Statistical modelling and data analysis
Syllabus of a short course of lectures (30 hrs)

1. Aims and general principles of modelling **2 hrs**
2. Mathematical toolbox of statistical modelling **8 hrs**
   - Occurrence. Operations on occurrences. Elements of combinatorics 2 hrs
   - Probability and its properties 1 hr
   - Conditional probability. Total probability. Bayes' formula 1 hr
   - Discrete random variable 1 hr
   - Continuous random variable 1 hr
   - Random vectors 2 hrs
3. Some important distributions and their properties **8 hrs**
   - Geometric and binomial distributions. Poisson distribution 2 hrs
   - Uniformly distributed random variable. Gaussian (normal) distribution 2 hrs
   - χ^2 distribution. Student, Cauchy, Breit-Wigner and Fisher distributions 2 hrs
   - Generating a random variable with a pre-defined distribution 2 hrs
4. Elements of mathematical statistics **2 hrs**
5. Monte Carlo method **3 hrs**
   - General features 1 hr
   - Calculating a definite integral using Monte Carlo method 1 hrs
   - Random number generators. Pseudo-random numbers 1 hrs
6. Classic example: modelling the propagation of neutrons through matter **2 hrs**
7. Methods of analysing experimental data distributions **5 hrs**
   - Maximum likelihood method. Method of least squares 3 hrs
   - Measurement uncertainties. Estimating uncertainties in indirect measurements. Combining independent uncertainties. Interpretation of measurement uncertainties 2 hrs

Prerequisites: full course in calculus.

Main literature: **The course of lectures given below**.

Additional literature:

1. Frodesen, Skjeggestad and Tofte, "Probability ad Statistics in Particle Physics", Columbia University Press, 1979.

2. G. Mania, "Probability theory and mathematical statistics" (in Georgian), Tbilisi, 1976.

3. D. Hudson, "Statistics for Physicists" (translated into Russian), Moscow, 1970.

4. I. M. Sobol, "Numerical Monte Carlo methods" (in Russian), Moscow, 1973.

5. A. Taylor, "Theory of errors" (translated into Russian), Moscow, 1992.

1 Aims and general principles of modelling

The aim of this course is to learn how to use the language of mathematics to formulate and solve various problems that emerge in realistic practical situations, including those in physics. In general, this process can be called *modelling*. The object of modelling is a *system* which consists of a number of functioning and interacting objects. The state of the system is defined through a collection of values taken by the variables necessary to describe the system at any particular moment in time. Depending on the nature of the system, these variables can be *discrete* or *continuous*. Examples of continuous systems can be found in physics, while discrete systems can be found in banks. Describing a system mathematically would allow us to improve our understanding of its main properties and help create correct predictions for various future developments.

In any modern experiment in physics, the formulation of its main physical idea is followed by a modelling stage. The aim of this stage is to figure out optimal conditions and parameters of the experiment, such as types and sizes of the detectors, their placement, occupancy etc. In this sense, modelling is often called a *computational experiment*.

Modelling starts with the formulation of the problem, which is then being solved based on certain ideas. The formulation of the problem is usually a non-trivial task, since the system rarely has well-defined edges, thus making it difficult to separate its parts from external objects. In other words, no system is perfectly isolated from the outside world, but we need to formulate our problem in a way that would allow us to consider it as isolated. As an example, consider the task of optimizing the air traffic in Europe after a volcanic eruption: if the eruption took place somewhere in the Pacific, its effects can be ignored, while an eruption in Iceland would have an important influence on the solution of the problem (which was indeed the case in 2010).

As the problem is being formulated, the main parameters characterising the system are determined. This implies some degree of *idealisation*, without which no problem can be solved. For example, when solving the motion of a pendulum, we use a mathematical model with a massless and unstretchable thread. At this stage, no account is taken of the shape of the weight or its colour, and air resistance is also ignored. So, at the idealisation stage it's important to separate the factors and parameters that drive the system from those that can be neglected, since an idealised problem can be solved much more easily. While observing a real pendulum, it's noticed that the amplitude of its oscillations decreases in time, and after some time – say, a couple of hours – the pendulum stops. The mathematical model does not predict this behaviour. However, on a shorter time-scale of, say, several seconds, the model "works" well. Hence, once a model is chosen, the range of its applicability also needs to be specified. Another example would be the ideal gas model applied to real gas. In these and similar cases, a mathematical model can be designed based on the laws of physics

governing these phenomena. But some other systems may appear to be too complicated to be described by a mathematical model. Such examples include activities of a group of human beings, or, say, various problems in economics. Such complex systems are studied experimentally and the models are built based on the statistical analysis of the obtained experimental data. The models of this type are sometimes called statistical (simulational) models.

Once the model is built, one needs to check that the model provides an *adequate* description of the real system. One would start by checking the dimensions of the physical quantities entering the mathematical expression describing the model. The model should be free of internal contradictions, and thus should obey the laws of mathematical logic. Note however, that the decision whether the model is adequate or not is itself, to some degree, subjective!

So the mathematical model is a simplified picture of reality, obtained by some kind of idealisation of this reality. The purpose of the model could be some kind of calculation, system design, control of various systems and processes etc. Modelling can also reveal new, previously unknown properties of system, and predict future developments. In cases where an experimental study is impossible or impractical, modelling is the only way of studying a system. Analysis of various situations for space exploration is a good example.

A mathematical model needs to be translated into a procedure (*algorithm*) that will be performed on a computer. At this stage of the model development, a *platform* needs to be selected. This could be a high-level language such as FORTRAN, C or C++, or a software package within the Windows operating system, such as MATHLAB or LABVIEW. After the model is created and solved on a computer, it's good practice to have some means of *visualisation* of the results of simulation. This will help understand the numerical or analytical output.

Once a model is developed, the expected *precision* of the model is usually implicitly defined. For example, if the model was built based on some experimental input which was known to the precision at the level of 5%, trying to obtain results with 1% precision will be a waste of time and effort. If one can identify some components in the calculation process which happen to be negligible compared to other terms, one can sometimes achieve major savings in the computing time if these components are neglected at an early stage.

At an early stage of modelling it is often necessary to decide on the types of variables used in the model. Usually two main categories are considered: *deterministic* variables whose values can be reliably measured and/or calculated theoretically, and *stochastic* variables whose values can be random. If a model contains stochastic variables, this fact needs to be reflected in the description of the model, and hence the model in this case needs to be based on the laws of probability theory and mathematical statistics.

A model describing a physical system almost always contains random variables, and in order to be able to manipulate those quantities it is necessary to be familiar with respective mathematical apparatus. For this reason, the introduc-

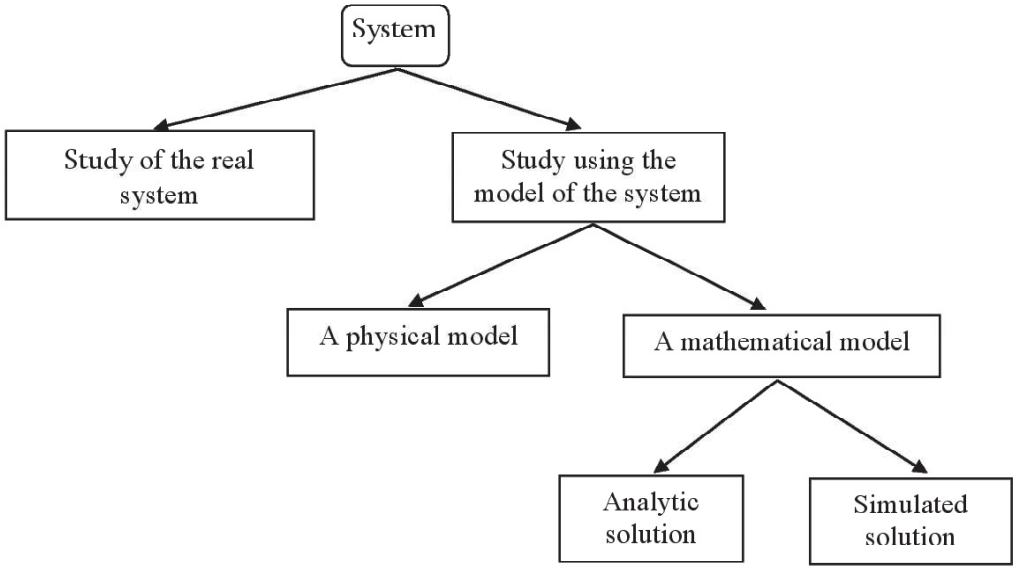
tory part of this course contains the description of random variables and their characteristics.

An important part of the modelling process is the *interpretation* of its results, which incorporates the translation of mathematical results back to the language describing the real world. Without this it would be impossible to make any conclusions on the validity of the model.

The creation process of the model can be compared to the evolution of a child learning to speak. Simply put, the language is a reflection of the real world, and the improvement in the child's speaking ability happens simultaneously with the improvement in his/her cognition of the world. Similarly, a model starts with a description of the simplest situation and becomes more and more sophisticated as our understanding of the system improves.

The philosophy of modelling is very well explained by a Chinese proverb: "I hear and I forget, I see and I remember, I do and I understand".

The diagram in Figure 1 shows various ways of studying a system.



2 Basics of probability theory

2.1 Occurrences. Operations on occurrences.

No natural phenomenon is free of a random influence of some sort. For this reason, no matter how precisely one defines the conditions of an experiment, it will never yield the same result twice. So every process is subject to some random variations, but the role and degree of randomness will be different for different phenomena. In some cases, those random variations may be negligibly small, but there are processes where randomness plays a major role. A good example of the latter is the Brownian motion, where the movement of particles is totally chaotic, which is in turn determined by the chaotic motion of the molecules of the liquid. In such cases, the randomness itself becomes a regularity.

It has been found that if one observes a random event many times, one can determine certain specific regular features that characterise this randomness. The *probability theory* is a field of mathematics that studies such random variables. Starting from definitions and axioms, probability theory is built using deduction – darting from general statements and applying mathematical logic and derivation rules.

An uncertainty of a measurement is a simple example of a random variable. There is no such thing as an exact measurement; this becomes more and more obvious when the precision of the instrument is improved. The results of individual measurements are different numbers, which are usually close to each other. If these results are plotted in a graph, they are not aligned along a smooth curve, but are instead scattered within a certain range. The scatter is caused by the measurement errors, but also by various random factors affecting the process. Another example of a random variable is the scatter of artillery shells around a target. Despite being aimed at the same spot, the shells never hit the same point twice. This is caused by the dynamic nature of the atmosphere, i.e. the fact that the parameters describing the atmosphere vary in time. The atmosphere affects the flight of the shell, and the variation of the atmospheric parameters at every point of the shell's trajectory, which cannot be taken into account precisely, causes the random scatter in the final position of the shell.

In probability theory, the term *occurrence* is used to describe a result of an experiment or an observation. The occurrence describes the fact of an event taking place, so it is neither a number nor a quantity. Occurrences are denoted by capital Latin letters (with or without subscripts). For example, if a dice is rolled, some possible occurrences are:

$$A\{\text{get a six}\} = \{6\}, B\{\text{get a three}\} = \{3\}, C\{\text{get an even number}\} = \{2, 4, 6\}.$$

The occurrence $D\{\text{get a six and a three}\}$ is impossible, because {a six is thrown up} and {a three is thrown up} are mutually exclusive – *incompatible* – occurrences. If, however, two dice are rolled, the above occurrence becomes perfectly

possible. Also possible is the occurrence $F\{\text{sum of two dice is } 4\} = \{2,2;1,3;3,1\}$ which can happen in three possibilities. Among the occurrences listed above, C and F are *composite* and can be split into simpler occurrences. A result of an experiment, which cannot be decomposed further, is represented by an *elementary* occurrence. All possible results of an experiment comprise the *space* of the occurrences, which is usually denoted by E, while individual elementary occurrences are said to be the *points* in this space. When a single dice is rolled, the space contains six points:

$$A_1\{\text{get a one}\}, A_2\{\text{get a two}\}, A_3\{\text{get a three}\},$$
$$A_4\{\text{get a four}\}, A_5\{\text{get a five}\}, A_6\{\text{get a six}\},$$

and hence the space E is $E = \{1,2,3,4,5,6\}$.

One can speak about an occurrence A only if it is known, for every experiment, whether A took place or not. The set of points, which includes all possible results of experiments where the occurrence A took place, fully defines this occurrence. And vice-versa, if the point belongs to the set A, one would say that occurrence A took place. In this sense, *occurrence is defined as a term that stands for a set of elementary occurrences*. So the terms "elementary occurrence" and "occurrence" are equivalent to the concepts of a point and a set of points, respectively. These terms belong to the primary, and hence undefined, concepts of the probability theory.

If an elementary occurrence B causes another occurrence A, then the former is said to be facilitating the latter. If an experiment results in one of the occurrences facilitating A, then occurrence A has taken place. In an earlier example, occurrence $C\{\text{get an even number}\}$ happens, when the dice throw up a $\{2\}$, or a $\{4\}$ or a $\{6\}$.

An occurrence that contains all possible elementary occurrences for a given experiment is said to be *necessary* for this experiment, and is denoted by the symbol Ω. An occurrence which does not contain any of the elementary occurrences for the current experiment is called *impossible*, and is denoted by the symbol $\emptyset$. or the case of a single dice, a number between 1 and 6 is a necessary occurrence, but a number outside this range, say larger than 6, is impossible. In other words, a necessary occurrence will certainly happen if the experiment is performed, while an impossible occurrence will not take place in any number of such experiments. An occurrence which is neither necessary, nor impossible – i.e. an occurrence which may or may not happen – is called a possible, or a *random* occurrence.

Two occurrences are said to be equiprobable, if, based on the symmetry of the problem, there is no reason to believe that one is more likely to happen than the other. When a dice is thrown, any number between 1 and 6 is equiprobable. When a coin is tossed, the chances of getting heads and tails are equal. Two occurrences are said to be *compatible*, if one of them does not exclude the other. If one occurrence excludes the other, than the two are *incompatible*. Again, in the

example of a single dice, occurrences $A\{\text{get a six}\}$ and $C\{\text{get an even number}\}$ are compatible, but the occurrences $B\{\text{get a three}\}$ and $C\{\text{get an even number}\}$ are not (since 3 is not an even number).

Consider an experiment, which must result in one of the following set of occurrences $A_1, A_2, \ldots, A_n$, $(n \leq \infty)$, where these occurrences are mutually incompatible. Such a set is said to form a *complete set of occurrences*. So, by definition, the sum of the complete set of occurrences is a necessary occurrence:

$$A_1 + A_2 + \cdots + A_n = \Omega$$

In the example of rolling dice, the complete set is given by $E\{1, 2, 3, 4, 5, 6\}$.

The following *theorem* is true: using the full set of occurrences, any occurrence can be presented as (decomposed into) a sum of mutually incompatible occurrences.

Proof: Let A_i form the complete set of occurrences, and A is an occurrence which happens together with a certain A_k. Then

$$A = A \cdot \Omega = A \cdot \sum_{i=1}^{n} A_i = A \cdot A_k + \sum_{i=1, i\neq k}^{n} A_i = A + \emptyset = A \qquad \text{Q.E.D.}$$

If every elementary occurrence that facilitates occurrence A causes occurrence B, then A is said to cause B. In this case, A is said to be a included in B, which is written as $A \subset B$ (see Figure 1). This operation is called *inclusion*. It is obvious that A is a subset of B. Consider, for example, two sets: $A\{\text{all mothers}\}$ and $B\{\text{all women}\}$. All mothers are women, but not all women are mothers; here B includes A, in other words, A is a subset of B.

Every occurrence includes itself, $A \subset A$; it also includes the impossible occurrence, $\emptyset \subset A$.

If $A \subset B$ and $B \subset A$, then A and B are *equivalent* occurrences, and one can write: $A = B$.

Consider again the example of dice. Let $A =\{\text{get a three}\}$ and $B =\{\text{get an odd number}\}$, then $A \subset B$, since 3 is an odd number. For a single dice, it is also clear that E and Ω are equivalent occurrences.

The inclusion operation is *transitive*: if $A \subset B$ and $B \subset C$, then $A \subset C$.

The sum (*union*) of two occurrences is an occurrence which takes place if and only if the first, the second or both occurrences take place. In other words, the occurrence $A + B = A \cup B$ contains all facilitating occurrences for both A and B. In the above examples, if $C =\{\text{get an even number}\}$, then $A + B = \{1, 3, 5\}$, while $A + C = \{2, 3, 4, 6\}$.

The product (*intersection*) of two occurrences is an occurrence which takes place only if both occurrences take place: $A \cdot B = A \cap B$. In the above examples, $A \cdot B = \{3\}$, $C \cdot A = \emptyset$.

The *difference* of occurrences A and B is an occurrence that happens when A takes place and B does not. Clearly, for incompatible occurrences one has

$A - B = A$, and also $B - A = B$, since B does not take place if A takes place, and vice versa.

The occurrence $\overline{A}$ is a *complement* to occurrence A if it only happens when A does not. The following rules are valid for complementary occurrences:

- Occurrences A and $\overline{A}$ are incompatible, i.e. cannot happen simultaneously.
- Either A or $\overline{A}$ must take place.

From these it is clear that $A + \overline{A}$ is a necessary occurrence, and that A and $\overline{A}$ are each-others' complements. So $A + \overline{A} = \Omega$ and $A \cdot \overline{A} = \emptyset$. Also, $A + \emptyset = A, A \cdot \emptyset = \emptyset, A + \Omega = \Omega, A \cdot \Omega = A$, and $\overline{\overline{A}} = A$.

In the above examples, $A = \{3\}, \overline{A} = \{1, 2, 4, 5, 6\}$, while $C = \{2, 4, 6\}, \overline{C} = \{1, 3, 5\}$.

Complementary occurrences are uniquely defined, i.e. if $A = B$ then $\overline{A} = \overline{B}$. It is also easy to show that

$$\overline{A \cdot B} = \overline{A} + \overline{B}, \qquad \overline{A + B} = \overline{A} \cdot \overline{B}, \tag{1}$$

In general, a sum of two occurrences can be decomposed into incompatible occurrences in the following way:

$$A + B = A \cdot B + A \cdot \overline{B} + \overline{A} \cdot B \tag{2}$$

Exercise: prove identities (1) and (2).

Venn's diagrams, shown in Figure 1, give simple geometric interpretation of the relations between an occurrence and its complement, and various operations on occurrences: the sum, the product, and the inclusion.

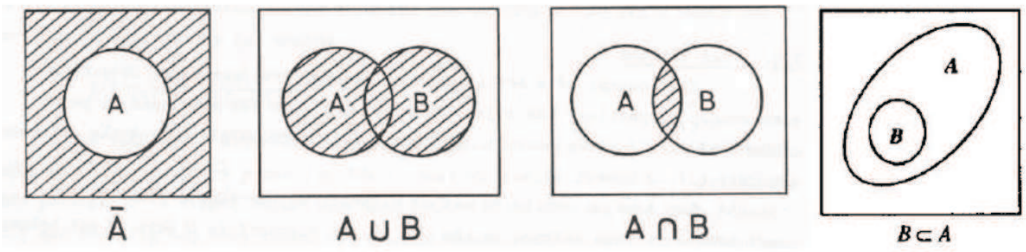


Figure 1:

Here are some other properties of occurrences:

- For any A, $A + A = A$ and also $A \cdot A = A$.

- The sum and the product of two occurrences is commutative:

$$A \cup B = B \cup A, \qquad A \cap B = B \cap A$$

- Sum and product are associative operations:

$$(A \cup B) \cup C = A \cup (B \cup C) = (A \cup C) \cup B = A \cup B \cup C$$
$$(A \cap B) \cap C = A \cap (B \cap C) = (A \cap C) \cap B = A \cap B \cap C$$

- Also, the following expression is true:

$$(A \cup B) \cap C = (A \cap C) \cup (B \cap C)$$

2.2 Elements of combinatorics

A set of n elements can be grouped into subsets of arbitrary k elements from the set in a variety of ways, called *groupings*. The number of distinct subsets of the set A that have exactly k elements is

$$C_n^k = \frac{n!}{k!(n-k)!}$$

The order of elements in subset k is irrelevant. The numbers C_n^k are called *binomial coefficients*; they have the following properties:

$$0! = 0, \qquad C_n^k = C_n^{n-k}, \qquad C_n^k = C_{n-1}^{k-1} + C_{n-1}^k (\text{Pascal}'\text{s triangle}), \qquad \sum_{k=0}^{n} C_n^k = 2^n.$$

The last identity means, that the number of all subsets in a set of n elements is 2^n.

The sets which consist of the elements from set A, but in different order, are called *permutations* of the set A. If A consists of n identical elements, there are $n!$ possible permutations.

Consider various possible groupings of k-element subsets from an n-element set, where the elements can be distinguished from each other, e.g. are numbered. There will be $k!$ permutations in each k-element subset. Hence the total number of such subsets is

$$A_n^k = k! C_n^k = \frac{n!}{(n-k)!}$$

Each of these is called a *partial permutation* of k non-identical elements out of n. Individual orderings differ from each other by the order of elements.

Consider a set A which consists of n different elements, and we want to construct k-element subsets which differ by the type of elements and their order.

Such subsets are called *permutations with repetitions*. Number of such permutations is $\overline{A_n^k} = n^k$.

Example: we have three digits: 1,2 and 3. How many different numbers can be composed out of these? Here $n = 3$ and $k = 1, 2, 3$; also, clearly, the order matters. Hence we have $3^1 + 3^2 + 3^3 = 3 + 9 + 27 = 39$ different numbers. The number of '1 out of 3' groupings is

$$C_3^1 = \frac{3!}{1!(3-1)!} = \frac{3!}{1!2!} = 3$$

These are 1,2 and 3. The number of 2-digit groupings is

$$C_3^2 = \frac{3!}{2!(3-2)!} = \frac{3!}{2!1!} = 3$$

with the number of possible permutations being $2! = 2$, so there are $3 \times 2 = 6$ such numbers: 12, 13, 23, 21, 31, 32. In addition, there are three numbers containing 2 identical digits: 11, 22, 33. Hence, overall we have $6 + 3 = 9$ 2-digit numbers. Following similar consideration, one ends up with 27 3-digit numbers: 123, 213, 312, 132, 232, 321, 122, 133, 112, 121, 131, 111, 211, 233, 221, 212, 223, 232, 222, 311, 322, 331, 313, 332, 323, 333.

2.3 Probability and its properties

A quantitative measure of an occurrence to take place is called its *probability* and is denoted by the letter P. An occurrence which has probability is *measurable* (in general, not all occurrences are measurable). Consider the space of all measurable occurrences $\pounds$, which has the following properties:

a) if $A \in \pounds$ then $\overline{A} \in \pounds$.

b) if $A \in \pounds$ and $B \in \pounds$ then $\overline{A} \cap B \in \pounds$.

The space $\pounds$ that satisfies these two conditions forms the *algebra* of the occurrences. From properties a) and b) it follows that

c) $A \cup B \in \pounds$ (here we used the identities $A + B = \overline{\overline{A} \cdot \overline{B}}$ and $\overline{\overline{A}} = A$).

d) $\Omega \in \pounds$ and also $\emptyset \in \pounds$.

In addition let's assume that if a certain occurrence A_k belongs to $\pounds$, i.e. $A_k \in \pounds$, then any countable union of such occurrences also belongs to $\pounds$, $\cup_{k=1}^{\infty} A_k \in \pounds$. The space of occurrences which has this property is called σ-algebra, and also *Borelev's space*. This property is necessary for proving certain complicated problems in probability theory.

Consider an occurrence space $\pounds$ which forms a σ-algebra. Now we can formulate the axioms of the probability theory, as formulated by the Russian mathematician Kolmogorov:

1. The probability of a random occurrence $A_k \in \mathcal{L}$ is a non-negative number, $P(A_k) \geq 0$.

2. The probability of a necessary occurrence is equal to 1, $P(\Omega) = 1$.

3. The probability of the sum of mutually exclusive occurrences is equal to the sum of probabilities of these occurrences:

$$P(A_1 + A_2 + \cdots + A_n) = P(A_1) + P(A_2) + \cdots + P(A_n)$$

The last axiom also holds for $n = \infty$. It follows from these axioms that the sum and the product of measurable occurrences are also measurable.

Probabilities have the following properties:

1. The probability of an impossible occurrence is equal to zero. Indeed:

$$\Omega + \emptyset = \Omega \quad \Rightarrow \quad P(\Omega) + P(\emptyset) = P(\Omega) \quad \Rightarrow \quad P(\Omega) = 0.$$

2. The probability $P(A)$ of any occurrence A lies within the range $0 \leq P(A) \leq 1$.

3. If $A \subset B$ then $P(A) \leq P(B)$.

4. The probability of the complete set of occurrences is equal to 1, $\sum_{i=1}^{n} P(A_i) = 1$. Indeed:

$$A + \overline{A} = \Omega \quad \Rightarrow \quad P(A) + P(\overline{A}) = P(\Omega) \equiv 1 \quad \Rightarrow \quad P(A) = 1 - P(\overline{A}).$$

5. For any two occurrences A and B, $P(A + B) = P(A) + P(B) - P(A \cdot B)$ (see Figure 1 for the geometric interpretation of the sum of occurrences). This formula can be used for calculating the probability of the sum of any two occurrences.

