Statistical Methods for Physicists

Lecture 1: parameter estimation, statistical tests

`www.pp.rhul.ac.uk/~cowan/stat/granada20`

`(see also www.pp.rhul.ac.uk/~cowan/stat_course.html)`

University of Granada
4,5 May 2020

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Outline

→ Lecture 1: Introduction and review of fundamentals

- Probability, random variables, pdfs
- Parameter estimation, maximum likelihood
- Introduction to statistical tests

Lecture 2: More on statistical tests

- Multivariate methods
- Neural networks

Lecture 3: Framework for full analysis

- *p*-values, discovery, limits
- Tests from likelihood ratio

Lecture 4: Further topics

- Nuisance parameters and systematic uncertainties
- More parameter estimation, Bayesian methods
- Experimental sensitivity

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

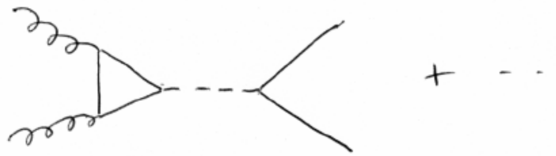
S. Brandt, *Statistical and Computational Methods in Data Analysis*, Springer, New York, 1998 (with program library on CD)

M. Tanabashi et al. (PDG), Phys. Rev. D 98, 030001 (2018); see also **`pdg.lbl.gov`** sections on probability, statistics, Monte Carlo

Theory ↔ Statistics ↔ Experiment

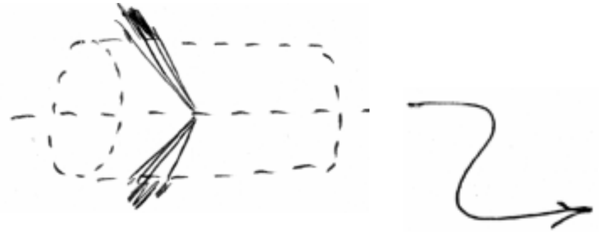
Theory (model, hypothesis):

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + i\bar{\psi}\not{D}\psi + \cdots$$

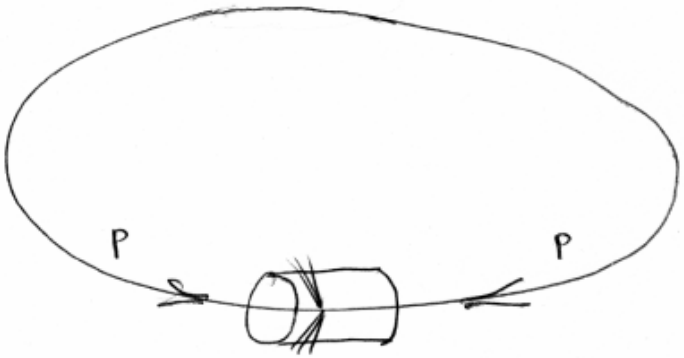


$$\sigma = \frac{G_F\,\alpha_s^2\,m_H^2}{288\sqrt{2\pi}} \times \sim$$

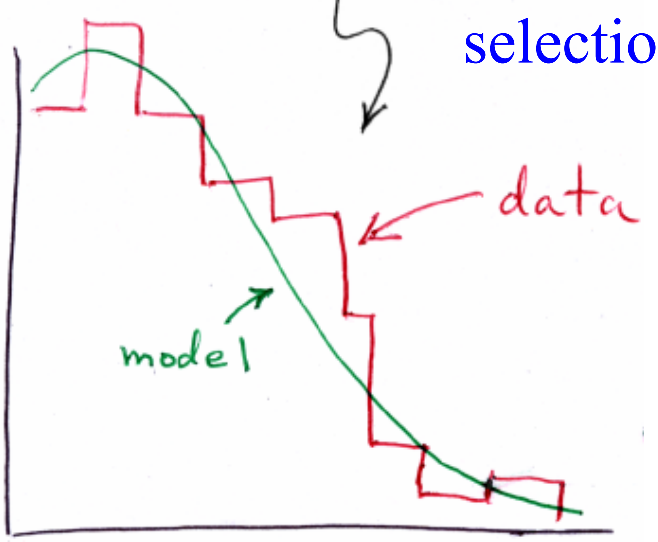
+ simulation of detector and cuts



Experiment:



+ data selection



Data analysis in particle physics

Observe events (e.g., pp collisions) and for each, measure a set of characteristics:

particle momenta, number of muons, energy of jets,...

Compare observed distributions of these characteristics to predictions of theory. From this, we want to:

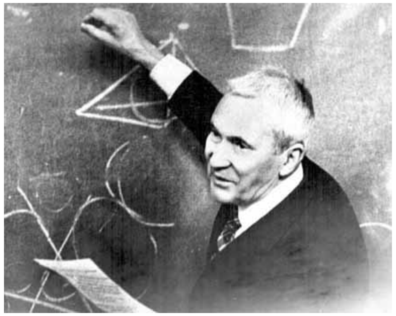
Estimate the free parameters of the theory: $m_H = 125.4$

Quantify the uncertainty in the estimates: ± 0.4 GeV

Assess how well a given theory stands in agreement with the observed data: 0^+ good, 2^+ bad

To do this we need a clear definition of PROBABILITY

A definition of probability



Consider a set *S* with subsets *A*, *B*, ...

$$\text{For all } A \subset S, P(A) \geq 0$$

$$P(S) = 1$$

$$\text{If } A \cap B = \emptyset, P(A \cup B) = P(A) + P(B)$$

Kolmogorov axioms (1933)

Also define conditional probability of *A* given *B*:

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

Subsets *A*, *B* independent if: $P(A \cap B) = P(A)P(B)$

If *A*, *B* independent, $P(A|B) = \frac{P(A)P(B)}{P(B)} = P(A)$

Interpretation of probability

I. Relative frequency

A, *B*, ... are outcomes of a repeatable experiment

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

cf. quantum mechanics, particle scattering, radioactive decay...

II. Subjective probability

A, *B*, ... are hypotheses (statements that are true or false)

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

- Both interpretations consistent with Kolmogorov axioms.
- In particle physics frequency interpretation often most useful, but subjective probability can provide more natural treatment of non-repeatable phenomena:

systematic uncertainties, probability that Higgs boson exists,...

Bayes' theorem

From the definition of conditional probability we have,

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

but $P(A \cap B) = P(B \cap A)$, so

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

Bayes' theorem

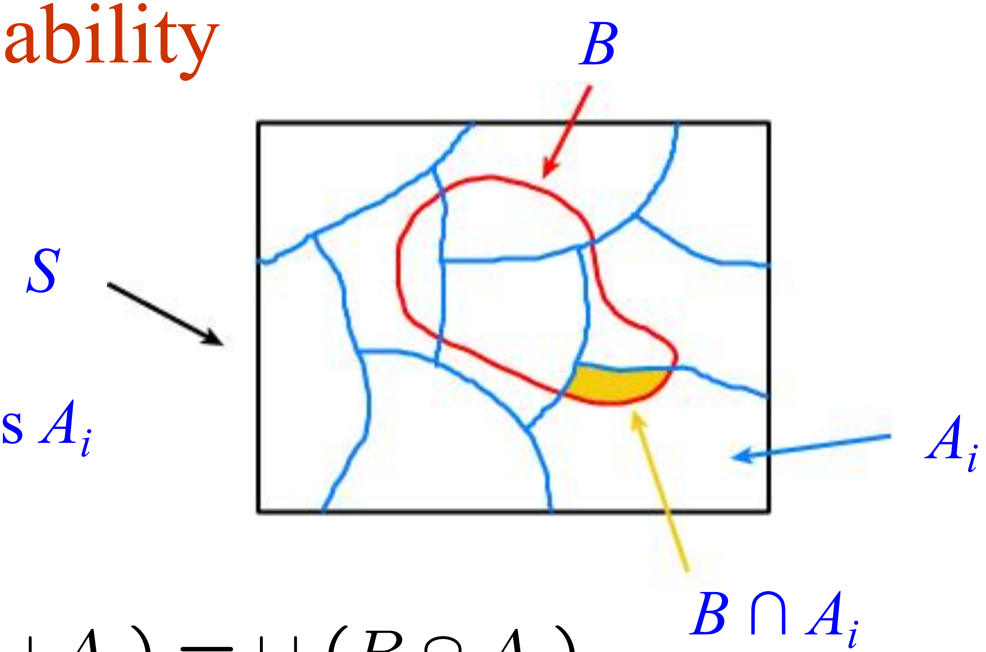
First published (posthumously) by the Reverend Thomas Bayes (1702−1761)

An essay towards solving a problem in the doctrine of chances, Philos. Trans. R. Soc. **53** (1763) 370; reprinted in Biometrika, **45** (1958) 293.

The law of total probability

Consider a subset B of the sample space S,

divided into disjoint subsets A_i such that $\cup_i A_i = S$,



$$\rightarrow \quad B = B \cap S = B \cap (\cup_i A_i) = \cup_i (B \cap A_i),$$

$$\rightarrow \quad P(B) = P(\cup_i (B \cap A_i)) = \textstyle\sum_i P(B \cap A_i)$$

$$\rightarrow \quad P(B) = \textstyle\sum_i P(B|A_i) P(A_i)$$ law of total probability

Bayes' theorem becomes

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

An example using Bayes' theorem

Suppose the probability (for anyone) to have a disease D is:

$$P(\mathrm{D}) = 0.001$$
$$P(\mathrm{no\ D}) = 0.999$$

← prior probabilities, i.e., before any test carried out

Consider a test for the disease: result is + or –

$$P(+|\mathrm{D}) = 0.98$$
$$P(-|\mathrm{D}) = 0.02$$

← probabilities to (in)correctly identify a person with the disease

$$P(+|\mathrm{no\ D}) = 0.03$$
$$P(-|\mathrm{no\ D}) = 0.97$$

← probabilities to (in)correctly identify a healthy person

Suppose your result is +. How worried should you be?

