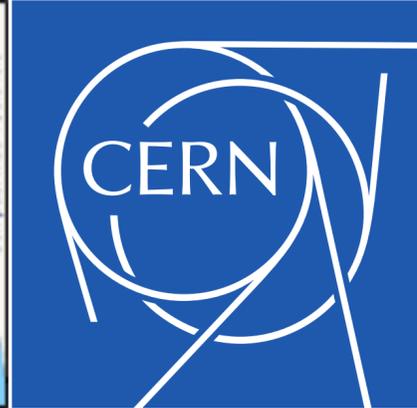




University
of Split



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INTRODUCTION TO MACHINE LEARNING METHODS

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LECTURES OUTLINE

- 1) Introduction to Statistics
- 2) Statistics and Machine Learning
- 3) Classical Machine Learning
- 4) Introduction to Deep Learning
- 5) Advanced Deep Learning

INTRODUCTION TO STATISTICS

WHAT IS DATA ANALYSIS?

*“Data analysis is a process for obtaining **raw data** and converting it into information useful for decision-making by users. Data are collected and analyzed to answer questions, test hypotheses or disprove theories.”*

RAW DATA



USABLE INFORMATION

- Data analysis uses statistics for presentation and interpretation (explanation) of data
- A mathematical foundation for **statistics** is the **probability theory**

DATA ANALYSIS GENERAL PICTURE



1

Physical phenomena
Described by a theory

$$e(W_\mu^- W_\nu^+ - W_\mu^+ W_\nu^-)|^2 -$$
$$- W_\nu^+ A_\mu) + ig' c_w (W_\mu^+ Z_\nu -$$
$$- \partial_\nu Z_\mu + ig' c_w (W_\mu^- W_\nu^+ - W$$

Described by PDFs,
depending on unknown parameters
with true values

$$\theta^{\text{true}} = (m_H^{\text{true}}, \Gamma_H^{\text{true}}, \dots, \sigma^{\text{true}})$$

3

Data sample
 $x = (x_1, x_2, \dots, x_N)$

x is a multivariate random variable



5

Results

- parameter estimates
- confidence limits
- hypothesis tests

PROBABILITY DEFINITION

What is probability anyway?

“Unfortunately, statisticians do not agree on basic principles.”
- Fred James

Mathematical (axiomatic) definition

Classical definition

Frequentist definition

Bayesian (subjective) definition



- Developed in 1933 by Kolmogorov in his “Foundations of the Theory of Probability”
- Define an exclusive set of all possible elementary events x_i
 - Exclusive means the occurrence of one of them implies that none of the others occurs
- For every event x_i , there is a probability $P(x_i)$ which is a real number satisfying the Kolmogorov Axioms of Probability:
 - I) $P(x_i) \geq 0$
 - II) $P(x_i \text{ or } x_j) = P(x_i) + P(x_j)$
 - III) $\sum P(x_i) = 1$
- From these properties more complex probability expressions can be deduced
 - For non-elementary events, i.e. set of elementary events
 - For non-exclusive events, i.e. overlapping sets of elementary events
- Entirely free of meaning, does not tell what probability is about

FREQUENTIST DEFINITION

● Experiment performed N times, outcome x occurs $N(x)$ times

● Define probability:
$$P(x) = \lim_{N \rightarrow \infty} \frac{N(x)}{N}$$

● Such a probability has big restrictions:

- depends on the sample, not just a property of the event
- experiment must be repeatable under identical conditions
- For example one can't define a probability that it'll snow tomorrow

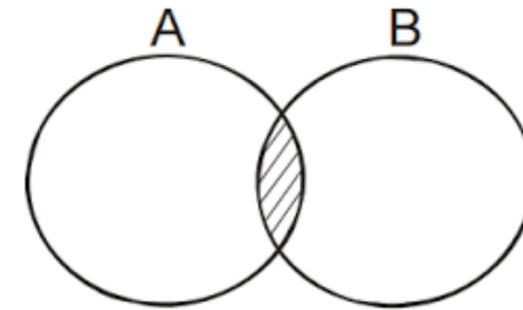
● Probably the one you're implicitly using in everyday life

● Frequentist statistics is often associated with the names of *Jerzy Neyman* and *Egon Pearson*

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- Define probability: $P(x)$ = **degree of belief** that x is true
 - It can be quantified with betting odds:
 - What's amount of money one's willing to bet based on their belief on the future occurrence of the event
 - In particle physics frequency interpretation often most useful, but Bayesian probability can provide more natural treatment of non-repeatable phenomena

BAYES' THEOREM

- Define conditional probability: $P(A|B) = P(A \cap B) / P(B)$
 - probability of A happening given B happened
 - for independent events $P(A|B) = P(A)$, hence $P(A \cap B) = P(A)P(B)$



- From the definition of conditional probability Bayes' theorem states:

$$P(T|D) = \frac{P(D|T)P(T)}{P(D)}$$

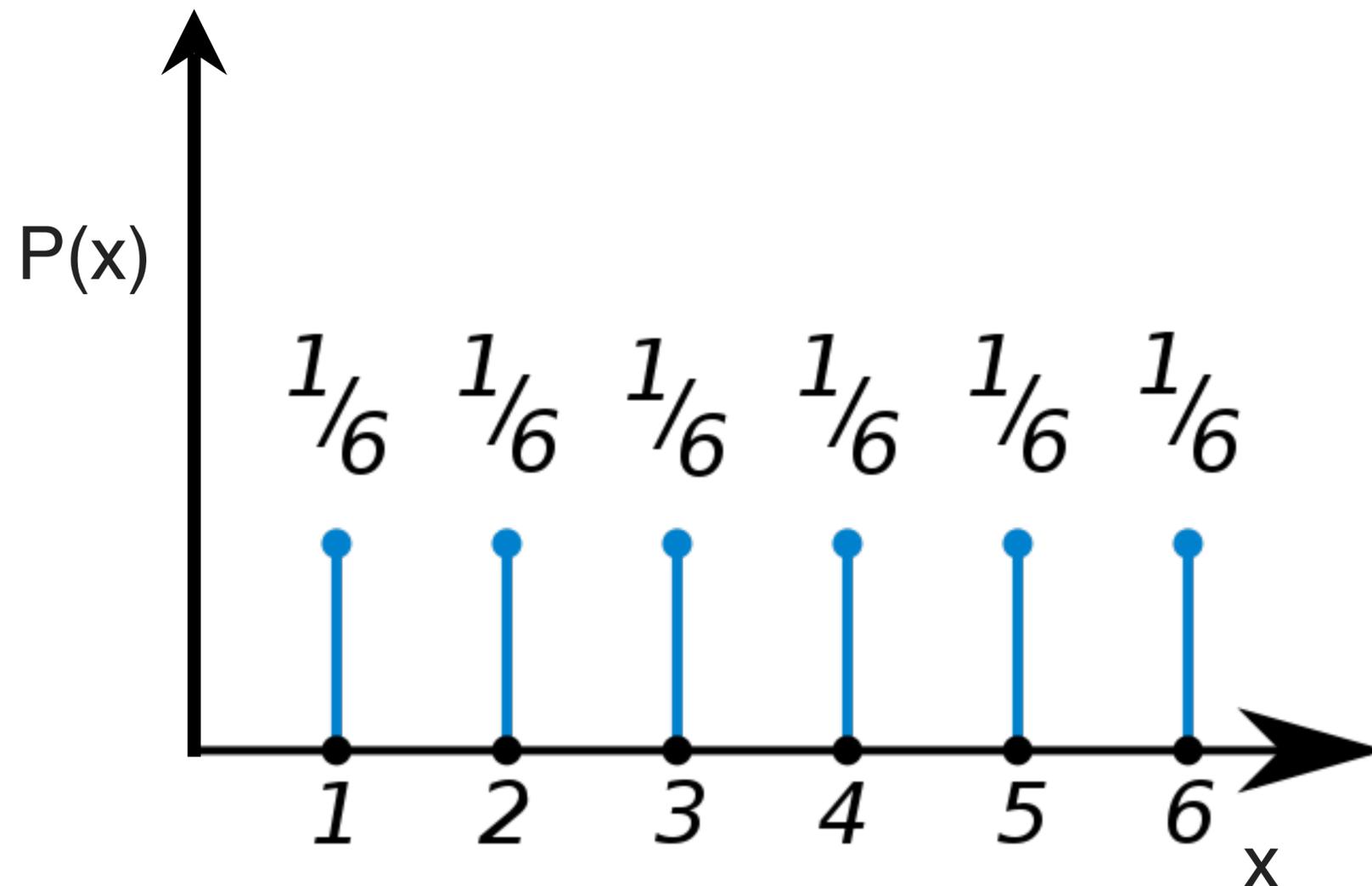
- T is a **theory** and D is the **data**
- P(T) is the **prior probability** of T: the probability that T is correct before the data D was seen
- P(D|T) is the **conditional probability** of seeing the data D given that the theory T is true.
 - P(D|T) is called the likelihood.
- P(D) is the **marginal probability** of D.
 - P(D) is the prior probability of witnessing the data D under all possible theories
- P(T|D) is the **posterior probability**: the probability that the theory is true, given the data and the previous state of belief about the theory

