# Statistical analysis of experimental data
# **Measurements and their uncertainties**

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**Lecture 03**

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## Measurements and their uncertainties

**Probability distribution function** (PDF)
also called "Probability density function" in some books

For given random variable $X$, probability distribution function, $f(x)$, describes the probability to obtain given numerical result $x$ (in single experiment). For infinitesimal interval $dx$:

$$P(x < X < x + dx) = f(x)\, dx$$

For arbitrary interval $[x_1, x_2]$:

$$P(x_1 < X < x_2) = \int_{x_1}^{x_2} dx\, f(x)$$

This can be considered an alternative definition of $f(x)$

## Cumulative distribution function

We can also define cumulative distribution function $F(x)$, which is the probability that an experiment will result in a value not grater than $x$:

$$F(x) \;=\; P(X < x)$$

Probability distribution function can be then written as the derivative:

$$f(x) \;=\; \frac{dF(x)}{dx}$$

Probability that the $X$ value observed is in the range from $x_1$ to $x_2$:

$$P(x_1 < X < x_2) \;=\; F(x_2) - F(x_1) \;=\; \int_{x_1}^{x_2} dx\, f(x)$$

**Moment** of order $n$ ($n^{th}$ moment) is defined as

$$\mu_n = \mathbb{E}(X^n) = \langle x^n \rangle = \int_{-\infty}^{+\infty} dx\, x^n\, f(x) \qquad = \sum_i x_i^n\, f(x_i)$$

Mean value is, by definition, the first ($n = 1$) moment of the probability distribution, $\mu \equiv \mu_1$.

**Central moment** of order n is defined as

$$m_n = \mathbb{E}\left((X-\mu)^n\right) = \langle (x-\mu)^n \rangle = \int_{-\infty}^{+\infty} dx\, (x-\mu)^n\, f(x)$$

$$= \sum_i (x_i-\mu)^n\, f(x_i)$$

By calculating moments of the (unknown) probability distribution we can get information about its shape.

## Moments of distribution functions

For the lowest order moments we have:

| | | |
|---|---|---|
| $\mu_0 \equiv 1$ | $m_0 \equiv 1$ | normalization of $f(x)$ |
| $\mu_1 \equiv \mu$ | $m_1 \equiv 0$ | definition of mean value of $f(x)$ |

The first moment which gives us information about the shape of $f(x)$ is **Variance**, which is the second central moment:

$$\sigma^2 = \mathbb{V}(X) = m_2 = \langle (x-\mu)^2 \rangle = \int_{-\infty}^{+\infty} dx \, (x-\mu)^2 \, f(x)$$

$$= \sum_i (x_i - \mu)^2 \, f(x_i)$$

The square root of the variance is referred to as the standard deviation $\sigma$.
Describes the average difference between measurements $x_i$ and the mean $\mu$

## Measurements and their uncertainties

# Measurements

So far, we considered different properties of probability density functions and random variables assuming PDF parameters are known.

But this is not the case in most measurements.

We do experiments to extract parameters of the distribution!
Or even to reconstruct the shape of the PDF, if not predicted by theory.

We can constrain shape of the PDF by measuring its moments.

Mean $\mu$ and standard deviation $\sigma$ are often of primary importance.
How do we reconstruct them? What is the precision of our estimate?

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How do we reconstruct them? What is the precision of our estimate?

Let us assume that random variable $X$ is described by probability distribution $f(x)$. We perform $N$ experiments resulting in set of $N$ measurements $x_i$, $i = 1 \ldots N$ (our sample).

## Sample mean

Mean of the obtained numerical results

$$\bar{x} = \frac{1}{N} \sum_i x_i$$

Expected value of the sample mean:

$$\mathbb{E}(\bar{x}) = \frac{1}{N}\,\mathbb{E}(x_1 + \ldots x_N) = \frac{1}{N}\,N\,\mu = \mu$$

The sample mean is an unbiased estimator of the true mean $\mu$.

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## Law of Large Numbers

"under suitable conditions"

The sample mean tends to the mean of the distribution

$$\lim_{N\to\infty}\;\frac{1}{N}\sum_{i=1}^{N} x_i \;=\; \mu$$

In the limit $N \to \infty$ sample mean is no longer a random variable...

## Variance of sample mean

In the limit $N \to \infty$ we can obtain exact value of $\mu$.

How precise is our estimate $\bar{x}$ of the true mean $\mu$ for finite $N$?

We can calculate variance of sample mean:

$$\begin{aligned}
\mathbb{V}(\bar{x}) &= \langle\, (\bar{x} - \mu)^2 \rangle \;=\; \langle\; \overline{(x-\mu)}^{\,2} \;\rangle \\
&= \frac{1}{N^2} \left\langle \sum_i (x_i - \mu) \;\cdot\; \sum_j (x_j - \mu) \right\rangle \\
&= \frac{1}{N^2} \sum_i \langle (x_i - \mu)^2 \rangle \;+\; \frac{1}{N^2} \sum_{i,\, j \neq i} \langle (x_i - \mu)(x_j - \mu) \rangle \\
&= \frac{1}{N^2}\, N\, \sigma^2 \;+\; 0 \;=\; \frac{\sigma^2}{N}
\end{aligned}$$

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\end{aligned}$$

Sample mean is a random variable with mean $\mu$ and standard deviation $\frac{\sigma}{\sqrt{N}}$

## Variance estimate

Consider the value for the mean squared difference:

$$
\begin{aligned}
d^2 &= \frac{1}{N}\sum_i (x_i - \bar{x})^2 \; = \; \frac{1}{N}\sum_i (x_i - \mu - (\bar{x} - \mu))^2 \\
&= \frac{1}{N}\sum_i \left[(x_i - \mu)^2 - 2(x_i - \mu)(\bar{x} - \mu) + (\bar{x} - \mu)^2\right] \\
&= \frac{1}{N}\sum_i (x_i - \mu)^2 - 2(\bar{x} - \mu)\frac{1}{N}\sum_i (x_i - \mu) + (\bar{x} - \mu)^2 \\
&= \frac{1}{N}\sum_i (x_i - \mu)^2 - (\bar{x} - \mu)^2
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&= \frac{1}{N}\sum_i (x_i - \mu)^2 - (\bar{x} - \mu)^2
\end{aligned}
$$

Expected value:

$$
\langle d^2 \rangle = \mathbb{V}(x_i) - \mathbb{V}(\bar{x}) = \sigma^2 - \frac{\sigma^2}{N} = \frac{N-1}{N}\,\sigma^2
$$

$d^2$ is NOT an unbiased estimator of the standard deviation $\sigma^2$ !!!

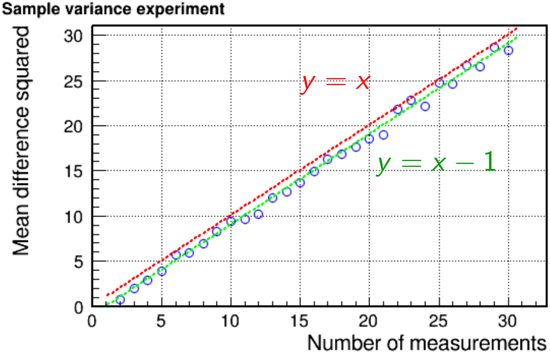
## Variance estimate

Run multiple numerical experiments to calculate expected value for

$$Nd^2 = \sum_i (x_i - \bar{x})^2$$

for $x_i$ being gaussian random variables with $\mu = 0$ and $\sigma = 1$

100 experiments



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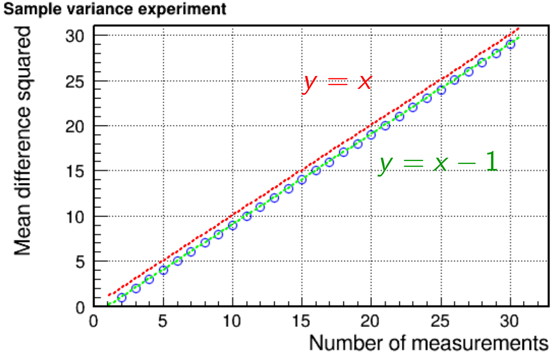

## Sample mean variance

Sample variance for a sample of $N$ measurements $x_i$ is defined as

$$s^2 = \frac{1}{N-1} \sum_i (x_i - \bar{x})^2$$

where Bessel's correction factor

$$\frac{\sigma^2}{\langle d^2 \rangle} = \frac{N}{N-1}$$

is applied to obtain an unbiased estimator of the standard deviation:

$$\langle s^2 \rangle = \sigma^2$$

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Bessel's correction is crucial for proper (unbiased) estimate of the sample mean variance:

$$\mathbb{V}(\bar{x}) = \frac{\sigma^2}{N} = \left\langle \frac{1}{N(N-1)} \sum_i (x_i - \bar{x})^2 \right\rangle$$

## Measurements and their uncertainties

For full description of the unknown probability distribution function $f(x)$ we need to know all its moments. Relation between moments and PDF can be also conveniently described by introducing

