B. Probability and statistical distributions

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1. Probability and permutations
2. Random variables and distributions
3. Standard distributions
4. Central limit theorem
5. Transformations (Error propagation)
6. Multidimensional distributions

1. Probability

"The theory of probability and statistics is concerned with situtations in which an observation is made and which contains an element of inherent variability outwith the observer's control. He knows that if he repeated the observation under conditions which were identical in so far as he could control them, the second observation would not necessarily agree exactly with the first." (S.D. Silvey, Statistical inference)

Historically the interest in statistical problems started with investigations of games of chance.

In games of chance there are often many different outcomes, which a-priori are equally likeli (tossing a coin, throwing a dice); this can be used to make a *combinatorical* definition of probability.

Similarly one can give an *empiricial* definition of probability/frequency.

Game of chance and statistics

Christiaan Huygens, "De Ratiociniis in Ludo Aleae", 1657

Jakob Bernoulli, "Ars Conjectandi, 1705

Pascal, in 'Oevres III', 307:

> " ...res hactenus erravit incerta; nunc autem quae experimento rebellis fuit rationis dominium effugere non potuit. Eam quippe tanta securitate in artem per geometricam reduximus, ut certitudinis eius particeps facta, iam audacter prodeat; et si metheseos demonstrationes cum aleae incertitudine iungendo, et quae contraria videntur conciliando, ab ultraque nominationem suam accipiens, stupendum hunc titulum iure sibi arrogat: aleae Geometrica."

Pascal – Geometrie des Würfels

" ...die Sache (d.h. das Glückspiel) war bisher ungewiß; nun aber, nachdem sie sich gegenüber dem Experiment unzugänglich gezeigt hatte, hat sie sich dem Verstand unterwerfen müssen. Wir haben es nämlich durch geometrische Argumentation auf eine berechenbare Kunst zurückgeführt, so daß es Teil an der Strenge der Geometrie hat und zuversichtlich vorangeht; es vereinigt die mathematische Gewißheit mit der Ungewißheit des Würfels, was vorher unvereinbar schien. Es nimmt nun den Namen beider an, und beansprucht den staunenerregenden Titel: Geometrie des Würfels."

Definition of probability

Combinatorical definition. If an event can happen in n different ways, which are all equal probable, and if k of the different ways have the probability $\mathcal{A}$, then the probability for event $\mathcal{A}$ is given by

$$P(\mathcal{A}) = \frac{k}{n} \,.$$

Empirical definition of probability. An observation is repeated independently under identical conditions n times; if property $\mathcal{A}$ is observed in k of the n cases, the ratio k/n is the empirical probability for $\mathcal{A}$. The probability $P(\mathcal{A})$ can be defined as the ratio in the limit for n going to infinity:

$$P(\mathcal{A}) = \lim_{n \to \infty} \frac{k}{n}.$$

Both definitions can be critisized: the first one can be considered as a vicious circle, and the second one is based on an impossible experiment.

Formal definition of probability – Kolmogorov 1931

Elementary events e_i are considered, which *exclude* each other:

$$\begin{aligned} e_i &= \text{elementary event} \\ \Omega &= \text{set of all elementary events} \\ P(e_i) &= \text{probability of event } e_i \end{aligned}$$

The probability for elementary events has to follow the following rules:

1. $P(e_i) \geq 0$ for all i
2. $P(e_i \vee e_j) = P(e_i) + P(e_j) \quad (\vee = \text{or})$
3. $\sum_\Omega P(e_i) = 1$

Non-elementary events $\mathcal{A}$ and $\mathcal{B}$ are formed from elementary events.

Combination of probability

Given two types of events, $\mathcal{A}$ and $\mathcal{B}$. $P(\mathcal{A})$ is the probability for the occurence of event $\mathcal{A}$ and $P(\mathcal{B})$ is the probability for the occurence of event $\mathcal{B}$.

$$
\begin{array}{rll}
P(\mathcal{A} \text{ or } \mathcal{B}) = & P(\mathcal{A}) + P(\mathcal{B}) - P(\mathcal{A} \text{ and } \mathcal{B}) & \mathcal{A} \text{ or } \mathcal{B} \\
P(\mathcal{A} \text{ and } \mathcal{B}) = & 0 & \text{if } \mathcal{A} \text{ and } \mathcal{B} \text{ exclude each other} \\
P(\mathcal{A} \text{ or } \mathcal{B}) = & P(\mathcal{A}) + P(\mathcal{B}) & \text{if } \mathcal{A} \text{ and } \mathcal{B} \text{ exclude each other} \\
P(\mathcal{A} \text{ or } \overline{\mathcal{A}}) = & P(\mathcal{A}) + P(\overline{\mathcal{A}}) = 1 & (\overline{\mathcal{A}} = \text{not } \mathcal{A}) \\
P(\mathcal{A} \text{ and } \mathcal{B}) = & P(\mathcal{A}) \cdot P(\mathcal{B}|\mathcal{A}) = P(\mathcal{B}) \cdot P(\mathcal{A}|\mathcal{B}) & \mathcal{A} \text{ and } \mathcal{B} \\
P(\mathcal{A} \text{ and } \mathcal{B}) = & P(\mathcal{A}) \cdot P(\mathcal{B}) & \text{if } \mathcal{A} \text{ and } \mathcal{B} \text{ independent}
\end{array}
$$

$P(\mathcal{B}|\mathcal{A})$ is the probability for event $\mathcal{B}$, if event $\mathcal{A}$ has happened, and is called *conditional* probability.

Bayes' theorem

It relates the two conditional probabilities $P(\mathcal{A}|\mathcal{B})$ and $P(\mathcal{B}|\mathcal{A})$:

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

which follows directly from

$$P(\mathcal{A} \text{ and } \mathcal{B}) = P(\mathcal{A}) \cdot P(\mathcal{B}|\mathcal{A}) = P(\mathcal{B}) \cdot P(\mathcal{A}|\mathcal{B})$$

Generalized to n classes of events with properties $\mathcal{A}_i$, $(i = 1, 2, \ldots n)$ and $P(\mathcal{B}) = \sum_i P(\mathcal{B}|\mathcal{A}_i) \cdot P(\mathcal{A}_i)$

$$P(\mathcal{A}_i|\mathcal{B}) = \frac{P(\mathcal{B}|\mathcal{A}_i)P(\mathcal{A}_i)}{\sum_{i=1}^{n} P(\mathcal{B}|\mathcal{A}_i) \cdot P(\mathcal{A}_i)}$$

There is a special interpretation of the Bayes' theorem with controversial discussions $\rightarrow$ subjective probability

Reverend Thomas Bayes (1702-1761), "An essay towards solving a problem in the doctrine of chances, Philos. Trans. R. Society **53** (1763) 370, reprinted in Biometrika **45** (1958) 293

Application of Bayes theorem

A test for a rare, very dangerous illnes K is made.
The result is positive! What does it mean?