-
- **Random event** is an event having more than one possible outcome
 - Each outcome may have associated probability
 - Outcome not predictable, only the probabilities known
 - Different possible outcomes may take different possible numerical values x_1, x_2, \dots
 - The corresponding probabilities $P(x_1), P(x_2), \dots$ form a **probability distribution**
 - If observations are independent the distribution of each random variable is unaffected by knowledge of any other observation
 - When an experiment consists of N repeated observations of the same random variable x , this can be considered as the single observation of a random vector \mathbf{x} , with components x_1, x_2, \dots, x_N

DISCRETE RANDOM VARIABLES

- Rolling a die:
 - Sample space = $\{1,2,3,4,5,6\}$
 - Random variable x is the number rolled

- Discrete probability distribution:



- Let x be a possible outcome of an observation and can take any value from a continuous range
- We write $f(x;\theta)dx$ as the probability that the measurement's outcome lies between x and $x + dx$
- The function **$f(x;\theta)dx$** is called the **probability density function (PDF)**
 - And may depend on one or more parameters θ
- If $f(x;\theta)$ can take only discrete values then $f(x;\theta)$ is itself a probability
- The p.d.f. is always normalised to a unit area (unit sum, if discrete)
- Both \mathbf{x} and $\boldsymbol{\theta}$ may have multiple components and are then written as vectors

$$P(x \in [x, x + dx] | \theta) = f(x; \theta)dx$$

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

-
- Probability density function (PDF) = $f(x)dx$
 - Expectation:
 - Expectation of any random function $g(x)$: $E(g) = \int g(x)f(x)dx$
 - Expectation of x is the **mean**: $\mu = E(x) = \int xf(x)dx$
 - **Variance**: $V(x) = \sigma^2 = E[(x - \mu)^2] = \int (x - \mu)^2 f(x)dx$
 - $E(x)$ is usually a measure of the **location** of the distribution
 - $V(x)$ is usually a measure of the **spread** of the distribution

- The most important distribution in statistics because of the Central Limit Theorem:

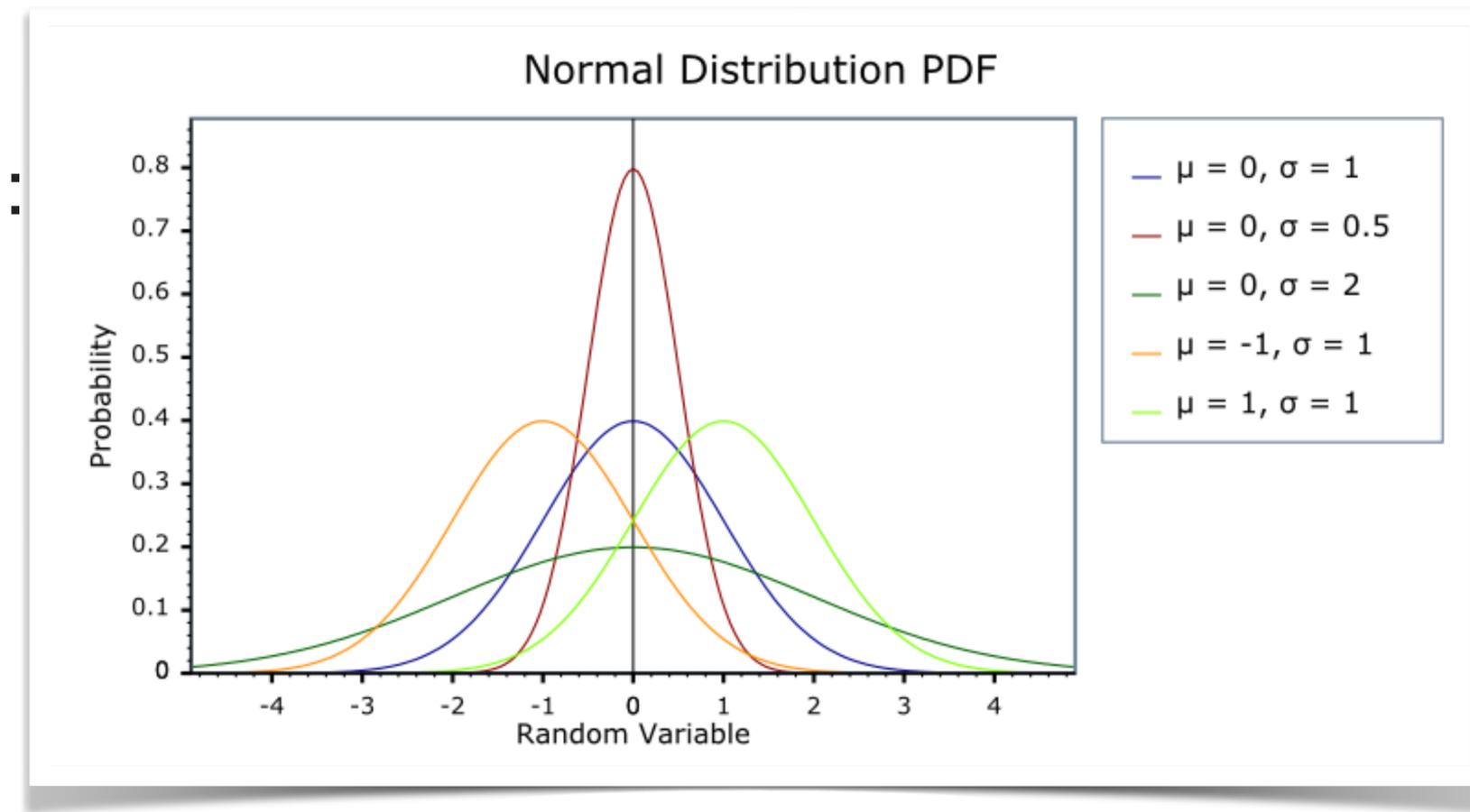
$$N(x; \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

