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Iosif Refulyevich Entinzon

Theory of Errors

Lectures

English Edition · Complete

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Theory of Errors (Lectures)

English edition — complete translation

Original work: Iosif Refulyevich Entinzon, *Теория ошибок (Лекции)*, Kyiv, 2023. Entinzon remains the author and owner of his work.

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Authoritative source: sealed Russian Word manuscript SHA-256 `ed3b1d8829ee06501115e1c85df763e9731eaf7e58d09a2895bce7fda7738abd`. Visual/structural reference: approved Russian complete PDF SHA-256 `a0cfe2d88d2ec5a8d54e7ecb4ca347f23ffb8e3545aae72524f29031a7b4fbb6` (74 pages).

Section 1 terminology follows the approved English preview. Contents page numbers are those of the 2023 Russian original; they are not the page numbers of this English edition.

Appendix statistical tables are facsimile plates from the author's original; numerical values are unchanged. English titles are supplied for each plate.

I. R. Entinzon

Theory of Errors

(Lectures)

Kyiv — 2023

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1. Introduction

Repeated measurements of any quantity always lead to different numerical values. Suppose that a true value of the measured quantity exists. We will then call the difference between the measurement result x and the true value a of the measured quantity the measurement error ε. That is, we set

$$\varepsilon = x - a \tag{1.1}$$

Depending on the causes that produce them, measurement errors are divided into random errors, systematic errors, and gross errors (blunders). Random errors are those whose values change from one measurement to another. The magnitude of these errors cannot be established before the experiment. They arise from inaccuracy of measurement — random errors of the measuring instruments, random errors of the experimenter, and inexact adherence to the measurement procedure — and from the measured quantity itself not being constant.

Systematic errors differ from random errors in that their value remains constant through a series of measurements of the same kind. They can therefore be excluded from the final result if their magnitude has been determined by a prior study of the measurement procedure.

The division of errors into systematic and random is plainly conditional, because the same errors should be treated as random in some cases and as systematic in others. For example, a series of measurements made at the same temperature will contain a systematic error which arose because the temperature correction is not taken into account (or is taken into account incorrectly). However, in a series of measurements made at different (not fixed) temperatures, those same errors will be random in character. Likewise, an unaccounted error of a standard (errors of calibration) will be systematic in character for a given laboratory; however, when results obtained in different laboratories are processed, that error must be regarded as random.

Gross errors (blunders) are also random, but their character differs substantially from that of random measurement errors. This difference is due to the fact that if random measurement errors arise when the apparatus is working properly and the experimenter is acting correctly, then gross errors are caused by faulty measuring equipment or by errors in the experimenter's work. If the gross errors are considerable, the results stand out sharply from the others and should be discarded. If that is not the case, the results may also be discarded, but only after special quantitative criteria have been applied.

If the quantity measured is the one that directly interests the experimenter, the measurements are called direct. If the quantity to be determined is calculated, through a given functional relation, from quantities obtained by direct measurement, the measurements are called indirect. When several measured quantities are connected by a

known functional relation — for example, the three angles of a triangle; the temperature, volume, and pressure of a gas; and so on — the values obtained will, because of measurement errors, generally contradict one another. Such measurements are called conditional.

In direct, indirect, and conditional measurements, the errors may be systematic, random, or gross.

Any real measuring instrument, working in real situations, is subject, as is the situation itself (the setup), to the uncontrolled influence of many external and internal factors. The measured quantity can therefore take different numerical values.

Statisticians joke about this, saying that the measured quantity α is a function of an infinite number of parameters Φi:

$$\alpha = \alpha(\Phi 1, \Phi 2, \Phi 3, \Phi 4, \ldots, \Phi 40, \ldots, \Phi 400, \ldots, \Phi\infty). \tag{1.2}$$

In theory, an infinite (∞) number of parameters have an effect; in practice, 400. Of these, the experimenter can name 40, if he thinks the situation through from all sides. He is able to control — to hold fixed — only 4 parameters, and even those only to within the accuracy of the measuring instrument.

That joke contains the chief feature of any measurement. The number of factors that affect the measured quantity is enormous, and their influence is uncontrolled and random. The measured quantity should therefore be regarded as a random variable. The true quantity, as is evident, cannot be obtained from the experiment, and so statistics has no concept of a "true quantity."

Yet, "there is no harm without some good" — the fact that the number of influencing parameters is infinite (or enormous) turned out to be decisive in formulating objective principles for discussing the results of direct measurements. These lectures are devoted to considering these principles.

We will call a random variable a quantity that, as the result of an experiment, can take different numerical values. A random variable is the possibility that a number appears on the screen. A particular number on the screen is a realization of the random variable. A random variable may take discrete values, or any values in a given interval: it may be a discrete or a continuous random variable. From here on, only continuous random variables will be considered.

In the theory of errors, random variables are the principal object of study. The principal mathematical apparatus of the theory is therefore probability theory, and the mathematical statistics that follows from it.

2. The Concept of Probability

In the modern theory no attempt is made to define the concept of probability; it is regarded as a fundamental (undefined) notion that satisfies certain axioms, which may be viewed as experimental facts:

1. To every random event A there corresponds a number P(A), $0 \leq P(A) \leq 1$, called the probability of the event A.

2. The probability of the certain event U is equal to 1;

$$P(U) = 1 \tag{2.1}$$

3. The axiom of additivity: if A_1 and A_2 are incompatible random events, that is, their intersection $A_1 \cap A_2 = V$ (where V is the impossible event), then

$$P(A_1 \cup A_2) = P(A_1) + P(A_2) \tag{2.2}$$

that is, the probability of the union of incompatible events equals the sum of the probabilities of those events. In particular it follows that

$$P(U \cup V) = P(U) + P(V) = 1 + P(V) \leq 1 \tag{2.3}$$

Therefore $P(V) = 0$: the probability of the impossible event is zero. But not conversely! If the probability of some event A equals 0, $P(A) = 0$, that does not mean that the event A is impossible, $A \neq V$!

3. Random Variables

A real variable which, depending on the outcome of an experiment — that is, depending on chance — takes different values is called a random variable. A random variable is denoted by a capital letter, for example X. The distribution function (or distribution law) of the random variable X is the function

$$F(x) = P\{X < x\} \tag{3.1}$$

This function completely characterizes the random variable.

The function f(x) is called the density of the distribution, or the differential distribution function, if the distribution function F(x) can be represented in the form

$$F(x) = \int_{-\infty}^{x} f(t)\,dt \tag{3.2}$$

The distribution function F(x) of an arbitrary random variable has the following properties:

$$\lim_{x\to+\infty} F(x) = 1, \quad \lim_{x\to-\infty} F(x) = 0 \tag{3.3}$$

and we note that

$$\int_{-\infty}^{+\infty} f(t)\,dt = 1 \tag{3.4}$$

2) F(x) is monotonically non-decreasing: if $x_1 < x_2$, then

$$F(x_1) \le F(x_2) \tag{3.5}$$

3) F(x) is continuous from the left:

$$\lim_{x\to x_0-0} F(x) = F(x_0) \tag{3.6}$$

From the axioms it follows that the probability that the random variable falls in a given half-open interval equals

$$P\{a \le X < b\} = F(b) - F(a) = \int_a^b f(x)\,dx \tag{3.7}$$

Note that here $P(X = a) = 0$. It does not follow, however, that the event $X = a$ is impossible!

4. Numerical Parameters

The functions F(x) and f(x) are by no means always known, and in many problems it is possible to restrict oneself to an approximate characterization of the probability density by specifying certain numerical parameters that convey the general properties of that function. As such parameters it is often convenient to choose the quantities called, in probability theory, the initial and central moments of various orders of the random variable X.

Initial moments:

$$m_k = \int_{-\infty}^{+\infty} x^k f(x)\,dx, \quad \text{where } k = 1, 2, \ldots \tag{4.1}$$

Central moments:

$$\mu_l = \int_{-\infty}^{+\infty} (x - m_1)^l f(x)\,dx, \quad \text{where } l = 1, 2, \ldots \tag{4.2}$$

The most important among this infinite set of moments are the following two: the first initial moment of the random variable X, also called the mathematical expectation of X,

$$m_1 = \bar{x} = M(X) = \int_{-\infty}^{+\infty} x f(x)\,dx \tag{4.3}$$

and the second central moment of X, also called the variance of X,

$$\mu_2 = \sigma_X^2 = D(X) = \int_{-\infty}^{+\infty} (x - \bar{x})^2 f(x)\,dx \tag{4.4}$$

which characterizes the spread of the random variable about its mathematical expectation.

Note that if c is a constant, then

$$M(cX) = c\,M(X) \tag{4.5}$$

$$D(cX) = c^2\,D(X) \tag{4.6}$$

5. The Normal Distribution Law

Consider a concrete probability density — the normal probability distribution law (the normal law, Gauss's law). It will be shown later that all the practically important results are obtained using the normal law.