The illness K is rare: a-priori $P(K) = 0.001 \qquad P(\bar{K}) = 0.999$

The test result is not safe, their are known error probabilities:

in case of illness	$P(+\|K) = 0.98$	$P(-\|K) = 0.02$
no illness	$P(+\|\bar{K}) = 0.03$	$P(-\|\bar{K}) = 0.97$

Application of Bayes theorem to calculate $P(K|+)$:

$$P(K|+) = \frac{P(+|K) \cdot P(K)}{P(+|K) \cdot P(K) + P(+|\bar{K}) \cdot P(\bar{K})} = \frac{0.98 \cdot 0.001}{0.98 \cdot 0.001 + 0.03 \cdot 0.999}$$
$$= 0.033$$

Thus the probability to have illness K after a positive test is 3.3 %.

Subjective probability – the Bayesian view

A, $B, \ldots$ are hypotheses, i.e. statements, that are either true of false

$P(A) =$ degree of belief that A is true.

This definition of "probability" is consistent with the Kolmogorov axioms.
Subjective probability allows a more natural treatment of phenomena that are not repeatable.

Examples for hypotheses:

the particle is a K meson
nature is supersymmetric
the Higgs mass is 115 GeV
it will rain tomorrow

Sometimes one has to take decisions on the basis of degree of belief (take an umbrella or not).

Relative frequency – the Frequentists view

$A, B, \ldots$ are outcomes of a repeatable experiment

$P(A)$ is limit of frequency

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

This frequency interpretation is often most natural for data analysis in physics.

Examples for frequencies:

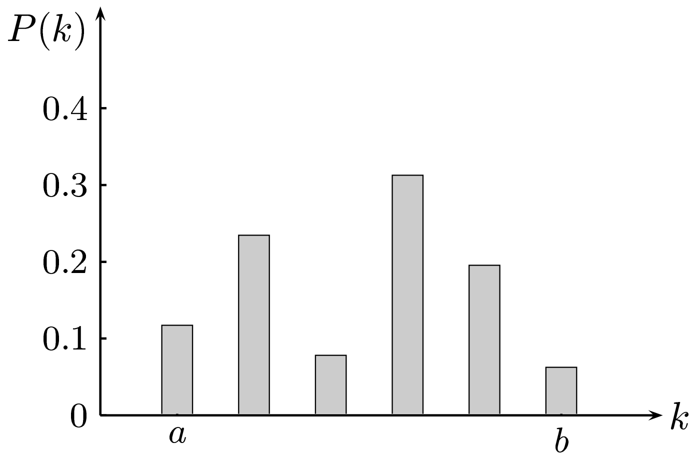
decay probability of $J/\Psi \to \mu^+\mu^-$ $(\Gamma_i/\Gamma = 6.01\%)$
detector acceptance
upper limit of electron neutrino mass is 3 eV (95 % C.L.)

The probability of hypotheses $A, B, \ldots$ is either 1 (true) of 0 (false).

Discrete random variables

A discrete variable k can take on a finite or infinite number of values k_i with $i = a, a+1, \ldots b$. The probability for the value k_i is $P(k_i)$ with the normalization

$$\sum_{i=a}^{b} P(k_i) = 1 \; .$$



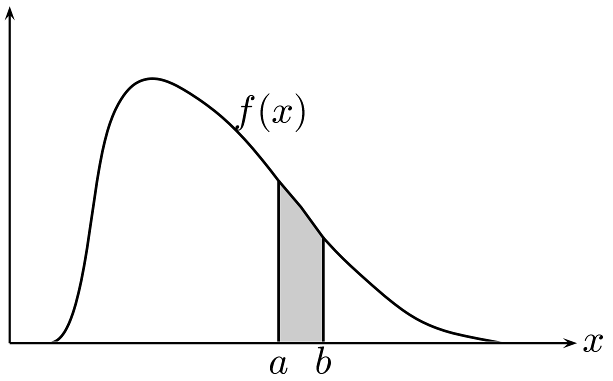
Continuous random variables

A continuous random variables x can take on values from a continuum. The probability for x to fall in the interval $a \leq x < b$ is

$$P\,(a \leq x < b) = \int_a^b f(x)\,\mathrm{d}x$$

where the function $f(x)$ is called *probability density* of the random variable x; the density is non-negative and is normalized to 1:

$$f(x) \geq 0 \qquad \int_{-\infty}^{+\infty} f(x)\,\mathrm{d}x = 1$$



Continuous random variables contnd.

The *distribution function* $F(x)$ is defined by

$$F(x) = \int_{-\infty}^{x} f(x')\,\mathrm{d}x' \qquad \text{with} \quad F(-\infty) = 0 \quad \text{and} \quad F(+\infty) = 1\,.$$

The distribution function and the probability density function are related also by $f(x) = \mathrm{d}F(x)/\,\mathrm{d}x$.

Expectation values

The *expectation value* of the function $h(x)$, where x is a random variable from a density $f(x)$, is defined by

$$E[h] = \int_{-\infty}^{+\infty} h(x)\, f(x)\, \mathrm{d}x \qquad E[h] = \sum_{i=a}^{b} h(r_i)\, P(r_i)\,.$$

Important special cases are the expectation value of x or k, or mean value, and the *variance* of x or k:

$$E[x] = \int_{-\infty}^{+\infty} x\, f(x)\, \mathrm{d}x = \langle x \rangle \qquad E[k] = \sum_{i=a}^{b} k_i P(k_i) = \langle k \rangle$$

$$V[x] = \int_{-\infty}^{+\infty} (x - \langle x \rangle)^2\; f(x)\, \mathrm{d}x \qquad V[k] = \sum_{i=a}^{b} (k_i - \langle k \rangle)^2\, P(k_i)$$

$$\text{standard deviation} \qquad \sigma = \sqrt{V}$$

Expectation and variance

The expectation of a random variable x is often called μ, it is the standard parameter describing the "center of mass" of a distribution of a random variable. The variance of a random variable is non-negative; the square root is called the standard deviation σ and is the standard measure of the "width" of a distribution.

The expectation is a linear operator:

$$E[a \cdot g(x) + b \cdot h(x)] = a \cdot E[g(x)] + b \cdot E[h(x)]$$

For the variance operator

$$V[a \cdot g(x)] = a^2 \cdot V[g(x)]$$

is valid.

Algebraic and central moments

Moments:

$$\begin{aligned} n\text{-th algebraic moment} &= \alpha_n = E[x^n] \\ n\text{-th central moment} &= m_n = E[(x - \langle x \rangle)^n] \end{aligned}$$

Central moments are defined with respect to the mean value.

