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Lecture's Notes

**METHODS OF COMPUTATIONAL MATHEMATICS AND
MATHEMATICAL PHYSICS, P.1**

MINISTRY OF EDUCATION AND SCIENCE OF UKRAINE
ODESSA STATE ENVIRONMENTAL UNIVERSITY

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There are considered the fundamental questions of modern calculational methods, which are used in in solving some important and complicated classes of problems in computational mathematics, mathematical physics, quantum geometry and mechanics, geophysics and so on.

For magisters and PhD students of the the specialities: "Calculational Mathematics", "Mathematical Physics", "Optics and Laser Physics" and so on.

В книзі 1 викладені фундаментальні питання сучасних обчислювальних методів, що використовуються у розв'язанні декотрих важливих і складних класів задач обчислювальної математики, математичної фізики, квантової геометрії та механіки, а також геофізики тощо. Для магістрів та аспірантів спеціальностей «Обчислювальна математика», «Оптика та лазерна фізика» «Математична фізика», тощо.

Навчальне видання

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Методи обчислювальної математики та математичної фізики, Ч.1
Конспект лекцій

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Introducing Remarks

Modern computers and personal computers gave researchers in various fields of science and technology reliable and durable tool for mathematical modeling of the most toughest problems. This contributed to a significant development and progress in various spheres of human activity. Realization of mathematical models on computers is using methods of computational mathematics, which, of course, constantly being improved with advances in computer technology.

Solution mathematical model of the problem, which is to ensure efficiency and optimality criterion can be obtained quickly by a corresponding efficient numerical algorithm.

Any reduction of problems of mathematical physics or engineering course reduced to the solution of algebraic equations with one or other structure. As a result, most methods of computational mathematics related to reducing the problem to a system of algebraic equations and their subsequent decisions.

One fairly common methods for solving problems of mathematical physics is the method of finite differences. In recent years, the problem is very actual widespread use different methods for constructing difference schemes in problems of quantum and geo-physics, modern hydrometeorology, etc.

These notes present a brief consideration of the classical questions of calculational mathematics, in particular, the numerical interpolation, differentiation and integration of functions, numerical methods for solving algebraic equations and their systems of ordinary differential equations, finite difference method and a series of new numerical methods used in solving a number of problems of theoretical and mathematical physics, quantum physics, etc.

Chapter 1 MATHEMATICAL MODELS AND NUMERAL METHODS

1.1 A Role of mathematical design is in decision of tasks of outward things

Stormy development of ECM was instrumental in the wide process of matematizacii of science, technique and economy, on the whole. Exactly development and application of mathematical methods of decision of the applied tasks on the base of ECM is the article of the modern applied mathematics. Mathematics — one of the oldest sciences — arose out of practical necessities of man.

Development of mathematics was instrumental in general scientific and technical progress of civilization, and the necessities of natural history, technique and practical activity of people, put before mathematics new tasks and stimulated its development.

On the role of mathematics in society the level of development of mathematical vehicle of science and degree of perfection of knowledges influences about probed object, possibility to describe it the most substantial lines and properties by the language of mathematical concepts, that possibility to build the mathematical model of probed object.

A mathematical model is built on the basis of some simplifications and idealization of object and that is why always his close description is. But due to replacement of real object it a mathematical model is possibility to formulate the task of his study as mathematical, for decision which apply a mathematical vehicle which does not depend on nature of probed object. Mathematical models — it, as a rule, various equalizations, which are the records of natural laws which manage probed by us object or by the phenomenon.

The study of the real phenomena or processes often conduces to the necessity of decision of differential equalization or system of such equalizations. Therefore differential equalizations which arise up as a result of research of these phenomena or processes name differential models. Differential equalizations are the special case of that plural of mathematical models which arise up in the process of study of the real world. A mathematical design is widely used in geophysics, chemistry, geology, biology, economy, sociology, ecology, medicine, psychology, linguistics and other sciences.

At the same differential model can describe processes or phenomena of different nature. Yes, model which is set equalization of type of $y' = ky$, the radioactive-decay of matter describes, and change of atmospheric pressure with

the change of height above an earthly surface, and cooling of body as a result of convective heat exchange with an environment.

And oscillation of bullet, suspended to pruzhinya can describe a model which is set equalization of $y'' + W^2 Y = 0$, and swing of the mathematical pendulum, and change of charge of condenser, the plates of which will lock on inductance, and turning vibrations, and others like that. Vibrations are different (mechanical, electromagnetic), but fundamental essence them identical, that is why they are described that mathematical model. Consequently, the same mathematical model can have many real prototypes.

However for description of different sides of one phenomenon sometimes there is a requirement in the use of other mathematical model. Such models mostly mutually complement each other.

Science history knows many examples, when within the limits of the successfully built mathematical model by calculations and reasonings, as they say, "on the tag of peer", it was succeeded to foresee existence of the new physical phenomena and object.

Yes, leaning on differential models, after implementation of difficult calculations there are astronomers of John Adams (England) in September in 1845 and Urbain Leverrier (France) in September in 1846 independent of each other came to the conclusion about existence of unknown until then planets and its placing specified. After the calculations of Leverrier an astronomer Galle (Germany) found this planet it was named Neptune.

This opening led to justice of heliocentric theory of M. Kopernik (1473-1543), which to it during three hundred years remained a hypothesis, to a great extent credible, but all the same by a hypothesis. Like on the "tag of peer" P. Lovell (USA) foresaw existence of ninth planet of the planetary system, which after his calculations in 1930y. opened K. Tombo (USA) and which was called Pluto.

English physicist John Maksvell (1831-1879) in labour the "Dynamic theory of the electromagnetic field" (1864) showed out the system of differential equalizations which in number link between itself to tension of the electric and magnetic fields. A conclusion about existence of hertzian waves and electromagnetic nature of light swam out from these equalizations.

G. Gertz (Germany) in 1883 extracted experimental hertzian waves, learned their nature, and in 1895 O. S. Popov (Russia) used these waves for transferrableness and acceptance of signals without send-offs on distance, putting beginning of development of technique of radio contact. This opening is basis of development of radio, television, radio-location.

The English physicist of P. Dirac in 1928 built mechanical equalization of electron quantum. Existence of elementary particle with a positive charge, mass of which equals mass of electron, swam out from his decision.

A physicist Anderson (USA) opened such particle in 1932 in composition ultrarayss and named it a positron. This was the first anti-particle. At present time different computational methods are widely used in modern particles and nuclear physics.

The method of mathematical design played a large role in shipbuilding and aircraft building. The mathematical models of constructions of ships are developed the Russian scientist, academician O. M. Krilevim (1863-1945), became basis of domestic shipbuilding.

Aircraft construction a long ago ran into negative, and at certain terms and by the harmful effect of vibrations of separate parts of aircrafts. When an aircraft arrives at certain speed which is named critical, there are samozbudni vibrations of wings and plumages in him. These vibrations which got the name of flatera often were reason of catastrophes of airplanes midair.

Developed the mathematical theory of flatera airplane in 30th of our age by then yet young mathematician M. V. Keldish (1911-1978), which became an academician later. He developed not only the methods of numeral calculation of flatera and his design in wind-channels but also offered the effective practical methods of fight against him. Then M. V. Keldish learned nature of other phenomenon which often was reason of failures of airplanes, speech goes about the phenomenon of shimi — samozbudni vibrations of nasal wheel of the three-wheeled undercarriage of airplane during rulinnya, running approach and run.

Such examples, when a differential model is certain enabled to foresee existence in nature of the certain phenomena or object, in science it is known much. All of them testify to the forecasting role of mathematics in science. Mathematics became the instruments of cognition of the material world. Surely they are actively used in modern geophysics, environmental sciences, sciences about the Earth.

1.2 Calculable experiment and the technological stages

The method of mathematical design is an effective mean of research of real object and phenomena. But with their complication mathematical models the calculations of which require enormous calculable work become complicated. It restrained the use of models in a scitech. as mathematical tasks of decision by hand. Application of fast-acting ECM for decision of the intricate

applied problems formed the new method of leadthrough of theoretical researches on the base of mathematical models is a calculable (or mathematical) experiment.

His basis is a mathematical design, by a theoretical base is the applied mathematics, technical are mighty ECM. A calculable experiment became the mean of decision of the thorny applied problems. Now select the five stages of technological cycle of calculable experiment: a construction of mathematical model of task, development of method of decision of mathematical model, programming, calculations, is on electronic calculable machines, analysis of results of calculations and application. Schematically the technological cycle of calculable experiment is represented on a Fig.1.1.

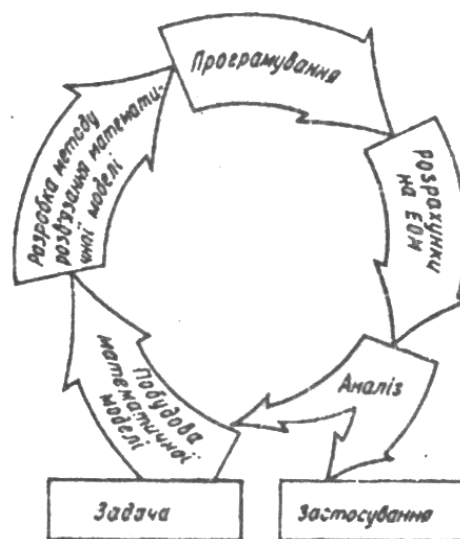


Figure 1.1.

On the first stage study essence of the probed phenomenon or process, find out his composition, conformities to law and interconnections of his separate parts. Select basic and second-rate factors in the phenomenon. On the initial stage of researches ignore the last. Basic factors and conformities to law of the probed phenomenon write down as mathematical formulas. More frequent all are differential or integral equalizations. At the same time set the limits of application of the built model, as not a single mathematical model is adequate reality.

Nature is considerably more rich and more various in the displays, than any mathematical models, that they are described. In the applied tasks construction of mathematical model - one of the most difficult and responsibility is stages of calculable experiment. Complication consists in that he requires combination of mathematical and special knowledges. Therefore above creation of mathematical model mathematicians and specialists of that industry which probed object belongs to work jointly.

When a mathematical model is built, proceed to its theoretical analysis: to probe how correctly a task is put, whether it has decision, unique he or not and others like that. Often decision the intricate applied problems begin and without an exhaustive analysis them mathematical properties, as it is possible to squander time for such analysis, which exceeds taken for decision of the applied task term.

The second stage of calculable experiment is link with the searches of method of decision of mathematical model. As a rule, the applied tasks are described models, decision which can not be found as analytical formulas. Then from the known numeral methods pick up most effective for the search of close decision model or develop a new method. The method of decision model is written down as an algorithm. It is possible to make for one mathematical task, as a rule, a few algorithms.

Determination of criteria for the estimation of quality of computational algorithms is the article of theory of numeral methods. Its primary purpose is a construction of effective numeral methods which would enable to find decision of the put mathematical task with the beforehand set exactness with the as possible less expenses of machine time. Estimating efficiency of numeral method, such his qualities take into account, as universality, simplicity of organization of calculable process to control of his exactness, speed of convergence, and firmness of calculable process.

During a calculable experiment it is important to use effective numeral methods, as for one tasks often it will be to execute plenty of calculations, changing some parameters only.

1.3 Some applications of calculable experiment

A mathematical design and leadthrough on his basis of calculable experiment is a mighty and economic advantageous mean for the leadthrough of not only scientific researches but also implementation of the most various experimental and designer works. Yes, leadthrough of calculable experiments at planning of airplanes and ships economic more advantageous from creation of experimental standards leadthroughs of model experiments, which can be dangerous for testers. In addition, a calculable experiment can be conducted for research of such situations which can not be reproduced in the real terms. Exactly with the help of calculable experiment study the evolution of Universe, evolution of life, on Earths or evolution of some populyacy, that the phenomena.

Will notice that calculable experiment not it can fully after to change the real, as he deals not with the phenomenon, but only with his mathematical model. But a calculable experiment can result in opening of the new real phenomena. Confirmation of it is opening of physical effect of T-layer by the group of scientists of Institute of the applied mathematics of Academy of

Sciences of the former USSR under the direction of A.M.Tikhonova and O.A. Samarskogo (1968).

Essence of this effect consists in that in plasma which co-operates with the magnetic field, at certain terms there can be areas in relation to a high temperature. These areas name thermal layers or 7- layers. An electric current which warms up plasma and supports a high temperature is concentrated in them. In a model experiment it was succeeded to find out the effect of T-layer only in a few years after his opening by a calculable experiment.

One of typical tasks for a calculable experiment is a problem of laser thermonuclear synthesis — inexhaustible source of receipt of energy. To take under control the process of thermonuclear synthesis (confluence of deuterons or tritium) and to learn them to lead — means decision power problem.