## Moment Generating Function

The moment generating function of a random variable $X$ is defined as

$$M(t) \;=\; \mathbb{E}(e^{tX}) \;=\; \int_{-\infty}^{+\infty} dx\, f(x)\, e^{tx}$$

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By using Taylor series expansion near $t = 0$ we get

$$M(t) = \int_{-\infty}^{+\infty} dx \; f(x) \; \left( 1 + tx + \frac{(tx)^2}{2!} + \dots \right) \; = \; 1 + t\mu_1 + \frac{t^2}{2!}\mu_2 + \dots$$

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$\Rightarrow$ all moments can be now obtained as derivatives at $t = 0$:

$$\mu_k = \left.\frac{\partial^k M(t)}{\partial t^k}\right|_{t=0}$$

## Moment Generating Function

If $X$ and $Y$ are two independent variables and $Z = X + Y$ then

$$M_z(t) = M_x(t) \cdot M_y(t)$$

where $M_x$, $M_y$ and $M_z$ are moment generating functions for $X$, $Y$ and $Z$

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$$\frac{\partial M(t)}{\partial t} = (\mu + \sigma^2 t)\ M(t) \qquad \to \mu \text{ for } t = 0$$

$$\frac{\partial^2 M(t)}{\partial t^2} = \left[\sigma^2 + (\mu + \sigma^2 t)^2\right]\ M(t) \qquad \to \sigma^2 + \mu^2$$

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PDF described by generating function of this form is by definition gaussian

## Central Limit Theorem

Consider the sum of $N$ independent variables $X_i$:

$$Y = \sum_{i=1}^{N} X_i$$

For simplicity, let us assume mean values are zero, $\mathbb{E}(X_i) \equiv 0 \Rightarrow \mu_y = 0$

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and increases with increasing $N$...

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$\Rightarrow$ let us consider scaled random variable $(\mu_z = 0,\ \sigma_z = 1)$

$$Z = \frac{1}{\sigma} Y = \sum_{i=1}^{N} \frac{X_i}{\sigma}$$

which should tend to a fixed distribution in $N \to \infty$ limit. What is it?

## Central Limit Theorem

Moment generating function for $Z$:

$$M_Z(t) = \prod_{i=1}^{N} M_i\left(\frac{t}{\sigma}\right)$$

where moment generating function of variables $X_i$ can be written as

$$M_i\left(\frac{t}{\sigma}\right) = 1 + \frac{\sigma_i^2}{2}\left(\frac{t}{\sigma}\right)^2 + \frac{\mu_{3(i)}}{3!}\left(\frac{t}{\sigma}\right)^3 + \ldots$$

where the term linear in $t$ vanishes because of $\mu_i \equiv 0$

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Logarithm of moment generating function for Z

$$\ln M_Z(t) \;=\; \sum_{i=1}^{N} \ln M_i\left(\frac{t}{\sigma}\right) \;=\; \sum_{i=1}^{N} \ln\left(1 + \frac{\sigma_i^2}{2}\left(\frac{t}{\sigma}\right)^2 + \ldots\right)$$

## Central Limit Theorem

Distribution is defined by shape of $M(t)$ for $t \approx 0$, we can expand

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ignoring terms $\frac{1}{\sigma^3}$ and higher: $$\approx \sum_{i=1}^{N} \frac{\sigma_i^2}{2}\left(\frac{t}{\sigma}\right)^2 = \frac{1}{2}\,t^2$$

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We conclude that in the limit $N \to \infty$

$$M_Z(t) \;=\; \exp\left(\frac{1}{2}\,t^2\right)$$

and $Z$ has gaussian distribution function with unit deviation $(\sigma = 1)$

## Central Limit Theorem (2)

If we assume that all $X_i$ have same variance $\sigma_x^2$ $\Rightarrow \sigma = \sigma_x \cdot \sqrt{N}$

$$
\begin{aligned}
M_i\left(\frac{t}{\sigma}\right) &= 1 + \frac{\sigma_x^2}{2}\left(\frac{t}{\sigma_x\sqrt{N}}\right)^2 + \frac{\mu_{3(i)}}{3!}\left(\frac{t}{\sigma_x\sqrt{N}}\right)^3 + \dots \\
&= 1 + \frac{t^2}{2N} + \frac{\mu_{3(i)}}{3!\sigma_x^3} \cdot \frac{t^3}{N^{3/2}} + \dots
\end{aligned}
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$$= 1 + \frac{t^2}{2N} + \frac{\mu_{3(i)}}{3!\sigma_x^3} \cdot \frac{t^3}{N^{3/2}} + \ldots$$

Then the moment generating function for $Z$ can be written as:

$$M_Z(t) = \prod_{i=1}^{N} M_i\left(\frac{t}{\sigma}\right) = \left(1 + \frac{t^2}{2N} + \ldots\right)^N$$

and in the limit $N \to \infty$ we get:

$$M_Z(t) = \exp\left(\frac{1}{2}\, t^2\right)$$

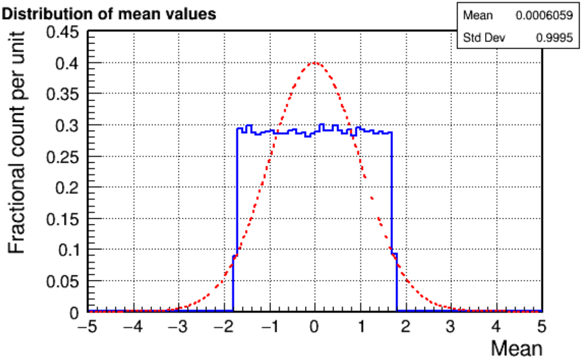
## Example (1)

Simplest case: $X_i$ are random numbers from uniform distribution

Distribution of the mean of $N$ values:
compared with normal distribution

scaling to $\sigma = 1$ applied

N = 1



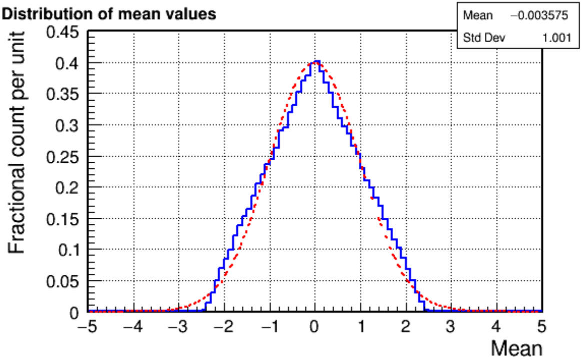
## Example (1)

Simplest case: $X_i$ are random numbers from uniform distribution

Distribution of the mean of $N$ values:
compared with normal distribution

scaling to $\sigma = 1$ applied

N = 2



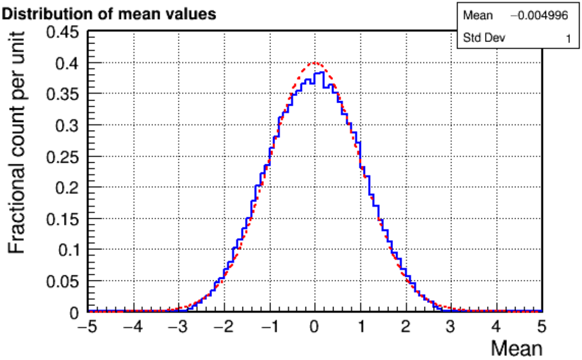
## Example (1)

Simplest case: $X_i$ are random numbers from uniform distribution

Distribution of the mean of $N$ values:
compared with normal distribution

scaling to $\sigma = 1$ applied

$N = 3$



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Simplest case: $X_i$ are random numbers from uniform distribution

Distribution of the mean of $N$ values:

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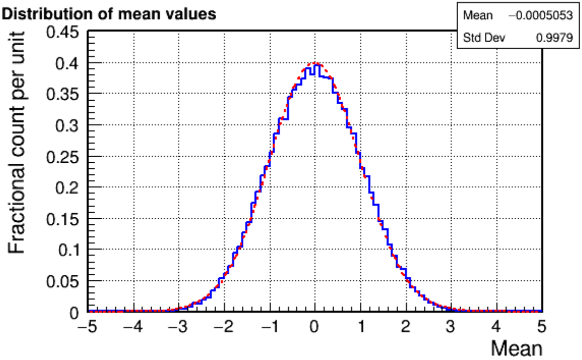
scaling to $\sigma = 1$ applied

N = 5



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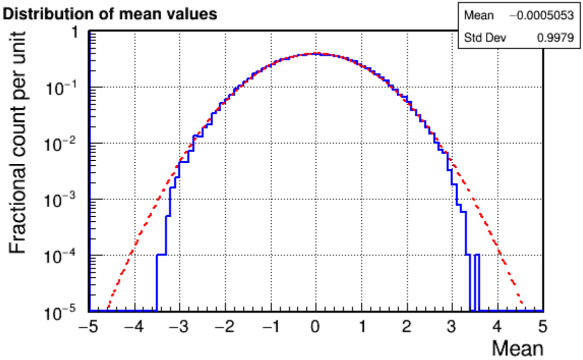