- $N(0,1)$ is called standard Normal density

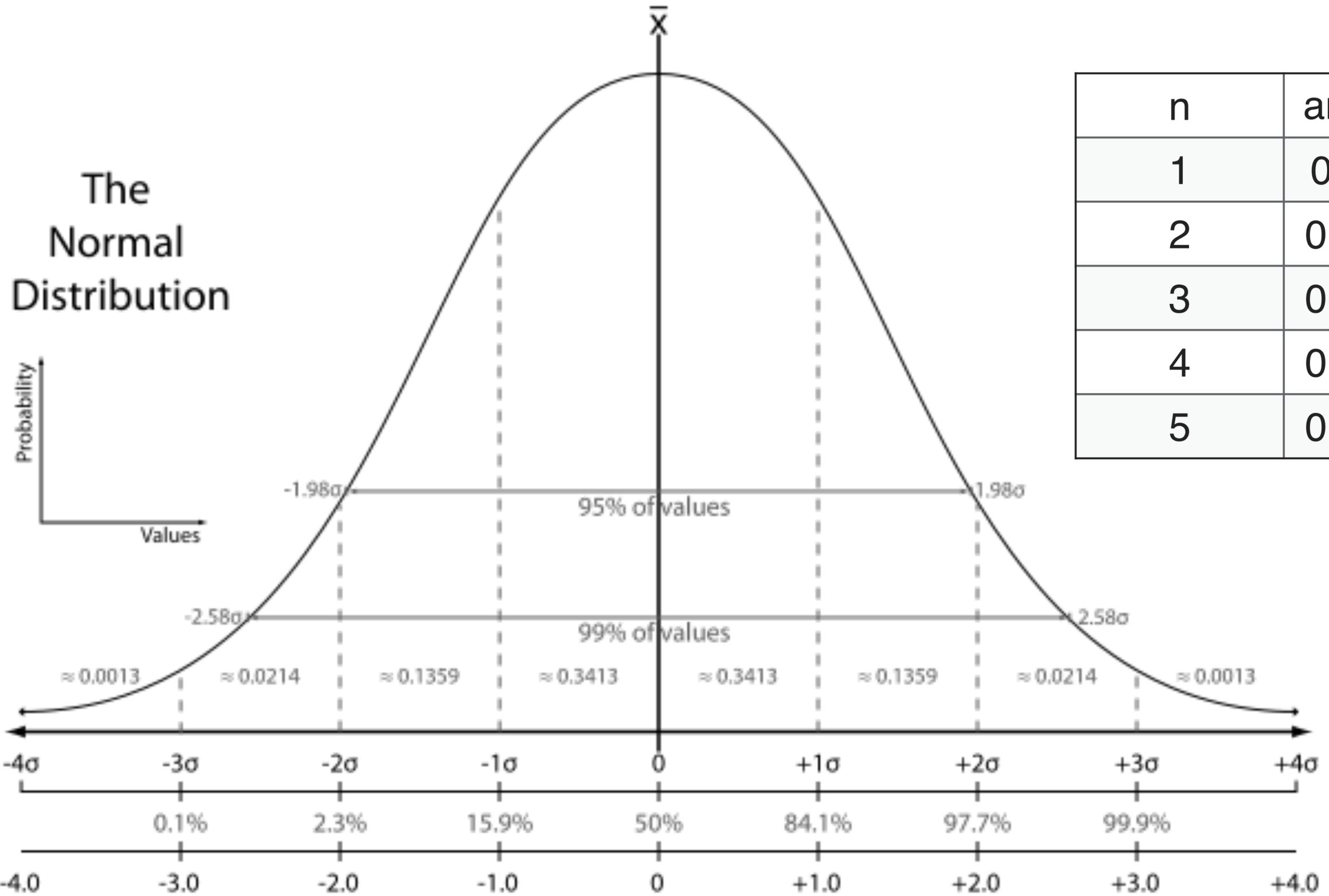
- Properties of the Gaussian distribution:

- Mean: $\langle r \rangle = E(r) = \mu$

- Variance: $V(r) = \sigma^2$

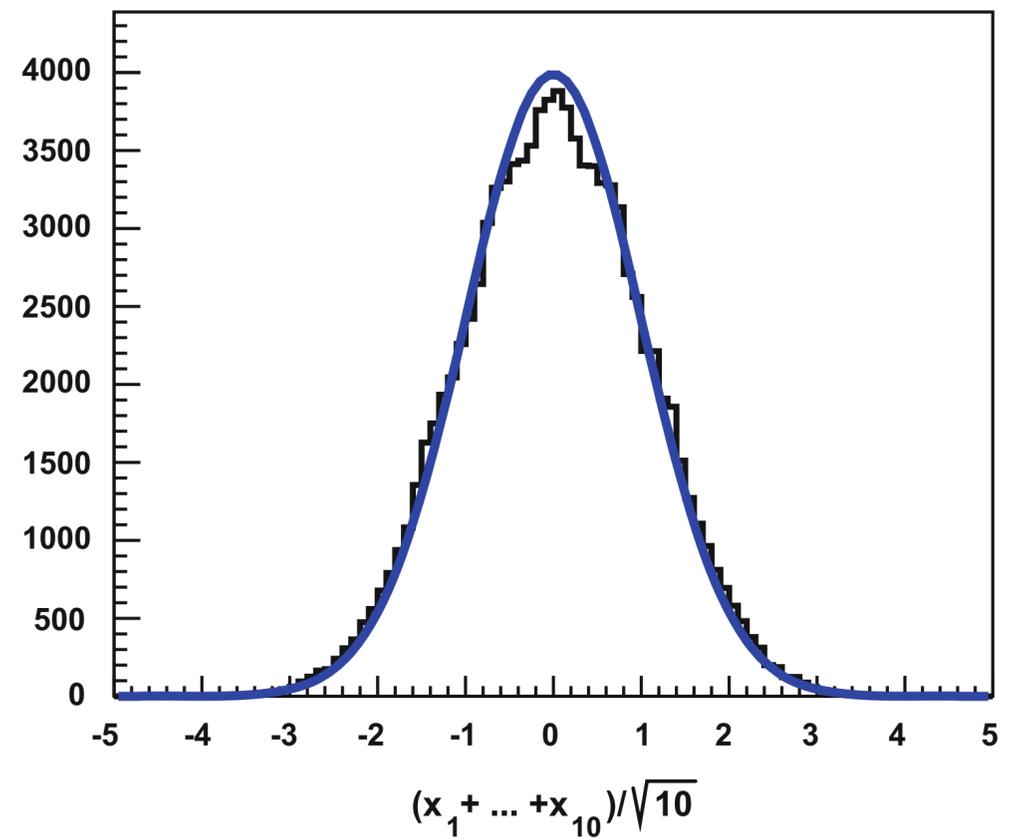
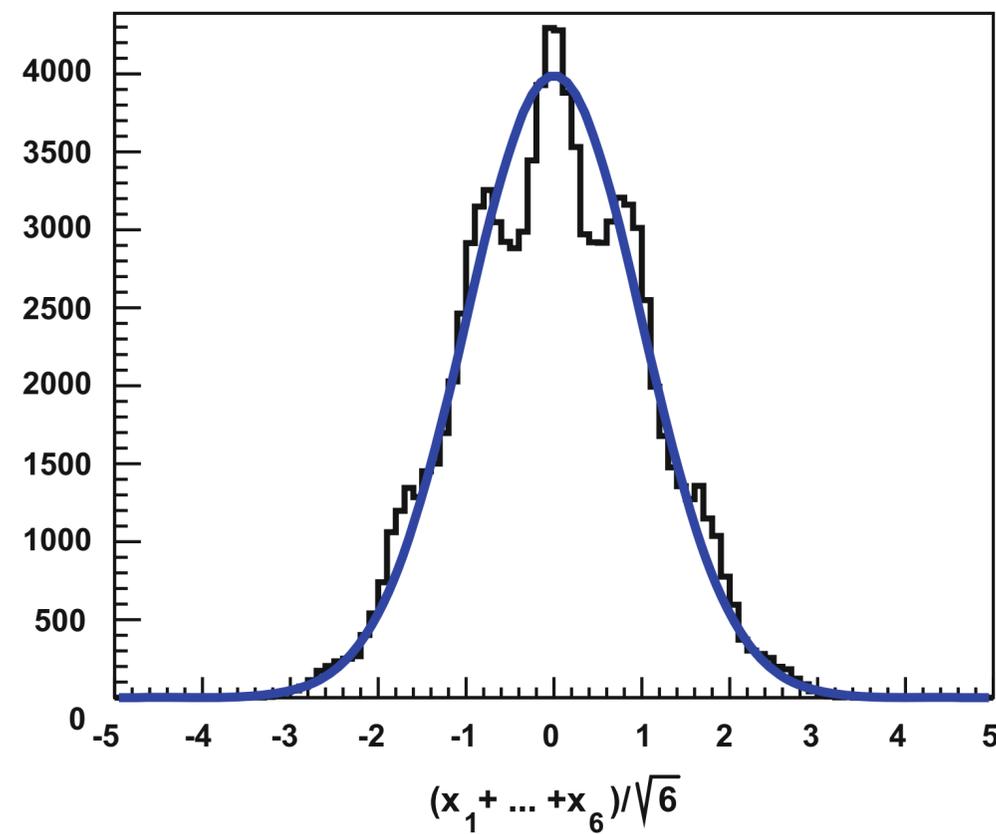
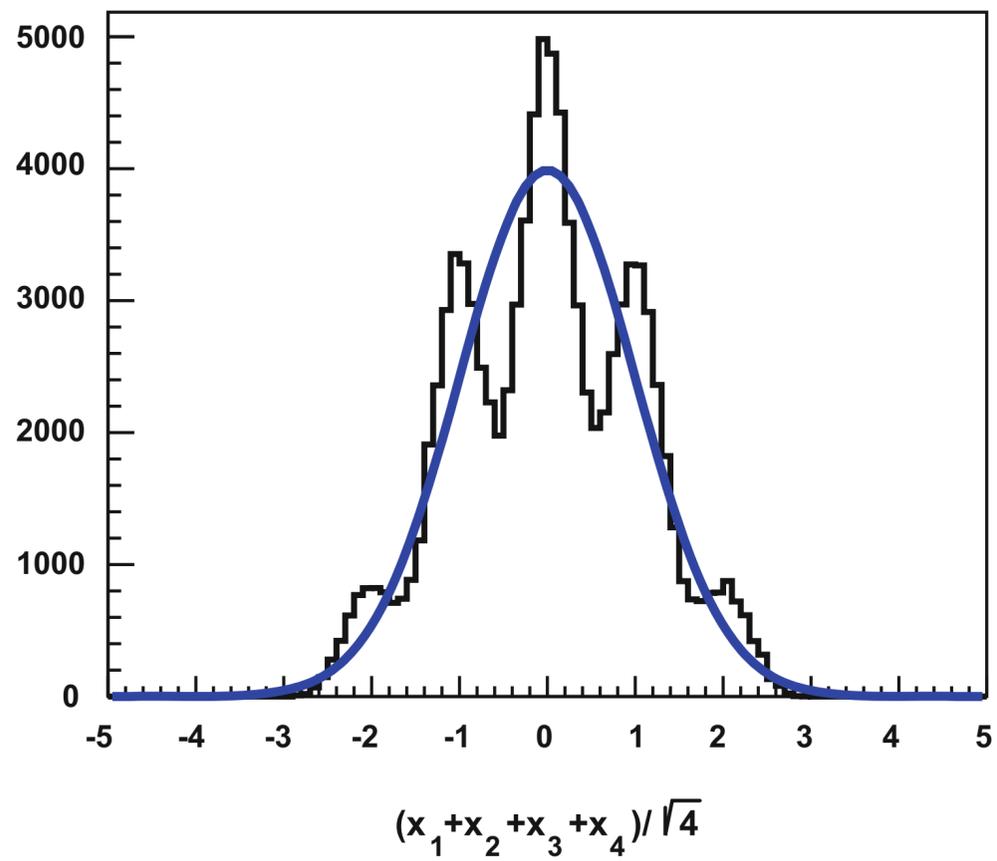
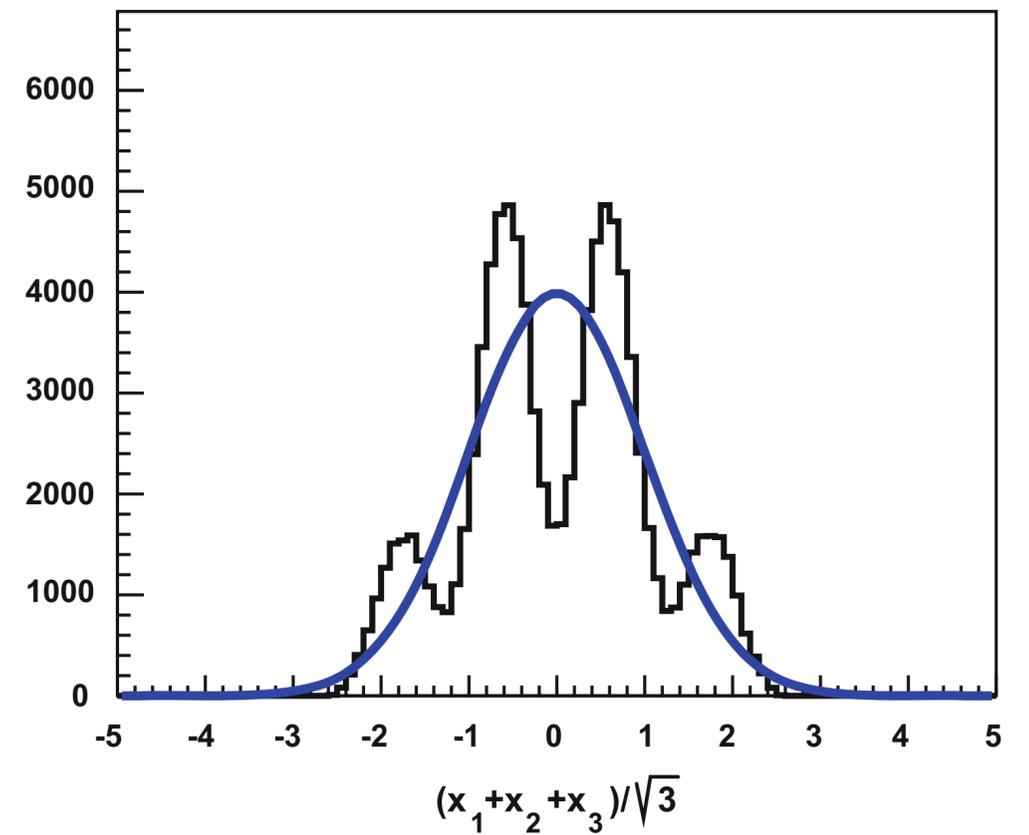
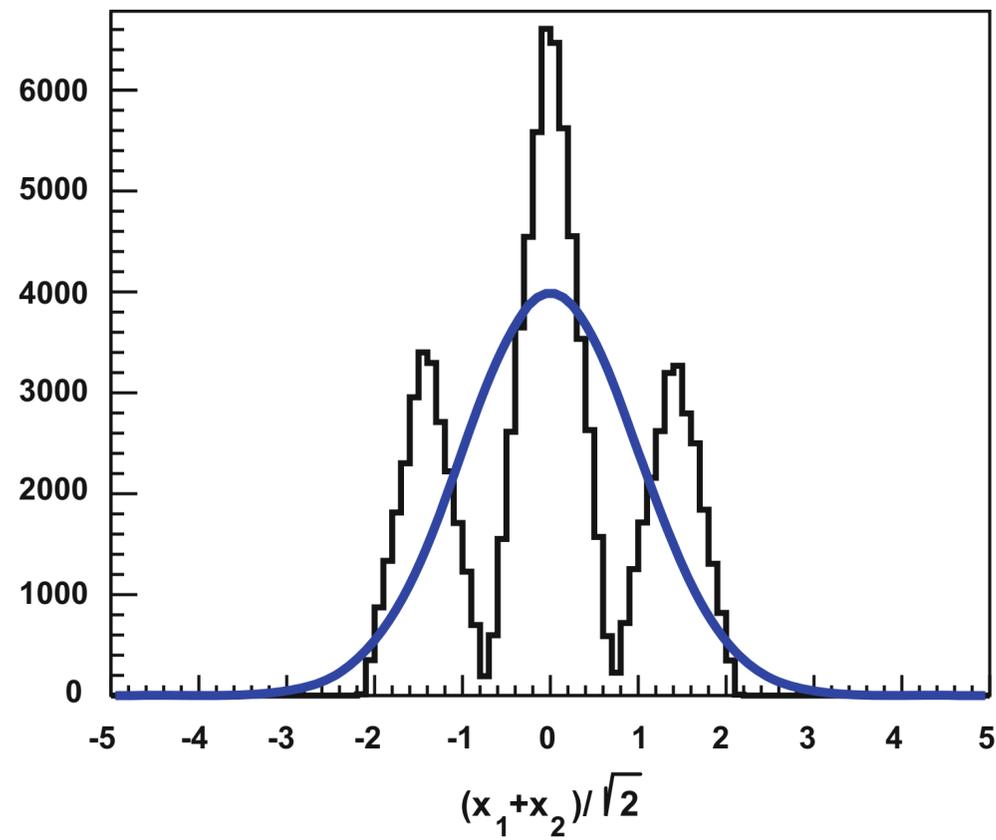
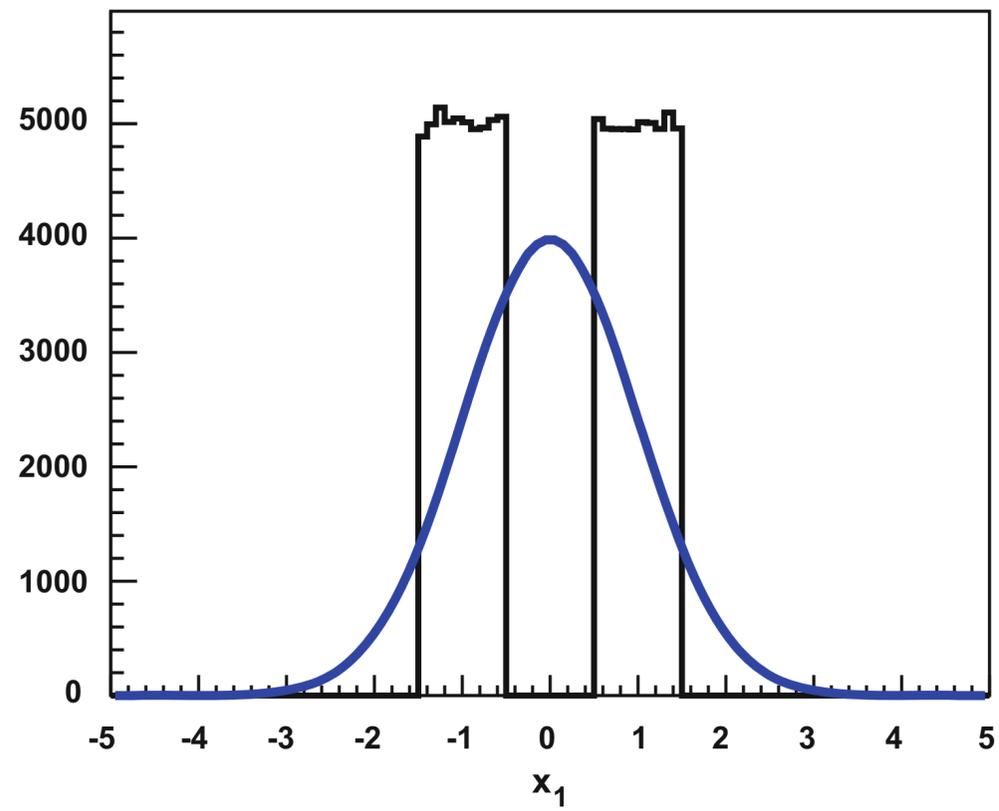