In 1962 the soviet scientists M. Basov and O. Krokhin advanced idea inflammation of thermonuclear reaction by lasers. It consists in that by a laser ray for very short time (10^{-9} c) to charge high energy small hard marble from the frozen mixture of heavy hydrogen and tritium (thermonuclear target). Energy of laser impulse will create in a thermonuclear target a high temperature which is pre-condition for the beginning of thermonuclear reaction. How here do processes flow in a target, are terms arrived at for the origin of thermonuclear reaction, how these terms depend on pair of meters of target, power of laser radiation, pulsewidth? To learn these and other questions today in a model experiment it is impossible even because there are not lasers with the proper descriptions.

Therefore the unique way of research is a calculable experiment, by which it was succeeded to set such details of laser thermonuclear synthesis, which scarcely will be set and measured even then, when the modern proper lasers will appear.

Due to a calculable experiment decision was succeeded not only many important applied tasks but also to check up some hypotheses of classic mathematics. The known topological task is a problem of four paints, formulated as early as 1852 London student Gutri. He discovered that by four paints it is possible to paint the map of England so, that each two nearby counties will be painted out in different colors, and pulled out a hypothesis that for painting of any map on a plane sufficiently four paints. This hypothesis was confirmed only in 1976 the American mathematicians of K.Appelem and V.Khakenom by ECM.

In modern a science by facilities of calculable experiment of rozv'yazuyut' task, decision with cosmonautics, technological processes, prognostication and

management, study of geo-, the ecological systems, and the astrophysical phenomena, by the study of fundamental problems in industry of genetics, biotechnology, chemistry, physics and economy.

1.4 Structure of error of decision of task

Building a mathematical model, try to find its decision. For the intricate applied problems, as a rule, there is not exact decision as obvious formulas or complete sequence of arithmetic operations, each of which is executed exactly. Then come running to the numeral methods — mighty mathematical mean of decision tasks.

The simplest numeral methods arose up and widely used long before appearance of ECM. But there are many applied tasks for which to find decision it are practically impossible without application of ECM.

Modern fast-acting ECM became a stimulus for development of new numeral methods. To apply numeral methods for decision of the applied tasks on the base of ECM it is needed carefully, as exactness of found decision depends on many factors. Thus it follows to be able to estimate the error of numerous decisions and calculations.

The error of decision task consists of error of mathematical model, not removed error, error of method and calculable error. Error of mathematical model of decision with that a model is described by the phenomenon approximately, with suppositions and simplifications. It is therefore needed to know about exactness end-point, to simplify the construction of mathematical model.

A not removed error is predefined errors in the datains of task. It depends on the method of decision task. But, correctly to choose a method and define exactness of calculations, it is important to know the limits of not removed error.

Error of method connection with the necessity of replacement of continuous model discrete or with the precipice of endless iteration process after the complete amount of iterations.

An error which is reached from replacement of continuous model discrete is named the error of sampling (or by the error of approximation).

Except for the error of sampling, there is other type of error of numeral methods any methods the idea of iteration process during which the sequence of approaching is built by certain rule to the decision of task is underlaid. If this sequence has border, when the amount of members of sequence heads for endlessness, then this border will be decision of this task. But on ECM it is

possible to calculate the complete amount of members of sequence only. An error, caused the precipice of iteration process, is named the error of convergence. It is tried to erect the error of method to the size which in once or twice less from the error of datains.

Consequently, the errors of sampling or error of convergence can form the error of numeral method or for some methods both types of errors simultaneously.

All these errors and also the methods of their analysis and adjusting are examined at the construction of concrete numeral methods.

Calculable errors conection with errors of rounding off of numbers. Calculation, both hand and on ECM, execute with the certain amount of meaningful numbers. It brings in in a result a trunsaction error which accumulates during calculations. Errors of rounding off of numbers can variously influence on end-point. As a result of implementation of millions of operations, each of which brings in a small error, the total error of rounding off can considerably exceed the sought after result of calculations. But in the separate operations of error of rounding off can have different signs and partly to compensate each other.

Therefore, if there are not systematic reasons, the casual piling up of trunsaction errors is insignificant.

Systematic reason of piling up of errors is deduction of near after a size numbers, for example,, as at the small absolute error of numbers of x_1 and x_2 relative error $(\Delta x_1 + \Delta x_2) / |x_1 - x_2|$ can become large a result.

Calculable errors arise up and during transformation of numbers from one scale of notation in other, if basis of one scale of notation is not the degree of basis other. It can result in a volume, which in the new scale of notation a number will become irrational.

The loss of exactness can happen and at adding to the large number of very small numbers. For diminishing of error adding numbers costs in order of their growth. In machine arithmetic the commutative and distributive laws of algebra are not always executed. A computational algorithm needs to be built so that an error of rounding off was considerably less from all other errors.

1.5 Absolute and relative errors

Absolute error of close number. If a_0 is some number (it is known exactly or not exactly), and a - is a number, accepted for the close value of number of a_0 , by the error of close number a name the difference of $a_0 - a$. The exact number of a_0 is not known usually, that is why error of close number a defining is impossible. nevertheless it is always possible to specify a number which estimates this error. Number $\Delta(a) > 0$, that satisfies inequalities

$$|a_0 - a| < \Delta(a), \quad (1.1)$$

named the absolute error of close number a .

Obviously, such determination of absolute error is not synonymous.

Yes, if $a_0 = \pi$, and for a close value to take $a = 3,14$, taking into account, that $3,140 < \pi < 3,142$, it is possible to write down:

$$\begin{aligned} |\pi - a| &< 0.002, \\ |\pi - a| &< 0.01, \\ |\pi - a| &< 0.1 \end{aligned}$$

Each of numbers 0,002, 0,01, 0,1 will be the absolute error of number a . But than nearer between itself number $|a_0 - a|$ and $\Delta(a)$, the more precisely an absolute error estimates an actual error.

How absolute error $\Delta(a)$ close number and take on possibility least from numbers which satisfy inequalities (1.1). Inequality (1.1) is tantamount inequalities:

$$a - \Delta(a) < a_0 < a + \Delta(a), \quad (1.2)$$

An absolute error is sometimes named the estimation of exactness of close number.

Relative error of close number. Absolute error $\Delta(a)$ numbers of the number of a_0 accepted for close value, not always is comfortable description of degree of exactness a , but as approaching to a_0 . An error in one meter is a flagrant error at measuring of length of apartment, but it can be examined as a small error at measuring of distance between two remote points of earthly surface. Consequently, except for the size of absolute error, it is necessary yet to know its attitude toward measureable (whether that is calculated) a size, mainly expressed in percents.

By the relative error of close number a is the relation of absolute error named $\Delta(a)$ to the module of this number. A relative error is reflected through $\delta(a)$:

$$\delta(a) = \Delta(a)/|a| \text{ or}$$

$$\text{in \% } \delta(a) = \Delta(a)/|a| \cdot 100\%.$$

Yes, relative error of number 3,14, number accepted for a close value π , at $\Delta(3,14)=0,002$ evened

$$\delta(3,14)=0,00064.$$

In technical calculations exactness of measurings is usually characterized a relative error. A result is considered beautiful, if a relative error does not exceed 0,1%.

Rule rounding off of numbers. Rounding off of number consists in a casting-out in it of all numbers which swim out after some digit. Thus if round-off number unit, the throw-away numbers of whole part deputize zeros. Rounding off ordinary is done by following rule:

If the first number which is cast aside, less than p'yati, a previous number does not change.

If the first number which is cast aside, anymore five, a previous number is increased on unit.

At rounding off of integers usually in place of throw-away numbers write down not zeros, but number 10, in the proper degrees.

If at rounding off of number the last zeros which are kept numbers, it costs to write down them. Yes, a number 1,2997, round-off to 0,001, assumes an air 1,300.

There is an additional error — transaction which does not excel the half of unit of digit of the last number error at rounding off of number. An absolute error of round-off number is the sum of it primitive absolute error and transaction error.

Meaningful, faithful and doubtful numbers. The Meaningful number of close number is naming any his number, beginning from the first (to unzero). For example, in a number 0,00030900 the first four zeros are not meaningful numbers. All other numbers (including next three zeros) are meaningful.

By the faithful number (by a faithful sign) of close number and is any named it meaningful number which an absolute error is for $\Delta(a)$ does not exceed the half of digit of this number. Other meaningful numbers of number a are named doubtful.

Faithful numbers over are brought in the mathematical tables of values of functions only. Absolute error of tabular values, for example, in three-digit tables not exceeds $0,5 \cdot 10^3$, in sevenvalue — $0,5 \cdot 10^7$.

Exactness of close number depends not on the amount of meaningful numbers, but from the amount of faithful numbers.

A final close result is usually rounded off to his faithful numbers, abandoning one doubtful. At calculations with close numbers in intermediate results keep one, two, and sometimes and three doubtful numbers.

1.6 Concept of firmness and correctness

Errors in the datains of task — not removed. A calculator can not decrease them, but must know how they influence on exactness of end-point. One tasks have an error of result of the same order, as well as order of error of datains, in other tasks the error of result can on a few orders exceed the error of datains. The sensitiveness of task to inaccuracies in datains is characterized the concepts of firmness.

Is a task named a bar from entrance data, if it decision the continuous depends on datains, that to the small increase Δx entrance size does a small increase answer Δy sought after decision.

In other words, the small errors of datains are caused by the small errors of decision task.

If this condition is not executed, a task is considered unsteady from entrance data. It means that even the insignificant errors of datains can result in the large errors of decision, that decision can be quite distorted.

Therefore to apply directly to such tasks numeral methods it is impossible, as errors of rounding off at application of method will catastrophically accumulate during calculations. Will make an example of unsteady task which belongs Wilkinson. The roots of polynomia

$$P(x) = (x - 1)(x - 2) \dots (x - 20) = x^{20} - 210x^{19} + \dots \quad (1.3)$$

are numbers $x_1=1, x_2=2, \dots, x_{20}=20$.

Let one of roots of polynomial (1.3) be calculated with an insignificant error. For example, coefficient -210 at x_{19} it is transferable on a coefficient $-210 + 2^{-23}$. Then something the changed polynomial of $P(x) = P(x) - 2^{-23}x^{19}$ has to two decimal (after a comma) signs have such round-off scolded:

$$x_1=1,00; x_2=2,00; \dots; x_8=8,01; x_9=8.92;$$

$$x_{10,11} = 10,10 \pm 0.64i; x_{12,13} = 11,79 \pm 1,65i; \dots;$$

$$x_{18,19} = 19.50 \pm 1.94i; x_{20} = 20.85.$$

Insignificant error, in a coefficient -210 this polynomial caused other values of roots. Reason of it is instability of task, as roots calculated within 11 meaningful numbers the error of rounding off is insignificant. Sometimes during decision of proof from entrance data task not proof there can be a method of it decision.

We will enter the concept of correctness of task. A task is named correctly put, if for any datains from some class there is the unique and proof from entrance data it decision.

The task of calculation of roots of polynomial (1.3) is above-mentioned is uncorrectly put. For decision of grey tasks to apply classic numeral methods it does not cost, as errors of rounding off at calculations can catastrophic to grow and result in a result, to distant from shukanogo of decision. For decision of not reasonably tasks use the so-called methods of regularization, which replace this task correctly put.

Chapter 2 INTERPOLATION OF FUNCTIONS

2.1 Raising of task

Let on a segment $[a; b]$ certainly certain class of functions $\{P(x)\}$, for example class of polynomials of algebra, and in points x_0, x_1, \dots, x_n this interval the value of some function is set $y_0 = f(x_0), y_1 = f(x_1), \dots, y_n = f(x_n)$. Close replacement of function of f on a segment $[a; b]$ one of functions of $P(x)$ of this class so that a function of $P(x)$ is in points x_0, x_1, \dots, x_n acquired those values, that and function of f , that $P(x_i) = y_i$ ($i = 0, 1, \dots, n$), name interpolation, or by interpolation. Points of x_0, x_1, \dots, x_n name the knots of interpolation, function of $P(x)$ — by an interpolating function, and formula of $f(x) \approx P(x)$ by which calculate the value of function of f in an interval $[a; b]$, — by an interpolation formula.

From the geometrical point of view the task of interpolation consists in finding of curve $y = P(x)$ of certain class, which passes through the points of plane with co-ordinates (x_i, y_i) ($i = 0, 1, \dots, n$) (Fig. 2.1).