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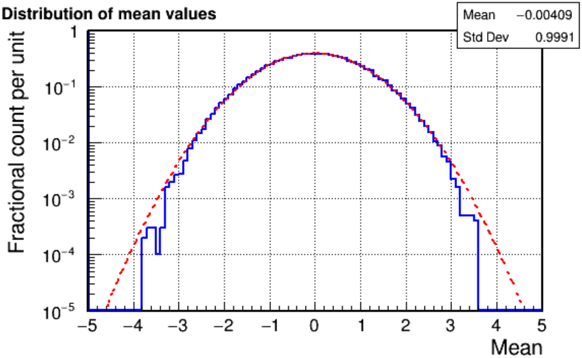
Distribution of the mean of $N$ values:
compared with normal distribution scaling to $\sigma = 1$ applied

N = 7



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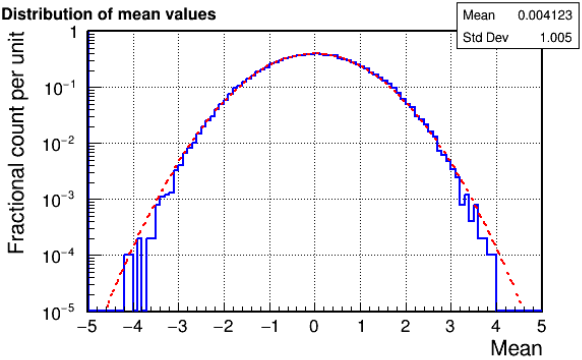
Simplest case: $X_i$ are random numbers from uniform distribution

Distribution of the mean of $N$ values:
compared with normal distribution

scaling to $\sigma = 1$ applied

$\mathrm{N} = 10$



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Distribution of the mean of $N$ values:
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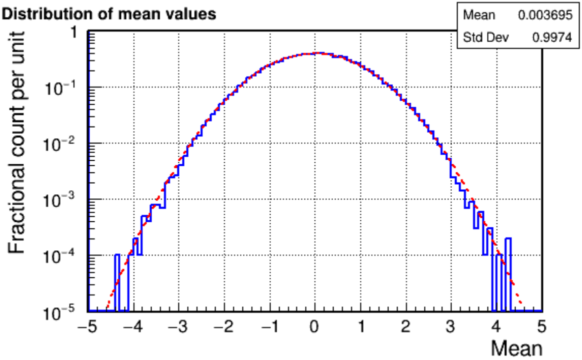
N = 20



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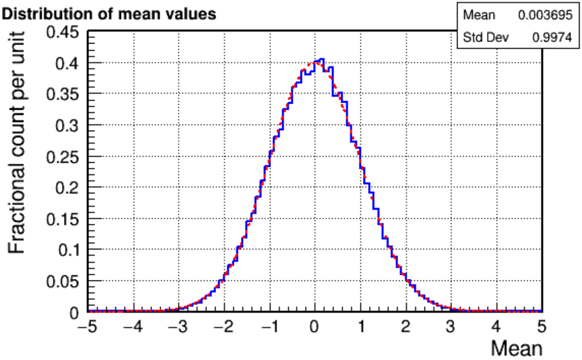


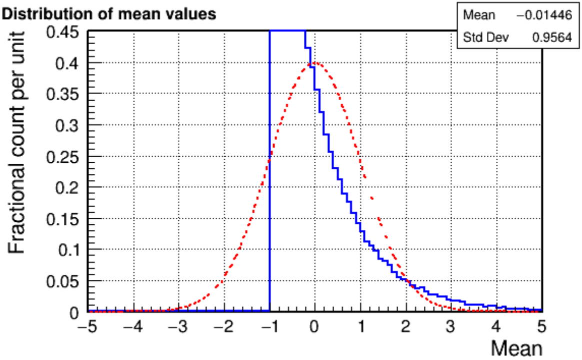
## Example (2)

More problematic: $X_i$ are random numbers from exponential distribution

Distribution of the mean of $N$ values:
compared with normal distribution

scaling to $\sigma = 1$ applied

N = 1



## Example (2)

More problematic: $X_i$ are random numbers from exponential distribution

Distribution of the mean of $N$ values:
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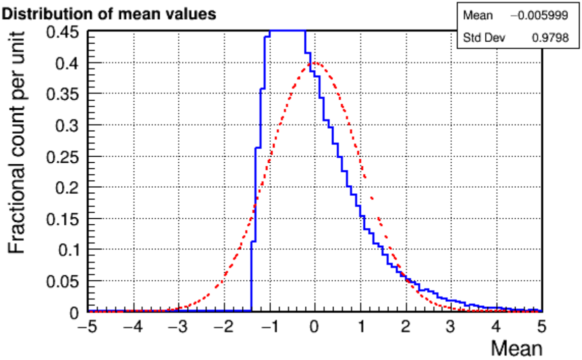
N = 2



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compared with normal distribution

scaling to $\sigma = 1$ applied

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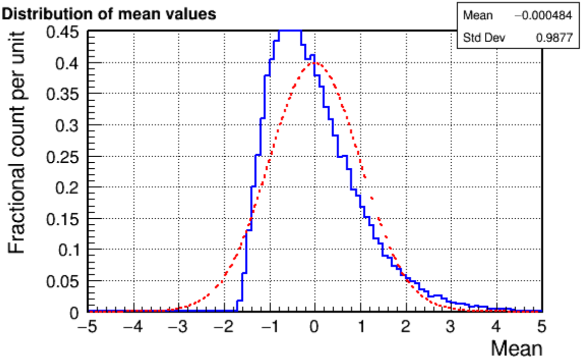

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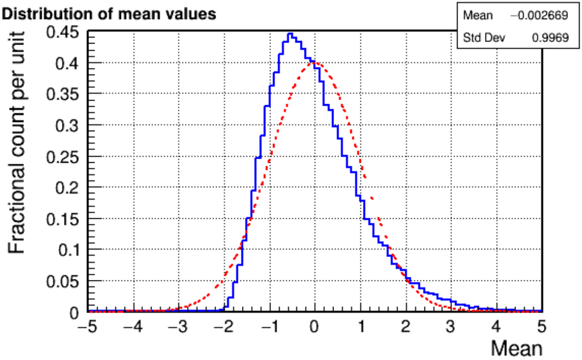
scaling to $\sigma = 1$ applied

N = 5

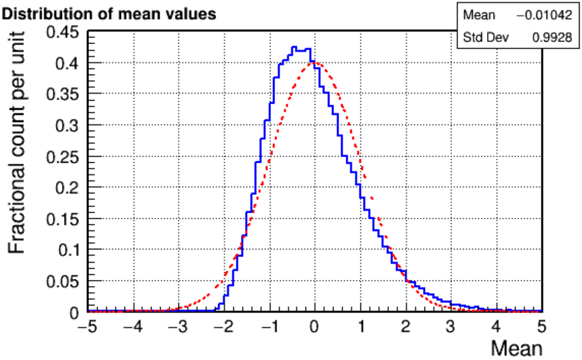


## Example (2)

More problematic: $X_i$ are random numbers from exponential distribution

Distribution of the mean of $N$ values:
compared with normal distribution    scaling to $\sigma = 1$ applied

N = 7



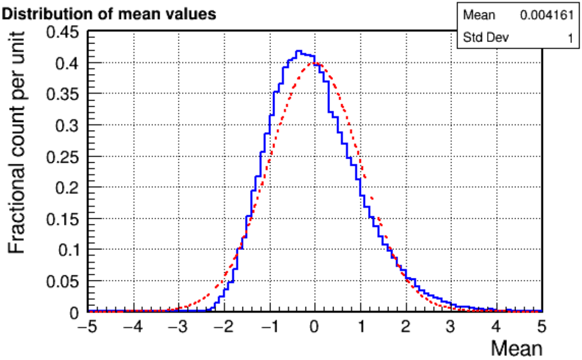
## Example (2)

More problematic: $X_i$ are random numbers from exponential distribution

Distribution of the mean of $N$ values:
compared with normal distribution

scaling to $\sigma = 1$ applied

N = 10

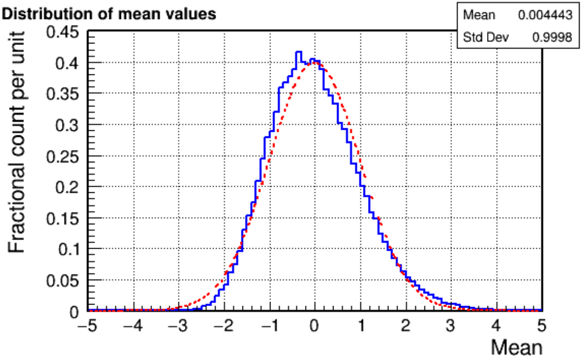


## Example (2)

More problematic: $X_i$ are random numbers from exponential distribution

Distribution of the mean of $N$ values:
compared with normal distribution scaling to $\sigma = 1$ applied

