Statistical Methods for Particle Physics

Lecture 1: probability, random variables, MC

www.pp.rhul.ac.uk/~cowan/stat_aachen.html

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Outline

→ 1 Probability

Definition, Bayes' theorem, probability densities and their properties, catalogue of pdfs, Monte Carlo

2 Statistical tests

general concepts, test statistics, multivariate methods, goodness-of-fit tests

3 Parameter estimation

general concepts, maximum likelihood, variance of estimators, least squares

4 Hypothesis tests for discovery and exclusion

discovery significance, sensitivity, setting limits

5 Further topics

systematic errors, Bayesian methods, MCMC

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.

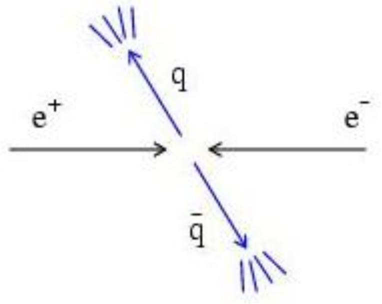
L. Lyons, *Statistics for Nuclear and Particle Physics*, CUP, 1986

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)

J. Beringer et al. (Particle Data Group), *Review of Particle Physics*, Phys. Rev. D86, 010001 (2012) ; see also `pdg.lbl.gov` sections on probability, statistics, Monte Carlo

Data analysis in particle physics



Observe events of a certain type

Measure characteristics of each event (particle momenta, number of muons, energy of jets,...)

Theories (e.g. SM) predict distributions of these properties up to free parameters, e.g., α, G_{F}, M_{Z}, α_{s}, m_{H}, ...

Some tasks of data analysis:

Estimate (measure) the parameters;

Quantify the uncertainty of the parameter estimates;

Test the extent to which the predictions of a theory are in agreement with the data.

Dealing with uncertainty

In particle physics there are various elements of uncertainty:

final theory not known,

that's why we search further

theory is not deterministic,

quantum mechanics

random measurement errors,

present even without quantum effects

things we could know in principle but don't,

e.g. from limitations of cost, time, ...

We can quantify the uncertainty using PROBABILITY

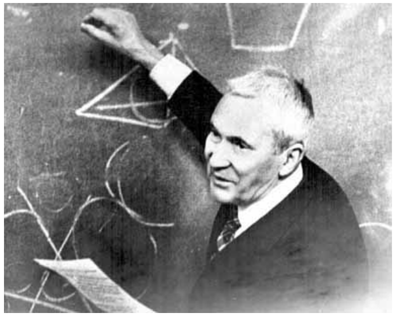
A definition of probability

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

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

$$P(S) = 1$$

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



Kolmogorov axioms (1933)

From these axioms we can derive further properties, e.g.

$$P(\overline{A}) = 1 - P(A)$$
$$P(A \cup \overline{A}) = 1$$
$$P(\emptyset) = 0$$
$$\text{if } A \subset B, \text{ then } P(A) \leq P(B)$$
$$P(A \cup B) = P(A) + P(B) - P(A \cap B)$$

Conditional probability, independence

Also define conditional probability of *A* given *B* (with $P(B) \neq 0$):

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

E.g. rolling dice: $P(n < 3 \,|\, n\,\text{even}) = \frac{P((n<3) \cap n\,\text{even})}{P(\text{even})} = \frac{1/6}{3/6} = \frac{1}{3}$

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

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

N.B. do not confuse with disjoint subsets, i.e., $A \cap B = \emptyset$

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

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

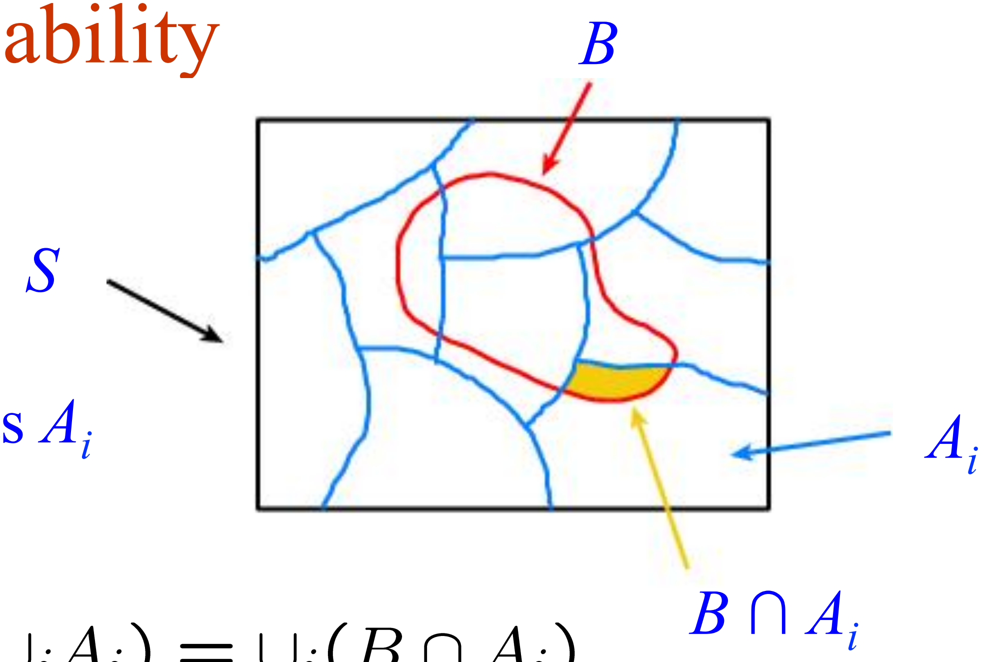
Bayes' theorem

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 AIDS is:

$$P(\text{AIDS}) = 0.001$$

$$P(\text{no AIDS}) = 0.999$$

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

Consider an AIDS test: result is + or −

$$P(+|\text{AIDS}) = 0.98$$

$$P(-|\text{AIDS}) = 0.02$$

← probabilities to (in)correctly identify an infected person

$$P(+|\text{no AIDS}) = 0.03$$

$$P(-|\text{no AIDS}) = 0.97$$

← probabilities to (in)correctly identify an uninfected person

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

Bayes' theorem example (cont.)

The probability to have AIDS given a + result is

$$P(\text{AIDS}|+) = \frac{P(+|\text{AIDS})P(\text{AIDS})}{P(+|\text{AIDS})P(\text{AIDS}) + P(+|\text{no AIDS})P(\text{no AIDS})}$$

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

$$= 0.032$$ ← posterior probability

i.e. you're probably OK!

Your viewpoint: my degree of belief that I have AIDS is 3.2%

Your doctor's viewpoint: 3.2% of people like this will have AIDS

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.

The preferred theories (models, hypotheses, ...) are those for which our observations would be considered 'usual'.

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!)

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

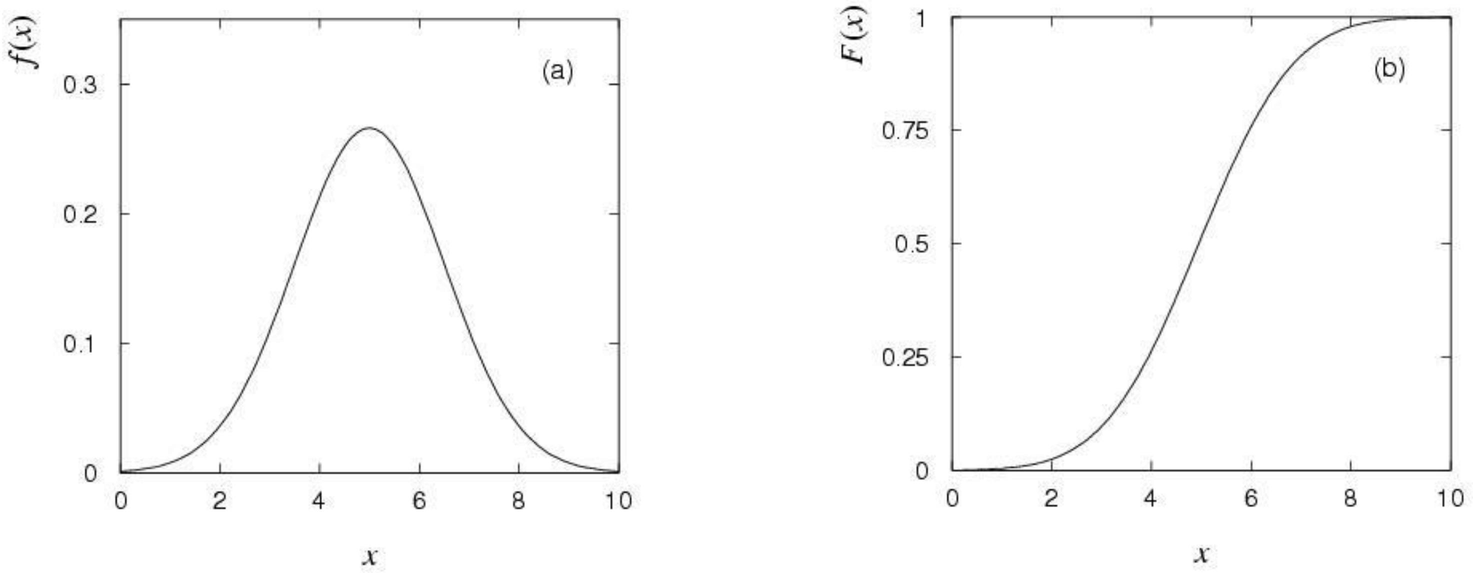
$$\sum_i P(x_i) = 1$$

x must take on one of its possible values

Cumulative distribution function

Probability to have outcome less than or equal to *x* is

$$\int_{-\infty}^{x} f(x')\,dx' \equiv F(x)$$ cumulative distribution function



Alternatively define pdf with $f(x) = \dfrac{\partial F(x)}{\partial x}$

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.

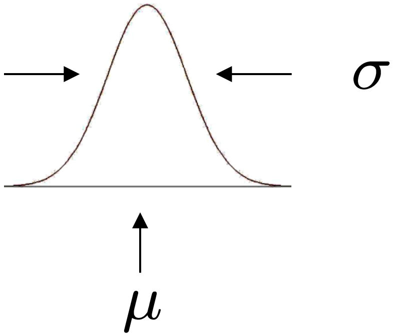
For a function $y(x)$ with pdf $g(y)$,

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

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

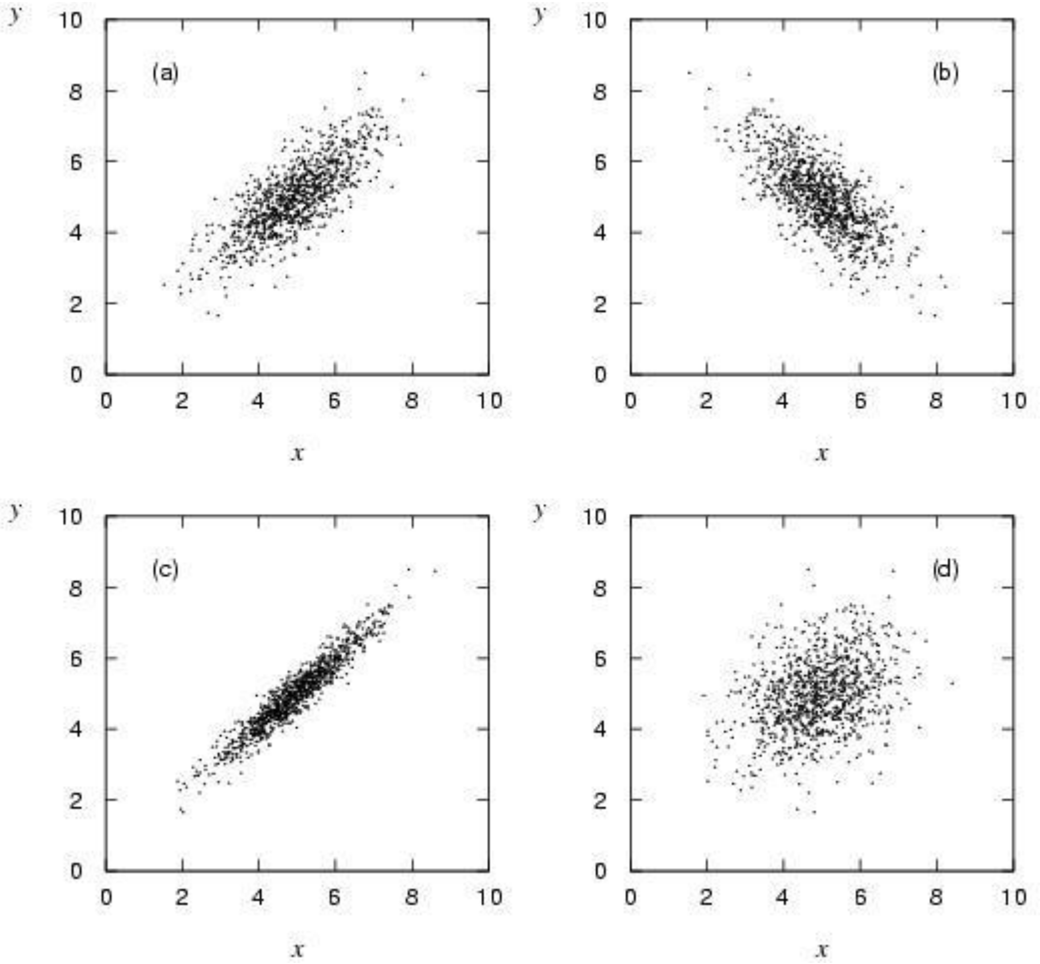
If x, y, independent, i.e., $f(x,y) = f_x(x)f_y(y)$, then