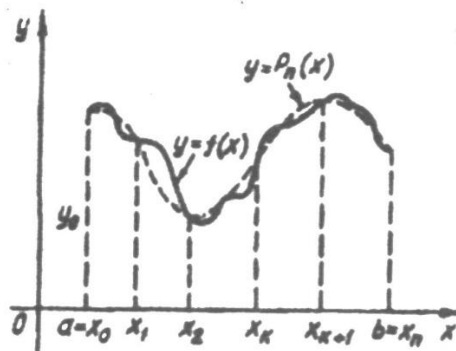


Figure 2.1 - Function $f(x_i, y_i)$ in the co-ordinates (x_i, y_i)

If the function of $P(x)$ belongs to the class of polynomials of algebra, interpolation is named parabolic.

Parabolic interpolation more comfortable in all, as polynomials, what simple after a form and does not have the special points, can acquire arbitrary values, easily to calculate them, to differentiate and integrate.

In some cases more expedient to use other classes of interpolating functions.

If, for example, the function of f is periodic, naturally to choose the function of $P(x)$ from the class of trigonometric polynomials, and if the function of f grows into endlessness in the set points or f near-by them, it is expedient to choose the function of $P(x)$ from the class of rational functions.

Will examine the task of parabolic interpolation only, which will formulate so: in $n+1$ different points X_0, X_1, \dots, X_n the value of function is set $f: Y_0 = f(X_0), Y_1 = f(X_1), \dots, Y_n = f(X_n)$ and it is needed to build a polynomial

$$P_n(x) = q_0 x^n + q_1 x^{n-1} + \dots + q_n, \quad (2.1)$$

degree of n , which would satisfy terms

$$f(x_i) = P_n(x_i), \quad i=0, 1, \dots, n \quad (2.2)$$

Polynomial of $P_n(x)$, which satisfies terms (2.2), does name an *interpolation polynomial* close equality of $f(x) \approx P_n(x)$ — by an *interpolation formula*, and difference of $R_n(f, x) = f(x) - P_n(x)$ — by *the remaining member* of interpolation formula.

Though interpolation polynomial which satisfies terms (2.2), and unique, the different forms of his record are however possible.

An interpolation polynomial is built then, when:

- 1) a function is set tabular for some values of argument, and it is needed to find its value for the values of argument, which are not in a table;
- 2) a function is set graphically, for example by a self-recording device, and it is needed to find its analytical expression is close;
- 3) a function is set analytical, but its expression is difficult enough and uncomfortable for implementation of different mathematical operations (differentiation, integration, and others like that).

2.2 Interpolation polynomial of Lagrange

Let in points x_i ($i = 0, 1, \dots, n$), where $X_0 < X_1 < \dots < X_n$ the value of function is set $f: Y_0 = f(X_0), Y_1 = f(X_1), \dots, Y_n = f(X_n)$. It is needed to build a polynomial $L_n(x)$ degree n , what in knots x_i ($i=0, 1, \dots, n$) acquires those values, that and function of f , that

$$L_n(x_i) = y_i, \quad i = 0, 1, 2, \dots, n. \quad (2.3)$$

Will search the interpolation polynomial of $P_n(x)$ will be by the polynomial of L_n in such kind:

$$L_n(x, x_i) = \frac{(x-x_0)(x-x_1) \dots (x-x_{i-1})(x-x_{i+1}) \dots (x-x_n)}{(x_i-x_0)(x_i-x_1) \dots (x_i-x_{i-1})(x_i-x_{i+1}) \dots (x_i-x_n)} \quad (2.4)$$

where

$$L_n(x_k, x_i) = \begin{cases} 0, & \text{if } k \neq i \\ 1, & \text{if } k = i \end{cases} \quad (2.5)$$

Then expression of interpolation polynomial $P_n(x)$ has

$$\begin{aligned} P_n(x) &= \sum L_n(x, x_i) y_i = L_n(x, x_0) y_0 + L_n(x, x_1) y_1 + \dots + L_n(x, x_n) y_n = \\ &= \frac{(x-x_1) \dots (x-x_n)}{(x_0-x_1) \dots (x_0-x_n)} y_0 + \frac{(x-x_1)(x-x_2) \dots (x-x_n)}{(x_1-x_0)(x_1-x_2) \dots (x_1-x_n)} y_1 + \dots + \frac{(x-x_0) \dots (x-x_{n-1})}{(x_n-x_0) \dots (x_n-x_{n-1})} y_n \end{aligned} \quad (2.6)$$

where polynomial of degree of n , answers, to the terms (2.5) and terms (2.3).

Is the polynomial of $P_n(x)$ of kind (2.6) named *the interpolation polynomial of Lagrange*, and close equality of $f(x) \approx P_n(x)$ — by *the interpolation formula of Lagrange*. $L_n(x, x_i)$ ($i=0, 1, \dots, n$) in the polynomial of Lagrange name the *coefficients of Lagrange*.

Will consider the two special cases of interpolation formula of Lagrange (2.6).

Let $n=1$, that value of function f it is set in two knots x_0 i x_1 . Will designate these values y_0 i y_1 .

Then from a formula (5.6) will get

$$P_1(x) = L_n(x, x_0) y_0 + L_n(x, x_1) y_1 = \frac{(x-x_1)}{(x_0-x_1)} y_0 + \frac{(x-x_0)}{(x_1-x_0)} y_1 \quad (2.7)$$

A formula (2.7) is named the formula of *linear interpolation*. At linear interpoluvanni arc of curve $y=f(x)$ on the segment $[x_0; x_1]$ replaced the segment of line (2.7) which lies between points $(x_0; y_0)$ i $(x_1; y_1)$.

2. Let $n=2$. Function f it is set in three knots x_i ($i=0, 1, 2$) by values y_i ($i=0, 1, 2$). In this case a formula (5.6) assumes an air

$$P_2(x) = L_2(x, x_0) y_0 + L_2(x, x_1) y_1 + L_2(x, x_2) y_2 \quad (2.8)$$

A formula (5.11) is named the formula of quadratic interpolation. At quadratic interpolating arc of curve $y = f(x)$ on the segment $[x_0; x_2]$ replaced the arc of parabola which passes through points $(x_i; y_i)$, $i=0, 1, 2$.

Estimation of error of interpolation formula of Lagrange, If a function of f is on a segment $[a; b]$ it is the polynomial of degree, that less or n is evened, from the unicity of interpolation polynomial swims out, that interpolation polynomial $L_n(x)$ evened identically f , that

$$f(x) - P_n(x) \equiv 0, x \in [a; b].$$

If f on a segment $[a; b]$ which contains the knots of interpolation x_i ($i=0, 1, \dots, n$), it is not the polynomial of degree, that less or n is evened, difference

$$R_n(f, x) = f(x) - P_n(x) \quad (2.9)$$

will equal a zero only in the knots of interpolation x_i ($i=0, 1, \dots, n$), and in other points of segment $[a; b]$ it is different from an identical zero.

Function $R_n(f, x)$, what characterizes exactness of approaching of function of f an interpolation polynomial $P_n(x)$, name the remaining *member of interpolation formula of Lagrange* (2.6), or *error of interpolation*.

If analytical expression of function of f is known, it is possible to estimate $R_n(f, x)$. Such theorem is just.

Theorem. If the knots of interpolation x_i ($i=0, 1, \dots, n$) are different and belong to the segment $[a; b]$, and the function of f is differentiated $n+1$ time on a segment $[a; b]$, for any point of $x \in [a; b]$ there is such point of $\xi \in [a; b]$, that for the error of interpolation just equality

$$|R_n(x)| \leq M_{n+1} \frac{|(x-x_0)(x-x_1)\dots(x-x_n)|}{(n+1)!} \quad (2.10)$$

where

$$M_{n+1} = \max |f^{(n+1)}(\xi)|.$$

From a formula (2.10) evidently, that the absolute error of interpolation formula of Lagrange is proportional work of two multipliers M_{n+1} and $|(x-x_0)(x-x_1)\dots(x-x_n)|$, from which M_{n+1} depends only on the function of f , and size of the second $|(x-x_0)(x-x_1)\dots(x-x_n)|$, it is determined exceptionally the choice of knots of interpolation. Is decreasing the size of absolute error of

interpolation formula of Lagrange possible such choice of knots of interpolation, which a multiplier is for $|(x-x_0)(x-x_1)\dots(x-x_n)|$ acquires the least maximal value on a segment $[a;b]$.

Example 1. To build the interpolation polynomial of Lagrange for the function of $f(x)=\ln x$ with the knots of $x=2,3,4$ and to estimate the error of interpolation polynomial at $x=2,5$. A value of function is in the knots of interpolation

Table 2.1

x	2,	3	4
$F(x)$	0,6931	1,0986	1,3863

Will build the polynomial of Lagrange on the following formula:

$$P_n(x) = \sum L_n(X, X_i) * Y_i = L_n(x, x_0) y_0 + L_n(x, x_1) y_1 + \dots + L_n(x, x_n) y_n =$$

$$= \frac{(x-x_1)\dots(x-x_n)}{(x_0-x_1)\dots(x_0-x_n)} y_0 + \frac{(x-x_1)(x-x_2)\dots(x-x_n)}{(x_1-x_0)(x_1-x_2)\dots(x_1-x_n)} y_1 + \dots + \frac{(x-x_0)\dots(x-x_{n-1})}{(x_n-x_0)\dots(x_n-x_{n-1})} y_n$$

where $n=2$ i

$$P_2(x) = 0.6931 \frac{(x-3)(x-4)}{(2-3)(2-4)} + 1.0986 \frac{(x-2)(x-4)}{(3-2)(3-4)} + 1.3863 \frac{(x-2)(x-3)}{(4-2)(4-3)} =$$

$$= -0.4713 + 0.7000x - 0.0589x^2.$$

For the estimation of error will take advantage of inequality

$$|R_2(2,5)| < M_3(2; 4) - \frac{|A_3(2,5)|}{3!}$$

where

$$|A_3(2,5)| = 0.5 * 0.5 * 1.5 = 0.375,$$

$$f(x) = \ln x, f'(x) = 1/x, f''(x) = -1/x^2, f'''(x) = 2/x^3$$

From here accordingly $M_3(2; 4) = 1/4$, and finally

$$|R_2(2,5)| < 0.25 \frac{0.375}{3!} = 0.0156.$$

In actual fact error less than. Determining $\ln 2,5$ chetiriznachnim tables, will find

$$\ln 2,5 - P_2(2,5) = 0,9163 - 0,9103 = 0,0057.$$

The interpolation polynomial of Lagrange can be built at any the location of knots of interpolation. Odnako, if it will be needed for the improvement of approaching to promote on unit the number of knots (that degree of polynomial) by addition of new knot, a polynomial of Lagrange will be pereobchisliti anew. In this relation considerably to use interpolation polynomial of Newton to the construction of which we pass.

2.3 Eventual differences and their properties

Let y_i ($i = 0, 1, \dots, n$) — a value is functions, $y = f(x)$, calculated for the equidistant values of argument x_i ($i = 0, 1, \dots, n$), $X_1 = X_0 + h$, $X_2 = X_0 + 2h, \dots$, $X_n = X_{n-1} + h = X_0 + nh$, де h — step of table.

Eventual, by the or tabular differences of the first order, or first differences, name numbers which equal the increases of values of functions:

$$\begin{aligned} y_1 - y_0 &= \Delta y_0 \\ y_2 - y_1 &= \Delta y_1 \\ &\dots\dots\dots \\ y_{i+1} - y_i &= \Delta y_i \\ &\dots\dots\dots \\ y_n - y_{n-1} &= \Delta y_{n-1} \end{aligned} \quad (2.11)$$

To grow on differences of the first order name *the differences of the second* an order, or by *the second differences*:

$$\Delta y_1 - \Delta y_0 = \Delta^2 y_0, \Delta y_2 - \Delta y_1 = \Delta^2 y_1, \dots, \Delta y_{n-1} - \Delta y_{n-2} = \Delta^2 y_{n-2} \quad (2.12)$$

In general, differences of any order k appear through the differences of $k-1$ of the order after formulas

$$\Delta^{k-1} y_{i+1} - \Delta^{k-1} y_i = \Delta^k y_i \quad (k=1, \dots, n, i=0, \dots, n-(k-1)) \quad (2.13)$$

Comfortably to write down successive differences as tables. Use two forms of tables: diagonal and horizontal.

The diagonal table of differences is reached then, when tabular differences in every column write down between the proper values diminished and difference. In a horizontal table tabular differences write down in one line from difference.

Both in diagonal and in horizontal tables will arrange to write down the eventual differences of all orders in units of lower digit of values of functions in the knots of interpolation. Farther will toe this line.