A random variable X obeys the normal law if its probability density f(x) can be written in the form

$$f(x) = (1/(\sigma_X\sqrt{(2\pi)})) \exp(-(x - \bar{x})^2/(2\sigma_X{}^2)) \tag{5.1}$$

One can show that this function is constructed so as to exhibit all the properties of a probability density and has two parameters, namely the mathematical expectation and the variance:

$$M(X) = \bar{x}, \quad D(X) = \sigma_X{}^2 \tag{5.2}$$

For the distribution function of a normal variable we have

$$F(x) = \int_{-\infty}^{x} f(t)\,dt \tag{5.3}$$

After a change of variables one arrives at the form

$$F(x) = ½\,[1 + \Phi((x - \bar{x})/\sigma_X)] \tag{5.4}$$

where $\Phi(Z)$ is the integral Laplace function of the argument Z, defined by (Pierre-Simon Laplace, 1749–1827)

$$\Phi(Z) = (2/\sqrt{(2\pi)}) \int_0^Z e^{-t^2/2}\,dt \tag{5.5}$$

This function is odd,

$$\Phi(-Z) = -\Phi(Z) \tag{5.6}$$

and as $Z \to \infty$ it tends to 1. If the normal distribution is centered ($\bar{x} = 0$) and normalized ($\sigma_X = 1$), then

$$\Phi(x) = 2F(x) - 1 \tag{5.7}$$

Note that if the distribution law of the random variable is normal, the problem reduces to finding, from the experimental results, the two parameters $\bar{x}$ and $\sigma_X{}^2$.

As an example, determine the probability that a normal random variable deviates from its mathematical expectation in absolute value by no more than σ, 2σ, 3σ, … — that is, falls in the interval $[\bar{x} - k\sigma, \bar{x} + k\sigma]$:

$$P\{|X - \bar{x}| \leq k\sigma\} = \Phi(k) \tag{5.8}$$

We obtained the answer knowing only the form of the probability distribution and without knowing particular values of $\bar{x}$ and σ. The result is therefore valid for any $\bar{x}$ and σ.

Values of the function Φ are tabulated; for $k = 1, 2, 3$ and 4 they are given in Table 5.1:

Table 5.1

$k\sigma$	k	$P = \Phi(k)$
1σ	1	0.6827
2σ	2	0.9545
3σ	3	0.9973
4σ	4	0.99994

The numbers in the third column equal the probability that the deviation of a normal random variable from its mathematical expectation does not exceed, in absolute value, one, two, etc., root-mean-square deviations. In many problems that assume a normal law of errors one may approximately regard deviations exceeding 3σ as so improbable that the possibility of their occurrence (in those problems) may be disregarded. This recommendation is called the "3σ rule." Values of the functions Φ, f and F are given in the tables; see the Appendix.

6. Problems of Mathematical Statistics

Mathematical statistics treats problems in which one must formulate statements about the properties of a set of elements called the general population, using information about some properties of a subset of elements from that population. In mathematical statistics that subset is a random sample of n elements from the general population, the selection of individual elements being independent.

Here we consider the processing of the results of direct measurements, which is the foundation of the whole theory of errors.

The result of n direct measurements of one and the same quantity is a series of numbers

$$x_1, x_2, \ldots, x_n \tag{6.1}$$

The aim of processing this series is to find an approximate value of the measured quantity with the greatest possible accuracy, to estimate that accuracy, and, in some cases, to determine the form of the distribution law.

The series $x_1, \ldots, x_n$ obtained in n trials is a random sample of size n from the general population — the set of all possible realizations of the random variables $X_1, \ldots, X_n$.

(schematic array of repeated samples; $m \to \infty$) (6.2)

Note that the distribution laws of the random variables $X_1, \ldots, X_n$ are unknown, as are the parameters of those laws:

$$f_1(x), \ldots, f_n(x) \quad \Rightarrow \quad ? \tag{6.3}$$

$$\bar{x}_1, \ldots, \bar{x}_n \quad \Rightarrow \quad ? \tag{6.4}$$

$$\sigma_{X_1}^2, \ldots, \sigma_{X_n}^2 \quad \Rightarrow \quad ? \tag{6.5}$$

The spread σ_X is also unknown; it is also called the standard deviation and the root-mean-square (quadratic) deviation.

Since the repeated measurements are of the same kind, one should regard all the random variables $X_1, \ldots, X_n$ as having the same distribution law

$$f_1(x) = f_2(x) = \ldots = f_n(x) = f(x) \tag{6.6}$$

and the same parameters

$$\bar{x}_1 = \bar{x}_2 = \ldots = \bar{x}_n = \bar{x} \tag{6.7}$$

$$\sigma_{X_1}^2 = \ldots = \sigma_{X_n}^2 = \sigma_X^2 \tag{6.8}$$

We therefore regard the sample $x_1, \ldots, x_n$ as a realization of independent random variables $X_1, \ldots, X_n$ with identical distributions. The n-dimensional random vector $(X_1, \ldots, X_n)$, whose components are independent and all have distribution f(x), is called a mathematical sample of size n. Each realization $(x_1, \ldots, x_n)$ of that vector is a sample.

7. The Concept of an Estimate

We call an approximate value of the quantity being estimated its estimate.

We agree to denote an estimate by the same letter as the estimated quantity, but with a wavy line (tilde) above it: a — a numerical parameter of the distribution law; $\tilde{a}$ — an estimate of that value; $\tilde{A}$ — the random variable of which the estimate $\tilde{a}$ is a realization.

Examples of estimates of numerical parameters: $\tilde{x}$ — an estimate of the mathematical expectation $\bar{x}$ of the random variable X; $\tilde{\sigma}_X^2$ — an estimate of the variance σ_X^2; $\tilde{\sigma}_X$ — an estimate of the spread σ_X.

The numbers

$$\tilde{x}, \quad \tilde{\sigma}_X^2, \quad \tilde{\sigma}_X \tag{7.1}$$

are concrete realizations of new random variables

$$\tilde{X}, \quad \tilde{\Sigma}_X^2, \quad \tilde{\Sigma}_X \tag{7.2}$$

with their own distribution densities

$$f_{\tilde{X}}(x), \quad f_{\tilde{\Sigma}^2}(\sigma^2), \quad f_{\tilde{\Sigma}}(\sigma) \tag{7.3}$$

as well as mathematical expectations

$$M(\tilde{X}), \quad M(\tilde{\Sigma}_X^2), \quad M(\tilde{\Sigma}_X) \tag{7.4}$$

and variances

$$D(\tilde{X}), \quad D(\tilde{\Sigma}_X^2), \quad D(\tilde{\Sigma}_X) \tag{7.5}$$

The new random variables $\tilde{X}$, $\tilde{\Sigma}_X^2$, $\tilde{\Sigma}_X$ are usually defined as functions of the mathematical sample $(X_1, \ldots, X_n)$.

For example, consider the sample function

$$\tilde{X} = (1/n)\, \Sigma_{i=1}^{n} X_i \tag{7.6}$$

If the mathematical sample is realized, the sample function

$$\tilde{x} = (1/n)\, \Sigma_{i=1}^{n} x_i \tag{7.7}$$

is called a point estimate of the mathematical expectation $\bar{x}$ of the random variable X.

Properties of point estimates.

1) An estimate should be consistent: the variance (spread) of the random variable $\tilde{A}$ tends to zero in the limit,

$$\lim_{n\to\infty} D(\tilde{A}) = 0 \tag{7.8}$$

It then ensures small deviations of the estimate $\tilde{a}$ from its mathematical expectation.

2) An estimate should be unbiased, that is,

$$M(\tilde{A}) = a \tag{7.9}$$

the mathematical expectation of $\tilde{A}$ should equal the numerical parameter being estimated. Unbiasedness then guarantees the absence of systematic error: $\tilde{a} \to a$. In some cases one is content with asymptotic unbiasedness,

$$\lim_{n\to\infty} M(\tilde{a}) = a \tag{7.10}$$

Estimates of that type contain systematic errors, but their absolute magnitude decreases as the sample size grows and tends asymptotically to zero.

3) An estimate should be efficient — of two estimates of one parameter, the more efficient is the one with the smaller variance. It is the best estimate in the sense that it makes the best use of the information contained in the sample.

Two principal methods are used to obtain estimates: the method of moments and the method of maximum likelihood. Here we consider the method of moments, proposed by the English mathematician Karl Pearson (1857–1936). In the method of moments the parameters of the distribution law f(x) are expressed through the initial and central moments of the random variable under study. As their estimates one takes those mean values of the corresponding quantities that satisfy the requirements of consistency, unbiasedness, and efficiency.

8. Estimates of the Parameters of the Distribution Law: $\tilde{x}$, $\tilde{\sigma}_X^2$, $\tilde{\sigma}_X$

As an estimate of the mathematical expectation of the random variable X from the sample $x_1, \ldots, x_n$ one takes the ordinary arithmetic mean

$$\tilde{x} = (1/n) \Sigma_{i=1}^{n} x_i \tag{8.1}$$

which is a realization of the random variable

$$\tilde{X} = (1/n) \Sigma_{i=1}^{n} X_i \tag{8.2}$$

The appropriateness of that choice was justified in the mid-nineteenth century by Pafnuty Lvovich Chebyshev.

Chebyshev's theorem. If $X_1, \ldots, X_n$ are independent random variables with distribution laws having mathematical expectations $\bar{x}_i$ and finite variances, and if $\tilde{x}$ is the arithmetic mean of a sample from those variables (8.1), then for any $\varepsilon > 0$ the limit relation

$$\lim_{n\to\infty} P\{|\tilde{x} - \bar{x}| < \varepsilon\} = 1 \tag{8.3}$$

holds, where

$$\bar{x} = (1/n) \Sigma_{i=1}^{n} \bar{x}_i \tag{8.4}$$

Expression (8.3) states that $\tilde{x}$ tends to $\bar{x}$ in probability as $n \to \infty$. The theorem shows that for a sufficiently large number of terms the probability of a deviation of the arithmetic mean from the mean of the mathematical expectations by any small amount ε can be made arbitrarily small as n increases.

Thus for large n one may confidently use the arithmetic mean of the random variable as an approximate estimate of the mathematical expectation (even with different variances — that is, different instruments and setups).

This is a fundamental result, but it does not by itself give a path to the best estimates that satisfy the criteria for point estimates. It will be shown below that in a number of concrete cases the sample arithmetic mean is a point estimate of the mathematical expectation $\bar{x}$ of X.