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

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

N.B. converse not always true.

Correlation (cont.)



$\rho = 0.75$

$\rho = -0.75$

$\rho = 0.95$

$\rho = 0.25$

Error propagation

Suppose we measure a set of values $\vec{x} = (x_1, \ldots, x_n)$

and we have the covariances $V_{ij} = \mathrm{cov}[x_i, x_j]$

which quantify the measurement errors in the x_i.

Now consider a function $y(\vec{x})$.

What is the variance of $y(\vec{x})$?

The hard way: use joint pdf $f(\vec{x})$ to find the pdf $g(y)$,

then from $g(y)$ find $V[y] = E[y^2] - (E[y])^2$.

Often not practical, $f(\vec{x})$ may not even be fully known.

Error propagation (2)

Suppose we had $\vec{\mu} = E[\vec{x}]$

in practice only estimates given by the measured $\vec{x}$

Expand $y(\vec{x})$ to 1st order in a Taylor series about $\vec{\mu}$

$$y(\vec{x}) \approx y(\vec{\mu}) + \sum_{i=1}^{n} \left[\frac{\partial y}{\partial x_i} \right]_{\vec{x}=\vec{\mu}} (x_i - \mu_i)$$

To find $V[y]$ we need $E[y^2]$ and $E[y]$.

$$E[y(\vec{x})] \approx y(\vec{\mu}) \quad \text{since} \quad E[x_i - \mu_i] = 0$$

Error propagation (3)

$$E[y^2(\vec{x})] \approx y^2(\vec{\mu}) \; + \; 2y(\vec{\mu}) \sum_{i=1}^{n} \left[\frac{\partial y}{\partial x_i} \right]_{\vec{x}=\vec{\mu}} E[x_i - \mu_i]$$

$$+E \left[\left(\sum_{i=1}^{n} \left[\frac{\partial y}{\partial x_i} \right]_{\vec{x}=\vec{\mu}} (x_i - \mu_i) \right) \left(\sum_{j=1}^{n} \left[\frac{\partial y}{\partial x_j} \right]_{\vec{x}=\vec{\mu}} (x_j - \mu_j) \right) \right]$$

$$= y^2(\vec{\mu}) + \sum_{i,j=1}^{n} \left[\frac{\partial y}{\partial x_i} \frac{\partial y}{\partial x_j} \right]_{\vec{x}=\vec{\mu}} V_{ij}$$

Putting the ingredients together gives the variance of $y(\vec{x})$

$$\boxed{\sigma_y^2 \approx \sum_{i,j=1}^{n} \left[\frac{\partial y}{\partial x_i} \frac{\partial y}{\partial x_j} \right]_{\vec{x}=\vec{\mu}} V_{ij}}$$

Error propagation (4)

If the x_i are uncorrelated, i.e., $V_{ij} = \sigma_i^2 \delta_{ij}$, then this becomes

$$\sigma_y^2 \approx \sum_{i=1}^{n} \left[\frac{\partial y}{\partial x_i} \right]^2_{\vec{x}=\vec{\mu}} \sigma_i^2$$

Similar for a set of m functions $\vec{y}(\vec{x}) = (y_1(\vec{x}), \ldots, y_m(\vec{x}))$

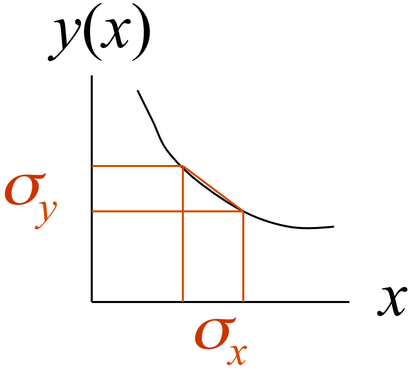
$$\boxed{U_{kl} = \mathrm{cov}[y_k, y_l] \approx \sum_{i,j=1}^{n} \left[\frac{\partial y_k}{\partial x_i} \frac{\partial y_l}{\partial x_j} \right]_{\vec{x}=\vec{\mu}} V_{ij}}$$

or in matrix notation $U = AVA^T$, where

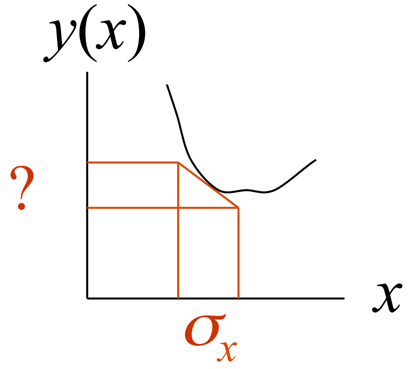
$$A_{ij} = \left[\frac{\partial y_i}{\partial x_j} \right]_{\vec{x}=\vec{\mu}}$$

Error propagation (5)

The ‘error propagation’ formulae tell us the covariances of a set of functions $\vec{y}(\vec{x}) = (y_1(\vec{x}), \ldots, y_m(\vec{x}))$ in terms of the covariances of the original variables.



Limitations: exact only if $\vec{y}(\vec{x})$ linear. Approximation breaks down if function nonlinear over a region comparable in size to the σ_i.



N.B. We have said nothing about the exact pdf of the x_i, e.g., it doesn’t have to be Gaussian.

Error propagation – special cases

$$y = x_1 + x_2 \quad \rightarrow \quad \sigma_y^2 = \sigma_1^2 + \sigma_2^2 + 2\,\mathrm{cov}[x_1, x_2]$$

$$y = x_1 x_2 \quad \rightarrow \quad \frac{\sigma_y^2}{y^2} = \frac{\sigma_1^2}{x_1^2} + \frac{\sigma_2^2}{x_2^2} + 2\frac{\mathrm{cov}[x_1, x_2]}{x_1 x_2}$$

That is, if the x_i are uncorrelated:

add errors quadratically for the sum (or difference),

add relative errors quadratically for product (or ratio).

⚠ But correlations can change this completely...

Error propagation – special cases (2)

Consider $y = x_1 - x_2$ with

$$\mu_1 = \mu_2 = 10, \quad \sigma_1 = \sigma_2 = 1, \quad \rho = \frac{\mathrm{cov}[x_1, x_2]}{\sigma_1 \sigma_2} = 0\,.$$

$$V[y] = 1^2 + 1^2 = 2, \rightarrow \sigma_y = 1.4$$

Now suppose $\rho = 1$. Then

$$V[y] = 1^2 + 1^2 - 2 = 0, \rightarrow \sigma_y = 0$$

i.e. for 100% correlation, error in difference → 0.

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 $\dfrac{N!}{n!(N-n)!}$

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

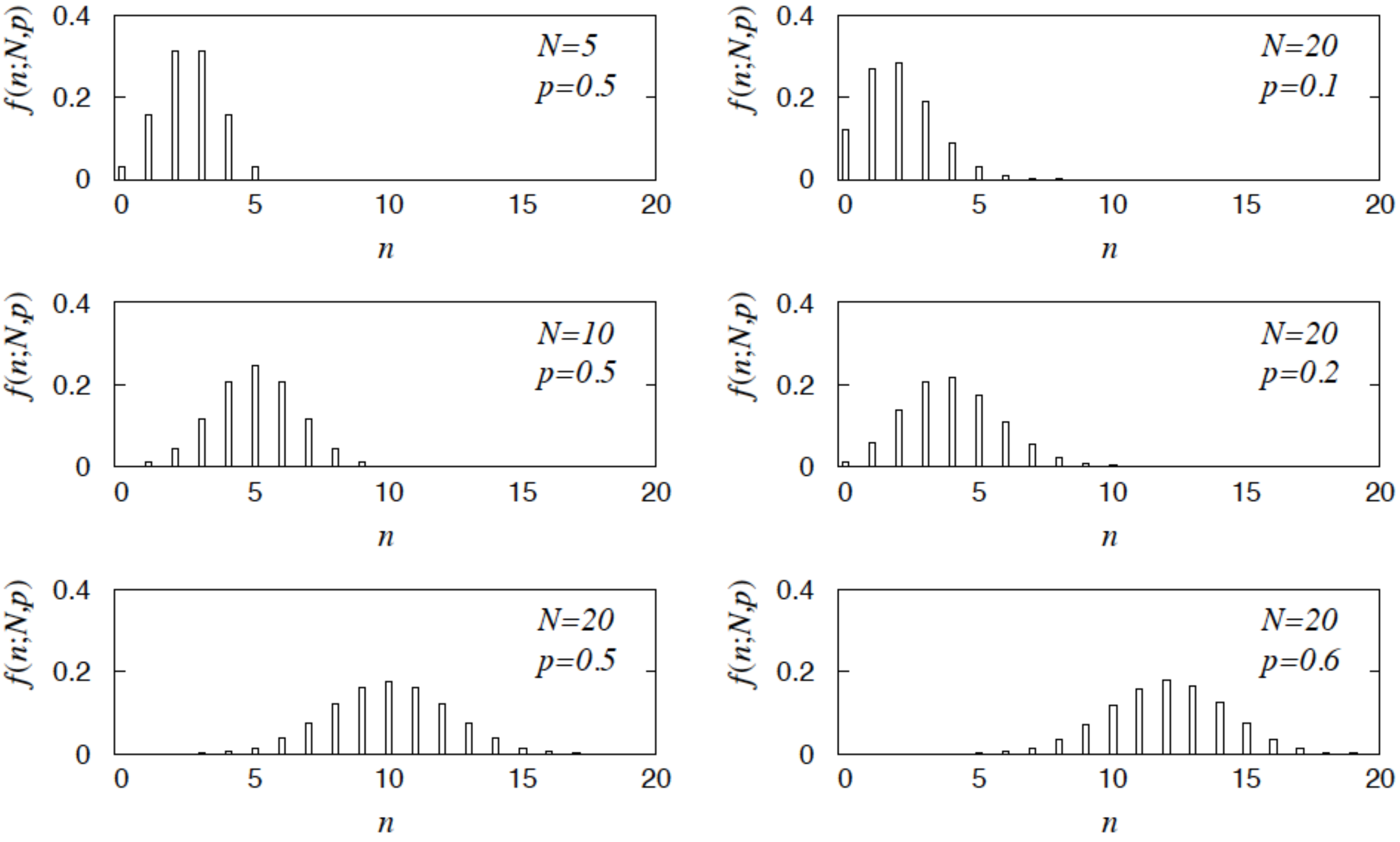
For the expectation value and variance we find:

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

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

Binomial distribution (3)

Binomial distribution for several values of the parameters:



Example: observe *N* decays of W$^\pm$, the number *n* of which are W→μν 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

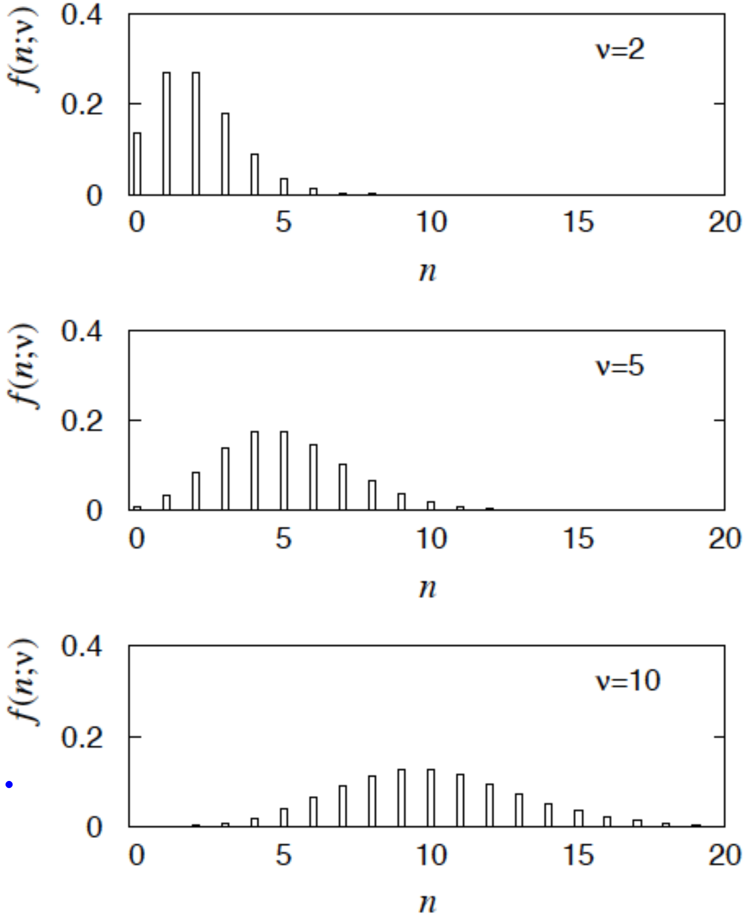
Consider binomial *n* in the limit

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

→ *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 $\nu = \sigma \int L \, dt$.

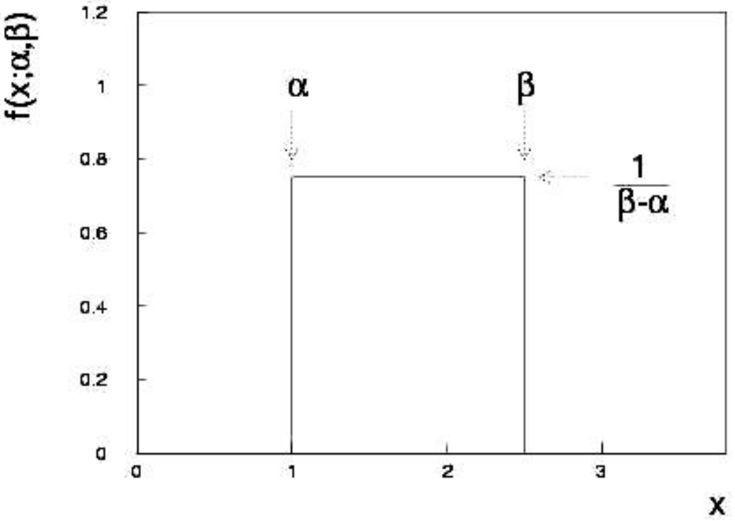
Uniform distribution

Consider a continuous r.v. *x* with −∞ < x < ∞ . 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

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

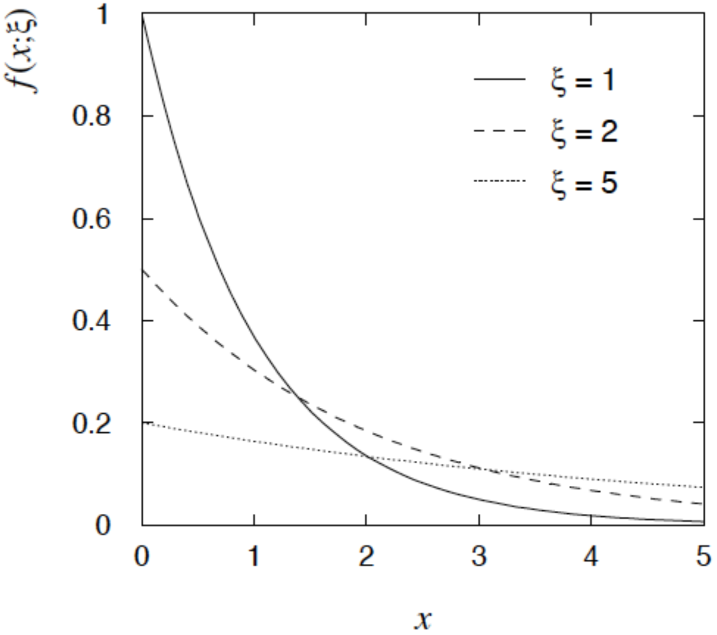
Exponential distribution

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

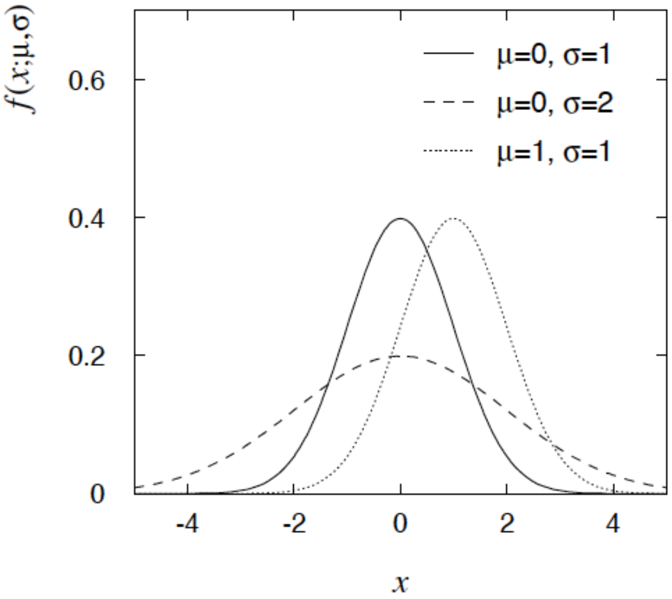
$$f(t;\tau) = \frac{1}{\tau} e^{-t/\tau} \qquad (\tau = \text{mean lifetime})$$

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 ~ 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

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

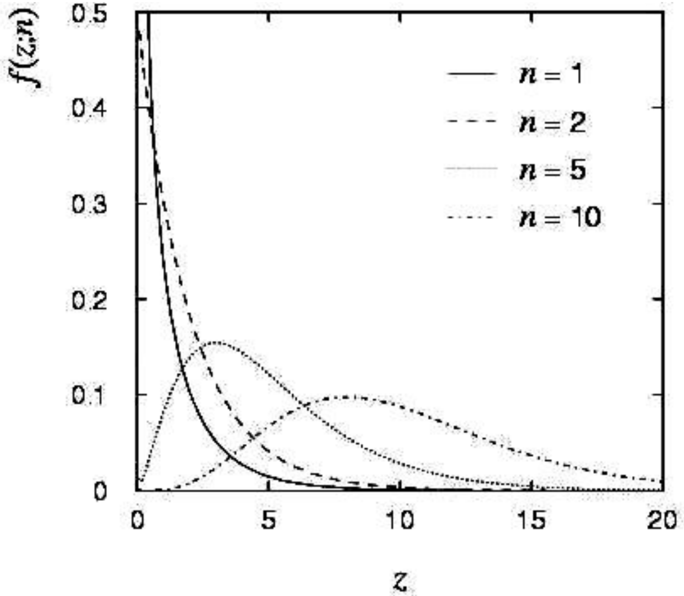
$$\times \exp\left\{-\frac{1}{2(1-\rho^2)}\left[\left(\frac{x_1-\mu_1}{\sigma_1}\right)^2 + \left(\frac{x_2-\mu_2}{\sigma_2}\right)^2 - 2\rho\left(\frac{x_1-\mu_1}{\sigma_1}\right)\left(\frac{x_2-\mu_2}{\sigma_2}\right)\right]\right\}$$

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, ... = number of 'degrees of freedom' (dof)

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

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.

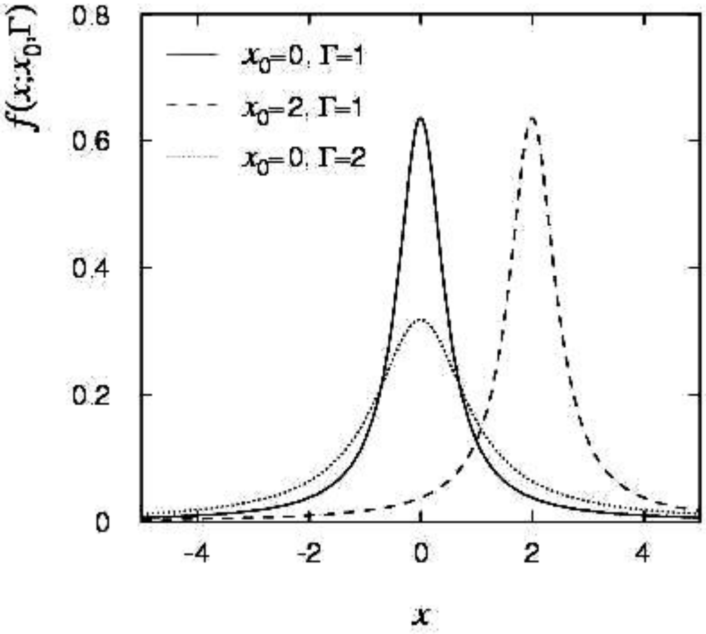
Example: goodness-of-fit test variable especially in conjunction with method of least squares.

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, $V[x] \rightarrow \infty$.