N = 20



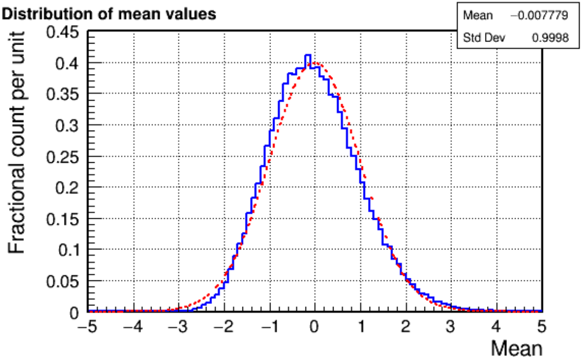
## Example (2)

More problematic: $X_i$ are random numbers from exponential distribution

Distribution of the mean of $N$ values:
compared with normal distribution

scaling to $\sigma = 1$ applied

N = 30



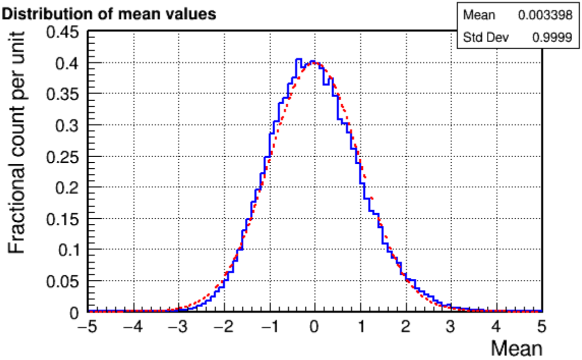
## Example (2)

More problematic: $X_i$ are random numbers from exponential distribution

Distribution of the mean of $N$ values:
compared with normal distribution

scaling to $\sigma = 1$ applied

N = 50



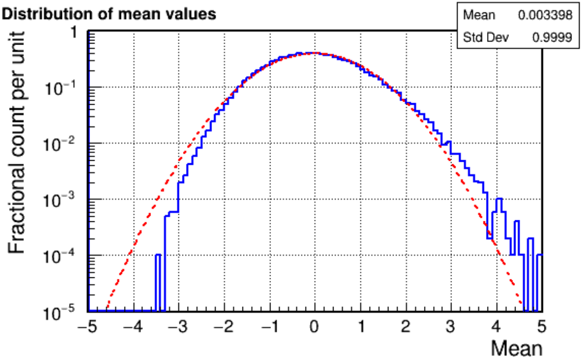
## Example (2)

More problematic: $X_i$ are random numbers from exponential distribution

Distribution of the mean of $N$ values:
compared with normal distribution

scaling to $\sigma = 1$ applied

N = 50



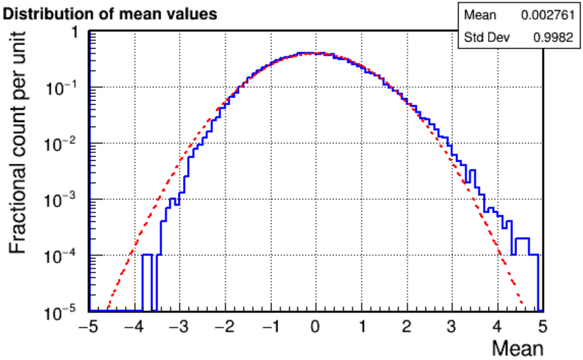
## Example (2)

More problematic: $X_i$ are random numbers from exponential distribution

Distribution of the mean of $N$ values:
compared with normal distribution

scaling to $\sigma = 1$ applied

N = 70

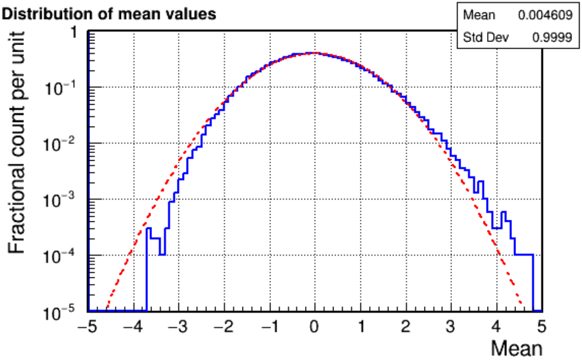


## Example (2)

More problematic: $X_i$ are random numbers from exponential distribution

Distribution of the mean of $N$ values:
compared with normal distribution — scaling to $\sigma = 1$ applied

N = 100



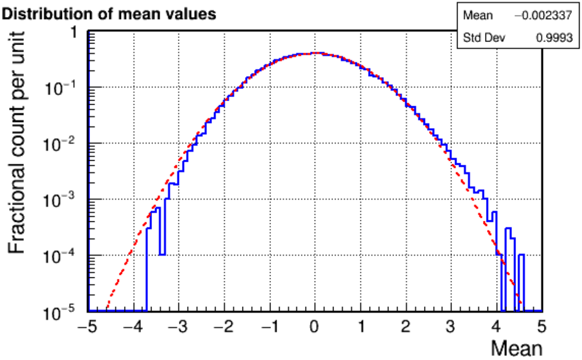
## Example (2)

More problematic: $X_i$ are random numbers from exponential distribution

Distribution of the mean of $N$ values:
compared with normal distribution

scaling to $\sigma = 1$ applied

N = 200



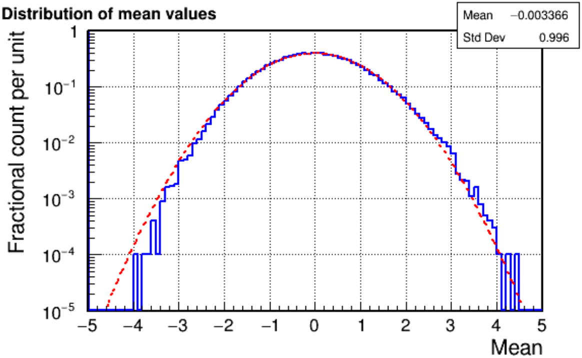
## Example (2)

More problematic: $X_i$ are random numbers from exponential distribution

Distribution of the mean of $N$ values:
compared with normal distribution

scaling to $\sigma = 1$ applied

$N = 300$

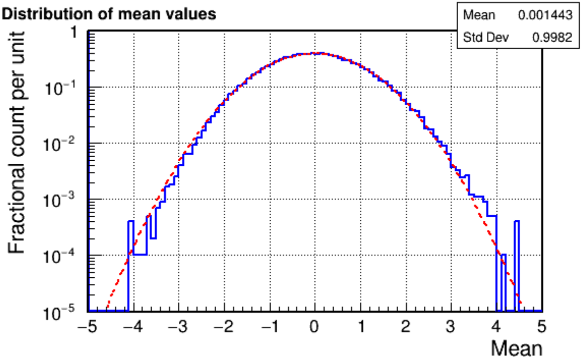


## Example (2)

More problematic: $X_i$ are random numbers from exponential distribution

Distribution of the mean of $N$ values:
compared with normal distribution scaling to $\sigma = 1$ applied

N = 500

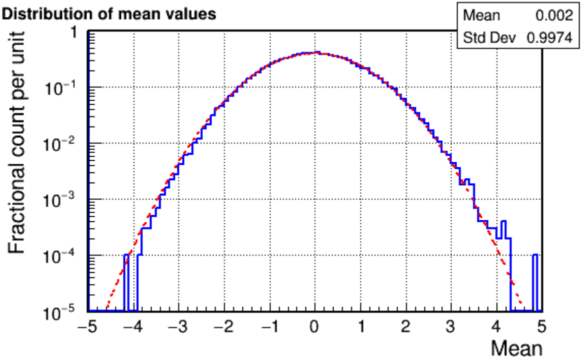


## Example (2)

More problematic: $X_i$ are random numbers from exponential distribution

Distribution of the mean of $N$ values:
compared with normal distribution scaling to $\sigma = 1$ applied

N = 1000



# Central Limit Theorem

**Central Limit Theorem** as presented by M. Bonamente

*The sum of a large number of independent random variables is approximately distributed as a Gaussian. The mean of the distribution is the sum of the means of the variables and the variance of the distribution is the sum of the variances of the variables. This result holds regardless of the distribution of each individual variable.*

**Central Limit Theorem** as presented by M. Bonamente

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This is a very strong statement!

It is true in most of the “physical” cases, but it is not true in general case...

In our proof we had to assume that $M(t)$ can be defined, that is all moments of the considered probability distribution can be calculated and are finite. This is not always the case...

## Example (3)

Consider random numbers $x_i$ from Cauchy distribution

$$f(x) = \frac{1}{\pi} \cdot \frac{1}{1+x^2}$$

It is properly normalized, but already its mean is not well defined:

$$\mathbb{E}(X) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{2x\,dx}{1+x^2}$$

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$$\mathbb{E}(X) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{2x\,dx}{1+x^2} = \frac{1}{2\pi} \ln(1+x^2)\Big|_{-\infty}^{+\infty}$$

Higher moments diverge even faster...