As an estimate of the variance of X when the mathematical expectation $\bar{x}$ is known one chooses

$$\tilde{\sigma}_X^2 = (1/n) \Sigma_{i=1}^{n} (x_i - \bar{x})^2 \tag{8.5}$$

for which it is also proved that $\tilde{\sigma}_X^2 \to \sigma_X^2$ in probability as $n \to \infty$: for any $\varepsilon > 0$,

$$\lim_{n\to\infty} P\{|\tilde{\sigma}_X{}^2 - \sigma_X{}^2| < \varepsilon\} = 1 \tag{8.6}$$

The estimate of the root-mean-square deviation

$$\tilde{\sigma}_X = \sqrt{\tilde{\sigma}_X{}^2} \tag{8.7}$$

is then also consistent, but it is no longer unbiased — only asymptotically unbiased (unbiased in the limit as $n \to \infty$).

9. The Central Limit Theorem

The distribution law of a sum of independent random variables (under fairly general conditions) tends, as the number of terms n grows, to the normal law, independently of the form of the distribution laws of the summands. A theorem of that type was first proved in 1730 by the English mathematician (French by origin) Abraham de Moivre (1667–1754). There is now a family of theorems establishing the limiting normality of sums of independent terms, differing in the additional conditions imposed on the laws of the summands.

Whatever the mathematical formulation, the physical meaning of those conditions reduces to this: no single summand should have a variance comparable with the variance of the whole sum as the number of terms increases — that is, no summand should dominate the sum. This means that the random variable X is normally distributed if it is a sum of independent random variables with $n \to \infty$,

$$X = X_1 + X_2 + \ldots + X_n \tag{9.1}$$

with variance

$$\sigma_X{}^2 = \sigma_{X_1}{}^2 + \ldots + \sigma_{X_n}{}^2 \tag{9.2}$$

and with

$$\sigma_{X_i}{}^2 / \sigma_X{}^2 \to 0 \quad (n \to \infty) \tag{9.3}$$

For the estimate of the mathematical expectation this condition is satisfied. Indeed

$$\tilde{X} = (1/n)X_1 + \ldots + (1/n)X_n \tag{9.4}$$

$$\sigma_{\tilde{X}}{}^2 = \sigma^2{}_{(1/n)X_1} + \ldots + \sigma^2{}_{(1/n)X_n} \tag{9.5}$$

$$\sigma_{\tilde{X}}{}^2 = (1/n^2)\sigma_{X_1}{}^2 + \ldots + (1/n^2)\sigma_{X_n}{}^2 \tag{9.6}$$

$$\sigma_{\tilde{X}}{}^2 = (1/n^2)\sigma_X{}^2 + \ldots + (1/n^2)\sigma_X{}^2 \tag{9.7}$$

$$\sigma_{\tilde{X}}{}^2 = (1/n)\,\sigma_X{}^2 \tag{9.8}$$

and moreover

$$\sigma^2{}_{X/n} = (1/n^2)\,\sigma_X{}^2 \tag{9.9}$$

Therefore

$$D(\tilde{X}) \gg D((1/n)X_i) \tag{9.10}$$

which was to be proved.

Regard the random variable X as the sum

$$X = \bar{x} + \xi_1 + \xi_2 + \ldots + \xi_n \tag{9.11}$$

where the ξ_i are random variables caused by various independent factors that could not be fixed with absolute accuracy.

Since the number of factors may be regarded as very large and the variances as comparable, we have the central-limit situation (9.12), and therefore X may be regarded as normally distributed.

When limit theorems are applied to concrete cases the basic condition that n tend to infinity is not fulfilled: n remains finite and sometimes not especially large. Limiting properties of sums usually appear already at comparatively small n, however, and although the theorems do not say from what n their results may be used, practice shows that in many cases those properties may be taken as holding already for comparatively small n ($n \sim 8 \div 10$).

That is why the normal law for X plays the decisive role in the study of experimental results. We shall use this fact below in analyzing one or another statistical procedure.

We next consider three fundamental problems of mathematical statistics that arise in processing experimental results. In all of them the sample is given, but in different problems additional information about X may be known, and the processing has different aims.

10. Problem 1. Find the Estimate $\tilde{x}$ when the Variance σ_X^2 Is Known

Find an estimate of the mathematical expectation $\bar{x}$ of the random variable X and determine the variance of that estimate, given the sample $x_1, \ldots, x_n$ and given that the variance of X equals σ_X^2. This problem arises when an unknown quantity is measured n times by a method free of systematic errors whose accuracy is characterized by a known variance.

$$X_1,\ldots,X_n \text{ — random variables;} \quad \text{parameters } \bar{x},\ \sigma_X^2 \text{ (known);} \quad \text{sample } x_1,\ldots,x_n \tag{10.1}$$

1. As the estimate $\tilde{x}$ of the mathematical expectation of $X_1, \ldots, X_n$ take the arithmetic mean

$$\tilde{x} = (1/n)\,\Sigma_{i=1}^{n}\, x_i \tag{10.2}$$

By construction $\tilde{x}$ is a realization of the random variable

$$\tilde{X} = (1/n)\,\Sigma_{i=1}^{n}\, X_i \tag{10.3}$$

2. Compute the variance of $\tilde{X}$, using the property of variance

$$D(cX) = c^2\, D(X) \tag{10.4}$$

$$D(\tilde{X}) = \sigma_{\tilde{X}}^2 = (1/n)\,\sigma_X^2 \tag{10.5}$$

The estimate (10.2) is consistent and unbiased. Indeed, letting $n \to \infty$ and using (10.5) we find

$$\lim_{n\to\infty} D(\tilde{X}) = 0 \tag{10.6}$$

so $\tilde{x}$ is a consistent estimate of the mathematical expectation. Taking the mathematical expectation of both sides of (10.2) yields

$$M(\tilde{X}) = \bar{x} \tag{10.7}$$

so the estimate is unbiased. As (10.5) shows, more efficient estimates are obtained by increasing the sample size n.

If X is normal, then $\tilde{X}$, being a sum of normal random variables, is also normal, and the probability density of the estimate is given by Gauss's formula

$$f_{\tilde{X}}(x) = (\sqrt{n}\,/(\sigma_X\sqrt{(2\pi)}))\,\exp(-n(x-\bar{x})^2/(2\sigma_X^2)) \tag{10.8}$$

with parameters $\bar{x}$ and $\sigma_{\tilde{X}}^2 = \sigma_X^2/n$. If the law of X is not normal but n is large enough, (10.8) may be used as an approximation by the central limit theorem. The accuracy then depends on the law of X and on the sample size.

11. Problem 2. Find the Estimate $\tilde{\sigma}_X^2$ when the Mathematical Expectation $\bar{x}$ Is Known

Find an estimate of the variance of X given the sample $x_1, \ldots, x_n$ and its mathematical expectation. This corresponds to processing measurements of a standard made to determine the accuracy of a measuring method. The measurement conditions are assumed unchanged, and any systematic error is absent or constant.

By definition the variance of X_i is the mathematical expectation of $(X_i - \bar{x})^2$, which in the i-th trial takes the value $(x_i - \bar{x})^2$. As an estimate of the variance take the arithmetic mean

$$\tilde{\sigma}_X^2 = (1/n)\,\Sigma_{i=1}^{n}\,(x_i - \bar{x})^2 \tag{11.1}$$

This estimate is unbiased, since taking mathematical expectations of both sides gives

$$M(\tilde{\sigma}_X^2) = \sigma_X^2 \tag{11.2}$$

It can also be shown to be consistent,

$$\lim_{n\to\infty} D(\tilde{\sigma}_X^2) = 0 \tag{11.3}$$

if the fourth central moment of X exists. When X is normal, the variance of the estimate takes the form

$$D(\tilde{\sigma}_X^2) = (2/n)\,\sigma_X^4 \tag{11.4}$$

Thus for a normal random variable the moment estimate $\tilde{\sigma}_X^2$ is consistent, and its efficiency is given by the simple formula (11.4).

If what is required is an estimate $\tilde{\sigma}_X$ of the root-mean-square deviation rather than of the variance, take

$$\tilde{\sigma}_X = \sqrt{\tilde{\sigma}_X^2} \tag{11.5}$$

This estimate is consistent but only asymptotically unbiased (unbiased in the limit as $n \to \infty$):

$$\lim_{n\to\infty} M(\tilde{\sigma}_X) = \sigma_X \tag{11.6}$$

If X is normal, an unbiased estimate of the root-mean-square deviation requires a correction factor k_{n+1}, rewriting (11.5) as

$$\tilde{\sigma}_X = k_{n+1}\,\sqrt{[(1/n)\,\Sigma_{i=1}^{n}\,(x_i - \bar{x})^2]} \approx \sqrt{[(1/(n - 0.45))\,\Sigma_{i=1}^{n}\,(x_i - \bar{x})^2]} \tag{11.7}$$

The correction coefficient k_{n+1} is given by

$$k_{n+1} = \sqrt{n} \cdot \Gamma(n/2) \,/\, (\sqrt{2} \cdot \Gamma((n+1)/2)) \tag{11.8}$$

where for positive integer n the gamma function satisfies

$$\Gamma(n) = (n-1)! \tag{11.9}$$

Table 11.1 gives values of the coefficient k_n (indexed by the subscript of k), showing that the approach to 1 as the index grows is fairly rapid. In (11.7)–(11.8) the sample size is n, so the tabulated entry used is that for index n+1.