NORMAL DISTRIBUTION PROPERTIES



● Central limit theorem:

- If we have a set of N independent variables x_i , each from a distribution with mean μ_i and variance σ_i^2 , then the distribution of the sum $X = \sum x_i$
 - has a mean $\langle X \rangle = \sum \mu_i$,
 - has a variance $V(X) = \sum \sigma_i^2$,
 - becomes Gaussian as $N \rightarrow \infty$.
- Therefore, no matter what the distributions of original variables may have been, their sum will be Gaussian in a large N limit
- Example:
 - measurements errors
 - human heights are well described by a Gaussian distribution, as many other anatomical measurements, as these are due to the combined effects of many genetic and environmental factors
 - student test scores



- The parameters of a PDF are constants that characterise its shape:

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

- where x is measured data, and θ are parameters that we are trying to estimate (measure)
- Suppose we have a sample of observed values $\vec{x} = (x_1, x_2, \dots, x_n)$
- Our goal is to find some function of the data to estimate the parameter(s)
 - we write the **parameter estimator** with a hat $\hat{\theta}(\vec{x})$
 - we usually call the procedure of estimating parameter(s): **parameter fitting**

● Consistent

- Estimate converges to the true value as amount of data increases

$$\hat{\theta} \xrightarrow{\text{more data}} \theta^{true}$$

● Unbiased

- Bias is the difference between expected value of the estimator and the true value of the parameter

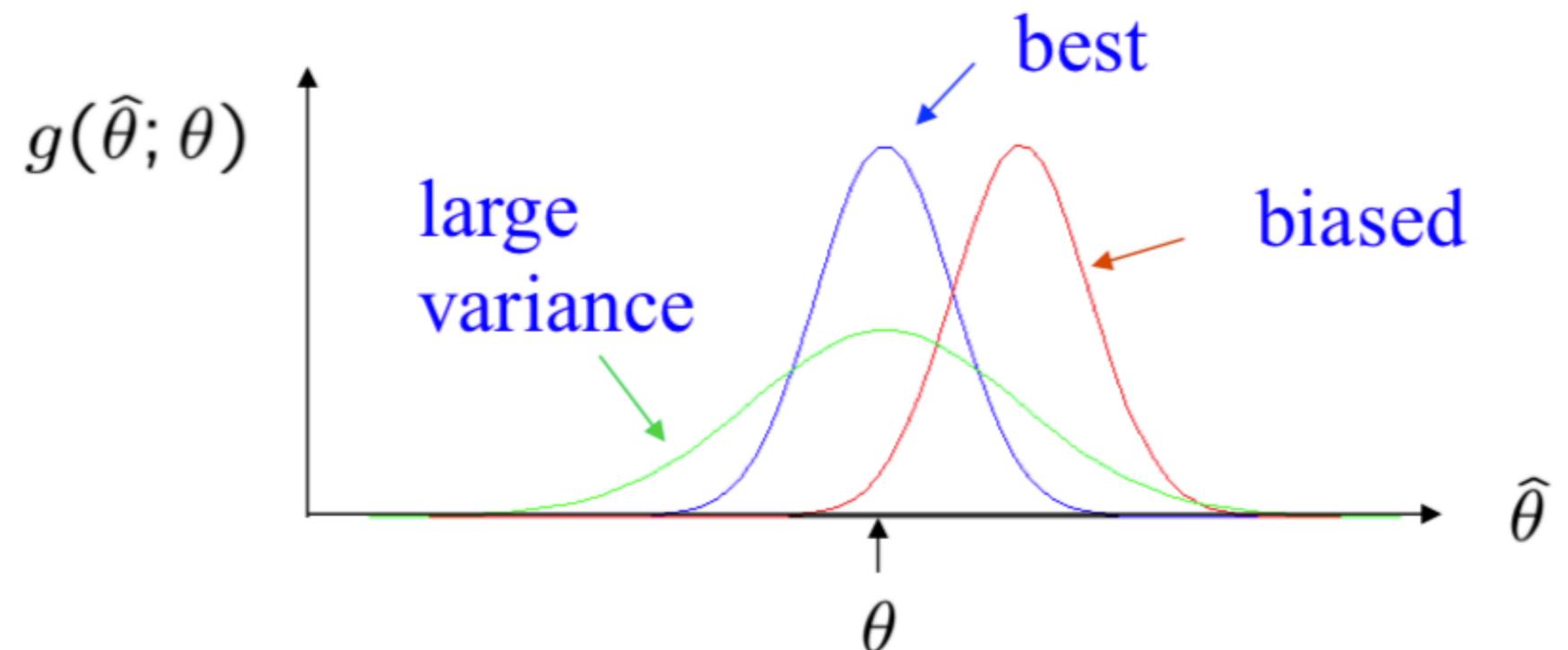
$$b = E(\hat{\theta}) - \theta^{true} = 0$$