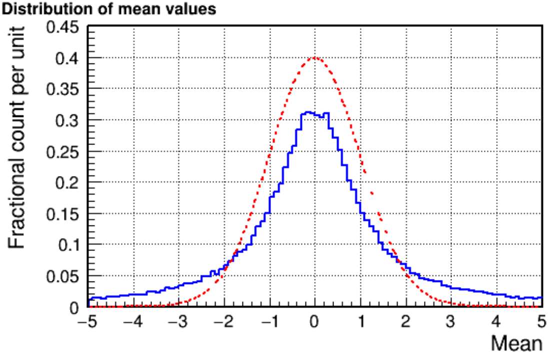
Our basic assumption is not fulfilled $\Rightarrow$ theorem does not hold !

## Example (3)

Consider random numbers $x_i$ from Cauchy distribution

Distribution of the mean of $N$ values: compared with normal distribution

$N = 1$

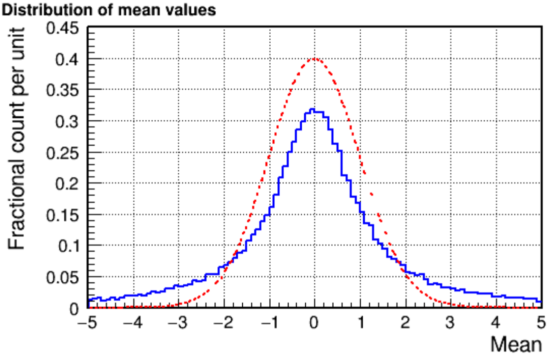


## Example (3)

Consider random numbers $x_i$ from Cauchy distribution

Distribution of the mean of $N$ values: compared with normal distribution

N = 10

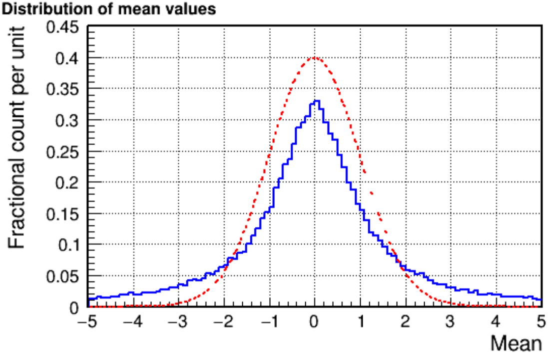


## Example (3)

Consider random numbers $x_i$ from Cauchy distribution

Distribution of the mean of $N$ values: compared with normal distribution

N = 100

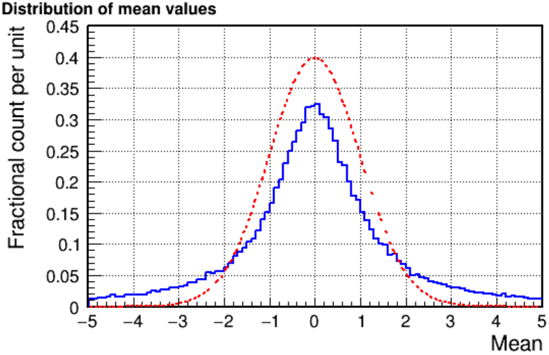


## Example (3)

Consider random numbers $x_i$ from Cauchy distribution

Distribution of the mean of $N$ values: compared with normal distribution

$\mathrm{N} = 1000$

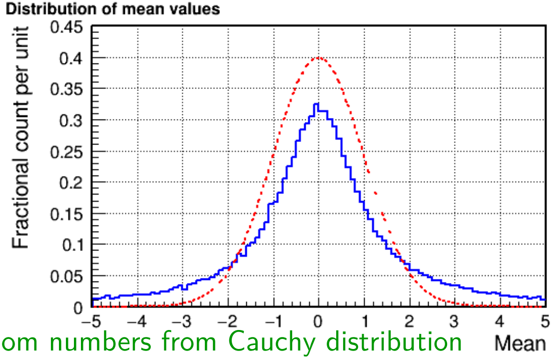


## Example (3)

Consider random numbers $x_i$ from Cauchy distribution

Distribution of the mean of $N$ values: compared with normal distribution

N = 10000




Mean of random numbers from Cauchy distribution has Cauchy distribution itself, even for $N \to \infty$

## Measurements and their uncertainties

## Multiple measurements

It is often the case that we measure two or more variables at the same time and we are interested in joint probability of obtaining given result.

So far we assumed that variables were independent, eg. coming from different measurements or from repeated experiment...

Let us consider two random variables $X$ and $Y$.
We can define joint probability function $h(x, y)$ by the relation:

$$P(x < X < x + dx \;\; \&\& \;\; y < Y < y + dy) \;\; = \;\; h(x, y)\, dx\, dy$$

which should be fulfilled for infinitesimal intervals $dx$ and $dy$, or:

$$P(x_1 < X < x_2 \;\; \&\& \;\; y_1 < Y < y_2) \;\; = \;\; \int_{x_1}^{x_2} dx \int_{y_1}^{y_2} dy\; h(x, y)$$

## Joint probability function

Joint probability function give full information on the measured set of variables. If we want to look only at one variable, we can consider marginal probability density functions defined as

$$f(x) = \int_{-\infty}^{+\infty} dy \; h(x,y)$$
$$g(y) = \int_{-\infty}^{+\infty} dx \; h(x,y)$$

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We can also directly extract parameters of $X$ and $Y$ distributions:

$$\mu_x = \mathbb{E}(X) = \int\int dx \; dy \; x \; h(x,y)$$

$$\sigma_x^2 = \mathbb{E}((X-\mu_x)^2) = \int\int dx \; dy \; (x-\mu_x)^2 \; h(x,y)$$

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\begin{aligned}
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\end{aligned}
$$

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$$
\begin{aligned}
\mu_y = \mathbb{E}(Y) &= \iint dx\ dy\ y\ h(x,y) \\
\sigma_y^2 = \mathbb{E}((Y-\mu_y)^2) &= \iint dx\ dy\ (y-\mu_y)^2\ h(x,y)
\end{aligned}
$$

## Covariance

Covariance of two random variables $X$ and $Y$ is defined as:

$$\mathbb{C}(X,Y) = Cov(X,Y) = \mathbb{E}((X-\mu_x)(Y-\mu_y)) = \sigma_{xy}$$

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which is the number between $-1$ and $+1$.

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When two variables are independent, their correlation is zero:

$$h(x,y) \;=\; f(x)\cdot g(y) \qquad \Rightarrow \quad Cov(X,Y) \;=\; \rho(X,Y) \;=\; 0$$

But the opposite statement is not true!
Vanishing correlation does not guarantee that variables are independent!

## Covariance

The role of covariance can be best shown on a simple example.
Let us consider random variable $Z = X + Y$. The expected value of $Z$:

$$\mathbb{E}(Z) = \mathbb{E}(X) + \mathbb{E}(Y) = \mu_x + \mu_y$$

The variance of $Z$:

$$\begin{aligned}\mathbb{V}(Z) &= \mathbb{E}((X + Y - \mu_x - \mu_y)^2) \\ &= \mathbb{E}((X - \mu_x)^2 + (Y - \mu_y)^2 + 2(X - \mu_x)(Y - \mu_y)) \\ &= \mathbb{V}(X) + \mathbb{V}(Y) + 2Cov(X, Y)\end{aligned}$$

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$$\sigma_z^2 = \sigma_x^2 + \sigma_y^2 + 2\rho_{xy}\sigma_x\sigma_y$$

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\sigma_z^2 &= \sigma_x^2 \;+\; \sigma_y^2 \;+\; 2\rho_{xy}\sigma_x\sigma_y
\end{aligned}$$

Correlation of input variables can have significant impact on result:

$$0 \;\leq\; \sigma_z^2 \;\leq\; (\sigma_x + \sigma_y)^2$$

## Sample covariance

The true covariance/correlation between variables is usually unknown.

We want to estimate it from the set of $N$ measurements $(x_i, y_i)$.
For unbiased estimate we should calculate sample covariance:

$$s_{xy}^2 = \frac{1}{N-1}\sum_i (x_i - \bar{x})(y_i - \bar{y})$$

The sample correlation coefficient is then defined as

$$r_{xy} = \frac{s_{xy}^2}{s_x \; s_y}$$

where $s_x$ and $s_y$ are sample variances (with Bessel's correction).

## 2D Gaussian distribution

Normal distribution for two correlated variables $X$ and $Y$:

$$h(x,y) = N \exp\left[\frac{-1}{2(1-\rho_{xy}^2)}\left(\frac{(x-\mu_x)^2}{\sigma_x^2} - \frac{2\rho_{xy}(x-\mu_x)(y-\mu_y)}{\sigma_x\sigma_y} + \frac{(y-\mu_y)^2}{\sigma_y^2}\right)\right]$$

where:

$$N = \frac{1}{2\pi\sigma_x\sigma_y\sqrt{1-\rho_{xy}^2}}$$

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where:

$$N = \frac{1}{2\pi\sigma_x\sigma_y\sqrt{1-\rho_{xy}^2}}$$

Due to correlation, distribution of $X$ for fixed $Y$ (and of $Y$ for fixed $X$) becomes narrower than the marginal distribution !