Table 11.1. Values of the coefficient k_n

n	3	4	5	6	7	10	15	25	50
k_n	1.128	1.085	1.064	1.051	1.042	1.028	1.018	1.010	1.005

The need for the correction factor in (11.7) shows that an estimate obtained by a nonlinear operation (here, extraction of a square root) ceases to be unbiased. That is a direct consequence of the fact that the mathematical expectation of a function of a random variable equals the function of the mathematical expectation only for a linear dependence,

$$M[\varphi(X)] = \varphi(M[X]) \quad \text{(when } \varphi \text{ is linear)} \tag{11.10}$$

12. Problem 3. Find the Estimates $\tilde{x}$ and $\tilde{\sigma}_X^2$ when $\bar{x}$ and σ_X^2 Are Unknown

Find estimates of the mathematical expectation $\bar{x}$ and the variance σ_X^2 of X from the sample. This situation is typical of physical measurements when neither the measured quantity nor the accuracy of the method is known.

The estimate of the mathematical expectation is again, by the method of moments,

$$\tilde{x} = (1/n)\,\Sigma_{i=1}^{n}\, x_i \tag{12.1}$$

As shown in Problem 1, it is consistent, unbiased, and efficient. In estimating the variance one cannot apply (11.1) directly, because that formula contains the unknown $\bar{x}$. Replacing $\bar{x}$ by $\tilde{x}$ gives

$$\tilde{\sigma}_X^2 = (1/n)\,\Sigma_{i=1}^{n}\,(x_i - \tilde{x})^2 \tag{12.2}$$

but this estimate is no longer unbiased: the same sample has been used twice, so the terms are not independent. One degree of freedom is effectively lost. The unbiased estimate is

$$\tilde{\sigma}_X^2 = (1/(n-1))\,\Sigma_{i=1}^{n}\,(x_i - \tilde{x})^2 \tag{12.3}$$

$$M(\tilde{\sigma}_X^2) = \sigma_X^2 \tag{12.4}$$

If the fourth central moment exists, (12.3) is consistent (in particular for a normal X):

$$\lim_{n\to\infty} D(\tilde{\sigma}_X^2) = 0 \tag{12.5}$$

The square root of (12.3) estimates the root-mean-square deviation and is only asymptotically unbiased. For a normal parent population an unbiased estimate may be written with a correcting factor,

$$\tilde{\sigma}_X = k_n \sqrt{[(1/(n-1))\,\Sigma\,(x_i - \tilde{x})^2]} \tag{12.6}$$

where the correcting factor is taken from (11.8) / Table 11.1 with index one less than in (11.7) (one element of the sample is effectively lost): for sample size n use k_n rather than k_{n+1}.

For the parameters of the law of $\tilde{X}$ one still has

$$M(\tilde{X}) = \bar{x} \tag{12.7}$$

$$D(\tilde{X}) = \sigma_X^2/n \tag{12.8}$$

and for the variance of the variance estimate,

$$D(\tilde{\sigma}_X^2) = 2\sigma_X^4/(n-1) \quad \text{(normal case)} \tag{12.9}$$

Because the relation between $\tilde{\sigma}_{\bar{X}}^2$ and $\tilde{\sigma}_X^2$ is linear, that estimate remains consistent and unbiased. Passage from the variance estimate to the root-mean-square estimate loses unbiasedness by nonlinearity; for a normal X one may restore unbiasedness via (12.6), writing

$$\tilde{\sigma}_{\bar{X}} = \tilde{\sigma}_X/\sqrt{n} \tag{12.10}$$

Thus when the mathematical expectation is unknown, estimates of variance differ from the known-$\bar{x}$ case by replacing n with (n−1) in a number of formulas. That replacement is unimportant for large n but can noticeably increase the variance estimate for small samples.

13. The Method of Confidence Intervals

Estimates of the parameters of a distribution law, obtained from the random values of the sample elements, are themselves random variables and should be regarded as approximate values of those parameters. A complete characterization of the accuracy of that approximation is given by the distribution laws of the estimates. Such a characterization is inconvenient, however: it is not transparent and is sufficiently complicated. Mathematical statistics therefore makes wide use of the method of confidence intervals.

Suppose one wishes to characterize the accuracy of an estimate $\tilde{a}$ of a parameter a. Choose a large probability α, so close to 1 that events of probability $1 - \alpha$ may practically be disregarded. In chemistry one most often chooses $\alpha = 0.95$. Determine an interval $(a - \varepsilon, a + \varepsilon)$ such that the probability of the random variable $\tilde{A}$ falling in it equals α:

$$\alpha = P\{|a - \tilde{A}| \le \varepsilon\} = \int_{a-\varepsilon}^{a+\varepsilon} f(\tilde{a})\, d\tilde{a} \tag{13.1}$$

where $f(\tilde{a})$ is the probability density of $\tilde{A}$. The interval is called the confidence interval corresponding to the confidence probability α. With probability α one then guarantees that the error in determining a does not exceed ε in absolute value; ε is called the measurement error or the width of the α-confidence interval.

The confidence probability α is chosen so that more critical cases have a greater guarantee that the error will not leave the interval, and less critical cases a smaller one. A certain indeterminacy in choosing α does not affect ε very strongly, because beyond some value α the width ε grows comparatively slowly.

Sometimes one prefers to fix the width of the confidence interval and determine the corresponding confidence probability, thereby establishing the percentage of cases in which the error will not exceed a value of interest.

Whether α or the interval width is taken as primary, relating α and ε requires knowing the distribution law of the estimate $\tilde{a}$, which depends essentially on the law of X and is usually unknown. The principal results for confidence intervals refer to samples from a normal general population.

In accordance with the central limit theorems (Section 9) we take the law of measurement errors as approximately normal, and in that approximation we compute confidence intervals for several estimates that occur most often in practice.

Procedures for computing confidence intervals and the corresponding presentation of experimental data are standardized by the state standards of all developed countries.

14. Problem 1. A Confidence Interval for the Estimate $\tilde{x}$ of the Mathematical Expectation when σ_X^2 Is Known (Normal X)

X is normal, so the estimate

$$\tilde{x} = (1/n)\,\Sigma_{i=1}^{n}\, x_i \tag{14.1}$$

being a sum of normal variables, is normal with mathematical expectation $\bar{x}$ and variance σ_X^2/n; its density is

$$f(\tilde{x}) = (1/(\sigma_{\tilde{X}}\sqrt{(2\pi)}))\,\exp(-(\tilde{x}-\bar{x})^2/(2\sigma_{\tilde{X}}^2)) \tag{14.2}$$

where $\sigma_{\tilde{X}} = \sigma_X/\sqrt{n}$. Hence

$$\alpha = P\{|\tilde{x}-\bar{x}| \le \varepsilon\} = \int_{\bar{x}-\varepsilon}^{\bar{x}+\varepsilon} f(\tilde{x})\,d\tilde{x} \tag{14.3}$$

With the substitution

$$Z = \varepsilon / \sigma_{\tilde{X}} = \varepsilon\,\sqrt{n} / \sigma_X \tag{14.4}$$

one obtains

$$\alpha = \Phi(Z) \tag{14.5}$$

where $\Phi(Z)$ is the Laplace function. Finally the relation between the confidence interval and the confidence probability is

$$\alpha = \Phi(\varepsilon / \sigma_{\tilde{X}}) = \Phi(\varepsilon\,\sqrt{n} / \sigma_X) \tag{14.6}$$

From a prescribed α and the Laplace table one obtains Z and then $\varepsilon = Z\,\sigma_{\tilde{X}} = Z\,\sigma_X/\sqrt{n}$. The result is written

$$\tilde{x} - \varepsilon \le \bar{x} \le \tilde{x} + \varepsilon \quad \text{or} \quad \bar{x} = \tilde{x} \pm \varepsilon \tag{14.7}$$

and one says that the random interval covers $\bar{x}$ with probability α, while a realized interval approximately contains $\bar{x}$ with probability α.

For integer arguments of Φ, using the relation $Z = \varepsilon/\sigma_{\tilde{X}}$,

$$\varepsilon = \sigma_{\tilde{X}}, \quad 2\sigma_{\tilde{X}}, \quad 3\sigma_{\tilde{X}}, \quad 4\sigma_{\tilde{X}} \tag{14.8}$$

the corresponding confidence probabilities (Table 5.1) are

$$\alpha = 0.683; \quad 0.954; \quad 0.9973; \quad 0.99994 \tag{14.9}$$

One often treats 0.9973 as practically 1 and writes

$$\bar{x} = \tilde{x} \pm 3\sigma_{\tilde{X}} \tag{14.10}$$

saying that the error “cannot leave three sigmas.” One should not forget that the “3σ rule” is rather artificial (there could be a “4σ rule”) and that the probability was obtained for a normal law of X. Raising the confidence probability from the “3σ rule” to the “4σ rule” increases the interval width by only one third.