6. Since $P(A \cdot B) \geq 0$, from property 5 one has:

$$P(A + B) \leq P(A) + P(B).$$

7. If A and B are equivalent occurrences, their probabilities are equal: $A = B \;\Rightarrow\; P(A) = P(B)$. Indeed, $A = B$ means that $A \subset B$ and also $B \subset A$. Then, from property 3, $A \subset B \;\Rightarrow\; P(A) \leq P(B)$ and also $B \subset A \;\Rightarrow\; P(B) \leq P(A)$. From these two inequalities one has $P(A) = P(B)$.

Let's now address the following practical question: how can we calculate an event occurrence probability?

Start with a simple case, when a set of n occurrences makes up a complete set, and each of these occurrences is equally expected to take place. If we want

to calculate the probability of a subset of m occurrences from the original set, then we need to sum the individual probability m times. The probability of a single occurrence is equal to $1/n$, so we have

$$P = \sum_{i=1}^{m} \frac{1}{n} = \frac{m}{n}. \tag{3}$$

In this definition, m is the number of occurrences facilitating our desired outcome, while n is the number of of all possible outcomes.

Returning to the example of dice, let's calculate the probability of getting an even number. The complete set is given by 6 elementary occurrences $\{1, 2, 3, 4, 5, 6\}$, out of which 3 are occurrences facilitating the desired outcome, $\{2, 4, 6\}$. Hence, the probability of getting an even number is $P = 3/6 = 0.5$.

When calculating the probability given by eq. (3), m and n do not have to be finite or even defined, as long as the ratio m/n can be calculated. For example, one has a large number of identical steel balls with the total weight of 50 kg, out of which 20 kg are red and 30 kg are blue. A single ball is picked at random. What's the probability of picking a blue ball? The total number of balls is not defined, but eq. (3) can still be used, because we know that the number of facilitating occurrences is proportional to 3, while the complete set of occurrences is proportional to 5. So the probability in question will be $P = 3/5 = 0.6$.

2.4 Conditional probability. Total probability and Bayes' formula

Let's figure out how to calculate the probability of a complicated occurrence. One frequently encountered problem is when the probability of occurrence A needs to be calculated under the condition that occurrence B, which has some probability, has taken place. This is called a *conditional probability* and is denoted by $P_B(A)$ or $P(A|B)$. It's intuitively clear that this probability is somehow related to the overlap of occurrences A and B. Consider an example of a group of N people, out of which N_B are men and N_A are smokers. A randomly selected person from this group happens to be a man. One needs to calculate the probability that this man is a smoker. Let A denote the occurrence that the selected person is a smoker, and B stands for the occurrence that the selected person is a man. Let N_C be the number of smoker men, i.e. both A and B occurrences are taking place. The Venn's diagram corresponding to this case is given in Figure 2. From the definition of probability one has

$$P(A) = \frac{N_A}{N}, \qquad P(B) = \frac{N_B}{N}, \qquad P(A \cdot B) = \frac{N_C}{N}. \tag{4}$$

Let's now calculate $P_B(A)$. We already know that the selected person is a man, so the overall number of cases is N_B, while facilitating cases are those where

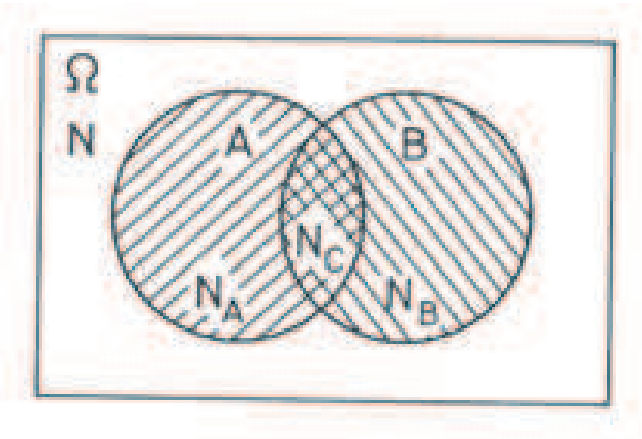


Figure 2: Venn's diagram illustrating the concept of conditional probability.

both A and B are taking place, the number of which is N_C. Hence we have:

$$P_B(A) = \frac{N_C}{N_B} = \frac{N_C/N}{N_B/N} = \frac{P(A \cdot B)}{P(B)} \tag{5}$$

This formula can be used for calculating conditional probabilities. It can also be used for calculating the probability of a product of occurrences:

$$P(A \cdot B) = P(B) \cdot P_B(A) \tag{6}$$

In analogy with eq. (6) one can write $P(B \cdot A) = P(A) \cdot P_A(B)$, hence $P(A) \cdot P_A(B) = P(B) \cdot P_B(A)$.

Two occurrences are said to be *mutually independent* if one does not affect the other. For such occurrences it is clear that $P_B(A) = P(A)$, and hence eq. (6) takes the form

$$P(A \cdot B) = P(A) \cdot P(B). \tag{7}$$

Eq. (7) is the necessary and sufficient condition of mutual independence of the two occurrences. This condition can be generalised for the case of 3 mutually independent occurrences:

$$P(A \cdot B \cdot C) = P(A) \cdot P(B) \cdot P(C). \tag{8}$$

Consider now two mutually independent occurrences A and B. Then one has

$$P(\overline{A}B) = P(B) - P(AB) = P(B) - P(A)P(B) = P(B)[1 - P(A)] = P(B)P(\overline{A})$$
$$B = \overline{A}B + AB \quad \Rightarrow \quad P(B) = P(\overline{A}B) + P(AB)$$

which means that in this case A's complement and B are independent as well.

Consider a collection of occurrences $H_1, H_2, \ldots, H_n$, which are mutually exclusive and form a complete set, and another occurrence A that can only happen together with one of the occurrences H_i. The individual probabilities $P(H_i)$ are known, as well as conditional probabilities $P_{H_i}(A)$. Our aim here is to calculate $P(A)$, the probability of occurrence A.

Occurrence A can be presented as the sum of occurrences H_i; since these form a complete set, their sum will be the necessary occurrence. Since A only happens with one of H_i, one can write:

$$A = A \cdot \Omega = A \cdot \sum_{i=1}^{n} H_i = \sum_{i=1}^{n} A \cdot H_i \quad \Rightarrow \quad P(A) = \sum_{i=1}^{n} P(A \cdot H_i),$$

and using eq. (6) one finally gets:

$$P(A) = \sum_{i=1}^{n} P(H_i) \cdot P_{H_i}(A). \tag{9}$$

Eq. (9) is known as the *full probability formula*.

Now let's imagine that, within the above problem, we know that occurrence A has taken place. How will the conditional probabilities $P(H_i)$ change? In other words, we would like to find the conditional probabilities for each of H_i with respect to the occurrence A, $P_A(H_i)$. Using eq. (6) one has $P(A \cdot H_i) = P(A) \cdot P_A(H_i) = P_{H_i}(A)$, hence

$$P_A(H_i) = \frac{P(H_i) \cdot P_{H_i}(A)}{P(A)} = \frac{P(H_i) \cdot P_{H_i}(A)}{\sum_{j=1}^{n} P(H_i) \cdot P_{H_j}(A)}, \qquad i = 1, 2, \ldots, n. \tag{10}$$

Eq. (10) is known as Bayes' formula. The probabilities $P(H_i)$ of the occurrences H_i are called *a priori probabilities* or *hypotheses*.

Complementary hypotheses always form a complete system of occurrences, so one can always write

$$P(A) = P(H) \cdot P_H(A) + P(\overline{H}) \cdot P_{\overline{H}}(A). \tag{11}$$

Eq. (11), which is often used in practice, is a special case of eq. (10).

Let's consider an example, which will help us understand the essence of eq. (10). A doctor is trying to diagnose a patient, based on the patient's blood test result. Initially, based on the symptoms, the doctor comes up with a set of hypotheses, which we will denote H_i. Let the blood test result be A. The probabilities $P_{H_i}(A)$ are known from the statistical analysis, i.e. from experimental data it is known what the blood test looks like for hypothesis H_i. The doctor applies eq. (10) and comes up with a set of probabilities $P_A(H_i)$. If one of these

is close to 1, then the matching hypothesis H_i looks likely and the patient can be treated accordingly.

The following is obviously true:

$$\sum_{i=1}^{n} P_A(H_i) == \frac{\sum_{i=1}^{n} P(H_i) \cdot P_{H_i}(A)}{\sum_{j=1}^{n} P(H_i) \cdot P_{H_j}(A)} = 1. \tag{12}$$

This formula can be used to check whether the calculations of various conditional probabilities are correct.

3 Random variables

3.1 Discrete random variables

Let's introduce the concept of a random variable. A random variable is defined when the range of its possible values is determined, and the probability of each value is known. A random variable ξ is *discrete* if it can take a value from a discrete set $x_1, x_2, \ldots, x_n$ and the probability of each value is given. The probability that ξ takes a value x_i is p_i:

$$P\{\xi = x_i\} = p_i \tag{13}$$

There are no restrictions on values $x_1, x_2, \ldots, x_n$, but the probabilities p_i must satisfy the properties

$$p_i > 0 \tag{14}$$

$$p_1 + p_2 + \cdots + p_n = 1. \tag{15}$$

Eq. (15) means that the random variable ξ must take some value out of the set $x_1, x_2, \ldots, x_n$, i.e., this set is *complete*.

Let's put the values x_i in an increasing order, and list respective probabilities p_i underneath. The resulting table is called the *distribution* of the random variable:

$$X = \left\{ \begin{array}{ccccc} x_1 & x_2 & x_3 & \ldots & x_n \\ p_1 & p_2 & p_3 & \ldots & p_n \end{array} \right. \tag{16}$$

There is another way of defining the random variable ξ. Instead of considering the occurrence $\{\xi = x_i\}$, one can consider occurrence $\{\xi \le x_i\}$, i.e. the occurrence that the variable ξ takes a value equal or less than x_i. The probability of the occurrence $\{\xi \le x_i\}$ is a function of the variable x, and is called the *distribution function* $F(x)$ of the random variable x. It is clear from the definition, that

$$F(x) = P\{\xi \le x_i\} = \left\{ \begin{array}{cc} 0, & x < x_1 \\ \sum_{k=1}^{i} p_k, & x_i \le x < x_{i+1}, \quad i = 1, 2, \ldots, n-1 \\ 1, & x \ge x_n \end{array} \right. \tag{17}$$

Sometimes $F(x)$ is called the *cumulative* distribution function. It's graph has a stepwise form, where the i-th step at $x = x_i$ has the height of p_i (see Figure 3).

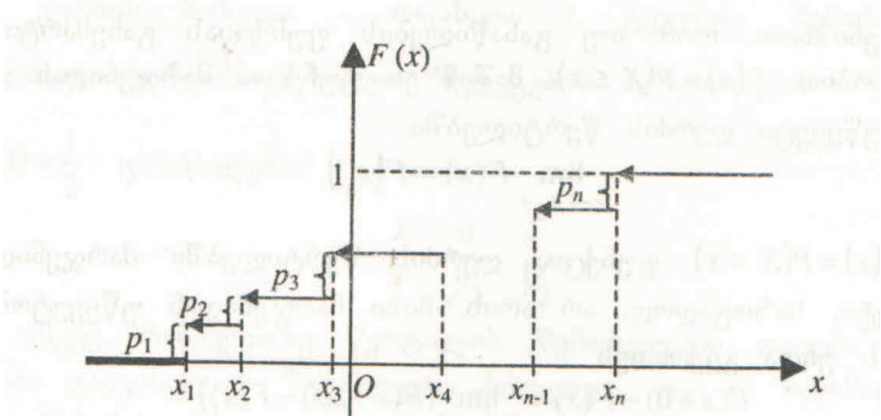


Figure 3: A graph representing the distribution function of a discrete random variable.

It's easy to calculate the probability $P\{\alpha \leq \xi < \beta\}$ that the random variable ξ falls into the semi-interval $[\alpha, \beta)$:

$$P\{\alpha \leq \xi < \beta\} = F(\beta) - F(\alpha), \tag{18}$$

where, clearly, $F(\beta) \geq F(\alpha)$ for $\beta > \alpha$. Using eq: (18) it's easy to show that $F(-\infty) = 0$ and $F(+\infty) = 1$.

In many cases, a random variable can be characterised by specific numerical values that define certain basic properties of its distribution. Two such parameters are mathematical expectation value and dispersion.

The mathematical *expectation value* $M\xi$ of a random variable ξ is defined as

$$M\xi \equiv \overline{\xi} = \sum_{i=1}^{n} x_i p_i \cdot \left(\sum_{i=1}^{n} p_i \right)^{-1}. \tag{19}$$

From this definition it is clear that $M\xi$ is the mean value of ξ, which we will denote by $\overline{\xi}$. Note that the more probable the values of ξ, the larger is its weight in Eq. (19).

The expectation value has the following properties:

a) The expectation value of a constant is equal to that constant:

$$Mc = c \tag{20}$$

b) For any constant c and a random variable ξ the following is true:

$$M(\xi + c) = (M\xi) + c, \qquad M(c\xi) = c(M\xi). \tag{21}$$

c) For any two random variables ξ and μ one has:

$$M(\xi + \mu) = M\xi + M\mu. \tag{22}$$

The *dispersion* $D\xi$ of a random variable ξ is defined as

$$D\xi = M(\xi - M\xi)^2 = M(\xi - \overline{\xi})^2 \tag{23}$$

It follows from this definition that

$$D\xi = M\xi^2 - 2 \cdot M\xi \cdot M\xi + (M\xi)^2 = M\xi^2 - (M\xi)^2 = \overline{\xi^2} - \left(\overline{\xi}\right)^2. \tag{24}$$

The dispersion is a measure of scatter of the random variable around its mean value. It has the following properties:

$$D(\xi + c) = D\xi, \qquad D(c\xi) = c^2(D\xi). \tag{25}$$

For two independent random variables ξ and μ the following two properties are true:

$$M(\xi\mu) = M\xi \cdot M\mu, \qquad D(\xi + \mu) = D(\xi) + D(\mu). \tag{26}$$

A square root of the dispersion is called a *root mean square deviation*, or, in short, r.m.s.:

$$\sigma\xi = \sqrt{D\xi}. \tag{27}$$

Here are some more definitions:

If a random variable can take $2n + 1$ possible values, which are ordered in their magnitude, then the number with index $n + 1$ is called the *median* m of the distribution:

$$m = x_{n+1} \tag{28}$$

If the sequence contains an even number of values $2n$, then the median is calculated as

$$m = 0.5 \cdot (x_n + x_{n+1}). \tag{29}$$

The value of a random variable, which corresponds to the highest probability, is called the *mode*: $x_m = \max(p_i)$.

3.2 Continuous random variable

A random variable that can take any value from an interval (a, b) is called a *continuous random variable*. An good example of a continuous random variable is the polar angle of an α-particle radiated in a decay of a radioactive isotope. It can take any value in the interval $(0, \pi)$.

A continuous random variable ξ is defined by the interval (a, b), which includes all possible values of the variable, and the distribution function $F(x)$, which is continuous and differentiable for all values of x from that interval. Using this property of $F(x)$ and a generalisation of eq. (18), one can calculate the probability of the random variable falling within the interval $(x, x + \Delta x)$:

$$P\{x \leq \xi < x + \Delta x\} = F(x + \Delta x) - F(x)$$

Divide the r.h.s. by Δx and take the limit $\Delta x \to 0$:

$$\lim_{\Delta x \to 0} \frac{P\{x \leq \xi < x + \Delta x\}}{\Delta x} = \lim_{\Delta x \to 0} \frac{F(x + \Delta x) - F(x)}{\Delta x} = F'(x) \equiv \rho(x). \quad (30)$$

The quantity $\rho(x)$ is called the *probability density function* or simply the probability density of the random variable ξ. It is clear from the definition that $P(\xi = x\} = 0$ (for this reason, $P\{x \leq \xi \leq x + \Delta x\} = P\{x < \xi < x + \Delta x\}$). Hence, the probability of ξ being equal to some value x is meaningless; it's the probability that ξ takes a value from an interval – even infinitesimally small – which contains x which has a direct physical meaning. Clearly, the probability is proportional to the length of this interval:

$$P\{x \leq \xi < x + \Delta x\} \approx \rho(x)\Delta x = \Delta F(x), \quad (31)$$

where $\rho(x)$ plays the role of the proportionality coefficient. Based on this formula, the probability density $\rho(x)$ can be given the following physical meaning: let (a', b') be an interval within the interval (a, b), i.e. $\leq a' < b' \leq b$. The probability that the variable ξ falls within (a', b') is then given by the integral

$$P\{a' < \xi < b'\} = \int_{a'}^{b'} \rho(x)dx \quad (32)$$

Based on this formula, one can give the following interpretation to the probability density: the probability is the area of the curvilinear trapeze under the density graph, between the limits of the interval.

In general, a random variable ξ can take its values from any interval, including the infinite range $(-\infty, \infty)$. In the latter case, similarly to the discrete variable, one has $F(-\infty) = 0$ and $F(+\infty) = 1$. As for the density, in analogy with eqs. (14,15) from the discrete case, it has the following properties:

$$\rho(x) > 0, \quad (33)$$

$$\int_a^b \rho(x)dx = 1 \quad (34)$$

Again in analogy with eq. (18), the distribution function $F(x)$ can be presented as the integral of the probability density:

$$F(x) = P\{\xi < x\} = P\{-\infty < \xi < x\} = \int_{-\infty}^{x} \rho(t)dt. \tag{35}$$

Differentiating eq. (35) one has $F'(x) = \rho(x)$, which confirms the interpretation that the probability density function is the derivative of the distribution function, and hence characterises the speed of its variation with x. It is clear that the distribution function is non-decreasing; it is defined through an integral with a variable upper limit, and hence it is continuous and differentiable on the whole interval of its definition.

The expectation value M and the dispersion D of the continuous random variable ξ are defined by

$$M\xi = \int_a^b x\rho(x)dx, \tag{36}$$

$$D\xi = \int_a^b (x - M\xi)^2\rho(x)dx. \tag{37}$$

As with the discrete random variable, the expectation value is equal to the mean of ξ:

$$M\xi = \int_a^b x\rho(x)dx = \frac{\int_a^b x\rho(x)dx}{\int_a^b \rho(x)dx}, \tag{38}$$

since $\int_a^b \rho(x)dx = 1$.

It can be shown that if the integral $\int_{-\infty}^{\infty} |x|\rho(x)dx$ converges, then the expectation value $M\xi$ is finite. In fact, the convergence of the above integral is the necessary and sufficient condition for the expectation value to be finite.

For a continuous random variable the median m is derided as the value of x such that $F(m) = 1/2$. Thus, the word 'median' is synonymous to 'middle', as it defines the point where the distribution function is equal to its middle value.

Let's define the *initial moments* of the random variable ξ:

$$\mu'_k = M(x^k) = \sum_{i=1}^{n} x_i^k p_i, \tag{39}$$

$$\mu'_k = \int_a^b x^k\rho(x)dx, \tag{40}$$

where the first expression is for the discrete case, and the second is for the continuous case. The k-th *central* moments are then defined as

$$\mu_k = M\left([x - \overline{\xi}]^k\right). \tag{41}$$

It is clear from these definitions that $\mu'_0 = 1$ and $\mu'_1 = \overline{\xi}$; also, $\mu_0 = 1$, $\mu_1 = 0$ and $\mu_2 = \sigma^2$; i.e. the first initial moment is equal to the expectation value, while the second central moment is equal to the dispersion.

An important characteristic of a distribution function is the *skewness* A defined as

$$A = \frac{\mu_3}{\sigma^3} \tag{42}$$

If the density $\rho(x)$ is stretched on the left-hand side of the mean, then the skewness is positive, and if the density is is stretched to the right, the skewness is negative. If the distribution density is symmetric with respect to $\overline{\xi}$, then the asymmetry is zero.

The *kurtosis* of the distribution is defined as

$$E = \frac{\mu_4}{\sigma^4} - 3. \tag{43}$$

As will be seen later, for a Gaussian distribution $\mu_4/\sigma^4 = 3$ and hence $E = 0$. So (for a symmetric distribution) the kurtosis tells us whether the distribution density is squashed (for $E < 0$) or stretched (for $E > 0$) when compared to the Gaussian distribution.

Consider a random variable ξ with distribution density $\rho(x)$, and an arbitrary *monotonous* function $f(x)$. We would like to know the distribution density for a random variable η which is related to ξ as $\eta = f(\xi)$. Using the definition eq. (35) we have:

$$F_\eta(x) = P\{\eta < x\} = P\{f(\xi) < x\} = P\{\xi < f^{-1}(x)\} = \int_{-\infty}^{f^{-1}(x)} \rho_\xi(t)dt. \tag{44}$$

Here we assumed that the function $f(x)$ is monotonously increasing. Now, from the definitions we have

$$\rho_\eta(x) = \frac{d}{dx}F_\eta(x) = \frac{d}{dx}\int_{-\infty}^{f^{-1}(x)} \rho_\xi(t)dt = \rho\left(f^{-1}(x)\right)\frac{d}{dx}\left(f^{-1}(x)\right). \tag{45}$$

If the function $f(x)$ is monotonously decreasing, then $g(x) = -f(x)$ will be an increasing function and the above derivation would still be valid for $g(x)$. So, in general, one can write for an arbitrary monotonous function $f(x)$:

$$\rho_{f(x)} = \rho\left(f^{-1}(x)\right)\left|\frac{d}{dx}\left(f^{-1}(x)\right)\right|. \tag{46}$$

As for the expectation value of the random variable η, it can be shown that

$$Mf(\xi) = \int_a^b f(x)\rho(x)dx. \tag{47}$$

Remember however, that $Mf(\xi) \neq f(M\xi)$.

3.3 Multi-dimensional random quantities (random vectors)

The description of some experiments or observations may require several random variables. In such cases, an occurrence will correspond to a point $N(\xi_1, \xi_2, \ldots, \xi_n)$ in n-dimensional space – or, equivalently, a vector that starts at the origin and ends at that point. The system of such random variables has some extra properties, in addition to the usual properties of the individual random variables. These extra properties are linked with the inter-dependence of the variables comprising the system.

Let's introduce the concepts of the distribution function and density for vectors of random variables, starting with the case of just two random variables X and Y. The distribution function $F(\alpha, \beta)$ is defined as the probability that the following two inequalities are satisfied simultaneously: $X < \alpha, Y < \beta$. I.e.:

$$F(\alpha, \beta) = P\{X < \alpha, Y < \beta\} \tag{48}$$

Geometrically, $F(\alpha, \beta)$ is the probability that a random point (X, Y) is inside the infinite rectangle which has the top-right corner at point $M(\alpha, \beta)$, as illustrated in Figure 4. The function $F(\alpha, \beta)$ has the following properties:

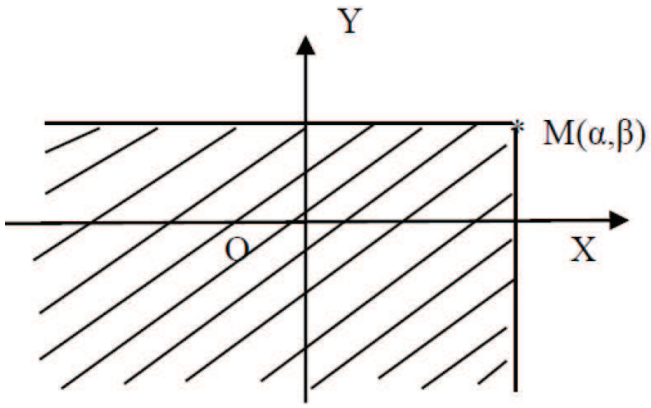


Figure 4: Geometric interpretation of the Equation (48).

1. If $\alpha_1 < \alpha_2$, then $F(\alpha_1, \beta) < F(\alpha_2, \beta)$. Also, if $\beta_1 < \beta_2$, then $F(\alpha, \beta_1) < F(\alpha, \beta_2)$.

2. The function equals zero everywhere at $-\infty$, i.e. $F(\alpha, -\infty) = F(-\infty, \beta) = F(-\infty, -\infty) = 0$.

3. If one of the arguments is equal to $+\infty$, the function is equal to the distribution function of the other variable: $F(\alpha, +\infty) = F_1(\alpha), F(+\infty, \beta) = F_2(\beta)$, where $F_1(\alpha)$ and $F_2(\beta)$ are the distribution functions of the variables X and Y, respectively.

4. If both arguments are equal to $+\infty$, the distribution function is equal to unity: $F(+\infty, +\infty) = 1$. Indeed, in this case the hatched rectangle in Figure 4 covers the whole plane, hence the probability to get inside is a certainty, a necessary occurrence.

