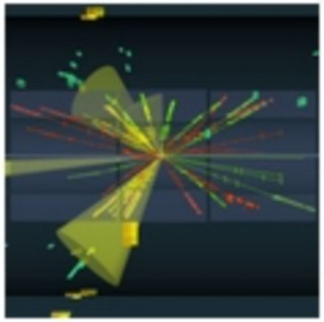
Statistics for Particle Physics
Lecture day 1



CENTRO DE CIENCIAS
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PEDRO PASCUAL

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Outline

→	Monday 9-11 :	Introduction
		Probability
		Hypothesis tests
		Machine Learning
	Tuesday 9-11 :	Parameter estimation
		Confidence limits
		Systematic uncertainties
		Experimental sensitivity
	Tuesday 15:30:	Tutorial on parameter estimation

Almost everything is a subset of the University of London course:

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

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.

Luca Lista, *Statistical Methods for Data Analysis in Particle Physics*, Springer, 2017.

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.

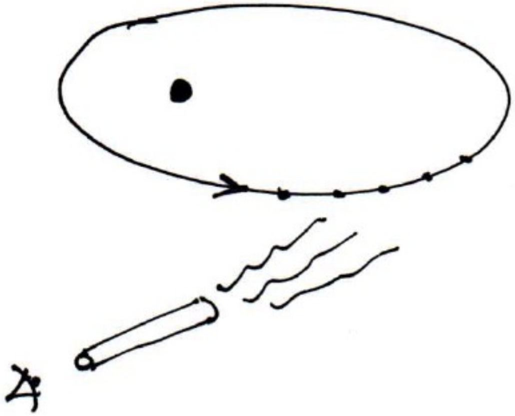
R.L. Workman et al. (Particle Data Group), Prog. Theor. Exp. Phys. 083C01 (2022); **`pdg.lbl.gov`** sections on probability, statistics, MC.

Theory ↔ Statistics ↔ Experiment

Theory (model, hypothesis):

Experiment (observation):

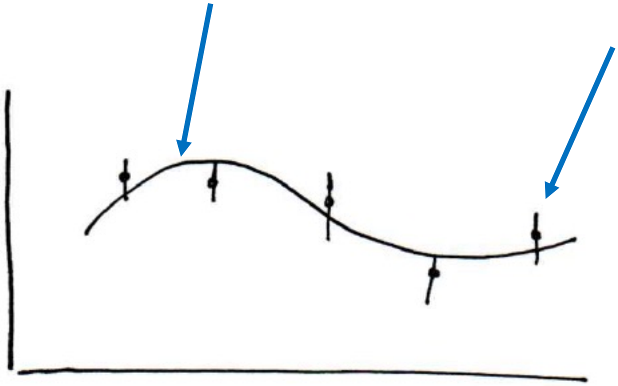
$$F = -G \frac{m_1 m_2}{r^2}, \ldots$$



+ response of measurement apparatus

= model prediction

data



Uncertainty enters on many levels

→ quantify with probability

A quick review of probability

Frequentist (A = outcome of repeatable observation)

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

Subjective (A = hypothesis)

$$P(A) = \text{degree of belief that } A \text{ is true}$$

Conditional probability:

$$P(A|B) = \frac{P(A \cap B)}{P(B)}$$

E.g. rolling a die,
outcome n = 1,2,...,6:

$$P(n \leq 3 | n \text{ even}) = \frac{P((n \leq 3) \cap n \text{ even})}{P(n \text{ even})} = \frac{1/6}{3/6} = \frac{1}{3}$$

A and B are independent iff:

$$P(A \cap B) = P(A)P(B)$$

I.e. if A, B independent, then

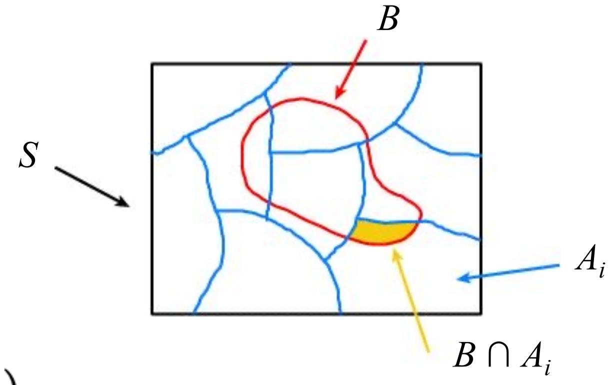
$$P(A|B) = \frac{P(A)P(B)}{P(B)} = P(A)$$

Bayes' theorem

Use definition of conditional probability and $P(A \cap B) = P(B \cap A)$

$$\rightarrow \quad P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$ (Bayes' theorem)

If set of all outcomes $S = \cup_i A_i$ with A_i disjoint, then law of total probability for $P(B)$ says



$$P(B) = \sum_i P(B \cap A_i) = \sum_i P(B|A_i)P(A_i)$$

so that Bayes' theorem becomes $$P(A|B) = \frac{P(B|A)P(A)}{\sum_i P(B|A_i)P(A_i)}$$

Bayes' theorem holds regardless of how probability is interpreted (frequency, degree of belief...).

Frequentist Statistics – general philosophy

In frequentist statistics, probabilities are associated only with the data, i.e., outcomes of repeatable observations (shorthand: $\boldsymbol{x}$).

Probability = limiting frequency

Probabilities such as

P (string theory is true),
P ($0.117 < \alpha_s < 0.119$),
P (Biden wins in 2024),

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.

Preferred theories (models, hypotheses, ...) are those that predict a high probability for data "like" the data observed.

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

normalization involves sum 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!)

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:

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

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

$P(\mathbf{x}|\boldsymbol{\theta}) = L(\boldsymbol{\theta})$ = 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 $\boldsymbol{x}$: $P(\boldsymbol{x}|H_0)$, $P(\boldsymbol{x}|H_1)$

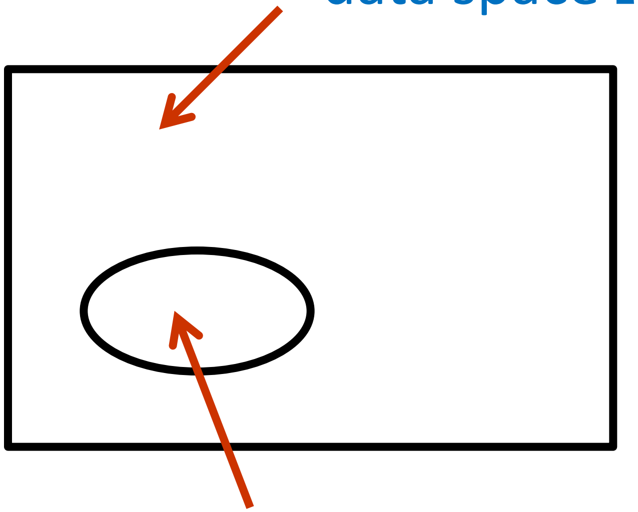
A test of H_0 is defined by specifying a critical region w of the data space such that there is no more than some (small) probability α, assuming H_0 is correct, to observe the data there, i.e.,

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

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.



data space Ω

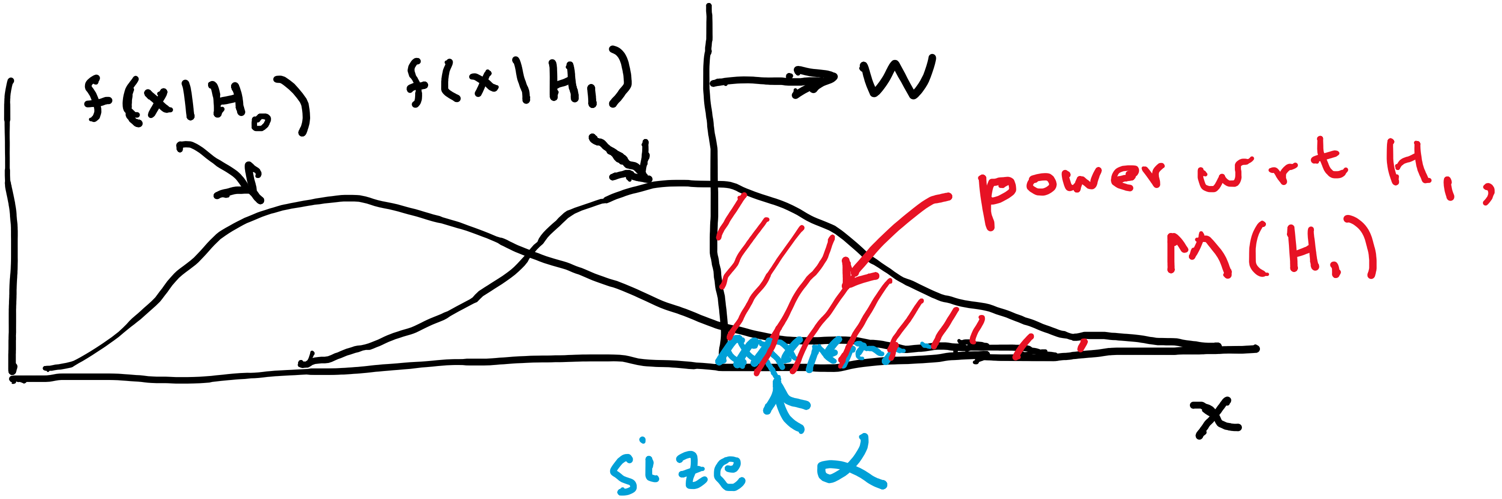
critical region w

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

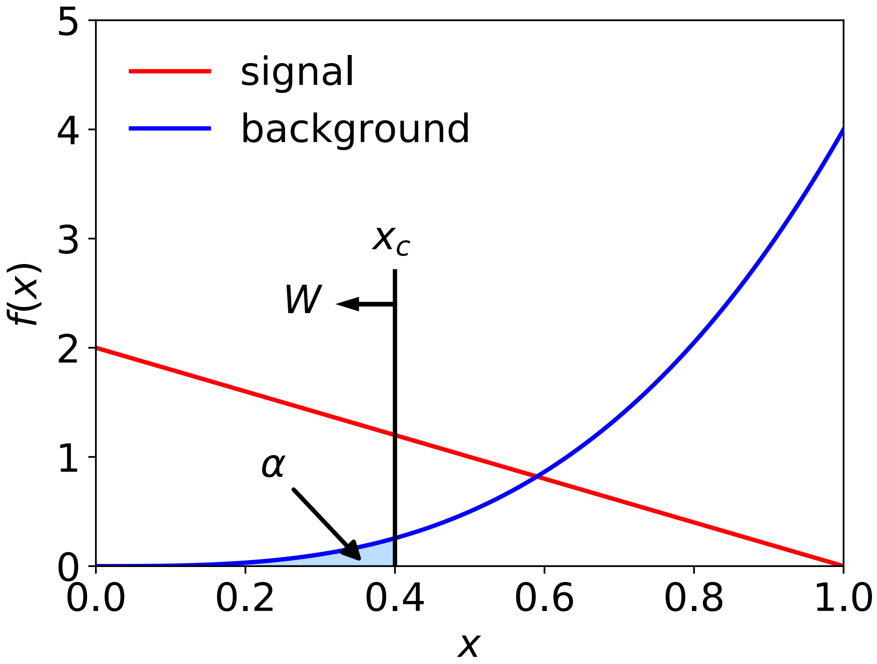
Example of a test for classification

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:

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

and therefore $x_{\mathrm{c}} = \alpha^{1/4} = 0.1$

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

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

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:

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

$$= 0.655$$

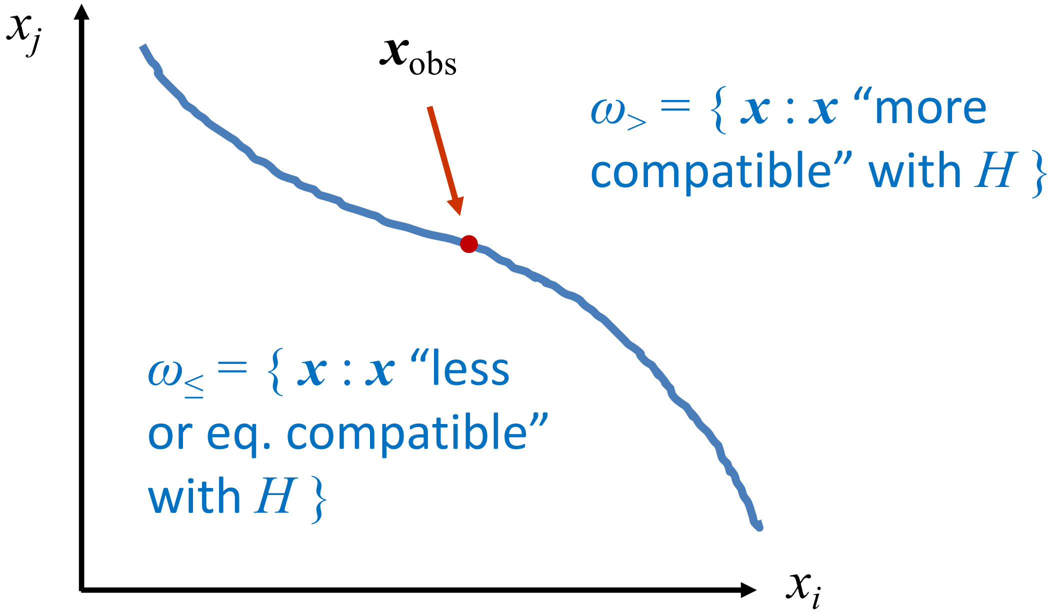
Testing significance / goodness-of-fit

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!)



$\omega_{>} = \{\, \boldsymbol{x} : \boldsymbol{x}$ "more compatible" with $H\,\}$

$\omega_{\leq} = \{\, \boldsymbol{x} : \boldsymbol{x}$ "less or eq. compatible" with $H\,\}$

p-values

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

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

= 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.