15. Problem 2. A Confidence Interval for the Estimate $\tilde{\sigma}_X^2$ when $\bar{x}$ Is Known (Normal X)

X is normal. By the method of moments the estimates

$$\tilde{\sigma}_X^2 = (1/n)\,\Sigma_{i=1}^{n}\,(x_i - \bar{x})^2 \tag{15.1}$$

$$\tilde{\sigma}_X = \sqrt{\tilde{\sigma}_X^2} \tag{15.2}$$

are realizations of corresponding random variables whose distributions are initially unknown. One seeks an explicit expression for the confidence probability

$$\alpha = P\{|\tilde{\sigma}_X^2 - \sigma_X^2| \le \varepsilon\} \tag{15.3}$$

and thereby the dependence of the interval width ε on α. Introduce the dimensionless random variable

$$\xi = n\,\tilde{\sigma}_X^2 / \sigma_X^2 \tag{15.4}$$

and the new dimensionless width

$$\delta = n\,\varepsilon / \sigma_X^2 \tag{15.5}$$

Multiplying the original inequality by n/σ_X^2 yields the equivalent inequality

$$|\xi - n| \le \delta \tag{15.6}$$

with the new dimensionless random variable ξ and width δ. Consequently

$$\alpha = P\{|\xi - n| \le \delta\} = P\{n - \delta \le \xi \le n + \delta\} \tag{15.7}$$

Using the notation and (15.1),

$$\xi = \Sigma_{i=1}^{n}\,((x_i - \bar{x})/\sigma_X)^2 = \Sigma_{i=1}^{n}\,((X_i - \bar{x})/\sigma_X)^2 \tag{15.8}$$

Introduce

$$Y_i = (X_i - \bar{x})/\sigma_X, \quad \text{so that} \quad \xi = \Sigma_{i=1}^{n}\,Y_i^2 \tag{15.9}$$

The Y_i are normal, centered, and normalized:

$$M(Y_i) = (M(X_i) - \bar{x})/\sigma_X = 0 \tag{15.10}$$

$$D(Y_i) = D(X_i)/\sigma_X^2 = 1 \tag{15.11}$$

Thus ξ is a sum of squares of independent standard normal variables and follows the χ^2 law with n degrees of freedom (see the Appendix). Hence

$$\alpha = \int_{n-\delta}^{n+\delta} f_n(\xi)\, d\xi \tag{15.12}$$

This formula contains none of the parameters of X. Tables of the integral as a function of α and n appear in handbooks (Table 15.1: from n and $1-\alpha$ one finds δ). The confidence interval for the variance is then

$$(n/(n+\delta))\, \tilde{\sigma}_X^2 \le \sigma_X^2 \le (n/(n-\delta))\, \tilde{\sigma}_X^2 \tag{15.13}$$

$$\sqrt{(n/(n+\delta))}\, \tilde{\sigma}_X \le \sigma_X \le \sqrt{(n/(n-\delta))}\, \tilde{\sigma}_X \tag{15.14}$$

The χ^2 density is asymmetric, so the probabilities of leaving the interval to the left and to the right need not be equal. One may equalize them by choosing boundaries δ_1 and δ_2 so that each tail probability equals $(1-\alpha)/2$:

$$P(\chi^2 < \delta_1) = P(\chi^2 > \delta_2) = (1-\alpha)/2 \tag{15.15}$$

with $\delta_1 = \chi^2_{(1+\alpha)/2}$ and $\delta_2 = \chi^2_{(1-\alpha)/2}$ (significance levels). For example, for $\alpha = 0.92$ and $m = 19$ the tables give $\delta_1 \approx 7.6$ and $\delta_2 \approx 36.2$. The numbers δ_1 and δ_2 are defined so that

$$P\{\delta_1 \le n\, \tilde{\sigma}_X^2/\sigma_X^2 \le \delta_2\} = \alpha \tag{15.16}$$

$$P\{(n/\delta_2)\, \tilde{\sigma}_X^2 \le \sigma_X^2 \le (n/\delta_1)\, \tilde{\sigma}_X^2\} = \alpha \tag{15.17}$$

Thus $(n/\delta_2)\, \tilde{\sigma}_X^2 \le \sigma_X^2 \le (n/\delta_1)\, \tilde{\sigma}_X^2$ is a confidence statement for σ_X^2 with reliability α. The α-confidence interval is written

$$(n/\delta_2)\, \tilde{\sigma}_X^2 \le \sigma_X^2 \le (n/\delta_1)\, \tilde{\sigma}_X^2 \tag{15.18}$$

and analogously for the root-mean-square deviation

$$\sqrt{(n/\delta_2)}\, \tilde{\sigma}_X \le \sigma_X \le \sqrt{(n/\delta_1)}\, \tilde{\sigma}_X \tag{15.19}$$

One then says that with approximate probability α the corresponding parameters lie in those intervals.

16. Problem 3. Confidence Intervals for $\tilde{x}$ and $\tilde{\sigma}_X^2$ when Both Are Unknown (Normal X)

From the sample $x_1, \ldots, x_n$ determine confidence intervals for the unknown parameters $\bar{x}$ and σ_X^2 of a normal X. The required statements are of the form

$$P\{|\tilde{x} - \bar{x}| \le \varepsilon\} = \alpha \tag{16.1}$$

$$P\{|\tilde{\sigma}_X^2 - \sigma_X^2| \le \varepsilon\} = \alpha \tag{16.2}$$

This is the most common experimental case. Neither (16.1) nor (16.2) can be evaluated as in Problems 1 and 2, because both parameters are unknown.

The English statistician Student (W. Gosset, 1876–1939) constructed the new random variable

$$T = (\tilde{X} - \bar{x}) / \sqrt{(\tilde{\Sigma}_{\tilde{X}}^2)} = (\tilde{X} - \bar{x})\,\sqrt{n} / \sqrt{(\tilde{\Sigma}_X^2)} \tag{16.3}$$

taking into account the relation

$$\tilde{\Sigma}_{\tilde{X}}^2 = \tilde{\Sigma}_X^2 / n \tag{16.4}$$

T has a distribution that does not depend on the parameters of the normal law. Replacing the estimates by their sample expressions

$$\tilde{X} = (1/n)\,\Sigma\, X_i, \quad \tilde{\Sigma}_X^2 = (1/(n-1))\,\Sigma\,(X_i - \tilde{X})^2 \tag{16.5}$$

gives

$$T = \sqrt{n}\,(\tilde{X} - \bar{x}) / \sqrt{[\,(1/(n-1))\,\Sigma\,(X_i - \tilde{X})^2\,]} \tag{16.6}$$

Linear transformations of the sums lead to a representation through new normal variables

$$\xi_0, \xi_1, \ldots, \xi_{n-1} \tag{16.7}$$

each centered ($M(\xi_i) = 0$) and normalized ($D(\xi_i) = 1$). The new form is

$$T = \sqrt{(n-1)} \cdot \xi_0 / \sqrt{(\Sigma_{i=1}^{n-1}\, \xi_i^2)} \tag{16.8}$$

which contains none of the parameters of X; the law of T depends only on the sample size n.

Student obtained the density of T — Student's law with $(n-1)$ degrees of freedom —

$$f_T(t) = C_n\,(1 + t^2/(n-1))^{-n/2} \tag{16.9}$$

where the normalizing constant involves the gamma function with

$$\Gamma(n) = (n-1)! \tag{16.10}$$

for natural numbers n. The confidence interval for $\bar{x}$ follows after the transformations

$$\alpha = P\{|\tilde{x} - \bar{x}| \le \varepsilon\} = P\{|T| \le t_\alpha\} = S(t_\alpha) \tag{16.11}$$

where $S(t_\alpha) = P\{|T| \le t_\alpha\}$ is the tabulated Student distribution function (see the Appendix), and

$$t_{\alpha;n-1} = \varepsilon \sqrt{n} / \sqrt{\tilde{\sigma}_X^2} = \varepsilon / \tilde{\sigma}_{\bar{X}} \tag{16.12}$$

From the Student tables, for prescribed α and $f = n - 1$ one finds $t_{\alpha;f}$ such that

$$P\{|T| \le t_{\alpha;f}\} = \alpha \tag{16.13}$$

$$\tilde{x} - t_{\alpha;f}\, \tilde{\sigma}_{\bar{X}} \le \bar{x} \le \tilde{x} + t_{\alpha;f}\, \tilde{\sigma}_{\bar{X}} \tag{16.14}$$

In chemistry results are customarily presented for $\alpha = 0.95$ (a 95% confidence interval). The complementary probability $1 - \alpha$ is the significance level, which some tables list instead.

For the variance, the random variable

$$\xi = (n-1)\, \tilde{\sigma}_X^2 / \sigma_X^2 \tag{16.15}$$

follows the χ^2 law with $m = n - 1$ degrees of freedom. Proceeding as in Problem 2, from α and $m = n - 1$ one finds δ_1 and δ_2 such that

$$P(\chi^2 < \delta_1) = P(\chi^2 > \delta_2) = (1 - \alpha)/2 \tag{16.16}$$

These numbers satisfy

$$P\{\delta_1 \le (n-1)\, \tilde{\sigma}_X^2/\sigma_X^2 \le \delta_2\} = \alpha \tag{16.17}$$

$$P\{(n-1)/\delta_2 \cdot \tilde{\sigma}_X^2 \le \sigma_X^2 \le (n-1)/\delta_1 \cdot \tilde{\sigma}_X^2\} = \alpha \tag{16.18}$$

The α-confidence interval is written

$$(n-1)/\delta_2 \cdot \tilde{\sigma}_X^2 \le \sigma_X^2 \le (n-1)/\delta_1 \cdot \tilde{\sigma}_X^2 \tag{16.19}$$

$$\sqrt{((n-1)/\delta_2)}\, \tilde{\sigma}_X \le \sigma_X \le \sqrt{((n-1)/\delta_1)}\, \tilde{\sigma}_X \tag{16.20}$$

where $\tilde{\sigma}_X$ is computed from (12.6) or approximately taken as $\sqrt{\tilde{\sigma}_X^2}$.

17. Procedures

Problem No. 1 (known variance).

1. Sample $x_1, \ldots, x_n$.

2. Compute $\tilde{x} = (1/n)\,\Sigma\, x_i$.

3. With known σ_X, form $\sigma_{\tilde{X}} = \sigma_X/\sqrt{n}$.

4. Prescribe α and find Z from the Laplace table so that $\Phi(Z) = \alpha$.

5. Compute the error $\varepsilon = Z\,\sigma_{\tilde{X}}$ at the prescribed confidence probability.

6. Present the result as $\bar{x} = \tilde{x} \pm \varepsilon$ (or the corresponding closed interval) at the stated α.

Problem No. 2 (known mathematical expectation).