Some moments and functions of moments have a special name:

Mean value = first algebraic moment	=	$E[x] = \mu = \alpha_1$
Variance = second central moment	=	$V[x] = m_2 = \sigma^2 = \alpha_2 - \mu^2$
Skewness	=	$\beta_1 = m_3^2/m_2^3$
Coefficient of skewness	=	$\gamma_1 = \sqrt{\beta_1} = m_3/\sigma^3$
Kurtosis	=	$\gamma_2 = m_4/m_2^2 - 3$

Tschebyscheff inequality

The probability for a deviation of a random variable from the mean value μ by k times the standard deviation σ depends on the specific distribution.

An upper limit is given, *independently* of the distribution, by the Tschebyscheff inequality:

$$\boxed{P\left(|x - \mu| \geq k\sigma\right) \leq \frac{1}{k^2}}$$

The statement is rather weak, but general and useful in special cases.

$$\begin{aligned} \sigma^2 &= \int_{-\infty}^{+\infty} (x - \langle x \rangle)^2 \cdot f(x)\,\mathrm{d}x \\ &= \left[\int_{-\infty}^{\langle x \rangle - k\sigma} + \int_{\langle x \rangle - k\sigma}^{\langle x \rangle + k\sigma} + \int_{\langle x \rangle + k\sigma}^{+\infty}\right] (x - \langle x \rangle)^2 \cdot f(x)\,\mathrm{d}x \end{aligned}$$

Tschebyscheff inequality contnd.

All three integrals are positive; removing the middle one an inequality is obtained:

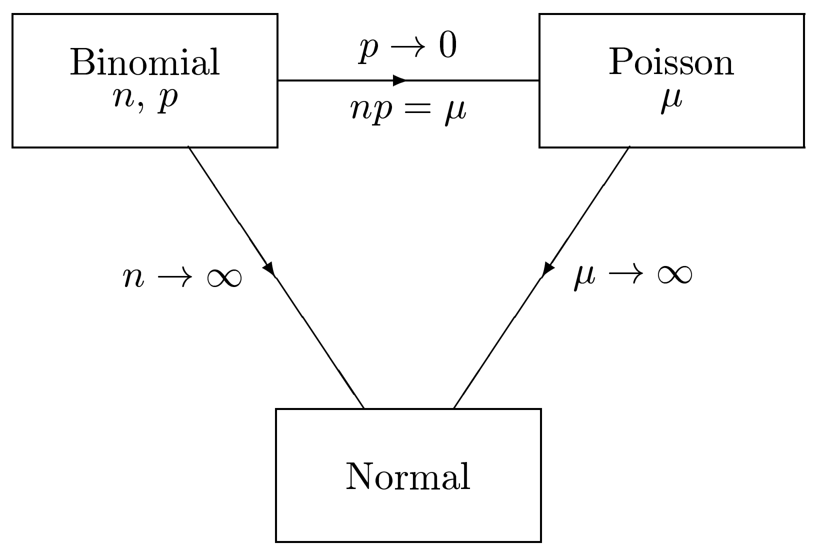
$$\sigma^2 \geq \int_{-\infty}^{\langle x\rangle - k\sigma} (x - \langle x\rangle)^2 \cdot f(x)\,\mathrm{d}x + \int_{\langle x\rangle + k\sigma}^{+\infty} (x - \langle x\rangle)^2 \cdot f(x)\,\mathrm{d}x\,.$$

Making use of the inequalities $x < \langle x\rangle - k\sigma$ bzw. $x > \langle x\rangle + k\sigma$ in the two remaining integrals the inequality

$$\begin{aligned} \sigma^2 &\geq k^2\sigma^2 \left[\int_{-\infty}^{\langle x\rangle - k\sigma} f(x)\,\mathrm{d}x + \int_{\langle x\rangle + k\sigma}^{+\infty} f(x)\,\mathrm{d}x\right] \\ &= P\left(|x - \mu| \geq k\sigma\right) \end{aligned}$$

is obtained. The expression in parentheses is the probability for $|x - \langle x\rangle| \geq k\sigma$, which proves the Tschebyscheff inequality.

3. Standard distributions



Binomial distribution

If the probability for a certain event is equal to p, the probability to observe in n experiments exactly k of the events, is given by the Binomial distribution:

$$\boxed{P_n(k) = \binom{n}{k} p^k \, (1-p)^{n-k} \qquad k = 0,\, 1,\, \ldots n}$$

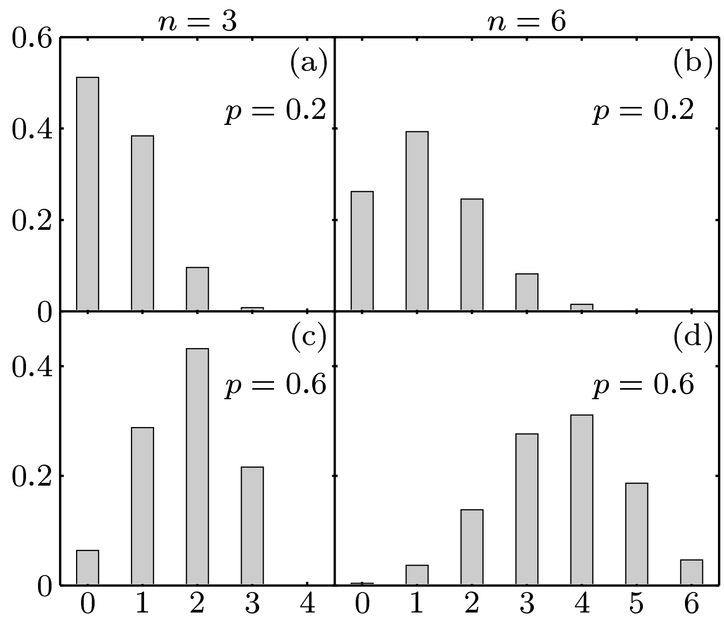
The factor $\binom{n}{k}$ ist the number of possibilities to select k elements out of total n different elements.

In a single event there are two possible outcomes, one (often called "success") with probability p and another (often called "failure") with probability $q = 1 - p$.

Expectation value $= E[k] = n\,p$ Variance $= V[k] = n\,p(1-p)$

Binomial distribution contnd.

Expectation value $= E[k] = n\,p$ Variance $= V[k] = n\,p(1-p)$



Law of large numbers

Estimate: If for an unknown value of p the values n and k are known from an experiment, the unknown value of the probability p can be estimated by $h = k/n$. An unbiased estimate of the variance of h is given by

$$V(h) = \frac{1}{n(n-1)} n \left(\frac{k}{n}\right)\left(1 - \frac{k}{n}\right)$$

The law of large numbers. The accuracy of an estimate h of the probability in an Binomial process increases with n.

$$V[h] = V[k/n] = \frac{1}{n^2} V[k] = \frac{1}{n^2} n\, p\, (1-p)$$

Because of $p\,(1-p) \leq 1/4$ for any value of p, one can estimate

$$V[h] \leq \frac{1}{4}\frac{1}{n} \qquad \sigma(h) \propto \frac{1}{\sqrt{n}}$$

The error of the estimate h can be made as small as required by choosing a sufficiently high value of n.