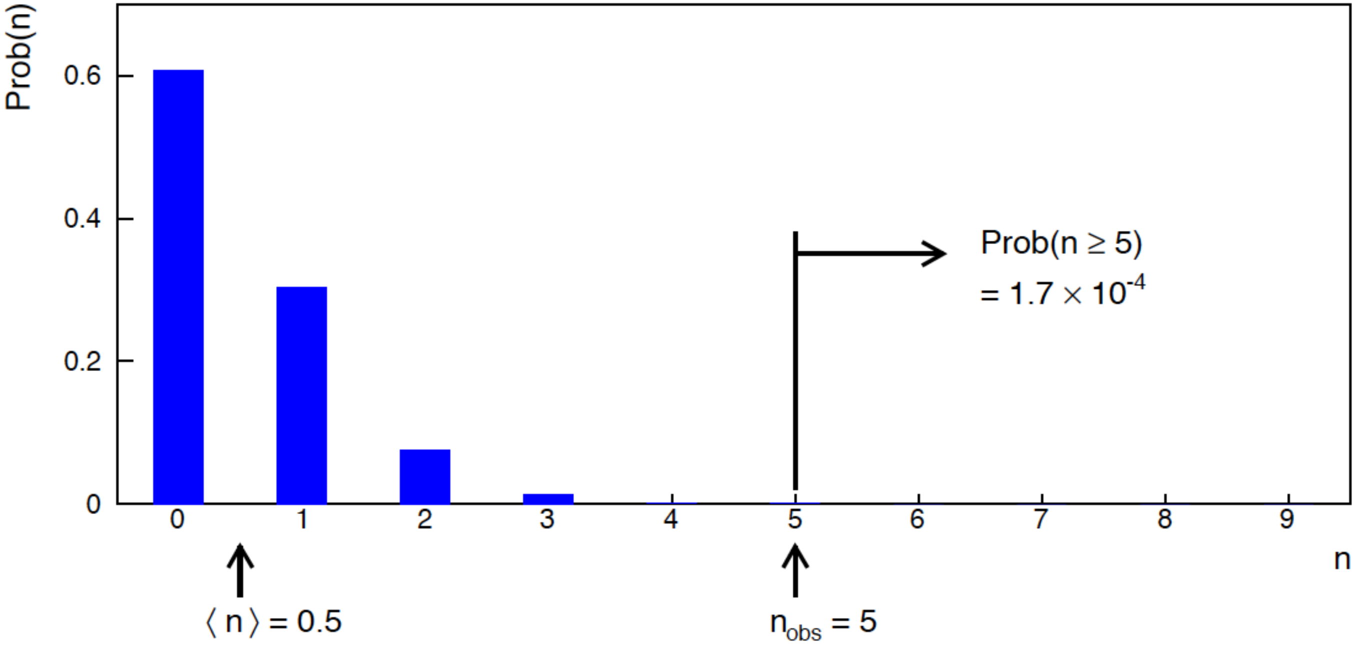
Poisson counting experiment: discovery p-value

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

Should we claim evidence for a new discovery?

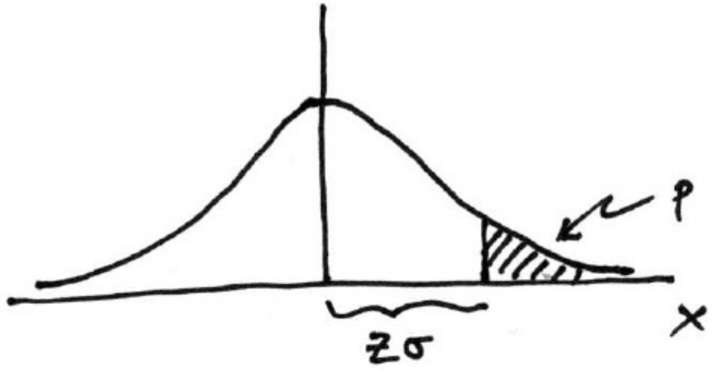
Give p-value for hypothesis $s = 0$, suppose relevant alt. is $s > 0$.