Bayes' theorem example (cont.)

The probability to have the disease given a + result is

$$p(\mathrm{D}|+) = \frac{P(+|\mathrm{D})P(\mathrm{D})}{P(+|\mathrm{D})P(\mathrm{D}) + P(+|\text{no D})P(\text{no D})}$$

$$= \frac{0.98 \times 0.001}{0.98 \times 0.001 + 0.03 \times 0.999}$$

$$= 0.032$$ ← posterior probability

i.e. you're probably OK!

Your viewpoint: my degree of belief that I have the disease is 3.2%.

Your doctor's viewpoint: 3.2% of people like this have the disease.

Frequentist Statistics − general philosophy

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

Probability = limiting frequency

Probabilities such as

P (Higgs boson exists),
$P\,(0.117 < \alpha_s < 0.121)$,

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.

A hypothesis is is preferred if the data are found in a region of high predicted probability (i.e., where an alternative hypothesis predicts lower probability).

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 value:

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

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 $\boldsymbol{\theta}$.

The likelihood function for i.i.d.*. data

* i.i.d. = independent and identically distributed

Consider n independent observations of x: $x_1, \ldots, x_n$, where x follows $f(x; \theta)$. The joint pdf for the whole data sample is:

$$f(x_1, \ldots, x_n; \theta) = \prod_{i=1}^{n} f(x_i; \theta)$$

In this case the likelihood function is

$$L(\vec{\theta}) = \prod_{i=1}^{n} f(x_i; \vec{\theta}) \qquad (x_i \text{ constant})$$

Frequentist parameter estimation

Suppose we have a pdf characterized by one or more parameters:

$$f(x;\theta) = \frac{1}{\theta} e^{-x/\theta}$$

random variable

parameter

Suppose we have a sample of observed values: $\vec{x} = (x_1, \ldots, x_n)$

We want to find some function of the data to estimate the parameter(s):

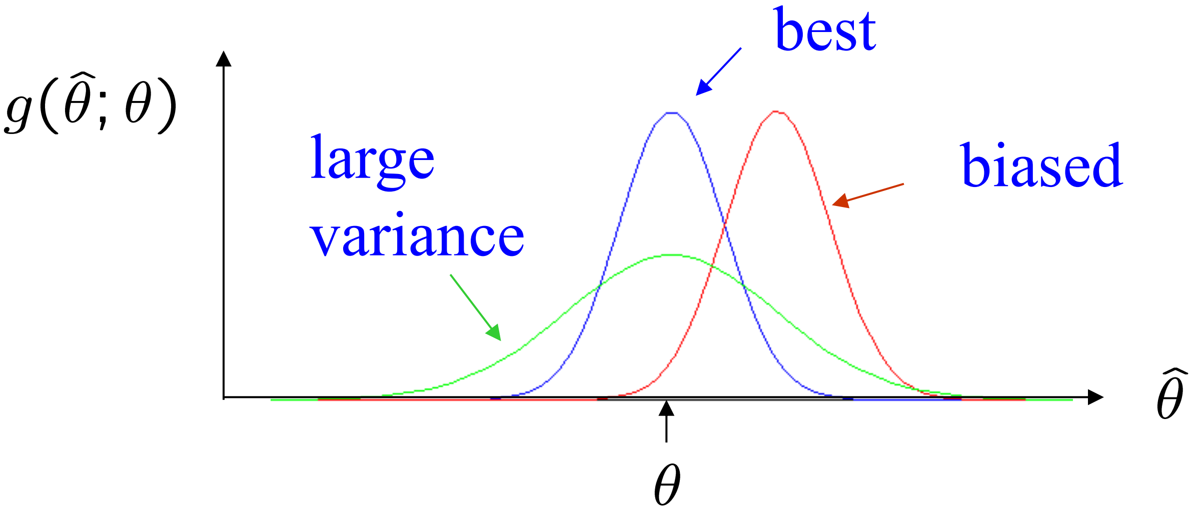
$$\boxed{\hat{\theta}(\vec{x})}$$

← estimator written with a hat

Sometimes we say 'estimator' for the function of $x_1, \ldots, x_n$; 'estimate' for the value of the estimator with a particular data set.

Properties of estimators

Estimators are functions of the data and thus characterized by a sampling distribution with a given (co)variance:

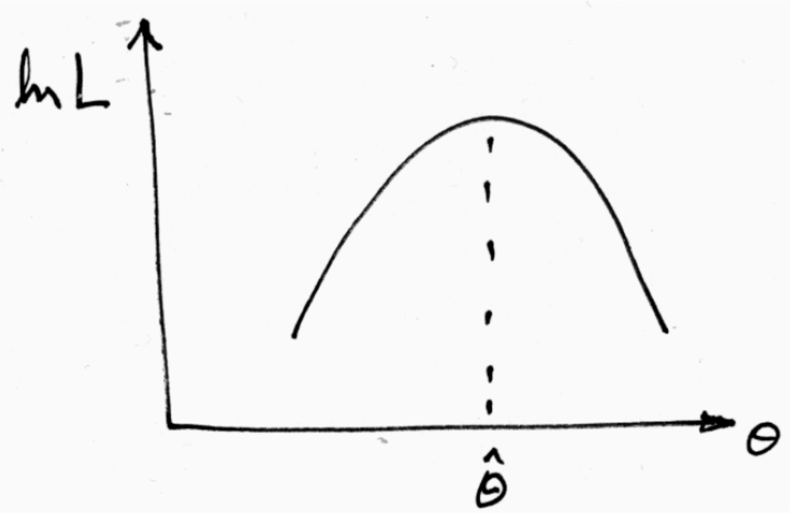


In general they may have a nonzero bias: $b = E[\hat{\theta}] - \theta$

Want small variance and small bias, but in general cannot optimize with respect to both; some trade-off necessary.

Maximum Likelihood (ML) estimators

The most important frequentist method for constructing estimators is to take the value of the parameter(s) that maximize the likelihood (or equivalently the log-likelihod):



$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}} \, L(x|\theta)$$

In some cases we can find the ML estimator as a closed-form function of the data; more often it is found numerically.

ML example: parameter of exponential pdf

Consider exponential pdf, $f(t;\tau) = \frac{1}{\tau} e^{-t/\tau}$

and suppose we have i.i.d. data, $t_1, \ldots, t_n$

The likelihood function is $L(\tau) = \prod_{i=1}^{n} \frac{1}{\tau} e^{-t_i/\tau}$

The value of τ for which $L(\tau)$ is maximum also gives the maximum value of its logarithm (the log-likelihood function):

$$\ln L(\tau) = \sum_{i=1}^{n} \ln f(t_i;\tau) = \sum_{i=1}^{n} \left(\ln \frac{1}{\tau} - \frac{t_i}{\tau} \right)$$

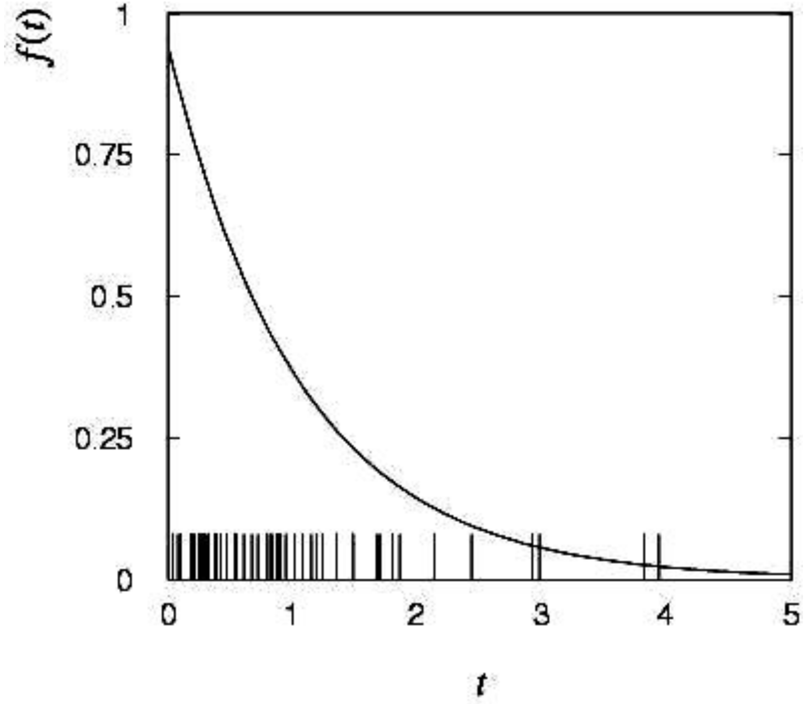
ML example: parameter of exponential pdf (2)

Find its maximum by setting $\dfrac{\partial \ln L(\tau)}{\partial \tau} = 0$,

$$\rightarrow \quad \hat{\tau} = \frac{1}{n} \sum_{i=1}^{n} t_i$$

Monte Carlo test:

generate 50 values
using $\tau = 1$:



We find the ML estimate:

$$\hat{\tau} = 1.062$$

ML example: parameter of exponential pdf (3)