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

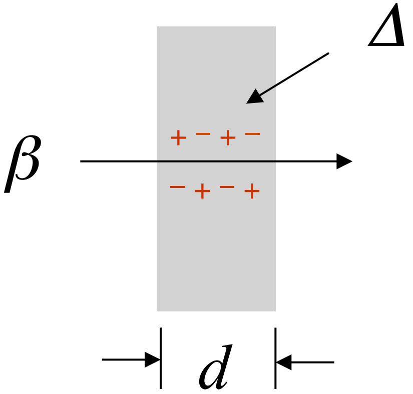
For a charged particle with *β* = *v* /*c* traversing a layer of matter of thickness *d*, the energy loss *Δ* follows the Landau pdf:

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

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

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

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



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

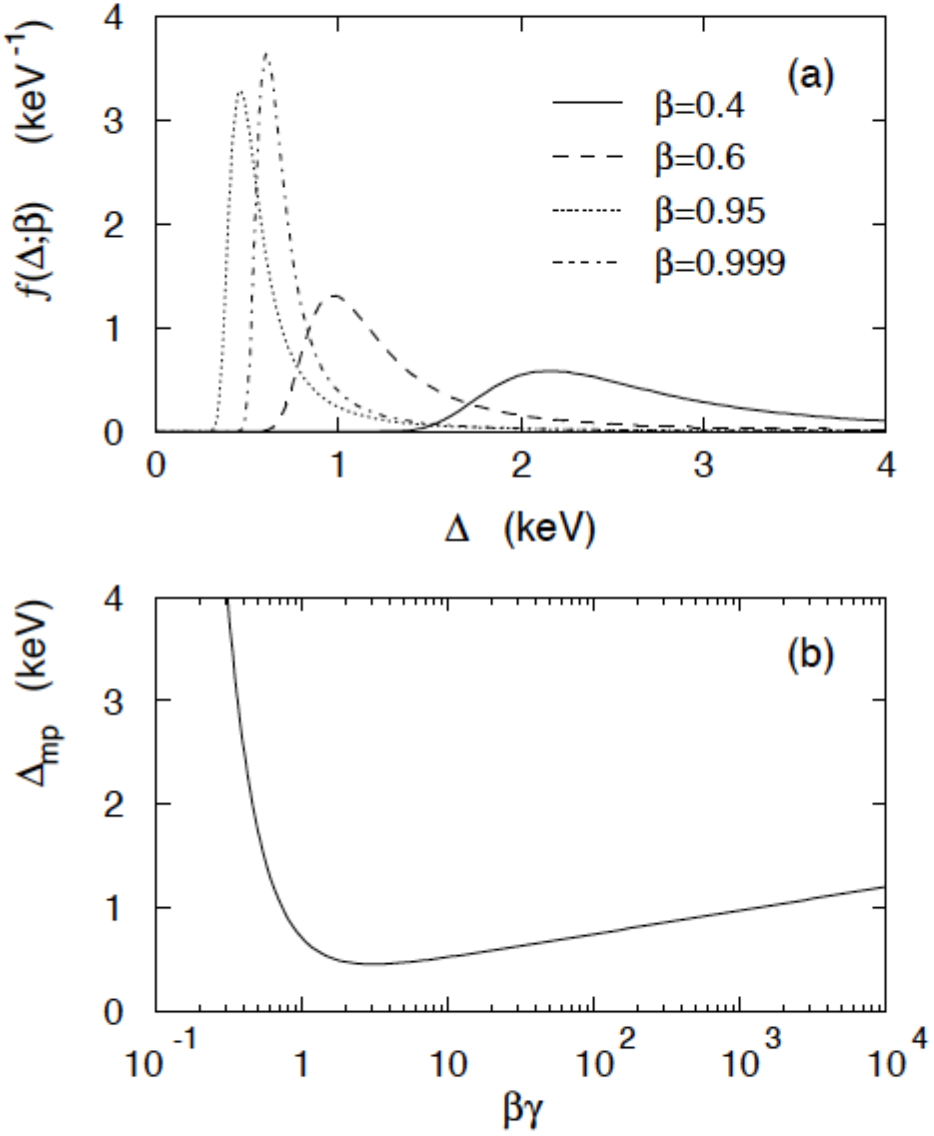
Landau distribution (2)

Long ‘Landau tail’

→ all moments ∞

Mode (most probable value) sensitive to β ,

→ particle i.d.

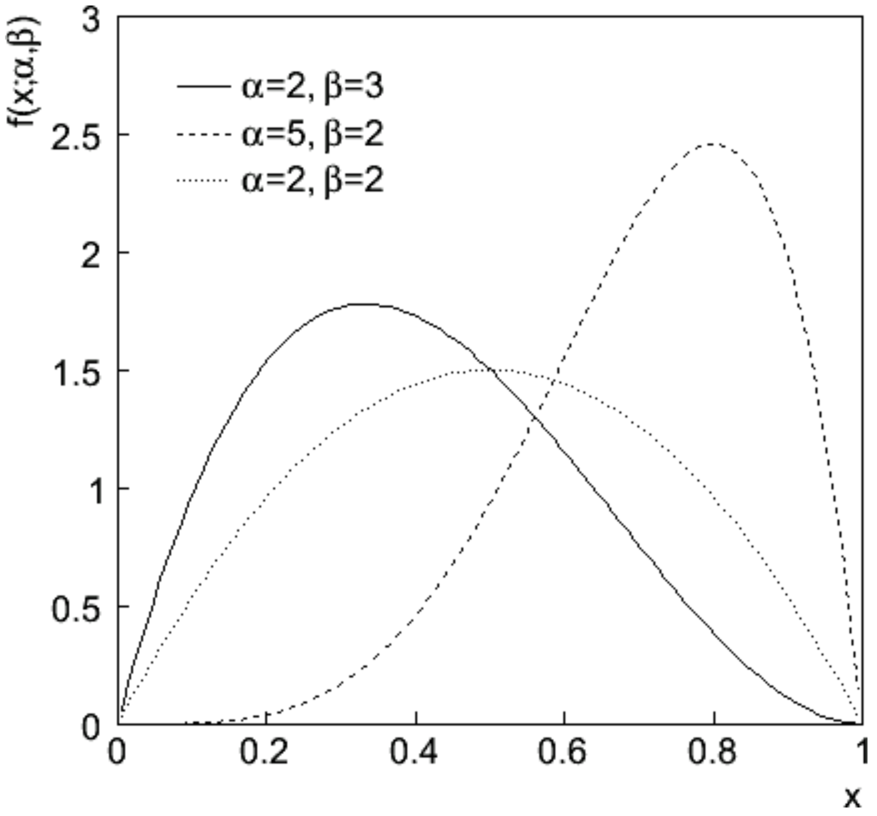


Beta distribution

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

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

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



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

Gamma distribution

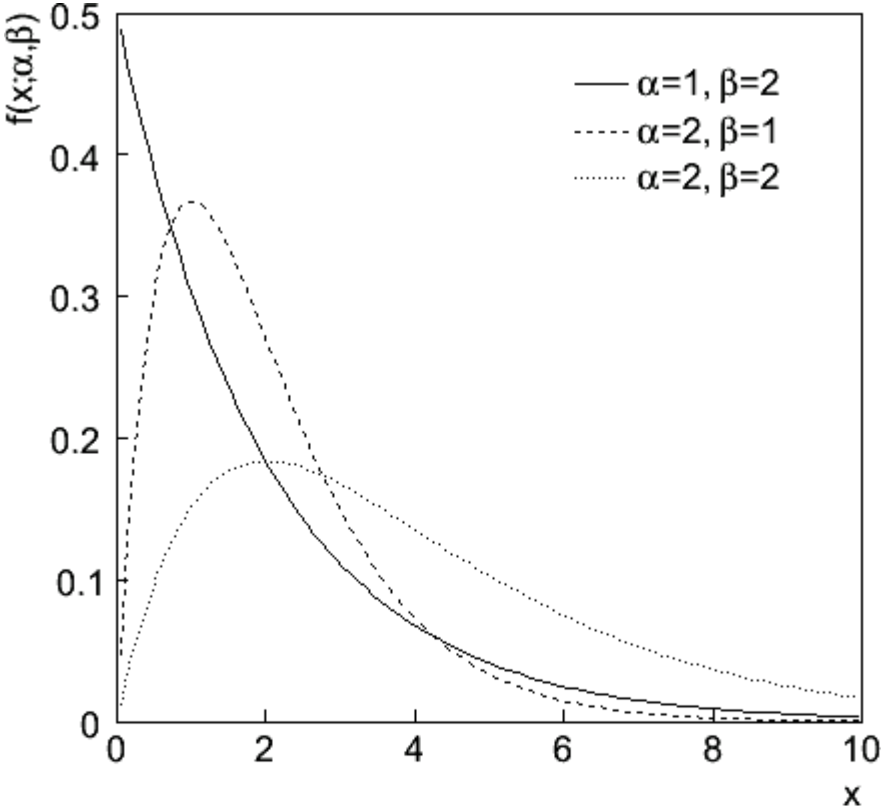
$$f(x;\alpha,\beta) = \frac{1}{\Gamma(\alpha)\beta^{\alpha}}\, x^{\alpha-1}\, e^{-x/\beta}$$

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

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

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

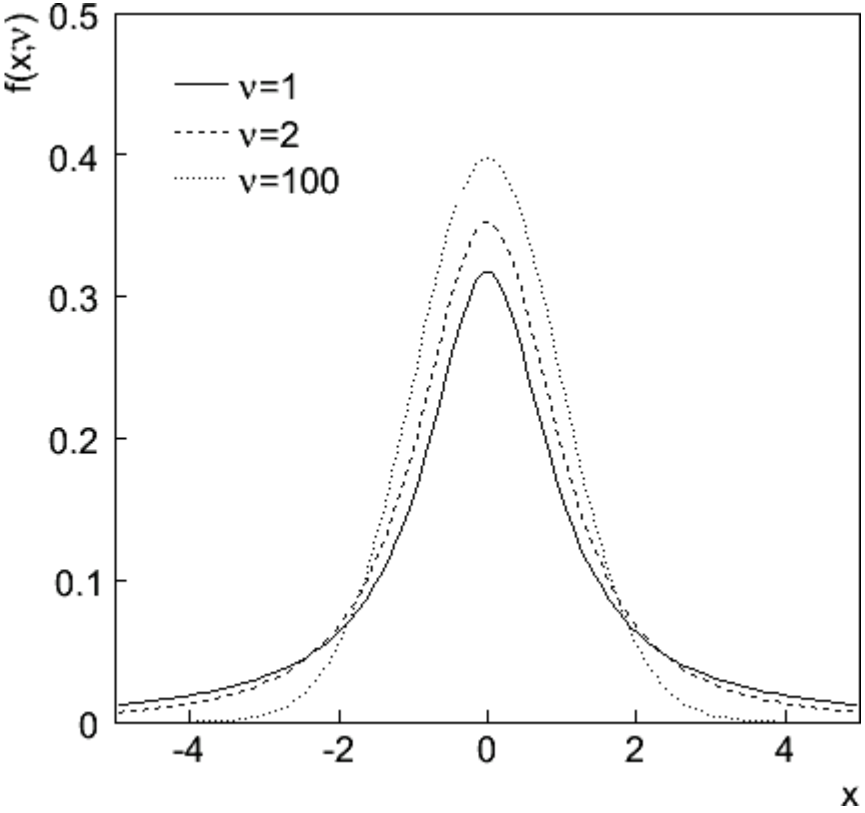


Student's *t* distribution

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

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

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



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

ν = 1 gives Cauchy,

$\nu \to \infty$ 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.

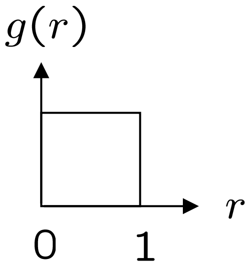
The Student's t provides a bell-shaped pdf with adjustable tails, ranging from those of a Gaussian, which fall off very quickly, ($\nu \to \infty$, but in fact already very Gauss-like for $\nu =$ two dozen), to the very long-tailed Cauchy ($\nu = 1$).

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

The Monte Carlo method

What it is: a numerical technique for calculating probabilities and related quantities using sequences of random numbers.

The usual steps:



(1) Generate sequence $r_1, r_2, \ldots, r_m$ uniform in [0, 1].

(2) Use this to produce another sequence $x_1, x_2, \ldots, x_n$ distributed according to some pdf $f(x)$ in which we're interested (x can be a vector).

(3) Use the x values to estimate some property of $f(x)$, e.g., fraction of x values with $a < x < b$ gives $\int_a^b f(x)\,dx$.

→ MC calculation = integration (at least formally)

MC generated values = 'simulated data'

→ use for testing statistical procedures

Random number generators

Goal: generate uniformly distributed values in [0, 1].

Toss coin for e.g. 32 bit number... (too tiring).

→ ‘random number generator’

= computer algorithm to generate $r_1, r_2, \ldots, r_n$.

Example: multiplicative linear congruential generator (MLCG)

$n_{i+1} = (a\, n_i) \bmod m$, where

n_i = integer

a = multiplier

m = modulus

n_0 = seed (initial value)

N.B. mod = modulus (remainder), e.g. 27 mod 5 = 2.

This rule produces a sequence of numbers $n_0, n_1, \ldots$

Random number generators (2)

The sequence is (unfortunately) periodic!