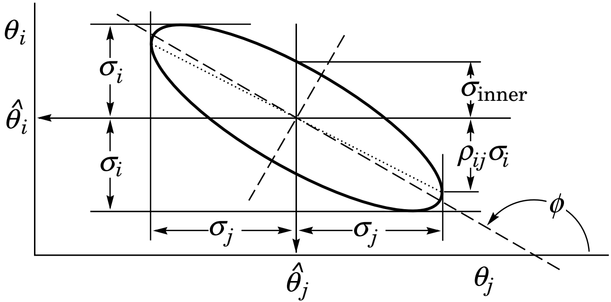
$$\mathbb{V}(X|Y) = (1-\rho_{xy}^2)\cdot\mathbb{V}(X)$$

## 2D Gaussian distribution

Graphical presentation of variable correlation: “one sigma” contour

R.L. Workman et al. (Particle Data Group), Prog. Theor. Exp. Phys. 2022, 083C01 (2022)

“One sigma” contour - $(x, y)$ values resulting in $h(x, y) = N \exp(-\frac{1}{2})$




$$\tan 2\phi = \frac{2\rho_{xy}\sigma_x\sigma_y}{\sigma_x^2 - \sigma_y^2}$$

Example case of negative correlation

## Multiple variable case

Definition of covariance can be generalized to the set of N variables $X_i$:

$$c_{ij} \; = \; Cov(X_i, X_j) \;\; = \;\; \mathbb{E}((X_i - \mu_i)(X_j - \mu_j))$$

## Multiple variable case

Definition of covariance can be generalized to the set of N variables $X_i$:

$$c_{ij} = Cov(X_i, X_j) = \mathbb{E}((X_i - \mu_i)(X_j - \mu_j))$$

We can present it in a form of the covariance matrix:

$$\mathbb{C} = \begin{pmatrix} c_{11} & c_{12} & \cdots & c_{1N} \\ c_{21} & c_{22} & \cdots & c_{2N} \\ \vdots & & & \vdots \\ c_{N1} & c_{N2} & \cdots & c_{NN} \end{pmatrix}$$

where diagonal elements correspond to variances of the variables

$$c_{ii} = Cov(X_i, X_i) \equiv \mathbb{V}(X_i)$$

## Multiple variable case

Let us now consider linear combination of $N$ random variables

$$Y = \sum_{i=1}^{N} a_i \, X_i$$

Expected value is given by (from the linearity of the mean)

$$\mu_y = \sum a_i \, \mu_i$$

The variance can be calculated as:

$$\sigma_y^2 = \mathbb{V}\left(\sum a_i \, X_i\right) = \mathbb{E}\left[\left(\sum a_i \, X_i - \sum a_i \, \mu_i\right)^2\right]$$

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$$= \mathbb{E}\left[\left(\sum_i a_i (X_i - \mu_i)\right)\left(\sum_j a_j (X_j - \mu_j)\right)\right] = \sum_{i,j} a_i a_j c_{ij}$$

## Multiple variable case

The variance of linear combination of variables

$$\sigma_y^2 = \sum_{i,j} a_i a_j \, c_{ij}$$

$$= \sum_i a_i^2 \sigma_i^2 + 2 \sum_{i,\, j>i} a_i a_j \, \sigma_i \sigma_j \, \rho_{ij}$$

factor 2 introduced due to $j > i$ condition

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factor 2 introduced due to $j > i$ condition

We can also write linear combination using vector notation:

$$y = \mathbf{a}^\mathsf{T} \cdot \mathbf{x}$$

where **a** and **x** are vectors $(a_1, \ldots, a_N)$ and $(x_1, \ldots, x_N)$, and then

$$\sigma_y^2 = \mathbf{a}^\mathsf{T} \, \mathbb{C} \, \mathbf{a}$$

## Measurements and their uncertainties

## Functions of Random Variables

So far, we have mainly discussed linear combinations of random variables...

Let us consider general case of functional dependence $Y = Y(X)$, where $X$ is a random variable with distribution $f(x)$.

Probability density function for dependent variable $Y$ is given by

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

assuming that y(x) is a single-valued function (one-to-one).

If the function considered is not single-valued (i.e. $y(x)$ can not be inverted), we need to divide $X$ domain into subdomains, where this condition is met...

## Functions of Random Variables

Change of Variables can be also considered in multi-dimensional case

$$\mathbf{y} = \mathbf{y}(\mathbf{x})$$

where components of vector $\mathbf{y}$ are given by functions $y_i(\mathbf{x})$, $i = 1, \ldots, N$

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where components of vector $\mathbf{y}$ are given by functions $y_i(\mathbf{x})$, $i = 1, \ldots, N$

Probability density function for dependent variables $\mathbf{y}$ is given by

$$g(\mathbf{y}) = f(\mathbf{x}(\mathbf{y}))\, |J|$$

assuming that function $\mathbf{y}(\mathbf{x})$ is one-to-one and can be inverted, with

$$J = \left( \frac{\partial x_i}{\partial y_j} \right)$$

being the Jacobian of the variable transformation (square matrix)

## Mean of Functions of Random Variables

It is important to notice that

$$\mu_y = \mathbb{E}(y(x)) \neq y(\mu_x)$$

this relation holds only for linear dependencies but not in general case

It is not sufficient to know $\mu_x$ (reconstructed value of $\bar{x}$)
$\Rightarrow$ we need to know the probability density function for the variable $X$ or have access to individual measurements of $X$

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$\Rightarrow$ we need to know the probability density function for the variable $X$ or have access to individual measurements of $X$

## Variance of Functions of Random Variables

In general, one has to calculate it from first principles, integrating over independent variable $x$ or summing over individual measurements.

However, if variance of $X$ is small, approximate formula can be used...

## Variance of Functions of Random Variables

We can use Taylor series expansion about the means of variables $\mathbf{x}$

$$y(\mathbf{x}) \approx \mu_y + \sum_i (x_i - \mu_i) \left.\frac{\partial y}{\partial x_i}\right|_{x_i=\mu_i} + \ldots$$

where we also approximate $y(\hat{\mu}_{\mathbf{x}}) \approx \mu_y$

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and, assuming the higher order terms can be neglected, we get

$$\mathbb{E}[(y-\mu_y)^2] = \mathbb{E}\left[\left(\sum_i (x_i - \mu_i) \left.\frac{\partial y}{\partial x_i}\right|_{x_i=\mu_i}\right)\left(\sum_j (x_j - \mu_j) \left.\frac{\partial y}{\partial x_j}\right|_{x_j=\mu_j}\right)\right]$$

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$$\begin{aligned}
\mathbb{E}[(y-\mu_y)^2] &= \mathbb{E}\left[\left(\sum_i (x_i - \mu_i) \left.\frac{\partial y}{\partial x_i}\right|_{x_i=\mu_i}\right)\left(\sum_j (x_j - \mu_j) \left.\frac{\partial y}{\partial x_j}\right|_{x_j=\mu_j}\right)\right] \\
&= \sum_{i,j} \left.\frac{\partial y}{\partial x_i}\right|_{x_i=\mu_i} \left.\frac{\partial y}{\partial x_j}\right|_{x_j=\mu_j} \mathbb{E}\left[(x_i-\mu_i)(x_j-\mu_j)\right] \\
&= \sum_{i,j} \frac{\partial y}{\partial x_i} \frac{\partial y}{\partial x_j} c_{ij}
\end{aligned}$$

## General form

Covariance matrix for $\mathbf{y} = \mathbf{y}(\mathbf{x})$ can be approximate as:

$$Cov(Y_k, Y_l) \;=\; \sum_{i,j} \frac{\partial y_k}{\partial x_i} \frac{\partial y_l}{\partial x_j} \, Cov(X_i, X_j)$$

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In matrix notation:

$$\mathbb{C}_{\mathbf{Y}} \;=\; A \, \mathbb{C}_{\mathbf{X}} \, A^{\mathsf{T}}$$

where $A$ is a matrix of partial derivatives:

$$A_{i,j} \;=\; \left. \frac{\partial y_i}{\partial x_j} \right|_{\hat{\mu}_{\mathbf{x}}}$$

**Example**

For a product of independent random variable powers:

$$y = \prod_i x_i^{\alpha_i}$$

we have

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as we assume variables are independent

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Relative variance of the product is a quadratic sum of relative variances:

$$\left( \frac{\sigma_y}{y} \right)^2 = \sum_i \left( \alpha_i \, \frac{\sigma_i}{x_i} \right)^2$$

## Measurements and their uncertainties

## Direct Method

Let us assume we have a large number of uniformly distributed random numbers corresponding to the uniform probability distribution:

$$u(r) = \begin{cases} 0 & \text{for } r < 0 \\ 1 & \text{for } 0 \leq r < 1 \\ 0 & \text{for } r \geq 1 \end{cases}$$

This type of uniform random number generators is commonly accessible in most systems and numerical libraries.