● Efficient

- Its variance is small

● Robust

- Insensitive to departures from assumptions in the PDF



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- Be careful: **statistic** is not **statistics**!
 - Any new random variable (f.g. T), defined as a function of a measured sample x is called a statistic $T = T(x_1, x_2, \dots, x_N)$
 - For example, the sample mean $\bar{x} = \frac{1}{N} \sum x_i$ is a statistic!
 - A statistic used to estimate a parameter is called an **estimator**
 - For instance, the **sample mean** is a statistic and an estimator for the **population mean**, which is an unknown parameter
 - **Estimator** is a function of the data
 - **Estimate**, a value of estimator, is our “best” guess for the true value of parameter
 - Some other example of statistics (plural of statistic!): sample median, variance, standard deviation, t-statistic, chi-square statistic, kurtosis, skewness, ...

THE MAXIMUM LIKELIHOOD METHOD

- Gives consistent and asymptotically unbiased estimators
- Widely used in practice

THE LEAST SQUARES (CHI-SQUARE) METHOD

- Gives consistent estimator
- Linear Chi-Square estimator is unbiased
- Frequently used in histogram fitting

- Assume that observations (events) are independent
 - With the PDF depending on parameters $\theta: f(x_i; \theta)$
- The **probability that all N events will happen** is a product of all single events probabilities:
 - $P(x; \theta) = P(x_1; \theta)P(x_2; \theta) \cdots P(x_N; \theta) = \prod P(x_i; \theta)$
- When the variable **x is replaced by the observed** data x^{OBS} , then P is no longer a PDF
- It is usual to denote it by L and called $L(x^{\text{OBS}}; \theta)$ **the likelihood function**
 - Which is now a function of θ only $L(\theta) = P(x^{\text{OBS}}; \theta)$
- Often in the literature, it's convenient to keep X as a variable and continue to use notation $L(X; \theta)$

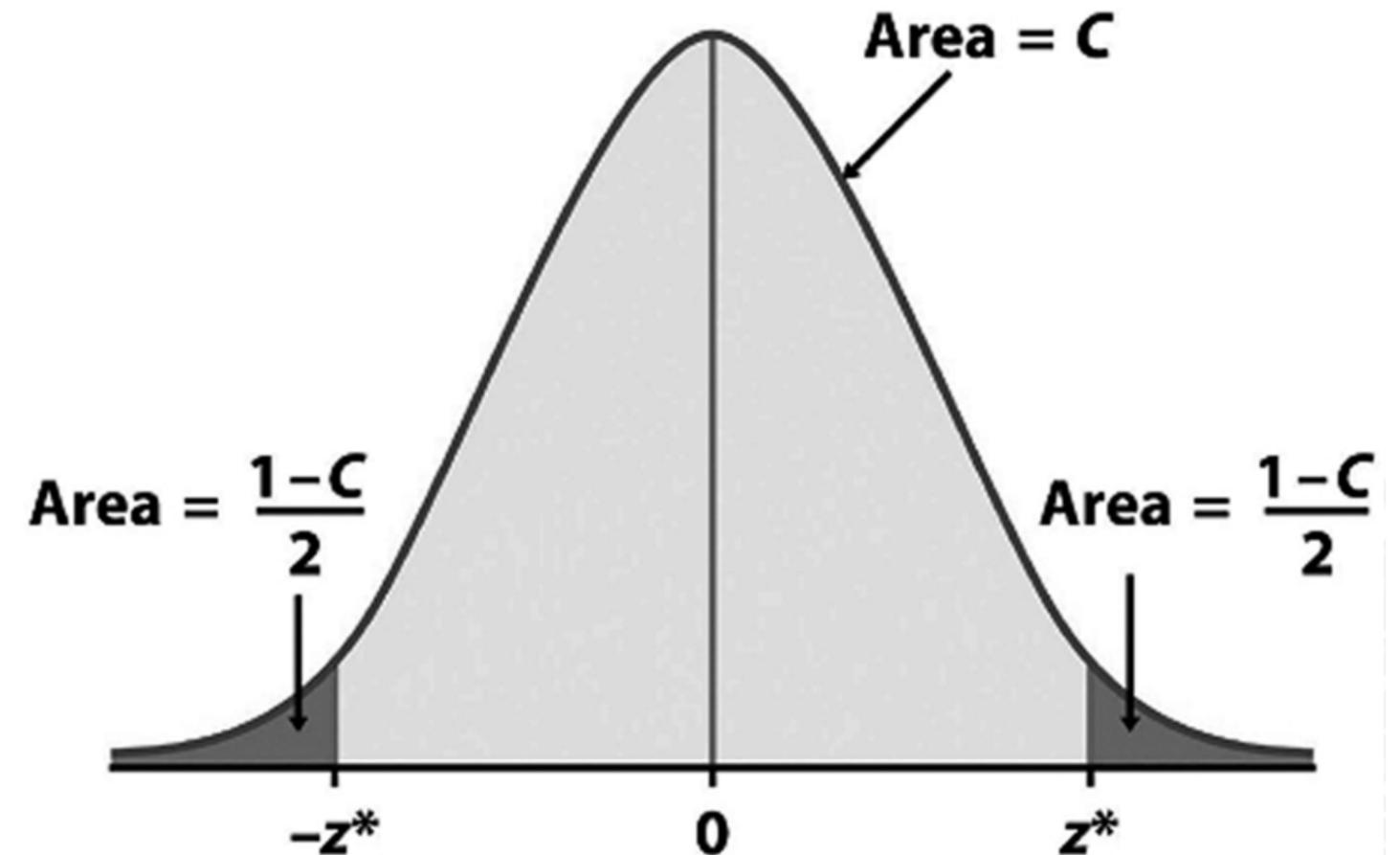
- The probability that all N independent events will happen is given by the likelihood function $L(x; \theta) = \prod f(x_i; \theta)$
- The principle of maximum likelihood (ML) says: **The maximum likelihood estimator $\hat{\theta}$ is the value of θ for which the likelihood is a maximum!**
- In words of R. J. Barlow: “You determine the value of θ that makes the probability of the actual results obtained, $\{x_1, \dots, x_N\}$, as large as it can possibly be.”
- In practice it's easier to maximize the **log-likelihood function**
 $\ln L(x; \theta) = \sum \ln f(x_i; \theta)$
- For p parameters we get a set of p **likelihood equations**: $\frac{\partial \ln L(x; \theta)}{\partial \theta_j} = 0$
- It is often more convenient to **minimise $-\ln L$ or $-2\ln L$**