Example (see Brandt Ch 4): $a = 3$, $m = 7$, $n_0 = 1$

$$\begin{aligned}
n_1 &= (3 \cdot 1)\mathrm{mod}7 = 3 \\
n_2 &= (3 \cdot 3)\mathrm{mod}7 = 2 \\
n_3 &= (3 \cdot 2)\mathrm{mod}7 = 6 \\
n_4 &= (3 \cdot 6)\mathrm{mod}7 = 4 \\
n_5 &= (3 \cdot 4)\mathrm{mod}7 = 5 \\
n_6 &= (3 \cdot 5)\mathrm{mod}7 = 1
\end{aligned}$$

← sequence repeats

Choose a, m to obtain long period (maximum = $m - 1$); m usually close to the largest integer that can represented in the computer.

Only use a subset of a single period of the sequence.

Random number generators (3)

$r_i = n_i/m$ are in [0, 1] but are they ‘random’?

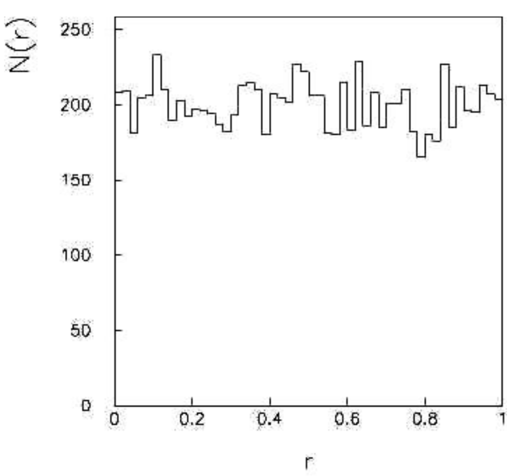
Choose a, m so that the r_i pass various tests of randomness:

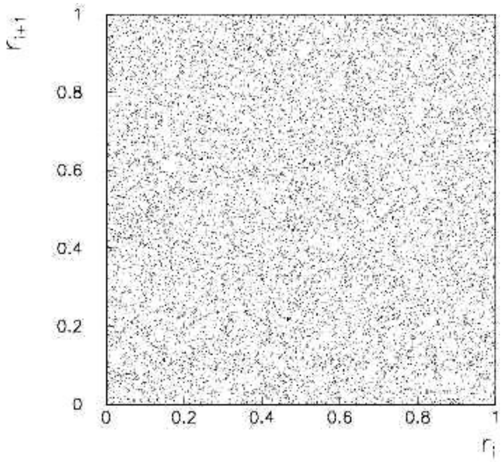
uniform distribution in [0, 1],

all values independent (no correlations between pairs),

e.g. L’Ecuyer, Commun. ACM **31** (1988) 742 suggests

$a = 40692$
$m = 2147483399$



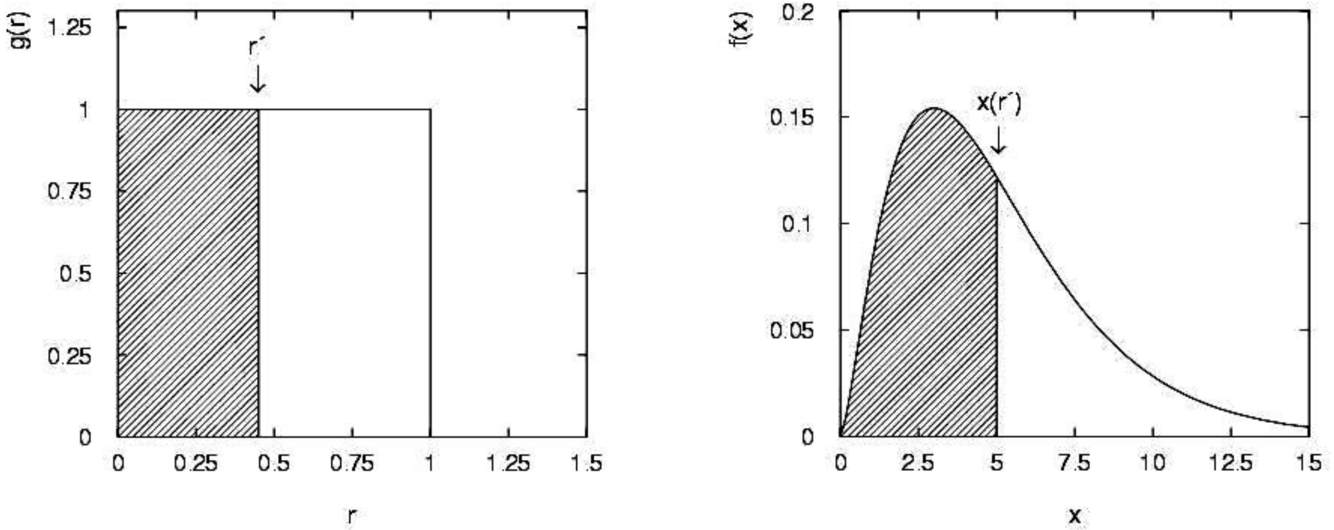


Far better generators available, e.g. `TRandom3`, based on Mersenne twister algorithm, period = $2^{19937} - 1$ (a “Mersenne prime”).

See F. James, Comp. Phys. Comm. 60 (1990) 111; Brandt Ch. 4

The transformation method

Given $r_1, r_2, \ldots, r_n$ uniform in [0, 1], find $x_1, x_2, \ldots, x_n$ that follow $f(x)$ by finding a suitable transformation $x(r)$.



Require: $P(r \le r') = P(x \le x(r'))$

i.e. $$\int_{-\infty}^{r'} g(r)\,dr = r' = \int_{-\infty}^{x(r')} f(x')\,dx' = F(x(r'))$$

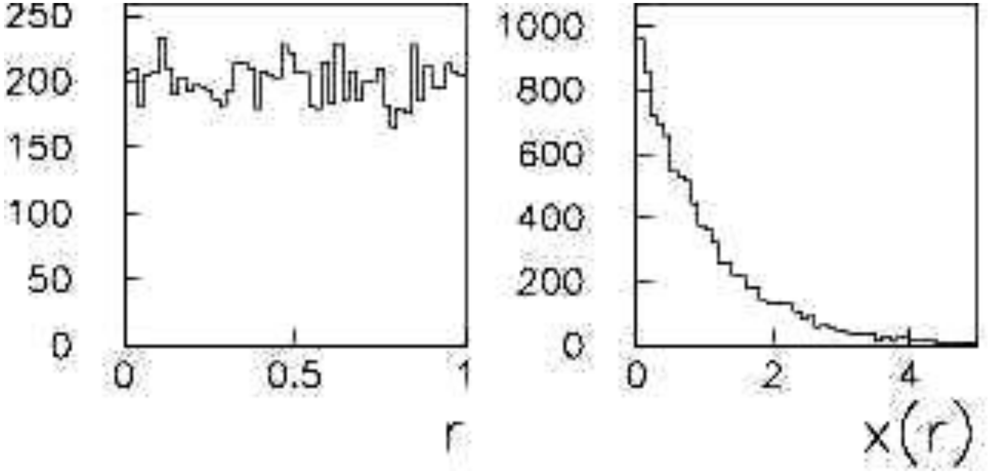
That is, $\boxed{\text{set } F(x) = r \text{ and solve for } x(r).}$

Example of the transformation method

Exponential pdf: $f(x;\xi) = \frac{1}{\xi} e^{-x/\xi} \quad (x \geq 0)$

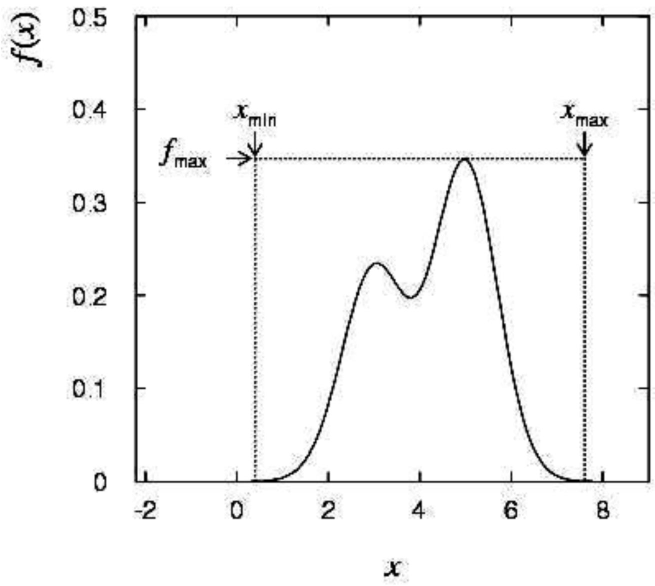
Set $\int_0^x \frac{1}{\xi} e^{-x'/\xi} \, dx' = r$ and solve for $x\,(r)$.

→ $x(r) = -\xi \ln(1-r)$ ($x(r) = -\xi \ln r$ works too.)



The acceptance-rejection method

Enclose the pdf in a box:



(1) Generate a random number x, uniform in $[x_{\text{min}}, x_{\text{max}}]$, i.e. $x = x_{\mathsf{min}} + r_1(x_{\mathsf{max}} - x_{\mathsf{min}})$, r_1 is uniform in [0,1].

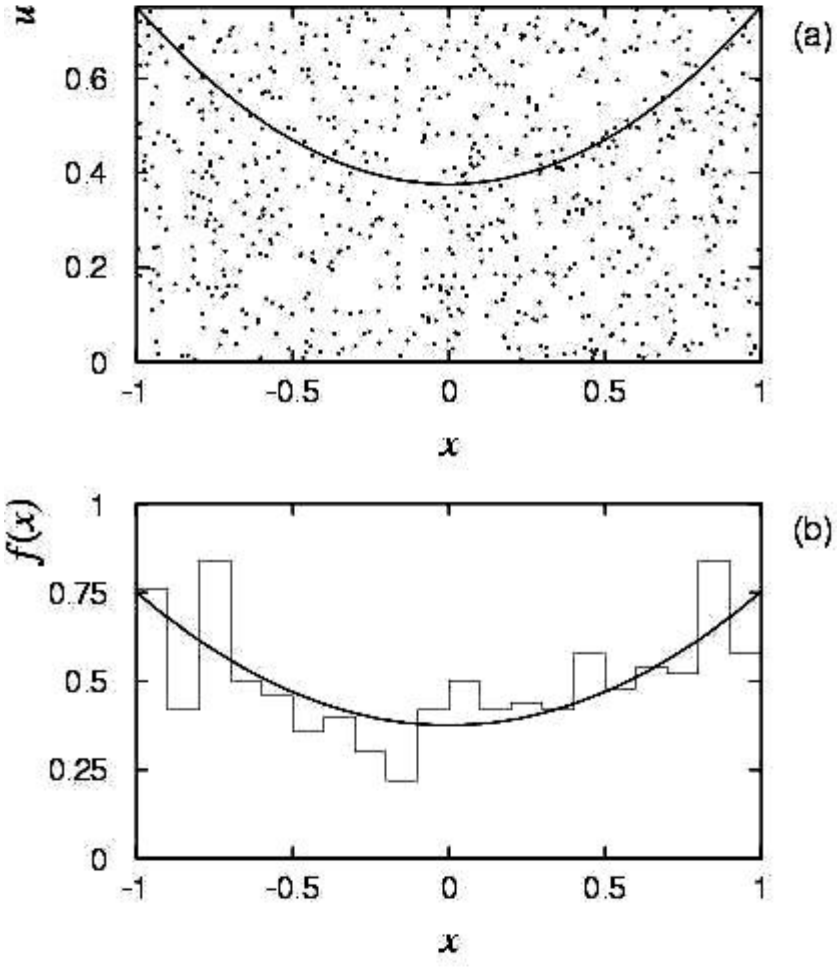
(2) Generate a 2nd independent random number u uniformly distributed between 0 and f_{max}, i.e. $u = r_2 f_{\mathsf{max}}$.