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



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)
```

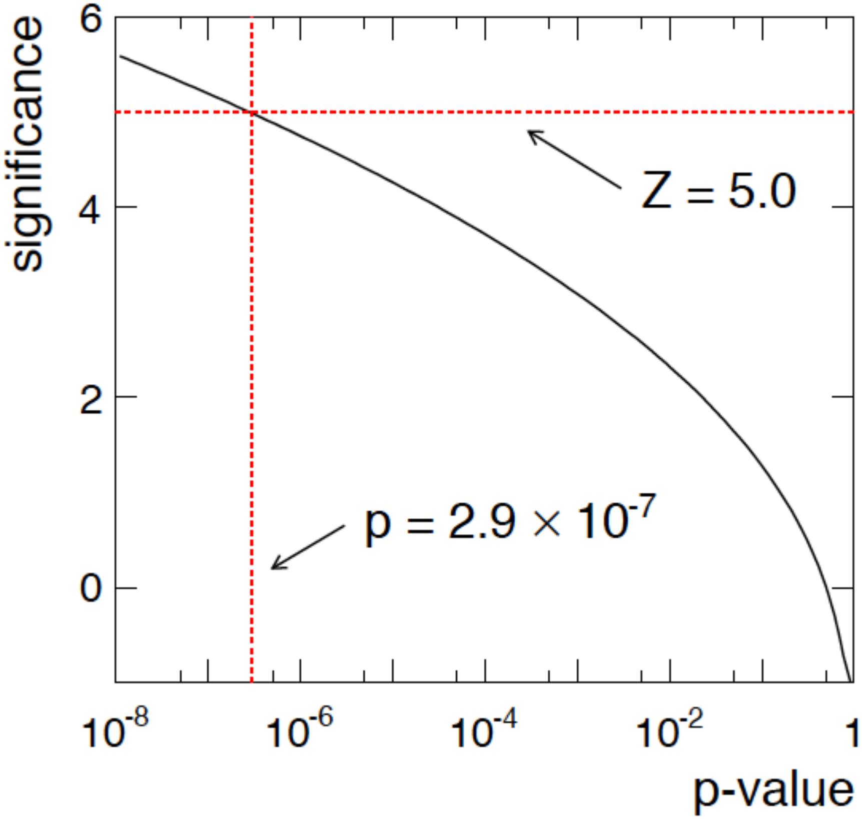
```
in python (scipy.stats):
p = 1 - norm.cdf(Z) = norm.sf(Z)
Z = norm.ppf(1-p)
```

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 $p = 1.7 \times 10^{-4}$: $Z = \Phi^{-1}(1-p) = 3.6$

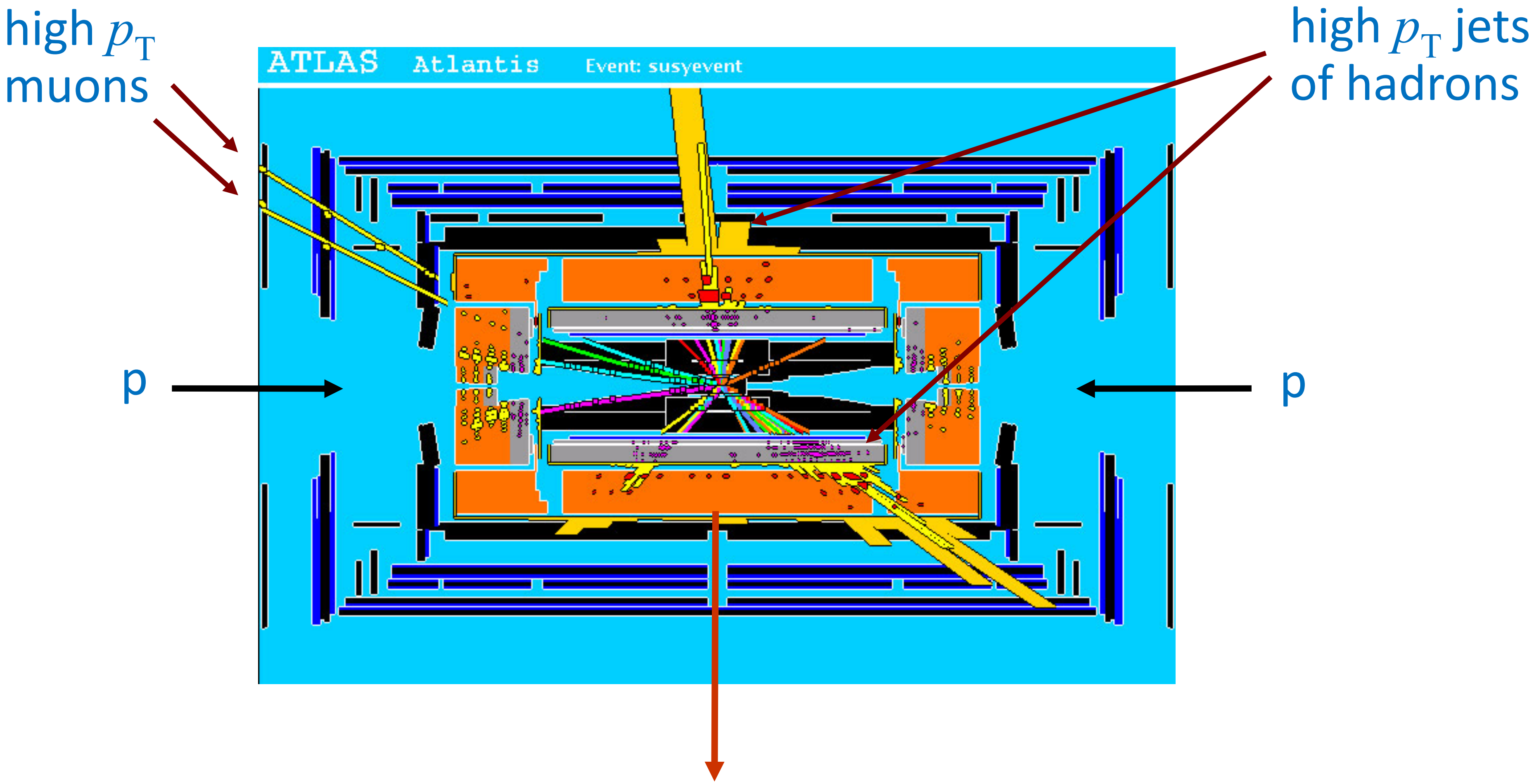
Often claim discovery if $Z > 5$ ($p < 2.9 \times 10^{-7}$, i.e., a "5-sigma effect")



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" (~multiple testing), etc.

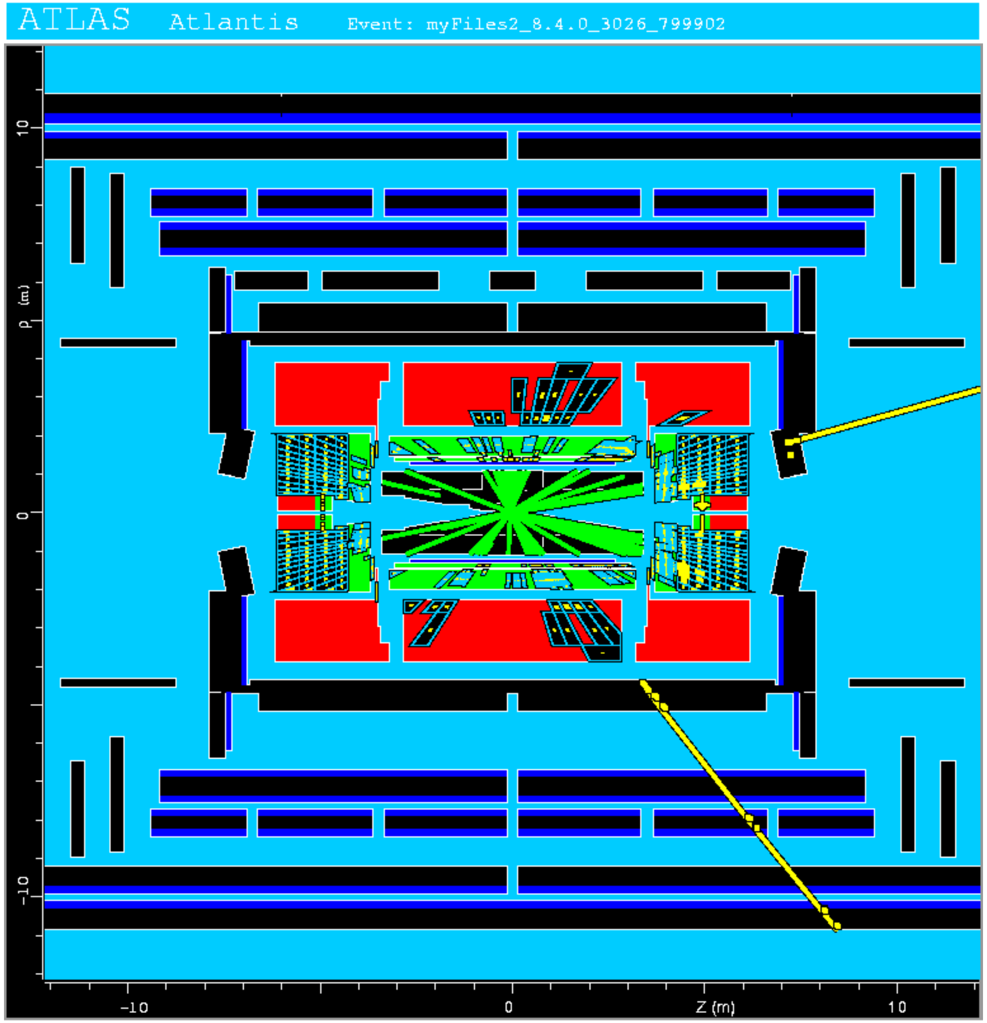
Particle Physics context for a hypothesis test

A simulated SUSY event ("signal"):


ATLAS
Atlantis
Event: susyevent
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 = ...

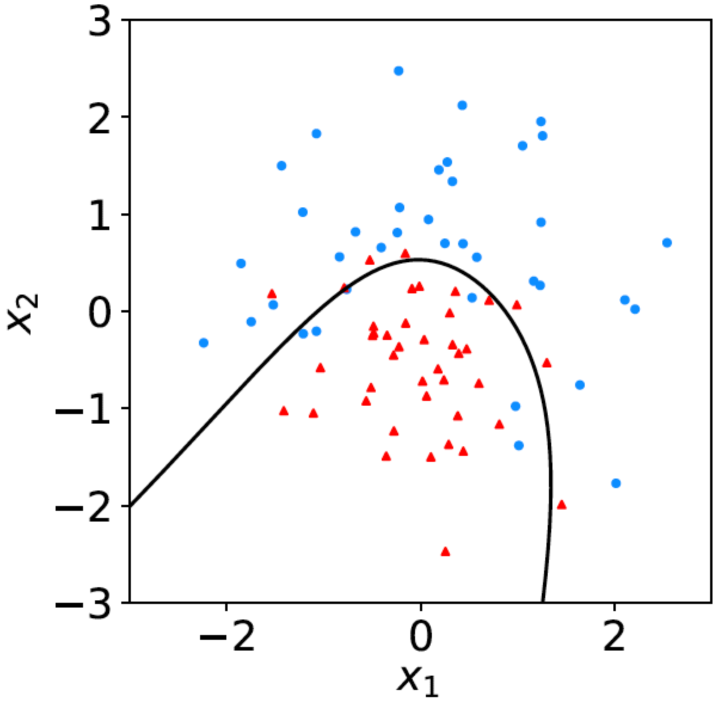
The real events don't come with true class labels, but computer-simulated events do. So we can have a set of simulated events that consist of a feature vector $\boldsymbol{x}$ and true class label y (0 for background, 1 for signal):

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

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

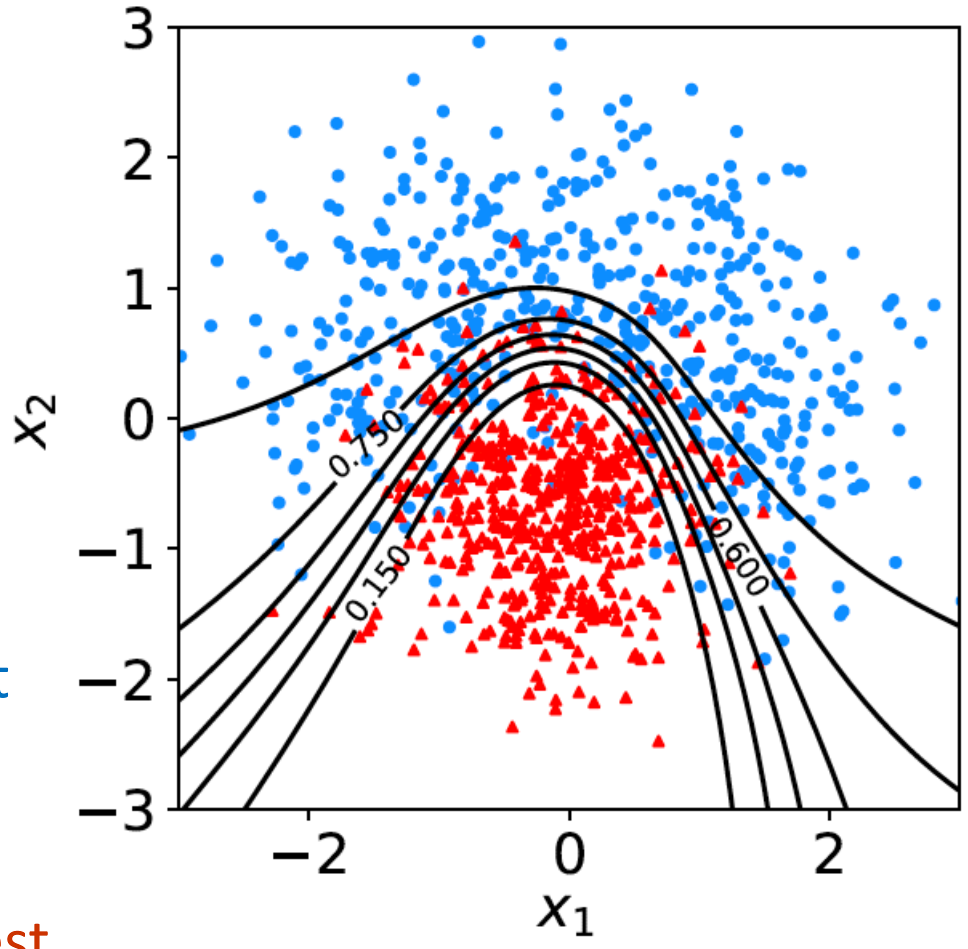
$$t(x_1, \ldots, x_n) = t_c$$

scalar function

constant

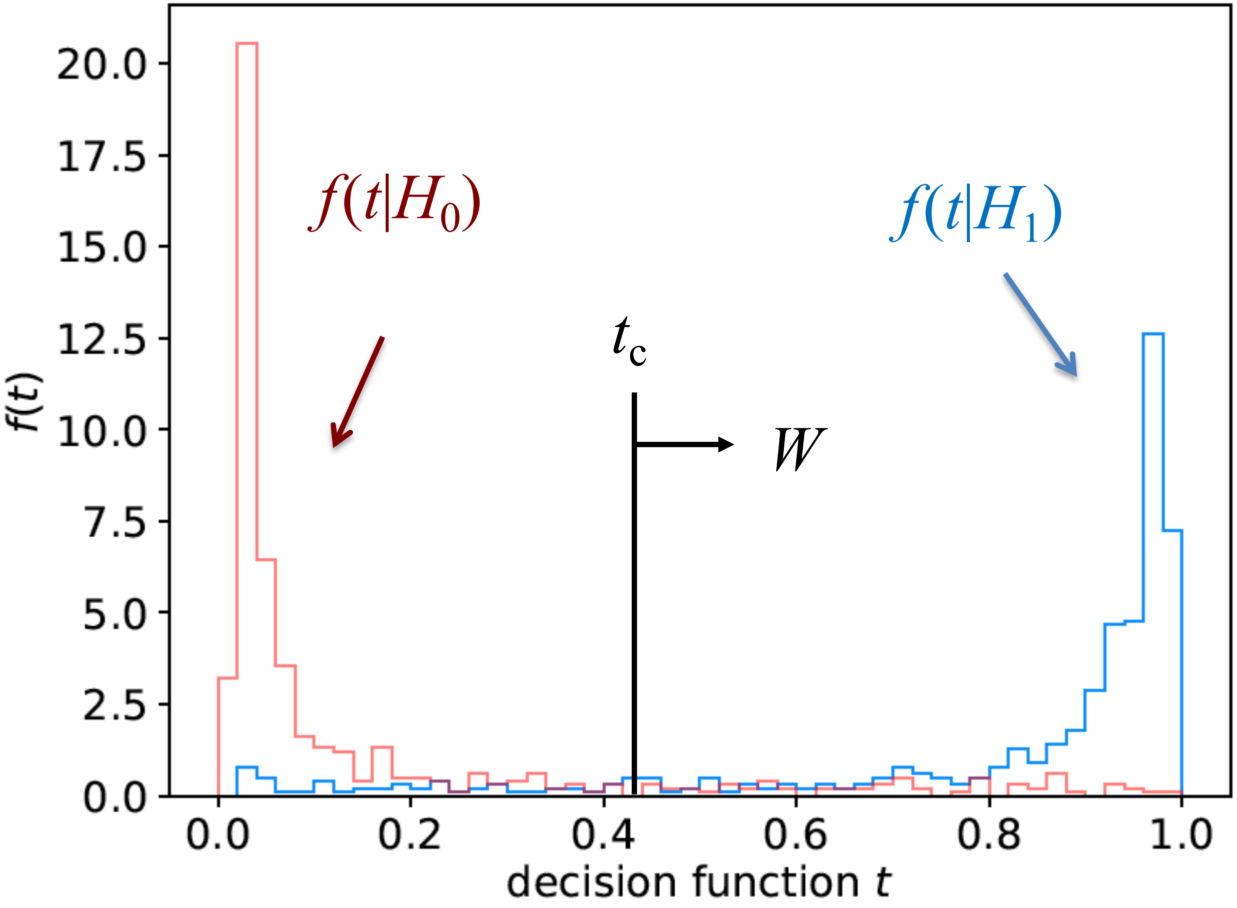
Different values of the constant t_c result in a family of surfaces.

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.

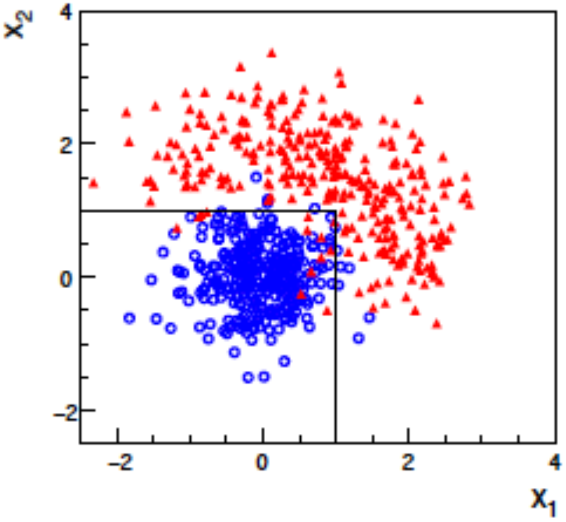


Types of decision boundaries

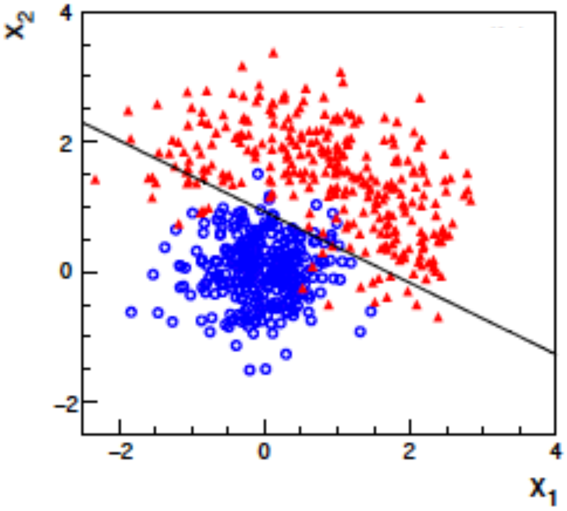
So what is the optimal boundary for the critical region, i.e., what is the optimal test statistic $t(\boldsymbol{x})$?

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

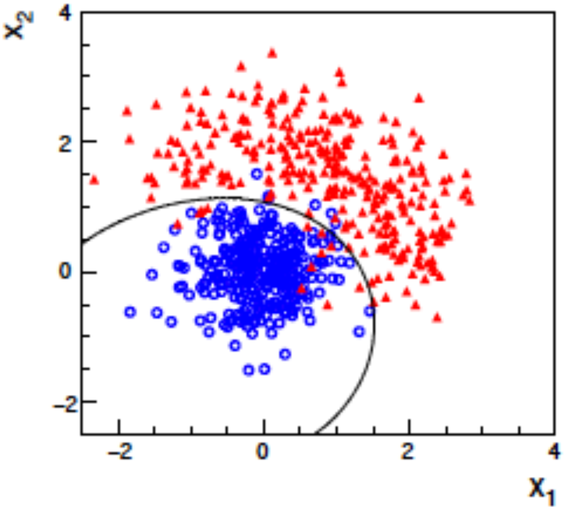
Remember $\boldsymbol{x}$-space can have many dimensions.



“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

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

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 $\boldsymbol{x} \sim f(\boldsymbol{x}|\mathrm{s}) \quad \to \quad \boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$

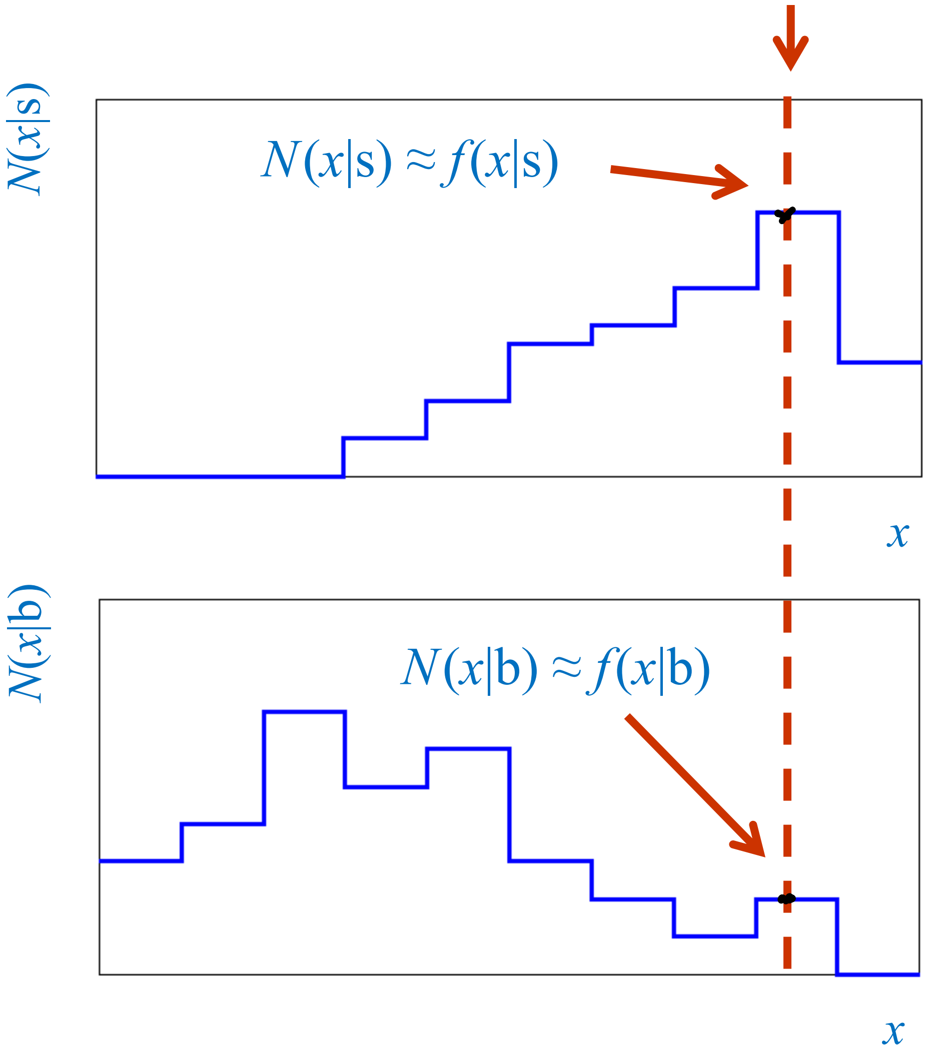
generate $\boldsymbol{x} \sim f(\boldsymbol{x}|\mathrm{b}) \quad \to \quad \boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$

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.

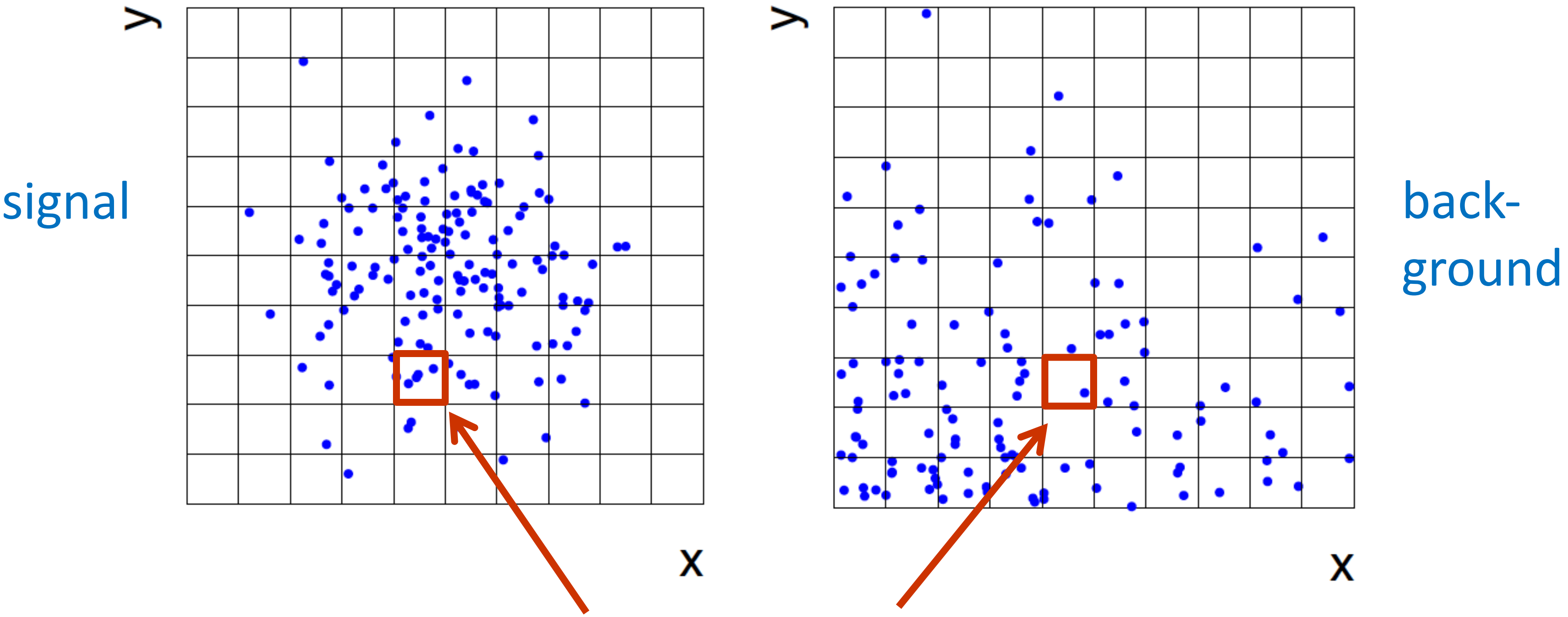
Use (normalized) histogram values to approximate LR:

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

Can work well for single variable.

Approximate LR from 2D-histograms

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



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:

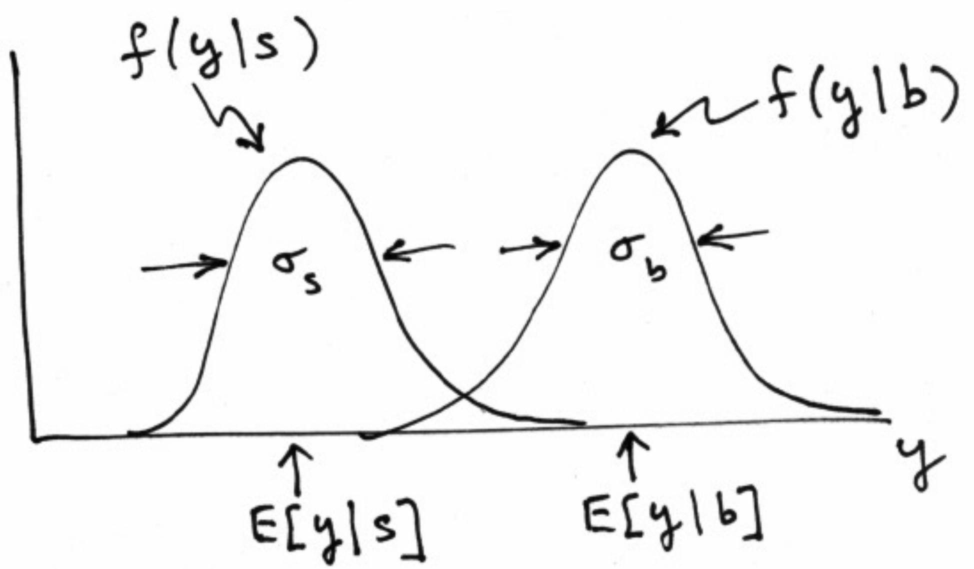
- Fisher discriminant
- (Deep) Neural Networks
- Kernel density methods
- Support Vector Machines
- Decision trees
  - Boosting
  - Bagging

Linear test statistic

Suppose there are n input variables: $\boldsymbol{x} = (x_1,\ldots, x_n)$.

Consider a linear function:
$$y(\mathbf{x}) = \sum_{i=1}^{n} w_i x_i$$

For a given choice of the coefficients $\boldsymbol{w} = (w_1,\ldots, w_n)$ we will get pdfs $f(y|\mathrm{s})$ and $f(y|\mathrm{b})$:



Linear test statistic

Fisher: to get large difference between means and small widths for $f(y|\mathrm{s})$ and $f(y|\mathrm{b})$, maximize the difference squared of the expectation values divided by the sum of the variances:

$$J(\mathbf{w}) = \frac{(E[y|s] - E[y|b])^2}{V[y|s] + V[y|b]}$$

Setting $\partial J / \partial w_i = 0$ gives:

$$\mathbf{w} \propto W^{-1}(\boldsymbol{\mu}_{\mathrm{b}} - \boldsymbol{\mu}_{\mathrm{s}})$$

$$W_{ij} = \mathrm{cov}[x_i, x_j|\mathrm{s}] + \mathrm{cov}[x_i, x_j|\mathrm{b}]$$

$$\mu_{i,\mathrm{s}} = E[x_i|s], \qquad \mu_{i,\mathrm{b}} = E[x_i|b]$$

The Fisher discriminant

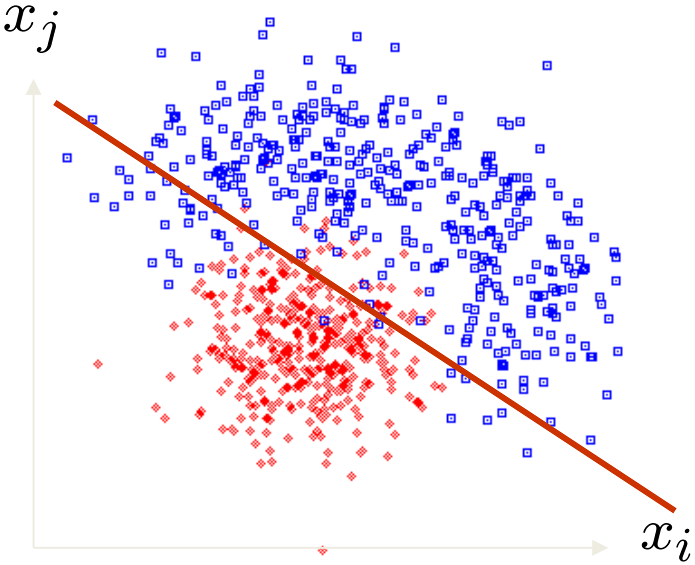
The resulting coefficients w_i define a Fisher discriminant.

Coefficients defined up to multiplicative constant; can also add arbitrary offset, i.e., usually define test statistic as

$$y(\mathbf{x}) = w_0 + \sum_{i=1}^{n} w_i x_i$$

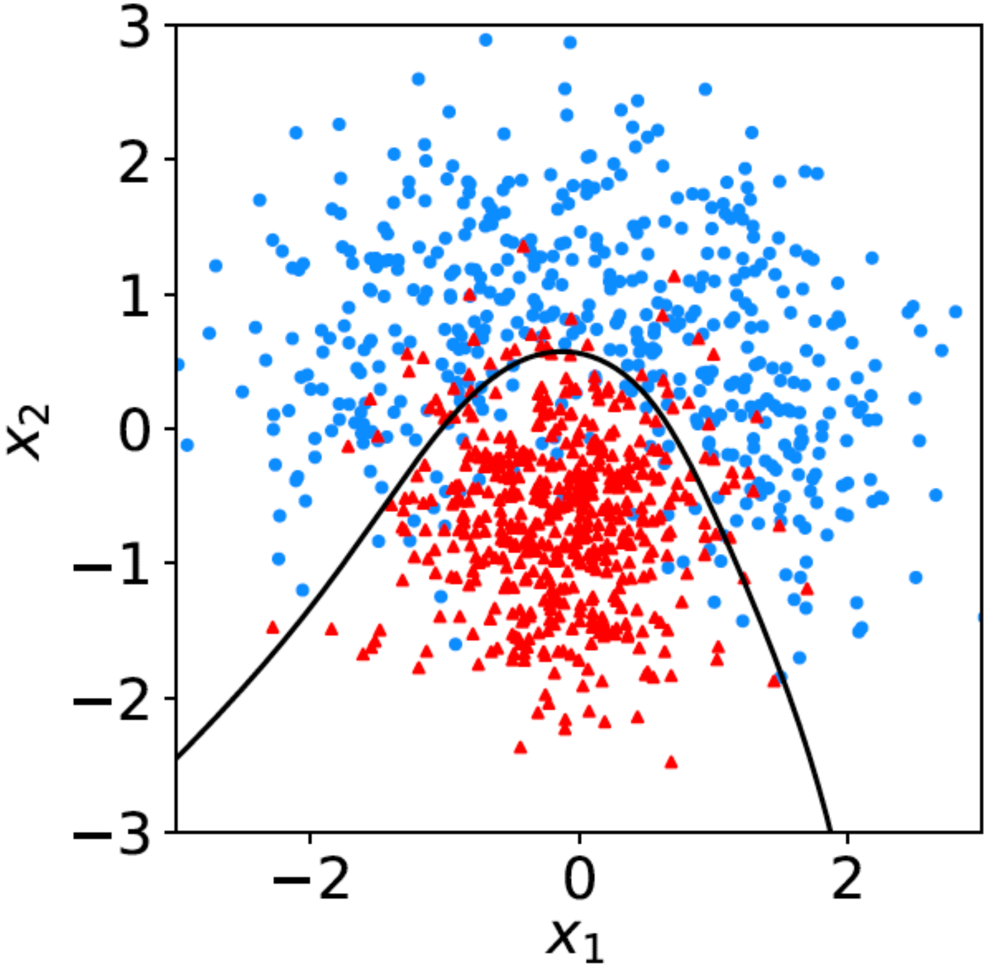
.

Boundaries of the test's critical region are surfaces of constant $y(\boldsymbol{x})$, here linear (hyperplanes):



Nonlinear decision boundaries

From the scatter plot below it's clear that some nonlinear boundary would be better than a linear one:



And to have a nonlinear boundary, the decision function $t(\boldsymbol{x})$ must be nonlinear in $\boldsymbol{x}$.

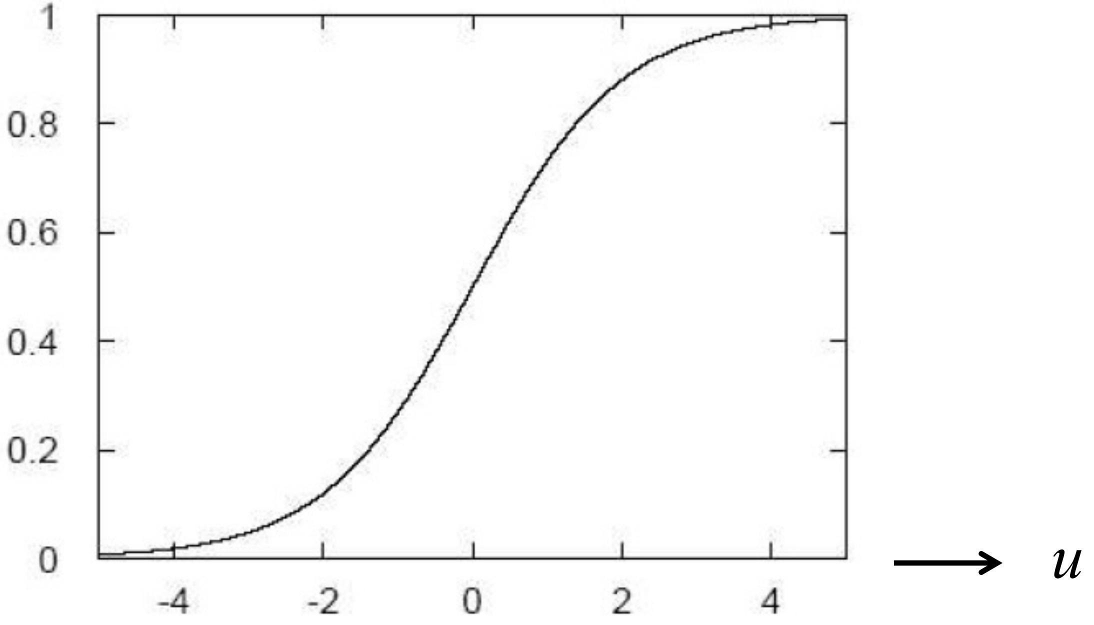
Neural Networks

A simple nonlinear decision function can be constructed as

$$t(\mathbf{x}) = h\left(w_0 + \sum_{i=1}^{n} w_i x_i\right)$$

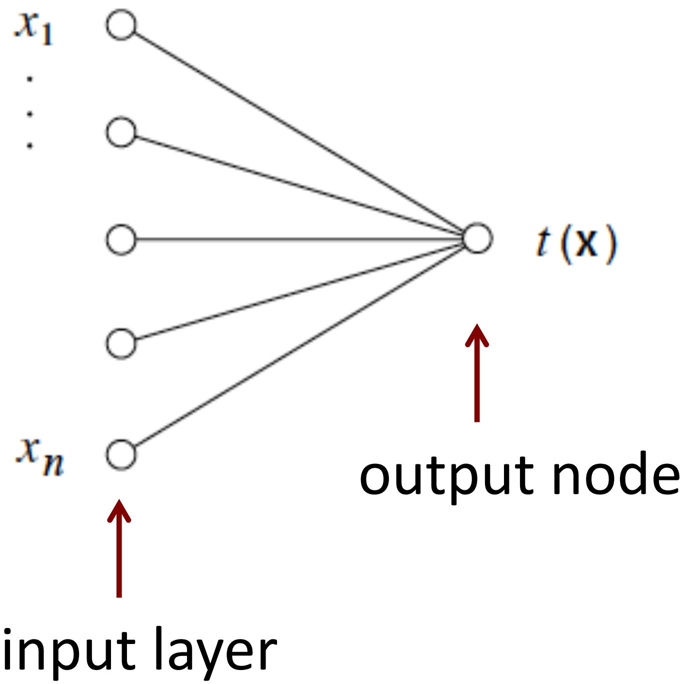
where h is called the “activation function”. For this one can use, e.g., a logistic sigmoid function,

$$h(u) = \frac{1}{1+e^{-u}}$$



Single Layer Perceptron

In this form, the decision function is called a Single Layer Perceptron – the simplest example of a Neural Network.



output node

input layer

But the surface described by $t(\boldsymbol{x}) = t_c$ is the same as by

$$h^{-1}(t(\mathbf{x})) = w_0 + \sum_{i=1}^{n} w_i x_i = h^{-1}(t_c)$$

So here we still have a linear decision boundary.

Multilayer Perceptron

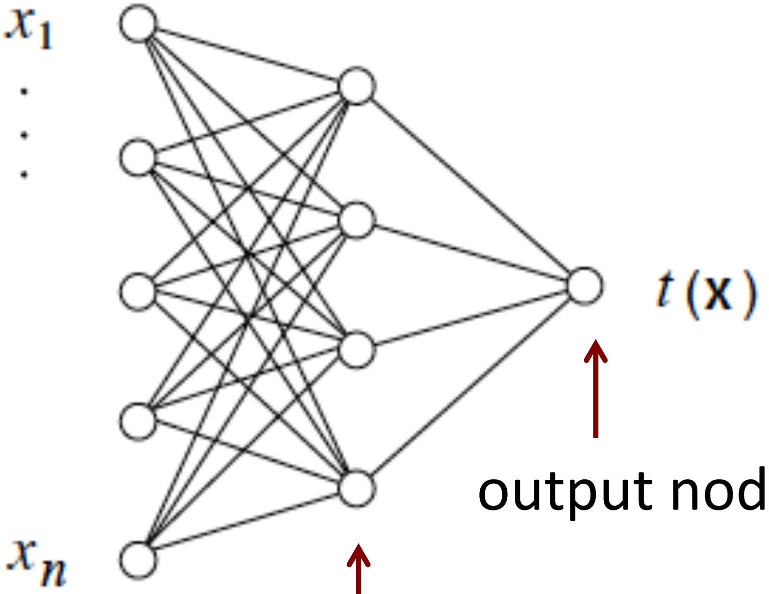
The Single Layer Perceptron can be generalized by defining first a set of functions $\varphi_i(\boldsymbol{x})$, with $i = 1,\ldots, m$:

$$\varphi_i(\mathbf{x}) = h\left(w_{i0}^{(1)} + \sum_{j=1}^{n} w_{ij}^{(1)} x_j\right) \qquad i = 1, \ldots, m$$

The $\varphi_i(\boldsymbol{x})$ are then treated as if they were the input variables, in a perceptron, i.e., the decision function (output node) is

$$t(\mathbf{x}) = h\left(w_{10}^{(2)} + \sum_{j=1}^{n} w_{1j}^{(2)} \varphi_j(\mathbf{x})\right)$$

Multilayer Perceptron (2)



output node

hidden layer with m nodes
$\varphi_1(\boldsymbol{x}),\ldots,\varphi_m(\boldsymbol{x})$

input
layer

Each line in the graph represents one of the weights $w_{ij}^{(k)}$, which must be adjusted using the training data.

Training a Neural Network

To train the network (i.e., determine the best values for the weights), define a loss function, e.g.,

$$E(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N} |t(\mathbf{x}_i) - y_i|^2$$

where $\boldsymbol{w}$ represents the set of all weights, the sum is over the set of training events, and y_i is the (numeric) true class label of each event (0 or 1).

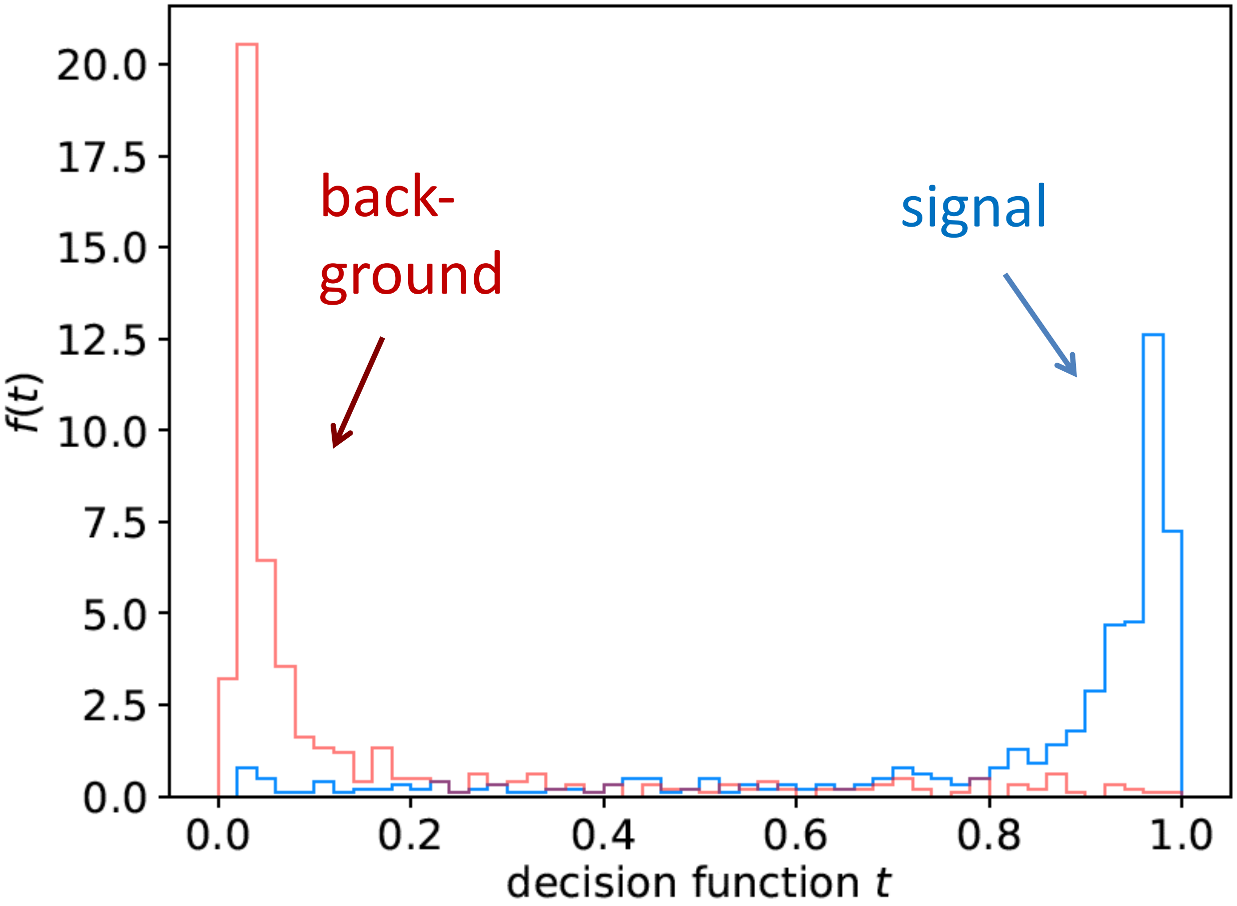
The optimal values of the weights are found by minimizing $E(\boldsymbol{w})$ with respect to the weights (non-trivial algorithms: backpropagation, stochastic gradient descent,...).

The desired result for an event with feature vector $\boldsymbol{x}$ is:

if the event is of type 0, want $t(\boldsymbol{x}) \sim 0$,
if the event is of type 1, want $t(\boldsymbol{x}) \sim 1$.

Distribution of neural net output

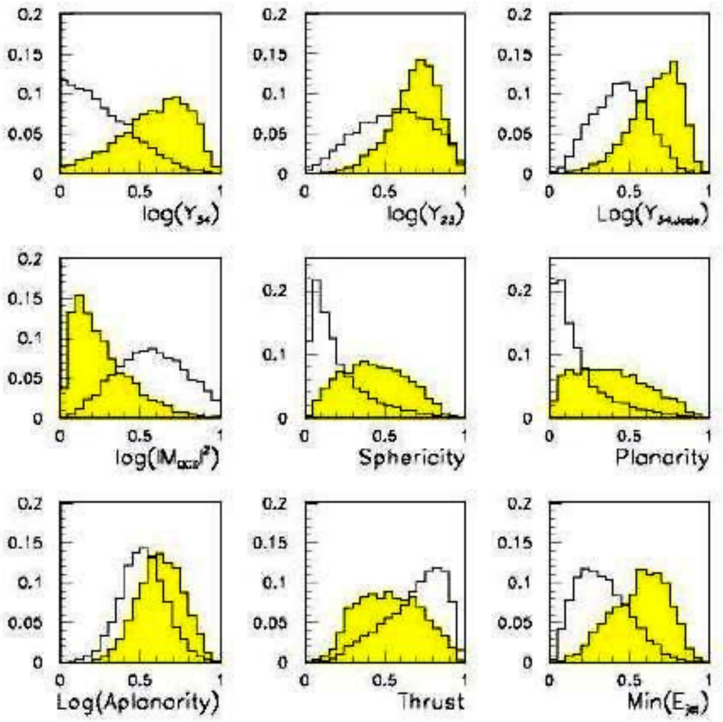
Degree of separation between classes now much better than with linear decision function:



Neural network example from LEP II

Signal: $e^+e^- \rightarrow W^+W^-$ (often 4 well separated hadron jets)