Can we use uniform random number generator to generate random numbers from arbitrary probability distribution $f(x)$?

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Very simple procedure can be used.
Let us consider cumulative distribution function for $X$, $F(x)$:

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$$f(u) = \frac{dF(u)}{du} = 1$$

If cumulative distribution function $F(x)$ can be inverted, we can generate random numbers from $f(x)$ by using relation:

$$x = F^{-1}(r)$$

where $r$ is uniformly distributed random number (from $u(r)$)

## Direct Method example

Nice example is Cauchy distribution:

$$f(x) = \frac{1}{\pi} \cdot \frac{1}{1+x^2} \quad \Rightarrow \quad F(x) = \frac{1}{\pi} \cdot \arctan(x) + \frac{1}{2}$$

which can be easily inverted, resulting in:

$$x \;\; = \;\; \tan\left(\pi\left(r - \frac{1}{2}\right)\right)$$

where $r$ is uniformly distributed random number

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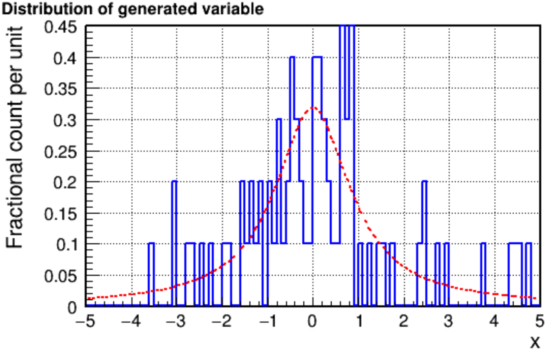
Example generation, $\mathrm{N} = 100$



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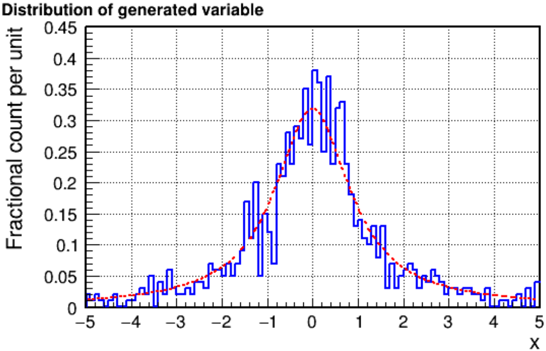

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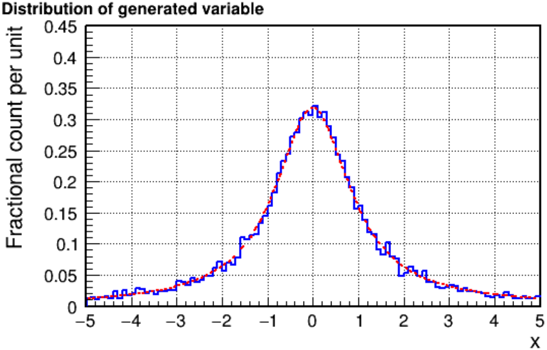

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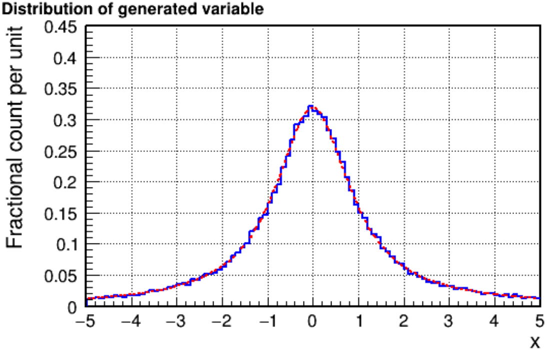
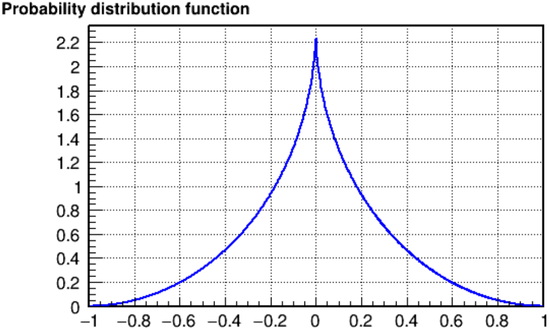


## von Neumann method

The direct method is very elegant and efficient, but requires that the invert function to cumulative distribution is known.
This is not the case in many problems - solution is not general.
We need an alternative...

Example problem:



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Example problem:

$$f(x) = \begin{cases} 0 & \text{for } x < -1 \\ N\left[1 - \sqrt{1-(1-|x|)^2}\right] & \text{for } -1 \le x \le 1 \\ 0 & \text{for } x > 1 \end{cases}$$

where normalization factor

$$N = \frac{2}{4-\pi}$$

## von Neumann method

We can notice that

$$f_{\max} = \max_x f(x) = N$$

Assume $f(x)$ is non-zero only for $a \leq x \leq b$.

We can then apply the following procedure:

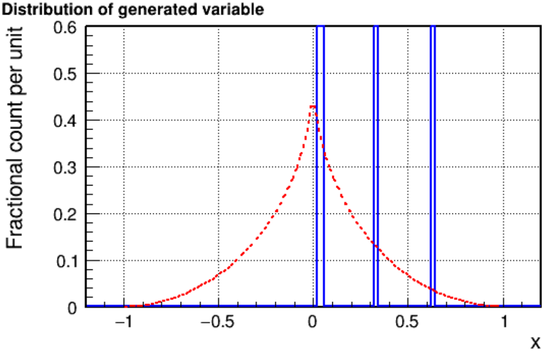
- generate value $x$ uniformly distributed in $[a, b]$
- generate test variable $r$ from uniform distribution ($[0, 1[$)
- accept generated value of $x$, if $r \cdot f_{\max} < f(x)$
  otherwise repeat from the beginning

This procedure is called von Neumann Acceptance–Rejection Technique

## von Neumann method

Acceptance–Rejection Technique applied to the example problem:

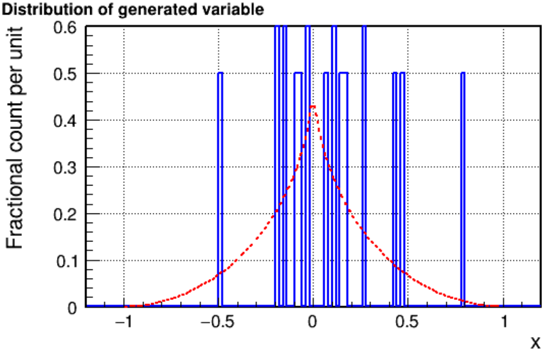
Test generation, $N = 10$



## von Neumann method

Acceptance–Rejection Technique applied to the example problem:

Test generation, $N = 100$



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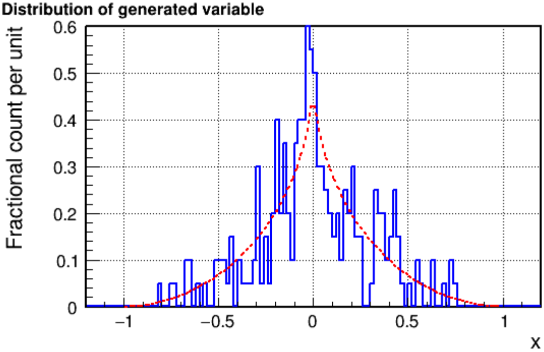

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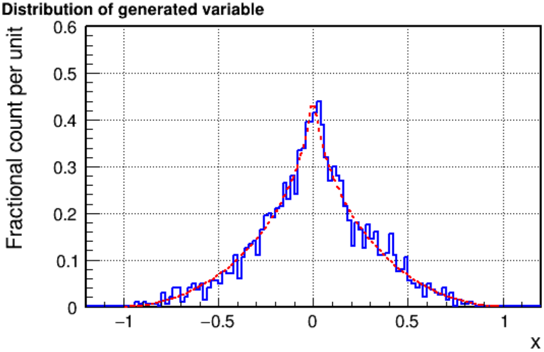