(3) If $u < f(x)$, then accept x. If not, reject x and repeat.

Example with acceptance-rejection method

$$f(x) = \frac{3}{8}(1 + x^2)$$

$$(-1 \leq x \leq 1)$$



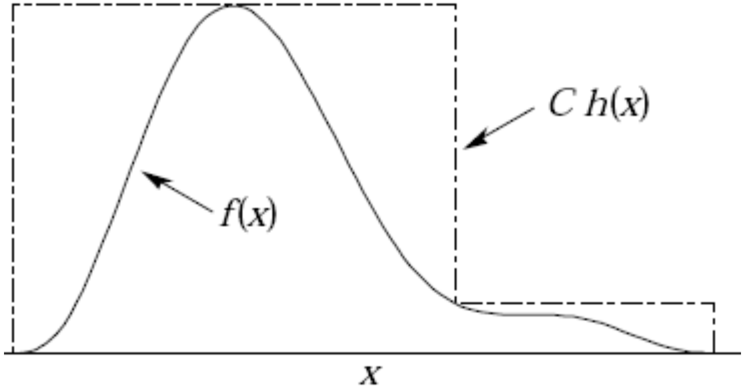
If dot below curve, use *x* value in histogram.

Improving efficiency of the acceptance-rejection method

The fraction of accepted points is equal to the fraction of the box's area under the curve.

For very peaked distributions, this may be very low and thus the algorithm may be slow.

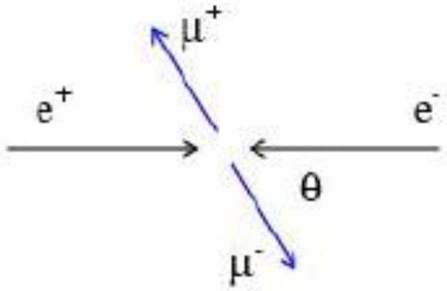
Improve by enclosing the pdf $f(x)$ in a curve $C\,h(x)$ that conforms to $f(x)$ more closely, where $h(x)$ is a pdf from which we can generate random values and C is a constant.



Generate points uniformly over $C\,h(x)$.

If point is below $f(x)$, accept x.

Monte Carlo event generators



Simple example: $e^+e^- \to \mu^+\mu^-$

Generate $\cos\theta$ and ϕ:

$$f(\cos\theta; A_{\rm FB}) \propto (1 + \frac{8}{3}A_{\rm FB}\cos\theta + \cos^2\theta) \ ,$$

$$g(\phi) = \frac{1}{2\pi} \quad (0 \le \phi \le 2\pi)$$

Less simple: ‘event generators’ for a variety of reactions:

$e^+e^- \to \mu^+\mu^-$, hadrons, ...

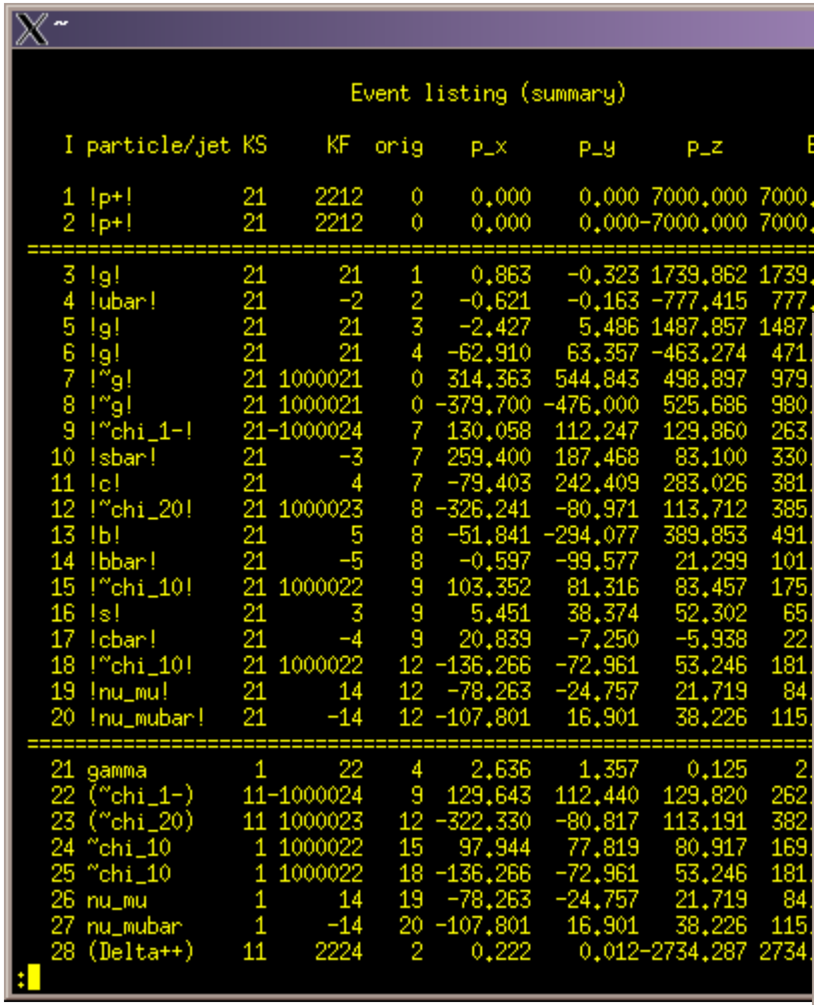
pp → hadrons, D-Y, SUSY,...

e.g. PYTHIA, HERWIG, ISAJET...

Output = ‘events’, i.e., for each event we get a list of generated particles and their momentum vectors, types, etc.

A simulated event

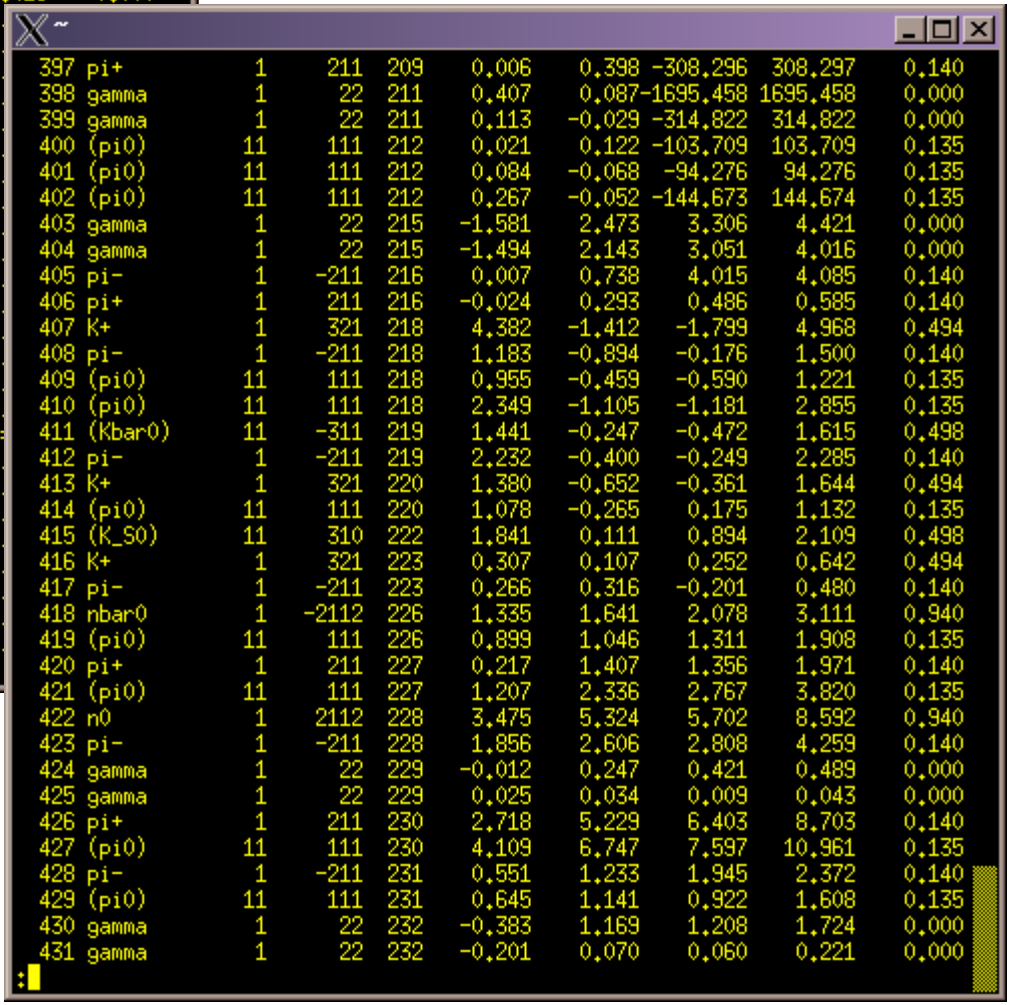
⋮



```
                        Event listing (summary)

    I particle/jet KS     KF  orig    p_x      p_y      p_z       E        m

    1 !p+!         21    2212    0    0.000    0.000 7000.000 7000.000    0.938
    2 !p+!         21    2212    0    0.000    0.000-7000.000 7000.000    0.938
 ==============================================================================
    3 !g!          21      21    1    0.863   -0.323 1739.862 1739.862    0.000
    4 !ubar!       21      -2    2   -0.621   -0.163 -777.415  777.415    0.000
    5 !g!          21      21    3   -2.427    5.486 1487.857 1487.
    6 !g!          21      21    4  -62.910   63.357 -463.274  471.
    7 !~g!         21 1000021    0  314.363  544.843  498.897  979.
    8 !~g!         21 1000021    0 -379.700 -476.000  525.686  980.
    9 !~chi_1-!    21-1000024    7  130.058  112.247  129.860  263.
   10 !sbar!       21      -3    7  259.400  187.468   83.100  330.
   11 !c!          21       4    7  -79.403  242.409  283.026  381.
   12 !~chi_20!    21 1000023    8 -326.241  -80.971  113.712  385.
   13 !b!          21       5    8  -51.841 -294.077  389.853  491.
   14 !bbar!       21      -5    8   -0.597  -99.577   21.299  101.
   15 !~chi_10!    21 1000022    9  103.352   81.316   83.457  175.
   16 !s!          21       3    9    5.451   38.374   52.302   65.
   17 !cbar!       21      -4    9   20.839   -7.250   -5.938   22.
   18 !~chi_10!    21 1000022   12 -136.266  -72.961   53.246  181.
   19 !nu_mu!      21      14   12  -78.263  -24.757   21.719   84.
   20 !nu_mubar!   21     -14   12 -107.801   16.901   38.226  115.
 ===========================================================
   21 gamma         1      22    4    2.636    1.357    0.125    2.
   22 (~chi_1-)    11-1000024    9  129.643  112.440  129.820  262.
   23 (~chi_20)    11 1000023   12 -322.330  -80.817  113.191  382.
   24 ~chi_10       1 1000022   15   97.944   77.819   80.917  169.
   25 ~chi_10       1 1000022   18 -136.266  -72.961   53.246  181.
   26 nu_mu         1      14   19  -78.263  -24.757   21.719   84.
   27 nu_mubar      1     -14   20 -107.801   16.901   38.226  115.
   28 (Delta++)    11    2224    2    0.222    0.012-2734.287 2734.
:
```



```
  397 pi+           1     211  209    0.006    0.398 -308.296  308.297    0.140
  398 gamma         1      22  211    0.407    0.087-1695.458 1695.458    0.000
  399 gamma         1      22  211    0.113   -0.029 -314.822  314.822    0.000
  400 (pi0)        11     111  212    0.021    0.122 -103.709  103.709    0.135
  401 (pi0)        11     111  212    0.084   -0.068  -94.276   94.276    0.135
  402 (pi0)        11     111  212    0.267   -0.052 -144.673  144.674    0.135
  403 gamma         1      22  215   -1.581    2.473    3.306    4.421    0.000
  404 gamma         1      22  215   -1.494    2.143    3.051    4.016    0.000
  405 pi-           1    -211  216    0.007    0.738    4.015    4.085    0.140
  406 pi+           1     211  216   -0.024    0.293    0.486    0.585    0.140
  407 K+            1     321  218    4.382   -1.412   -1.799    4.968    0.494
  408 pi-           1    -211  218    1.183   -0.894   -0.176    1.500    0.140
  409 (pi0)        11     111  218    0.955   -0.459   -0.590    1.221    0.135
  410 (pi0)        11     111  218    2.349   -1.105   -1.181    2.855    0.135
  411 (Kbar0)      11    -311  219    1.441   -0.247   -0.472    1.615    0.498
  412 pi-           1    -211  219    2.232   -0.400   -0.249    2.285    0.140
  413 K+            1     321  220    1.380   -0.652   -0.361    1.644    0.494
  414 (pi0)        11     111  220    1.078   -0.265    0.175    1.132    0.135
  415 (K_S0)       11     310  222    1.841    0.111    0.894    2.109    0.498
  416 K+            1     321  223    0.307    0.107    0.252    0.642    0.494
  417 pi-           1    -211  223    0.266    0.316   -0.201    0.480    0.140
  418 nbar0         1   -2112  226    1.335    1.641    2.078    3.111    0.940
  419 (pi0)        11     111  226    0.899    1.046    1.311    1.908    0.135
  420 pi+           1     211  227    0.217    1.407    1.356    1.971    0.140
  421 (pi0)        11     111  227    1.207    2.336    2.767    3.820    0.135
  422 n0            1    2112  228    3.475    5.324    5.702    8.592    0.940
  423 pi-           1    -211  228    1.856    2.606    2.808    4.259    0.140
  424 gamma         1      22  229   -0.012    0.247    0.421    0.489    0.000
  425 gamma         1      22  229    0.025    0.034    0.009    0.043    0.000
  426 pi+           1     211  230    2.718    5.229    6.403    8.703    0.140
  427 (pi0)        11     111  230    4.109    6.747    7.597   10.961    0.135
  428 pi-           1    -211  231    0.551    1.233    1.945    2.372    0.140
  429 (pi0)        11     111  231    0.645    1.141    0.922    1.608    0.135
  430 gamma         1      22  232   -0.383    1.169    1.208    1.724    0.000
  431 gamma         1      22  232   -0.201    0.070    0.060    0.221    0.000
:
```