1. Sample $x_1, \ldots, x_n$.

2. Compute $\tilde{\sigma}_X{}^2 = (1/n)\,\Sigma\,(x_i - \bar{x})^2$ and $\tilde{\sigma}_X = \sqrt{\tilde{\sigma}_X{}^2}$.

3. For prescribed α and $m = n$ find δ_1, δ_2 in the χ^2 tables.

4. Present the result for $\sigma_X{}^2$: $(n/\delta_2)\tilde{\sigma}_X{}^2 \le \sigma_X{}^2 \le (n/\delta_1)\tilde{\sigma}_X{}^2$ at α.

5. Present the result for σ_X: $\sqrt{(n/\delta_2)}\tilde{\sigma}_X \le \sigma_X \le \sqrt{(n/\delta_1)}\tilde{\sigma}_X$ at α.

Problem No. 3 (both parameters unknown).

1. Sample $x_1, \ldots, x_n$.

2. Compute $\tilde{x}$ and $\tilde{\sigma}_X{}^2 = (1/(n-1))\,\Sigma\,(x_i - \tilde{x})^2$ (and $\tilde{\sigma}_X$ as needed).

3. From Student's tables at $\alpha = 0.95$ and $m = n - 1$ find $t_{\alpha;m}$.

4. Compute the α-confidence error $\varepsilon = t_{\alpha;m} \cdot \tilde{\sigma}_X/\sqrt{n}$ (if S denotes $\tilde{\sigma}_X$, use the same formula with S).

5. Present $\bar{x} = \tilde{x} \pm \varepsilon$, or the closed interval, at α.

6. From the χ^2 tables at the same α and $m = n - 1$ find δ_1, δ_2.

7–8. Present the intervals for $\sigma_X{}^2$ and σ_X as in (16.19)–(16.20).

18. A Numerical Example

Guessing at a distance the length of a 30-centimeter ruler by different people.

Problem No. 2 (known mathematical expectation $\bar{x} = 30$ cm; estimate σ_X).

X_1	X_2	X_3	X_4	X_5
42	17	33	45	25

$n = 5$. Values restored from the Russian original (pp. 57–60) and independently recomputed.

2. Variance about the known mean:

$$\tilde{\sigma}_X^2 = (1/n)\,\Sigma\,(x_i - 30)^2 = 114.4 \cong 114$$

$$\tilde{\sigma}_X = k_{n+1}\sqrt{\tilde{\sigma}_X^2} \cong k_6 \cdot 10.696 \cong 1.051 \cdot 10.696 \cong 11.24 \cong 11$$

3. For $\alpha = 0.95$ and $m = n = 5$, from the χ^2 tables: $\delta_1 = \chi^2_{0.975} = 0.831$, $\delta_2 = \chi^2_{0.025} = 12.8$.

4. Result for σ_X^2:

$$44.5 \le \sigma_X^2 \le 685 \quad \text{at } \alpha = 0.95$$

5. Result for σ_X:

$$6.7 \le \sigma_X \le 26.2 \quad \text{at } \alpha = 0.95$$

Problem No. 1 (same sample; known $\sigma_X = 11$; estimate $\bar{x}$).

2. Sample mean:

$$\bar{x} = (1/5)(42+17+33+45+25) = 32.4 \cong 32$$

3. Standard error:

$$\sigma_{\bar{x}} = \sigma_X/\sqrt{n} = 11/\sqrt{5} = 4.92 \cong 5$$

4. For $\alpha = 0.95$, $Z_{0.95} = 1.96$.

5. Error:

$$\varepsilon_{0.95} = 1.96 \cdot 4.92 = 9.64 \cong 10$$

6. Result:

$$22 \le \bar{x} \le 42; \quad \bar{x} = 32 \pm 10 \quad \text{at } \alpha = 0.95$$

7. “3σ rule”:

$\tilde{x} \pm 3\sigma_{\tilde{x}} = 32 \pm 15$ with probability $\alpha = 0.9973$

Problem No. 3 (same sample; both parameters unknown).

2. $\tilde{x} = 32$ (as above). Unbiased variance estimate:

$\tilde{\sigma}_X^2 = (1/(n-1)) \Sigma (x_i - \tilde{x})^2 = 544/4 = 136$

$\sqrt{\tilde{\sigma}_X^2} = \sqrt{136} \cong 11.7; \quad \tilde{\sigma}_X = k_5\sqrt{136} = 1.064 \cdot 11.7 = 12.45 \cong 12$

3. For $\alpha = 0.95$ and $n-1 = 4$, $t = 2.77$.

4. Confidence error for the mean:

$\varepsilon_{0.95} = (11.7/\sqrt{5}) \cdot 2.77 = 14.49 \cong 14$

5. Result for $\bar{x}$:

$18 \le \bar{x} \le 46$ at $\alpha = 0.95$

$\tilde{x} = 32; \quad S_0 \cong 11.7; \quad n = 5$ at $\alpha = 0.95$

6. For $m = 4$ and $\alpha = 0.95$: $\delta_1 = \chi^2_{0.975} = 0.484$, $\delta_2 = \chi^2_{0.025} = 11.1$.

7. Result for σ_X^2:

$49 \le \sigma_X^2 \le 1124$ at $\alpha = 0.95$

8. Result for σ_X:

$7 \le \sigma_X \le 33$ at $\alpha = 0.95$

> *Translator/editor note (LCC Research Lab).* In Problem 2 the mathematical expectation is known, so (11.7)–(11.8) use k_{n+1}; for $n = 5$ that is $k_6 \approx 1.051$ from Table 11.1. In Problem 3 both parameters are unknown, so (12.6) uses the table entry with index one less, $k_n = k_5 = 1.064$. The two factors are not interchangeable; they belong to different estimation conditions in the Russian original.

Verification note. The sample, rounded intermediates, and final intervals match the Russian original plates (pp. 57–60). Independent recomputation confirms the arithmetic; Problem 2 uses $\bar{x} = 30$ from the ruler length in the example title. $\sqrt{1124} \approx 33.5$ (source rounds to 33).

19. The Method of Least Squares

If a functional dependence of known form exists between measured quantities, known up to the numerical values of certain parameters, those parameters are estimated by the method of least squares.

Consider two quantities y and x related by

$$y = \varphi(x; a_1, a_2, \ldots, a_m) \tag{19.1}$$

where the form of φ is known and the constants a_l ($l = 1, \ldots, m$) are to be determined from experiment. Suppose that for n values ξ_i of the argument, n measurements η_i of the function are made ($i = 1, \ldots, n$). Because of measurement errors one obtains not the ideal pairs but values distorted by error. If the measured pairs were free of error they would satisfy

$$\eta_i = \varphi(\xi_i; a_1, \ldots, a_m), \quad i = 1, \ldots, n \tag{19.2}$$

In reality (19.1) is not satisfied strictly; those relations are therefore called conditional equations. The difference between the left- and right-hand sides of the i-th conditional equation is the residual (discrepancy) of the i-th measurement,

$$\varepsilon_i = \eta_i - \varphi(\xi_i; a_1, \ldots, a_m), \quad i = 1, \ldots, n \tag{19.3}$$

If $n < m$ the number of conditional equations is smaller than the number of unknown parameters and the estimates cannot be determined. If $n = m$ the problem reduces to solving a system of equations. If $n > m$ one must use the excess equations to obtain the best estimates of the a_j. In practice this arises when increasing the number of measurements is used to compensate for the inevitable error of each measurement.

In the method of least squares the constants a_l are chosen so that the sum of squared residuals is minimized:

$$S = \sum_{i=1}^{n} \varepsilon_i^2 = \min \tag{19.4}$$

S is a function of the unknown parameters, so (19.4) implies that all first partial derivatives vanish:

$$\partial S/\partial a_j = 0, \quad j = 1, \ldots, m \tag{19.5}$$

The system (19.5), called the system of normal equations, contains as many equations as unknown parameters, so a solution $a_1, \ldots, a_m$ exists. The method does not in general guarantee the most efficient estimates, but it is justified by the simplicity of the computational scheme and by the fact that in a number of cases it does give the best estimates.

In science and engineering experimental data are often described by approximating equations of the form

$$Y = a_0x_0 + a_1x_1 + \ldots + a_lx_l = \Sigma\, a_q\, x_q \tag{19.6}$$

where Y is the function under study and $x_0, \ldots, x_l$ are the variables.

Consider the first two cases: measurement of a constant $Y = a_0$ ($x_0 = 1$ and the remaining $a_q = 0$), and the linear equation $Y = a + bx$.