Connection between the derivatives of function and eventual differences. Let the function of f have on a segment $[a;b]$ continuous derivatives to the order of p inclusive. The determinations of derivative swim out, that

$$f'(x) = \lim_{h \rightarrow 0} \frac{\Delta f(x)}{h}$$

where

$$\Delta f(x) = f(x+h) - f(x), x, x+h \in [a;b].$$

For the small values of h a close formula swims out from here

$$f'(x) \approx \frac{\Delta f(x)}{h} \quad (2.14)$$

Find now

$$\lim_{h \rightarrow 0} \frac{\Delta^2 f(x)}{h^2} = \lim_{h \rightarrow 0} \frac{f(x+2h) - 2f(x+h) + f(x)}{h^2}$$

where $x, x+h, x+2h \in [a;b]$. At the permanent value of x i $h \rightarrow 0$ numerator and denominator of this shot head for a zero. For opening $\frac{0}{0}$ of vagueness of type will apply twice rule by L'opital. One will get

$$\lim_{h \rightarrow 0} \frac{\Delta^2 f(x)}{h^2} = \lim_{h \rightarrow 0} \frac{2f'(x+2h) - 2f'(x+h)}{2h} = \lim_{h \rightarrow 0} \frac{2f''(x+2h) - f''(x+h)}{1} = f''(x)$$

From here for small enough h one has a close formula

$$f'' = \Delta^2 f(x) / h^2 \quad (2.15)$$

For any natural p it is possible the analogical reasonings to get a close formula

$$f^{(n)} = \Delta^n f(x) / h^n \quad (2.16)$$

After formulas (2.14) — (2.16) it is possible to calculate the close value of profitable, but their exactness (for $n > 1$) is low enough. Therefore in calculable practice use more exact formulas.

From formulas (2.14) — (2.16) does swim out, that with diminishing of step of table of h in λ once do the first differences diminish approximately in λ once, second — in λ^2 , third — in λ^3 times et cetera/ If, in addition, with growth of order of derivative their modules grow slowly (not too quickly), and the step of table is small enough, the modules of differences will diminish with growth of their order. Therefore are there l differences at some $\Delta^l y$ will become less than half of unit more low comfort of tabular values of functions, and that is why it follows to consider with the accepted exactness, that they equal a zero, and to the difference $(l-1)$ of th order — steel.

But the values of function in a table give mostly approximately, that is why at the calculation of eventual differences an error grows. If for example, a transaction of tabular values of function error equals the half of unit of lower digit, the error of the first differences will equal one unit of lower digit (at implementation of operation of addition of algebra of error added) already, error of the second differences — to 2 units of lower digit, third — to 4 units et cetera, and the errors of eventual differences of order of l are evened 2^{l-1} units of lower digit of tabular values of function are evened.

From it swims out, that, when, for example, the fourth differences of the exact meanings of function differ one from other less than, than on the half of unit of lower digit, these differences, but the functions (the absolute error of which equals the half of unit of lower digit) calculated for a close value, can differ one from other already on $2^4=16$ units of lower digit of tabular values of function.

Therefore there are grounds to give such determination practically of permanent differences: if on some part of table all eventual differences of l -go order differ one from other no more than on 2^l units of lower digit of tabular values of function, these differences are named *practically permanent*.

Then differences $(l+1)$ of th order it is not needed to calculate, because they will consist only of doubtful numbers, but that is why within the limits of this exactness consider that they equal a zero and does not accept them in attention.

Properties of eventual differences:

1. Do the eventual differences of permanent C equal a zero, that $\Delta^k C = 0$.

2. Can the permanent multiplier of S be taken away for the sign of eventual difference $\Delta^k(Cf(x))=C\Delta^k f(x)$.

3. The eventual differences of sum of algebra of functions equal the sum of algebra of eventual differences of these functions, that

$$\Delta^k(f(x) \pm g(x)) = \Delta^k f(x) \pm \Delta^k g(x).$$

These mastivosgi swim out from determination of eventual differences.

4. Eventual difference of function $(x)=x^n$

$$\Delta(x^n) = nhx^{n-1} + \frac{n(n-1)}{2!}h^2x^{n-2} + \dots + nh^{n-1}x + h^n \quad (2.17)$$

Really,

$$\Delta(x^n) = (x+h)^n - x^n$$

Decomposing after the formula of binomial Newton expression $(x+h)^n$; will get a formula (2.17)

By 4 properties easily to get the successive eventual differences of polynomial

$$y = a_0x^n + a_1x^{n-1} + \dots + a_n$$

After properties 1-4 have

$$\Delta y = a_0nhx^{n-1} + (a_0\frac{n(n-1)}{2!}h^2 + a_1(n-1)h)x^{n-2} + \dots + a_{n-1}h$$

Consequently, the first difference of polynomial of n-go degree with the senior member of a_0x^n is the polynomial (n-1) of th degree with the senior member of a_0x^n

Calculating the successive differences of polynomial of any order like, make sure in justice of such theorem:

Theorem 1. If $f(x)$ — polynomial of n-go degree relatively x with a senior member a_0x^n , that difference $\Delta^k f(x)$ at $k < n$ is by the polynomial (n-k) of th degree with a senior member $a_0n(n-1)\dots(n-k+1)h^kx^{n-k}$, when $k=n$, $\Delta^n f(x) = a_0n!h^n$ i at $k > n$ difference $\Delta^k f(x) = 0$.

Theorem 2. If n-1 differences of function of f of steel are for any step of n, this function is the polynomial of n-go degree.

Theorem 2 widely apply in calculable practice. Due to it for finding of intermediate values of function by the table of differences with the permanent

step of h limited to the calculation of values of interpolation polynomials, the degree of which equals an order practically permanent differences .

Properties of eventual differences are formulated higher just only for the exact differences of function. But in the process of calculations of value become round, that is why order practically permanent differences substantially depends on exactness with which calculate the value of function, and from the size of step of table.

2.4 First interpolation polynomial of Newton

Let the value of function be set for the equidistant values of argument $x_0, x_1 = x_0 + h, x_2 = x_0 + 2h, \dots, x_n = x_0 + nh$.

Will designate these values of function accordingly through $y_0, y_1, y_2, \dots, y_n$.

Will build the interpolation polynomial of n -go degree of kind:

$$P_n(x) = q_0 + q_1 (x - x_0) + \dots + q_k (x - x_0) \dots (x - x_{k-1}) + \dots + q_n (x - x_0) \dots (x - x_{n-1}) \quad (2.18)$$

so that in the knots of interpolation x_i ($i = 0, 1, \dots, n$) he acquired the values of y_i (and $= 0, 1, \dots, n$), that satisfied terms

$$P_n(x_i) = y_i \quad (i = 0, 1, \dots, n) \quad (2.19)$$

It was before well-proven that the unique interpolation polynomial of degree of n is, which satisfies terms (2.19). There is an interpolation polynomial of Lagrange them. However, as a formula (2.18) shows, the interpolation polynomial of n -go degree can be written down in a kind, different from the interpolation polynomial of Lagrange. If in the polynomial of Lagrange each of elements is the polynomial of n -go degree and all elements between itself are equal in rights, in a polynomial (2.18) elements are polynomials the orders of which with a removal from the beginning rise on unit.

Using terms (2.19), will define coefficients $q_0, q_1, \dots, q_k, \dots, q_n$ polynomial (2.18).

Let in (2.18) $x = x_0$. From (2.19) will get

$$P_n(x_0) = q_0 = y_0.$$

If $x = x_1$, have

$$P_n(x_1) = q_0 + q_1 (x_1 - x_0) \quad \text{or}$$

$$q_1=(y_1-y_0)/(x_1-x_0)=\Delta y_0/h$$

Like, putting the found values of coefficients in a formula

$$q_2=\Delta^2 y_0/2h^2, \quad q_3=\Delta^3 y_0/3!h^3, \dots, q_n=\Delta^n y_0/n!h^n$$

Putting the found values of coefficients in (2.18), will get

$$\begin{aligned} P_n(X)=y_0+\Delta y_0/h*(X-X_0)+\Delta^2 y_0/2h^2*(X-X_0)(X-X_1)+\dots+ \\ +\Delta^n y_0/n!h^n*(X-X_0)(X-X_1)*\dots*(X-X_{n-1}) \end{aligned} \quad (2.20)$$

This polynomial is named the *first interpolation polynomial of Newton*. Replacing the function of $f(x)$ proper it by the interpolation polynomial of $R_r(x)$ of Newton, will get close equality

$$f(x) \approx P_n(x). \quad (2.21)$$

This formula is named the first interpolation formula of Newton. The polynomial (and formula) of Newton differs from the polynomial (and formulas) of Lagrange. But if these polynomials are built for the that function of f and the same system of knots of x_i ($i = 0, 1 \dots, n$), after a theorem about the unicity of decide of interpolation task they identically will be evened each other.

If to the set system of equidistant knots of interpolation to add another, the proper interpolation polynomial of Lagrange needs to be built anew, and one new element is added in the interpolation polynomial of Newton only, and the already calculated elements are kept without changes. From a formula (2.21) for $n=1$ will get the formula of linear interpolation

$$f(x) \approx y_0 + \Delta y_0/h * (X-X_0) \quad (2.22)$$

and for $n=2$ — formula of quadratic interpolation

$$f(x) \approx y_0 + \Delta y_0/h * (X-X_0) + \Delta^2 y_0/2h^2 * (X-X_0)(X-X_1). \quad (2.23)$$

In calculable practice more comfortable to use other form of record of polynomial of Newton (2.20). If to put $t=(x-x_0)/h$

$$x - x_0 = th, \quad x - x_1 = x - x_0 - h = th - h = (t-1)h, \quad x - x_2 = (t-2)h, \dots, \quad x - x_{n-1} = (t - (n-1))h$$

and (2.24) will get

$$P_n(x) = P_n(x_0 + th) = y_0 + \Delta y_0 t + 1/2! \Delta^2 y_0 t(t-1) + \dots + 1/n! \Delta^n y_0 t(t-1) \dots (t-(n-1)). \quad (2.24)$$

and the first interpolation formula of Newton (2.21)

$$f(x) \approx P_n(x_0 + th). \quad (2.25)$$

Difference

$$f(x) - P_n(x_0 + th) = R_n(x) \quad (2.26)$$

name the remaining member of the first interpolation formula of Newton.

As for this function of f and this system of equidistant knots of $(i=0, 1, \dots, n)$ there is the unique interpolation polynomial of degree of n , interpolation polynomials of Lagrange and Newton will coincide between itself, that $L_n(x)$ in $P_n(x)$. And that is why and the remaining member of interpolation formula of Newton (2.21) will coincide with the remaining member of formula of Lagrange. With introduction of variable of t a remaining member R_n acquires a kind

$$|R_n(x)| = |R_n(x_0 + th)| <$$

$$h^{n+1} \frac{|t(t-1) \dots (t-n)|}{(n+1)!} M_{n+1}$$

where $M_{n+1} = \max |f^{(n+1)}(x)|$

Formula (2.21) or (2.25) name also the interpolation formula of Newton for interpolation forward.

If the first differences of function practically to steel, use the formula of linear interpolation, and if the second differences of function practically to steel, use the formula of quadratic interpolation

2.5 Second interpolation polynomial of Newton

If the value of argument lies nearer to the end segment interpolation, to apply the first interpolation formula of Newton unprofitably, because the eventual differences of function of higher orders will not be enough. If, for example, it is needed to calculate the value of function in the point of $x \in [x_{n-1}, x_n]$, for the first interpolation polynomial of Newton there are only the first and second differences of function.

Therefore in the end segment interpolation use the polynomial of kind

$$P_n(x) = b_0 + b_1(x - x_n) + b_2(x - x_n)(x - x_{n-1}) + \dots + u_n(u - x_n) \dots (x - u_{m-(n-1)}) + \dots + u_m(u - u_m) \dots (u - u_1) \quad (2.27)$$

Coefficients of b_0, b_1, \dots, b_n polynomial (2.27) determine so that a yogo value in the equidistant knots of interpolation coincided with the value of the proper function, that the terms of P_n were executed $P_n(X_i) = Y_i$ ($i=0, 1, \dots, n$).