Poisson distribution

Consider Binomial distribution with $n \to \infty$, $p \to 0$, but $n \cdot p \to \mu$ (fixed):

$$\boxed{P_\mu(k) = \frac{\mu^k}{k!} e^{-\mu} \qquad k = 0, 1, \ldots}$$

Expectation value $E[k] = \mu$ Variance $V[k] = \mu$

For rate of events, which is constant in time t: number of events k follows a Poisson distribtion, and time difference t follows exponential distribution:

$$f(t;\tau)\,\mathrm{d}t = \frac{1}{\tau} e^{-t/\tau}\,\mathrm{d}t$$

Normal distribution

The normal distribution ist the most important continous distribution; almost anything which is a sum of many random contributions, follows (approximately) the normal distribution ($\rightarrow$ central limit theorem).

$$\boxed{f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \qquad x \in (-\infty, \infty)}$$

Expectation value $E[x] = \mu$ Variance $V[x] = \sigma^2$

$$\begin{aligned} P(|x-\mu| < 1\cdot\sigma) &= 68.26\% \\ P(|x-\mu| < 2\cdot\sigma) &= 95.45\% \\ P(|x-\mu| < 3\cdot\sigma) &= 99.73\% \end{aligned}$$

4. Central limit theorem

In the limit of large n the sum $\sum_i x_i$ becomes a random variable with mean $\sum_i \mu_i$ and with variance $\sum_i \sigma_i^2$, which follows the normal distribution, regardless of the distribution *of the individual variables x_i.*

- Characteristic functions
- Sum of independent random variables
- Normal distribution
- Proof
- Numerical examples

For finite n: theorem is valid, if sum is not dominated by one (few) terms

- velocity component v_x of gas molecules (good example)
- energy loss of charged particles traversing thin gas layer (bad example, Landau distribution)

Characteristic functions

Given a random variable x with probability density $f(x)$, the characteristic function $\phi(t)$ (or Fourier transform) is defined as the expectation of e^{itx}

$$\phi(t) = E\left[e^{itx}\right] = \int_{-\infty}^{+\infty} e^{itx} \cdot f(x)\,\mathrm{d}x$$

with the inverse operation

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-itx} \cdot \phi(t)\,\mathrm{d}t\,.$$

The characteristic function for a random variable x can be expanded in a Taylor series by

$$\phi(t) = \sum_{n=0}^{\infty} \left.\frac{\mathrm{d}^n\phi}{\mathrm{d}t^n}\right|_{t=0} \frac{t^n}{n!} = \sum_{n=0}^{\infty} \frac{(it)^n}{n!} E\left[x^n\right] \qquad E\left[x^n\right] = \alpha_n$$

Special case: $t = 0$

$$\begin{aligned}
\phi(0) &= 1 \qquad \text{(Normalization)} \\
\left.\frac{d\phi(t)}{dt}\right|_{t=0} &= \left.\int_{-\infty}^{+\infty} ixe^{itx} f(x)\mathrm{d}x\right|_{t=0} = i\langle x\rangle \\
\left.\frac{d^2\phi(t)}{dt^2}\right|_{t=0} &= -\left.\int_{-\infty}^{+\infty} x^2 e^{itx} f(x)\mathrm{d}x\right|_{t=0} = -E\left[x^2\right] = -\left(\sigma^2 + \langle x\rangle^2\right)
\end{aligned}$$

or more general for the n-th derivative:

$$\left.\frac{d^n\phi(t)}{dt^n}\right|_{t=0} = i^n \int_{-\infty}^{+\infty} x^n f(x)\mathrm{d}x = i^n\,\alpha_n$$

Thus it may be simple to calculate all the moments of a distribution $f(x)$ defined by the characteristic function $\phi(t)$.
In the special case of a mean value of 0 the first few terms are

$$\phi(t) = 1 - \frac{1}{2!}t^2\sigma^2 - \frac{i}{3!}t^3 E\left[x^3\right]\ldots$$

Sum of independent random variables

The characteristic function $\phi_z(t)$ for a *sum* $z = \sum_i x_i$ of n independent random variables $x_1, x_2 \ldots x_n$ with probability densities $f_1(x_1), f_2(x_2) \ldots f_n(x_n)$ with characteristic functions $\phi_1(t), \phi_2(t) \ldots \phi_n(t)$ is given by the *product* of the individual characteristic functions:

$$\boxed{\phi_z(t) = \phi_1(t) \cdot \phi_2(t) \cdots \phi_n(t)}$$

This relation follows simply from the definition of the characteristic function:

$$\phi_z(t) = \int \ldots \int \exp\left(it \sum_{i=1}^{n} x_i\right) f_1(x_1)\, f_2(x_2) \cdots f_n(x_n)\, \mathrm{d}x_1\, \mathrm{d}x_2 \cdots \mathrm{d}x_n$$
$$= \int e^{itx_1} f_1(x_1)\, \mathrm{d}x_1 \cdots \int e^{itx_n} f_n(x_n)\, \mathrm{d}x_n$$

Normal distribution

Density $f(x)$ and the characteristic function $\phi(t)$ are:

$$f(x)\, \mathrm{d}x = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{\sigma^2}\right) \mathrm{d}x \qquad \phi(t) = \exp\left(i\mu t - \frac{1}{2}\sigma^2 t^2\right)$$

The addition theorem can be used to prove, that the sum $z = x + y$ of two random numbers x and y from the normal distribution with mean values μ_x and μ_y and with standard deviations σ_x and σ_y is a random number with mean $\mu_x + \mu_y$ and standard deviation $\sqrt{\sigma_x^2 + \sigma_y^2}$, which again follows the normal distribution:

$$\phi_z(t) = \phi_x(t) \cdot \phi_y(t) = \exp\left(i\mu_x t - \frac{1}{2}\sigma_x^2 t^2\right) \cdot \exp\left(i\mu_y t - \frac{1}{2}\sigma_y^2 t^2\right)$$
$$= \exp\left[i\left(\mu_x + \mu_y\right) t - \frac{1}{2}\left(\sigma_x^2 + \sigma_y^2\right) t^2\right]$$

Central limit theorem

In the limit of large n the sum $\sum_i x_i$ becomes a random variable with mean $\sum_i \mu_i$ and with variance $\sum_i \sigma_i^2$, which follows the normal distribution, regardless of the distribution *of the individual variables x_i.*

Proof: case of equal variances σ_i^2 is assumed, with fixed value of n, and the transformed sum

$$z = \sum_{i=1}^{n} \frac{x_i - \mu_i}{\sqrt{n}}$$

is considered; each term in the sum has a mean value of zero and a variance of σ^2/n. The characteristic function of the sum z can be expressed in terms of a Taylor expansion:

$$\phi_z(t) = \prod_{i=1}^{n} \phi_i(t) = \prod_{i=1}^{n} \left(1 - \frac{1}{2!} t^2 \frac{\sigma^2}{n} - \frac{i}{3!} t^3 \frac{E\left[(x_i - \mu_i)^3 \right]}{n^{3/2}} + \ldots \right)$$

Central limit theorem contnd.