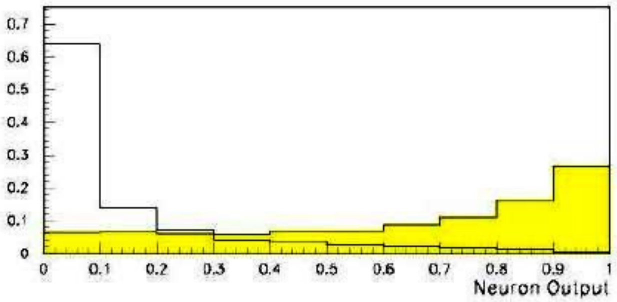
Background: $e^+e^- \rightarrow qqgg$ (4 less well separated hadron jets)



← input variables based on jet structure, event shape, ...

none by itself gives much separation.

Neural network output:



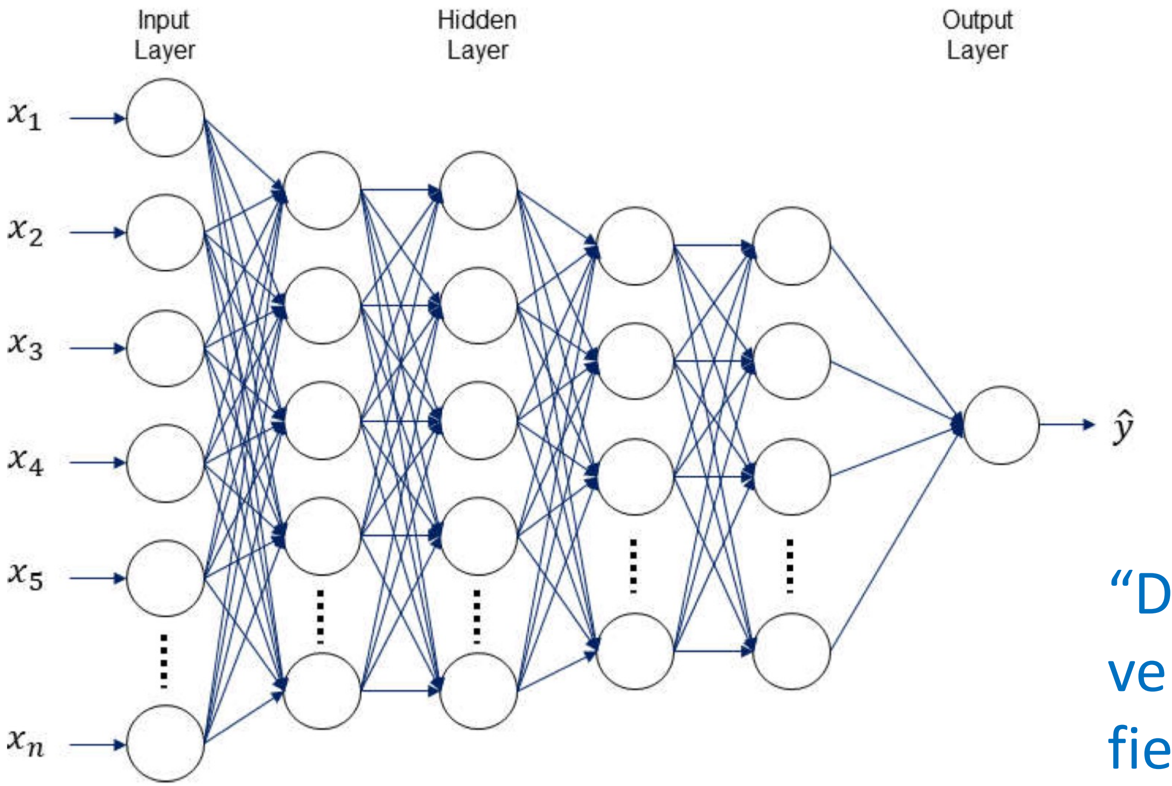
(Garrido, Juste and Martinez, ALEPH 96-144)

H.I. Kim and K.Y. Han, *Water* **2020**, *12*(3), 899

Deep Neural Networks

The multilayer perceptron can be generalized to have an arbitrary number of hidden layers, with an arbitrary number of nodes in each (= “network architecture”).

A “deep” network has several (or many) hidden layers:



“Deep Learning” is a very recent and active field of research.

Comments on network training

The algorithms for adjusting the network parameters have become a very active field of research (and beyond the scope of this course).

Recent ideas include:

“Deep” neural nets, use of ReLU activation function

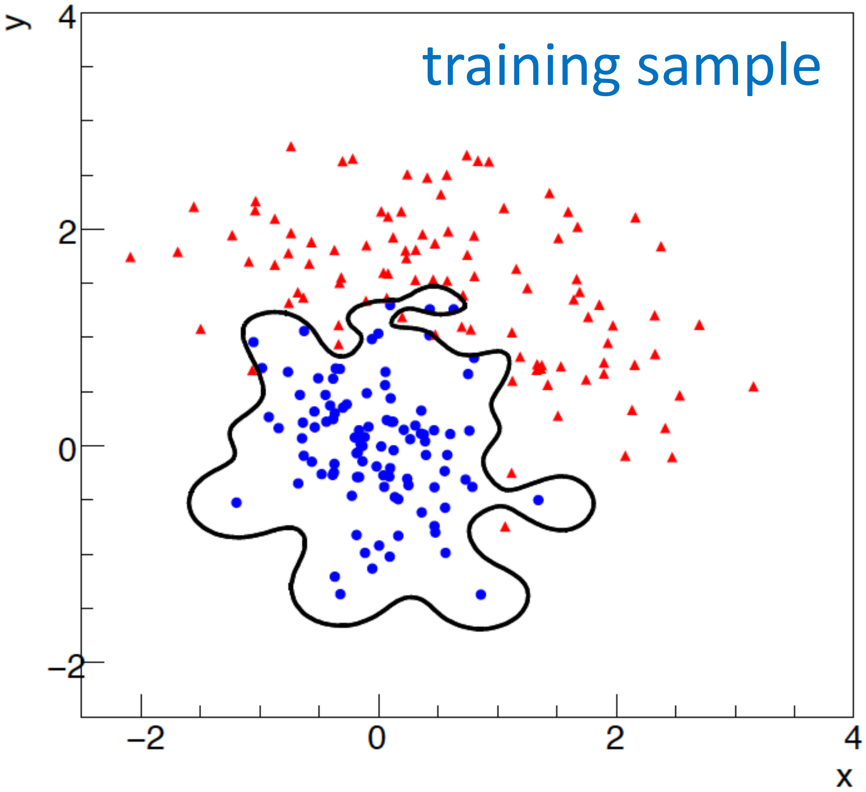
Stochastic gradient descent: estimate of gradient approximated by a randomly selected subset of the data.

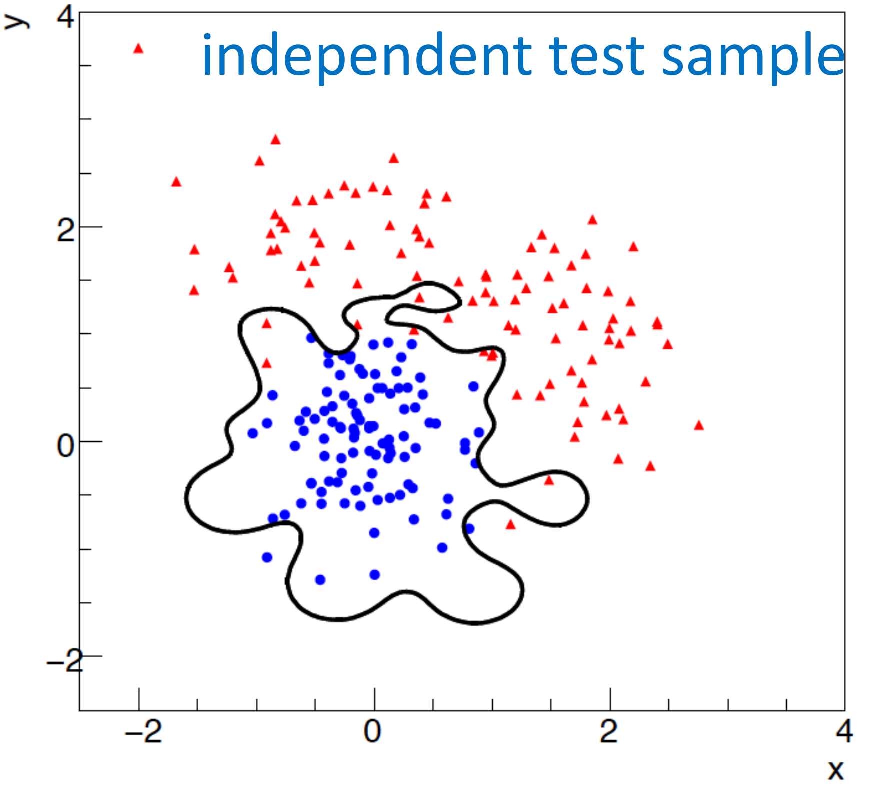
Dropout: randomly exclude nodes during training (prevents “overtraining”)

Overtraining

Including more parameters in a classifier makes its decision boundary increasingly flexible, e.g., more nodes/layers for a neural network.

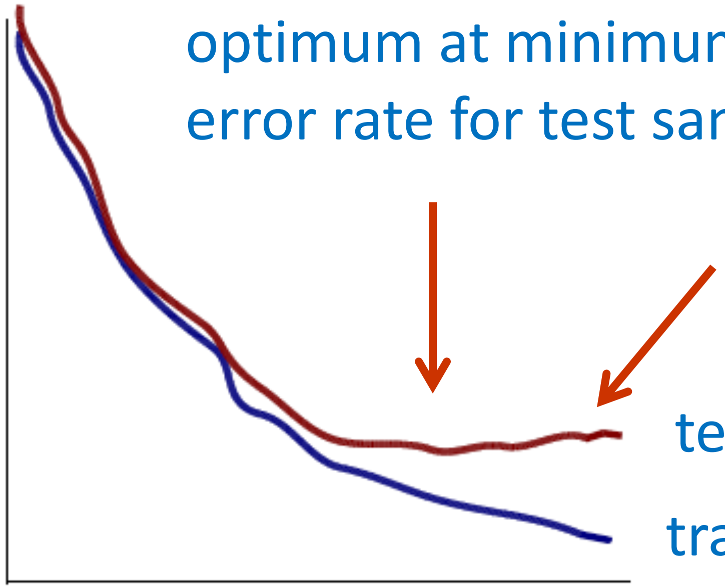
A “flexible” classifier may conform too closely to the training points; the same boundary will not perform well on an independent test data sample (→ “overtraining”).





Monitoring overtraining

If we monitor the fraction of misclassified events (or similar, e.g., error function $E(\mathbf{w})$) for test and training samples, it will usually decrease for both as the boundary is made more flexible:



error rate

optimum at minimum of error rate for test sample

increase in error rate indicates overtraining

test sample

training sample

flexibility (e.g., number of nodes/layers in MLP)

Other types of classifiers

We have seen only two types of classifiers:

Linear (Fisher discriminant)

Neural Network

There are many others:

Support Vector Machine

Boosted Decision Tree

K-Nearest Neighbour

...

The field is rapidly developing with advances, e.g., that allow one to use feature vectors of very high dimension, such as the pixels of an image.

$\rightarrow$ face/handwriting recognition, driverless cars...

Extra slides

Some distributions

Distribution/pdf	Example use in Particle Physics
Binomial	Branching ratio
Multinomial	Histogram with fixed N
Poisson	Number of events found
Uniform	Monte Carlo method
Exponential	Decay time
Gaussian	Measurement error
Chi-square	Goodness-of-fit
Cauchy	Mass of resonance
Landau	Ionization energy loss
Beta	Prior pdf for efficiency
Gamma	Sum of exponential variables
Student's t	Resolution function with adjustable tails

Binomial distribution

Consider N independent experiments (Bernoulli trials):

outcome of each is ‘success’ or ‘failure’,

probability of success on any given trial is p.

Define discrete r.v. n = number of successes ($0 \leq n \leq N$).

Probability of a specific outcome (in order), e.g. ‘ssfsf’ is

$$pp(1-p)p(1-p) = p^n(1-p)^{N-n}$$

But order not important; there are $\dfrac{N!}{n!(N-n)!}$

ways (permutations) to get n successes in N trials, total probability for n is sum of probabilities for each permutation.

Binomial distribution (2)

The binomial distribution is therefore

$$f(n; N, p) = \frac{N!}{n!(N-n)!} p^n (1-p)^{N-n}$$