For the exponential distribution one has for mean, variance:

$$E[t] = \int_0^\infty t \, \frac{1}{\tau} e^{-t/\tau} \, dt = \tau$$

$$V[t] = \int_0^\infty (t-\tau)^2 \, \frac{1}{\tau} e^{-t/\tau} \, dt = \tau^2$$

For the ML estimator $\widehat{\tau} = \frac{1}{n} \sum_{i=1}^{n} t_i$ we therefore find

$$E[\hat{\tau}] = E\left[\frac{1}{n}\sum_{i=1}^{n} t_i\right] = \frac{1}{n}\sum_{i=1}^{n} E[t_i] = \tau \quad \longrightarrow \quad b = E[\hat{\tau}] - \tau = 0$$

$$V[\hat{\tau}] = V\left[\frac{1}{n}\sum_{i=1}^{n} t_i\right] = \frac{1}{n^2}\sum_{i=1}^{n} V[t_i] = \frac{\tau^2}{n} \quad \longrightarrow \quad \sigma_{\hat{\tau}} = \frac{\tau}{\sqrt{n}}$$

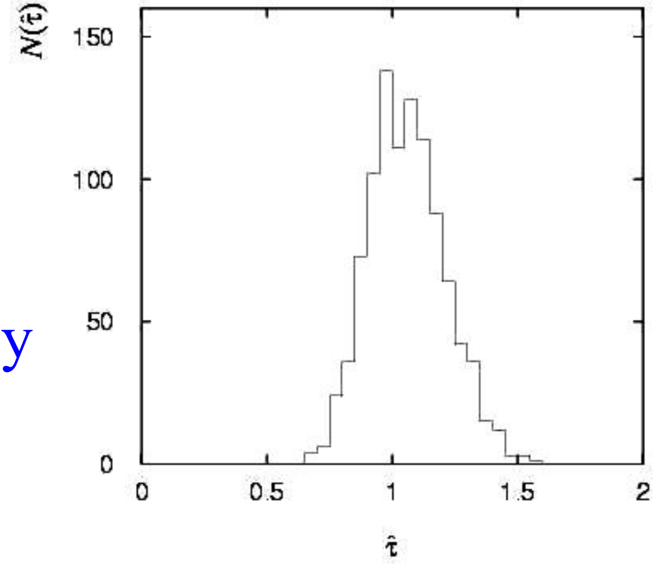
Variance of estimators: Monte Carlo method

Having estimated our parameter we now need to report its ‘statistical error’, i.e., how widely distributed would estimates be if we were to repeat the entire measurement many times.

One way to do this would be to simulate the entire experiment many times with a Monte Carlo program (use ML estimate for MC).

For exponential example, from sample variance of estimates we find:

$$\widehat{\sigma}_{\widehat{\tau}} = 0.151$$



Note distribution of estimates is roughly Gaussian − (almost) always true for ML in large sample limit.

Variance of estimators from information inequality

The information inequality (RCF) sets a lower bound on the variance of any estimator (not only ML):

$$V[\widehat{\theta}] \geq \left(1 + \frac{\partial b}{\partial \theta}\right)^2 \Big/ E\left[-\frac{\partial^2 \ln L}{\partial \theta^2}\right]$$

Minimum Variance Bound (MVB)

$$(b = E[\widehat{\theta}] - \theta)$$

Often the bias *b* is small, and equality either holds exactly or is a good approximation (e.g. large data sample limit). Then,

$$V[\widehat{\theta}] \approx -1 \Big/ E\left[\frac{\partial^2 \ln L}{\partial \theta^2}\right]$$

Estimate this using the 2nd derivative of ln *L* at its maximum:

$$\widehat{V}[\widehat{\theta}] = -\left(\frac{\partial^2 \ln L}{\partial \theta^2}\right)^{-1}\Bigg|_{\theta=\widehat{\theta}}$$

Variance of estimators: graphical method

Expand ln $L(\theta)$ about its maximum:

$$\ln L(\theta) = \ln L(\widehat{\theta}) + \left[\frac{\partial \ln L}{\partial \theta}\right]_{\theta=\widehat{\theta}} (\theta - \widehat{\theta}) + \frac{1}{2!}\left[\frac{\partial^2 \ln L}{\partial \theta^2}\right]_{\theta=\widehat{\theta}} (\theta - \widehat{\theta})^2 + \ldots$$

First term is ln $L_{\max}$, second term is zero, for third term use information inequality (assume equality):

$$\ln L(\theta) \approx \ln L_{\max} - \frac{(\theta - \widehat{\theta})^2}{2\widehat{\sigma^2}_{\widehat{\theta}}}$$

i.e., $$\ln L(\widehat{\theta} \pm \widehat{\sigma}_{\widehat{\theta}}) \approx \ln L_{\max} - \frac{1}{2}$$

→ to get $\widehat{\sigma}_{\widehat{\theta}}$, change θ away from $\widehat{\theta}$ until ln L decreases by 1/2.

Example of variance by graphical method

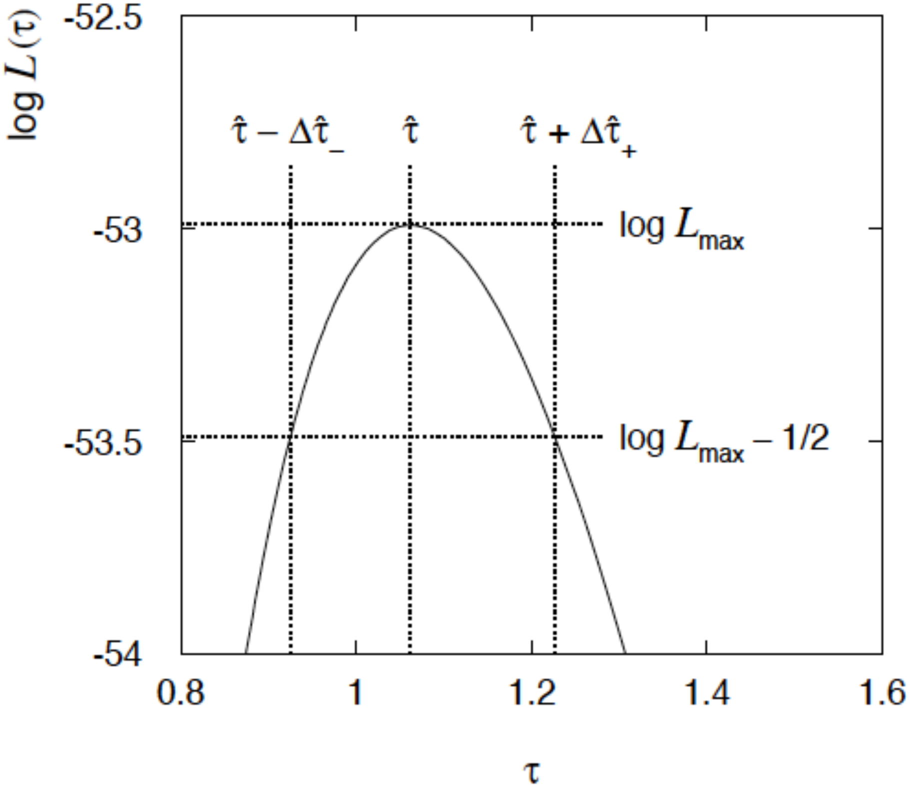
ML example with exponential:

$$\hat{\tau} = 1.062$$

$$\Delta\hat{\tau}_- = 0.137$$

$$\Delta\hat{\tau}_+ = 0.165$$

$$\hat{\sigma}_{\hat{\tau}} \approx \Delta\hat{\tau}_- \approx \Delta\hat{\tau}_+ \approx 0.15$$



Not quite parabolic ln L since finite sample size (n = 50).

Information inequality for N parameters

Suppose we have estimated N parameters $\vec{\theta} = (\theta_1, \ldots, \theta_N)$.

The (inverse) minimum variance bound is given by the Fisher information matrix:

$$I_{ij} = -E\left[\frac{\partial^2 \ln L}{\partial\theta_i \partial\theta_j}\right] = -\int \frac{\partial^2 \ln L}{\partial\theta_i \partial\theta_j} P(\mathbf{x}|\boldsymbol{\theta})\, d\mathbf{x}$$

The information inequality then states that $V - I^{-1}$ is a positive semi-definite matrix, where $V_{ij} = \mathrm{cov}[\hat{\theta}_i, \hat{\theta}_j]$. Therefore

$$V[\hat{\theta}_i] \geq (I^{-1})_{ii}$$

Often use I^{-1} as an approximation for covariance matrix, estimate using e.g. matrix of 2nd derivatives at maximum of L.

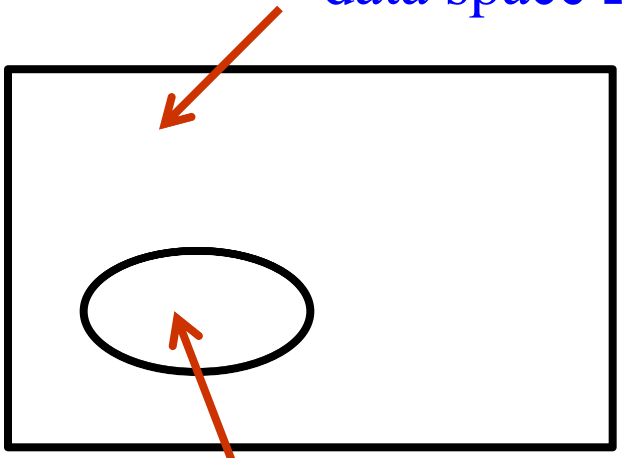
Frequentist statistical tests

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

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

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.,

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



data space Ω

critical region w

Need inequality if data are discrete.