The first case was treated above as Problem No. 3: for a constant,

$$\tilde{y} \pm t_{0.05} \cdot S_0/\sqrt{n} \tag{19.7}$$

where $\tilde{y} = (1/n)\Sigma\, y_i$, $S_0^2 = (1/(n-1))\Sigma(y_i - \tilde{y})^2$, and $t_{0.05}$ is Student's coefficient for $f = n - 1$ degrees of freedom at significance level 0.05 (95% probability). If one does not standardize the 95% interval as the measure of error, the result may be presented as the triple of numbers

$$\tilde{y}, \quad S_0^2, \quad n \tag{19.8}$$

The second case is the linear equation $Y = a + bx$ that smooths the data (y_i, x_i) under condition (19.4). It is equivalent to

$$Y = \tilde{y} + b(x - \tilde{x}) \tag{19.9}$$

with $\tilde{y} = (1/n)\Sigma\, y_i$, $\tilde{x} = (1/n)\Sigma\, x_i$, $b = (1/B)\,\Sigma\, y_i(x_i - \tilde{x})$, and $B = \Sigma(x_i - \tilde{x})^2$. (Note that here $a = \tilde{y} - b\,\tilde{x}$.) The measurement result should therefore be presented either as a "95% confidence road" in the xOy-plane,

$$Y = \tilde{y} + b(x - \tilde{x}) \pm t_{0.05}\, S_0\, \sqrt{[1/n + (x - \tilde{x})^2/B]} \tag{19.10}$$

or as the six numbers

$$\tilde{y}, \quad n, \quad \tilde{x}, \quad b, \quad B, \quad S_0^2 \tag{19.11}$$

where

$$S_0^2 = (1/(n-2))\,\Sigma\,(y_i - Y_i)^2 \tag{19.12}$$

The number of degrees of freedom in this case is $f = n - 2$. The quantity $t_{0.05}$ is the two-sided Student critical value at significance level 0.05; for $f \geq 8$–12 it differs little from 2. Hence the recommendation to take enough measurements that $f > 8$–12, in which case $t_{0.05} \cdot S_0 \approx 2\, S_0$.

Source note. Section 19 appears in the sealed Word manuscript principally as embedded page images. The English text above was prepared from Vision OCR of those plates (Russian PDF pages 61, 63–65) and checked against the plate content; equation numbers (19.1)–(19.12) continue the edition's sectional numbering (the plates themselves number (1)–(12) locally).

20. References

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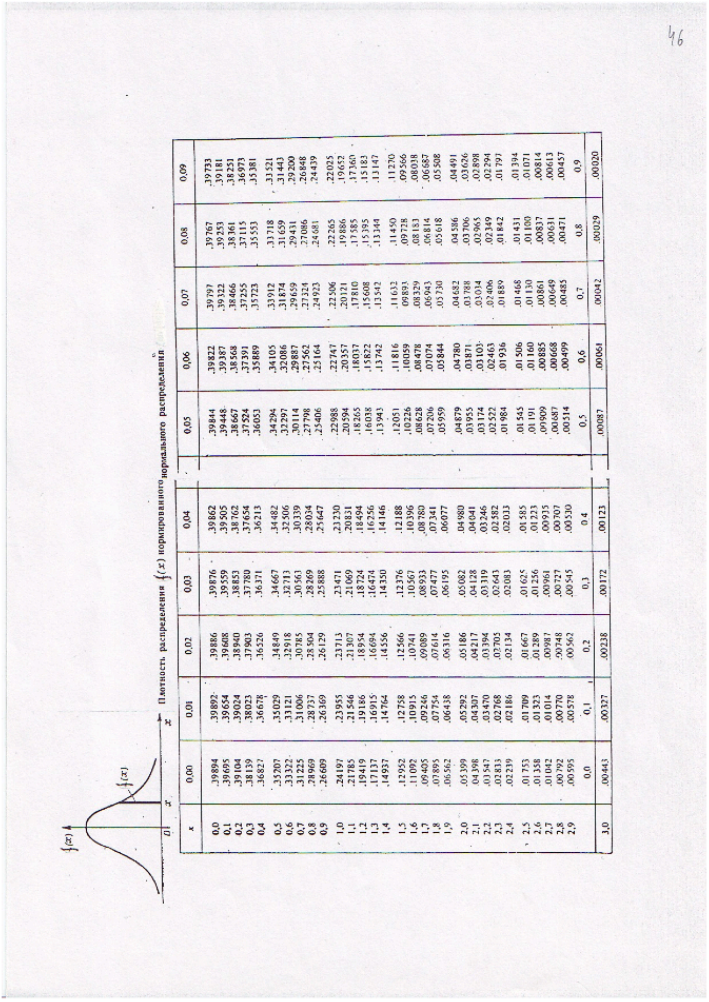
21. Appendix

On pages 74 and 75 of the 2023 Russian original the letter α denotes the significance level, which in the text is written as 1 − (confidence probability). In the literature one finds tables constructed both with the confidence probability and with the significance level 1 − α.

The statistical tables and figures of the Appendix are reproduced as facsimile plates from the author's original Russian edition (numerical values unchanged). English titles are supplied above each plate.

Appendix · Plate A

Appendix plate A — Probability density f(x) of the standardized normal distribution (facsimile of the author's table and figure).

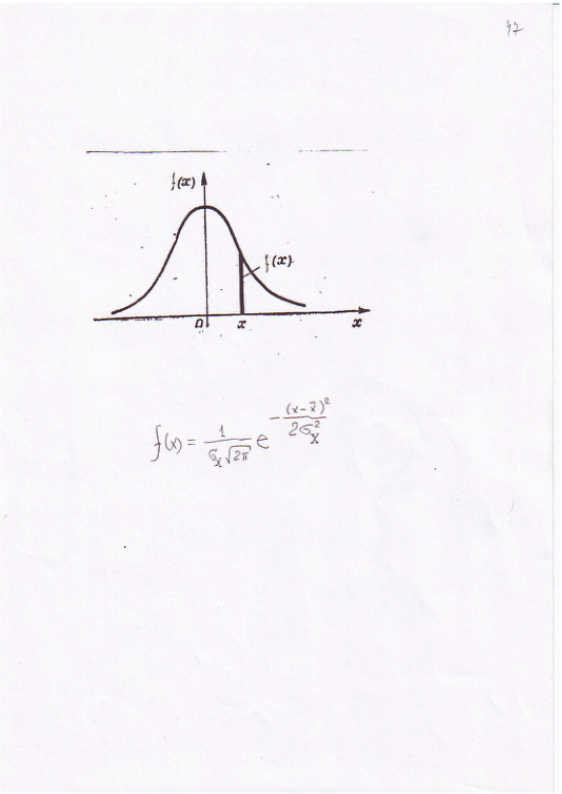


Плотность распределения $f(x)$ нормированного нормального распределения.

x	0,00	0,01	0,02	0,03	0,04	0,05	0,06	0,07	0,08	0,09
0,0	,39894	,39892	,39886	,39876	,39862	,39844	,39822	,39797	,39767	,39733
0,1	,39695	,39654	,39608	,39559	,39505	,39448	,39387	,39322	,39253	,39181
0,2	,39104	,39024	,38940	,38853	,38762	,38667	,38568	,38466	,38361	,38251
0,3	,38139	,38023	,37903	,37780	,37654	,37524	,37391	,37255	,37115	,36973
0,4	,36827	,36678	,36526	,36371	,36213	,36053	,35889	,35723	,35553	,35381
0,5	,35207	,35029	,34849	,34667	,34482	,34294	,34105	,33912	,33718	,33521
0,6	,33322	,33121	,32918	,32713	,32506	,32297	,32086	,31874	,31659	,31443
0,7	,31225	,31006	,30785	,30561	,30339	,30114	,29887	,29658	,29431	,29200
0,8	,28969	,28737	,28504	,28269	,28034	,27798	,27562	,27324	,27086	,26848
0,9	,26609	,26369	,26129	,25888	,25647	,25406	,25164	,24923	,24681	,24439
1,0	,24197	,23955	,23713	,23471	,23230	,22988	,22747	,22506	,22265	,22025
1,1	,21785	,21546	,21307	,21069	,20831	,20594	,20357	,20121	,19886	,19652
1,2	,19419	,19186	,18954	,18724	,18494	,18265	,18037	,17810	,17585	,17361
1,3	,17137	,16915	,16694	,16474	,16256	,16038	,15822	,15608	,15395	,15183
1,4	,14973	,14764	,14556	,14350	,14146	,13943	,13742	,13542	,13344	,13147
1,5	,12952	,12758	,12566	,12376	,12188	,12001	,11816	,11633	,11450	,11270
1,6	,11092	,10915	,10741	,10567	,10396	,10226	,10059	,09893	,09728	,09566
1,7	,09405	,09246	,09089	,08933	,08780	,08628	,08478	,08329	,08183	,08038
1,8	,07895	,07754	,07614	,07477	,07341	,07206	,07074	,06943	,06814	,06687
1,9	,06562	,06438	,06316	,06195	,06077	,05959	,05844	,05730	,05618	,05508
2,0	,05399	,05292	,05186	,05082	,04980	,04879	,04780	,04682	,04586	,04491
2,1	,04398	,04307	,04217	,04128	,04041	,03955	,03871	,03788	,03706	,03626
2,2	,03547	,03470	,03394	,03319	,03246	,03174	,03103	,03034	,02965	,02898
2,3	,02833	,02768	,02705	,02643	,02582	,02522	,02463	,02406	,02349	,02294
2,4	,02239	,02186	,02134	,02083	,02033	,01984	,01936	,01889	,01842	,01797
2,5	,01753	,01709	,01667	,01625	,01585	,01545	,01506	,01468	,01431	,01394
2,6	,01358	,01323	,01289	,01256	,01223	,01191	,01160	,01130	,01100	,01071
2,7	,01042	,01014	,00987	,00961	,00935	,00909	,00885	,00861	,00837	,00814
2,8	,00792	,00770	,00748	,00727	,00707	,00687	,00668	,00649	,00631	,00613
2,9	,00595	,00578	,00562	,00545	,00530	,00514	,00499	,00485	,00471	,00457
3,0	,00443	,00327	,00238	,00172	,00123	,00087	,00064	,00042	,00029	,00020

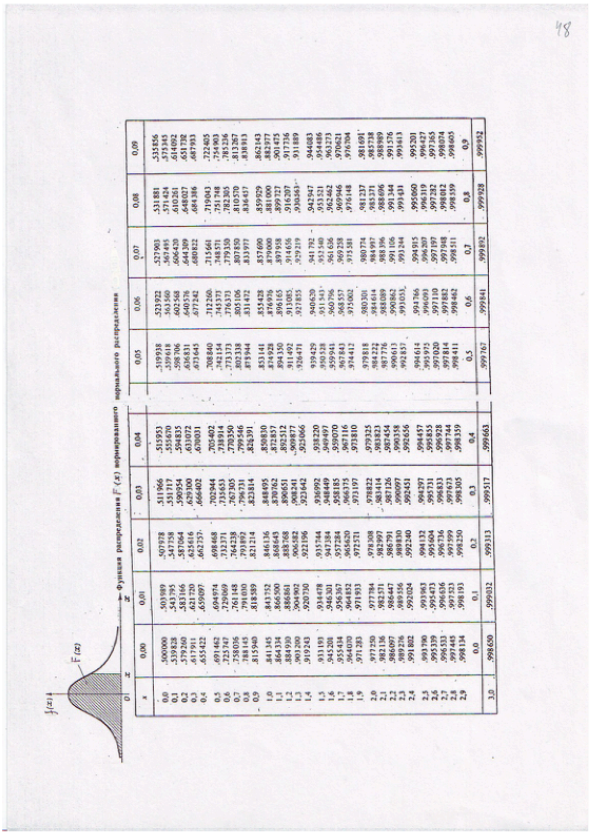
Appendix · Plate B

Appendix plate B — Normal density curve and formula for f(x) (facsimile).