random variable

parameters

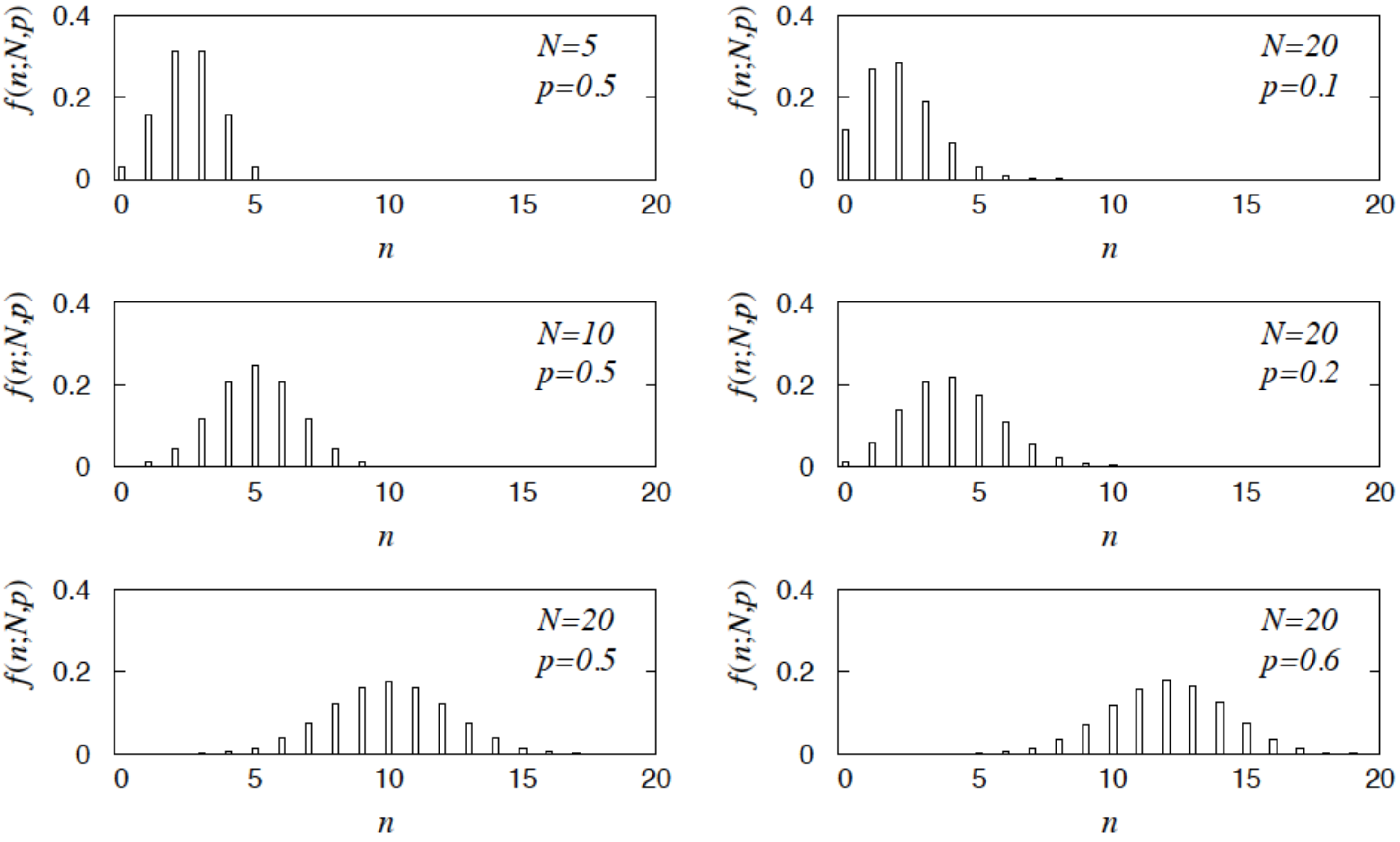
For the expectation value and variance we find:

$$E[n] = \sum_{n=0}^{N} n f(n; N, p) = Np$$

$$V[n] = E[n^2] - (E[n])^2 = Np(1-p)$$

Binomial distribution (3)

Binomial distribution for several values of the parameters:



Example: observe N decays of $\mathrm{W}^{\pm}$, the number n of which are $\mathrm{W}\rightarrow\mu\nu$ is a binomial r.v., p = branching ratio.

Multinomial distribution

Like binomial but now m outcomes instead of two, probabilities are

$$\vec{p} = (p_1, \ldots, p_m)\,, \quad \text{with} \sum_{i=1}^{m} p_i = 1\,.$$

For N trials we want the probability to obtain:

n_1 of outcome 1,
n_2 of outcome 2,
$\vdots$
n_m of outcome m.

This is the multinomial distribution for $\vec{n} = (n_1, \ldots, n_m)$

$$f(\vec{n}; N, \vec{p}) = \frac{N!}{n_1! n_2! \cdots n_m!} p_1^{n_1} p_2^{n_2} \cdots p_m^{n_m}$$

Multinomial distribution (2)

Now consider outcome i as ‘success’, all others as ‘failure’.

→ all n_i individually binomial with parameters N, p_i

$$E[n_i] = Np_i, \qquad V[n_i] = Np_i(1 - p_i) \qquad \text{for all } i$$

One can also find the covariance to be

$$V_{ij} = Np_i(\delta_{ij} - p_j)$$

Example: $\vec{n} = (n_1, \ldots, n_m)$ represents a histogram

with m bins, N total entries, all entries independent.

Poisson distribution

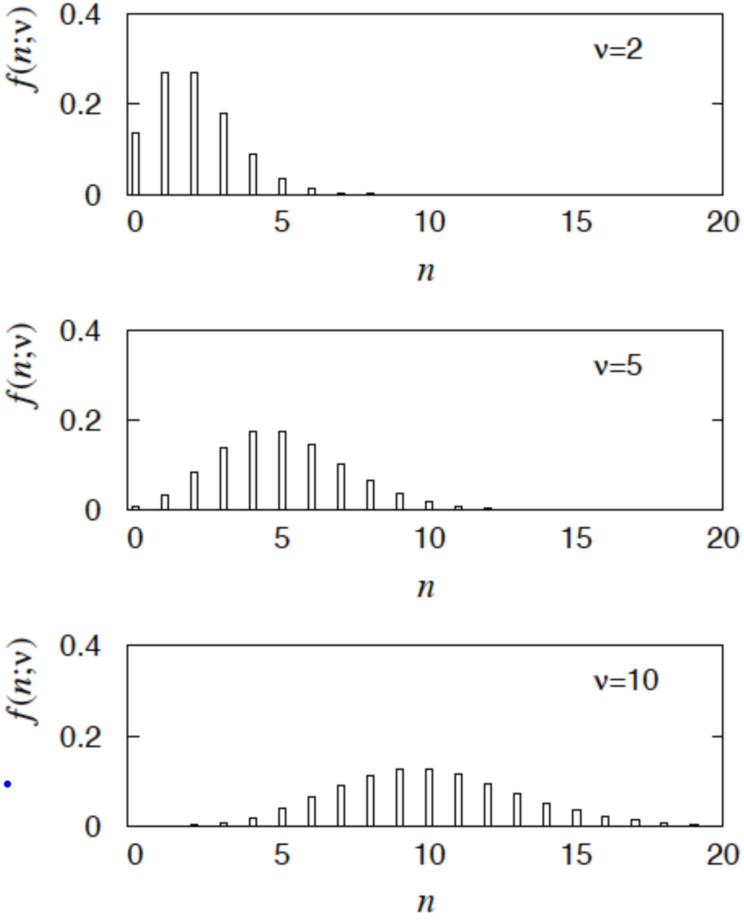
Consider binomial n in the limit

$$N \to \infty, \qquad p \to 0, \qquad E[n] = Np \to \nu \; .$$

→ n follows the Poisson distribution:

$$f(n;\nu) = \frac{\nu^n}{n!} e^{-\nu} \qquad (n \geq 0)$$

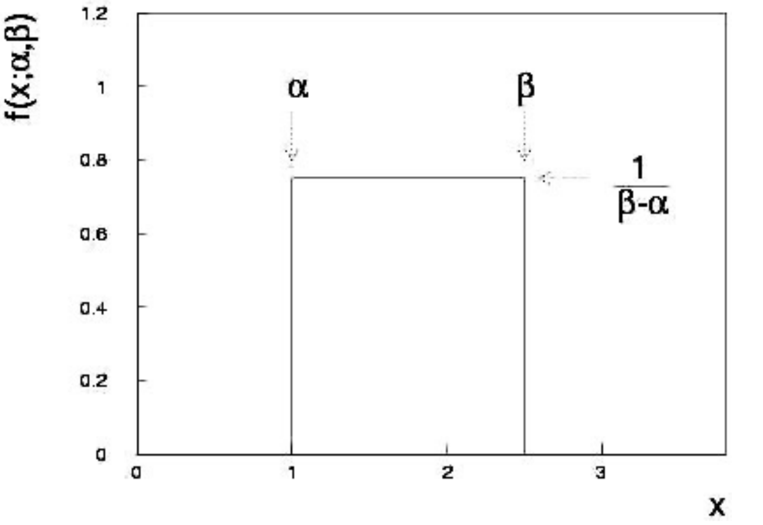
$$E[n] = \nu \, , \qquad V[n] = \nu \; .$$



Example: number of scattering events n with cross section σ found for a fixed integrated luminosity, with $\nu = \sigma \int L \, dt$.

Uniform distribution

$$f(x;\alpha,\beta) = \begin{cases} \frac{1}{\beta-\alpha} & \alpha \le x \le \beta \\ 0 & \text{otherwise} \end{cases}$$



$$E[x] = \frac{1}{2}(\alpha+\beta)$$

$$V[x] = \frac{1}{12}(\beta-\alpha)^2$$

Notation: x follows a uniform distribution between α and β

write as: $x \sim \mathrm{U}[\alpha,\beta]$

Uniform distribution (2)

Very often used with $\alpha = 0$, $\beta = 1$ (e.g., Monte Carlo method).

For any r.v. x with pdf $f(x)$, cumulative distribution $F(x)$, the function $y = F(x)$ is uniform in $[0,1]$:

$$g(y) = f(x)\left|\frac{dx}{dy}\right| = \frac{f(x)}{|dy/dx|}$$

$$= \frac{f(x)}{|dF/dx|} = \frac{f(x)}{f(x)} = 1\,, \quad 0 \leq y \leq 1$$

because $f(x) = dF/dx = dy/dx$

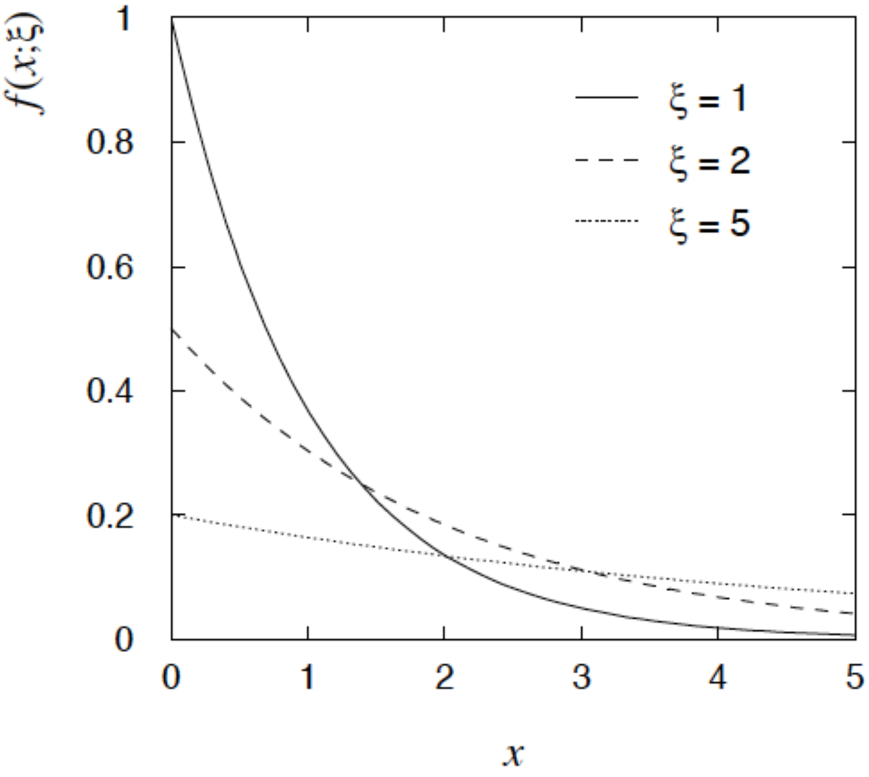
Exponential distribution

The exponential pdf for the continuous r.v. x is defined by:

$$f(x;\xi) = \begin{cases} \frac{1}{\xi} e^{-x/\xi} & x \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

$$E[x] = \xi$$

$$V[x] = \xi^2$$



Exponential distribution (2)

Example: proper decay time t of an unstable particle

$$f(t;\tau) = \frac{1}{\tau} e^{-t/\tau} \qquad (\tau = \text{mean lifetime})$$

Lack of memory (unique to exponential): $f(t - t_0 | t \geq t_0) = f(t)$

Question for discussion:

A cosmic ray muon is created 30 km high in the atmosphere, travels to sea level and is stopped in a block of scintillator, giving a start signal at t_0. At a time t it decays to an electron giving a stop signal. What is distribution of the difference between stop and start times, i.e., the pdf of $t - t_0$ given $t > t_0$?

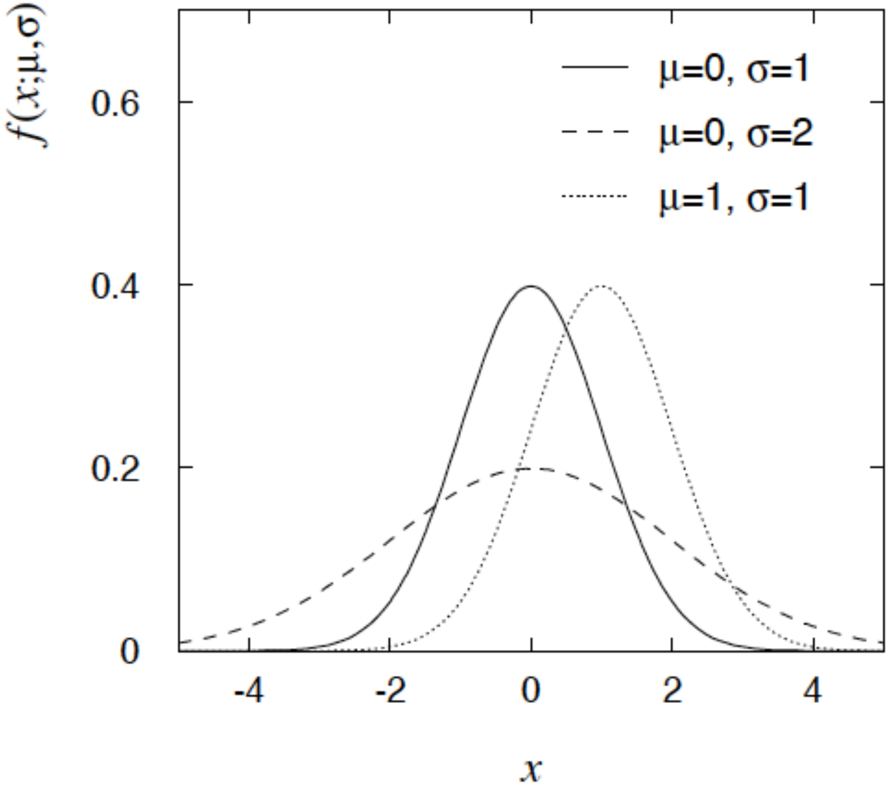
Gaussian (normal) distribution

The Gaussian (normal) pdf for a continuous r.v. x is defined by:

$$f(x;\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-(x-\mu)^2/2\sigma^2}$$

$$E[x] = \mu$$

$$V[x] = \sigma^2$$



N.B. often μ, σ^2 denote mean, variance of any r.v., not only Gaussian.

Standardized random variables

If a random variable y has pdf $f(y)$ with mean μ and std. dev. σ, then the *standardized* variable

$$x = \frac{y-\mu}{\sigma}$$ has the pdf $$g(x) = f(y(x)) \left| \frac{dy}{dx} \right| = \sigma f(\mu + \sigma x)$$

has mean of zero and standard deviation of 1.

Often work with the *standard* Gaussian distribution (μ = 0. σ = 1) using notation:

$$\varphi(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \, , \qquad \Phi(x) = \int_{-\infty}^{x} \varphi(x') \, dx'$$

Then e.g. $y = \mu + \sigma x$ follows

$$f(y) = \frac{1}{\sigma} \varphi\left(\frac{y-\mu}{\sigma}\right) = \frac{1}{\sqrt{2\pi}\sigma} e^{-(y-\mu)^2/2\sigma^2}$$

Multivariate Gaussian distribution

Multivariate Gaussian pdf for the vector $\vec{x} = (x_1, \ldots, x_n)$:

$$f(\vec{x}; \vec{\mu}, V) = \frac{1}{(2\pi)^{n/2}|V|^{1/2}} \exp\left[-\frac{1}{2}(\vec{x}-\vec{\mu})^T V^{-1}(\vec{x}-\vec{\mu})\right]$$

$\vec{x}$, $\vec{\mu}$ are column vectors, $\vec{x}^T$, $\vec{\mu}^T$ are transpose (row) vectors,

$$E[x_i] = \mu_i, \ , \qquad \mathrm{cov}[x_i, x_j] = V_{ij} \ .$$

Marginal pdf of each x_i is Gaussian with mean μ_i, standard deviation $\sigma_i = \sqrt{V_{ii}}$.

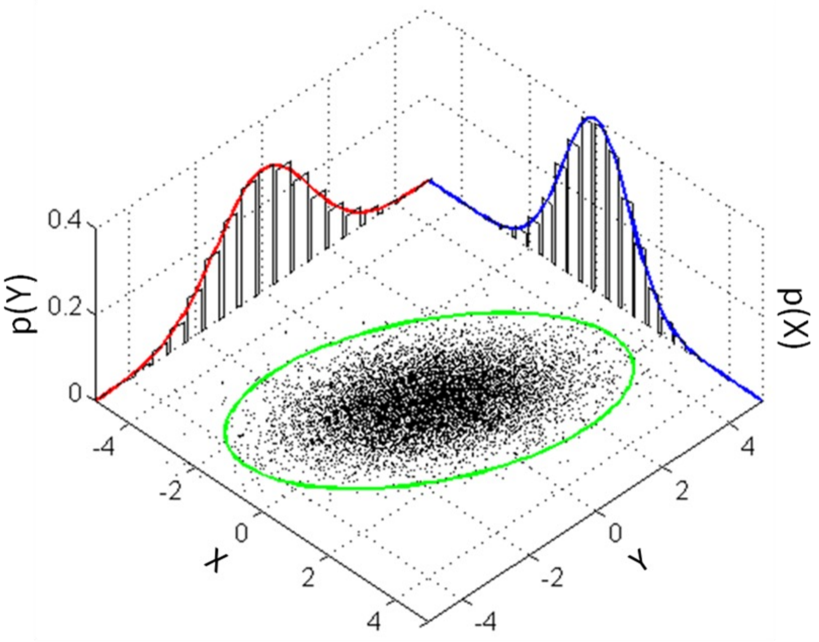
https://en.wikipedia.org/wiki/Multivariate_normal_distribution

Two-dimensional Gaussian distribution

$$f(x_1, x_2, ; \mu_1, \mu_2, \sigma_1, \sigma_2, \rho) = \frac{1}{2\pi\sigma_1\sigma_2\sqrt{1-\rho^2}}$$

$$\times \exp\left\{ -\frac{1}{2(1-\rho^2)} \left[\left(\frac{x_1-\mu_1}{\sigma_1}\right)^2 + \left(\frac{x_2-\mu_2}{\sigma_2}\right)^2 - 2\rho\left(\frac{x_1-\mu_1}{\sigma_1}\right)\left(\frac{x_2-\mu_2}{\sigma_2}\right)\right]\right\}$$

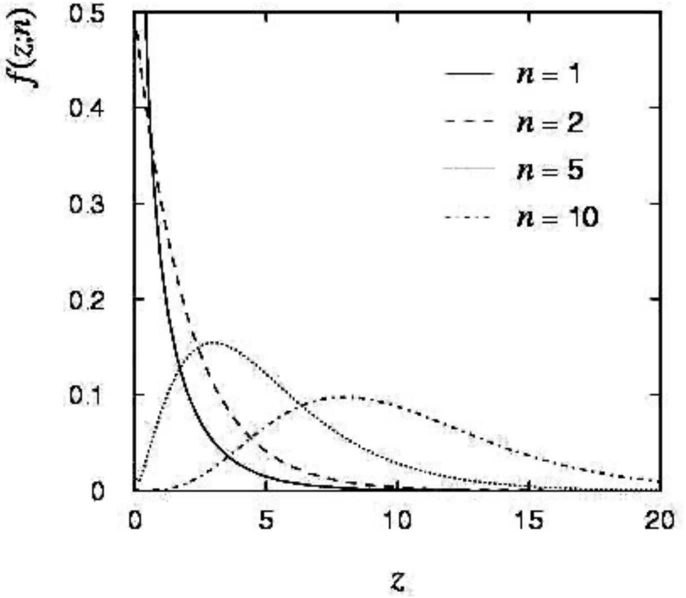
where $\rho = \mathrm{cov}[x_1, x_2]/(\sigma_1\sigma_2)$
is the correlation coefficient.



Chi-square (χ^2) distribution

The chi-square pdf for the continuous r.v. z ($z \geq 0$) is defined by

$$f(z;n) = \frac{1}{2^{n/2}\Gamma(n/2)} z^{n/2-1} e^{-z/2}$$



n = 1, 2, ... = number of 'degrees of freedom' (dof)

$$E[z] = n\,, \quad V[z] = 2n\,.$$

For independent Gaussian x_i, i = 1, ..., n, means μ_i, variances σ_i^2,

$$z = \sum_{i=1}^{n} \frac{(x_i - \mu_i)^2}{\sigma_i^2}$$

follows χ^2 pdf with n dof.

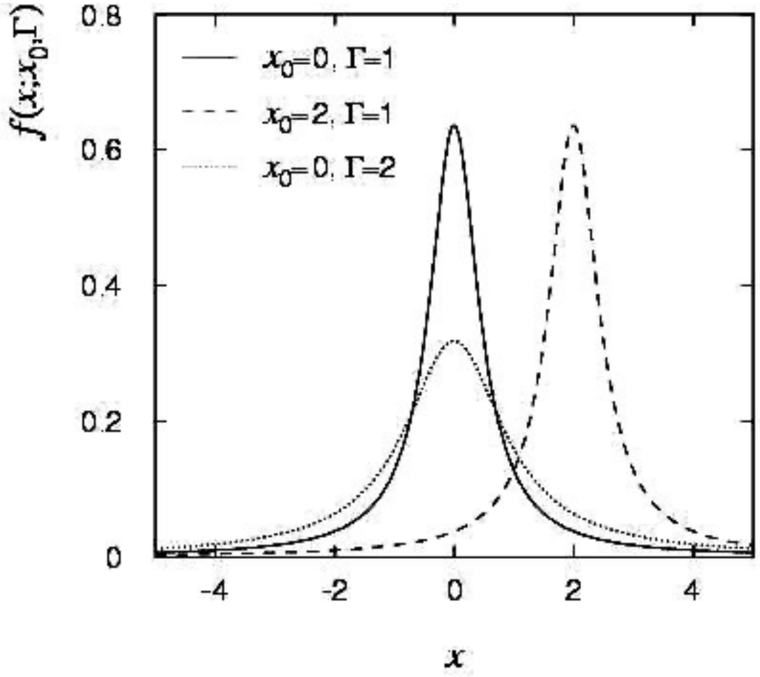
Example: goodness-of-fit test variable especially in conjunction with method of least squares.

Cauchy (Breit-Wigner) distribution

The Breit-Wigner pdf for the continuous r.v. x is defined by

$$f(x;\Gamma,x_0) = \frac{1}{\pi}\frac{\Gamma/2}{\Gamma^2/4+(x-x_0)^2}$$

($\Gamma = 2$, $x_0 = 0$ is the Cauchy pdf.)



$E[x]$ not well defined, $V[x] \to \infty$.

x_0 = mode (most probable value)

Γ = full width at half maximum

Example: mass of resonance particle, e.g. ρ, K^*, φ^0, ...

Γ = decay rate (inverse of mean lifetime)

Landau distribution

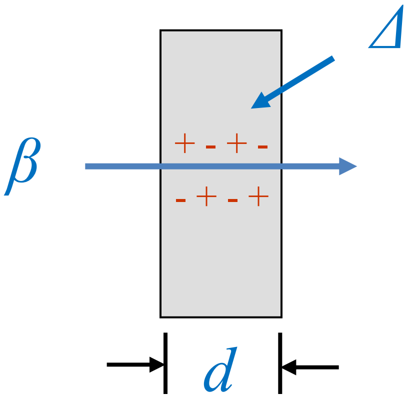
For a charged particle with $\beta = v/c$ traversing a layer of matter of thickness d, the energy loss Δ follows the Landau pdf:

$$f(\Delta;\beta) = \frac{1}{\xi}\phi(\lambda) \;,$$

$$\phi(\lambda) = \frac{1}{\pi}\int_0^\infty \exp(-u\ln u - \lambda u)\sin \pi u \, du \;,$$

$$\lambda = \frac{1}{\xi}\left[\Delta - \xi\left(\ln\frac{\xi}{\epsilon'} + 1 - \gamma_{\mathrm{E}}\right)\right] \;,$$