If the function $F(\alpha, \beta)$ is continuous and differentiable, then the function

$$\rho(\alpha, \beta) = \frac{\partial F(\alpha, \beta)}{\partial \alpha \partial \beta} \tag{49}$$

is the density of the distribution function F. It can be used to find the probability of finding the point inside some area D:

$$P\{(X, Y) \subset D\} = \int\int_D \rho(\alpha, \beta)\, d\alpha\, d\beta. \tag{50}$$

The density $\rho(\alpha, \beta)$ must be non-negative, and the normalisation condition needs to be satisfied:

$$\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \rho(\alpha, \beta)\, d\alpha\, d\beta = 1. \tag{51}$$

The distribution function F and its density ρ are related through the formula

$$F(\alpha, \beta) = \int_{-\infty}^{\alpha} \int_{-\infty}^{\beta} \rho(\gamma, \delta)\, d\gamma\, d\delta. \tag{52}$$

Using equation (52) and the property 3, one can obtain the distribution functions of individual variables:

$$F_1(\alpha) = \int_{-\infty}^{\alpha} \int_{-\infty}^{+\infty} \rho(\gamma, \delta)\, d\gamma\, d\delta \qquad \Rightarrow \qquad \rho_1(\alpha) = \int_{-\infty}^{+\infty} \rho(\alpha, \beta)\, d\beta, \tag{53}$$

$$F_2(\beta) = \int_{-\infty}^{+\infty} \int_{-\infty}^{\beta} \rho(\gamma, \delta)\, d\gamma\, d\delta \qquad \Rightarrow \qquad \rho_2(\beta) = \int_{-\infty}^{+\infty} \rho(\alpha, \beta)\, d\alpha. \tag{54}$$

So, for a our system of two random variables, in order to obtain the distribution function for one random variable, the density should be integrated within infinite limits over the other random variable.

If the two random variables are mutually independent, then

$$\rho(\alpha, \beta) = \rho(\alpha)\rho(\beta). \tag{55}$$

In analogy with equations (39-41) one can define *initial moments* μ' and *central moments* μ of order k, s:

$$\begin{aligned} \mu'_{k,s} &= M(x^k y^s), \\ \mu_{k,s} &= M\left([x - Mx]^k [y - My]^s\right) \\ &= M\left([x - \overline{X}]^k [y - \overline{Y}]^s\right) \end{aligned} \tag{56}$$

Similarly, for a 2-dimensional discrete variable one has:

$$\begin{aligned} \mu'_{k,s} &= \sum_i \sum_j x_i^k y_i^s p_{ij}, \\ \mu_{k,s} &= \sum_i \sum_j [x_i - \overline{X}]^k [y_j - \overline{Y}]^s p_{ij}, \end{aligned} \tag{57}$$

where $p_{ij} = P\{X = x_i, Y = y_j\}$ is the probability that the system (X, Y) takes the values x_i, y_j, while the summation in made over all possible values x_i, y_j.

For continuous random variables one has:

$$\begin{aligned} \mu'_{k,s} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} x^k y^s \rho(x, y)\, dx\, dy, \\ \mu_{k,s} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} (x - \overline{X})^k (y - \overline{Y})^s \rho(x, y)\, dx\, dy, \end{aligned} \tag{58}$$

where $\rho(x, y)$ is the probability density of the system.

Apart from the expectation values $\mu'_{1,0} = MX, \mu'_{0,1} = MY$, which define the average values of coordinates x and y, and the respective dispersions $\mu_{2,0} = DX, \mu_{0,2} = DY$, which define the spread of the values with respect to their averages, there is an additional important characteristic, the mixed second-order central moment

$$\begin{aligned} \mu_{1,1} &= M\left([x - \overline{X}][y - \overline{Y}]\right) \\ &= M(XY) - M(X)M(Y), \end{aligned} \tag{59}$$

which is called *covariance*. This quantity characterises not just the scatter of the values of x and y, but also their connection. For independent variables, the covariance is equal to zero.

The *correlation coefficient* is defined as

$$R(X, Y) = \frac{\mu_{1,1}}{\sigma_x \sigma_y} = \frac{M(XY) - M(X)M(Y)}{\sqrt{D(X)D(Y)}}. \tag{60}$$

It can be shown that the absolute value of R cannot exceed unity. If the variables X and Y are independent, one has $R(X, Y) = 0$, although uncorrelated does not necessarily mean independent. To illustrate this, consider a random variable X

such that $M(X) = 0$ and $M(X^3) = 0$, while $Y = X^2$. The covariance between X and Y is

$$\mu_{1,1} = M\left([x - 0][y - M(Y)]\right) = M(X^3) - M(X)M(X^2) = 0, \qquad (61)$$

and, hence, the correlation coefficient is also zero, despite the fact that X and Y are functionally linked and clearly cannot be independent.

A correlation is a probabilistic and/or statistical relationship between two variables, somewhere in-between the functional dependence and statistical dependence/independence. For random variables corresponding to mutually exclusive occurrences, the correlation coefficient is equal to -1.

Everything that was said above about 2-dimensional random variables can be generalised to the case when the number of dimensions $n > 2$.

Let $\rho(x, y)$ be the probability density of a pair of random variables X and Y, and consider the sum $Z = X + Y$. What is the probability density for Z? Say, $z_1 < Z < z_2$ and hence $z_1 < X + Y < z_2$, which means that a random point with coordinates (X, Y) lies within the shaded area D in Figure 5, which is limited by

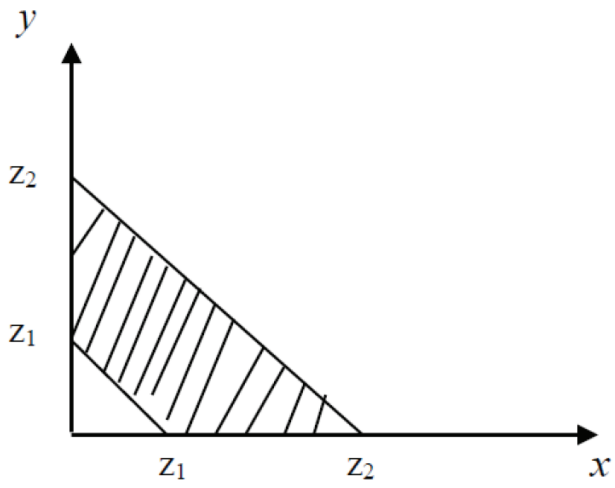


Figure 5: Integration limits for a sum of two random variables.

the straight lines $y = z_1 - x$ and $y = z_2 - x$. So the probability of occurrence $z_1 < Z < z_2$ is:

$$\begin{aligned} P(z_1 < Z < z_2) &= \int\int_D \rho(x, y)\, dx\, dy = \int_{-\infty}^{+\infty} dx \int_{z_1 - x}^{z_2 - x} \rho(x, y)\, dy = \\ &= \int_{-\infty}^{+\infty} dx \int_{z_1}^{z_2} \rho(x, z - x)\, dz \\ &= \int_{z_1}^{z_2} \left\{ \int_{-\infty}^{+\infty} \rho(x, z - x)\, dx \right\} dz \qquad (62) \end{aligned}$$

where the change of integration variable was made, $y = z - x$, followed by the change in the order of integration. From equation (62) one can see, that Z is a random variable with the following distribution density:

$$\rho_Z(z) = \int_{-\infty}^{+\infty} \rho(x, z - x)\, dx. \tag{63}$$

The case where the two variables X and Y are mutually independent is of special interest, since in this case $\rho(x, y) = \rho(x)\rho(y)$ and equation (63) takes the form

$$\rho_Z(z) = \int_{-\infty}^{+\infty} \rho(x)\rho(z - x)\, dx. \tag{64}$$

Equation (64), which combines the two distributions in this particular way, is called a *convolution* of the distributions $\rho(x)$ and $\rho(y)$.

Let X and Y be two independent random variables distributed uniformly in the interval $(0, 1)$. Let's find the probability density of the random variable $Z = X + Y$. We have

$$\begin{aligned} \rho_X(x) &= \begin{cases} 1, & 0 \le x \le 1 \\ 0, & x < 0 \cup x > 1 \end{cases} \\ \rho_Y(z - x) &= \begin{cases} 1, & 0 \le z - x \le 1 \\ 0, & z - x < 0 \cup z - x > 1 \end{cases} \end{aligned} \tag{65}$$

The density of the distribution $\rho_Z(z)$ is only non-zero for $0 < x < z, z \subset (0, 1) \cup z - 1 < x < 1, z \subset (1, 2)$, hence

$$\rho_Z(z) = \begin{cases} 0, & 0 < z \cup z > 2 \\ \int_0^z dx = z, & 0 \le z \le 1 \\ \int_{z-1}^1 dx = 2 - z, & 1 \le z \le 2 \end{cases}$$

Geometrically, this is an isosceles triangle with the ends of the base at points with coordinates $(0, 0)$ and $(2, 0)$, while the tip has coordinates $(1, 1)$. It is easy to check that the area of this triangle is equal to 1, which satisfies the normalisation condition.

Some important distributions in probability theory retain their form under composition. The Gaussian distribution and the Gamma distribution are the examples of such distributions. We will discuss them in the following section.

4 Some important distributions and their properties

We have seen in the previous section that a discrete random variable is fully defined by its distribution, while a continuous random variable is fully defined by its distribution function or its density. Here we will study the properties of several distributions, which are frequently needed in practice, in particular in physics.

4.1 Geometric and binomial distributions

Consider an experiment that is carried out an indefinite number of times in perfectly identical conditions, and the results of each try are totally independent from each other. Throwing dice or tossing a coin would be good examples of such distributions. Let $p = P(A)$ be the probability of getting a particular outcome, occurrence A (e.g. 'heads' in a coin toss) in each individual experiment. Then the probability of *not* getting occurrence A is $P(\overline{A}) = 1 - p = q$.

Consider a game of tossing a ring, aiming to land it on a vertical pole. Let $p \in (0, 1)$ be the probability of an individual try being a success. Let's determine the probability that the success is achieved at the n-th try. The tries are considered to be independent, and the number of tries X until the first success is a discrete random variable taking values $1, 2, 3, \ldots, n$:

$$\begin{aligned} P\{X = 1\} &= p \\ P\{X = 2\} &= (1 - p) \cdot p = q \cdot p, \qquad q \equiv 1 - p \\ P\{X = 3\} &= = q^2 \cdot p \\ &\ldots \\ P\{X = n\} &= q^{n-1} \cdot p, \qquad n = 1, 2, 3, \ldots \end{aligned}$$

This is called the *geometric distribution*. Let us add up individual probabilities:

$$\begin{aligned} p + q \cdot p + q^2 \cdot p + \cdots + q^{n-1} \cdot p + \ldots &= p(1 + q + q^2 + \cdots + q^{n-1} + \ldots) \\ &= \frac{p}{1 - q} = 1, \end{aligned}$$

since the expression in brackets is a geometric progression, with the sum equal to $1/(1 - q)$. So the normalisation condition is satisfied:

$$\sum_{n=1}^{\infty} p_n = 1$$

The expectation value of this distribution is

$$M(X) = \sum_{n=1}^{\infty} n \cdot p \cdot q^{n-1} = p \cdot \left(\sum_{n=1}^{\infty} q^n \right)' = p \cdot \left(\frac{q}{1 - q} \right)' = \frac{p}{(1 - q)^2} = \frac{p}{p^2} = \frac{1}{p},$$

since $(q^n)' = nq^{n-1}$ and

$$\sum_{n=1}^{\infty} q^n = q \sum_{n=1}^{\infty} q^{n-1} = \frac{q}{1 - q}.$$

Let's study a more general problem: what's the probability of getting m successes (i.e. m cases of occurrence A) in n tries? Since the tries are independent,

the probability that A happens in each of m tries and does not happen in any of $n-m$ tries is equal to the product of individual probabilities $p^m \cdot q^{n-m}$. This combination, however, is not unique, the total number of such combinations is $C_n^m = \frac{n!}{m!(n-m)!}$, and they are all mutually exclusive. The number C_n^m describes the number of possibilities to select m elements out of n elements. So the probability in question will be the sum of individual probabilities:

$$P_n(m) = \frac{n!}{m!(n-m)!} p^m \cdot q^{n-m}. \tag{66}$$

This equation describes Bernoulli's *binomial* distribution. It is characterised by two parameters: n and p. The distribution is called binomial, because the individual terms $P_n(m)$ show up in the expansion of the expression $(p+q)^n$.

Once again, let p be the probability of occurrence A taking place, i.e. $p = P(A)$. Let's introduce the concept of the indicator I_A of occurrence A, which equals 1 if A took place, and equals zero if it did not. Then the indicator is a random variable with the following distribution:

$$X = I_A = \left\{ \begin{array}{cc} 1, & 0 \\ p, & 1-p \end{array} \right\}.$$

This is a special case of the binomial distribution with $n = 1$, first introduced by Bernoulli. Let's calculate its mean and variance:

$$\begin{aligned} M(I_A) &= 1 \cdot p + 0 \cdot q = p, \\ D(I_A) &= M[I_A - M(I_A)]^2 = M(I_A - p)^2 = (1-p)^2 p + (0-p)^2 q = pq \end{aligned}$$

Calculating the mean of the binomial distribution directly is somewhat awkward, so we will present the binomial occurrence X (number of positive outcomes from n tries) as a sum of simple, indicator-type occurrences X_k: each of these is equal to 1 if the occurrence took place on the k-th attempt, and is equal to 0 otherwise. Then

$$X = X_1 + X_2 + X_3 + \cdots + X_n.$$

This sum contains only ones and zeroes, and the number of ones is equal to the number of successful occurrences in n attempts. Since these occurrences are independent, one has

$$\begin{aligned} M(X) &= M(X_1) + M(X_2) + M(X_3) + \cdots + M(X_n) = n \cdot p, \\ D(X) &= D(X_1) + D(X_2) + D(X_3) + \cdots + D(X_n) = n \cdot p \cdot q. \end{aligned}$$

So the mean of the binomial distribution is $n \cdot p$ and its dispersion is $n \cdot p \cdot q$. The skewness A is

$$A = \frac{q-p}{\sqrt{n \cdot p \cdot q}} = \frac{1-2p}{\sqrt{n \cdot p \cdot (1-p)}}.$$

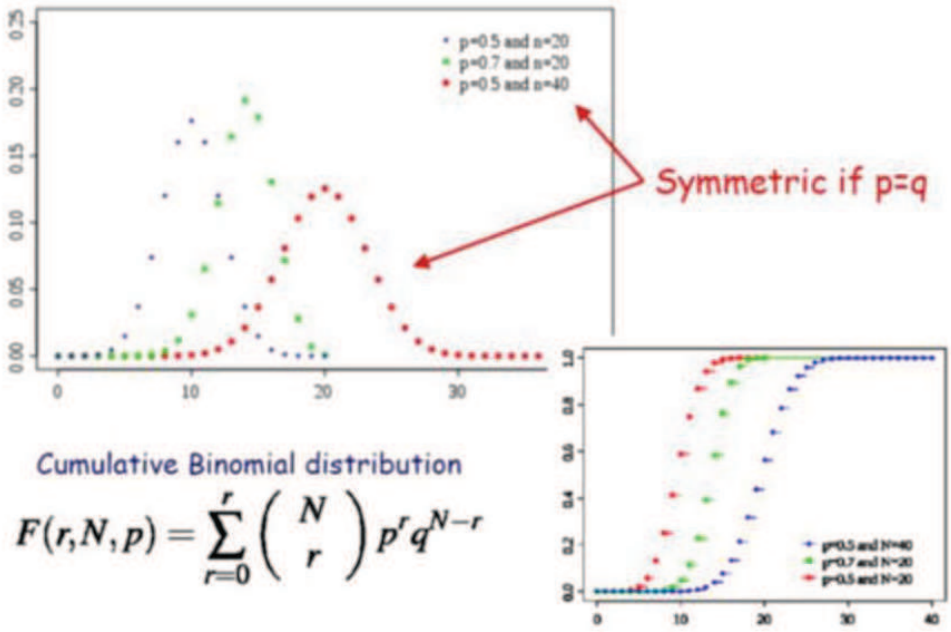


Figure 6: Examples of binomial distributions. Corresponding cumulative functions are shown at bottom right.

You can see that $A < 0$ if $p < \frac{1}{2}$, $A = 0$ if $p = \frac{1}{2}$ and $A > 0$ if $p > \frac{1}{2}$.

Three examples of the binomial distribution are shown in Figure 6. Blue points describe the number of female babies in 20 newborns. In this example, the probability p of a girl being born in a "single attempt" is $p = \frac{1}{2}$, the number of girls m can be any number between 0 and 20, while n is fixed to 20. From the plot you can see that the curve has a maximum at $m = 10$; probabilities of having 6 or 14 girl babies are about 6 times smaller than the maximum and are equally probable; the distribution is symmetric with respect to the mean at $n \cdot p = 20 \cdot 0.5 = 10$.

For large n equation (66) is difficult to use, because $n!$ can be a very big number. In these cases one should use limiting forms of the binomial distribution: for fixed p and $n \to \infty$ it is the Gaussian distribution, while for $n \cdot p$ fixed and $n \to \infty$ it is the Poisson distribution. In the latter case it is clear that $p \ll 1$. The overview of these distributions is given below.

4.2 Poisson distribution

In practice we have to deal with events that happen randomly in time. Let's demand that the probability of the event happening within certain time interval τ

does not depend on whether the event has happened in any other non-overlapping time interval. The probability that the event happens within a small time interval $(t, t+\Delta t)$ is also small and proportional to the length of the time interval Δt, while the probability that two events happen within this time interval is an even smaller number of higher order in Δt. Let $p_m(t_1, t_2)$ be the probability that m events happen within the time interval (t_1, t_2). Then, the above conditions can be written in the following way:

$$\begin{aligned} p_m(t, t+\Delta t) &= \lambda(t)\Delta t + o(\Delta t), \\ \sum_{k=2}^{\infty} p_k(t, t+\Delta t) &= o(\Delta t), \end{aligned} \tag{67}$$

where $\lambda(t)$ is a non-negative function of time, while

$$\lim_{\Delta t \to 0} \frac{o(\Delta t)}{\Delta t} = 0$$

. Let's try to determine the distribution law for a random variable that satisfies these conditions.

Let's start counting time at $t = t_0$. The probability only depends on the length of the time interval; the occurrence did not happen within time interval $(t_0, t+\delta t)$ if it did not happen within intervals (t_0, t) and $(t, t+\delta t)$. Let p_0 be the probability that the occurrence did *not* take place. Then

$$p_0(t+\delta t) = p_0(t_0, t) \cdot p_0(t, t+\delta t) \equiv p_0(t) \cdot p_0(\delta t).$$

From conditions (67) and the completeness condition for the interval $(t, t+\delta t)$, during that interval the occurrence can happen either 0 times, or once, or twice, or more times. Hence:

$$\begin{aligned} p_0(\delta t) + p_1(\delta t) + \sum_{k=2}^{\infty} p_k(\delta t) &= 1, \\ p_0(\delta t) &= 1 - \lambda \cdot \delta t + o(\delta t) \end{aligned}$$

For the probability at starting point, $t_0 = t, \delta t \to 0$ we get $p_0(t_0) = 1$.

Assume for simplicity that λ is a constant function of time, $\lambda(t) = \lambda = \text{const}$ (this would be the case, for example, for the number of electrons per unit time emitted from a cathode). Then

$$\begin{aligned} p_0(t+\delta t) &= p_0(t) \cdot [1 - \lambda \cdot \delta t + o(\delta t)], \\ \frac{p_0(t+\delta t) - p_0(t)}{\delta t} &= -\lambda \cdot p_0(t) + p_0(t)\frac{o(\delta t)}{\delta t}. \end{aligned}$$

In the limit $\delta t \to 0$ we get

$$\begin{aligned} p_0(t) &= -\lambda \cdot p_0(t), \\ p_0(t) &= e^{-\lambda t}. \end{aligned}$$

Similarly, the probability of a single occurrence taking place is

$$p_1(t+\delta t) = p_1(t)\cdot[1-\lambda\cdot\delta t+\mathcal{o}(\delta t)] + p_0(t)\cdot[\lambda\cdot\delta t+\mathcal{o}(\delta t)],$$

since the event will take place either within $(0,t)$ or within $(t,t+\delta t)$ intervals. Hence

$$\frac{p_1(t+\delta t)-p_1(t)}{\delta t} \;=\; -\lambda\cdot p_1(t) + p_0(t)\cdot\left[\frac{\mathcal{o}(\delta t)}{\delta t}\right],$$

and in the limit $\delta t\to 0$ we get the equation

$$\begin{aligned} p_1(t) &= -\lambda\cdot p_1(t)+\lambda\cdot p_0(t), \\ p_1(t) &= (\lambda\cdot t)\cdot e^{-\lambda t}. \end{aligned}$$

Along the same lines one can show that

$$\begin{aligned} p_2(t) &= \frac{1}{2}(\lambda\cdot t)^2\cdot e^{-\lambda t}, \\ p_3(t) &= \frac{1}{2\cdot 3}(\lambda\cdot t)^3\cdot e^{-\lambda t},\ldots \end{aligned}$$

For a general term one gets the differential equation

$$p'_m(t) = \lambda\cdot[p_{m-1}(t)-p_m(t)], \qquad m=0,1,2,\ldots$$

with initial conditions $p_0=1, p_m=0$, with a solution

$$p_m(t) = \frac{(\lambda\cdot t)^m}{m!}\cdot e^{-\lambda t} \qquad m=0,1,2,\ldots$$

In a more general case when $\lambda=\lambda(t)$ is not a constant, the differential equation for the probability looks like this:

$$p'_m(t) = \lambda(t)\cdot[p_{m-1}(t)-p_m(t)], \qquad m=0,1,2,\ldots$$

Define an independent variable $\mu=\int_{t_0}^{t}\lambda(\tau)d\tau$. Then the solution can be shown to be

$$p_m(t) = \frac{\mu^m}{m!}\cdot e^{-\mu}, \qquad m=0,1,2,\ldots \tag{68}$$

Equation (68) defines the Poisson distribution, which describes the probability of $m=0,1,2,\ldots$ events taking place within the interval (t_0,t). It clearly satisfies the normalisation condition:

$$\sum_{m=0}^{\infty} p_m = \sum_{m=0}^{\infty}\frac{\mu^m}{m!}\cdot e^{-\mu} = e^{-\mu}\cdot\sum_{m=0}^{\infty}\frac{\mu^m}{m!} = e^{-\mu}\cdot e^{\mu} = 1.$$

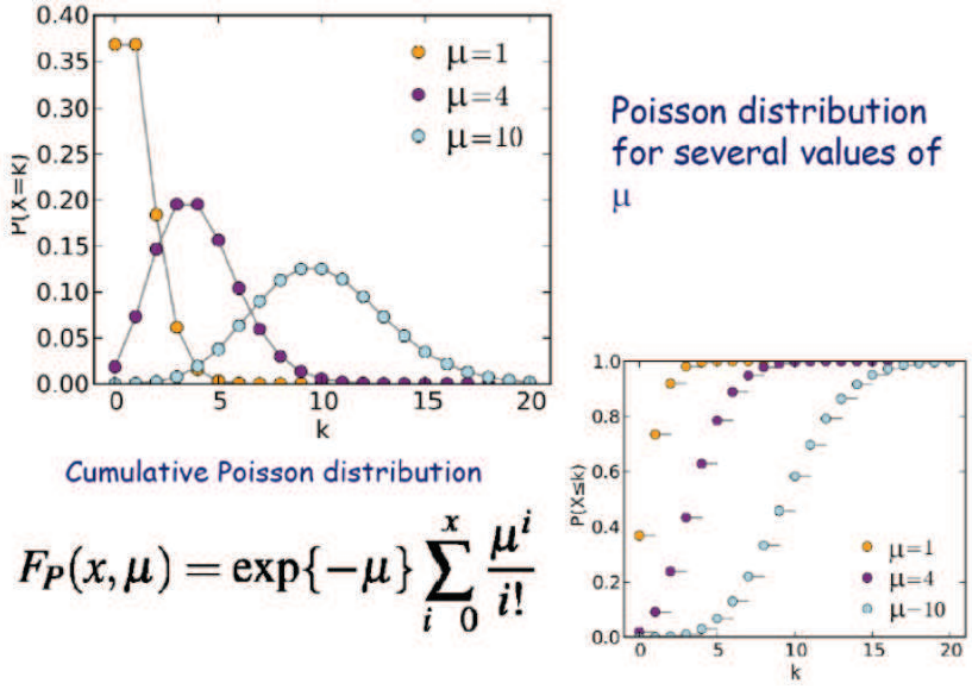


Figure 7: Examples of Poisson distribution, together with their respective cumulative distributions.

Figure 7 shows examples of Poisson distributions for three values of parameter μ, together with the respective cumulative distribution functions.