Neglecting terms with the third and higher moments in the limit of large n the characteristic function of the sum z is

$$\phi_z(t) = \prod_{i=1}^{n} \phi_i(t) \approx \prod_{i=1}^{n} \left(1 - \frac{1}{2!} t^2 \frac{\sigma^2}{n} \right) = \left(1 - \frac{1}{2!} t^2 \frac{\sigma^2}{n} \right)^n$$

for which in the limit $n \to \infty$

$$\lim_{n\to\infty} \left(1 - \frac{1}{2!} t^2 \frac{\sigma^2}{n} \right)^n = \exp\left(-\frac{1}{2} \sigma^2 t^2 \right)$$

follows; this is the characteristic function of the normal distribution with mean zero and variance σ^2.

$$\lim_{n\to\infty} \left(1 + \frac{u}{n} \right)^n = \lim_{n\to\infty} \left(1 + \binom{n}{1} \frac{u}{n} + \binom{n}{2} \left(\frac{u}{n} \right)^2 + \ldots \right)$$
$$= \lim_{n\to\infty} \left(1 + u + \frac{1}{2} \frac{n-1}{n} u^2 + \ldots \right) = e^u$$

5. Transformation (error propagation)

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

Suppose x follows a pdf $f_x(x)$ and the transformation

$$y = y(x) \tag{1}$$

of x into a variable y is given; what is the pdf $f_y(y)$?

Transformation of a single variable

Consider intervals $(x, x + \mathrm{d}x)$ and $(y, y + \mathrm{d}y)$. For intervals

$$f_x(x)\,|\,\mathrm{d}x| = f_y(y)\,|\,\mathrm{d}y|$$

$$f_y(y) = f_x\left(x\left(y\right)\right)\left|\frac{\mathrm{d}x}{\mathrm{d}y}\right| = f_x\left(x\left(y\right)\right)\left|\frac{1}{\mathrm{d}y/\,\mathrm{d}x}\right|$$

If the inverse of $y(x)$ is not unique, include all branches.

Example: $y = x^2$ $\qquad x = \pm\sqrt{y} \qquad \mathrm{d}x = \pm\frac{\mathrm{d}y}{2\sqrt{y}}$

Transformed distribution:

transf. distribution $\qquad f_y(y) = \dfrac{1}{2\sqrt{y}}\left(f_x(+\sqrt{y}) + f_x(-\sqrt{y})\right)$

Example: Linear transformation $y = ax + b \qquad x = (y - b)/a$

transf. distr. $f_y(y) = \dfrac{1}{a} f_x\left(\dfrac{y-b}{a}\right) \qquad E[y] = a{\cdot}E[x]{+}b \qquad V[y] = a^2 V[x]$

Error propagation

Nonlinear transformation $y = y(x)$ may be complicated.

Simpler: transform mean and variance based on expansion

$$y(x) = y(\langle x \rangle) + (x - \langle x \rangle) \left. \frac{\mathrm{d}y}{\mathrm{d}x} \right|_{x=\langle x \rangle} + \frac{1}{2}(x - \langle x \rangle)^2 \left. \frac{\mathrm{d}^2 y}{\mathrm{d}x^2} \right|_{x=\langle x \rangle} + \dots$$

Taking terms up to second order with correction term

$$\text{mean} \quad \langle y \rangle \approx y(\langle x \rangle) \qquad + \frac{1}{2}\sigma_x^2 \left. \frac{\mathrm{d}^2 y}{\mathrm{d}x^2} \right|_{x=\langle x \rangle}$$

$$\text{Variance} \qquad V[y] \approx \left(\frac{\mathrm{d}y}{\mathrm{d}x} \right)^2 \cdot V[x] \qquad \text{error propagation}$$

6. Multidimensional distributions

Starting with two random variables x and y ...

The two-dimensional probability density $f(x, y)$ is defined by the probability to find (x, y) in intervals $a \leq x < b$ and $c \leq y < d$:

$$P(a \leq x < b \, , c \leq y < d) = \int_c^d \int_a^b f(x, y) \, \mathrm{d}x \, \mathrm{d}y \, .$$

Normalisation:

$$\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(x, y) \, \mathrm{d}x \, \mathrm{d}y = 1 \, .$$

Marginal distributions:

$$f_x(y) = \int_{-\infty}^{\infty} f(x, y) \, \mathrm{d}x \qquad f_y(x) = \int_{-\infty}^{\infty} f(x, y) \, \mathrm{d}y \, .$$

They represent the probability density of the random variables x and y, resp., if the other variable is ignored.

Two-dimensional distributions

For a given $x = x_0$ the conditional probability density function is given by

$$f(y|x_0) = \frac{f(x_0, y)}{\int f(x_0, y)\,\mathrm{d}y} = \frac{f(x_0, y)}{f_y(x_0)}.$$

From the marginal and the conditional p.d.f. the joint p.d.f. is obtained:

$$f(x, y) = f(y|x)\; f_y(x)$$

For independent variables the joint p.d.f. factorizes:

$$f(x, y) = f_x(x) \cdot f_y(y)$$

Expectation, variance and covariance

$$\begin{aligned}
E[x] &= \iint x f(x,y)\,\mathrm{d}x\,\mathrm{d}y = \int x f_y(x)\,\mathrm{d}x \\
E[y] &= \iint y f(x,y)\,\mathrm{d}x\,\mathrm{d}y = \int y f_x(y)\,\mathrm{d}y \\
V[x] &= \iint (x - \langle x \rangle)^2 f(x,y)\,\mathrm{d}x\,\mathrm{d}y = \sigma_x^2 \\
V[y] &= \iint (y - \langle y \rangle)^2 f(x,y)\,\mathrm{d}x\,\mathrm{d}y = \sigma_y^2 \,.
\end{aligned}$$