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

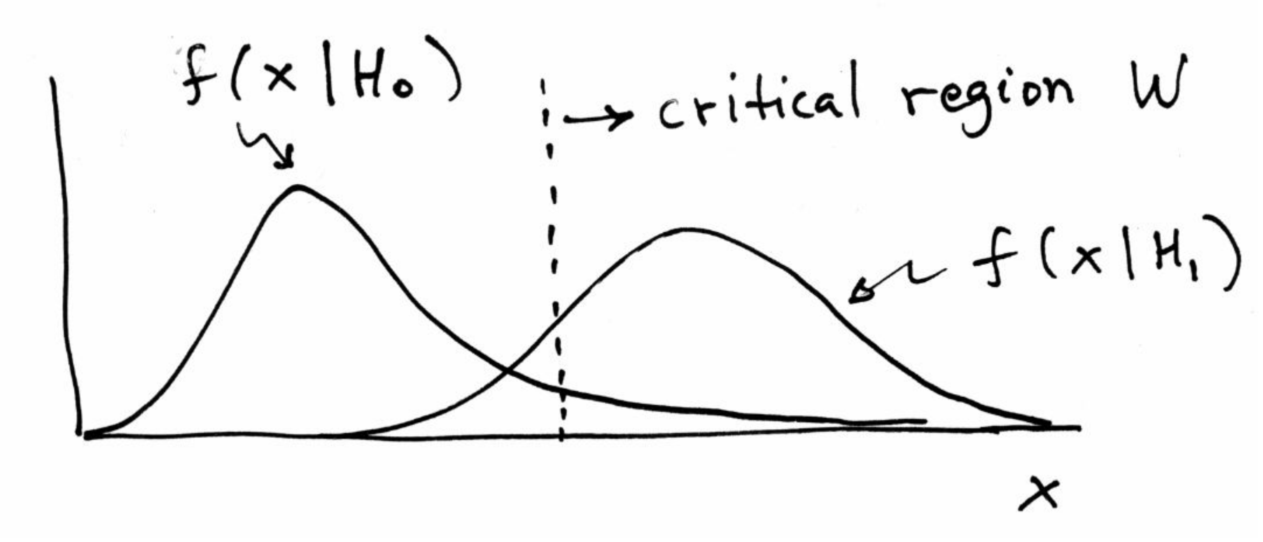
If x is observed in the critical region, reject H_0.

Definition of a test (2)

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

So the choice of the critical region for a test of H_0 needs to take into account the alternative hypothesis H_1.

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



Efficiencies, purity

Let H_0 = b (event is background, H_1 = s (event is signal).

For each event test b. If b rejected, "accept" as candidate signal.

background efficiency = $\varepsilon_b = P(\boldsymbol{x} \in W \mid \mathrm{b}) = \alpha$

signal efficiency = ε_s = power = $P(\boldsymbol{x} \in W \mid \mathrm{s}) = 1 - \beta$

To find purity of candidate signal sample, use Bayes' theorem:

prior probability

ε_s

Here W is signal region

$$P(\mathrm{s}|\mathbf{x} \in W) = \frac{P(\mathbf{x} \in W|\mathrm{s})P(\mathrm{s})}{P(\mathbf{x} \in W|\mathrm{s})P(\mathrm{s}) + P(\mathbf{x} \in W|\mathrm{b})P(\mathrm{b})}$$

ε_b

posterior probability = signal purity

Physics context of a statistical test

Event Selection: data = individual event; goal is to classify

Example: separation of different particle types (electron vs muon) or known event types (ttbar vs QCD multijet).
E.g. test H_0 : event is background vs. H_1 : event is signal.
Use selected events for further study.

Search for New Physics: data = a sample of events. Test null hypothesis

H_0 : all events correspond to Standard Model (background only),

against the alternative

H_1 : events include a type whose existence is not yet established (signal plus background)

Many subtle issues here, mainly related to the high standard of proof required to establish presence of a new phenomenon. The optimal statistical test for a search is closely related to that used for event selection.

Extra slides

Random variables and probability density functions

A random variable is a numerical characteristic assigned to an element of the sample space; can be discrete or continuous.

Suppose outcome of experiment is continuous value x

$$P(x \text{ found in } [x, x+dx]) = f(x)\,dx$$

→ $f(x)$ = probability density function (pdf)

$$\int_{-\infty}^{\infty} f(x)\,dx = 1$$

x must be somewhere

Or for discrete outcome x_i with e.g. $i = 1, 2, \ldots$ we have

$$P(x_i) = p_i$$

probability mass function

$$\sum_i P(x_i) = 1$$

x must take on one of its possible values

Other types of probability densities

Outcome of experiment characterized by several values,
e.g. an n-component vector, $(x_1, \ldots x_n)$

→ joint pdf $f(x_1, \ldots, x_n)$

Sometimes we want only pdf of some (or one) of the components

→ marginal pdf $f_1(x_1) = \int \cdots \int f(x_1, \ldots, x_n)\, dx_2 \ldots dx_n$

x_1, x_2 independent if $f(x_1, x_2) = f_1(x_1) f_2(x_2)$

Sometimes we want to consider some components as constant

→ conditional pdf $g(x_1|x_2) = \dfrac{f(x_1, x_2)}{f_2(x_2)}$

Expectation values

Consider continuous r.v. x with pdf $f(x)$.

Define expectation (mean) value as $E[x] = \int x\, f(x)\, dx$

Notation (often): $E[x] = \mu$ ~ "centre of gravity" of pdf.

For a function $y(x)$ with pdf $g(y)$,

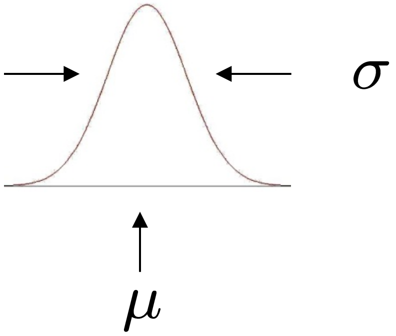
$$E[y] = \int y\, g(y)\, dy = \int y(x) f(x)\, dx$$ (equivalent)

Variance: $V[x] = E[x^2] - \mu^2 = E[(x-\mu)^2]$

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

Standard deviation: $\sigma = \sqrt{\sigma^2}$

σ ~ width of pdf, same units as x.



Covariance and correlation

Define covariance cov[x,y] (also use matrix notation V_{xy}) as

$$\mathrm{cov}[x,y] = E[xy] - \mu_x \mu_y = E[(x-\mu_x)(y-\mu_y)]$$

Correlation coefficient (dimensionless) defined as

$$\rho_{xy} = \frac{\mathrm{cov}[x,y]}{\sigma_x \sigma_y}$$

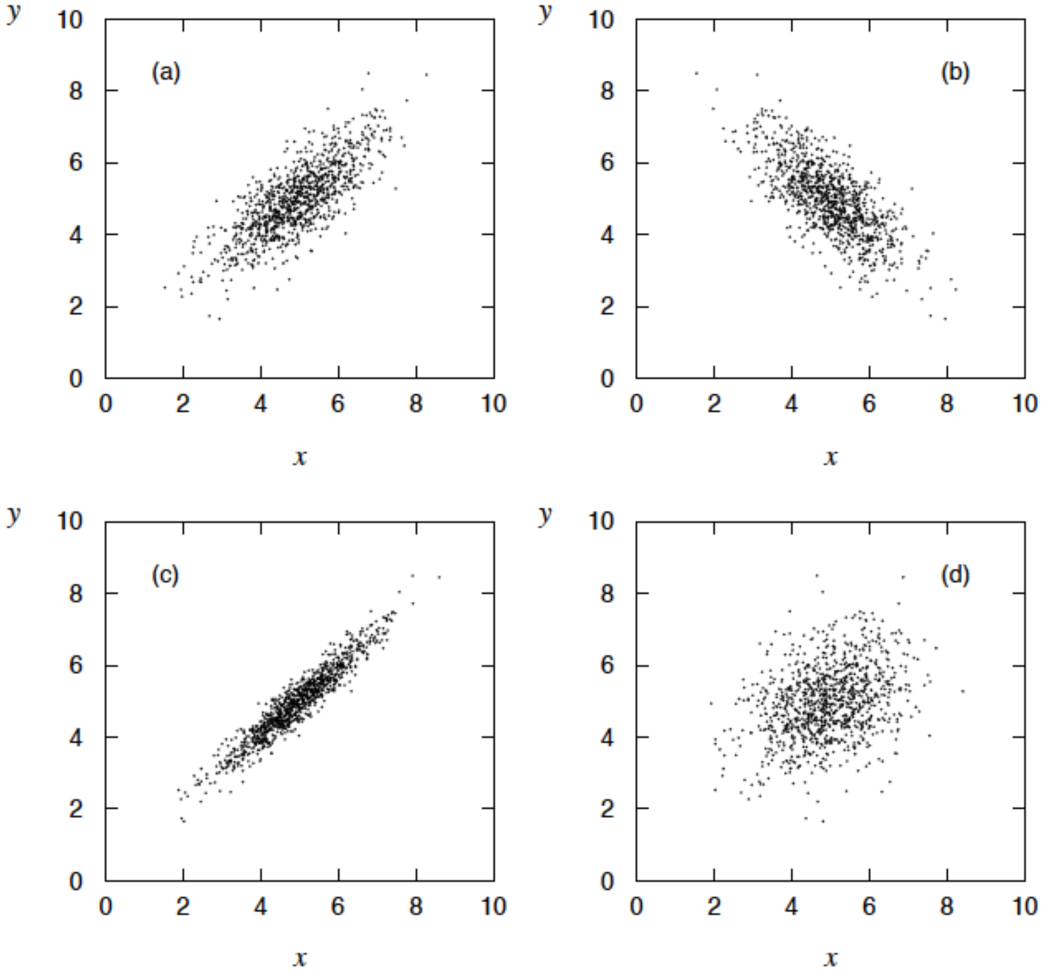
If x, y, independent, i.e., $f(x,y) = f_x(x) f_y(y)$, then

$$E[xy] = \int\int xy\, f(x,y)\, dx dy = \mu_x \mu_y$$

→ $\mathrm{cov}[x,y] = 0$ x and y, ‘uncorrelated’

N.B. converse not always true.