Let's calculate the mean of the Poisson distribution:

$$M(X) = \sum_{m=0}^{\infty} m \frac{\mu^m}{m!} \cdot e^{-\mu} = \mu e^{-\mu} \cdot \sum_{m=1}^{\infty} \frac{\mu^{m-1}}{(m-1)!} = \mu e^{-\mu} \cdot e^{\mu} = \mu.$$

This result clarifies the physical meaning of the parameter μ: it is equal to the mean number of events taking place within the interval (t_0, t).

In order to calculate the dispersion of the Poisson distribution, let's calculate first the quantity

$$\begin{aligned} M(X(X-1)) &= \sum_{m=0}^{\infty} m(m-1) \frac{\mu^m}{m!} \cdot e^{-\mu} = \mu^2 e^{-\mu} \cdot \sum_{m=2}^{\infty} \frac{\mu^{m-2}}{(m-2)!} = \mu^2 e^{-\mu} \cdot e^{\mu} \\ &= \mu^2. \end{aligned}$$

Hence we have

$$\begin{aligned} M(X^2) &= M(X(X-1)) + M(X) = \mu^2 + \mu, \\ D(X) &= M(X^2) - (M(X))^2 = (\mu^2 + \mu) - \mu^2 = \mu \end{aligned}$$

So both the mean and the dispersion of the Poisson distribution are equal to μ. The skewness A and the kurtosis E of the Poisson distribution can also be calculated: $A = 1/\sqrt{\mu}, E = 1/\mu$.

It appears that for small values of the probability p the Binomial distribution can at large n be approximated by the Poisson distribution:

$$P_n(m) \approx \frac{(n \cdot p)^m}{m!} e^{-n \cdot p}. \tag{69}$$

Figure 8 illustrates how the binomial distribution transforms in the limit into the

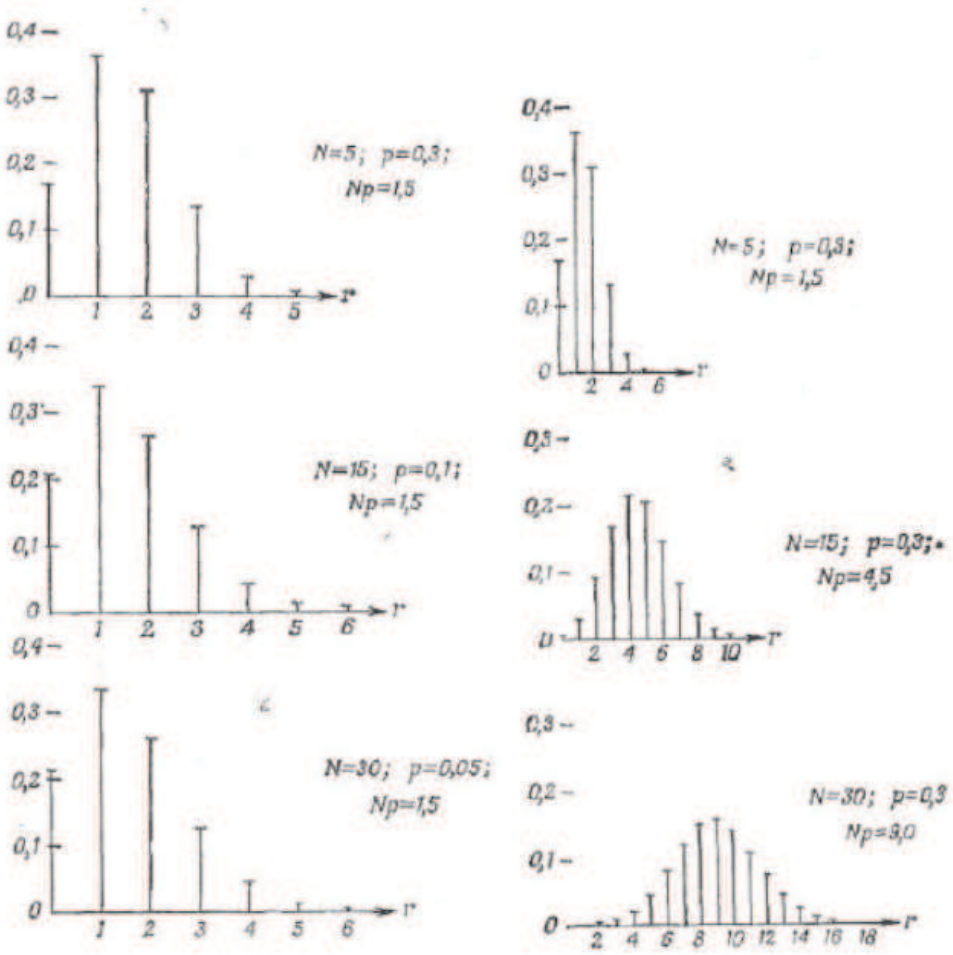


Figure 8: Left column: transformation of the binomial distribution into the Poisson distribution in the limit $n \cdot p = \text{const}, n \to \infty$. Right column: transformation of the binomial distribution into the Gaussian distribution in the limit of fixed p, $n \to \infty$.

Poisson (left column) and Gaussian (right column) distributions. One can also

see that for larger values of μ the Poisson distribution is close to the Gaussian distribution.

4.3 Uniformly distributed random variable

Consider a random variable r defined on the interval $x \in [0, 1]$ with probability density $\rho(x) = 1$. This variable is said to be *uniformly* distributed over the interval $[0, 1]$. The graph of this distribution is shown in Figure 9. The probability

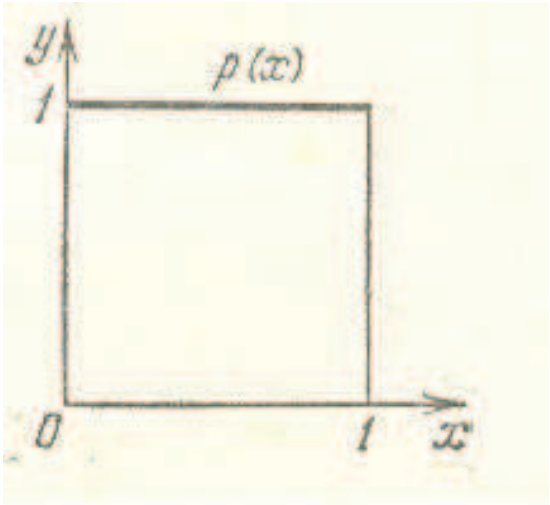


Figure 9: Random variable uniformly distributed over the interval $[0, 1]$.

of x falling within an interval a', b' is

$$P\{a' < x < b'\} = \int_{a'}^{b'} \rho(x)\, dx = b' - a', \tag{70}$$

i.e. it is equal to the length of the interval. If we divide the interval $[0, 1]$ into any number n of sub-intervals of equal length, the probability of x falling into any of the subintervals is equal to $1/n$. It is easy to show by direct calculation that the mean Mr of the variable uniformly distributed on the interval $[0, 1]$ is equal to $1/2$, while its dispersion Dr is equal to $1/12$.

In practical calculations the quantity $1 - r$ is sometimes used instead of r, with the same distribution function as for r. Sometimes the symbol γ is used instead or r.

More generally, for a uniform distribution over the interval $[a, b]$, one has:

$$a \le x \le b, \qquad \rho(x) = \frac{1}{b-a}, \qquad Mr = \frac{a+b}{2}, \qquad Dr = \frac{(a+b)^2}{12}.$$

The plots illustrating the uniform distribution density and its respective cumulative distribution are shown in Figure 10.

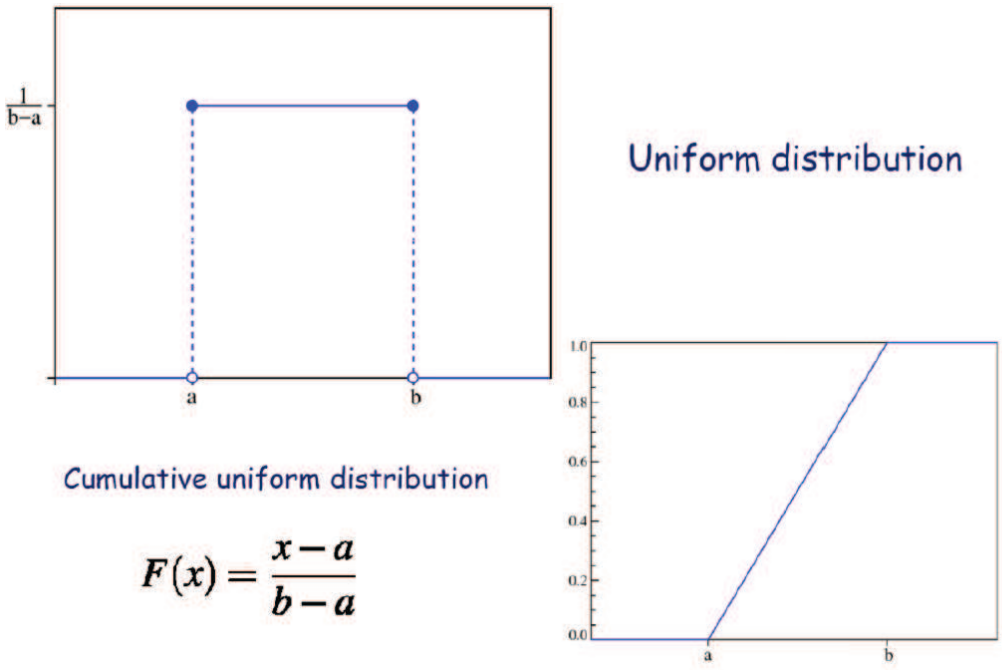


Figure 10: The density of a uniformly distributed random variable and its cumulative distribution.

4.4 Gaussian (normal) distribution

Random variables distributed according to the Gaussian (otherwise known as *normal* distribution play an important role in probability theory. This distribution is defined on the whole axis $(-\infty, +\infty)$ and has the following density:

$$\rho(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x-a)^2}{2\sigma^2}\right], \tag{71}$$

where a and $\sigma > 0$ are numerical parameters. The parameter a has no influence on the shape of the curve $y = \rho(x)$ but rather simply shifts the curve along the x axis, while parameter σ defines the shape of the curve. In particular,

$$\max \rho(x) = \rho(a) = \frac{1}{\sigma\sqrt{2\pi}},$$

so that decreasing σ means increasing the height of the distribution. Since the area under the distribution (71) is normalised, the increase in height must be

compensated by the narrowing of the distribution. Figure 11 shows examples of the Gaussian distribution for various values of its parameters: for larger σ

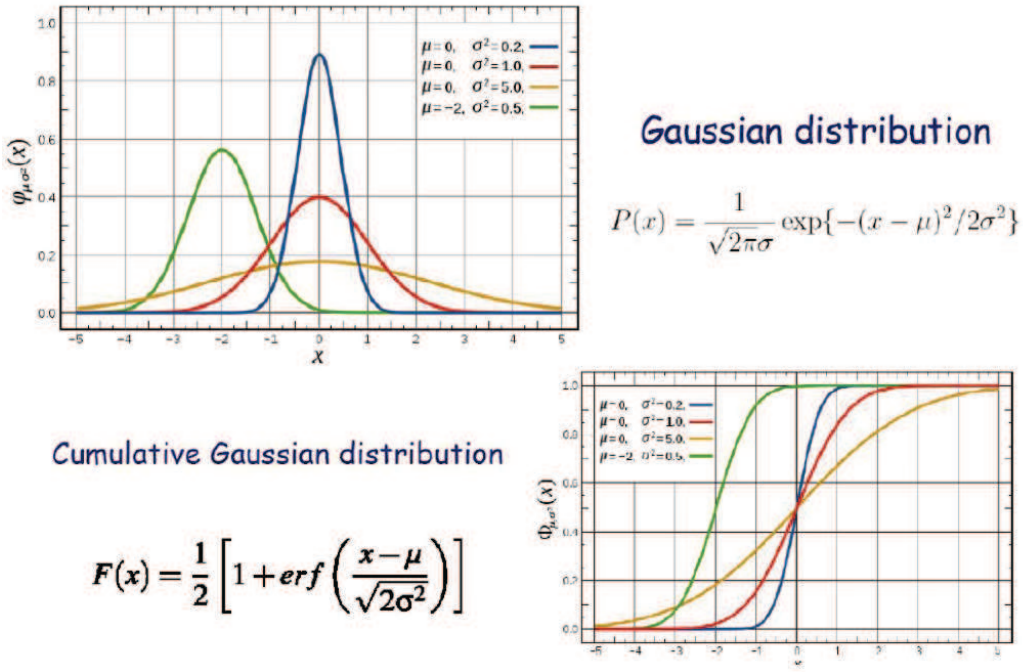


Figure 11: The Gaussian (normal) distribution density and its matching cumulative distribution for 4 different sets of parameter values.

the distribution becomes wider and lower. The *standard Gaussian distribution* corresponds to the choice of parameters $a = 0, \sigma = 1$:

$$\rho(x) = \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{x^2}{2}\right].$$

This function has the following properties:

a) it is symmetric with respect to $x = 0$, i.e. $\rho(x) = \rho(-x)$;

b) $\max \rho(x) = \frac{1}{\sqrt{2\pi}} \approx 0.40$;

c) the inflection points lie at $x = \pm 1$, where the probability density ρ is equal to $\rho(\pm 1) = \frac{1}{\sqrt{2\pi e}} \approx 0.24$;

d) the probability falls sharply with increasing $|x|$: $\rho(|2|) = 0.05, \rho(|3|) = 0.003$ etc.

It can be shown that the mean $M\xi$ of the Gaussian distribution (71) is equal to a, the dispersion $D\xi$ is equal to σ^2 and its skewness $A = 0$, since it is symmetric w.r.t. its mean.

Another example of the Gaussian distribution is shown in Figure 8 (bottom left), as a limiting case of the binomial distribution. In this example the mean value is 9.

When dealing with the Gaussian distribution, any probability of the type $P\{x' < \xi < x''\}$ can be calculated using special tables where the values of the *Laplace function* (otherwise sometime known as the probability integral) are tabulated. The latter is defined as

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_0^x e^{-\frac{t^2}{2}} \tag{72}$$

Indeed, using equation (32) we have

$$P\{x' < \xi < x''\} = \frac{1}{\sigma\sqrt{2\pi}} \int_{x'}^{x''} \exp\left[-\frac{(x-a)^2}{2\sigma^2}\right] dx.$$

Substituting $x - a = \sigma t$ we get

$$P\{x' < \xi < x''\} = \frac{1}{\sqrt{2\pi}} \int_{t_1}^{t_2} \exp\left[-\frac{t^2}{2}\right] dt,$$

where $t_1 = (x' - a)/\sigma$ and $t_2 = (x'' - a)/\sigma$. Hence

$$P\{x' < \xi < x''\} = \Phi(t_2) - \Phi(t_1).$$

Note that $\Phi(-t) = -\Phi(t)$.

Let's look at specific examples. First, choose $x' = a - 3\sigma, x'' = a + \sigma$, which corresponds to $t_1 = -3, t_2 = +3$. From the table of integral (72) we can calculate the probability

$$P\{a - 3\sigma < \xi < a + 3\sigma\} = 2\Phi(3) = 0.997. \tag{73}$$

This probability is quite close to unity. Its interpretation goes like this: the probability that a measured value falls outside $\pm 3\sigma$ of the mean is less than 0.3%, i.e. is usually negligibly small (that is, of course, if the variable in question is distributed according to a Gaussian distribution!).

One also has:

$$P\{a - \sigma < \xi < a + \sigma\} = 2\Phi(1) \approx 0.68.$$

If $r = 0.6745$ then one has from the same table:

$$P\{a - r\sigma < \xi < a + r\sigma\} = 2\Phi(0.6745) = 0.5. \tag{74}$$

This means that $P\{|\frac{\xi-a}{\sigma}| < r\} = 0.5$ and $P\{|\frac{\xi-a}{\sigma}| > r\} = 0.5$, with, of course, $P\{|\frac{\xi-a}{\sigma}| = r\} = 0$. Hence, the deviation of the normally distributed random variable is equally probable by less than and more than $r \cdot \sigma$. The value $r \cdot \sigma$ is sometimes called the *probable error*.

Results of experimental measurements in physics are often presented in the form $y \pm \Delta y$, where Δy is the root-mean-square deviation. For a Gaussian-distributed random variable, this would be σ. Hence, this result has a fairly modest *confidence level* of about 68%, meaning that there is (only) a 68% probability that the value lies within the *confidence interval* $(y - \Delta y, y + \Delta y)$, so in about 1/3 of cases the result will fall outside this interval.

The topic of confidence levels and confidence intervals will be discussed in more detail in the following section.

4.5 χ^2 distribution

Consider a random variable ξ which obeys the standard Gaussian distribution $\rho(x) = \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{x^2}{2}\right]$, and we need to determine how the random variable $\eta = \xi^2$ is distributed. We can achieve this task using the equation (46), with $f(x) = x^2$ and hence $f^{-1}(x) = x^{\frac{1}{2}}$, so that $\frac{d}{dx}\left[f^{-1}(x)\right] = \frac{1}{2}x^{-\frac{1}{2}}$. So the density of variable η is

$$\rho_\eta(x) = \frac{1}{2\sqrt{2\pi x}} \exp\left[-\frac{x}{2}\right], \qquad x > 0. \tag{75}$$

Consider now a set of random variables $\xi_1, \xi_2, \ldots \xi_n$ distributed according to the standard Gaussian. Then the random variable

$$\chi^2_n = \sum_{i=1}^{n} \xi_i^2 \tag{76}$$

is distributed according to the χ^2 *distribution* with n degrees of freedom. It can be shown that its density is

$$\rho_n(x) = C_n x^{\frac{n}{2}-1} \exp\left(-\frac{x}{2}\right), \qquad x > 0. \tag{77}$$

where $C_n = \left[2^{\frac{n}{2}}\Gamma\left(\frac{n}{2}\right)\right]^{-1}$, with Euler's Γ function defined as $\Gamma(p) = \int_0^1 x^{p-1}e^{-x}dx$. Some examples of this distribution are shown in Figure 12.

The χ^2 distribution has one parameter n, number of degrees of freedom, and hence it can be easily tabulated. Its mean M is equal to n and its dispersion D is equal to $2n$, skewness A is $2\sqrt{2/n}$ and kurtosis $E = 12/n$.

Note that the distribution shown in equation (75) corresponds to the χ^2 distribution with one degree of freedom. In the limit of large n the χ^2 distribution can be approximated by a Gaussian with mean n and dispersion $2n$.

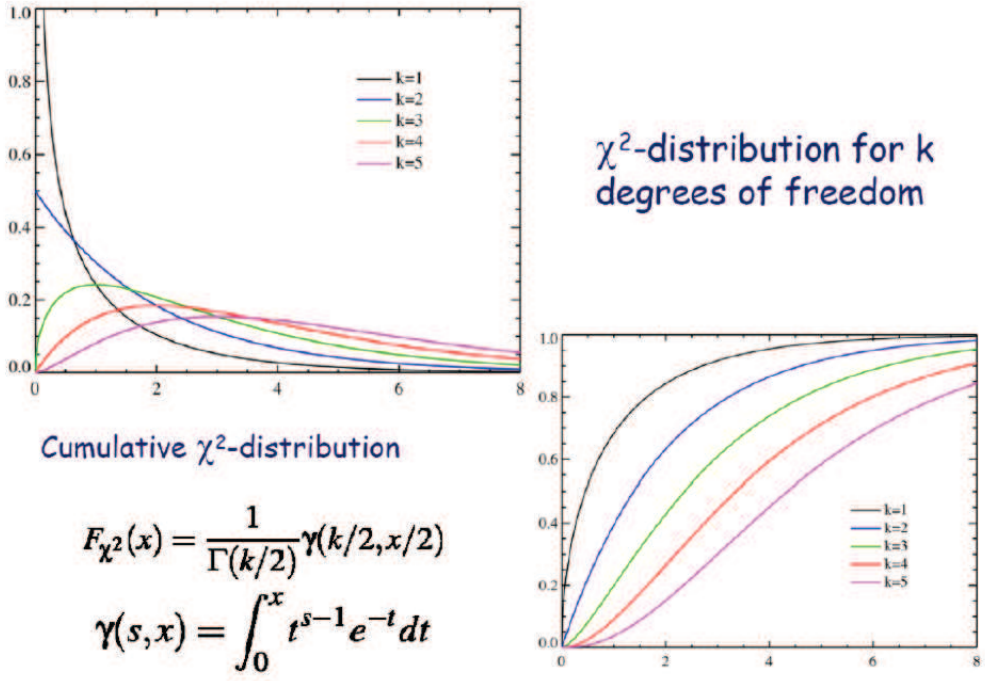


Figure 12: Examples of χ^2 distributions for different values of parameter n, together with its respective cumulative distributions.

Let ξ be a standard Gaussian-distributed random variable, while variable χ obeys a χ^2 distribution with $k = n-1$ degrees of freedom. Then the combination $t = \xi\sqrt{n}/\chi$ is a random variable distributed according to *Student's distribution* with density

$$\rho(t) = \frac{1}{\sqrt{k\pi}} \frac{\Gamma\left(\frac{k+1}{2}\right)}{\Gamma\left(\frac{k}{2}\right)} \left(1 + \frac{t^2}{k}\right)^{\frac{k+1}{2}}. \tag{78}$$

Student's distribution plays an important role in the studies of validity of various statistical hypotheses.

In the special case $n = 2$ the Student's distribution (76) becomes *Cauchy's distribution* with density

$$\rho(t) = \frac{1}{\pi \cdot (1 + t^2)}. \tag{79}$$

Both the mode and the median of this distribution are equal to zero, but the mean, dispersion and higher moments do not exist, since the corresponding integrals are divergent. To quantify the width of the distribution, its full width

at half maximum (FWHM) is used, which is equal to 2. If θ is a uniformly distributed random variable on interval $(-\pi/2, +\pi/2)$ then $x = \tan\theta$ will be distributed according to equation (79). Also, if y and z are two independent normally distributed variables, then the variable $x = y/z$ will follow the Cauchy distribution.

The Lorentz distribution, also called the Breit-Wigner distribution, is a more general form of equation (79), which is often used to describe resonances in high energy physics. Its density is

$$f(x) = \frac{1}{\pi} \frac{\Gamma/2}{(x - x_0)^2 + \Gamma^2/4}, \tag{80}$$

where x_0 is the mode and Γ is full height at half maximum. In the relativistic limit, where the momenta of particles are much larger than their masses, one often uses a relativistic version of the Breit-Wigner distribution, which is slightly asymmetric and has a longer 'tail' at high x:

$$f(x) \propto \frac{1}{(x^2 - M_0^2)^2 + M_0^2\Gamma^2}. \tag{81}$$

Here x is the centre-of-mass energy of the resonance, M_0 is its mass, and γ is its decay width, the reciprocal of its decay time τ: $\Gamma = 1/tau$. In general, Γ has some dependence on the energy x, the fact which may become important if the width Γ is not much smaller than the mass M_0 (for example, in the decay of the Z boson into a fermion-antifermion pair, $Z^0 \to f\overline{f}$). Sometimes the term $M_0^2\Gamma^2$ in equation (80) is replaced by $\Gamma^2 E^4/M_0^2$.

In Figure 13 some examples of Cauchy distributions are shown for a number of parameter values.