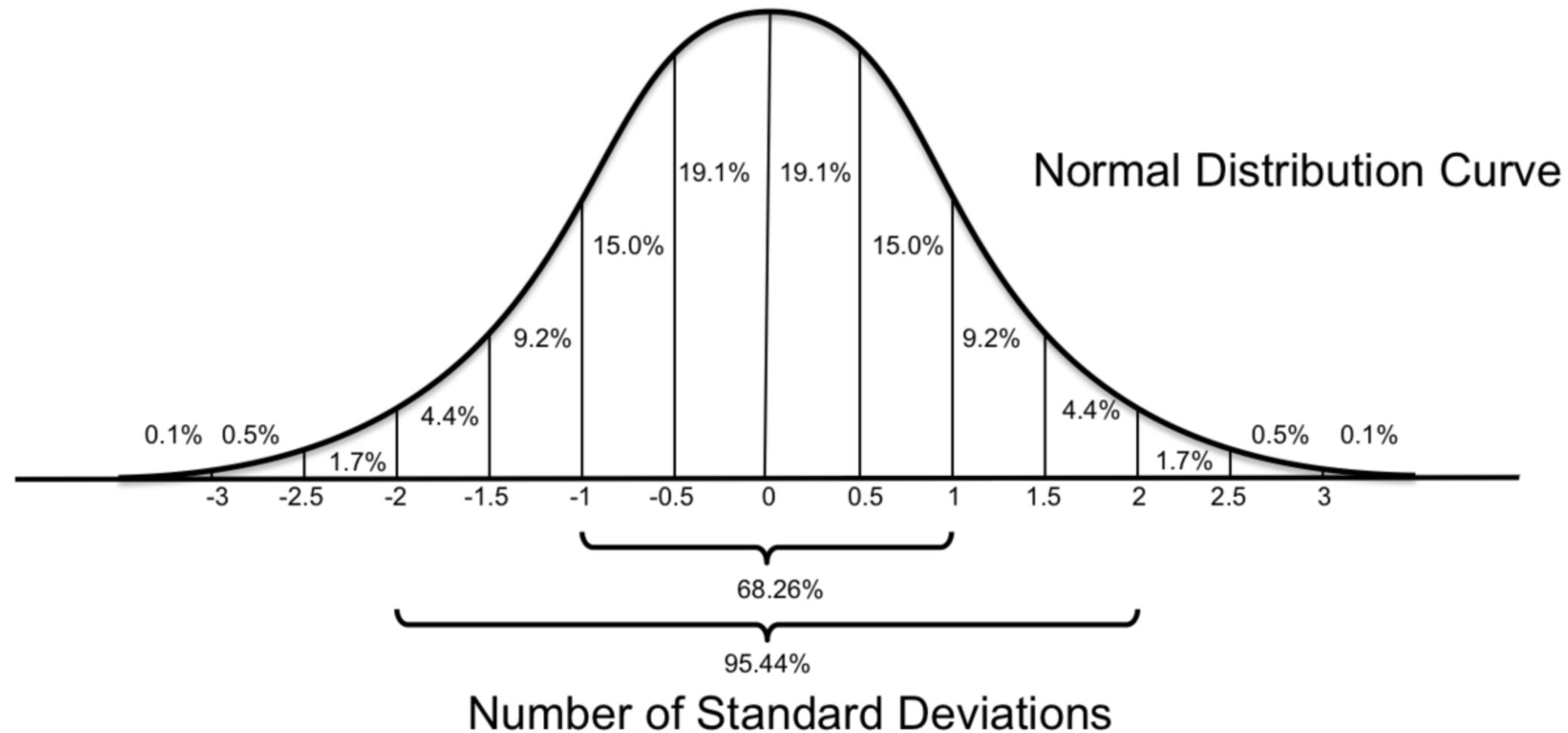
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- Never ever (really, don't ever do it!) quote measurements without confidence intervals
 - In addition to a “point estimate” of a parameter we should report an interval reflecting its statistical uncertainty.
 - Desirable properties of such an interval:
 - communicate objectively the result of the experiment
 - have a given probability of containing the true parameter
 - provide information needed to draw conclusions about the parameter
 - communicate incorporated prior beliefs and relevant assumptions
 - Often use \pm the estimated standard deviation (σ) of the estimator
 - In some cases, however, this is not adequate:
 - estimate near a physical boundary
 - if the PDF is not Gaussian

- Let some measured quantity be distributed according to some PDF $f(x; \theta)$, we can determine the probability that x lies within some interval, with some confidence C :

$$P(x_- < x < x_+) = \int_{x_-}^{x_+} f(x; \theta) dx = C$$

- We say that x lies in the interval $[x_-, x_+]$ with confidence C





● If $f(x; \theta)$ is a Gaussian distribution with mean μ and variance σ^2 :

● $x_{\pm} = \mu \pm 1 \cdot \sigma \quad C = 68 \%$

● $x_{\pm} = \mu \pm 2 \cdot \sigma \quad C = 95.4 \%$

● $x_{\pm} = \mu \pm 1.64 \cdot \sigma \quad C = 90 \%$

● $x_{\pm} = \mu \pm 1.96 \cdot \sigma \quad C = 95 \%$

- In a measurement two things involved:
 - True physical parameters: θ^{true}
 - Measurement of the physical parameter (parameter estimation): $\hat{\theta}$
- Given the measurement $\hat{\theta} \pm \sigma_{\theta}$ what can we say about θ^{true} ?
- Can we say that θ^{true} lies within $\hat{\theta} \pm \sigma_{\theta}$ with 68% probability?
 - **NO!!!**
 - θ^{true} is **not a random variable!** It lies in the measured interval or it does not!
- We can say that if we repeat the experiment many times with the same sample size, construct the interval according to the same prescription each time, in 68% of the experiments $\hat{\theta} \pm \sigma_{\theta}$ interval will cover θ^{true} .

- There are two ways to obtain confidence intervals for the parameter estimated by the Maximum Likelihood method

- **Analytical way:**

- If we assume the **Gaussian approximation** we can estimate the confidence interval by matrix inversion:

$$\text{cov}^{-1}(\theta_i, \theta_j) = \frac{\partial^2 \ln L}{\partial \theta_i \partial \theta_j} \Bigg|_{\theta = \hat{\theta}}$$