Correlation (cont.)



$\rho = 0.75$

$\rho = -0.75$

$\rho = 0.95$

$\rho = 0.25$

Some distributions

Distribution/pdf	Example use in HEP
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 $\displaystyle \frac{N!}{n!(N-n)!}$

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

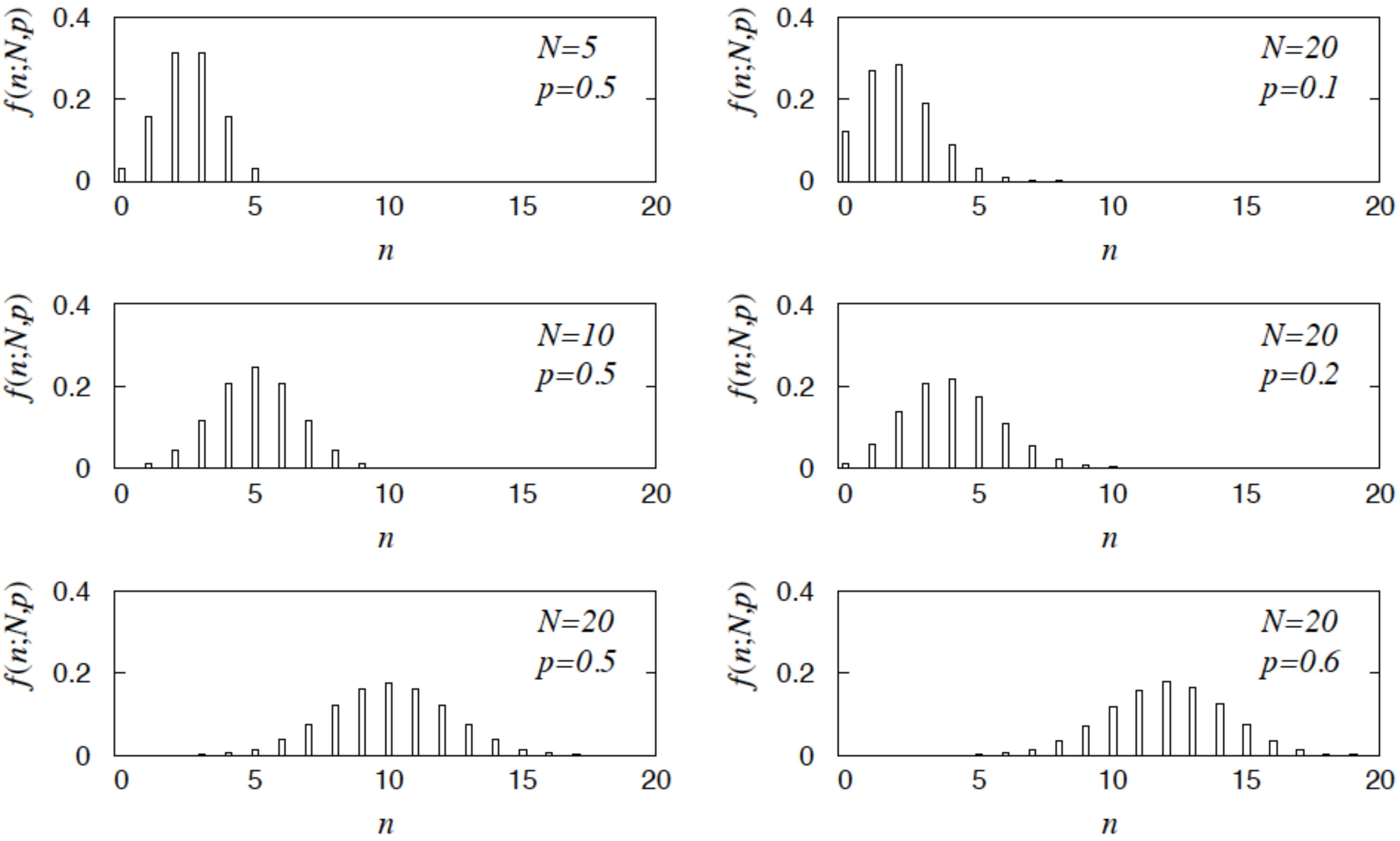
For the expectation value and variance we find:

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

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

Binomial distribution (3)

Binomial distribution for several values of the parameters:



Example: observe N decays of $W^{\pm}$, the number n of which are $W \rightarrow \mu\nu$ 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,
⋮
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

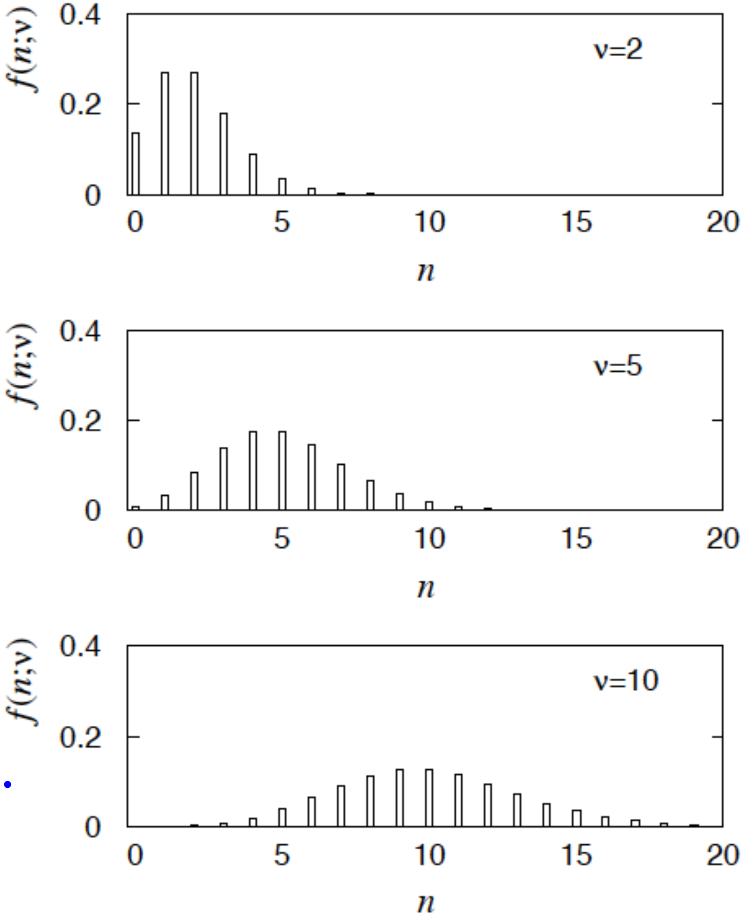
Consider binomial *n* in the limit

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

→ *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 $\nu = \sigma \int L\, dt$.

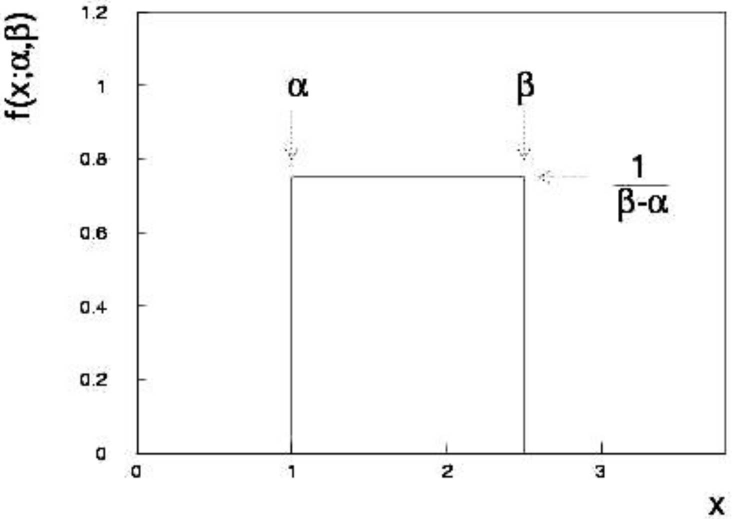
Uniform distribution

Consider a continuous r.v. x with $-\infty < x < \infty$. Uniform pdf is:

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

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

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



N.B. For any r.v. x with cumulative distribution $F(x)$, $y = F(x)$ is uniform in [0,1].