A new quantity:

covariance $\qquad \sigma_{xy} = \mathrm{cov}(x, y) = \iint (x - \langle x \rangle)\,(y - \langle y \rangle)\, f(x,y)\,\mathrm{d}x\,\mathrm{d}y\,.$

correlation coefficient ρ_{xy} $\qquad \sigma_{xy} = \rho_{xy}\, \sigma_x \sigma_y \qquad -1 \le \rho \le +1$

$$\begin{aligned}
x \text{ and } y \text{ independent} \quad &\rightarrow \quad \rho = 0 \\
\rho = 0 \quad &\rightarrow \quad x \text{ and } y \text{ independent or dependent} \\
\rho = +1 \text{ or } -1 \quad &\rightarrow \quad x \text{ and } y \text{ completely correlated}
\end{aligned}$$

Vectors

A n-vector $\boldsymbol{x}$ has n elements $x_1, x_2, \ldots x_n$ in a column; the *transposed* vector $\boldsymbol{x}^T$ is a row vector:

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \qquad \boldsymbol{x}^T = (x_1, x_2, \ldots x_n) \ .$$

The *scalar* product of two vectors $\boldsymbol{x}$ und $\boldsymbol{y}$ is defined by

$$\boldsymbol{x}^T \boldsymbol{y} = \sum_{i=1}^{n} x_i \, y_i = x_1 \, y_1 + x_2 \, y_2 + \ldots + x_n \, y_n \ .$$

with $\boldsymbol{x}^T \boldsymbol{y} = \boldsymbol{y}^T \boldsymbol{x}$. The *norm* of a vector is defined by

$$|\boldsymbol{x}| = \left(\boldsymbol{x}^T \boldsymbol{x}\right)^{1/2} \ .$$

Matrices

A $m \times n$ Matrix $\boldsymbol{A}$ is a scheme of m rows and n columns; the element A_{ij} is the element in row i and column j:

$$\boldsymbol{A} = (A_{ij}) = \begin{pmatrix} A_{11} & A_{12} & \ldots & A_{1n} \\ A_{21} & A_{22} & \ldots & A_{2n} \\ . & . & \ldots & . \\ A_{m1} & A_{m2} & \ldots & A_{mn} \end{pmatrix} \ .$$

The *transposed* of matrix $\boldsymbol{A}$ is $\boldsymbol{A}^T$ and has the elements $(\boldsymbol{A}^T)_{ij} = (\boldsymbol{A})_{ji}$. The matrix is called *symmetric* if $\boldsymbol{A} = \boldsymbol{A}^T$.

The elements A_{ii} of a *square* matrix are called *diagonal elements* of matrix $\boldsymbol{A}$; the sum of the diagonal elements is called *trace* of the matrix: $\text{trace}(\boldsymbol{A}) = \sum_i A_{ii}$.

The *unit* matrix $\mathbf{1}$ has all diagonal elements equal to 1, all other elements are 0.

Addition and subtraction of vectors and matrices is done elementwise; the operands have to agree in their dimensions.

Proof of inequality for correlation coefficient

Correlation coefficient ρ defined by $\sigma_{xy} = \rho\sigma_x\sigma_y$:

$$|\rho_{xy}| = \frac{|\sigma_{xy}|}{\sqrt{\sigma_x^2\sigma_y^2}} \leq 1$$

Consider expectation value

$$E\left[(a(x - \langle x\rangle) + b(y - \langle y\rangle))^2\right] = a^2\sigma_x^2 + b^2\sigma_y^2 + 2ab\sigma_{xy} \geq 0$$

. . . for any values of a and b.

Written with matrices: quadratic form

$$\begin{pmatrix} a & b \end{pmatrix} \begin{pmatrix} \sigma_x^2 & \sigma_{xy} \\ \sigma_{xy} & \sigma_y^2 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = a^2\sigma_x^2 + b^2\sigma_y^2 + 2ab\sigma_{xy} \geq 0$$

$$\begin{vmatrix} \sigma_x^2 & \sigma_{xy} \\ \sigma_{xy} & \sigma_y^2 \end{vmatrix} = \sigma_x^2\sigma_y^2 - \sigma_{xy}^2 \geq 0$$

which proves the inequality.

n-dimensional random variable

Consider random vector $\boldsymbol{x}$ with components x_i, $(i = 1, 2, \ldots n)$.

Probability density function:

$$f(x_1, x_2, \ldots x_n) = f(\boldsymbol{x})$$

Expectation values with $\langle\boldsymbol{x}\rangle = E[\boldsymbol{x}]$:

$$\begin{aligned} E[x_i] = \langle x_i\rangle &= \int x_i f(x_1, x_2, \ldots, x_n)\,\mathrm{d}x_1\,\mathrm{d}x_2 \ldots \mathrm{d}x_n \\ &= \int x_i \cdot f(\boldsymbol{x})\,\mathrm{d}x_1\,\mathrm{d}x_2 \ldots \mathrm{d}x_n\ . \end{aligned}$$

Variance

Generalization of the variance:

$$\text{covariance matrix} \quad \boldsymbol{V} = \boldsymbol{V}[\boldsymbol{x}] = E\left[(\boldsymbol{x} - E[\boldsymbol{x}])(\boldsymbol{x} - E[\boldsymbol{x}])^T\right]$$

with diagonal and not-diagonal elements:

$$\begin{aligned} V_{ii} &= \operatorname{var}(x_i) = \int (x_i - \langle x_i \rangle)^2 \cdot f(\boldsymbol{x}) \, \mathrm{d}x_1 \, \mathrm{d}x_2 \ldots \mathrm{d}x_n \\ V_{ij} &= \operatorname{cov}(x_i, x_j) = \int (x_i - \langle x_i \rangle)(x_j - \langle x_j \rangle) \cdot f(\boldsymbol{x}) \, \mathrm{d}x_1 \, \mathrm{d}x_2 \ldots \mathrm{d}x_n \, . \end{aligned}$$

Multivariate normal distribution

Generalization of the one-dimensional normal distribution to the case of n dimensions.
The random variable is a n-vector $\boldsymbol{x}$, the density depends on the n-vector μ_x of mean values and on the n-by-n covariance matrix V_x.

$$\boxed{f(\boldsymbol{x}) = \frac{|\boldsymbol{W}|^{1/2}}{(2\pi)^{n/2}} \exp\left(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu_x})^T \boldsymbol{W} (\boldsymbol{x} - \boldsymbol{\mu_x})\right)}$$

with $\boldsymbol{W} = \boldsymbol{V}^{-1}$ and $|\boldsymbol{W}| = \det \boldsymbol{W} = |\boldsymbol{V}^{-1}|$.

The n-dimensional normal distribution is often used as approximation to other n-dimensional distributions; the parameters of the n-dimensional normal distribution are just

- the first moment (mean $\boldsymbol{\mu}$), and
- the second central moment (covariance matrix $\boldsymbol{V}$).