Putting consistently in a formula (2.27) in place of x value of x_n, x_{n-1}, \dots, x_1 , find the coefficients of b_0, b_1, \dots, b_n . If in (2.27) to put $x = x_n$, that will get

$$P_n(X_n) = b_0, \quad b_0 = P_n(X_n) = Y_n.$$

Let $x = x_{n-1}$, have

$$P_m(x_{m-1}) = u_0 + u_1(x_{m-1} - x_m) = u_0 - u_1 p \quad \text{that} \quad u_1 = \Delta u_{m-1} p$$

Putting in (2.27) $x = x_{n-2}$ and replacing the coefficients of b_0, b_1, \dots, b_n by their values, will get

$$b_2 = \Delta^2 y_{n-2} / 2h^2$$

In general, when $x = x_0$ from (2.27) find

$$b_n = \Delta^n y_0 / n! h^n$$

Putting the value of these coefficients in (2.27), have

$$P_n(X) = y_n + \Delta y_{n-1} / h (X - X_n) + \dots + \Delta^n y_0 / n! h^n (X - X_n) \dots (X - X_1) \quad (2.28)$$

This polynomial and name the *second interpolation polynomial of Newton*. Replacing the function of $f(x)$ the second interpolation polynomial of Newton, will get close equality

$$f(x) \approx P_n(x). \quad (2.29)$$

Equality (2.28) is named the second interpolation formula of Newton, and difference $f(x) - P_n(x) = R_n(x, f)$ — *remaining by the member of this formula*. From formulas (2.28) and (2.29) for $n=1$ will get the formula of linear interpolation

$$f(x) \approx y_n + \Delta y_{n-1}/h (X - X_n),$$

and for $n = 2$ — quadratic interpolation

$$f(x) \approx P_n(X) = y_n + \frac{1}{h} \Delta y_{n-1} (X - X_n) + \frac{1}{2!h^2} \Delta y_{n-2} (X - X_n) (X - X_{n-1})$$

In practical calculations more comfortable to use other record of polynomial (2.28). If to enter such denotation $t = (x - x_n)/h$ or $th = (x - x_n)$

And a polynomial (2.28) assumes an air then

$$\begin{aligned} P_n(x) = P_n(x_n + th) = & y_n + \Delta y_{n-1}t + \frac{1}{2!} \Delta^2 y_{n-2} t(t+1) + \\ & + \frac{1}{n!} \Delta^n y_0 t(t+1)(t+n-1) \end{aligned} \quad (2.30)$$

Are differences included in expressions of polynomial (2.28) (2.30) $\Delta y_{n-1}, \Delta^2 y_{n-2}, \dots, \Delta^n y_0$, what take place in the diagonal table of differences bias from below upwards, that is why a formula (2.30) is used for interpolation at the end of table. If is it needed to calculate the value of function in the point of x , after x_n take the nearest, but anymore than kh value of argument from a table, so that $x \in (x_{n-1}; x_n)$ i $|t| < 1$.

Therefore a formula (2.30) is named also the interpolation formula of Newton for interpolationa back.

As interpolation polynomials of Lagrange and Newton is the different forms of record of the same interpolation polynomial, an estimation of remaining member of formula of Newton will be the same, as well as for the formula of Lagrange, built for a that function and that system of knots.

Therefore for the absolute error of interpolation formula (2.30) there is a just estimation

$$|R_n(x)| = |R_n(x_n + th)| < \quad (2.31)$$

$$h^{n+1} \frac{|t(t+1) \cdots (t+n)|}{(n+1)!} M_{n+1}$$

where $M_{n+1} = \max |f^{(n+1)}(x)|$

If the derivative of function is unknown, but there are tabular differences of function to $(n+1)$ the th order, remaining member $R_n(x;f)$ interpolation formula (2.31) it is possible to give approximately a formula

$$R_n(x;f) \approx \Delta^{n+1} y \frac{|t(t+1)\cdots(t+n)|}{(n+1)!}$$

Example 2. To build the interpolation polynomial of Newton for a function $f(x)=\ln x$ with knots $x=2, 3, 4, 5$. A value of function is in the knots of interpolation

Table 2.2

x	2	3	4	5
y	0,6931	1.0986	1,3863	1.6094

Will build a table for the calculation of differences

Table 2.3

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$
2	0.6931	4055	—1178	532
3	1,0986	2877	—646	
4	1,3863	2231		
5	1.6094			

Here $n=3$, $h = 1$ and in force (2.20):

$$P_3(x)=0,6931+0,4055(x-2)-0,78/2*(x-2)(x-3)+0,0532/6**(x-2)(x-3)(x-4).$$

Example 3. In a previous example to estimate the error of interpolation polynomial of Newton at $x=3,5$

For the estimation of error will take advantage of inequality

$$|R_3(3,5)| \leq M_4(2; 5) - \frac{|A_4(3,5)|}{4!}$$

Accordingly $A_4(x) = (x-2)(x-3)(x-4)(x-5)$

and $|A_4(3,5)| = 1,5 * 0,5 * 0,5 * 1,5 = 0,5625$,

$$f(x) = \ln x, f'(x) = 1/x, f''(x) = -1/x^2, f'''(x) = 2/x^3, f(4) = -6/x^4$$

From $M_4(2; 5) = 3/8$ and finally $|R_3(3,5)| \leq 3/8 * 0,5625/4 = 0,0088$.

In actual fact error a bit less than. Determining $\ln 3,5$ on chetiriznachnikh tables, will find $\ln 3,5 - P_3(3,5) = 1,2528 - 1,2552 = 0,0024$.

Example 4. To calculate in points $x = 0.1, 0.9$ value of function of $y = f(x)$, set table. 2.4, comfortably to erect the process of calculations in a table. 2. Every next eventual difference goes out by deduction in previous the column of overhead line from nizhnei.

Table 2.4

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$
0	1.2715	1.1937	-0.0146	0.0007	-0.0001	0.0000
0.2	2.4652	1.1791	—0.0139	0.0006	-0.0001	
0.4	3.6443	1.1652	—0.0133	0.0005		
0.6	4.8095	1.1519	—0.0128			
0.8	5.9614	1.1391				
1.0	7.1005					

At $x = 0.1$ have $t = (x - x_0)/h = (0,1 - 0)/0.2 = 0.5$. On a formula (2.24) will get

$$f(0,1) = P_4(0,1) = 1.2715 + 0.5 * 1.1937 + \frac{0,5(0,5-1)}{2!} (-0.0146) + \frac{0,5(0,5-1)(0,5-2)}{3!} * 0.0007 + \frac{0,5(0,5-1)(0,5-2)(0,5-3)}{4!} (-0.00004) = -1.8702.$$

For comparison on the formula of linear interpolation get

$$f(0,1) = 1.8684$$

A value of function is in a point $x = 0.9$ it is needed to calculate on a formula (2.30). In this case have $t = (x - x_n)/h = (0.9 - 1) / 0.2 = -0.5$. Than

$$\begin{aligned} F(0,9) = P_n(0.9) &= 7.1,005 - 0.5 \cdot 1.1391 - \frac{0.5(-0.5+1)}{2!} (-0.0128) - \\ &- \frac{0.5(-0.5+1)(-0.5+2)}{3!} 0.0005 - \frac{0.5(-0.5+1)(-0.5+2)(-0.5+3)}{4!} (-0.0001) = \\ &= 7.1005 - 0.5698 + 0.0016 - 0.00003 + 0.000004 = 6.5325 \end{aligned}$$

We considered the construction of interpolation polynomial of Newton for equidistant knots.

Chapter 3 NUMERICAL DIFFERENTIATION OF FUNCTIONS

3.1 Introduction

By numerical differentiation of functions resort when asked tabular function, so

methods of differential calculus simply inapplicable or function when asked quite complex analytical expression and therefore the calculation of derivatives associated with considerable difficulties.

To build numerical differentiation formulas defined on the interval $[a; b]$ replace function f corresponding interpolation polynomial $P(x)$. Then

$$f(x) - P(x) = R(x, f), \quad (3.1)$$

where $R(x; f)$ - the error term interpolation formula.

If the function f on $[a; b]$ is derived to the n -th order inclusive, then differentiating the identity (3.1) in x , are

$$\begin{aligned} f'(x) - P'(x) &= R'(x, f), \\ f''(x) - P''(x) &= R''(x, f), \\ &\dots\dots\dots \\ f^{(k)}(x) - P^{(k)}(x) &= R^{(k)}(x, f) \end{aligned}$$

The approximate value of derivatives of f are the first terms of the right sides of equations:

$$f'(x) \approx P'(x), \quad f''(x) \approx P''(x), \dots, f^{(k)}(x) \approx P^{(k)}(x), \quad x \in [a, b] \quad (3.2)$$

Then the remaining members of $r_i(x)$ ($i = 1, 2, \dots, K$) numerical differentiation formulas (3.2) will be derived from the remaining member interpolation formula (5.55), ie

$$r_i(x) = f^{(i)}(x) - P^{(i)}(x) \quad (3.3)$$

It should be noted that the smallness of the remainder term interpolation formula $R(x; f)$ does not mean the smallness of the remaining members of the original (the error of numerical differentiation) $r_i(x)$, as derived from small functions can be quite large. For example, the function $y_1(x) = f(x)$ $y_2(x) = f(x) + \frac{\cos n^3 x}{n^2}$ for large values of n may vary in arbitrarily small

$$|y_1 - y_2| \leq \frac{|\cos n^3 x|}{n^2} \leq \frac{1}{n^2}.$$

But derivatives for some values of x and large values of n can vary significantly among themselves:

$$|y'_1 - y'_2| \leq \frac{n^3 |\sin n^3 x|}{n^2} \leq n |\sin n^3 x| \leq n$$

This shows that the continuous dependence of values of the derivative of the function does not exist. Therefore the problem of numerical differentiation, in general, are less accurate in operation compared to interpolation is ill-posed problems. Fig. 3.1 at the point x_i ordinates polynomial function f and R are the same, however tangential angular coefficients are significantly different.

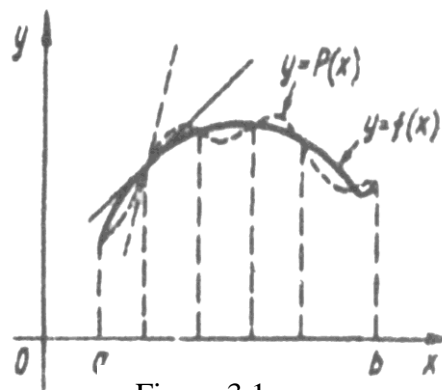


Figure 3.1

If interpolation polynomial P in a particular area with sufficient accuracy brings the function f , and she fairly smooth function f varies smoothly in this region, we can expect that at sufficiently small step interpolation polynomial interpolation derivatives as little different from original function f .

But we should not forget that with increasing order derivative precision numerical differentiation mostly falling sharply.

Therefore, in practice, numerical differentiation formulas for derivatives of higher second order is used infrequently.

3.2 Numerical differentiation formulas based on Newton's first interpolation formula

Let the function f given as equidistant points $X_i (i = 0, 1, \dots, n)$ segment $[a; b]$ values $Y_i = f(x_i) (i = 0, 1, \dots, n)$. To find the derivative f' i f'' a point x to close x_0 , function f approximate polynomial interpolation replace the first Newton (5.34),

built by nodes x_0, x_1, \dots, x_n .

$$P_n(x) = P_n(x_0 + th) = y_0 + \Delta y_0 t + \frac{1}{2!} \Delta^2 y_0 t(t-1) + \dots + \frac{1}{n!} \Delta^n y_0 t(t-1) \dots (t-(n-1)),$$

where $t = (x - x_0)/h$. Taking into account that the derivatives

$$df/dx = df/dt * dt/dx = 1/h * df/dt$$

prodyferentsiyuvavshy on t approximate equality (5.58), we receive:

$$\frac{d^2 f}{dx^2} = \frac{d}{dx} \left(\frac{1}{h} \frac{df(x)}{dt} \right) = \frac{1}{h^2} \frac{d^2 f}{dt^2}$$

$$y' \approx \frac{1}{h} (\Delta y_0 + \frac{2t-1}{2!} \Delta^2 y_0 + \frac{3t^2-6t+2}{3!} \Delta^3 y_0 + \dots) \quad (3.4)$$

$$y'' \approx \frac{1}{h^2} (\Delta^2 y_0 + \frac{6t-6}{3!} \Delta^3 y_0 + \dots) \quad (3.5)$$

Similarly, we can calculate higher order derivatives. If derivatives are calculated by formulas (3.4), (3.5) at x , then choose the closest point h_0 brief argument value that is less than the numerical differentiation formulas (3.4), greatly simplified if the values of the derivatives calculated at the nodes of interpolation. Since each tabulated values can be taken as h_0 then. putting in formulas (3.4) and (3.5), $t = 0$, we obtain

$$y' \approx \frac{1}{h} (\Delta y_0 - \frac{1}{2!} \Delta^2 y_0 + \frac{2}{3!} \Delta^3 y_0 + \dots) \quad (3.6)$$

$$y'' \approx \frac{1}{h^2} (\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12} \Delta^4 y_0 - \frac{5}{6} \Delta^5 y_0 + \dots) \quad (3.7)$$

Using equality (3.3), see the error of numerical differentiation formulas. Since the error term first interpolation formula

$$|R_n(x)| = |R_n(x_0 + th)| <$$

$$\text{where } M_{n+1} = \max |f^{(n+1)}(x)| \frac{h^{n+1} |t(t-1) \dots (t-n)|}{(n+1)!} M_{n+1}$$

Hence, if $t = 0$ ($x = x_0$) for remainder term numerical differentiation formula (3.6) we have

$$R_1(x) = (-1)^n \frac{h^n}{(n+1)!} f^{(n+1)}(\xi)$$

But the original $f^{(n+1)}(\xi)$ in many cases it is difficult to assess. Therefore, when sufficiently small h suggest that

Then the error term for derivative at $x = x_0$ is

$$R_1(x_0) = \frac{(-1)^n \Delta^{n+1} y_0}{h(n+1)}$$

The formulas of numerical differentiation, based on the second Newton interpolation formula.