Yet another important distribution, often used for checking various hypotheses, is Fisher's distribution. If χ_1 and χ_2 are random variables governed by the χ^2 distributions with n_1 and n_2 degrees of freedom respectively, then the combination $f = (\chi_1/n_1)/(\chi_2/n_2) = (n_2\chi_1)/(n_1\chi_2)$ follows Fisher's distribution. Its density is

$$\rho(f) = \frac{C \cdot f^{(n_1-2)/2}}{(n_1 f + n_2)(n_1 + n_2)/2}, \tag{82}$$

where the normalisation constant C is equal to

$$C = \frac{\Gamma\left(\frac{n_1}{2} + \frac{n_2}{2}\right)}{\Gamma\left(\frac{n_1}{2}\right) \cdot \Gamma\left(\frac{n_2}{2}\right)} \cdot n_1^{n_1/2} \cdot n_2^{n_2/2}.$$

4.6 Generating a random variable with a given distribution

Our task is to develop a way of obtaining a random variable ξ with a given probability distribution density $\rho(x)$ defined on an interval (a, b), based on a

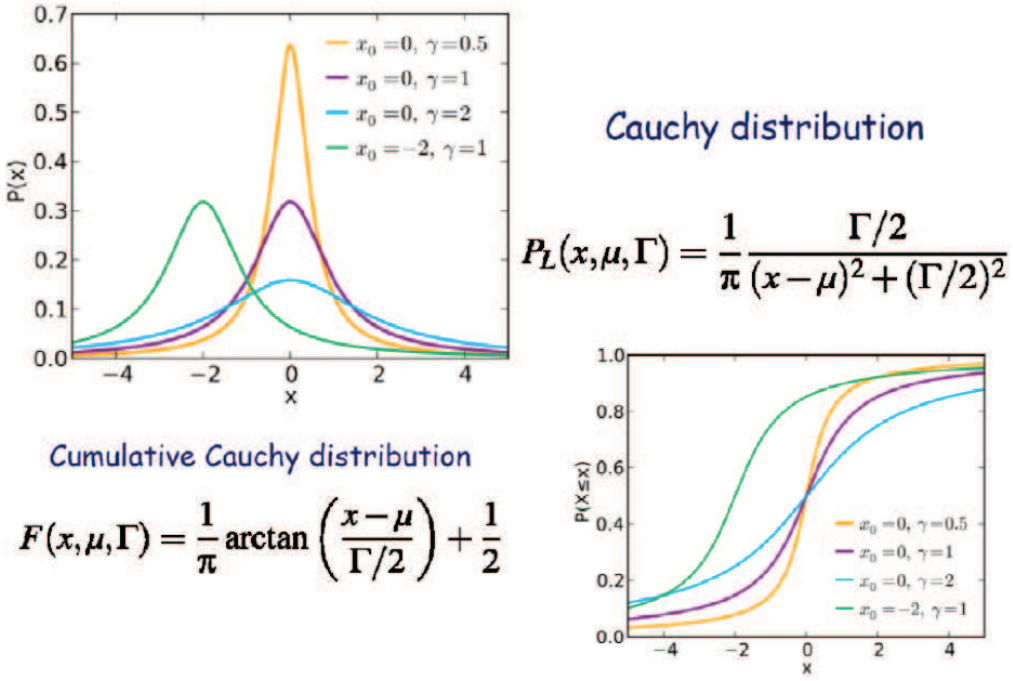


Figure 13: Examples of Cauchy/Lorentz/Breit-Wigner distributions for different values of parameters, together with their respective cumulative distributions.

uniformly distributed variable r defined on the interval $[0, 1]$. This procedure is based on Monte Carlo method, and is sometimes also referred to as *sampling* of the variable ξ.

The sought relationship between the variables x and r can be obtained from the definition $F(x) = \int_{-\infty}^{x} \rho(x)dx$ (see equation (35), if we can solve the equation

$$F(x) = r \tag{83}$$

If the inverse function F^{-1} exists, then the solution of equation (83) can be written as

$$x = F^{-1}(r) \tag{84}$$

Indeed, we know that r is distributed uniformly on interval $[0, 1]$, and equation (83) states that $F(x)$ is also distributed in the same way. But for the uniform distribution the probability that $F(x)$ falls within the interval $[F(x), F(x) + dF(x)]$ is equal to the length of that interval, $dw = dF(x)$. On the other hand, from equation (35) we have:

$$dF(x) = \rho(x)\, dx \qquad \Rightarrow \qquad dw = \rho(x)\, dx,$$

which means that the random variable x is distributed with density $\rho(x)$, as required. Hence, in order to obtain a random variable with distribution density $\rho(x)$, we need to solve equation (84).

Figure 14 illustrates how a uniform variable u defined on an interval $[0, 1]$ can

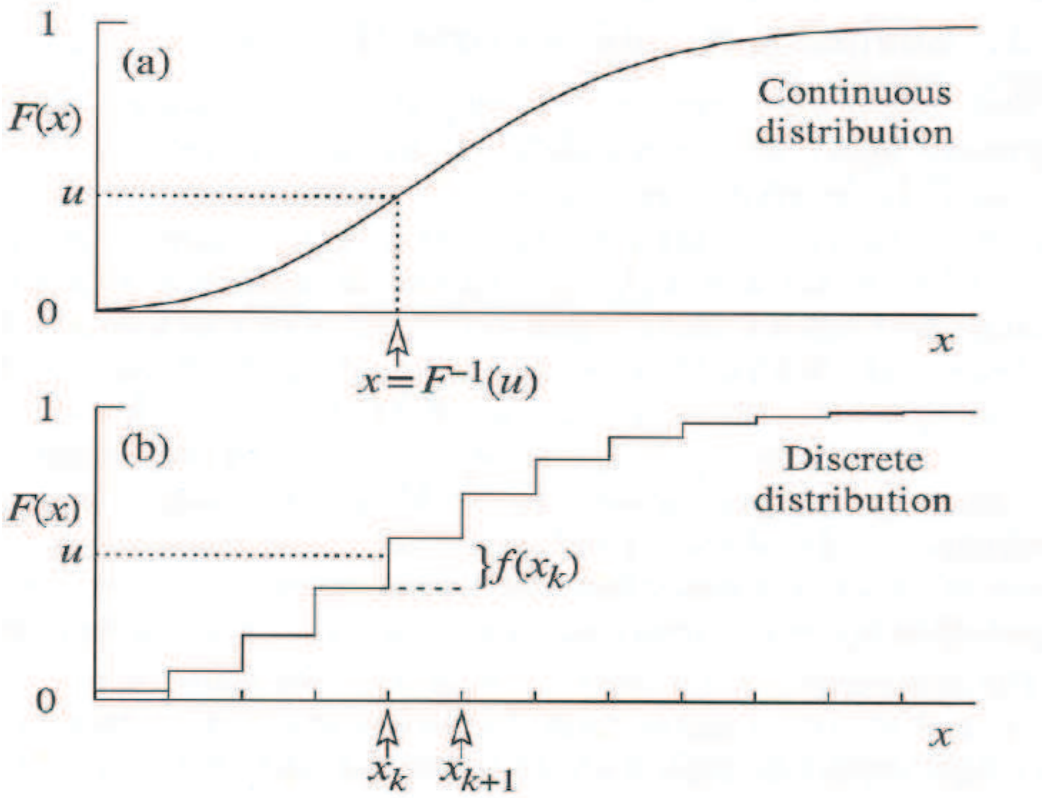


Figure 14: Geometric interpretation of equations (83) and (84) for a continuous (top) and discrete (bottom) cases.

be used to obtain the variable x with a pre-defined cumulative distribution $F(x)$. The top figure refers to a continuous random variable, while the bottom figure describes the procedure for a discrete random variable. In the latter case $f(x_k)$ is the probability of x falling within the interval (x_k, x_{k+1}), and the sought values of x_k are obtained from the conditions

$$F(x_{k-1}) < u < F(x_k) \equiv P\{x \leq x_k\} = \sum_{i=1}^{k} f(x_i),$$

where $F(x_0) \equiv 0$.

As an example, consider a random variable ξ distributed uniformly in the interval (a, b). Then, from equation (70), its probability density is $\rho(x) = 1/(b - a)$. Use equations (83) to obtain the sampling formula for ξ:

$$\int_a^\xi \frac{dx}{b-a}, \qquad \Rightarrow \qquad \frac{\xi - a}{b-a} = r \qquad \Rightarrow \qquad \xi = a + r(b-a). \tag{85}$$

This expression allows us to generate a random variable uniformly distributed in the interval (a, b).

Another example would be to model the process of the radioactive decay of an unstable isotope in the time interval $t = (a, b)$. We know that the decay probability follows the exponential law, $f(t) = \frac{1}{\tau}\exp(-\frac{t}{\tau})$, where τ is the mean life of the isotope.

In order to simulate this process, we need to calculate in advance the quantities $\alpha = \exp(-\frac{a}{\tau})$ and $\beta = \exp(-\frac{b}{\tau})$ and use them to generate, for each value of r, the quantity

$$t = -\tau \ln[\beta + r(\alpha - \beta)]. \tag{86}$$

Thus obtained values of t will have the required distribution $f(t)$.

In practice it is often necessary to generate decays which are isotropic in space, such as α-decays of various nuclei. Isotropic is the decay with the spherical symmetry, i.e. where the direction of flight of the radiated α particle is uniformly distributed over the surface of the sphere whose centre is placed at the origin of the decay. This means that if the decay directions are characterised with unit vectors, the density of these unit vectors on the surface of the sphere of unit radius is proportional to the solid angle. The direction in a 3-dimensional space is characterised by two angles: the azimuthal angle ϕ which varies in the interval $0, 2\pi$ and the polar angle θ which varies within $0, \pi$. The solid angle element $d\Omega$ in polar coordinates is calculated as $d\Omega = \sin\theta d\theta d\phi = d(\cos\theta)d\phi$. Isotropy will be achieved, if the angle ϕ is generated uniformly in the interval $(0, 2\pi)$ and $\cos\theta$ is generated uniformly within $(-1, 1)$. This will be achieved if we generate two independent uniform random numbers r_1 and r_2 from the interval $[0, 1]$ and then calculate ϕ as $2\pi r_1$ and $\cos\theta$ as $(2r_2 - 1)$.

What do we do if the explicit form of the function $F(x)$ cannot be found? This can happen if the r.h.s. in expression (35) and/or the inverse function in equation (84) can only be obtained numerically. This is often the case, for example, for Gaussian-distributed variables. Here we consider two ways of tackling this problem.

In the next section we will show that a normally distributed random variable can be obtained based on the central limit theorem. Consider a random variable ζ which is a (normalised) sum of n uniformly-distributed random variables:

$$\zeta^{(n)} = \sqrt{\frac{3}{n}} \cdot \sum_{i=1}^{n} (2r_i - 1). \tag{87}$$

It appears that with n as low as 12, the distribution is acceptably close to the standard Gaussian distribution:

$$\zeta \approx \zeta^{(12)} = \sum_{i=1}^{1} 2r_i - 6. \tag{88}$$

In practice a modified formula is usually used, which increases the sampling speed and improves convergence:

$$\zeta \approx 0.0109\zeta^{(5)} \left[97 + (\zeta^{(5)})^2\right]. \tag{89}$$

The other method of generating Gaussian-distributed variables is the Box-Müller method. Consider two independent variables ξ and η, each sampled from the standard normal distribution. Then, in Cartesian coordinate system (on the XOY plane) the density of points with coordinates (ξ, η) is given by the product of the two Gaussian distributions:

$$\rho(x, y) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \cdot \frac{1}{\sqrt{2\pi}} e^{-y^2/2} = \frac{1}{2\pi} e^{-(x^2+y^2)/2}. \tag{90}$$

In polar coordinates (r, ϕ) one has $x = r\cos\phi$ and $y = r\sin\phi$. Let (ζ, θ) be the coordinates of the random point (ξ, η) in terms of the new (polar) coordinates. Obviously, $\xi = \zeta\cos\theta, \eta = \zeta\sin\theta$. The transformation of a distribution from one system of coordinates to another is done using the Jacobian of the transformation, J:

$$\hat{\rho}(r, \phi)\, dr\, d\phi = J\, \rho(x, y)\, dx\, dy, \tag{91}$$

where the Jacobian is

$$J = \left|\frac{\partial(x, y)}{\partial(r, \phi)}\right| = \begin{vmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \phi} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \phi} \end{vmatrix} = \begin{vmatrix} \cos\phi & \sin\phi \\ -r\sin\phi & r\cos\phi \end{vmatrix} = r(\cos^2\phi + \sin^2\phi) = r.$$

Hence, the distribution density (91) takes the form

$$\hat{\rho}(r, \phi) = \frac{1}{2\pi} r e^{-r^2/2}. \tag{92}$$

As we see, in polar coordinates the dependences on variables r and ϕ are separated:

$$\begin{gathered} \hat{\rho}(r, \phi) = \rho_1(r) \cdot \rho_2(\phi), \\ \rho_1(r) = r e^{-r^2/2}, \qquad \rho_2(\phi) = \frac{1}{2\pi}. \end{gathered} \tag{93}$$

Sampling the distributions $\rho_1(r)$ and $\rho_2(\phi)$ is not a problem, one just needs to apply the equation (35) with the correct limits, $(0 < r < \infty)$ and $(0 < \phi < 2\pi)$, and then solve equation (83) for each case. The integrations lead to the functions

$$F_1(r) = 1 - e^{-r^2/2}, \qquad F_2(\phi) = \frac{\phi}{2\pi}. \tag{94}$$

The distributions for random variables ζ and θ are obtained from equations

$$F_1(\zeta) = 1 - \gamma_1, \qquad F_2(\phi) = \gamma_2,$$

where γ_1 and γ_2 are random variables uniformly distributed in the interval $[0, 1]$. In particular

$$\zeta = \sqrt{-2\ln\gamma_1}, \qquad \theta = 2\pi\gamma_2. \tag{95}$$

Finally, for the random variables ξ and η we get

$$\xi = \sqrt{-2\ln\gamma_1}\cos(2\pi\gamma_2), \qquad \eta = \sqrt{-2\ln\gamma_1}\sin(2\pi\gamma_2). \tag{96}$$

These are distributed according to the standard Gaussian (normal) distributions. The random variables

$$x = m + \sigma\xi, \qquad y = n + \sigma\eta \tag{97}$$

will have Gaussian distributions with widths σ, centered at m and n respectively.

Let's get back now to the problem of generating a variable with an arbitrary probability density distribution $\rho(x)$ defined in the interval (a, b). In the most general case, one can use von Neumann's *rejection sampling* method. Find an *envelope* function T(x) which satisfies the condition $T(x) > \rho(x)$ for all $x \in (a, b)$. For simplicity, $T(x)$ can be chosen as a constant C which is as close as possible to the maximum of $\rho(x)$, as this helps improve the *rejection efficiency*. Now let's generate two random numbers r_1 and r_2, the first uniformly distributed in the interval (a, b), and the other uniformly distributed in the interval $(0, C)$. If the condition $r_2 > \rho(r_1)$ is satisfied, then the number r_1 is rejected; if not, then it is stored. This procedure is repeated multiple times, and the collection of stored numbers r_1 is distributed according to the desired density function $\rho(x)$ defined in the interval (a, b). The method is illustrated by Figure 15 (a).

If the input function $\rho(x)$ is varying strongly, then the rejection method as defined above can be inefficient. In such cases one can use a piecewise constant density function as the envelope, or use some kind of variable transformation. There is no universal recipe for efficiency optimisation, the exact recipe will depend on the problem at hand and the experience of the user. Figure 15 (b) illustrates how the efficiency of the method can be improved by choosing a different constant function for different subintervals of the variable x.

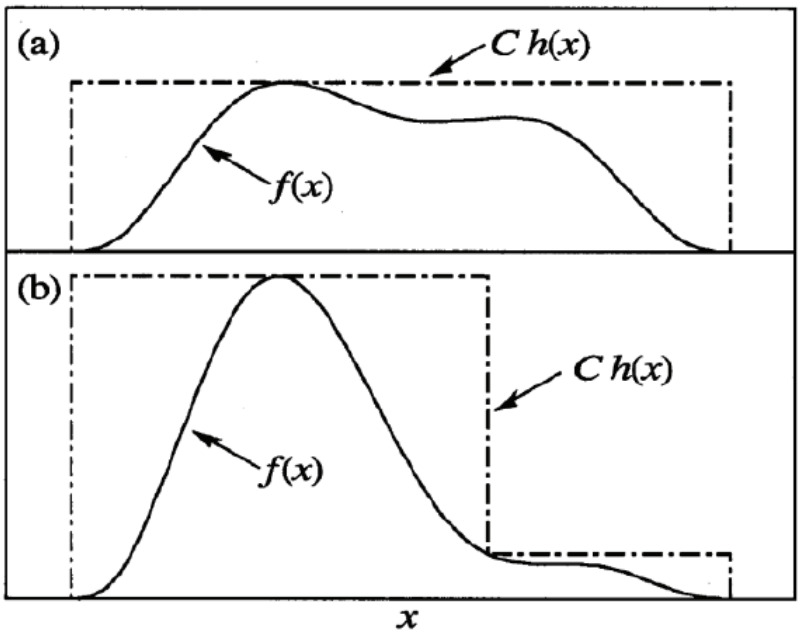


Figure 15: The illustration of Neumann's method of generating a random variable with an arbitrary density. Here $f(x)$ is the required density $\rho(x)$, $h(x)$ is a uniform distribution normalised to unity, and C is a constant.

This method is used to obtain a fast sampling of Gaussian-distributed random variables, since the method explained above requires calculating trigonometric functions (see equation (35)) which are rather expensive in CPU time. Instead, two uniformly distributed random variables r_1 and r_2 are used to calculate variables $v_1 = 2r_1 - 1$ and $v_2 = 2r_2 - 1$, which, of course, are distributed uniformly in the interval $(-1, +1)$. Now calculate $R^2 = v_1^2 + v_2^2$. If $R^2 > 1$, reject the sampling and start again. For those R^2 which are less than 1, calculate

$$z_1 = v_1\sqrt{\frac{-2\ln R^2}{R^2}}, \qquad z_2 = v_2\sqrt{\frac{-2\ln R^2}{R^2}}. \tag{98}$$

Variables z_1 and z_2 are independent, and are each distributed according to the Gaussian distribution with mean of zero and unit width.

5 Elements of mathematical statistics

Consider a collection of similar elements which are united into a single group by one common property, but can be separated into a number of subgroups with

respect to some other properties. Such set of elements is called a *general set*, while the elements of the general set are said to be its *members*. The number of members defines the *volume* of the general set. The properties (characteristics) which are used to sub-divide the general set into subsets are called the *arguments* of the set, while the numbers of elements contributing to individual subsets are called variation frequencies.

For example, the collection of scientists working in a research institute forms a general set consisting of 100 people. These are divided into two subsets, theorists and experimentalists, with numbers of 30 and 70 respectively. Here 100 is the volume of the general set, while "theorist" and "experimentalist" are arguments, with respective variation frequencies of 30 and 70. We could have subdivided the scientists into a number of groups according to their age, in which case age would have become one of the arguments. The general property that unites all members of the set is that they all are scientists and hence participate in some kind of research activity, e.g. publish papers in scientific journals.

If the volume of the general set is large, it is practically impossible to study in detail each element of the set (which would have given us the exhaustive information about the set). In such cases a random subset (a *sample*) of the general set is selected, with the number of elements of the sample being its volume. The selected ('sampled') elements are studied in detail, and, based on these studies, conclusions are made about the composition and properties of the general sample. The main aim of the *mathematical statistics* is just that: estimating various numerical characteristics (in particular, things like the expectation value, dispersion etc.) of the general set, based on a subset sample. We will consider this task in this chapter. Mathematical statistics has another aim as well, to asses the validity of various hypotheses; we do not cover this topic in our lecture course.

In some sense, the problems of mathematical statistics are the inverse of the problems of the probability theory. In probability theory we know the model and we try to describe (or predict) the variety of possible developments, whereas in mathematical statistics we start from experimental observations and try to figure out the model. Because of this link, many methods and tools used in the probability theory are also used in mathematical statistics. Mathematical statistics is part of the field of applied mathematics, which is developed using induction.

Consider a random sampling of n values $x_1, x_2, \ldots, x_n$ of a random variable X, which are obtained from n independent experiments. Mathematical statistics views these as n random variables $X_1, X_2, \ldots, X_n$ which belong to the same distribution as X, and hence have the same numerical characteristics such as mean, dispersion etc.

Let's try to estimate the value of some parameter θ which characterises the theoretical distribution, based on experimental data. The parameter in question can be the mean of the distribution, its dispersion, or something else. If the value $\hat{\theta}_n$ of the parameter, calculated with the sample $x_1, x_2, \ldots, x_n$, comes closer and

closer to the true θ with increasing n, so that

$$\lim_{n\to\infty} P(\{|\hat{\theta}_n - \theta| < \varepsilon\} = 1, \tag{99}$$

where $\varepsilon > 0$ is an infinitesimally small number, then $\hat{\theta}_n$ is said to be a *consistent estimator* of θ. Clearly, since $\hat{\theta}_n$ is calculated by random sampling of a random variable, it itself is a random variable, and hence should be treated as such.

With a small sample, an *unbiased* estimator is usually used. This is an estimator $\hat{\theta}_n$ whose expectation value $M(\hat{\theta}_n)$ is equal to the true value θ.

A consistent and unbiased estimator is sometimes called a *point estimator*, which can be considered to be 'the best guess' based on available data. For a small sample, a point estimator can deviate substantially from the true value, so it will only make sense if one can assign some uncertainty limits to its value. In other words, one needs to establish an interval of values which, with a certain probability, will contain the true value of the parameter. It is called the *confidence interval*.

We will now state, without proof, a hugely important theorem in the theory of random variables. For further information, please see reference [2], pp. 159-168.

Consider a large number N of mutually independent variables $\xi_1, \xi_2, \ldots, \xi_N$ which share the same probability distribution function. Then their means and dispersions will also be the same:

$$\begin{aligned} M\xi_1 = M\xi_2 = \cdots = M\xi_N &\equiv m, \\ D\xi_1 = D\xi_2 = \cdots = D\xi_N &\equiv \sigma^2. \end{aligned} \tag{100}$$

Consider now the *sample mean*

$$\overline{\xi} = \frac{1}{n}\sum_{i=1}^{n} \xi_i$$

for a subset of n variables, and calculate its expectation value:

$$M(\overline{\xi}) = \frac{1}{n} M\left(\sum_{i=1}^{n} \xi_i\right) = \frac{1}{n}\sum_{i=1}^{n} M\left(\xi_i\right) = \frac{1}{n}\cdot n \cdot M(\xi) = M(\xi) = m \tag{101}$$

It appears that in the limit of large n, the sample mean is equal to the true mean of the variable ξ:

$$P\{|\overline{\xi} - m| < \varepsilon\} \to 1, \quad \text{or} \quad \lim_{n\to\infty} P\left\{\left|\frac{1}{n}\sum_{i=1}^{n} \xi_i - m\right| < \varepsilon\right\} = 1, \tag{102}$$

where ε is infinitesimally small, and hence the sample mean is a consistent and unbiased estimator of the true mean of the variable ξ. This statement is often

called *the law of large numbers*, which was first introduced in this form by *Markov*. This is an extremely important theorem, which in fact states that the net result of a large number of random factors, although a random variable by its nature, is not that random any more and can be predicted with high confidence. So it is sometimes also referred to as the law of *stability of the mean*. Chebyshev subsequently proved a more general form of the law, where it is no longer necessary for the random variables to belong to the same distribution, they just need to be mutually independent, and each should have a finite mean and dispersion:

$$\lim_{n\to\infty} P\left\{\left|\frac{1}{n}\sum_{i=1}^{n}\xi_i - \frac{1}{n}\sum_{i=1}^{n}M(\xi_i)\right| < \varepsilon\right\} = 1. \tag{103}$$

Here the first term in brackets is a random variable, while the second term is a constant.

As for the dispersion of the sample mean, one has:

$$D(\overline{\xi}) = D\left(\frac{1}{n}\sum_{i=1}^{n}\xi_i\right) = \frac{1}{n^2}D\left(\sum_{i=1}^{n}\xi_i\right) = \frac{1}{n^2}\sum_{i=1}^{n}D(\xi_i) = \frac{n\sigma^2}{n^2} = \frac{\sigma^2}{n}, \tag{104}$$

i.e. the dispersion of the sample mean is n times smaller than the dispersion of the random variable ξ itself.

In analogy with sample mean, we can introduce the concept of *sample dispersion*:

$$s^2 = \frac{1}{n}\sum_{i=1}^{n}\left(\xi_i - \overline{\xi}\right)^2 = \frac{1}{n}\sum_{i=1}^{n}\xi_i^2 - \left(\overline{\xi}\right)^2. \tag{105}$$

Let's calculate the expectation value of the sample dispersion:

$$\begin{aligned} M(s^2) &= M\left[\frac{1}{n}\sum_{i=1}^{n}\xi_i^2 - \left(\overline{\xi}\right)^2\right] = \frac{1}{n}\sum_{i=1}^{n}M(\xi_i^2) - M\left[\left(\overline{\xi}\right)^2\right] \\ &= \frac{n}{n}M(\xi^2) - M\left[\left(\overline{\xi}\right)^2\right] = \left[D\xi + (M\xi)^2\right] - \left[D\overline{\xi} + \left(M\overline{\xi}\right)^2\right] \\ &= (\sigma^2 + m^2) - \left(\frac{\sigma}{n} + m^2\right) = \frac{n-1}{n}\sigma^2, \end{aligned} \tag{106}$$

where we used the result of equation (104) and the property $M\xi^2 = D\xi + (M\xi)^2$. From equation (106) you can see that if the sample dispersion is calculated like this:

$$\overline{s^2} = \frac{1}{n-1}\sum_{i=1}^{n}\left(\xi_i - \overline{\xi}\right)^2, \tag{107}$$

then $\overline{s^2}$ becomes a consistent and unbiased estimator of the true dispersion of ξ. The emergence of $(n-1)$ in the denominator instead of n reflects the fact that

the values ξ_i are no longer independent, since they were used to calculate the sample mean, which in its turn was used in equation (107).