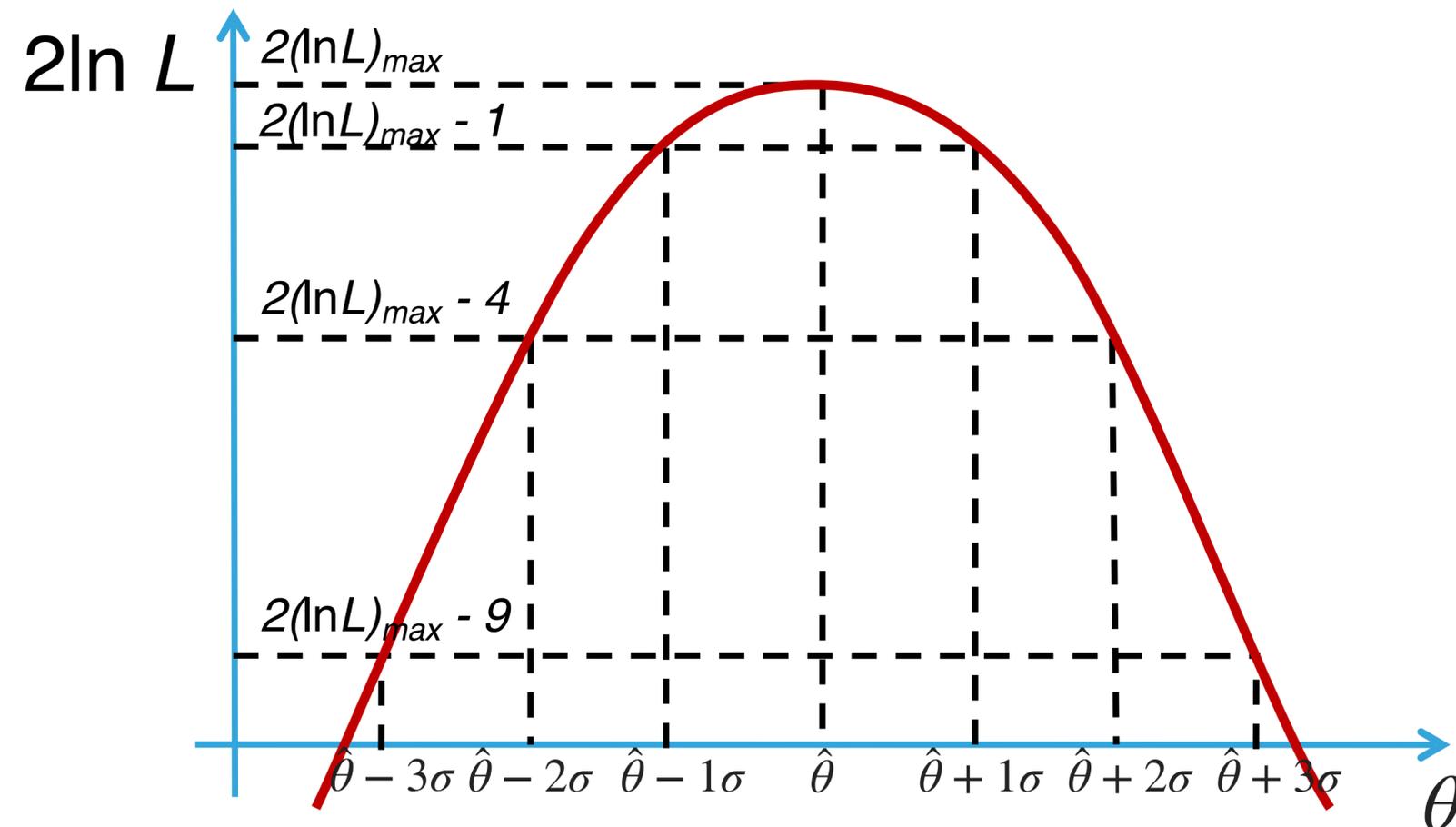
- If the likelihood function is non-Gaussian and in the limit of small number of events this approximation will give symmetrical interval while that might not be the case
- Possible to solve by hand only for very simple PDF cases, otherwise numerical solution needed
 - Matrix inversion done with HESSE/MINUIT algorithm in ROOT

- **From the Log-Likelihood curve**

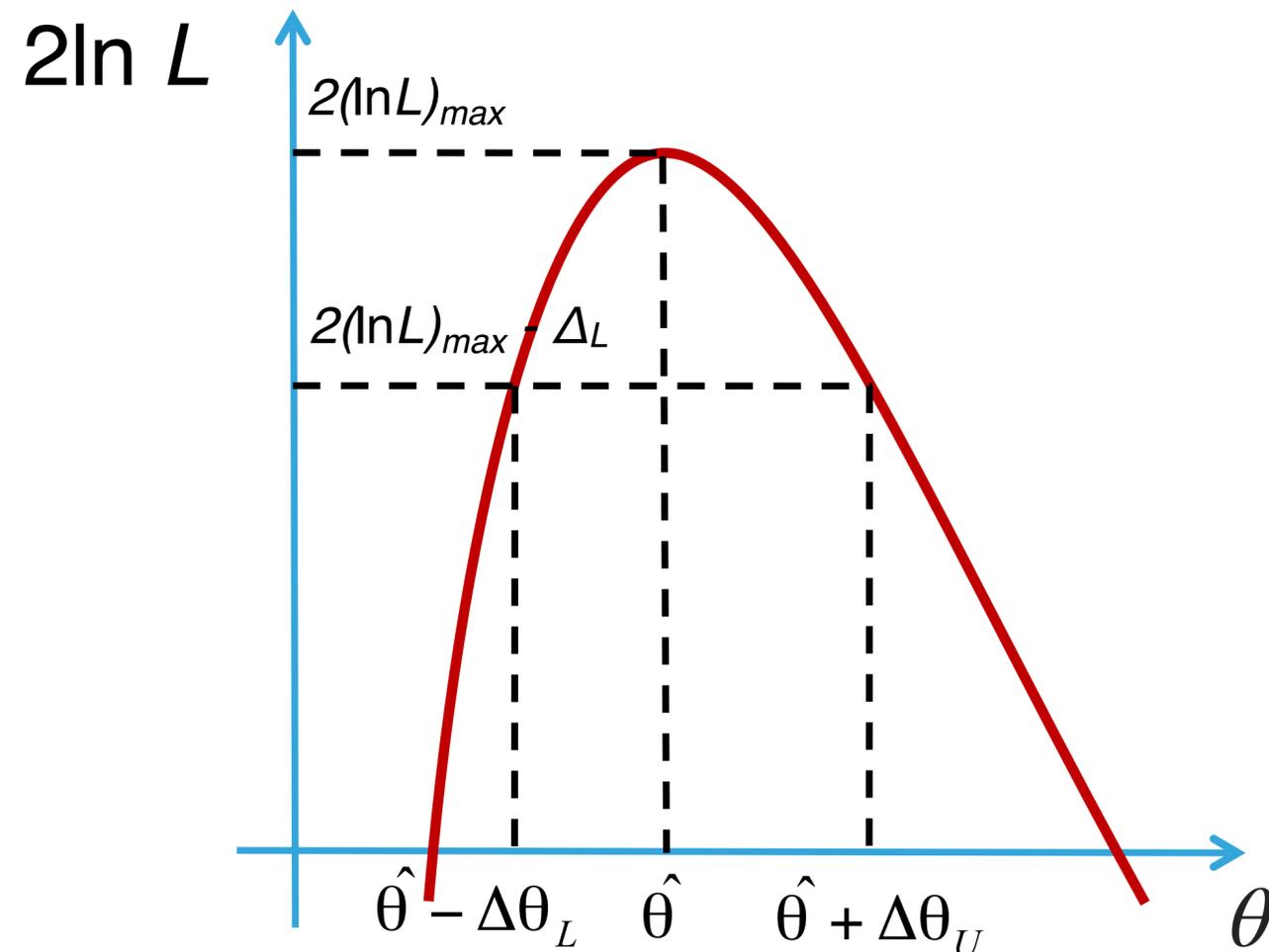
- Extract $\sigma_{\hat{\theta}}$ from log-likelihood scan using:

$$\ln L(\hat{\theta} \pm N \cdot \sigma_{\hat{\theta}}) = \ln L_{max} - \frac{N^2}{2}$$

- This is the same as looking for $2\ln L_{max} - N^2$



- The Log-Likelihood function can be asymmetric
 - for smaller samples, very non-Gaussian PDFs, non-linear problems,...
- The confidence interval is still extracted from the Log-Likelihood curve using the same prescription
 - This leads to asymmetrical confidence interval that should be used when quoting the final result



CL	Δ_L
68.27	1
95.45	4
99.73	9

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