$$\xi = \frac{2\pi N_{\mathrm{A}} e^4 z^2 \rho \sum Z}{m_{\mathrm{e}}c^2 \sum A}\frac{d}{\beta^2} \;, \qquad \epsilon' = \frac{I^2 \exp\beta^2}{2m_{\mathrm{e}}c^2\beta^2\gamma^2} \;.$$



L. Landau, J. Phys. USSR **8** (1944) 201; see also
W. Allison and J. Cobb, Ann. Rev. Nucl. Part. Sci. **30** (1980) 253.

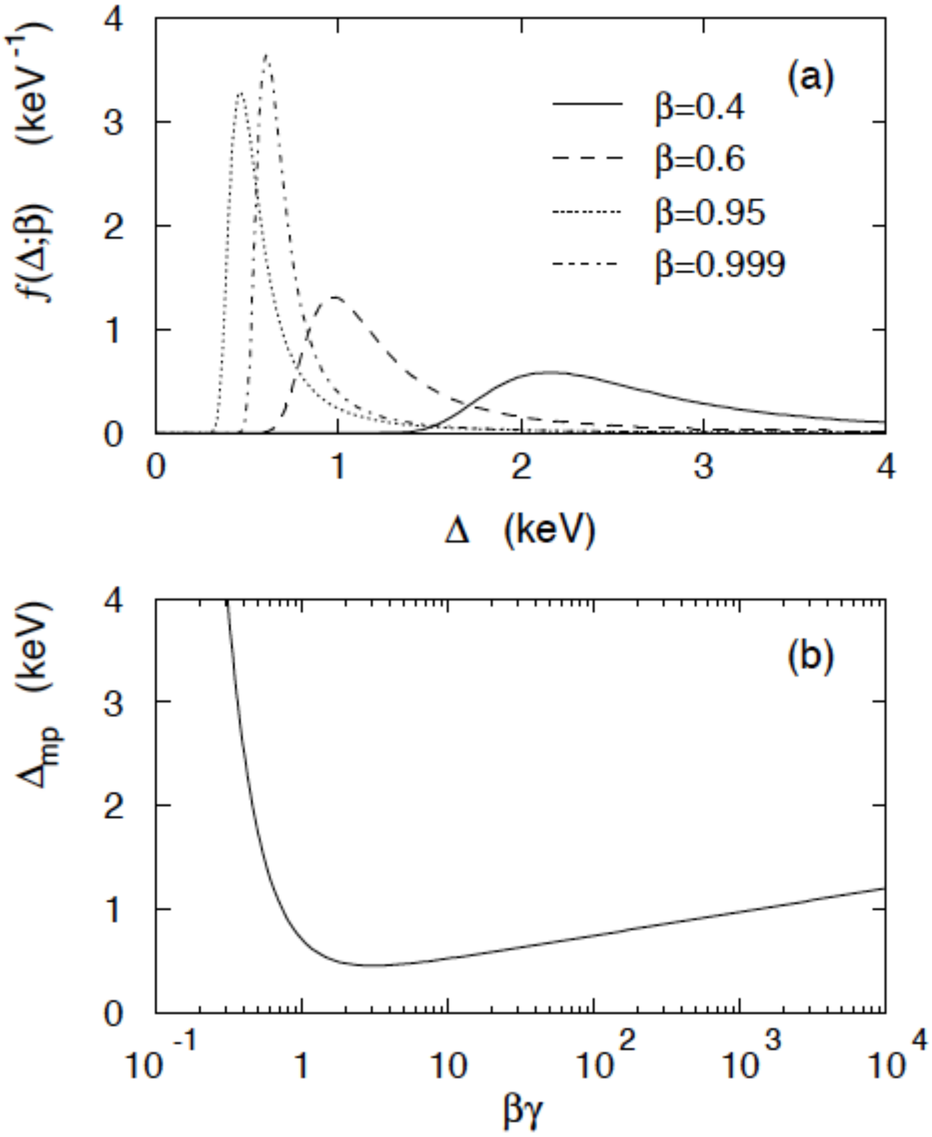
Landau distribution (2)

Long 'Landau tail'

→ all moments ∞

Mode (most probable value) sensitive to β ,

→ particle i.d.

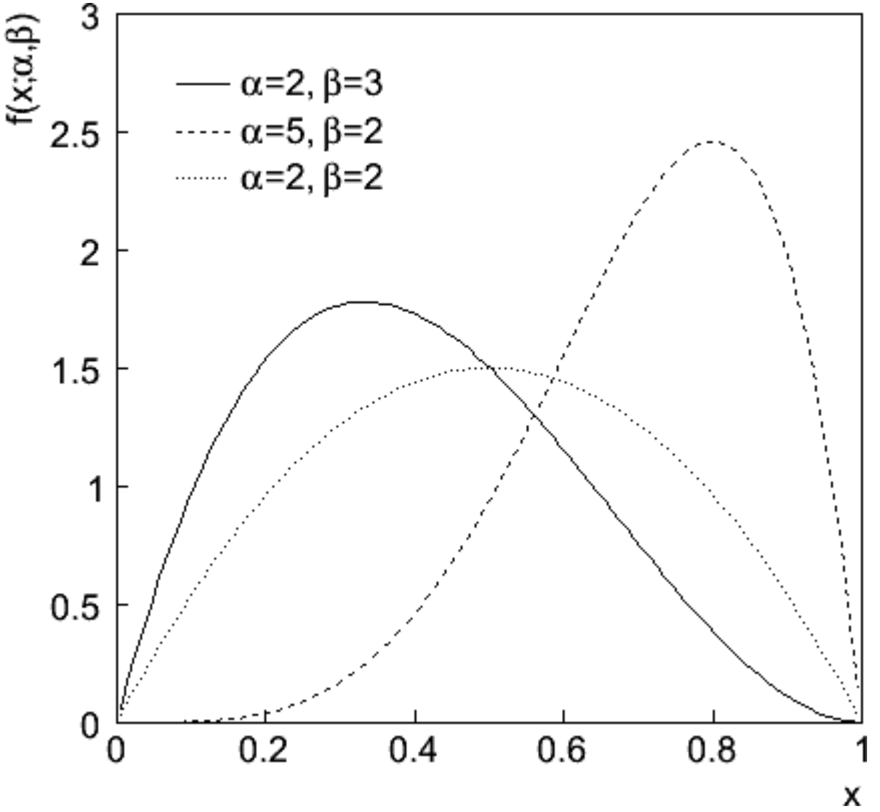


Beta distribution

$$f(x;\alpha,\beta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}\,x^{\alpha-1}(1-x)^{\beta-1}$$

$$E[x] = \frac{\alpha}{\alpha+\beta}$$

$$V[x] = \frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}$$



Often used to represent pdf of continuous r.v. nonzero only between finite limits, e.g.,

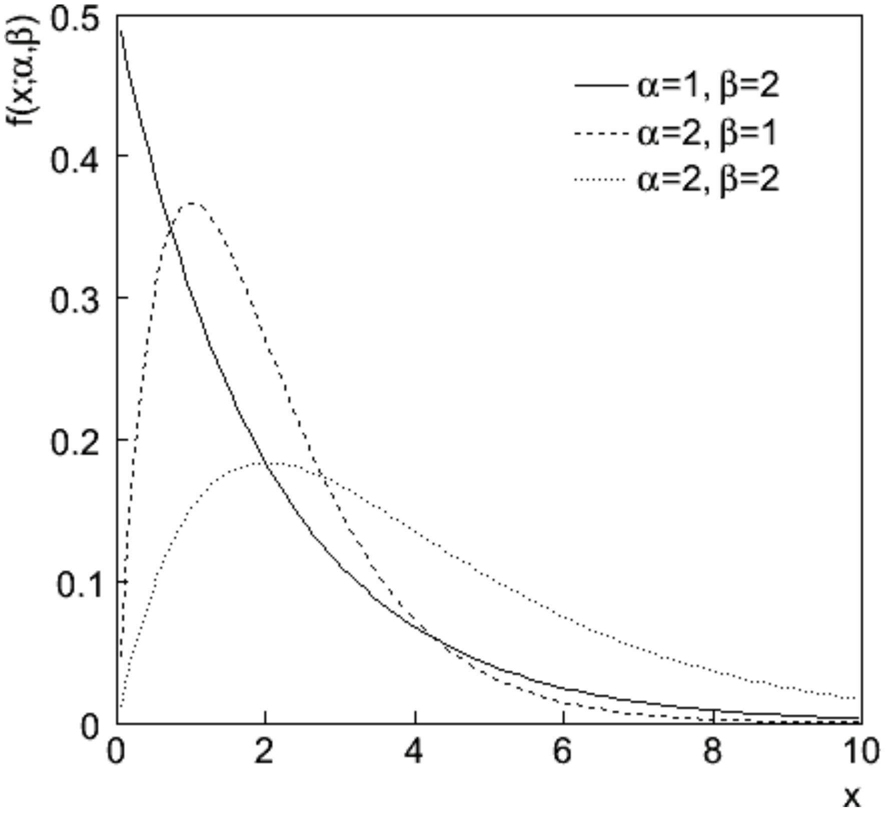
$y = a_0 + a_1 x, \quad a_0 \leq y \leq a_0 + a_1$

Gamma distribution

$$f(x;\alpha,\beta) = \frac{1}{\Gamma(\alpha)\beta^\alpha}\, x^{\alpha-1}\, e^{-x/\beta}$$

$$E[x] = \alpha\beta$$

$$V[x] = \alpha\beta^2$$



Often used to represent pdf of continuous r.v. nonzero only in $[0,\infty]$.

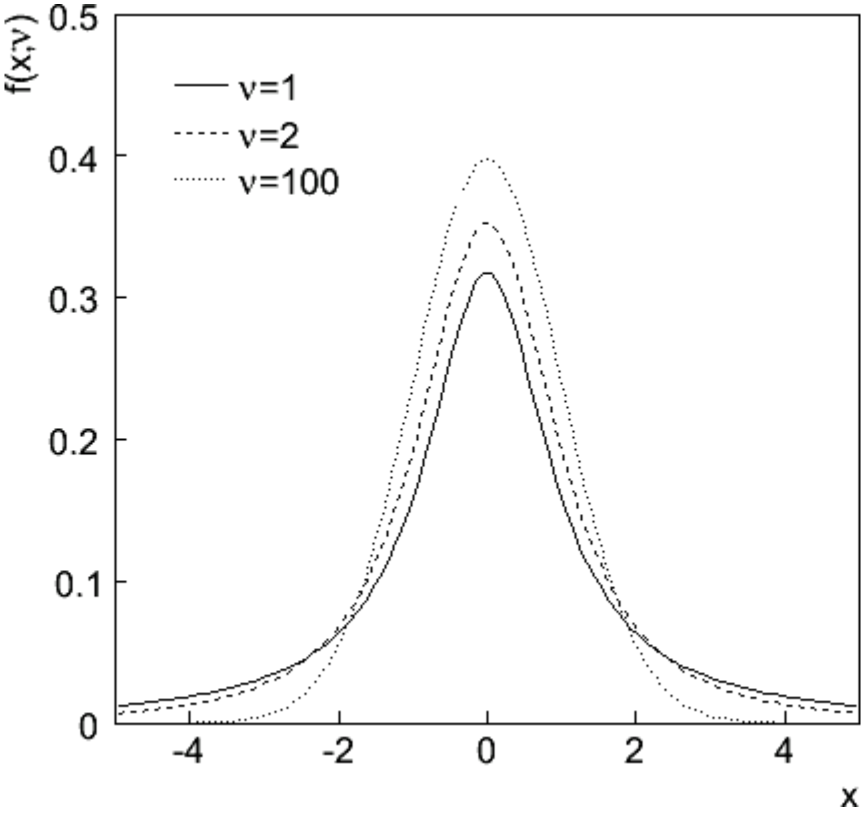
Also e.g. sum of n exponential r.v.s or time until nth event in Poisson process ~ Gamma

Student's t distribution

$$f(x;\nu) = \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\sqrt{\nu\pi}\,\Gamma(\nu/2)}\left(1+\frac{x^2}{\nu}\right)^{-\left(\frac{\nu+1}{2}\right)}$$

$$E[x] = 0 \quad (\nu > 1)$$

$$V[x] = \frac{\nu}{\nu-2} \quad (\nu > 2)$$



ν = number of degrees of freedom (not necessarily integer)

$\nu = 1$ gives Cauchy,

$\nu \rightarrow \infty$ gives Gaussian.

Student's *t* distribution (2)

If $x \sim$ Gaussian with $\mu = 0$, $\sigma^2 = 1$, and

$z \sim \chi^2$ with n degrees of freedom, then

$t = x \,/\, (z/n)^{1/2}$ follows Student's t with $\nu = n$.

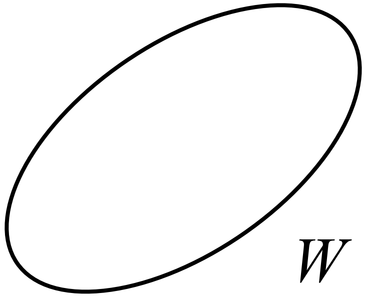
This arises in problems where one forms the ratio of a sample mean to the sample standard deviation of Gaussian r.v.s.

The Student's t provides a bell-shaped pdf with adjustable tails, ranging from those of a Gaussian, which fall off very quickly, ($\nu \rightarrow \infty$, but in fact already very Gauss-like for $\nu =$ two dozen), to the very long-tailed Cauchy ($\nu = 1$).

Developed in 1908 by William Gosset, who worked under the pseudonym "Student" for the Guinness Brewery.

Proof of Neyman-Pearson Lemma

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

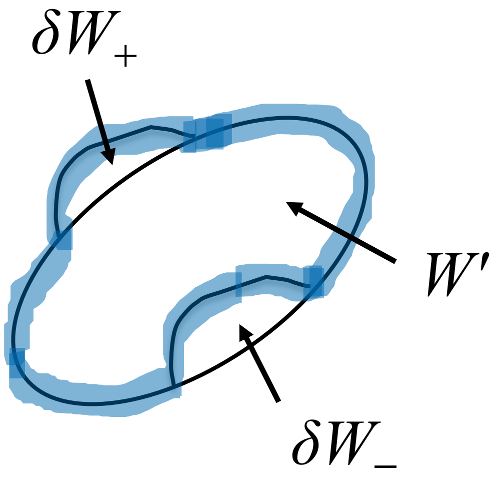


$P(\boldsymbol{x}|H_1)/P(\boldsymbol{x}|H_0) \geq c_\alpha$ for all $\boldsymbol{x}$ in W,

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

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

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

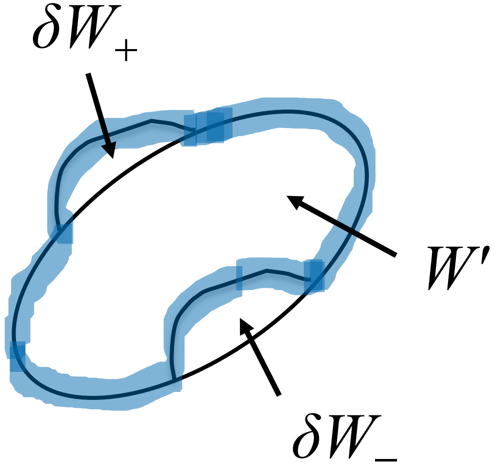


To do so add a part δW_+, but to keep the size α, we need to remove a part δW_-, i.e.,

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

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

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

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

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

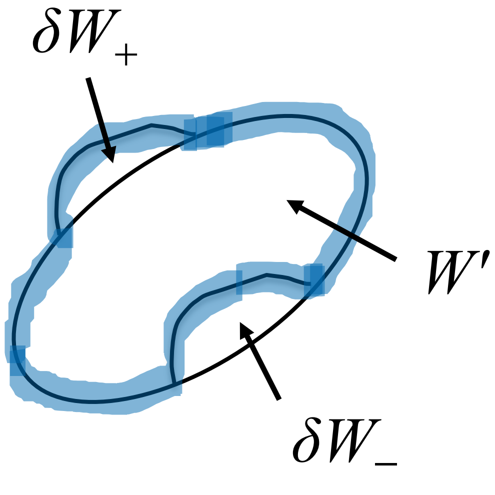
The right-hand sides are equal and therefore

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

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

$$P(\mathbf{x} \in W'|H_1) = P(\mathbf{x} \in W|H_1) + \underbrace{P(\mathbf{x} \in \delta W_+|H_1) - P(\mathbf{x} \in \delta W_-|H_1)}_{\leq 0}$$

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.