Let's now consider a different problem. Let ξ be the sum of N independent random variables $\xi_1, \xi_2, \ldots, \xi_N$ where ξ_i have the same probability distributions, $\chi = \xi_1 + \xi_2 + \cdots + \xi_N$. This sum is in itself a random variable, whose mean and dispersion can be easily calculated using equation (100) and properties (22) and (26):

$$M\chi = Nm, \qquad D\chi = N\sigma^2.$$

Now let ζ_N be a normally distributed random variable with the same mean Nm and the same dispersion $N\sigma^2$ as χ. It can be shown that for any interval (a, b) the following approximate equation is valid:

$$P\{a < \chi < b\} \approx \int_a^b \rho_\zeta(x)\, dx, \tag{108}$$

where ρ_ζ is the probability density of the variable ζ_N. This means that the sum of a large number of similar random variables is distributed as a normal (Gaussian) random variable. This statement is known as the *central limit theorem*, and was originally formulated by Laplace. Subsequently Chebyshev, Markov and Lyapunov showed that it is also true in a more general case: it is not necessary for the members of the sum χ to be independent and to belong to the same distribution, it's only required that individual terms do not play a significant role in the sum. The theorem explains why the Gaussian distribution are so often observed in nature: when a large number of minor factors are affecting a random variable, the resulting distribution tends to be a Gaussian.

Now consider a normally distributed general set, and let's try to estimate its expectation value and determine its confidence interval. Let's select a random sampling $\xi_1, \xi_2, \ldots, \xi_n$ which, of course, is also distributed normally, and our aim is to determine $M(\xi_i) = m$. We will consider separately two cases, when the dispersion of the general set is a) known and b) unknown.

a) The dispersion $D(\xi_i) = \sigma^2$ of the general set is known.

Consider the variable $z = \frac{\overline{\xi} - m}{\sigma/\sqrt{n}}$. Since ξ is distributed normally, so is z, except for z the following is true: $M(z) = 0, D(z) = 1$. Hence the probability distribution for z is $\rho_\xi(z) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right)$. Now, using equation (32) we can calculate the probability

$$P\left\{\left|\frac{\overline{\xi} - m}{\sigma/\sqrt{n}}\right| < \delta\right\} = \frac{1}{\sqrt{2\pi}} \int_{-\delta}^{\delta} e^{-z^2/2} dz = 2\Phi(\delta) = \gamma, \tag{109}$$

where Φ is Laplace's function, and using its tables for any δ one can estimate the value of γ, or vice-versa, for any given γ one can calculate the matching value of δ (which would correspond to the one-sided probability $\gamma/2$).

The inequality $\left|\frac{\overline{\xi}-m}{\sigma/\sqrt{n}}\right| < \delta$ can be rewritten as

$$\overline{\xi} - \frac{\sigma\delta}{\sqrt{n}} < m < \overline{\xi} + \frac{\sigma\delta}{\sqrt{n}}. \tag{110}$$

Hence the interval $\left(\overline{\xi} - \frac{\sigma\delta}{\sqrt{n}}, \overline{\xi} + \frac{\sigma\delta}{\sqrt{n}}\right)$ is the confidence interval for the expectation value of m, corresponding to the *confidence probability* γ calculated with equation (110). γ is usually quoted in % and is also sometimes called *confidence level* (C.L.).

Since the sample mean $\overline{\xi}$ is a random variable, the position of the confidence interval on the ξ axis will vary from one experiment to another. The meaning of equation (110) is the following: if a variety of random samplings are used, and $\overline{\xi}$ and $\sigma\delta/\sqrt{n}$ are calculated for each of these, then in γ% of cases the confidence interval will include the value of the true mean m (which, of course, is unknown).

b) The dispersion of the general set is unknown.

Once again, the task is to obtain an estimate of the confidence interval for the expectation value m of a normally distributed random variable, except this time the dispersion (and hence σ) is unknown. Consider again the variable $z = \frac{\overline{\xi}-m}{\sigma/\sqrt{n}}$, which is also normally distributed. The quantity

$$V^2 = \sum_{i=1}^{n} \left(\frac{\xi_i - \overline{\xi}}{\sigma}\right)^2 = \frac{n \cdot s^2}{\sigma^2},$$

where s^2 is the sample dispersion, has the χ^2 distribution with $n-1$ degrees of freedom (see equation (75)). Consequently, the variable

$$t = \frac{z\sqrt{n-1}}{V} = \frac{\overline{\xi} - m}{s/\sqrt{n-1}}$$

is distributed according to Student's distribution (see equation (76)), which only depends on the number of degrees of freedom. Hence, for any given value of γ, one can use the tables of Student's distribution to find a value t_γ such, that

$$P\{|t| < t_\gamma\} = P\{-t_\gamma < t < t_\gamma\} = \gamma.$$

. Remembering that $t = \frac{\overline{\xi}-m}{s/\sqrt{n-1}}$, one has

$$P\left\{\overline{\xi} - t_\gamma \frac{s}{\sqrt{n-1}} < m < \overline{\xi} + t_\gamma \frac{s}{\sqrt{n-1}}\right\} = \gamma. \tag{111}$$

If we use the unbiased estimator for the dispersion of the sample mean, $\overline{s^2} = \frac{n}{n-1}s^2$, then we obtain the following expression for the confidence interval for the expectation value m at the $\gamma - \%$ confidence level:

$$\left(\overline{\xi} - t_\gamma \frac{\overline{s}}{\sqrt{n}}, \overline{\xi} + t_\gamma \frac{\overline{s}}{\sqrt{n}}\right) \tag{112}$$

where t_γ is the number obtained from the tables of Student's distribution, defined by

$$\gamma = \int_{-t_\gamma}^{t_\gamma} \rho(t)\, dt. \tag{113}$$

As a practical example, consider the following *problem*: the working life of diodes manufactured in a particular factory is described by the normal distribution. On a sample of 16 diodes it was found that mean life $\overline{\xi}$ is equal to 3000 hours, with sample standard deviation $\sqrt{\overline{s^2}} = 20$ hours. Based on these numbers, let's estimate the 90% C.L. for the mean life of the diodes.

Solution: here the sample volume $n = 16$, the number of degrees of freedom for the Student's distribution is $k = n-1 = 15$, and $\gamma = 0.9$. Based on equation (113) we find from the table of the Student's distribution that $t_\gamma = 1.753$. Hence, using equation (112), we get

$$(3000 - 1.753\frac{20}{\sqrt{16}}, 3000 + 1.753\frac{20}{\sqrt{16}}) = (2991.235, 3008.765).$$

For a 95% C.L. interval we would get a wider range, $2989.35, 3010.65$. If a larger sample of diodes had been used (24 instead of the original 16), then for the 90% C.L. one would get a narrower interval, $2993.015, 3006.985$.

Finally, let us state another important equation, which allows to estimate the probability that a random variable ξ deviates from its expectation value $m = M\xi$ by more than a given value $\varepsilon > 0$, provided the dispersion of ξ is finite. This probability is obtained from *Chebyshev's inequality*:

$$P\{|\xi - m| \geq \varepsilon\} \leq \frac{D\xi}{\varepsilon^2} \tag{114}$$

we can see that this probability is smaller if the dispersion is small. Inequality (114) is very important for the probability theory. In particular, it can be used to prove Chebyshev's theorem.

6 Monte Carlo method

6.1 The general overview

The Monte Carlo method is a universal numerical method that can be used to calculate any quantity which cannot be calculated analytically. Although the

theoretical foundations of the method were established long time ago, it started to be widely used only after the proliferation of electronic computers. The method was pioneered by American scientists John von Neumann and Stan Ulam, who started using computers to solve probability-related problems in the process of designing nuclear reactors.

One of the main tasks of the Monte Carlo method is to estimate various parameters of a system by presenting the system as some kind of a random probabilistic model and determine those parameters from series of experiments on the model. Often the parameter in question is an expectation value of some variable and its dispersion. This process is sometimes called *statistical modelling*, with Kolmogorov's law of large numbers (equation (103)) at its foundation.

Suppose we need to calculate a scalar number m. Based on the law of large numbers and the central limit theorem, the value of m can be estimated by finding a random variable ξ whose expectation value $M\xi = m$, and the dispersion $D\xi = b^2$ is finite (in case of infinite dispersion a variable transformation is used, such that the dispersion becomes finite without changing the mean). Consider N independent random variables $\xi_1, \xi_2, \ldots, \xi_N$ which have the same distribution as ξ. If N is large enough then, according to the central limit theorem, the distribution of the sum $\zeta = \xi_1 + \xi_2 + \cdots + \xi_N$ will be approximately described by a Gaussian with the mean $a = Nm$ and width $\sigma = b\sqrt{N}$, where $\sigma = \sqrt{D}$.

Remember now the property of the Gaussian distribution (equation (73)) that it is almost totally concentrated within the interval $(a - 3\sigma, a + 3\sigma)$:

$$P\{Nm - 3b\sqrt{N} < \zeta < Nm + 3b\sqrt{N}\} \approx 0.997,$$

hence

$$P\left\{\frac{m - 3b}{\sqrt{N}} < \frac{\zeta}{N} < \frac{m + 3b}{\sqrt{N}}\right\} \approx 0.997.$$

The last inequality can be rewritten like this:

$$P\left\{\left|\frac{1}{N}\sum_{i=1}^{N}\xi_i - m\right| < \frac{3b}{\sqrt{N}}\right\} \approx 0.997. \tag{115}$$

Equation (115) is one of the most important for the Monte Carlo method, since it provides the method of calculating m (as the average of values ξ_i) as well as its uncertainty (as $\sigma = b/\sqrt{N}$). Note here, that in order to calculate σ one can use the formula for sample dispersion, equation (107).

In practice, instead of the upper limit of the uncertainty $3b/\sqrt{N}$ given by equation (115), one often uses the 'probable error' calculated as $0.6745 \cdot b/\sqrt{N}$. These formulae also illustrate the weakness of the Monte Carlo method: slow convergence. If you want to improve your estimate of m by reducing its uncertainty by a factor of 10, you need to increase the statistics N by a factor of $10^2 = 100$.

We said that equation (115) allows the estimation of the quantity m, however it does not specify how to choose the distribution of the random variable ξ, as there are many random variables of various distributions which have the same mean m. Practical guidance on the best choice of the distribution ξ is given in manuals on Monte Carlo method. Our general advice here would be to choose a variable with smallest dispersion D, as the uncertainty in m is proportional to $\sqrt{D}$.

Consider a simple example, which would help understand the essence of the Monte Carlo method. Let's try to calculate the area of a flat shape with of an arbitrary shape. One such shape, which fits within the square of unit area, is shown in Figure 16. Let's put N random points into the unit square. These

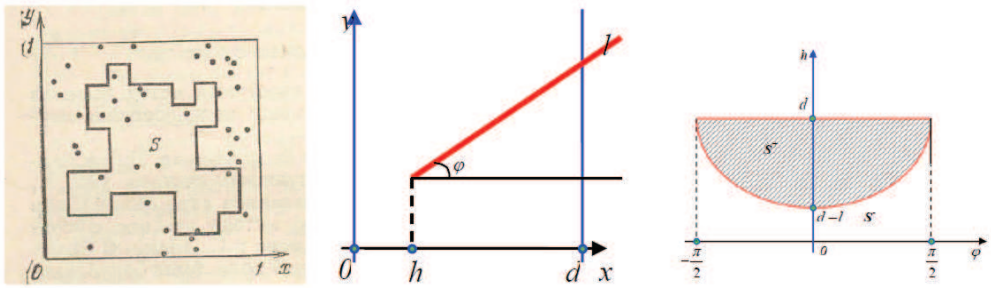


Figure 16: Left: calculating the area of a figure using the Monte Carlo method. Middle: the positioning of two parallel lines and a needle in Buffon's problem. Right: occurrence A – the condition that the line is crossed – in Buffon's problem.

could be generated by an amateur shooter from far away, if the picture is used as a target. Let the number of points that hit the square inside the shape is n. Then n/N is the area of the shape (relative to the unit area of the square itself). The higher is the number N, the more precise is our estimate, but it is crucially important that the distribution of points is uniformly random over the square. The amateur shooter from far away may not be the best solution here, it's probably better to use a computer to generate uniformly distributed random numbers. Each point will require 2 such numbers as its x and y coordinates. In Figure 16 (left) there are $N = 40$ points, out of which $n = 12$ fell inside the shape. Hence our estimate of the area of the shape is $s = 12/40 = 0.3$, with the true area being 0.35. By taking a significantly larger number of tries N, one can greatly improve the precision of the calculation, down to the level of 0.1% or even better.

In 1977 a French scientist Buffon used statistically independent tries to calculate the number π with great precision. The analysis of this problem will help understand the essence of the Monte Carlo approach even better.

Draw two parallel lines on a plane: $x = 0$ and $x = d$. Suppose that a needle of length $l \leq d$ is thrown randomly onto the plane. What is the probability that the needle will cross at least one of the lines?

After each throw, the position of the needle on the plane can be characterised by two numbers: the x-coordinate of one of its ends h and the angle ϕ relative to x axis. Clearly, h and ϕ are random variables, uniformly distributed in their respective intervals, $x \in [0, d]$ and $\phi \in [-frac\pi 2, \frac{\pi}{2}]$. Consider occurrence A – the needle crosses one of the lines:

$$A = \{(x, \phi) : h + l \cdot \cos(\phi) > d\}$$

The geometric interpretation of this occurrence is shown in Figure 16 (right), where the shaded area covers the parameter space where the condition is satisfied and hence the occurrence A takes place. Let's denote the shaded area by S^+. Clearly, the whole rectangle has the area $S = \pi d$. The difference between these two is has the area S^- which can be calculated through the double integral

$$S^- = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\phi \int_0^{d - l\cos\phi} dh = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} (d - l\cos\phi)\, d\phi = \pi d - 2l.$$

Hence, the probability in question is

$$P(A) = \frac{S^+}{S} = \frac{S^+}{S^+ + S^-} = 1 - \frac{S^-}{S^+ + S^-} = 1 - \frac{S^-}{S} = 1 - \frac{\pi d - 2l}{\pi d} = \frac{2l}{\pi d}$$

Suppose the needle was dropped on the plane N times, and every time it was recorded whether the occurrence A took place or not. Clearly, these attempts are mutually independent. Consider the random variable

$$\xi_i = \left\{ \begin{array}{cc} 1 & 0 \\ A & \overline{A} \end{array} \right\}$$

and calculate $S_N = \sum_{i=1}^N \xi_i$. Then the random variable $\{\frac{S_N}{N} \in \{\frac{0}{N}, \frac{1}{N}, \ldots, \frac{N}{N}\}$ has the binomial distribution with the following properties:

$$\begin{aligned} P\{\xi_i = 1\} &= p = \frac{2l}{\pi d} \\ P\{\xi_i = 0\} &= q = 1 - p = \frac{\pi d - 2l}{\pi d} \\ P\{\tfrac{S_N}{N} = \tfrac{m}{N}\} &= C_N^m p^m q^{N-m} \end{aligned}$$

The quantity $\frac{S_N}{N}$ can be considered as an estimate of the probability p of the occurrence A. It can be used to obtain an estimate of the value of π through the following calculation:

$$\hat{\pi} = \frac{2l}{S_N d} N$$

Let's find out how good this estimate is. The expectation value

$$M\left(\frac{S_N}{N}\right) = M\left(\frac{\sum_{i=1}^N \xi_i}{N}\right) = \frac{1}{N} M\left(\sum_{i=1}^N \xi_i\right) = \frac{1}{N}\sum_{i=1}^N M\left(\xi_i\right)$$
$$= \frac{1}{N}\sum_{i=1}^N (1\cdot p - 0\cdot 1) = p$$

is a consistent and unbiased estimate of the probability p. As for the dispersion, we have

$$D\left(\frac{S_N}{N}\right) = \frac{p\cdot q}{N} = \frac{\left(\frac{2l}{\pi d}\right)\left(1-\frac{2l}{\pi d}\right)}{N}.$$

The minimum of this expression, under the constraint $l \leq d$, is achieved at $l = d$. In this case, $M\left(\frac{S_N}{N}\right) = \frac{2}{\pi}$, hence $\hat{\pi} = \frac{2N}{S_N}$, with the dispersion $D\left(\frac{S_N}{N}\right) = \frac{2}{\pi N}\left(1-\frac{2}{\pi}\right)$.

6.2 Pseudorandom numbers and random number generators

How can we obtain random numbers? One of the simplest 'generators' of random numbers can be built like this: take a cubic dice with numbers 0,1,2,3,4 embedded on the sides (with the sixth side left blank), and a coin with numbers 0 and 5 embedded on its two faces. Throw the dice and the coin simultaneously, and write down the sum of the resulting numbers. The result will be a random number from 0 to 9, which could be used to create tables of multi-digit random numbers (with 0 allowed to take any position).

Assume we have used this method to create a list of 300 4-digit random numbers, and let's find out how random the resulting numbers are:

1. What is the frequency of each digit (0 to 9) in the list? Clearly, it should be close to 0.1, which is the probability of getting one of 10 digits in each try.

2. What is the frequency of getting each digit in the first, second, third and fourth place? These frequencies should also be close to 0.1, but the deviation can be larger than for the first case, because the statistics of 300 is smaller than the 1200 entries above.

One can use an electronic device, such as a diode or a triode, as a random number generator, because their output is not exactly constant even in a stationary situation. Thermal (and other random) processes are causing the output voltage to fluctuate around the nominal value. Count the number of times n

when the output was higher than the nominal, and if n is odd, assume the random number to be 1, while for n even assume it to be 0. This will give a single random binary digit. If the mean is not close to 0.5, then one can use the following way to stabilise the output: group the random digits into pairs, and assume the output to be 1 for 01 and 0 for 10, while 00 and 11 are simply ignored. This way, the mean should be closer to 0.5. The weakness of this method is that the output is hard to control, because the physical device can change its pattern and the randomness of the output is diminished.

In practice, so called *pseudorandom* (rather than truly random) numbers are used, which are obtained by some kind of recurrence relationship that imitates a random process. The first such algorithm, sometimes called the *middle-square method*, was suggested by von Neumann. It works like this: choose a 4-digit number n_0, say $n_0 = 9876$. Calculate its square $n_0^2 = 97535376$ and select 4 middle digits $n_1 = 5353$. Then do the same with n_1 to obtain n_2: $n_1^2 = 42850116$, $n_2 = 8501$ and so on. To get random numbers in the interval $(0, 1)$, divide the result by 10000 to obtain the sequence $0.9876, 0.5353, 0.8501, \ldots$. Unfortunately, the method did not work very well, giving far too many small numbers.

Better results were obtained using residuals. Let's assume our computer has a 32-bit processor. In order to obtain a sequence of random numbers within the interval $(0, 1)$, one can use the following recurrence relation:

$$m_0 = 1, \quad g = 5^{13}, \quad m_{k+1} = g \cdot m_k (\mathrm{mod} 2^{31}). \tag{116}$$

I.e the next member of the sequence, m_{k+1}, is obtained from the previous one, m_k: divide the product $g \cdot m_k$ by 2^{31} and take the residual to be m_{k+1}. The sequence of 31-bit-long numbers m_k, can be transformed into the set of pseudorandom numbers in the interval $[0.1]$ by the operation $\gamma_k = 2^{-31} \cdot m_k$. The first 100 numbers in this sequence do not look uniformly distributed, but after $k \sim 500$ this algorithm gives satisfactory results.

When using pseudorandom numbers, one should remember that sooner or later the sequence produce a number which was produced before. Then the sequence will start repeating itself, and hence is not random any more. Thus, any pseudorandom number generator has a period, which is equal to the maximum length of the sequence of random numbers it can produce. The period L of our last algorithm (equation (116)) is $L = 2^{29}$.

The period can be made longer if the number of bits is increased. For example, with a 42-bit 'word', the algorithm (116) can be improved like this:

$$m_0 = 1, \quad g = 5^{17}, \quad m_{k+1} = g \cdot m_k (\mathrm{mod} 2^{40}), \tag{117}$$

followed by $\gamma_k = 2^{-40} \cdot m_k$. The period of this sequence is $L = 2^{38}$. This algorithm was developed by Lehmer. Since then, algorithms with much longer periods have been developed. The longest so far belongs to the *Mersenne twister* algorithm, with $L = 2^{19937} - 1$.

6.3 Calculating definite integrals using Monte Carlo method

Let's use Monte Carlo method to estimate the integral

$$I = \int_a^b g(x)\,dx. \tag{118}$$

Choose a random variable ξ defined in the interval (a, b), with any probability density $\rho(x) = \rho_\xi(x)$ which satisfies the usual conditions

$$\rho(x) > 0 \tag{119}$$

$$\int_a^b \rho(x)\,dx = 1. \tag{120}$$

In addition to the variable ξ we will need another random variable with the distribution $\eta = g(\xi)/\rho(\xi)$. Using equation (47), we can write:

$$M\eta = \int_a^b \eta(x)\rho(x)\,dx = \int_a^b \frac{g(x)}{\rho(x)}\rho(x)\,dx = \int_a^b g(x)\,dx = I.$$

Now consider N identical independent random variables $\eta_1, \eta_2, \ldots, \eta_N$ and apply the central limit theorem to their sum. Then equation (115) takes the form:

$$P\left\{\left|\frac{1}{N}\sum_{i=1}^{N}\eta_i - I\right| < 3\sqrt{\frac{D\eta}{N}}\right\} \approx 0.997. \tag{121}$$

This equation means that if we choose N random variables $\xi_1, \xi_2, \ldots, \xi_N$, then for large N an approximate value of the integral I is given by

$$I \approx \frac{1}{N}\sum_{i=1}^{N}\frac{g(\xi_i)}{\rho(\xi_i)} \tag{122}$$

According to equation (121), the uncertainty of the result given by this equation almost never exceeds $3\sqrt{(D\eta/N)}$. Let's calculate the dispersion $D\eta$:

$$D\eta = M\eta^2 - I^2 = \int_a^b \frac{g^2(x)}{\rho(x)}\,dx - I^2. \tag{123}$$

Next we will show that the dispersion is minimal if $\rho(x)$ is proportional to $g(x)$. The following inequality is known from calculus:

$$\left(\int_a^b |u(x)v(x)|\,dx\right)^2 \le \int_a^b u^2(x)\,dx \int_a^b v^2(x)\,dx. \tag{124}$$

Denoting $u(x) \equiv g(x)/\sqrt{\rho(x)}$ and $v(x) \equiv \sqrt{\rho(x)}$, we can write using equation (120):

$$\left(\int_a^b |u(x)v(x)|\, dx\right)^2 \left(\int_a^b |g(x)|\, dx\right)^2 \leq$$
$$\int_a^b \frac{g^2(x)}{\rho(x)}\, dx \int_a^b \rho(x)\, dx = \int_a^b \frac{g^2(x)}{\rho(x)}\, dx. \tag{125}$$

So combining equations (123) and (125) we now have

$$D\eta \geq \left(\int_a^b |g(x)|\, dx\right)^2 - I^2. \tag{126}$$

Let's show that the dispersion is minimised for $\rho(x) = c|g(x)|$. Firstly, from the normalisation condition (34) we have:

$$c = \left(\int_a^b |g(x)|\, dx\right)^{-1}$$

Then, the integral in the r.h.s. of equation (123) becomes

$$\int_a^b \frac{g^2(x)}{\rho(x)}\, dx = \frac{1}{c}\int_a^b |g(x)|\, dx = \left(\int_a^b |g(x)|\, dx\right)^2.$$

I.e. when $\rho(x)$ is proportional to $g(x)$, the r.h.s. of equation (123) is equal to the r.h.s. of equation (126), which minimises the dispersion (123).

In practice it is not recommended to choose a very complicated distribution $\rho(x)$, because it will take a long time to generate the values of ξ. In general, Monte Carlo methods are not very efficient for single integrals: conventional numerical integration methods are far more efficient. However, the Monte Carlo method is more efficient than any other known method, and sometimes is the only method, when dealing with multiple integrals.

We will now present a practical example of calculating the integral

$$I = \int_0^{\pi/2} \sin x\, dx = 1$$

using Monte Carlo method, for two different distribution functions (see Figure 17).

First, we will use a constant distribution function $\rho(x) = 2/\pi$. In this case, using equation (85), we have $\xi = 0 + (\frac{\pi}{2} - 0) \cdot \gamma = \frac{\pi}{2}\gamma$ and hence

$$I \approx \frac{\pi}{2N} \sum_{j=1}^{N} \sin \xi_j,$$

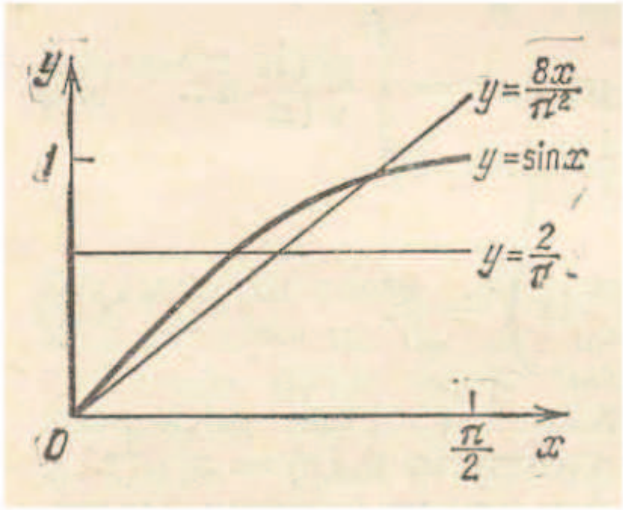


Figure 17: Illustration to the procedure of integration using Monte Carlo method.

where γ is the random variable uniformly distributed in the interval $[0, 1]$. $N = 10$ values of γ have been sampled and used to calculate ξ_j and corresponding $\sin \xi_j$. The numbers are presented in Figure 18 (top table). The resulting value of the integral is $I \approx 0.952$.