Example: for $\pi^0 \to \gamma\gamma$, E_γ is uniform in $[E_{\min}, E_{\max}]$, with

$$E_{\min} = \frac{1}{2}E_\pi(1-\beta)\,, \qquad E_{\max} = \frac{1}{2}E_\pi(1+\beta)$$

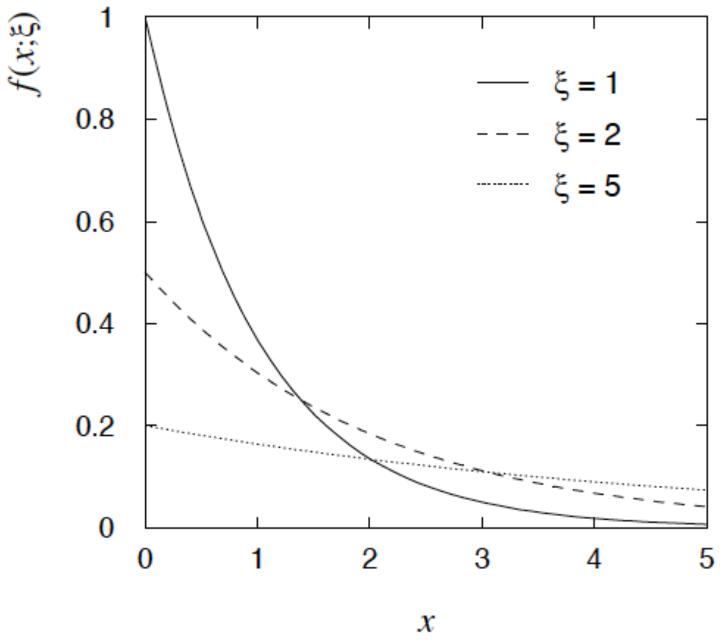
Exponential distribution

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

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

$$E[x] = \xi$$

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



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): $f(t - t_0 | t \geq t_0) = f(t)$

Gaussian distribution

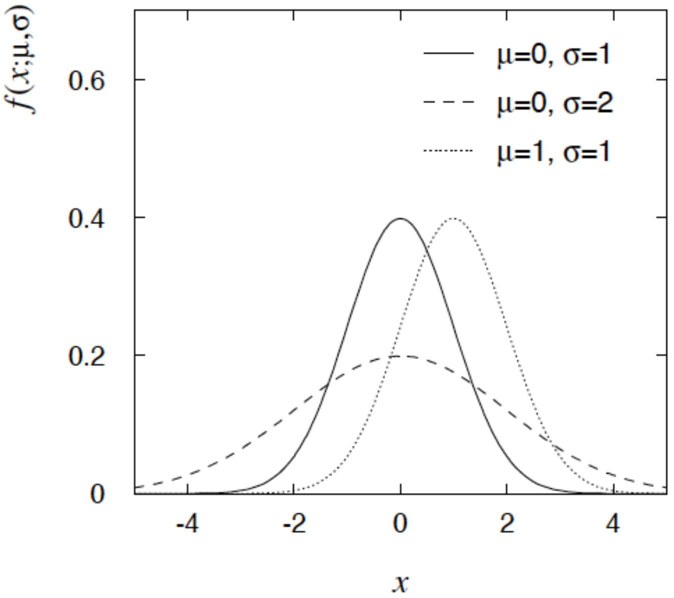
The Gaussian (normal) pdf for a continuous r.v. *x* is defined by:

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

$$E[x] = \mu$$

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

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



Special case: $\mu = 0$, $\sigma^2 = 1$ ('standard Gaussian'):

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

If $y \sim$ Gaussian with μ, σ^2, then $x = (y - \mu)/\sigma$ follows $\varphi(x)$.

Gaussian pdf and the Central Limit Theorem

The Gaussian pdf is so useful because almost any random variable that is a sum of a large number of small contributions follows it. This follows from the Central Limit Theorem:

For n independent r.v.s x_i with finite variances σ_i^2, otherwise arbitrary pdfs, consider the sum

$$y = \sum_{i=1}^{n} x_i$$

In the limit $n \to \infty$, y is a Gaussian r.v. with

$$E[y] = \sum_{i=1}^{n} \mu_i \qquad V[y] = \sum_{i=1}^{n} \sigma_i^2$$

Measurement errors are often the sum of many contributions, so frequently measured values can be treated as Gaussian r.v.s.

Central Limit Theorem (2)

The CLT can be proved using characteristic functions (Fourier transforms), see, e.g., SDA Chapter 10.

For finite n, the theorem is approximately valid to the extent that the fluctuation of the sum is not dominated by one (or few) terms.

⚠ Beware of measurement errors with non-Gaussian tails.

Good example: velocity component v_x of air molecules.

OK example: total deflection due to multiple Coulomb scattering. (Rare large angle deflections give non-Gaussian tail.)

Bad example: energy loss of charged particle traversing thin gas layer. (Rare collisions make up large fraction of energy loss, cf. Landau pdf.)

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,

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

For $n = 2$ this is

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

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

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

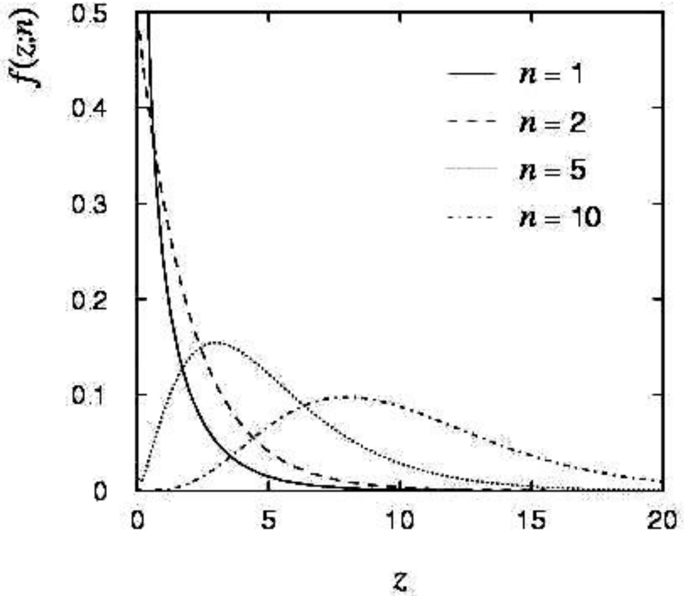
Chi-square (χ^2) distribution

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

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

$n = 1, 2, \ldots =$ number of ‘degrees of freedom’ (dof)

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



For independent Gaussian x_i, $i = 1, \ldots, n$, 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.

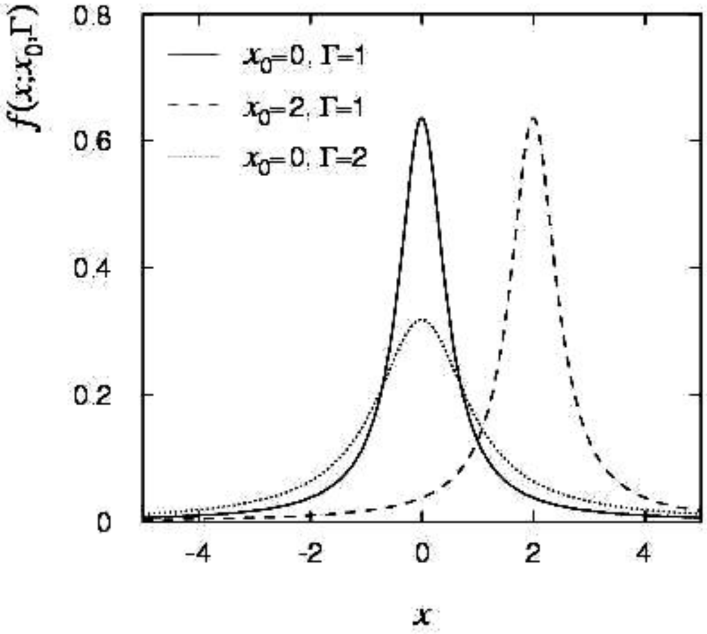
Example: goodness-of-fit test variable especially in conjunction with method of least squares.

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)

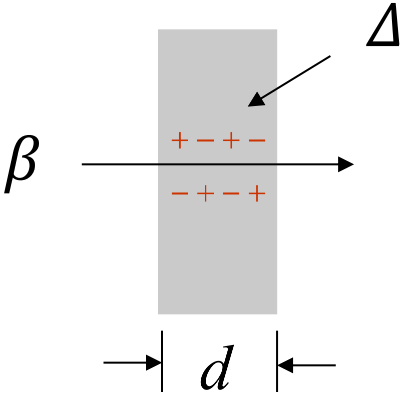
Γ = full width at half maximum

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:



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

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

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

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

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

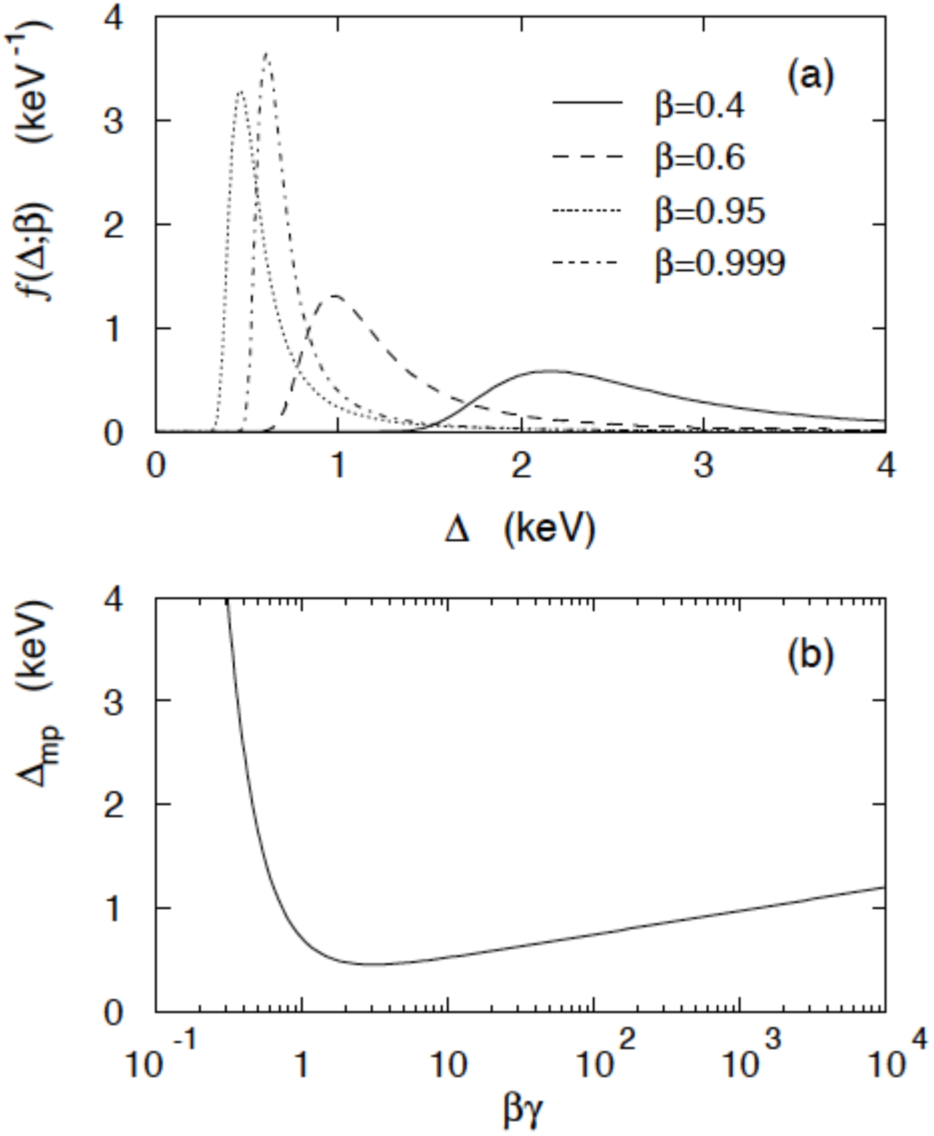
Landau distribution (2)

Long ‘Landau tail’

→ all moments ∞

Mode (most probable value) sensitive to β ,

→ particle i.d.

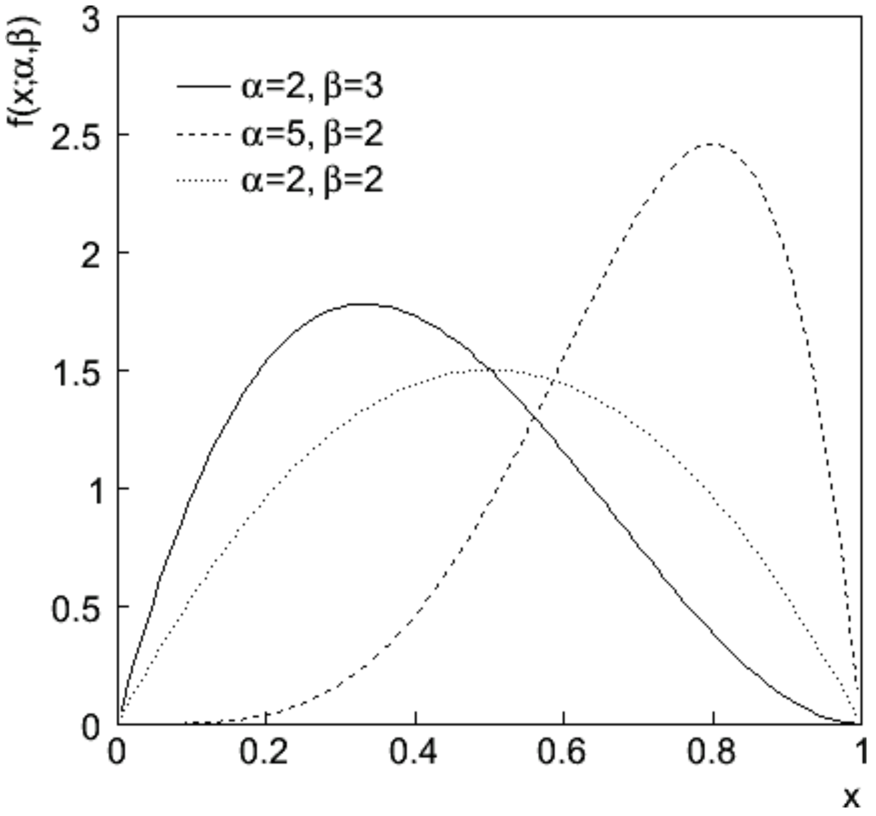


Beta distribution

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

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

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



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

Gamma distribution

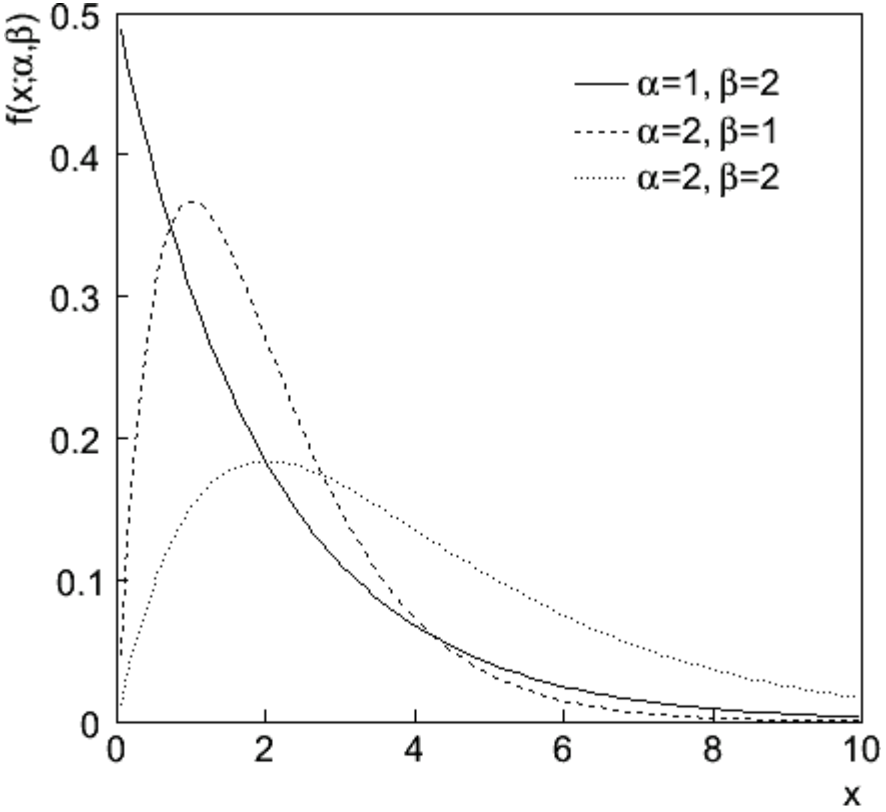
$$f(x;\alpha,\beta) = \frac{1}{\Gamma(\alpha)\beta^{\alpha}} x^{\alpha-1} e^{-x/\beta}$$

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

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

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

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



Student's *t* distribution

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

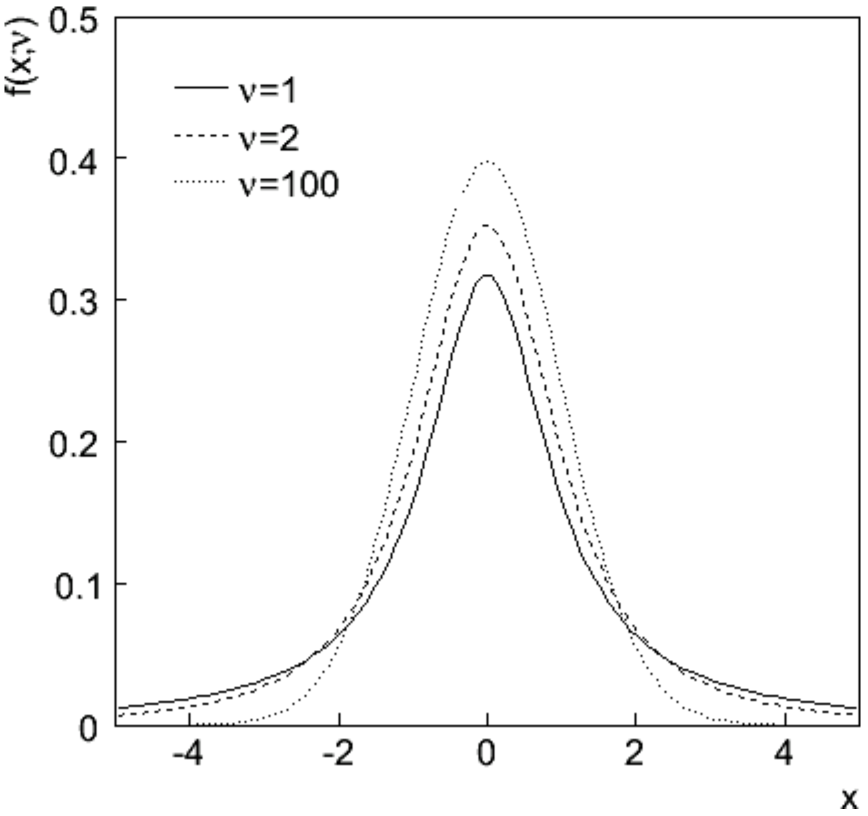
$$E[x] = 0 \quad (\nu > 1)$$

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

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

ν = 1 gives Cauchy,

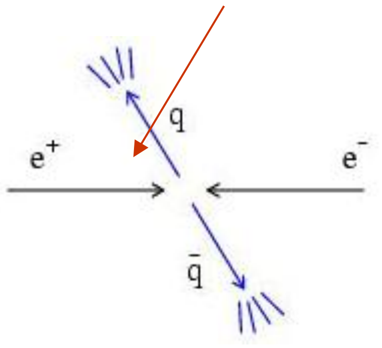
$\nu \rightarrow \infty$ gives Gaussian.