To find the derivative of a function given in tabular equidistant nodes x_0, x_1, \dots, x_n , at x contained at the end of the table, use a second Newton interpolation formula (2.30). Writing each term of this formula in a series of n , formula (2.30) takes as follows:

$$\begin{aligned} P_n(x) = P_n(x_n + th) = & y_n + \Delta y_{n-1} * t + \frac{t^2 + t}{2!} * \Delta^2 y_{n-2} + \\ & + \frac{t^3 + 3t^2 + 2t}{3!} * \Delta^3 y_{n-3} + \dots + \frac{1}{n!} * \Delta^n y_0 * t(t+1) \dots (t+n-1) \end{aligned} \quad (3.8)$$

because

$$df/dx = df/dt * dt/dx = 1/h * df/dt \quad (3.9)$$

$$\frac{d^2 f}{dx^2} = \frac{d}{dx} \left(\frac{1}{h} \frac{df}{dt} \right) = \frac{1}{h^2} \frac{d^2 f}{dt^2}$$

then differentiating with respect to t approximate equality (3.8), we obtain

$$f'(x) = \frac{1}{h} \left(\Delta y_{n-1} + \frac{2t+1}{2!} * \Delta^2 y_{n-2} + \frac{3t^2+6t+2}{3!} * \Delta^3 y_{n-3} + \dots \right) \quad (3.10)$$

Example 1. Compute a point $x = 0.1$ the first and second derivatives of functions given table (Table. 3.1).

Table 3.1

x	Y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$
0	1.2833	0.5274	0.0325	0.0047	0.0002	0.0000

0.1	1.8107	0.5599	0.0372	0.0049	0.0002	
0.2	2.3606	0.5971	0.0421	0.0051		
0.3	2.9577	0.6392	0.0472			
0.4	3.5969	0.6864				
0.5	4.2833					

There $h=0.1$, $t=(0.1-0)/0.1=1$. Using these formulas (3.4) we find

$$y' = 10 \left(0.5274 + \frac{2 \cdot 1 - 1}{2} \cdot 0.0325 + \frac{3 \cdot 1 - 6 \cdot 1 + 2}{6} \cdot 0.0047 + \frac{4 \cdot 1 - 18 \cdot 1 + 22 \cdot 1 - 6}{24} \cdot 0.0002 \right) = 5.436,$$

$$y'' = 100 \left(0.0325 + \frac{6 \cdot 1 - 6}{6} \cdot 0.0047 + \frac{12 - 36 + 22}{24} \cdot 0.0002 \right) = -3.25.$$

Newton interpolation polynomial expression to make a difference through derivatives $\Delta^k y$ ($k=1, 2, \dots$). However, in practice it is often advantageous to express the value of derivatives not because of the difference, and directly through the function values at the nodes. To obtain these formulas is convenient to use Lagrange equation with a uniform units ($X_i - X_{i-1} = h = \text{const}$, $i = 1, 2, \dots, n$).

Chapter 4 NUMERICAL INTEGRATION FUNCTIONS

4.1 Statement of the problem

If the function f is continuous on the interval $[a, b]$ and famous and

original $F'(x)=f(x)$, the Newton-Leibniz formula holds:

$$\int_a^b f(x)dx = F(b) - F(a). \quad (4.1)$$

However, this formula is difficult and even virtually impossible to use then. when the original F can not be expressed in elementary functions, such as in the following integrals $\int_0^1 e^{-x^2} dx$, $\int_0^1 \frac{\sin x}{x} dx$; integrand f asked tabular or graphical and analytical expression of the unknown; analytical expression of the original F very complex and difficult to calculate.

In these cases it is necessary to build a formula for approximate calculation of definite integrals. Particularly important are the methods of numerical integration of functions where to find an approximate value of certain integral values are used integrand and its derivatives in a finite number of points that are predominantly interval of integration. These formulas calculate the approximate value of certain integral equations called mechanical quadrature, or quadrature formulas.

The most common quadrature formula in which the values of the integrand f at some points of the segment of integration, ie formulas look

$$\int_a^b f(x)dx \approx \sum_{k=1}^n A_k f(x_k) \quad (4.2)$$

The amount of the right side of (4.2) is called the quadrature sum, real numbers x_k and A_k respectively nodes and coefficients quadrature formula. We assume that nodes quadrature formula (4.2) are numbered in ascending order $x_1 < x_2 < \dots < x_n$:

Equality (4.2) close. The difference between the definite integral and quadrature sum

$$R_n(f) = \int_a^b f(x)dx - \sum_{k=1}^n A_k f(x_k)$$

called the remainder term or accuracy of the quadrature formula (4.2).

In the error arising from the replacement of integral quadrature sum (error method $|R_n(f)|$), is the error that caused the execution of arithmetic operations on approximate numbers – values $f(x_k)$ equal Δ_f , the absolute error of the

quadrature sum $\sum_{k=1}^n A_k f(x_k)$ equal

$$\tilde{R} = \Delta_f \sum_{k=1}^n |A_k|$$

This so-called fatal error that caused the approximate values $f(x_k)$. While there is no computation error due to rounding of intermediate results. This error can be made much smaller compared to the immeasurable if intermediate calculations comply with spare figures who reject the final result. Estimating the error of numerical integration, we must also take into account the final rounding error Δ_o . Thus, the total error of numerical integration Δ_i is the sum of the above three errors, ie

$$\Delta_i = |Rn(f)| + \tilde{R} + \Delta_o = |R(f)| + \Delta_f \sum_{k=1}^n |A_k| + \Delta_o \quad (4.3)$$

To construct quadrature formulas of the form (4.2) is often used to parabolic interpolation integrand f . To do this, in the interval $[a; b]$ choose a finite sequence of points $x_0, x_1, x_2, \dots, x_n$ i buduyut interpolyatsiyny Lagrange polynomial

$$\begin{aligned} P_n(x) &= \sum L_n(X, X_i) * Y_i = L_n(x, x_0) y_0 + L_n(x, x_1) y_1 + \dots + L_n(x, x_n) y_n = \\ &= \frac{(x-x_1)\dots(x-x_n)}{(x_0-x_1)\dots(x_0-x_n)} y_0 + \frac{(x-x_1)(x-x_2)\dots(x-x_n)}{(x_1-x_0)(x_1-x_2)\dots(x_1-x_n)} y_1 + \dots + \frac{(x-x_0)\dots(x-x_{n-1})}{(x_n-x_0)\dots(x_n-x_{n-1})} y_n \\ f(x) &= \frac{(x-x_1)\dots(x-x_n)}{(x_0-x_1)\dots(x_0-x_n)} y_0 + \frac{(x-x_1)(x-x_2)\dots(x-x_n)}{(x_1-x_0)(x_1-x_2)\dots(x_1-x_n)} y_1 + \dots + \frac{(x-x_0)\dots(x-x_{n-1})}{(x_n-x_0)\dots(x_n-x_{n-1})} y_n + R_n(f, x) \end{aligned}$$

$R_n(f, x)$ — error term (error) interpolation.

After integration last equality in x , ranging from a to b , we obtain

$$\int_a^b f(x) dx \approx \sum_{k=1}^n A_k f(x_k) + R_n(f) \quad (4.4)$$

where

$$A_k = \int_a^b \left(\frac{(x-x_1)\dots(x-x_n)}{(x_0-x_1)\dots(x_0-x_n)} y_0 + \frac{(x-x_1)(x-x_2)\dots(x-x_n)}{(x_1-x_0)(x_1-x_2)\dots(x_1-x_n)} y_1 + \dots + \frac{(x-x_0)\dots(x-x_{n-1})}{(x_n-x_0)\dots(x_n-x_{n-1})} y_n \right) dx \quad (4.5)$$

$$R_n(f) = \int_a^b R_n(f, x) dx. \quad (4.6)$$

If the error term $R_n(f, x)$ interpolation function f is small throughout the period $[a; b]$, then in (4.4), which is an exact equality of terms $R_n(f)$ can be neglected. Then we obtain an approximate equality

$$\int_a^b f(x) dx \approx \sum_{k=0}^n A_k f(x_k) \quad (4.7)$$

Quadrature formula (4.7), the coefficients of which are calculated by formulas (4.5) is called interpolation. Odds interpolation quadrature formulas are dependent on the choice of interpolation nodes, but not on the type of the integrand. Fair theorem, served without proof.

4.2. Main theorems and methods

Theorem. To quadrature formula (4.7) with $n + 1$ nodes was interpolation, it is necessary and sufficient that it is accurate if f is a polynomial of degree not higher than n . If the limits of integration a and b are nodes of interpolation, the quadrature formula (4.7) is called a closed formula type, otherwise - open.

From the formula (4.5) to calculate the coefficients A_k quadrature formula (4.7) shows that the values of the coefficients A_k are independent of the choice of the integrand f , and are dependent on the choice of units x_k ($k = 0, 1, \dots, n$). Having calculated the values of the coefficients A_k ($k = 0, 1, \dots, n$) once the formula (4.7) can be used to calculate approximate values of various functions defined by integrals f .

Equation (4.7) for exact polynomial n -th degree, but then $f(x) \equiv L_n(x)$ (interpolation error $R_n(f, x) = 0$). In particular, the formula (6.7) exactly when $f(x) = x^k$ ($k = 0, 1, \dots, n$). However, $R_n(x^{n+1}) \neq 0$.

They say that the quadrature formula has algebraic degree of precision n , if it is accurate to $f(x) = x^k$ ($k = 0, 1, \dots, n$) (or, equivalently, for any polynomial of degree not higher than n), and does not give an accurate result for $f(x) = x^{n+1}$. Thus, interpolation quadrature formulas with $n + 1$ nodes must algebraic degree of accuracy not less than n .

Formula rectangle. The approximate value of the integral $\int_{x_0}^{x_0+h} f(x) dx$, where f is

continuous on $[x_0, x_0+h]$, You can search for a function f polynomial interpolation replace zero degree, ie for all $x \in [x_0, x_0+h]$ put $f(x) = f(c)$, де $c \in [x_0, x_0+h]$. Then we obtain an approximate equality

$$\int_{x_0}^{x_0+h} f(x) dx \approx hf(c). \quad (4.9)$$

If $f(x) > 0$ and continuous on $[x_0, x_0+h]$, the approximate equality (4.9) can be interpreted geometrically as follows: approximate value for the area of the curvilinear trapezoid ABCD (Fig. 4.1) is bounded from below the abscissa, top graph of f , and the sides straight $x = x_0$ i $x = x_0+h$, set value area of the rectangle MNCD. Therefore, formula (4.9) was called formula of rectangles.

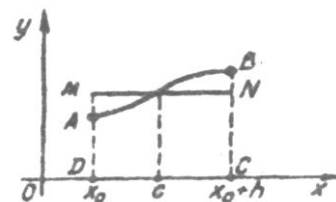


Figure 4.1

If $c = x_0$ або $c = x_0 + \frac{1}{2}h$, then (4.9) the formula is called left rectangles

$$\int_{x_0}^{x_0+h} f(x) dx = h_1 y_0 + h_2 y_1 + \dots + h_n y_{n-1} \quad (4.10)$$

If $c = x_0+h$, then (4.9) is called the formula right box

$$\int_{x_0}^{x_0+h} f(x) dx = h_1 y_1 + h_2 y_2 + \dots + h_n y_n \quad (4.11)$$

If $c = x_0 + \frac{1}{2}h$, then (4.9) the formula called medium rectangles.

$$\int_{x_0}^{x_0+h} f(x) dx = h \sum_{i=1}^n f\left(x_{i-\frac{1}{2}} + \frac{h}{2}\right) \quad (4.12)$$

Find the remaining members formulas rectangles, suggesting that the integrand function f on $[x_0; x_0+h]$ has continuous derivatives of the first order (in the case of formulas left and right rectangles) and continuous derivatives of the second order (in the case of formula medium rectangle).