In the second case, we choose $\rho(x) = \frac{8x}{\pi^2}$. Then, from equation (83)

$$\int_0^{\xi} \frac{8x}{\pi^2}\, dx = \gamma \qquad \Rightarrow \qquad \xi = \frac{\pi}{2}\sqrt{\gamma}.$$

So, from the equation (122) we now have

$$I \approx \frac{\pi^2}{8N} \sum_{j=1}^{N} \frac{\sin \xi_j}{\xi_j}.$$

The results are shown in Figure 18 (bottom table). The value of the integral in this case is $I \approx 1.016$, which is noticeably closer to the true value, than the first estimate.

From the tables shown in Figure 18 one can estimate the respective dispersions:

$$D\xi \approx \frac{\pi^2}{9 \cdot 4} \left[\sum_{j=1}^{10} (\sin \xi_j)^2 - \frac{1}{10} \left(\sum_{j=1}^{10} \sin \xi_j \right)^2 \right] = 0.256,$$

$$D\xi \approx \frac{\pi^4}{9 \cdot 64} \left[\sum_{j=1}^{10} \left(\frac{\sin \xi_j}{\xi_j} \right)^2 - \frac{1}{10} \left(\sum_{j=1}^{10} \frac{\sin \xi_j}{\xi_j} \right)^2 \right] = 0.016.$$

l	1	2	3	4	5	6	7	8	9	10
γ_l	0,865	0,159	0,079	0,566	0,155	0,664	0,345	0,655	0,812	0,332
ξ_l	1,359	0,250	0,124	0,889	0,243	1,043	0,542	1,029	1,275	0,521
$\sin \xi_l$	0,978	0,247	0,124	0,776	0,241	0,864	0,516	0,857	0,957	0,498

l	1	2	3	4	5	6	7	8	9	10
γ_l	0,865	0,159	0,079	0,566	0,155	0,664	0,345	0,655	0,812	0,332
ξ_l	1,461	0,626	0,442	1,182	0,618	1,280	0,923	1,271	1,415	0,905
$\frac{\sin \xi_l}{\xi_l}$	0,680	0,936	0,968	0,783	0,937	0,748	0,863	0,751	0,698	0,868

Figure 18: Results of the Monte Carlo integration with 10 points using two different distribution functions.

(the true values of the dispersions are 0.233 and 0.0166, respectively). So, even with a very modest number of points, $N = 10$, both methods of integration gave reasonably acceptable results. However, the second method is clearly preferable, giving a much smaller dispersion. As seen from Figure 17, the probability density chosen for the second method is much closer to the integrand, and hence is closer to satisfying the condition $\rho(x) = c|g(x)|$ and minimising the dispersion, as expected.

7 Modelling the propagation of neutrons through matter

Suppose a beam of monoenergetic neutrons with initial energy E_0 is normally incident onto an infinite and uniform plate of thickness h. Suppose also that only two processes are allowed when the neutrons interact with the atoms in the plate: the absorption of neutrons by the atom and the elastic scattering of neutrons, which is assumed to be isotropic. The latter assumption is often valid if the plate is formed by atoms with heavy nuclei. Yet another simplifying assumption is that the nuclei in the plate do not disintegrate as the result of the collision with

the neutrons. Out task is to obtain the probabilities of reflection, absorption and penetration in the framework of this simplified model.

Let the cross section of neutron absorption (capture) by the nuclei be σ_c and the cross section of the elastic scattering be σ_s. the total cross section will thus be $\sigma = \sigma_c + \sigma_s$. The physical meaning of the cross section is related to the probability of the process taking place, so σ_c/σ and σ_s/σ are capture and scattering probabilities in the event of the neutron interaction with a nucleus in the plate. The distance λ travelled by the neutron between two collisions is a random variable which is often called the *free path length*. This variable can take any arbitrary positive value with the distribution

$$\rho(x) = \sigma e^{-\sigma x} \tag{127}$$

where $x \in [0, h]$. For the mean free path length we then get

$$M\lambda = \int_0^\infty x\rho(x)\,dx = \int_0^\infty x\sigma e^{-\sigma x}\,dx = \frac{1}{\sigma}, \tag{128}$$

which clarifies the physical meaning of the parameter λ: it is inversely proportional to the total cross section. The bigger is the cross section, the shorter is the mean free path of the neutron in matter. In general, the cross section (and hence λ) depends on the initial energy of the neutron E_0.

For modelling neutron propagation it is enough to sample the free path length λ and the direction of the neutron after scattering. To generate λ with the correct distribution, use equation (83):

$$\int_0^\lambda \sigma e^{-\sigma x}\,dx = r, \qquad \Rightarrow \qquad \lambda = -\frac{1}{\sigma}\ln(1-r),$$

where r is a uniformly distributed random variable in the interval $[0, 1]$. Of course, $(1 - r)$ has the same distribution as r, so finally for λ we get:

$$\lambda = -\frac{1}{\sigma}\ln r, \tag{129}$$

The scattering process is assumed to be isotropic. Direct the x axis along the incident neutrons and let $\theta \in (0, \pi)$ be the angle between the velocity of the neutron after scattering and the x axis. The isotropy of the scattering process means that the quantity $\mu = \cos\theta$ is distributed uniformly in the interval $(-1, 1)$, so μ can be generated simply as $2r - 1$ which has the right distribution.

Let's now develop the algorithm of the simulation. The starting point is $x = 0, \mu = 1$, i.e. the neutrons are hitting the plate normally. Assume that the k-th act of scattering inside the plate happens at depth x_k, after which the neutron moves in the direction μ_k. Generate the free path length $\lambda_k = -(1/\sigma)\ln r$ and find the depth of the next point of scattering:

$$x_{k+1} = x_k + \lambda_k \cdot \mu_k. \tag{130}$$

If the resulting value $x_{k+1} > h$ then the neutron has penetrated the plate and the number of neutrons that went through the plate has to be increased by 1. If $x_{k+1} < h$ then the neutron was reflected back from the plate, and hence the number of reflected neutrons has to be increased by 1. In both of these cases this would be the end of the simulation process for this neutron. For the remaining values of x, i.e. $0 < x_{k+1} < h$ the neutron remains inside the plate, and another step of the simulation needs to be performed. In particular, the neutron capture hypothesis needs to be checked: generate r and if $r < \sigma_c/\sigma$ then the simulation for this neutron is over, the neutron is captured, and hence the number of captured neutrons has to be increased by 1. In the opposite case, the neutron is scattered, and another step has to be performed: new values of λ and μ are generated, and the cycle is repeated.

Figure 19 illustrates possible fates of the neutron, such as penetration of the

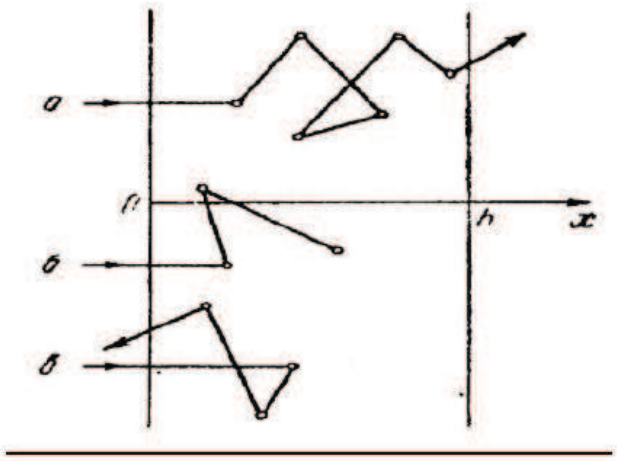


Figure 19: Three types of trajectories of a neutron hitting a solid plate.

plate (a), capture within the plate (b) and reflection from the plane (c). Suppose the total number of neutrons is N, out of which N^+ neutrons have one through, N^- were captured and N^0 were reflected. Then we get for respective probabilities:

$$p_1 = \frac{N^+}{N}, \quad p_1 = \frac{N^-}{N}, \quad p_1 = \frac{N^0}{N}, \tag{131}$$

and the problem is solved. A diagram illustrating the algorithm is shown in Figure 20, where the index j labels the trajectory of the neutron, while the index k goes over the collisions along a particular trajectory.

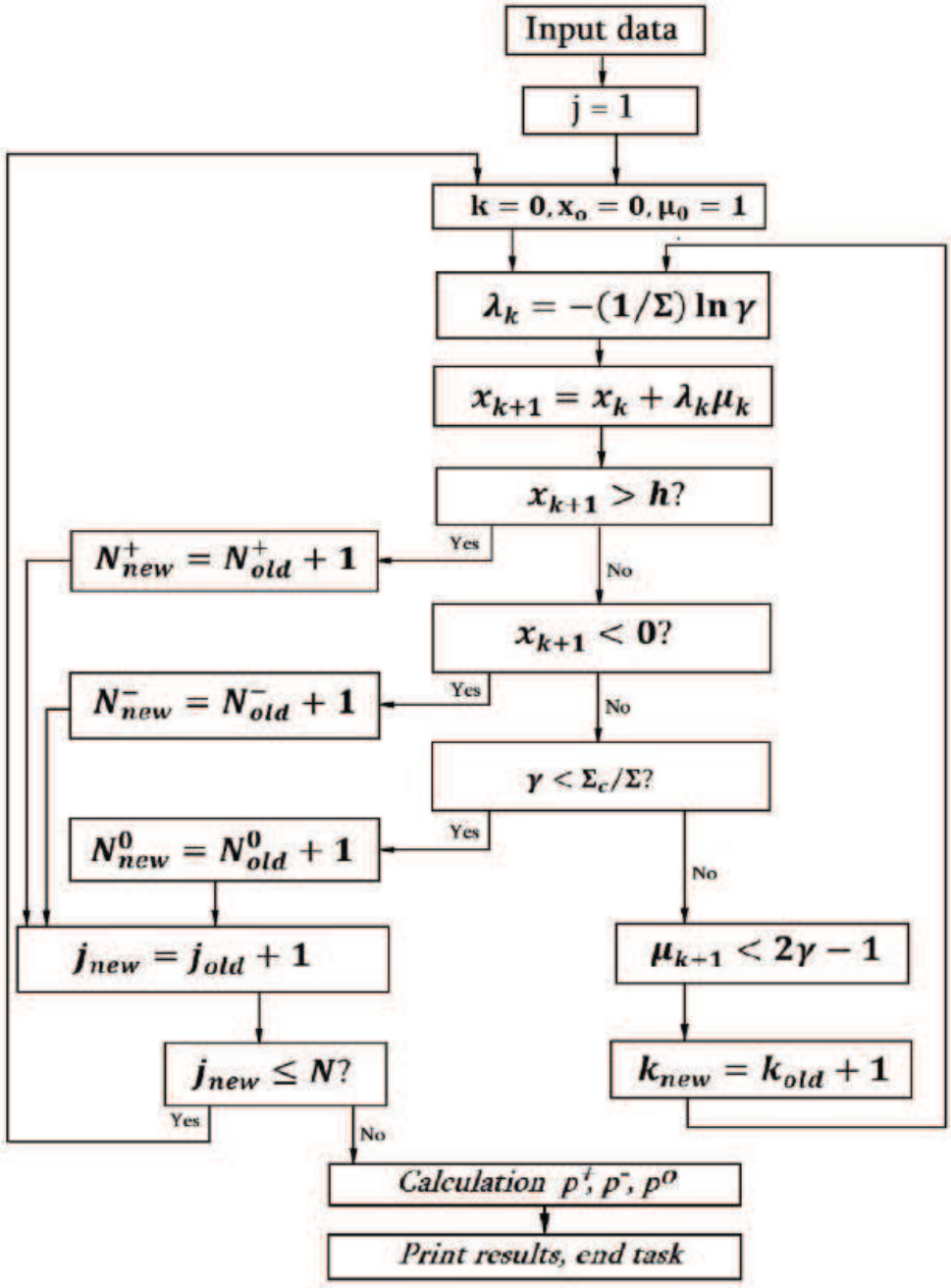


Figure 20: The diagram illustrating the algorithm of neutron simulation. The cross sections are denoted by Σ, while γ is the random variable distributed uniformly in $[0, 1]$.

8 Modelling methods of analysing experimental distributions

Physical processes taking place in Nature obey certain regularities, and the purpose of experimental studies is to discover or confirm these regularities. Limiting (asymptotic) distributions – distributions obtained in the limit of infinite number of measurements – are expected to be described by certain functions. However, the limiting distributions are our of practical reach, so the question is, how can we determine whether the results of a particular experiment obey the *expected* limiting distribution?

Here we only consider the case when the distribution law governing a particular experiment is known, however some of the parameters need to be determined. For example, we know that a radioactive decay obeys the exponential law, but we need to measure the mean life of this particular isotope, which in fact determines the nature of the decay.

Two methods of parameter estimation are described here: the method of *maximum likelihood*, and the method of *least squares*.

Before we start explaining these methods, let us familiarise ourselves with the way of presenting experimental data which is called a *histogram*. Suppose we have measured a quantity A which varies within the interval (a, b). Let's divide the interval into N subintervals (which, by the way, do not have to be equal), and calculate the frequencies of the quantity A falling within each subinterval (these subintervals are usually called *bins*). Let's plot the subinterval boundaries along the x axis, and draw the frequencies in each bin as the rectangles of appropriate height in the y dimension. So the experimental data are presented as a stepwise graph which consists of N rectangles with the bases equal to the bin widths, and heights proportional to the frequencies in the respective bins, like the one shown in Figure 21 (a). Sometimes the rectangles in the y direction are replaced by markers in the shape of a cross, with the horizontal bar (placed at the hight of the rectangle) showing the bin width and the vertical bar indicating the uncertainty of the measurement. If the range of frequencies in the y axis is too large, it is visually more appropriate to use the logarithmic scale on that axis (Figure 21 (c)). An example of a two-dimensional histogram is shown in Figure 21 (d).

Note the fact that the probability of an event ending up in a particular bin does not depend on whether the previous event fell in the same bin or not. The probability of falling in a bin is proportional to the width of that particular bin, and the probability of two events in a row falling into the same bin is a small number of a higher order. From the properties of the Poisson distribution (see subsection 4.2), it is clear that the number of entries in a bin is described by the Poisson distribution. If there are N entries in a bin, then the dispersion in that bin is also equal to N. Hence the statistical uncertainty on the number N is $\sigma = \Delta N = \sqrt{D} = \sqrt{N}$. This is an important property of a histogram.

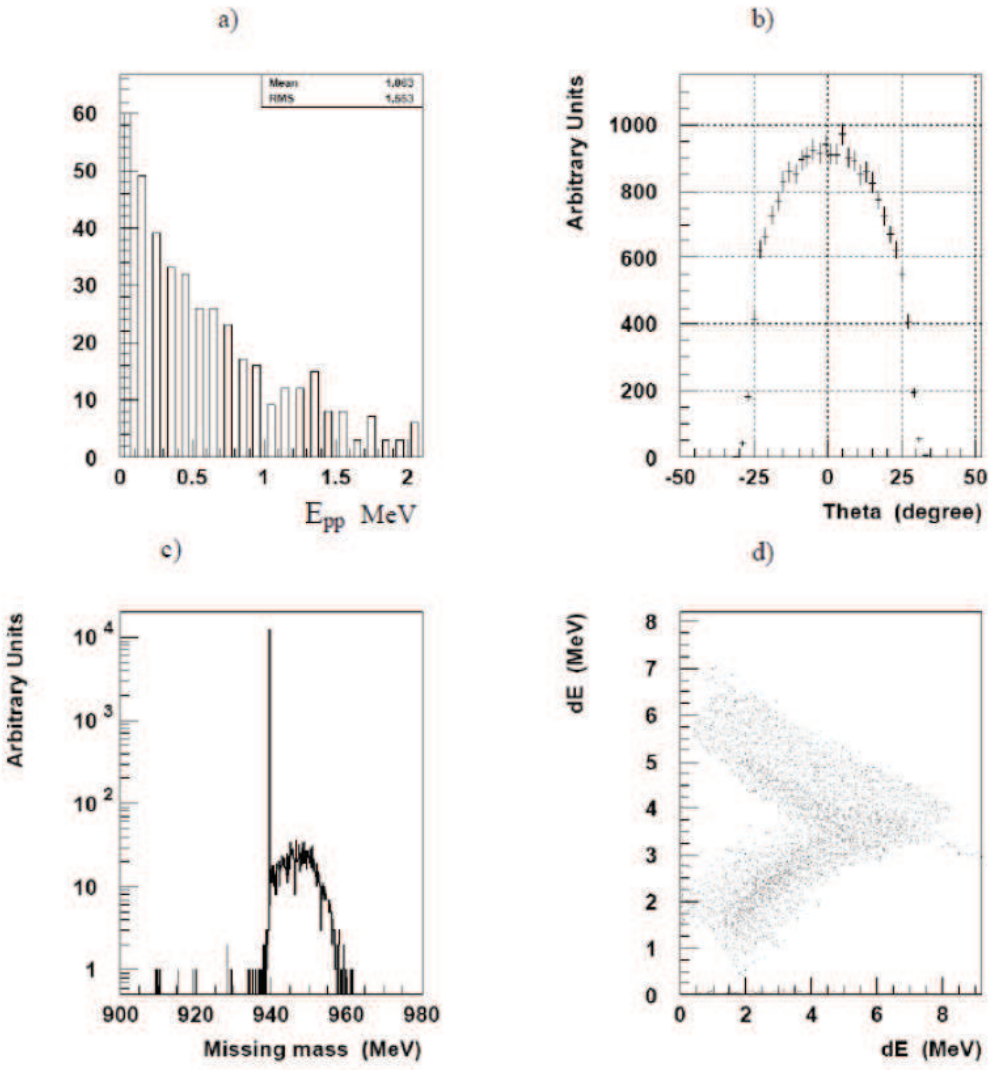


Figure 21: Examples of one-dimensional (a,b.c) and two-dimensional (d) histograms. Histogram (a) also shows the mean and σ of the distribution. Histogram (c) has a logarithmic scale on the y axis. In the two-dimensional histogram (d), a high concentration of dots indicates a larger number of entries in the respective bins. The distributions describe the process of the deuteron dissociation in the reaction $pd \to ppn$ with the proton beam energy of 49 MeV.

8.1 Method of maximum likelihood

Suppose a quantity is measured n times, with results $x_1, x_2, \ldots, x_n$. The distribution of the quantity is known to have the density $\rho(x; a)$ where a is an unknown parameter to be determined from the measurements. Since the measurement is a random process, the link between the value of a and the measurements $x_1, x_2, \ldots, x_n$ can only be established through the probability of observing this particular set of measurements. The latter can be calculated as the product $\rho(x_1, x_2, \ldots, x_n; a)\Delta x_1 \Delta x_2 \ldots \Delta x_n$, where $\rho(x_1, x_2, \ldots, x_n; a)$ is the probability density for n consecutive measurements x_i and Δx_i are the respective bin widths. If the measurements are independent – which is the case when the same quantity x is measured in the same conditions – then one has

$$\rho(x_1, x_2, \ldots, x_n; a) = \rho(x_1; a)\rho(x_2; a) \ldots \rho(x_n; a) \tag{132}$$

The above discussion is also valid in the case where the measured quantity is discrete and the results of the measurements are $v_1, v_2, \ldots, v_n$. In this case $\rho(v_1, v_2, \ldots, v_n; a)$ is the probability of measuring n consecutive values of variable v.

Let's define a functional $L(x_1, x_2, \ldots, x_n; \alpha)$ with the following properties:

1. It coincides with $\rho(x_1, x_2, \ldots, x_n; a)$ when $\alpha = a$, and hence contains the full information about the measurements and their distribution law.

2. For any value of α the unitarity condition is met:

$$\int dx_1 \int dx_2 \ldots \int dx_n \, L(x_1, x_2, \ldots, x_n; a) = 1 \tag{133}$$

   where the integration is performed over all possible x_i.

It can be shown that the best estimate of a is the value of α for which the functional $L(x_1, x_2, \ldots, x_n; \alpha)$ reaches its maximum. The functional L is called the *likelihood*, and hence this method of parameter estimation carries the name of maximum likelihood method.

In order to find the maximum of L we need to differentiate L with respect to α and equate the derivative to zero. Since $\ln L$ has the maxima at the same values of α as L, usually the following equation is solved:

$$\frac{\partial}{\partial \alpha} \ln L = 0. \tag{134}$$

Then, taking into account equation (132), one has:

$$\frac{\partial}{\partial \alpha} \ln \prod_{i=1}^{n} \rho(x_i; \alpha) = 0 \qquad \Rightarrow \qquad \frac{\partial}{\partial \alpha} \sum_{i=1}^{n} \ln \rho(x_i; \alpha) = 0. \tag{135}$$

Equation (135) explains the reason for introducing the logarithm into equation (134), as minimisation of the sum is much easier than minimisation of the product.

If the probability density ρ depends on 2 parameters, then equations (132) and (134) should be modified accordingly:

$$\begin{aligned} L(x_1, x_2, \ldots; \alpha_1, \alpha_2) &= \rho(x_1; \alpha_1, \alpha_2)\rho(x_2; \alpha_1, \alpha_2)\ldots, \\ \frac{\partial}{\partial \alpha_1} \ln L = 0 \qquad &\text{and} \qquad \frac{\partial}{\partial \alpha_2} \ln L = 0. \end{aligned} \tag{136}$$

Generalising the method further for the case of k parameters α_k should not be a problem.

In many cases it is not possible to find an analytic solution to equations (132) and (136). In these circumstances one can try using a different probability density function ρ, or solve the maximisation problem numerically.

To illustrate the use of the maximum likelihood method, consider an experiment that counts the number of particles registered by a detector. Suppose that N particles were detected during a time period t. The average number of particles per unit time, i.e. the average rate of particle detection ν, can then be calculated as

$$\nu = \frac{N}{t}.$$

Suppose now that the whole time interval t was divided into n subintervals $t_1, t_2, \ldots, t_n$ and the numbers of detected particles within each subinterval was $N_1, N_2, \ldots, N_n$, respectively. We know that in the counting experiments of this type, the number of detected particles obeys the Poisson distribution (see equation (68)):

$$\rho(N_i, \alpha) = \frac{(\alpha t_i)^{N_i}}{N_i!} e^{-\alpha t_i}.$$

Our task is to estimate the best value for parameter α. The likelihood function is constructed like this:

$$\begin{aligned} L(\alpha) &= \frac{(\alpha t_1)^{N_1}}{N_1!} e^{-\alpha t_1} \frac{(\alpha t_2)^{N_2}}{N_2!} e^{-\alpha t_2} \cdots \frac{(\alpha t_n)^{N_n}}{N_n!} e^{-\alpha t_n} \\ &= C \cdot \alpha^{\sum N_i} \cdot e^{-\alpha \sum t_i}. \end{aligned} \tag{137}$$

where C is a constant. Then

$$\ln L(\alpha) = \ln(C \cdot \alpha^{\sum N_i} \cdot e^{-\alpha \sum t_i}) = \ln C + \sum N_i \ln \alpha - \alpha \sum t_i.$$

Equating this to zero and solving for α we get

$$\begin{aligned} \frac{\partial}{\partial \alpha} \ln L &= \frac{1}{\alpha} \sum N_i - \sum t_i = 0, \\ \alpha &= \frac{\sum N_i}{\sum t_i} = \frac{N}{t} = \nu, \end{aligned}$$

which coincides with the expected result.