⋮

PYTHIA Monte Carlo
pp → gluino-gluino

Monte Carlo detector simulation

Takes as input the particle list and momenta from generator.

Simulates detector response:

multiple Coulomb scattering (generate scattering angle),
particle decays (generate lifetime),
ionization energy loss (generate Δ),
electromagnetic, hadronic showers,
production of signals, electronics response, ...

Output = simulated raw data → input to reconstruction software:

track finding, fitting, etc.

Predict what you should see at 'detector level' given a certain hypothesis for 'generator level'. Compare with the real data.

Estimate 'efficiencies' = #events found / # events generated.

Programming package: **`GEANT`**

Next time...

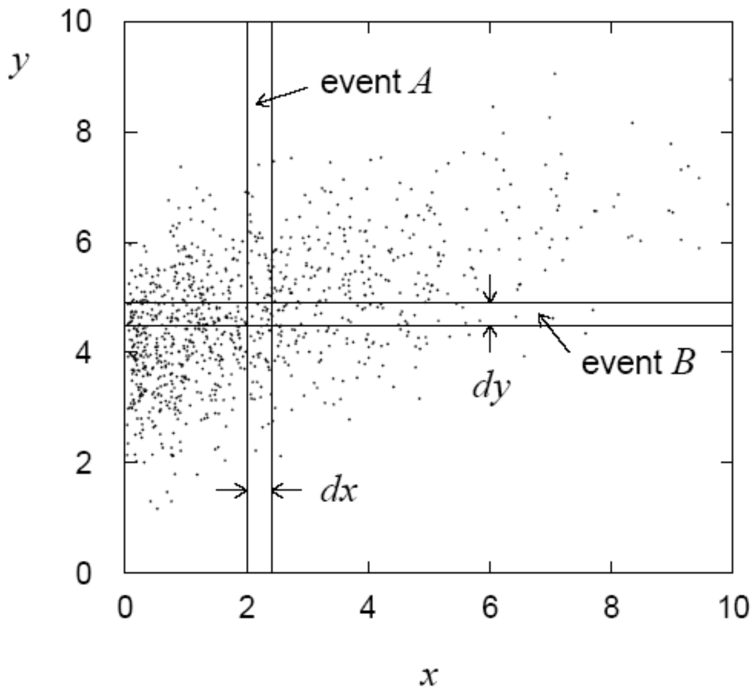
Today we have focused on probabilities, how they are defined, interpreted, quantified, manipulated, etc.

In the following lecture we will begin talking about *statistics*, i.e., how to make inferences about probabilities (e.g., probabilistic models or hypotheses) given a sample of data.

Extra slides

Multivariate distributions

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



$$P(A \cap B) = f(x,y)\,dx\,dy$$

joint pdf

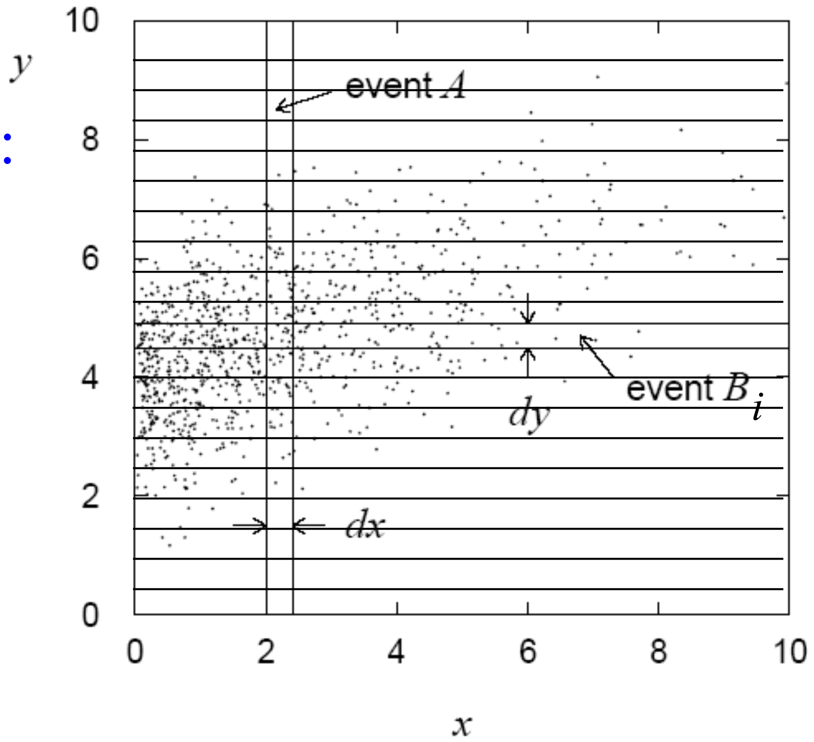
Normalization: $$\int \cdots \int f(x_1, \ldots, x_n) dx_1 \cdots dx_n = 1$$

Marginal pdf

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

$$
\begin{aligned}
P(A) &= \sum_i P(A \cap B_i) \\
&= \sum_i f(x, y_i)\, dy\, dx \\
&\to \int f(x, y)\, dy\, dx
\end{aligned}
$$

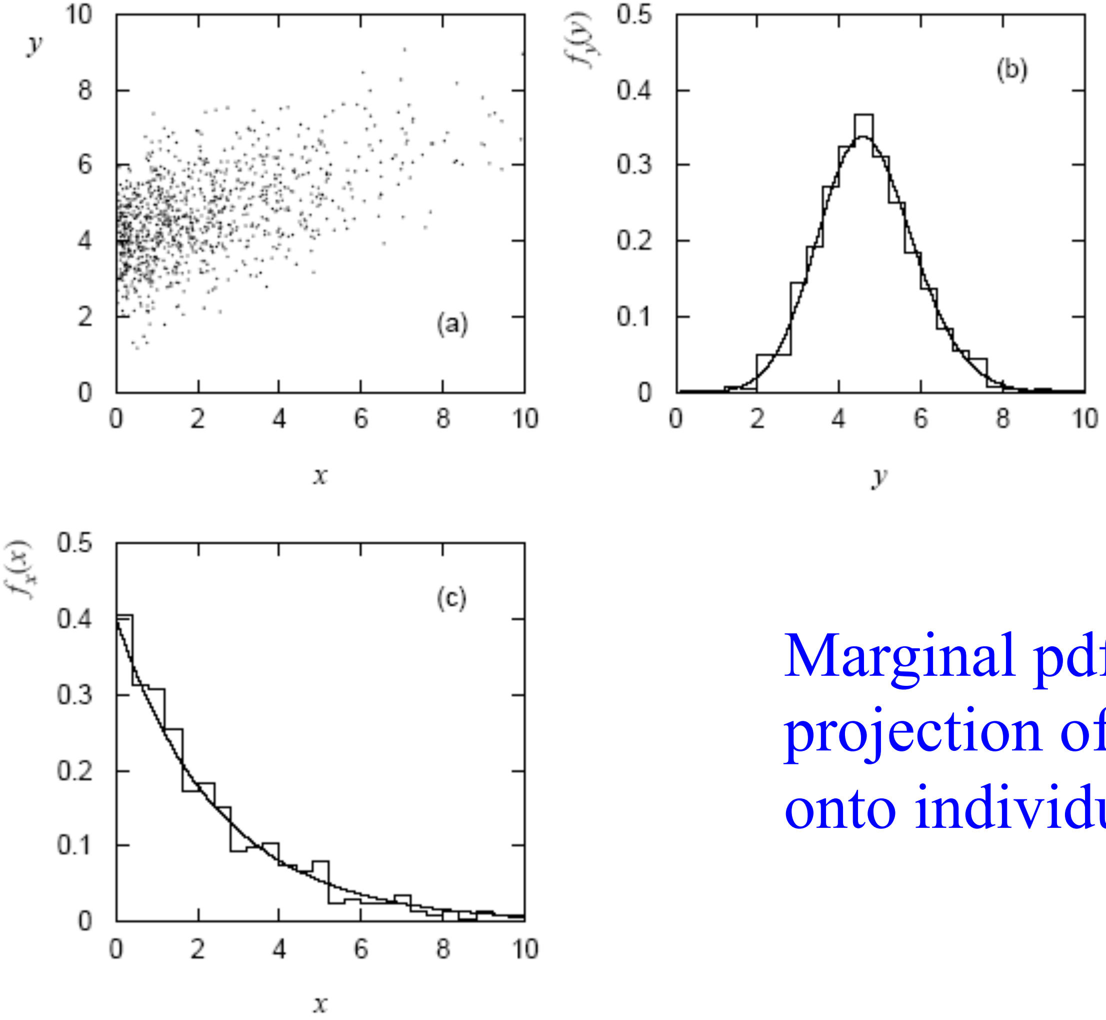
$$f_x(x) = \int f(x, y)\, dy$$



→ 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 $f(x_1, x_2) = f_1(x_1) f_2(x_2)$

Marginal pdf (2)



Marginal pdf ~ projection of joint pdf onto individual axes.