Covariance matrix

$$\begin{pmatrix} V_{11} & V_{12} & \cdots & V_{1n} \\ V_{21} & V_{22} & \cdots & V_{2n} \\ \cdots & \cdots & & \\ V_{n1} & V_{n2} & \cdots & V_{nn} \end{pmatrix} = \begin{pmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 & \cdots & \rho_{1n}\sigma_1\sigma_n \\ \rho_{12}\sigma_2\sigma_1 & \sigma_2^2 & \cdots & \rho_{2n}\sigma_2\sigma_n \\ \cdots & \cdots & & \\ \rho_{1n}\sigma_n\sigma_1 & \rho_{2n}\sigma_n\sigma_2 & \cdots & \sigma_n^2 \end{pmatrix}$$

Two-dimensional normal distribution

Covariance matrix $\boldsymbol{V}$ in terms of x and y:

$$\boldsymbol{V} = \begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix} = \begin{pmatrix} \sigma_x^2 & \rho\sigma_x\sigma_y \\ \rho\sigma_y\sigma_x & \sigma_y^2 \end{pmatrix}$$

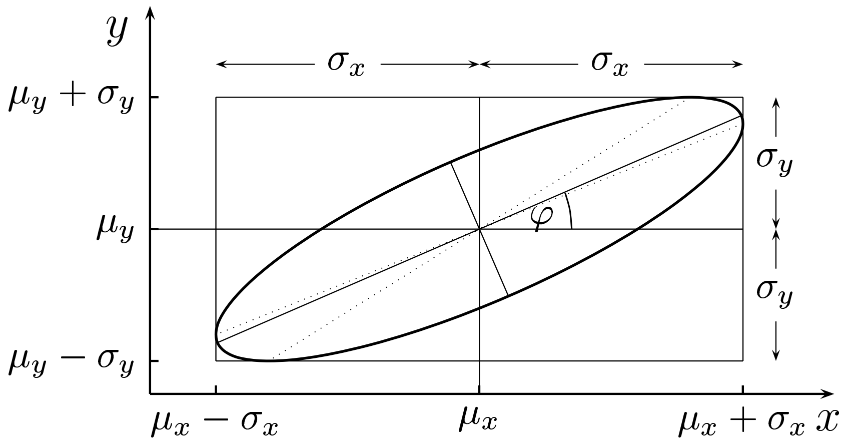
Inverse covariance matrix = weight matrix:

$$\boldsymbol{W} = \boldsymbol{V}^{-1} = \frac{1}{1-\rho^2} \begin{pmatrix} 1/\sigma_x^2 & -\rho/(\sigma_x\sigma_y) \\ -\rho/(\sigma_y\sigma_2) & 1/\sigma_y^2 \end{pmatrix}$$

$$f(x,y)\,\mathrm{d}x\,\mathrm{d}y = \frac{1}{2\pi\sigma_x\sigma_y\sqrt{1-\rho^2}} \cdot \exp\left\{-\frac{1}{2(1-\rho^2)}\right.$$
$$\left.\left[\left(\frac{x-\langle x\rangle}{\sigma_x}\right)^2 - 2\rho\left(\frac{x-\langle x\rangle}{\sigma_x}\right)\left(\frac{y-\langle y\rangle}{\sigma_y}\right) + \left(\frac{y-\langle y\rangle}{\sigma_y}\right)^2\right]\right\}\mathrm{d}x\,\mathrm{d}y$$

Two-dimensional normal distribution - contour

Elliptical 1σ contour (38 % probability content) with mean values μ_x, μ_y, standard deviations σ_x, σ_y and $\rho = +0.8$.



Main axes of the ellipse with the angles φ und $\varphi + \pi/2$ given by $\tan 2\varphi = \pm(2\rho\sigma_x\sigma_y)/(\sigma_x^2 - \sigma_y^2)$.
Dotted lines = conditional means $x - \mu_x = (y - \mu_y)\rho\sigma_x/\sigma_y$ and $y - \mu_y = (x - \mu_x)\rho\sigma_y/\sigma_x$.

Linear transformation

n-by-m matrix $\boldsymbol{B}$ with elements $B_{ik} = \partial y_i/\partial x_k$ transforms n-vector $\boldsymbol{x}$ with mean $\boldsymbol{\mu_x}$ and covariance matrix $\boldsymbol{V}(\boldsymbol{x})$ to m-vector $\boldsymbol{y}$

$$\langle \boldsymbol{y} \rangle = \boldsymbol{\mu_y} E[\boldsymbol{y}] = E[\boldsymbol{Bx}] = \boldsymbol{B} E[\boldsymbol{x}] = \boldsymbol{B}\boldsymbol{\mu_x}$$

(expectation is a linear operator)

Covariance matrix: "error" propagation

$$\begin{aligned}\boldsymbol{V}[\boldsymbol{y}] = E\left[(\boldsymbol{y} - \boldsymbol{\mu_y})(\boldsymbol{y} - \boldsymbol{\mu_y})^T)\right] &= E\left[(\boldsymbol{Bx} - \boldsymbol{B\mu_x})(\boldsymbol{Bx} - \boldsymbol{B\mu_x})^T\right] \\ &= E\left[\boldsymbol{B}(\boldsymbol{x} - \boldsymbol{\mu}_x)(\boldsymbol{x} - \boldsymbol{\mu}_x)^T \boldsymbol{B}^T\right] \\ &= \boldsymbol{B} \cdot E\left[(\boldsymbol{x} - \boldsymbol{\mu}_x)(\boldsymbol{x} - \boldsymbol{\mu}_x)^T\right] \boldsymbol{B}^T = \boldsymbol{BV}[\boldsymbol{x}]\,\boldsymbol{B}^T\end{aligned}$$

General transformation

$$y_i = y_i(x_1, x_2, \ldots x_n) = y_i(\boldsymbol{x})$$

In principle p.d.f. $f_y(\boldsymbol{y})$ can be calculated from $f_x(\boldsymbol{x})$ (assuming same dimensions):

$$f_x(\boldsymbol{x})\,\mathrm{d}x_1\,\mathrm{d}x_2 \ldots \mathrm{d}x_n = f_y(\boldsymbol{y})\,\mathrm{d}y_1\,\mathrm{d}y_2 \ldots \mathrm{d}y_n \;,$$

where $f_x(\boldsymbol{x})$ and $f_y(\boldsymbol{y})$ are multi-dimensional p.d.f's.

$$f_y(\boldsymbol{y}) = f_x(\boldsymbol{x}) \cdot J\left(\frac{x}{y}\right) \;, \qquad (2)$$

where the x_k have to be expressed by the y_i. $J\,(x/y)$ is Jakobi determinant:

$$J\left(\frac{x}{y}\right) = \left|\frac{\partial x_1 \partial x_2 \cdots \partial x_n}{\partial y_1 \partial y_2 \cdots \partial y_n}\right| \;.$$

Non-linear transformation

The approximate calculation of the covariance matrix uses the matrix $\boldsymbol{B}$ of derivatives:

$$\boldsymbol{B} = \begin{pmatrix} \partial y_1/\partial x_1 & \partial y_1/\partial x_2 & \ldots & \partial y_1/\partial x_n \\ \partial y_2/\partial x_1 & \partial y_2/\partial x_2 & \ldots & \partial y_2/\partial x_n \\ \ldots & & & \\ \ldots & & & \\ \partial y_m/\partial x_1 & \partial y_m/\partial x_2 & \ldots & \partial y_m/\partial x_n \end{pmatrix} \;,$$

(each element calculated for mean value $\boldsymbol{\mu}_y$).