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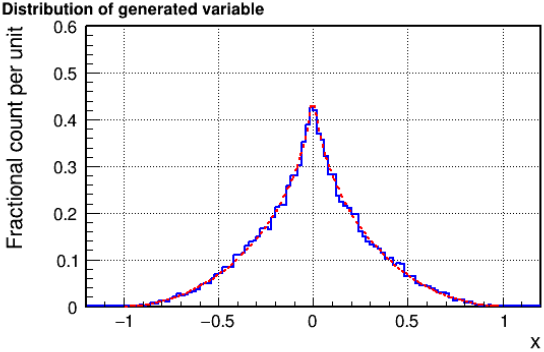
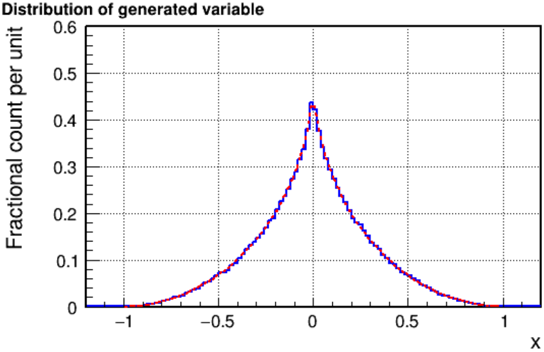



We can perfectly reproduce the assumed probability distribution

## von Neumann method

Acceptance–Rejection Technique applied to the example problem:

Test generation, $N = 1000000$

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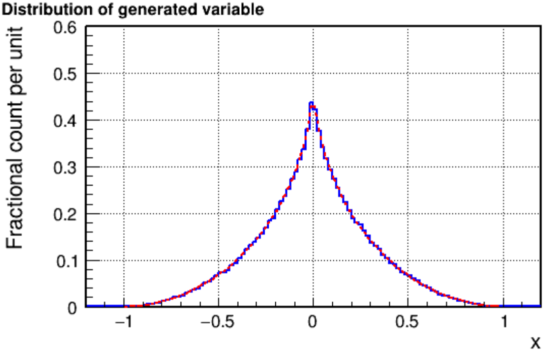


However, this procedure can not be directly applied if $a$ or $b \to \pm\infty$

## General method

For probability distributions with infinite domain we can combine direct and von Neumann methods.

**Example:** generate photon scattering angles for diffractive scattering

$$f(x) \quad = \quad N \cdot \frac{\sin^2 x}{x^2}$$

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$$f(x) \quad = \quad N \cdot \frac{\sin^2 x}{x^2}$$

One can check that this function is always smaller than:

$$g(x) \quad = \quad \frac{3}{2} N \cdot \frac{1}{1+x^2}$$

and both functions have similar asymptotic behavior.

Also, cumulative distribution function for $g(x)$ can be inverted, so we know how to generate random numbers with this distribution...

## General method

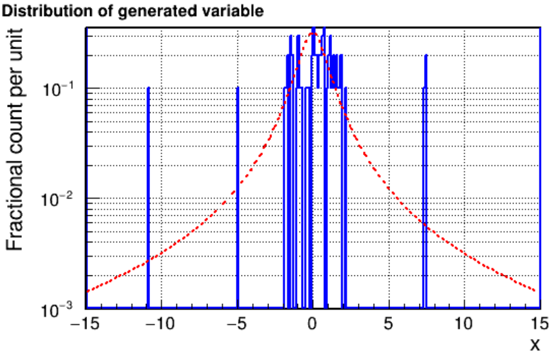
The following procedure can now be used:

- generate value $x$ distributed according to $g(x)$
- generate test variable $r$ from uniform distribution $([0, 1[)$
- accept generated value of $x$, if $r < f(x)/g(x)$
  otherwise repeat from the beginning

## General method

Described procedure applied to the diffractive problem:

Test generation, $N = 100$



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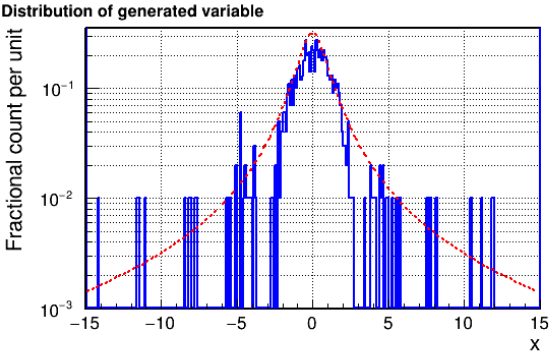

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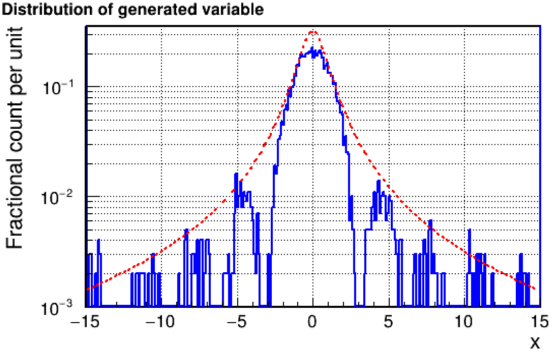

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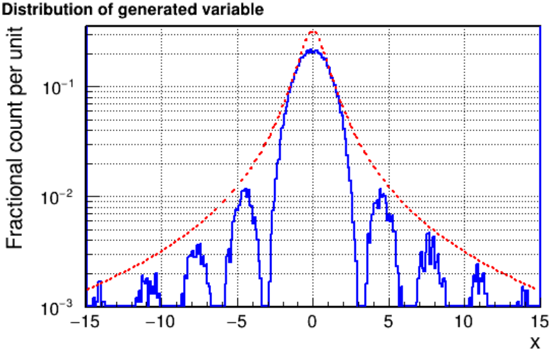

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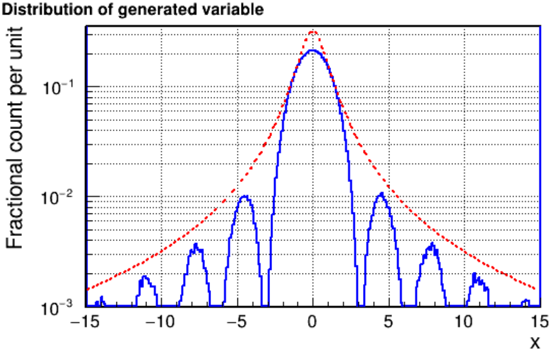


We reproduce the expected probability distribution

## Gaussian Variable

Cumulative distribution function can not be inverted analytically.
However, we can use a simple trick, consider 2-D distribution:

$$g(x,y) \;=\; \frac{1}{2\pi} \cdot \exp\left(-\frac{1}{2}(x^2+y^2)\right)$$

for simplicity we assume $\mu_x = \mu_y = 0$ and $\sigma_x = \sigma_y = 1$
and change variables to polar coordinates:

$$g(R,\theta) \;=\; \frac{1}{2\pi}\, R \;\exp\left(-\frac{1}{2}R^2\right) \;=\; h(R)\cdot t(\theta)$$

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$$g(R, \theta) = \frac{1}{2\pi} R \exp\left(-\frac{1}{2}R^2\right) = h(R) \cdot t(\theta)$$

Cumulative distribution functions can be now considered for $R$ and $\theta$:

$$H(R) = 1 - \exp\left(-\frac{1}{2}R^2\right) \qquad T(\theta) = \frac{1}{2\pi}\,\theta$$

where $R > 0$ and $0 \leq \theta \leq 2\pi$

## Gaussian Variable

Cumulative distribution functions for $r$ and $\theta$ can be inverted resulting in the following formula for generation of a pair of random variables:

$$R = \sqrt{-2\ln(1-r_1)}$$

$$\theta = 2\pi\ r_2$$

where $r_1$ and $r_2$ are two independent uniformly distributed random numbers

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We can now transform back to the $(x, y)$ plane:

$$x = R\;\cos\theta = \sqrt{-2\ln(1-r_1)} \cdot \cos(2\pi\; r_2)$$

$$y = R\;\sin\theta = \sqrt{-2\ln(1-r_1)} \cdot \sin(2\pi\; r_2)$$

$\Rightarrow$ from pair $(r_1, r_2)$ of uniform distributed numbers we get a pair $(x, y)$ of independent (!) random numbers from normal distribution

## Correlated 2D Gaussian

What, if we need to generate pair $(x, y)$ of correlated random numbers?

For 2-D Gaussian distribution it can be done by smart "rotation" of variables. Define "rotation angle":

$$\phi = \frac{1}{2} \arcsin(\rho_{xy})$$

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$$\phi = \frac{1}{2}\arcsin(\rho_{xy})$$

Then we can generate correlated pair of variables using the formula:

$$x = g_1 \cos\phi + g_2 \sin\phi$$
$$y = g_1 \sin\phi + g_2 \cos\phi$$

where $(g_1, g_2)$ is a pair of independent random numbers from Gaussian distribution (assuming $\sigma = 1$ in all cases)

## Measurements and their uncertainties

## Homework

Consider production of tables with length $l = 1.5\,\mathrm{m}$ and width $w = 1.0\,\mathrm{m}$.

Tolerance of production process (standard deviation) is 0.6 mm for length and 0.3 mm for width:

- what is the expected tolerance for the surface of the table assuming table length and width are independent?
- what should correlation between $l$ and $w$ be to result in surface precision (standard deviation) of $3\,\mathrm{cm}^2$?
- perform numerical experiment generating correlated numbers from Gaussian distribution to confirm the result.

Solutions should be uploaded until November 10.