Conditional pdf

Sometimes we want to consider some components of joint pdf as constant. Recall conditional probability:

$$P(B|A) = \frac{P(A \cap B)}{P(A)} = \frac{f(x,y)\,dx\,dy}{f_x(x)\,dx}$$

→ conditional pdfs: $h(y|x) = \dfrac{f(x,y)}{f_x(x)}\,, \qquad g(x|y) = \dfrac{f(x,y)}{f_y(y)}$

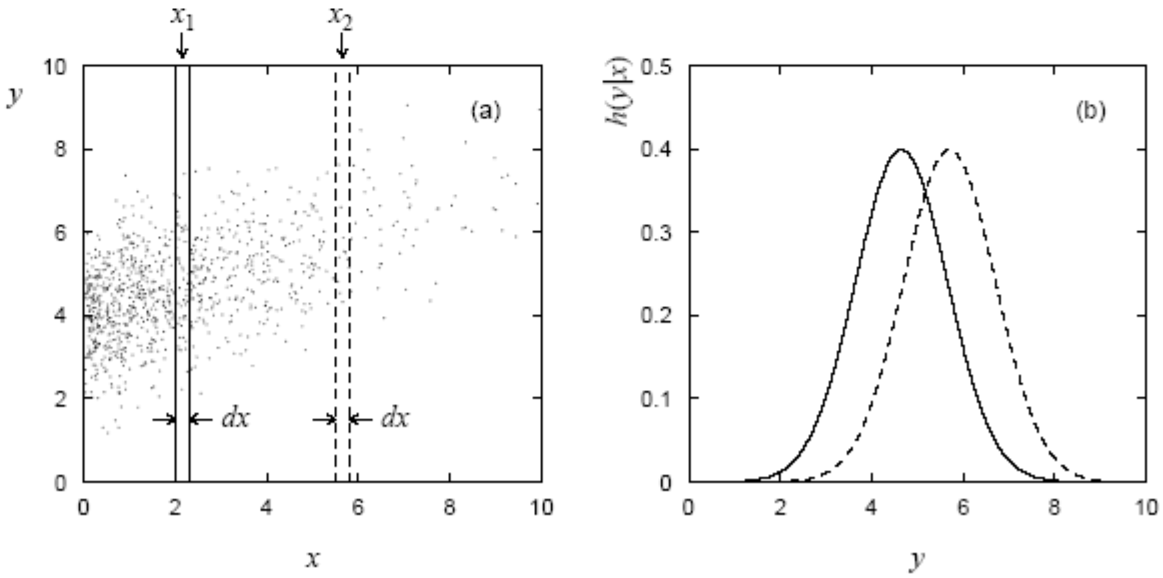
Bayes' theorem becomes: $g(x|y) = \dfrac{h(y|x) f_x(x)}{f_y(y)}\,.$

Recall *A*, *B* independent if $P(A \cap B) = P(A)P(B)\,.$

→ *x*, *y* independent if $f(x,y) = f_x(x) f_y(y)\,.$

Conditional pdfs (2)

E.g. joint pdf $f(x,y)$ used to find conditional pdfs $h(y|x_1)$, $h(y|x_2)$:



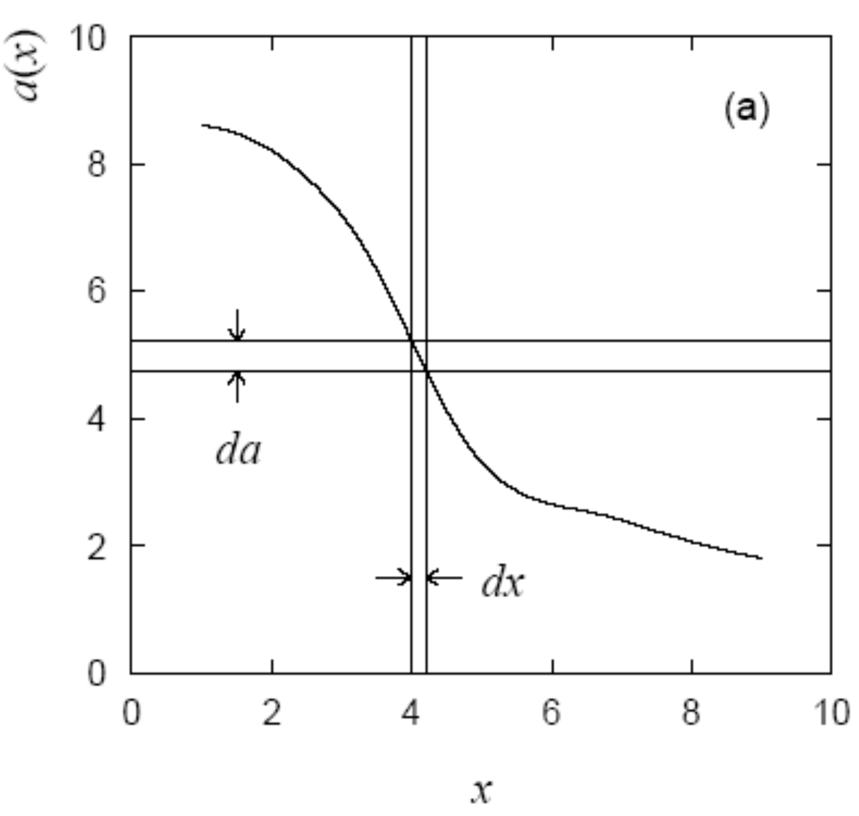
Basically treat some of the r.v.s as constant, then divide the joint pdf by the marginal pdf of those variables being held constant so that what is left has correct normalization, e.g., $\int h(y|x)\,dy = 1$.

Functions of a random variable

A function of a random variable is itself a random variable.

Suppose *x* follows a pdf *f*(*x*), consider a function *a*(*x*).

What is the pdf *g*(*a*)?



$$g(a)\,da = \int_{dS} f(x)\,dx$$

dS = region of *x* space for which *a* is in [*a*, *a*+*da*].

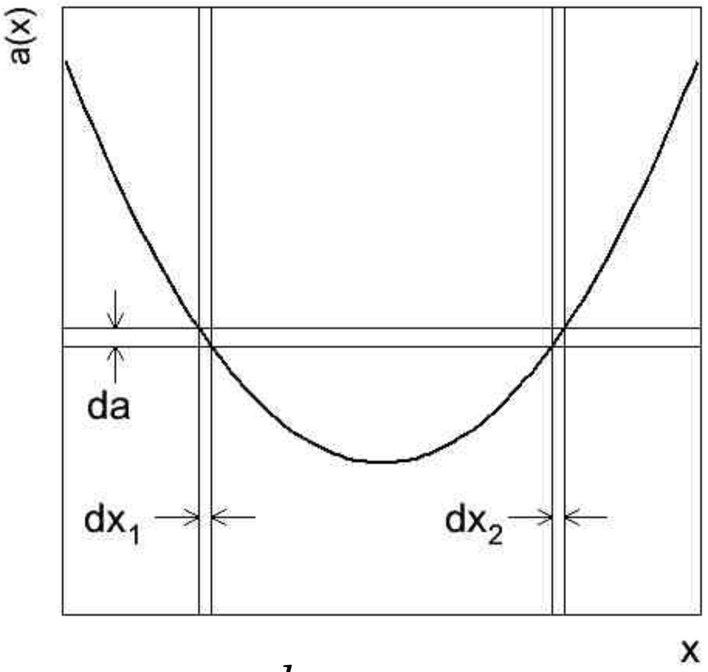
For one-variable case with unique inverse this is simply

$$g(a)\,da = f(x)\,dx$$

$$\rightarrow \quad g(a) = f(x(a)) \left|\frac{dx}{da}\right|$$

Functions without unique inverse

If inverse of *a*(*x*) not unique, include all *dx* intervals in *dS* which correspond to *da*:



Example: $$a = x^2, \;\; x = \pm\sqrt{a}, \;\; dx = \pm\frac{da}{2\sqrt{a}} \, .$$

$$dS = \left[\sqrt{a}, \sqrt{a} + \frac{da}{2\sqrt{a}}\right] \cup \left[-\sqrt{a} - \frac{da}{2\sqrt{a}}, -\sqrt{a}\right]$$

$$g(a) = \frac{f(\sqrt{a})}{2\sqrt{a}} + \frac{f(-\sqrt{a})}{2\sqrt{a}}$$

Functions of more than one r.v.

Consider r.v.s $\vec{x} = (x_1, \ldots, x_n)$ and a function $a(\vec{x})$.

$$g(a')da' = \int \ldots \int_{dS} f(x_1, \ldots, x_n) dx_1 \ldots dx_n$$

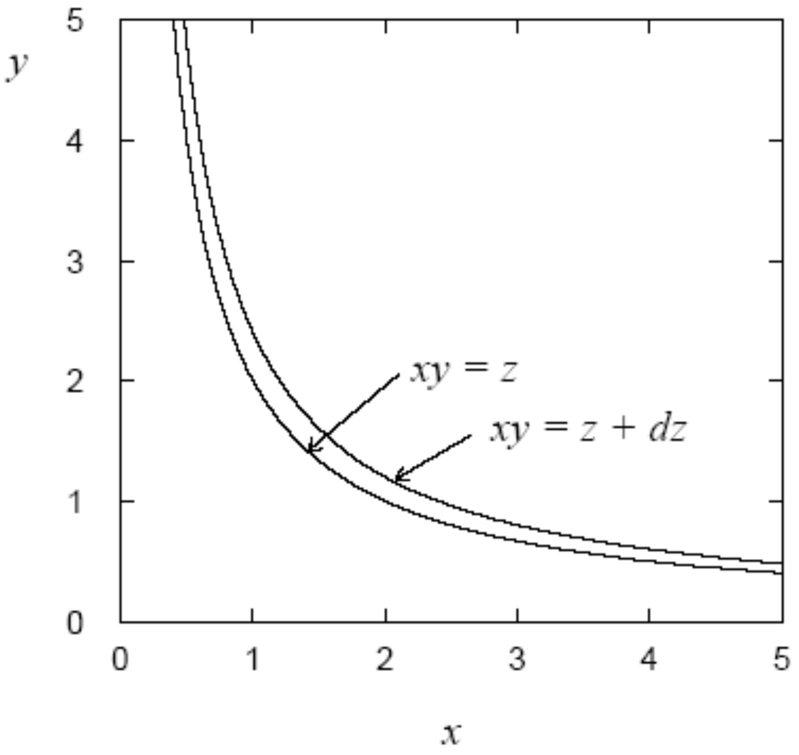
dS = region of *x*-space between (hyper)surfaces defined by

$$a(\vec{x}) = a', \; a(\vec{x}) = a' + da'$$

Functions of more than one r.v. (2)

Example: r.v.s x, $y > 0$ follow joint pdf $f(x,y)$,

consider the function $z = xy$. What is $g(z)$?



$$g(z)\,dz = \int \ldots \int_{dS} f(x,y)\,dx\,dy$$

$$= \int_0^\infty dx \int_{z/x}^{(z+dz)/x} f(x,y)\,dy$$

$$\rightarrow \quad g(z) = \int_0^\infty f(x, \frac{z}{x})\,\frac{dx}{x}$$

$$= \int_0^\infty f(\frac{z}{y}, y)\,\frac{dy}{y}$$

(Mellin convolution)

More on transformation of variables

Consider a random vector $\vec{x} = (x_1, \ldots, x_n)$ with joint pdf $f(\vec{x})$.

Form n linearly independent functions $\vec{y}(\vec{x}) = (y_1(\vec{x}), \ldots, y_n(\vec{x}))$

for which the inverse functions $x_1(\vec{y}), \ldots, x_n(\vec{y})$ exist.

Then the joint pdf of the vector of functions is $g(\vec{y}) = |J| f(\vec{x})$

where *J* is the Jacobian determinant:

$$J = \begin{vmatrix} \frac{\partial x_1}{\partial y_1} & \frac{\partial x_1}{\partial y_2} & \ldots & \frac{\partial x_1}{\partial y_n} \\ \frac{\partial x_2}{\partial y_1} & \frac{\partial x_2}{\partial y_2} & \ldots & \frac{\partial x_2}{\partial y_n} \\ \vdots & & & \vdots \\ & & \ldots & \frac{\partial x_n}{\partial y_n} \end{vmatrix}$$

For e.g. $g_1(y_1)$ integrate $g(\vec{y})$ over the unwanted components.