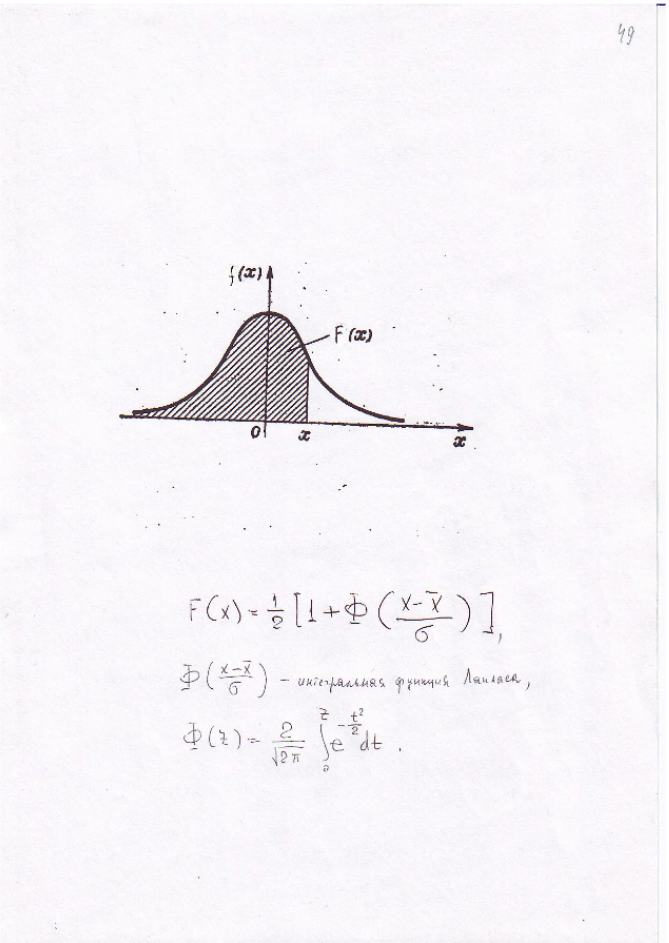
Appendix · Plate C

Appendix plate C — Distribution function F(x) of the standardized normal distribution (facsimile).



Appendix · Plate D

Appendix plate D — Normal integral illustration and Laplace-function formulae (facsimile).



Appendix · Plate E

Appendix plate E — Values of the integral Laplace function Φ(z) (facsimile).

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Значение интегральной функции Лапласа $\Phi(z)=\frac{2}{\sqrt{2\pi}}\int_0^z e^{-z^2/2}dz$

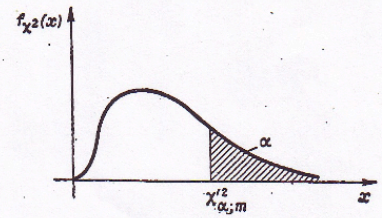
z	Φ (z)	z	Φ (z)
0	0	2.50	0.9876
0.25	0.1974	2.75	0.9940
0.50	0.3829	3.00	0.9973
0.75	0.5468	3.25	0.9988
1.00	0.6827	3.50	0.9995
1.25	0.7887	3.75	0.9998
1.50	0.8664	4.00	0.999937
1.75	0.9199	4.25	0.999965
2.00	0.9545	4.50	0.999993
2.25	0.9756	4.75	0.999997

Appendix · Plate F

Appendix plate F — Values of $\chi^2_{\alpha;m}$ and the χ^2 density sketch (facsimile).

Значения $\chi^2_{\alpha;m}$ для различных α и m

Число степеней свободы m	Уровень значимости α					
	0,99	0,975	0,95	0,05	0,025	0,01
1	0,00016	0,00098	0,0039	3,8	5,0	6,6
2	0,020	0,051	0,103	6,0	7,4	9,2
3	0,115	0,216	0,352	7,8	9,4	11,3
4	0,297	0,484	0,711	9,5	11,1	13,3
5	0,554	0 831	1,15	11,1	12,8	15,1
6	0,872	1,24	1,64	12,6	14,4	16,8
7	1,24	1,69	2,17	14,1	16,0	18,5
8	1,65	2,18	2,73	15,5	17,5	20,1
9	2,09	2,70	3,33	16,9	19,0	21,7
10	2,56	3,25	3,94	18,3	20,5	23,2
11	3,05	3,82	4,57	19,7	21,9	24,7
12	3,57	4,40	5,23	21,0	23,3	26,2
13	4,11	5,01	5,89	22,4	24,7	27,7
14	4,66	5,63	6,57	23,7	26,1	29,1
15	5,23	6,26	7,26	25,0	27,5	30,6
16	5,81	6,91	7,96	26,3	28,8	32,0
17	6,41	7,56	8,67	27,6	30,2	33,4
18	7,01	8,23	9,39	28,9	31,5	34,8
19	7,63	8,91	10,1	30,1	32,9	36,2
20	8,26	9,59	10,9	31,4	34,2	37,6
21	8,90	10,3	11,6	32,7	35,5	38,9
22	9.54	11,0	12,3	33,9	36,8	40,3
23	10,2	11,7	13,1	35,2	38,1	41,6
24	10,9	12,4	13,8	36,4	39,4	43,0
25	11,5	13,1	14,6	37,7	40,6	44,3
26	12,2	13,8	15,4	38,9	41,9	45,6
27	12,9	14,6	16,2	40,1	43,2	47,0
28	13,6	15,3	16,9	41,3	44,5	48,3
29	14,3	16,0	17,7	42,6	45,7	49,6
30	15,0	16,8	18,5	43,8	47,0	50,9



Appendix · Plate G

Appendix plate G — Values of Student's $t_{\alpha;m}$ and $t'_{\alpha;m}$ with density sketch (facsimile).

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Значения $t_{\alpha;\,m}$ и $t'_{\alpha;\,m}$ для различных α и m

Число степеней свободы m	Уровень значимости α (двусторонняя ограниченная)					
	0,10	0,05	0,02	0,01	0,002	0,001
1	6,31	12,7	31,82	63,7	318,3	637,0
2	2,92	4,30	6,97	9,92	22,33	31,6
3	2,35	3,18	4,54	5,84	10,22	12,9
4	2,13	2,78	3,75	4,60	7,17	8,61
5	2,01	2,57	3,37	4,03	5,89	6,86
6	1,94	2,45	3,14	3,71	5,21	5,96
7	1,89	2,36	3,00	3,50	4,79	5,40
8	1,86	2,31	2,90	3,36	4,50	5,04
9	1,83	2,26	2,82	3,25	4,30	4,78
10	1,81	2,23	2,76	3,17	4,14	4,59
11	1,80	2,20	2,72	3,11	4,03	4,44
12	1,78	2,18	2,68	3,05	3,93	4,32
13	1,77	2,16	2,65	3,01	3,85	4,22
14	1,76	2,14	2,62	2,98	3,79	4,14
15	1,75	2,13	2,60	2,95	3,73	4,07
16	1,75	2,12	2,58	2,92	3,69	4,01
17	1,74	2,11	2,57	2,90	3,65	3,96
18	1,73	2,10	2,55	2,88	3,61	3,92
19	1,73	2,09	2,54	2,86	3,58	3,88
20	1,73	2,09	2,53	2,85	3,55	3,85
21	1,72	2,08	2,52	2,83	3,53	3,82
22	1,72	2,07	2,51	2,82	3,51	3,79
23	1,71	2,07	2,50	2,81	3,49	3,77
24	1,71	2,06	2,49	2,80	3,47	3,74
25	1,71	2,06	2,49	2,79	3,45	3,72
26	1,71	2,06	2,48	2,78	3,44	3,71
27	1,71	2,05	2,47	2,77	3,42	3,69
28	1,70	2,05	2,46	2,76	3,40	3,66
29	1,70	2,05	2,46	2,76	3,40	3,66
30	1,70	2,04	2,46	2,75	3,39	3,65
40	1,68	2,02	2,42	2,70	3,31	3,55
60	1,67	2,00	2,39	2,66	3,23	3,46
120	1,66	1,98	2,36	2,62	3,17	3,37
∞	1,64	1,96	2,33	2,58	3,09	3,29
	0,05	0,025	0,01	0,005	0,001	0,0005
	Уровень значимости α (односторонне ограниченные)					