Example of ML with 2 parameters

Consider a scattering angle distribution with $x = \cos\theta$,

$$f(x;\alpha,\beta) = \frac{1 + \alpha x + \beta x^2}{2 + 2\beta/3}$$



or if $x_{\min} < x < x_{\max}$, need always to normalize so that

$$\int_{x_{\min}}^{x_{\max}} f(x;\alpha,\beta)\, dx = 1 \ .$$

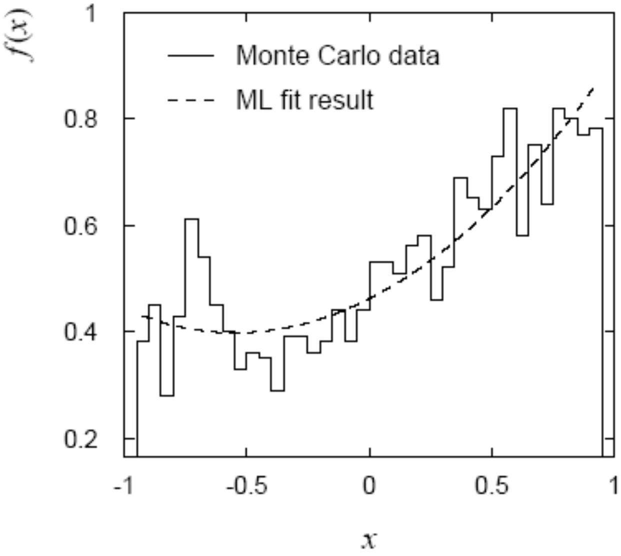
Example: $\alpha = 0.5$, $\beta = 0.5$, $x_{\min} = -0.95$, $x_{\max} = 0.95$, generate $n = 2000$ events with Monte Carlo.

Example of ML with 2 parameters: fit result

Finding maximum of ln $L(\alpha, \beta)$ numerically (**`MINUIT`**) gives

$$\hat{\alpha} = 0.508$$
$$\hat{\beta} = 0.47$$

N.B. No binning of data for fit, but can compare to histogram for goodness-of-fit (e.g. 'visual' or χ^2).

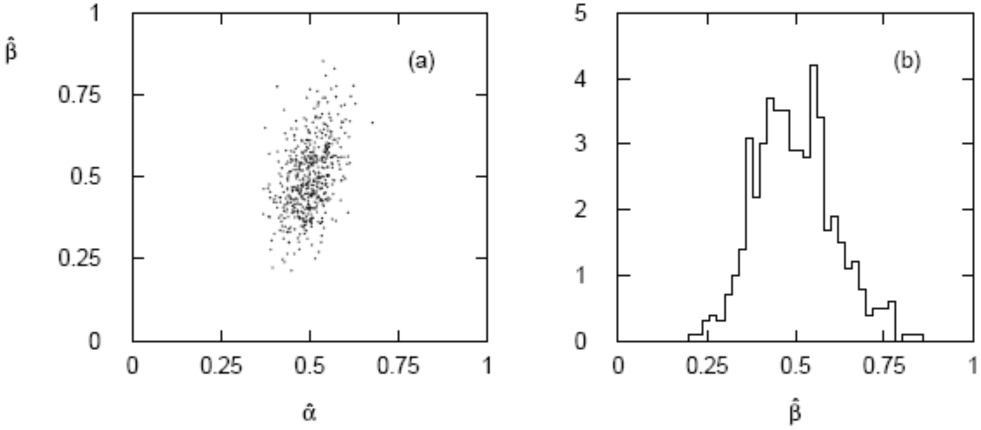


(Co)variances from $$(\widehat{V^{-1}})_{ij} = -\left.\frac{\partial^2 \ln L}{\partial\theta_i \partial\theta_j}\right|_{\vec{\theta}=\hat{\vec{\theta}}}$$ (**`MINUIT`** routine **`HESSE`**)

$$\hat{\sigma}_{\hat{\alpha}} = 0.052 \qquad \text{cov}[\hat{\alpha}, \hat{\beta}] = 0.0026$$
$$\hat{\sigma}_{\hat{\beta}} = 0.11 \qquad r = 0.46$$

Two-parameter fit: MC study

Repeat ML fit with 500 experiments, all with $n = 2000$ events:



$$\overline{\hat{\alpha}} = 0.499$$

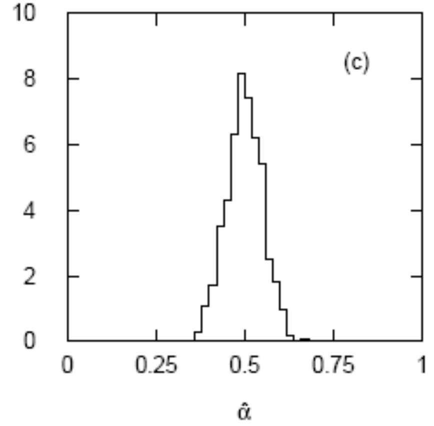
$$s_{\hat{\alpha}} = 0.051$$

$$\overline{\hat{\beta}} = 0.498$$

$$s_{\hat{\beta}} = 0.111$$

$$\widehat{\text{cov}}[\hat{\alpha}, \hat{\beta}] = 0.0024$$

$$r = 0.42$$



Estimates average to ~ true values;
(Co)variances close to previous estimates;
marginal pdfs approximately Gaussian.

The ln L_{max} – 1/2 contour

For large n, ln L takes on quadratic form near maximum:

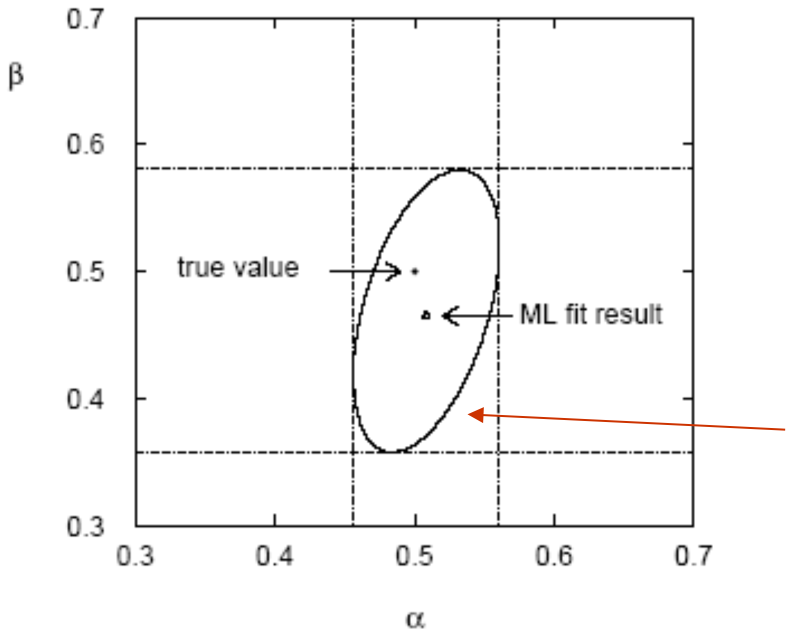
$$\ln L(\alpha,\beta) \approx \ln L_{\text{max}}$$

$$-\frac{1}{2(1-\rho^2)}\left[\left(\frac{\alpha-\widehat{\alpha}}{\sigma_{\widehat{\alpha}}}\right)^2+\left(\frac{\beta-\widehat{\beta}}{\sigma_{\widehat{\beta}}}\right)^2-2\rho\left(\frac{\alpha-\widehat{\alpha}}{\sigma_{\widehat{\alpha}}}\right)\left(\frac{\beta-\widehat{\beta}}{\sigma_{\widehat{\beta}}}\right)\right]$$

The contour $\ln L(\alpha,\beta) = \ln L_{\text{max}} - 1/2$ is an ellipse:

$$\frac{1}{(1-\rho^2)}\left[\left(\frac{\alpha-\widehat{\alpha}}{\sigma_{\widehat{\alpha}}}\right)^2+\left(\frac{\beta-\widehat{\beta}}{\sigma_{\widehat{\beta}}}\right)^2-2\rho\left(\frac{\alpha-\widehat{\alpha}}{\sigma_{\widehat{\alpha}}}\right)\left(\frac{\beta-\widehat{\beta}}{\sigma_{\widehat{\beta}}}\right)\right]=1$$

(Co)variances from ln L contour



The α, β plane for the first MC data set

$$\ln L(\alpha, \beta) = \ln L_{\max} - 1/2$$

→ Tangent lines to contours give standard deviations.

→ Angle of ellipse φ related to correlation: $\tan 2\phi = \frac{2\rho\sigma_{\hat{\alpha}}\sigma_{\hat{\beta}}}{\sigma_{\hat{\alpha}}^2 - \sigma\hat{\beta}^2}$

Correlations between estimators result in an increase in their standard deviations (statistical errors).