8.2 Method of least squares

Suppose that n measurements of a physical quantity were made with results $E_i \pm \Delta E_i, i = 1, 2, \ldots, n$. A theoretical model predicts that the measurements should be equal to the values T_i. It appears that, in the absence of systematic uncertainties, results of multiple measurements of each E_i are distributed normally with the expectation value T_i (if the theory is correct) and the standard deviation ΔE_i. In these conditions, the quantity

$$\chi^2(p_1, \ldots, p_k) = \sum_{i=1}^{n} \frac{[E_i - T_i(p_1, \ldots, p_k)]^2}{\Delta E_i^2} \tag{138}$$

is a sum of n normally-distributed random variables, and hence should obey the χ^2 distribution with n degrees of freedom. On the other hand, if the parameters of the theoretical model $p_1, \ldots, p_k$ are seen as free parameters, one can choose their values in such a way that the quantity (138) is minimised. The main purpose of this exercise is the estimation of these parameters, and this method is called the *method of least squares*, developed first by Legendre. The essence of the method is the following: given are the experimental measurements and their uncertainties, and a theoretical model which is supposed to describe the experimental points, but the values of the parameters of the model are unknown. Similarly to the maximum likelihood method, the least square method can be used to estimate the values of these parameters. The functional defined by equation (138) contains all the information about the experimental data as well as the theoretical model, and can be used for this purpose. Obviously, the smaller is the value of the functional (138), the closer is the theory to the experimental data. Naively one may expect that the ideal value for the minimum of χ^2 is zero. However the expectation value of the χ^2 distribution with n degrees of freedom is n, hence the 'best' value for the minimum of χ^2 is 1 per degree of freedom. For the set of n experimental points and k theoretical parameters, the number of degrees of freedom is $n - k$. Figure 22 shows the dependence of the confidence level (CL) on χ^2 for various numbers of degrees of freedom.

The general scheme of the process of minimisation of the functional (138) goes like this: take the derivative of the functional with respect to each parameter, and require it to be equal to zero. This yields k equations (as many as there are parameters) to be solved simultaneously to find the values of the parameters, as well as their uncertainties (see below). If the parameters enter the theoretical model linearly, then the simultaneous system of equations is linear with respect to parameters and can be solved either analytically, or using standard methods for such systems. However, in most cases it is practically advisable to use special computer programs to minimise the functional. A package called 'Minuit' is a good example of such programs.

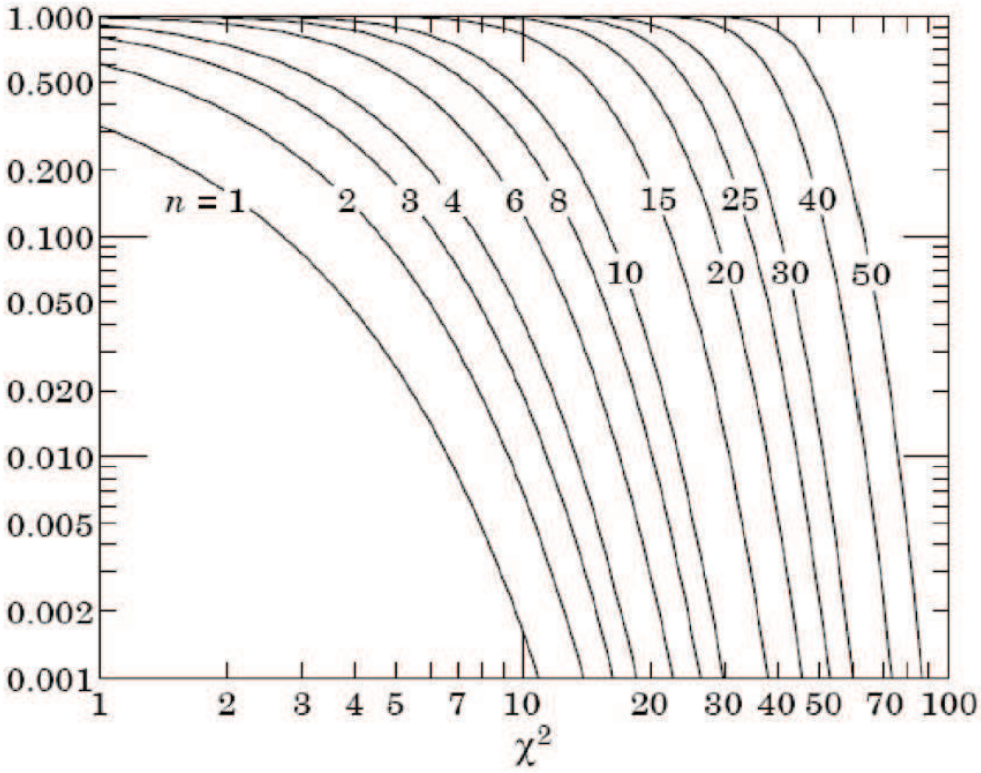


Figure 22: The confidence level (CL) as a function of χ^2 for n degrees of freedom.

Let's see how the method of least squares works on a simple example. Suppose that there is a linear dependence between two variables x and y, and that the uncertainty in x is negligibly small, while the uncertainty in y is independent of y and is constant at σ_y. We would like to present the measurement points (x_i, y_i) on a graph and try to determine the parameters a and b of a linear function $y = a + bx$ such that this function represents the best fit to the experimental data.

We will use the least square method to achieve this. Each measured value y_i is expected to be normally distributed with the mean at the 'true' value (i.e. the theoretical value $T_i = a + bx_i$) and with width σ_y, so that the probability of measuring some value y_i is given by

$$\rho_{a,b}(y_i) \sim \frac{1}{\sigma_y} \exp\left[-\frac{1}{2}\left(\frac{y_i - a - bx_i}{\sigma_y}\right)^2\right]. \tag{139}$$

The probability (139) clearly depends on parameters a and b. Since the measurements y_i are independent, the probability of measuring n values $y_1, y_2, \ldots, y_n$ is

the product of $\rho_{a,b}(y_i)$:

$$\rho_{a,b}(y_1, y_2, \ldots, y_n) \sim \frac{1}{\sigma_y^n} \exp\left(-\frac{\chi^2}{2}\right), \tag{140}$$

where

$$\chi^2 = \sum_{i=1}^{n} \frac{(y_i - a - bx_i)^2}{\sigma_y^2}. \tag{141}$$

Equation (141) is the specific case of equation (138), and hence represents the χ^2 distribution (see subsection 4.5).

We can now proceed to finding the minimum of the functional (141, which would correspond to the maximum of (140. At minimum the derivatives of (141) with respect to parameters a and b should be equal to zero:

$$\begin{aligned} \frac{\partial \chi^2}{\partial a} &= -\frac{2}{\sigma_y^2} \sum_{i=1}^{n} (y_i - a - bx_i) = 0 \\ \frac{\partial \chi^2}{\partial b} &= -\frac{2}{\sigma_y^2} \sum_{i=1}^{n} x_i (y_i - a - bx_i) = 0 \end{aligned} \tag{142}$$

The equations (142) can be rearranged to form the simultaneous system

$$\begin{aligned} a \cdot n + b \sum x_i &= \sum y_i \\ a \sum x_i + b \sum x_i^2 &= \sum x_i y_i \end{aligned} \tag{143}$$

which has the following solution:

$$a = \frac{\left(\sum x_i^2\right)\left(\sum y_i\right) - \left(\sum x_i\right)\left(\sum x_i y_i\right)}{\Delta}, \tag{144}$$

$$b = \frac{n\left(\sum x_i y_i\right) - \left(\sum x_i\right)\left(\sum y_i\right)}{\Delta}, \tag{145}$$

where $\Delta \equiv n\left(\sum x_i^2\right) - \left(\sum x_i\right)^2$. Equations (144) and (145) represent the best values for the parameters of the straight line $y = a + bx$ describing the data points (x_i, y_i).

Once the best values of the parameters are found, the next task is to assess the uncertainties of these values. The problem is that the spread of the experimental data cannot be directly used for this purpose, because the measurements y_i are not independent measurements of the same quantity, but change from point to point depending on x_i (for example, if h_i correspond to the heights of a body in freefall measured at different times t_i and our aim is to check the validity of the formula $h = gt^2/2$, then the distribution of values h_i carries little information on

the uncertainty in height measurement). On the other hand, we know that y_i are expected to be normally distributed around the 'true' value predicted by the theory, $a+bx_i$, with the width equal to σ_y. Hence, the values of y_i-a-bx_i belong to a Gaussian distribution with zero mean and the same width σ_y. Consider the quantity

$$\sigma_y^2 = \frac{1}{n-2}\sum_{i=1}^{n}(y_i - a - bx_i)^2. \tag{146}$$

According to the central limit theorem this expression can be used to find a corrected estimate of σ_y. Based on the maximum likelihood method it can be shown that the quantity (146) gives the best possible estimate of σ_y, which is consistent and unbiased. Indeed, by differentiating equation (140) with respect to σ_y we get

$$\frac{\partial\rho}{\partial\sigma} = \frac{e^{-\chi^2/2}}{\sigma^{n+3}}\left[\sum(y_i - a - bx_i)^2 - n\sigma^2\right] = 0, \tag{147}$$

which leads to equation (146), albeit with the factor $\frac{1}{n}$ instead of $\frac{1}{n-2}$. This difference is due to the fact that the parameters a and b were calculated from the measured values y_i using equations (144) and (145). As a consequence, the measured values of y_i are not independent any more, and the number of degrees of freedom is reduced by the number of parameters, 2. At high n the difference between n and $n-2$ is not that noticeable, but at smaller n the correct factor $1/(n-2)$ should be used for an unbiased estimate of σ_y. In the extreme case $n = 2$ there are just two points and it is always possible to put a straight line through these points without any approximation, hence no judgement can be made about the fit quality. In this case equation (146) gives an indeterminate answer $0/0$, while equation (147) would have given $0/2 = 0$, which is incorrect.

After this deliberation, we are ready to estimate the errors on the parameters a and b. These can be obtained using equations (152) and (153) from the following subsection, where the propagation of uncertainties in indirect measurements is discussed. We get

$$\begin{aligned} \sigma_a^2 &= \sigma_y^2\frac{\sum x_i^2}{\Delta}, \\ \sigma_b^2 &= \sigma_y^2\frac{n}{\Delta}. \end{aligned} \tag{148}$$

Thus, we solved our problem. We have found the values of parameters that produced the best linear approximation to the data points, and we also estimated the uncertainties in those values.

The method can be easily extended to the case when each measurement y_i has a different uncertainty σ_i. In this case it is convenient to introduce at each

point a weight $w_i = 1/\sigma_i^2$, and rewrite the equations (144) and (145) like this:

$$a = \frac{(\sum w_i x_i^2)(\sum w_i y_i) - (\sum w_i x_i)(\sum w_i x_i y_i)}{\Delta}, \quad (149)$$

$$b = \frac{(\sum w_i)(\sum w_i x_i y_i) - (\sum w_i x_i)(\sum w_i y_i)}{\Delta}, \quad (150)$$

where $\Delta = (\sum w_i)(\sum w_i x_i^2) - (\sum w_i x_i)^2$.

8.3 Propagation of uncertainties in indirect measurements

In physics it is often necessary to calculate the value of a physical quantity based on other variables which have been measured with certain precision. How can we assess the uncertainty in such calculations? For simplicity let's start with a simple case where we have two independent measured variables X and Y and we want to calculate the sum $Q = X + Y$ and its uncertainty.

Remembering equation (74) which defines the probable error, let's write the results of the measurements of X and Y as $x \pm \delta x$ and $y \pm \delta y$, where x and y are the measured values and δx and δy are their respective probable errors. Clearly, the largest probable value for $X + Y$ is $(x + \delta x) + (y + \delta y) = (x + y) + (\delta x + \delta y)$, while the smallest probable value is $(x - \delta x) + (y - \delta y) = (x + y) - (\delta x + \delta y)$. Based on these results one could say that the best estimate for the sum would be $q = x + y$, with estimated error $\delta q = \delta x + \delta y$. However, it is more-or-less obvious that this estimate for the error is incorrect, because its maximum is reached when both x and y errors are at maximum, which is quite improbable. In order to obtain a better estimate let's remind ourselves that any measurement which does not contain systematics is expected to be distributed as a Gaussian around the true value. So assuming for simplicity that the true values for X and Y are both 0, the measured values x and y will be distributed as $\rho(x) = \exp\left(-\frac{x^2}{2\sigma_x^2}\right)$ and $\rho(y) = \exp\left(-\frac{y^2}{2\sigma_y^2}\right)$, respectively. Since X and Y are independent, one has

$$\begin{aligned}\rho(x,y) &= \rho(x)\rho(y) = \exp\left(-\frac{x^2}{2\sigma_x^2}\right)\exp\left(-\frac{y^2}{2\sigma_y^2}\right) = \exp\left(-\frac{x^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2}\right) \\ &= \exp\left(-\frac{x^2+y^2}{2(\sigma_x^2+\sigma_y^2)}\right)\exp\left(-\frac{z^2}{2}\right) \equiv \rho(x+y,z)\end{aligned}$$

where we used the identity

$$\frac{x^2}{A} + \frac{y^2}{B} = \frac{(x+y)^2}{A+B} + \frac{(Bx - Ay)^2}{AB(A+B)} = \frac{(x+y)^2}{A+B} + z^2$$

The term containing z is irrelevant since it integrates into a constant coefficient $\sqrt{2\pi}$, so we finally get

$$\rho(x+y) \sim \exp\left[-\frac{x^2+y^2}{2(\sigma_x^2+\sigma_y^2)}\right].$$

It is obvious from here that the width of the distribution of the sum $x + y$ is $\sqrt{\sigma_x^2 + \sigma_y^2}$, and the probable error can be linked to this quantity.

If the means of X and Y, denoted by $\overline{x}$ and $\overline{y}$ respectively, are not equal to zero then one can write $x + y = (x - \overline{x}) + (y - \overline{y}) + (\overline{x} + \overline{y})$. Here the last term is a constant which cannot change the width of the distribution, while the first two terms are normally distributed with zero means and widths σ_x and σ_y, so for the width of their sum we could use the formula $\sqrt{\sigma_x^2 + \sigma_y^2}$.

Consider now a more general case where we would like to estimate the error on a quantity which is an arbitrary function of two measured quantities: $q = f(x, y)$. Let's assume that the mean $\overline{q} \approx f(\overline{x}, \overline{y})$ (which, strictly speaking, is not always true, since in general $M[f(\xi)] \neq f(M\xi)$). Under this assumption we can use equation (107) to obtain

$$\sigma_q^2 = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} (q_i - \overline{q})^2.$$

For any given measurement x_i the quantities $x_i - \overline{x}$ and $y_i - \overline{y}$ are expected to be small numbers, one can expand $q_i - \overline{q}$ into a series and only retain the leading terms:

$$q - \overline{q} = (x_i - \overline{x}) \frac{\partial f}{\partial x} + (y_i - \overline{y}) \frac{\partial f}{\partial y},$$

where the derivatives are calculated at the values $\overline{x}$ and $\overline{y}$ of the respective arguments. Then

$$\begin{aligned} \sigma_q^2 &= \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} \left[(x_i - \overline{x}) \frac{\partial f}{\partial x} + (y_i - \overline{y}) \frac{\partial f}{\partial y} \right]^2 \\ &= \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} \left[(x_i - \overline{x})^2 \left(\frac{\partial f}{\partial x} \right)^2 + (y_i - \overline{y})^2 \left(\frac{\partial f}{\partial y} \right) + 2(x_i - \overline{x})(y_i - \overline{y}) \frac{\partial f}{\partial x} \frac{\partial f}{\partial y} \right]. \end{aligned}$$

Now, taking into account that

$$\begin{aligned} \sigma_x^2 &= \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} (x_i - \overline{x})^2, \\ \sigma_y^2 &= \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} (y_i - \overline{y})^2, \\ \sigma_{xy}^2 &= \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} (x_i - \overline{x})(y_i - \overline{y}), \end{aligned}$$

we finally have:

$$\sigma_q^2 = \sigma_x^2 \left(\frac{\partial f}{\partial x} \right)^2 + \sigma_y^2 \left(\frac{\partial f}{\partial y} \right)^2 + 2\sigma_{xy}^2 \left(\frac{\partial f}{\partial x} \right) \left(\frac{\partial f}{\partial y} \right). \tag{151}$$

If the variables x and y are uncorrelated, then $\sigma_{xy} = 0$ and equation (151) is simplified.

Let's use equation (151) to calculate uncertainties for a sum and a difference of uncorrelated variables:

$$\begin{aligned} q &= (x+y)-(u+v), \\ \delta q &= \sqrt{(\delta x)^2+(\delta y)^2+(\delta u)^2+(\delta v)^2}. \end{aligned} \tag{152}$$

For a product and a ratio of uncorrelated variables we then have:

$$\begin{aligned} q &= \frac{x\cdot y}{u\cdot v}, \\ \frac{\delta q}{q} &= \sqrt{\left(\frac{\delta x}{x}\right)^2+\left(\frac{\delta y}{y}\right)^2+\left(\frac{\delta u}{u}\right)^2+\left(\frac{\delta v}{v}\right)^2}. \end{aligned} \tag{153}$$

In these equations δx etc. stand for the *absolute* uncertainty of the respective variable (x in this case); then the expression $\frac{\delta x}{x}$ is the *relative* uncertainty. We see that for a sum and/or a difference of variables their absolute uncertainties are added in quadrature, while for products and/or ratios it's the relative uncertainties that are added in quadrature.

Suppose that u and v are two measured variables, while a and b are numbers. Then, using equation (151), we can compile the following table:

$x = au \pm bv$	$\sigma_x^2 = a^2\sigma_u^2 + b^2\sigma_v^2 \pm 2ab\sigma_{uv}^2$
$x = avu$	$\sigma_x^2 = a^2v^2\sigma_u^2 + a^2u^2\sigma_v^2 + 2a^2uv\sigma_{uv}^2$
$x = \pm a\frac{u}{v}$	$\sigma_x^2 = \left[\frac{\sigma_u^2}{u^2} + \frac{\sigma_v^2}{v^2} + 2\frac{\sigma_{uv}^2}{uv}\right] x^2$
$x = au^{\pm b}$	$\sigma_x = b\frac{\sigma_u}{u}x$
$x = a\exp[\pm bu]$	$\sigma_x = b\sigma_u x$
$x = a\ln[\pm bu]$	$\sigma_x = a\frac{\sigma_u}{u}$

8.4 Combining independent measurements

Suppose that the same quantity x is measured in two independent parts of an experiment (or indeed in two independent experiments). How can we combine these results?

Specifically, we have measured:

$x = x_A \pm \sigma_A$ in experiment A;

$x = x_B \pm \sigma_B$ in experiment B.

Note that this question only makes sense if the difference between the two measurements $|x_A - x_B|$ is not much larger than their respective uncertainties; if it is, then something must be wrong and the combination does not make sense.

Assume that the measurements obey the Gaussian distribution, and denote the combination by X. The probability that experiment A results in measurement x_A is

$$\rho_X(x_A) \sim \frac{1}{\sigma_A} \exp\left[-\frac{(X - x_A)^2}{2\sigma_A^2}\right], \tag{154}$$

and similarly for experiment B:

$$\rho_X(x_B) \sim \frac{1}{\sigma_B} \exp\left[-\frac{(X - x_B)^2}{2\sigma_B^2}\right]. \tag{155}$$

The probabilities (154) and (155) depend on the combined value X which we are trying to determine. The probability that experiment A results in measurement x_A *and* experiment B results in measurement x_B is

$$\rho_X(x_A, x_B) \sim \frac{1}{\sigma_A \sigma_B} \exp\left(-\frac{\xi^2}{2}\right), \qquad \xi^2 \equiv \left(\frac{x_a - X}{\sigma_A}\right)^2 + \left(\frac{x_b - X}{\sigma_B}\right)^2. \tag{156}$$

According to the principle of maximum likelihood, the best estimate $\hat{x}$ for the parameter X is the value which maximises this probability. This is achieved when ξ^2 is minimised. At the minimum, the derivative of ξ^2 with respect to X must be zero:

$$2\frac{x_A - \hat{x}}{\sigma_A^2} + 2\frac{x_B - \hat{x}}{\sigma_B^2} = 0 \qquad \Rightarrow \qquad \hat{x} = \frac{x_A w_A + x_B w_B}{w_a + w_B} \tag{157}$$

where $w_A = \frac{1}{\sigma_A^2}, w_B = \frac{1}{\sigma_B^2}$.

The result (157) can be easily generalised for N independent measurements:

$$\hat{x} = \frac{\sum_{i=1}^N w_i x_i}{\sum_{i=1}^N w_i}, \qquad w_i = \frac{1}{\sigma_i^2}. \tag{158}$$

Using the error propagation formula (151), one gets for the uncertainty in $\hat{x}$:

$$\sigma_{\hat{x}} = \left(\sum_{i=1}^{N} w_i \right)^{-\frac{1}{2}} . \tag{159}$$

It is clear from equation (159) that the combination will be more precise than any individual measurement in the set.

8.5 Interpretation of the measurement uncertainties

Any experiment in physics implies some kind of measurement of a physical quantity or quantities. By its nature, the measurement is a random process, since it is impossible to get exactly identical results, no matter how precise the measurements are or how close are the conditions in each measurement. Hence, uncertainties – deviations from the 'exact true value' – exist in any measurement. Depending on the character of the uncertainty, it can be either random (*statistical*) or instrumental (*systematic*). Statistical errors are inevitable, however their effects can be minimised by repeating the measurements and averaging the results of a number of measurements. On the other hand, any measurement is performed using some kind of instrument which has a finite *sensitivity* and is subject to *calibration*. Imperfect calibration will give rise to systematic uncertainties; in some cases systematic uncertainties are due to the method of measurement (rather than the specific instrument) so it is important to choose the method wisely.

Measurements can be characterised by their *precision* – how close the repeated measurements are to each other – and *accuracy* – how close the measurements are to the true value of the measured variable. These concepts are illustrated in Figure 23: good precision means small statistical errors (small fluctuations),

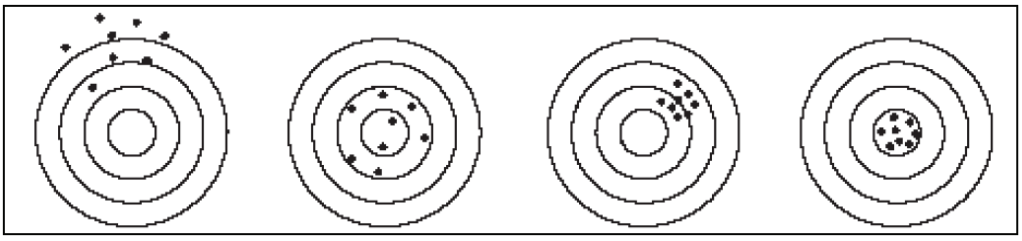


Figure 23: Illustration of the quality of measurement. From left to right: low precision, low accuracy; low precision, high accuracy; high precision, low accuracy; high precision, high accuracy.

while good accuracy means low systematic uncertainties.

The statistical uncertainty of the measurement of some quantity X can be estimated in the following way:

1. Measure the quantity n times and calculate the arithmetic mean $\overline{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$.
2. Calculate the sum of squares of the individual deviations of x_i from the mean $\overline{x}$.
3. Calculate the dispersion $D = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \overline{x})^2$.
4. Find the standard deviation $\sigma = \sqrt{D}$.
5. Find the standard uncertainty for the mean:

$$\sigma_{\text{stat}} = \frac{\sigma}{\sqrt{n}} = \sqrt{\sum_{i=1}^{n} \frac{(x_i - \overline{x})^2}{n(n-1)}} \tag{160}$$

6. The result of the measurement can now be written as $\overline{x} \pm \sigma_{\text{stat}}$.

For a direct measurement, the overall uncertainty can be estimated as

$$\Delta x = \sqrt{\sigma_{\text{stat}}^2 + \sigma_{\text{syst}}^2}, \tag{161}$$

where σ_{syst} is the instrumental – systematic – uncertainty. This could be the absolute resolving power of the measuring instrument (say, half of the smallest increment of the instrument scale), and/or some other uncertainty of a similar kind. Unless there are good reasons to do it differently, various sources of systematic uncertainties are added in quadrature to form the overall systematic error σ_{syst}.

As for the statistical uncertainty σ_{stat}, it can be calculated as $\sigma_x t_{\alpha,(n-1)}$. Here $t_{\alpha,(n-1)}$ is the quantile[1] of Student's distribution which depends on the number of degrees of freedom n and the required confidence level α.

If possible, the measurement is repeated until the statistical uncertainty σ_{stat} becomes as small as, or at least comparable to, the systematic error σ_{syst}. The final measurement result cab be presented as

$$\overline{x} \pm \Delta x \tag{162}$$

[1]For a random variable ζ with the cumulative distribution function $F(\zeta)$, the *quantile* of order p is defined as the value ζ_p for which

$$F(\zeta_p) \leq p, \quad F(\zeta_p + o) \geq p.$$

From this definition, $\zeta_{1/2}$ is the median of the distribution.

in which case the interval $(\overline{x} - \Delta x, \overline{x} + \Delta x)$ is the confidence interval of the measurement (see equation (110)). Sometimes the statistical and systematic errors are quoted separately:

$$\overline{x} \pm \Delta x_{\text{stat}}{}^{+\Delta x_{\text{syst}}}_{-\Delta x_{\text{syst}}}. \tag{163}$$

Since the systematic uncertainty can sometimes be asymmetric, in general the positive and negative systematic uncertainties do not have to be equal:

$$|+\Delta x_{\text{syst}}| \neq |-\Delta x_{\text{syst}}|. \tag{164}$$

If the measurement has several sources of systematic uncertainties, then in the expression (163) it may be advisable to quote these separately.