Errors method for evaluating formulas:

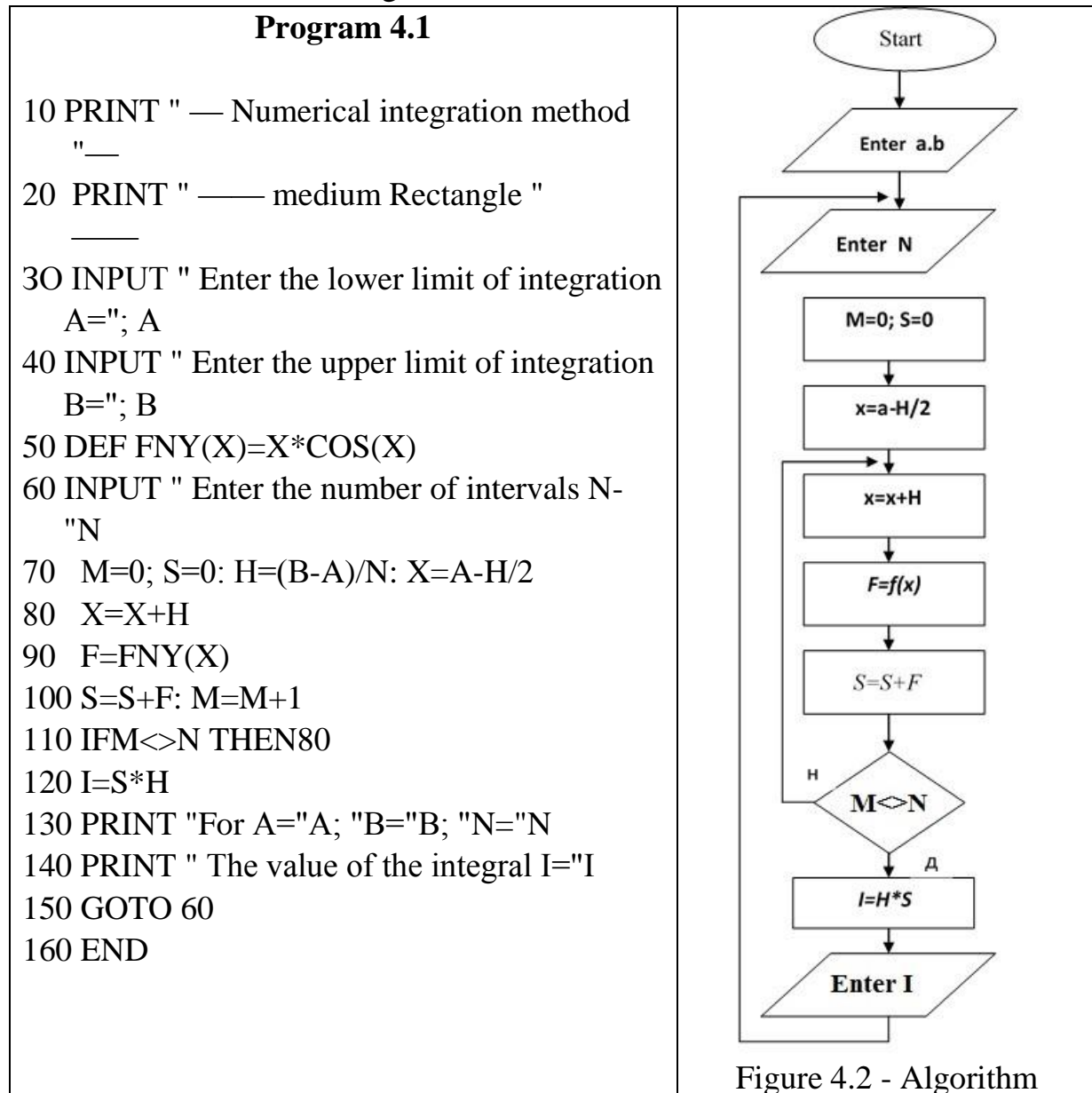
$$|R_1(f)| \leq h \frac{b-a}{2} M_1 = \frac{(b-a)^2}{2n} M_1, \quad (4.13)$$

$$|R_2(f)| \leq h^2 \frac{b-a}{24} M_2 = \frac{(b-a)^3}{24n^2} M_2, \quad (4.14)$$

where

$$M_1 = \max_{[a,b]} |f'(x)|, \quad M_2 = \max_{[a,b]} |f''(x)|,$$

Figure 4.2 presents the scheme of numerical integration algorithm functions by the formula medium rectangles.



Example 1. Method rectangles calculate the integral

$$I = \int_0^1 \frac{dx}{1+x^2}.$$

Formula "Left" rectangles (4.10). As we step constant $h = 0.1$, then the formula "Left" rectangles (4.10) have:

$$I = 0.1(1 + 0.990 + 0.962 + 0.917 + 0.862 + 0.800 + 0.735 + 0.671 + 0.610 + 0.552) = 0.8099$$

By formula "right" rectangles we obtain the following result:

$$I = 0.1(0.990 + 0.962 + 0.917 + 0.862 + 0.800 + 0.735 + 0.671 + 0.610 + 0.552 + 0.5) = 0.7599$$

The error in the calculation of the integral is $\Delta I_2 = I_2 - I = 0.00021$ (about 0.027%)

To calculate the integral in the formula "average" rectangles must first calculate the value of the function at points $X_{i+1/2}$

Table 4.1

$X_{i+1/2}$	0,05	0,15	0,25	0,35	0,45	0,55	0,65	0,75	0,85	0,95
$Y_{i+1/2}$	0,99	0,97	0,94	0,89	0,83	0,76	0,70	0,64	0,58	0,52

Then

$$\int_a^b f(x) dx = y_{1/2}h + y_{3/2}h + \dots + y_{i-1/2}h + \dots + y_{n-1/2}h = 0.7856$$

Formula Keystone. To calculate the approximate value $I = \int_{x_0}^{x_0+h} f(x) dx$ integrand f ,

is twice continuously differentiable on the interval $[x_0; x_0+h]$ ($h > 0$), replace interpolation Lagrange polynomial that passes through the points $(x_0; f(x_0))$ i $(x_0+h; f(x_0+h))$;

$$f(x) = \frac{x - x_0 - h}{x_0 - (x_0 + h)} f(x_0) + \frac{x - x_0}{x_0 + h - x_0} f(x_0 + h) + \frac{1}{2} f''(\xi)(x - x_0)(x - x_0 - h), \quad (4.15)$$

$$x_0 < \xi < x_0 + h$$

After integration this equality for x in the range of x_0 to $x_0 + h$, we obtain

$$\int_{x_0}^{x_0+h} f(x) dx = \frac{h}{2} (f(x_0) + f(x_0 + h)) + \frac{1}{2!} \int_{x_0}^{x_0+h} f''(\xi)(x - x_0)(x - x_0 - h) dx$$

Rejecting this equality in the error term

$$R_2(f) = \frac{1}{2!} \int_{x_0}^{x_0+h} f''(\xi)(x-x_0)(x-x_0-h)dx. \quad (4.16)$$

we obtain quadrature formulas

$$\int_{x_0}^{x_0+h} f(x)dx \approx \frac{h}{2} (f(x_0) + f(x_0+h)) \quad (4.17)$$

If $f(x)$ is continuous on the interval function is an integral $[x_0; x_0 + h]$, then the approximate equality (4.17) can be interpreted geometrically as follows: for the approximate value of the curvilinear trapezoid ABCD (Fig. 4.3) takes the shaded area of trapezoid ABCD. Therefore, the formula was called trapezoid formula.

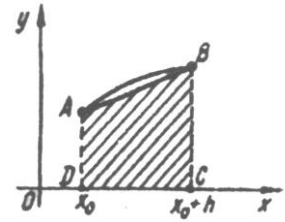


Figure 4.3

If $f'(x)$ continuous on the interval $[x_0; x_0+h]$, then applying generalized theorem to the integral of the mean (4.16), we find the absolute error estimate for numerical integration formula trapezoids:

$$|R_2(f)| \leq \frac{h^3}{12} M_2, \quad (4.18)$$

where

$$M_2 = \max_{[a,b]} |f''(x)|,$$

To calculate the approximate value of the integral $\int_{x_0}^{x_0+h} f(x)dx$, where f with continuous derivatives of first and second order in $[a; b]$, with reasonable accuracy, the interval $[a; b]$ is divided into n equal segments of length $h = (b - a)/n$ and each of the segments $[x_k, x_{k+1}]$, ($k = 0, 1, \dots, n-1$) apply a formula with remainder term trapezoids. While rejecting equality in the error term $R_2(f)$ obtain the quadrature formula

$$\int_a^b f(x)dx \approx \frac{1}{2} \sum_{i=1}^n h_i (y_{i-1} + y_i) \approx h \left(\frac{f(a) + f(b)}{2} + \sum_{k=1}^{n-1} f(a + kh) \right) \quad (4.19)$$

$$h = (b - a)/n$$

called general formula trapezoids.

Because $f''(x)$ continuous on the interval $[a; b]$, then there is a point $\eta \in [a; b]$ such that the error term of generalized formula shall become final form trapezoids

$$R_2(f) = -\frac{h^2}{12} (b-a) f''(\eta), \quad \eta \in [a; b] \quad (4.20)$$

From (4.20) it follows that the generalized trapezoid exact formula for the linear function for the second derivative of a linear function is zero. Calculate the error of numerical integration by general formula trapezoids impossible because point $\eta \in [a; b]$ Formula (4.20) is unknown. But it is easy to estimate the absolute error of the approximate integration formula (4.19)

$$|R_2(f)| \leq h^2 \frac{b-a}{12} M_2 = \frac{(b-a)^3}{12n^2} M_2, \quad (4.21)$$

where

$$M_2 = \max_{[a,b]} |f''(x)|, \quad h = (b-a)/n$$

Note: 1. The remaining members of the general formula rectangles and trapezoids medium (see. (4.14) and (4.20)) have opposite signs.

Thus, the formula approximating the integral of lack and excess, if $f''(x)$ keeps a sign on $[a; b]$. Therefore, the approximate value of the integral I can take pivsumu these bilateral approximations that put

$$I \approx 0,5(I_{cp} + I_{tp}) = I^*. \text{ Th}$$

en the absolute error of approximation I^*

$$|I - I^*| < \frac{1}{2} |I_{cp} - I_{tp}|.$$

Example 2. The method of trapezoids calculate the integral $\int_0^1 \frac{dx}{1+x^2}$,

Two faithful decimal digits.

To select a step, which we will calculate the values of the integrand, we estimate the magnitude of the correction member. Маємо:

$$f(x) = \frac{1}{1+x^2}, \quad f'(x) = \frac{-2x}{(1+x^2)^2}, \quad f''(x) = -2 * \frac{1-3x^2}{(1+x^2)^3}$$

and the interval $0 \leq x \leq 1$ $|f''(x)| \leq 2 |1-3x^2| \leq 4$.

By the condition of the task error should not exceed 0,005. We have:

$$\frac{1}{12n^2} 4 \leq 0.005 \quad \text{or} \quad n^2 \geq 200/3$$

For ease of computation it is desirable to step expressed a round number. Therefore, we take $n = 10$, then step $h = 0,1$. The error will be much less computation error formula, if ordinates are calculated to the nearest three decimal znakiv. Blank calculation will now type in Table 4.

Table 4.2

i	X_i	X_i^2	$1+X_i^2$	$Y_i=1/(1+X_i^2)$
0	0	0	1	1
1	0,1	0,01	1,01	0,990
2	0,2	0,04	1,04	0,962
3	0,3	0,09	1,09	0,917
4	0,4	0,16	1,16	0,862
5	0,5	0,25	1,25	0,800
6	0,6	0,36	1,36	0,735
7	0,7	0,49	1,49	0,671
8	0,8	0,64	1,64	0,610
9	0,9	0,81	1,81	0,552
10	1	1	2	0,5
				1,5 7,099

Hence, by virtue of formula (4.19) :

$$\int_0^1 \frac{dx}{1+x^2} \approx 0,1 (0,5*1,5+7.099) = 0,1*7,849 = 0,7854981.$$

For comp

arison, find the value given by the integral formula of Newton - Leibniz (to four decimal digits faithful):

$$\int_0^1 \frac{dx}{1+x^2} = \arctan x \Big|_0^1 = \arctan 1 - \arctan 0 = 0,7854.$$

Thus, in this case the formula trapezoids gave a more accurate result. The error here is $\Delta I_2 = -0.00042$ (about 0.054%).

Formula by Simpson. To build a three-point quadrature formula with equidistant nodes to calculate an approximate value $\int_{x_{i-1}}^{x_{i+1}} f(x) dx$, where $f(x)$ — continuous

on $[x_{i-1}; x_{i+1}]$ together with its derivatives up to fourth order inclusive, you can use interpolation Lagrange polynomial 2nd order, the schedule of which passes through the point:

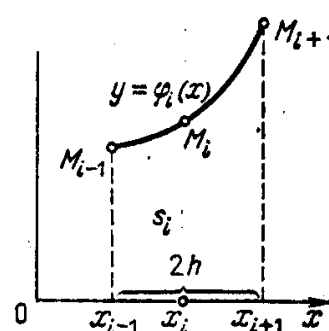


Figure 4.4.

$$M_{i-1}(x_{i-1}; f(x_{i-1})), M_i(x_i; f(x_i)), M_{i+1}(x_{i+1}; f(x_{i+1}))$$

and integrate it over x in the range of x_{i-1} to x_{i+1} , to $x_{i+1} - x_{i-1} = x_i - x_{i-1} = h$.