General law of "error" propagation:

$$\boldsymbol{V}\,[\boldsymbol{y}] = \boldsymbol{B}\boldsymbol{V}\,[\boldsymbol{x}]\,\boldsymbol{B}^T$$

χ^2 *distribution*

If $x_i \in N(0,1)$ for $i = 1,\, 2, \ldots n$, then the sum

$$u = \chi^2 = \sum_{i=1}^{n} x_i^2$$

follows a χ^2 distribution $f_n(u) = f_n(\chi^2)$ with n degrees of freedom.

$$\boxed{f_n(u) \;=\; \frac{\frac{1}{2}\left(\frac{u}{2}\right)^{n/2-1} e^{-u/2}}{\Gamma(n/2)}} \qquad \text{density}$$

Important for statistical tests ("goodness of fit").

Correlations between data points

Case of two *correlated* data points:

$$\text{Covariance matrix} \quad \boldsymbol{V} = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}$$

$$\begin{aligned} \sigma_{1,2} &= \text{standard deviations of the variables} \\ \rho &= \text{correlation coefficient} \qquad -1 < \rho < +1 \end{aligned}$$

The χ^2 value for a deviation $\boldsymbol{\Delta}$ from a theoretical prediction is given by:

$$\boxed{\chi^2 = \boldsymbol{\Delta}^T \left(\boldsymbol{V}^{-1}\right) \boldsymbol{\Delta}}$$

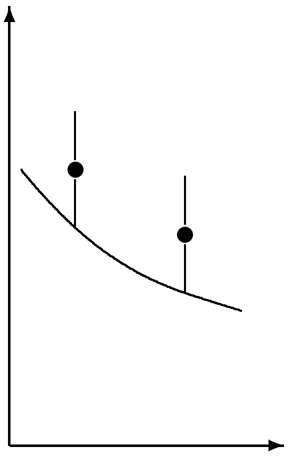
with the inverse of the covariance matrix

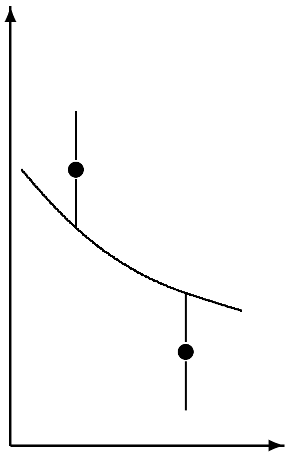
$$\boldsymbol{V}^{-1} = \frac{1}{(1-\rho^2)} \begin{pmatrix} 1/\sigma_1^2 & -\rho/\sigma_1\sigma_2 \\ -\rho/\sigma_1\sigma_2 & 1/\sigma_2^2 \end{pmatrix}$$

Numerical Example for deviations

$\sigma_1 = \sigma_2 = \sigma$ and two deviations $\Delta = \pm 1\,\sigma$

$$\chi^2 = \begin{cases} 2/(1+\rho) & \text{same sign of } \Delta \\ 2/(1-\rho) & \text{opposite sign of } \Delta \end{cases}$$





Numerical Example - averaging of two data points contnd.

Probability from χ^2

	same sign	opposite sign
$\rho = 0$	37 %	37 %
$\rho = +0.9$	59 %	0.0005 %
$\rho = -0.9$	0.0005 %	59 %

Conclusion: Difficult interpretation of *common* deviations of > 1 data point in case of *correlated* ($\rho \neq 0$) data points.

Numerical Example - averaging of two data points

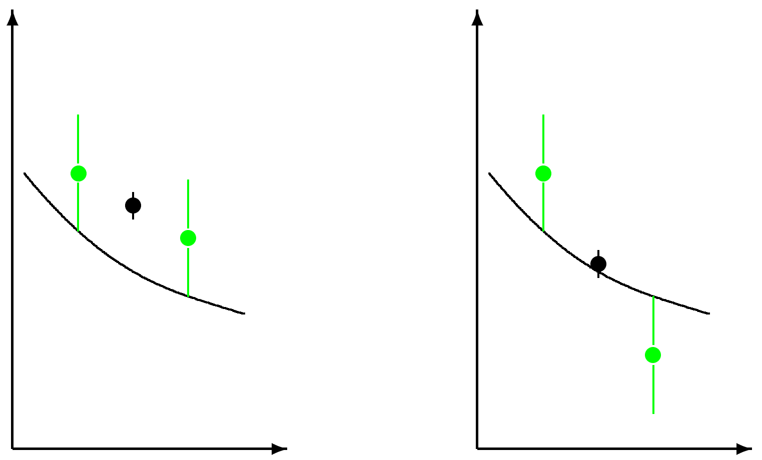
$\sigma_1 = \sigma_2 = \sigma$ and correlation coefficient ρ

Standard deviation of averaged data point:

	$\sqrt{\frac{1+\rho}{2}}\,\sigma$	comment
$\rho = 0$	$0.707\ \sigma$	$1/\sqrt{2}$
$\rho = +0.9$	$0.975\ \sigma$	same precison as single point
$\rho = -0.9$	$0.224\ \sigma$	much more accurate

Numerical Example - averaging of two data points contnd.

Averaging in case of negatively correlated data points:



Conclusion:

- Averaging of data points with large negative correlations results in very accurate values.
- Averaging of data points with large positive correlation reduces the number of data points without increasing their accuracy.

Multinomial distribution

The multinomial distribution is the generalization of the binomial distribtion to the case of m different possible outcomes.

There are n (non-negative) probabilities p_i with the constraint $\sum_i p_i = 1$. The probability to obtain k_1 events of type 1, k_2 events of type 2, $\ldots k_m$ events of type m for total n $(= \sum_i k_i)$ events is given by

$$P(k_1, \ldots, k_m; n, p_1, \ldots, p_m) = \frac{n}{k_1! k_2! \cdots k_m!} p_1^{k_1} \cdot p_2^{k_2} \cdots p_m^{k_m}$$

The factor is equal to the number of possibilities to select from total n elements k_1 elements of type 1, k_2 elements of type 2 ... and k_m elements of type m.

$$E[k_i] = n\, p_i \qquad V[\boldsymbol{k}]_{ij} = \begin{cases} -np_i p_j & i \neq j \\ np\,(1-p_i) & i = j \end{cases}$$