The unit area can be calculated by using the definite integral:

$$\begin{aligned} s_i &= \int_{x_{i-1}}^{x_{i+1}} \varphi_i(x) dx = \frac{1}{2h^2} \int_{x_{i-1}}^{x_{i+1}} [(x - x_i)(x - x_{i+1})y_{i-1} - 2(x - x_{i-1})(x - x_{i+1})y_i + (x - x_{i-1})(x - x_i)y_{i+1}] dx \\ &= \frac{h}{3} (y_{i-1} + 4y_i + y_{i+1}) \end{aligned}$$

After these calculations for each elementary segment $\{x_{i-1}, x_{i+1}\} (i=1, 2, \dots, n)$, summarize the equations:

$$S = \frac{1}{3} h (y_0 + 4y_1 + 2y_2 + 4y_3 + 2y_4 + \dots + 2y_{n-2} + 4y_{n-1} + y_n). \quad 4.22)$$

Thus, the formula can be written as:

$$\int_a^b f(x) dx \approx \frac{h}{3} [y_0 + 4(y_1 + y_3 + \dots + y_{n-1}) + 2(y_2 + y_4 + \dots + y_{n-2}) + y_n] + R(f) \quad (4.23)$$

This is Simpson's quadrature formula or formula with remainder term parabolas. It is exact for polynomials of the third degree, for the fourth order derivative of this polynomial is zero.

Assessment absolute error of numerical integration formula Simpson:

$$|R(f)| \leq h^4 \frac{b-a}{180} M_4 = \frac{(b-a)^5}{2880n^4} M_4, \quad (4.24)$$

where

$$M_4 = \max_{[a,b]} |f^{(4)}(x)|, \quad h = (b-a)/n$$

Example 3. Simpson's rule to calculate the integral $\int_0^1 \frac{dx}{1+x^2}$

All calculations will be carried out in Table 4.3

Table 4.3

i	X _i	Y _i =1/(1+x _i ²)		
		i=0, i=10	Непарні i	Парні i
0	0	1		
1	0,1		0,990	
2	0,2			0,962
3	0,3		0,917	
4	0,4			0,862
5	0,5		0,800	
6	0,6			0,735
7	0,7		0,671	
8	0,8			0,610
9	0,9		0,552	
10	1	0,5		

Find the value of the integral in formula (4.23):

$$\begin{aligned} \int_a^b f(x)dx &\approx \frac{0.1}{3} [1 + 4(0.990 + 0.917 + 0.800 + 0.671 + 0.552) \\ &\quad + 2(0.962 + 0.862 + 0.735 + 0.610) + 0.5] = 0.785398 \end{aligned}$$

If we compare the results of calculations of the integral obtained by three different methods then you can conclude the following:

Simpson's rule has higher accuracy; For Simpson's rule requires almost half the table of the function, because the method of rectangles need additional data in

secondary points.

Compare and practical error of quadrature formulas. Generalized formula trapezoids and Simpson - a formula of closed type. Medium Rectangle - open, and left and right rectangles - napivzamknutoho and semi-open type. As already stated, the exact value of the integral is determined by the formulas: left and right box if the integrand has become; rectangles and trapezoids medium if the integrand is linear, and the formula Simpson, if the integrand is a polynomial of degree not higher on the third.

The accuracy of the quadrature formula is characterized order remainder term $R(f)$ regarding the degree of integration step h . From formulas (4.13), (4.14), (4.21) and (4.23) shows that the error term $R(f)$ quadrature formulas depends on the integration step h i $R(f) \rightarrow 0$ ($h \rightarrow 0$). They say that the error term $R(f)$ the order p (p — integer) relatively h , if there is a finite boundary

$$\lim_{h \rightarrow 0} \frac{R(f)}{h^p} = M \neq 0$$

and record it so: $R(f) = O(h^p)$.

Thus, the remaining members formulas left and right rectangles h with respect to the first order: $R(f) = O(h)$, medium rectangles and trapezoids - second: $R(f) = O(h^2)$, and Simpson – fourth : $R(f) = O(h^4)$. Quadrature formulas considered the better, the more the order of the remaining member $R(f)$. With the previously quadrature formula is the most accurate formula Simpson, and the least accurate - formulas left and right rectangles. Accuracy formulas rectangles and trapezoids medium identical.

As noted above, sometimes estimate the error term quadrature formula is difficult or impossible, such as when asked function graphically or tabular and analytical expression of the unknown, or when asked difficult analytical function expression and its derivatives is difficult to assess. But if a certain order derivative is found, then evaluate it modulo the interval of integration is always possible by building using a computer spreadsheet values of the derivative. However, to estimate the error term $R(f)$ quadrature formula can and if you can not evaluate the top module of the original integrand. It is only important to know the order remainder term $R(f)$ relative integration step h For this purpose the double conversion.

Let the remaining members of some quadrature formulas of the order, the relative integration step A , ie $R(f) = O(h^p)$, $p \in N$. We also assume that the original, which is a remainder term $R(f)$ the interval of integration $[a; b]$ changes

little, so it can be considered approximately constant. Then the error term $R(f)$ come look

$$R(f) = Mh^p,$$

where M - some unknown constant.

If the interval $[a; b]$ divided by n and $2n$ equal parts

$$h = \frac{b-a}{n}, \quad \frac{h}{2} = \frac{b-a}{2n}$$

and calculate the approximate values of the quadrature formula I_n and I_{2n} , integral, and the corresponding residual denoted by members $R_n(f)$ and $R_{2n}(f)$, then we obtain two equal

$$\begin{aligned} I &= I_n + R_n(f) = I_n + Mh^p, \\ I &= I_{2n} + R_{2n}(f) = I_n + M(h/2)^p, \end{aligned} \quad (4.25)$$

This equality can be seen as a linear system of equations I and M . excluded from this system I , find the value for M

$$M = \frac{2^p}{2^p - 1} \frac{I_{2n} - I_n}{h^p}$$

Substituting this value M in the expression for $R_{2n}(f)$ we obtain

$$R_{2n}(f) = \frac{I_{2n} - I_n}{2^p - 1} \quad (4.26)$$

Thus, the error term quadrature formula is proportional difference of two integral approximate values calculated with the same quadrature formula with steps h and $h/2$. This estimation error quadrature formula called Runge rule. Now, if (4.26) to substitute into the second equation of (4.25), we find the revised values of the integral

$$I_{n,2n} = I_{2n} + \frac{I_{2n} - I_n}{2^p - 1} \quad (4.27)$$

Calculate the approximate value of the integral formula (4.27) is called by Richardson extrapolation. If $I_n \neq I_{2n}$ then revised values $I_{n,2n}$ never lies between I_n ,

I_{2n} . If $I_{2n} > I_n$ then the formula (4.27) implies that $I_{n,2n} > I_{2n} = \max \{I_n, I_{2n}\}$ And if $I_{2n} < I_n$ to $I_{n,2n} < I_{2n} = \min \{I_n, I_{2n}\}$ Consequently, the approach $I_{n,2n}$ determines the approximate I_n and I_{2n} a transaction extrapolation, because he himself method of calculating $I_{n,2n}$, called extrapolation.

To calculate the approximate value of the integral of accuracy is > 0 by double conversion should:

1. Calculate the approximate value of the integral I_n and I_{2n} increments h and $h/2$
2. Formula (4.26) to calculate the approximate value of the error $R_{2n}(f)$ numerical integration.
3. Compare $R_{2n}(f)$ with ε . If $|R_{2n}(f)| < \varepsilon$, then the formula (4.27) to calculate the revised values of the integral $I_{n,2n}$ and the calculation process to stop. If $|R_{2n}(f)| > \varepsilon$, then retaining value I_{2n} , interval $[a; b]$ $4n$ divided into equal parts and calculate $R_{2n}(f)$ Which again is compared to ε . This process of successive doubling of the number of nodes quadrature formula (halving integration step) continue until at some step k is executed inequality $|R_{2n}(f)| < \varepsilon$.

Chapter 5 NUMERAL METHODS OF DECISION OF EQUALIZATIONS WITH ONE VARIABLE

5.1 Raising of task

Let equalization is set with one variable $F(x)=0$ (5.1) where a function is $F(x)$ certain and continuous on some interval $[a; b]$

To decide of equalization means to find the plural of his roots, that such values $x \in [a; b]$, at which equalization (5.1) will grow into an identity. The root of equalization (5.1) is named yet the zero of function of $F(x)$. If a function is a polynomial of algebra, equalization (5.1) is named algebra. If the function of $F(x)$ contains trigonometric, to the index or logarithmic functions, then equalizations (5.1) name transcendent. Finding the exact meanings of roots of the set equalization is possible only for the simplest functions of $F(x)$: polynomials of algebra not higher fourth-degree, some polynomials of degree of $n \geq 5$ and some transcendent functions.

Universal methods do not exist for finding of the exact meanings of roots of equalizations of algebra of degree of $p=5$ and transcendent equalizations. In addition, deciding practical tasks, often reach equalizations with coefficients, which are close numbers. Then raising of task of finding of exact roots does not make sense. Therefore an important value is acquired by the close methods of finding of roots of equalization with sufficient for practice exactness. The task of finding of roots of equalization (5.1) is considered deciding, if roots are calculated with the beforehand set exactness.

Let x^* is an exact root, and \bar{x} — it close value. Talk, that a root \bar{x} is calculated with the beforehand set exactness is, if $|x^* - \bar{x}| < \varepsilon$. Let, for example, $x^* \in [a; b]$ and $b-a < \varepsilon$, then numbers but also b are close values of root of x^* accordingly with a shortage and surplus with exactness is. In this case for a close value with exactness it is possible to take any number from interval $[a; b]$.

Finding of close roots of equalization (5.1) consists of two stages:

- 1) separation of roots, that finding enough small cuttings-off on each of which one is and only one root of equalization;
- 2) a calculation of roots is with the beforehand set exactness. The first stage is named yet the task of determination of cuttings-off of isolation of roots, and second — by clarification of close roots. The first stage is more difficult of the second, as for a general case there are enough effective methods of separation of roots. For finding of roots with the beforehand set exactness apply methods which enable to specify the found approaching of roots.

Will mark that the scolded equalizations (5.1) can be actual and complex. The close methods of calculation only of actual roots of equalization are farther considered (5.1).

Separation of roots. a theorem is about estimation of error of close value of root. The root of x^* equalization (5.1) is considered separated on a segment $[a; b]$, if

$x \in [a; b]$ and on this segment this equalization does not have other roots. To separate the scolded equalizations (5.1), it is needed to break up the range of definition of this equalization on intervals on each of which one is and only one root or there is not a single root. Separate roots graphic and analytical methods, and also method of linear search. For the separation of roots build the chart of function of $y=F(x)$ a graphic method and find intersections chart with abscise axis and ends of cuttings-off of isolation of roots.

The analytical method of separation of roots is based on theorems from the course of mathematical analysis. Will formulate them.

Theorem 1 (theorem of existence of root). If a function is continuous on $[a; b]$ and acquires the vidrizka values of opposite signs on the ends of it, that $F(a)F(b) < 0$, inwardly segment $[a; b]$ exists even one root of equalization of $F(x) = 0$.

Will mark that a theorem does not give an answer for a question about the amount of roots of equalization (5.1), which belong $[a; b]$. At implementation of terms of theorem of equalization can have a few roots. On Fig.7.1 a plot of function of $y=F(x)$ is listed, which satisfies all requirements of theorem 1

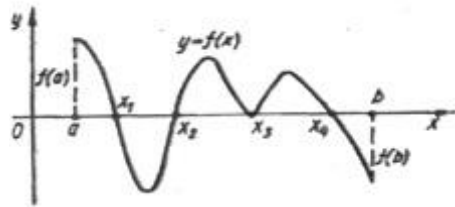


Figure 5.1.

and it had 4 zeros on $[a; b]$. In small enough near points, applying the xz, theorem of existence of root is impossible, because in transition from left to right through a point the x_3 sign of function of $F(x)$ does not change. A point of x_3 is a multiple root of equalization (5.1) and it can not be separated, using a theorem 1. Therefore will consider farther, that $F'(x) \neq 0$ is for all $x \in [a; b]$.

Theorem 2 (theorem of existence and unicity of root). If the function of $F(x)$, continuous and differentiated on $[a; b]$, acquires the vidrizka values of different signs on the ends of it, and the derivative of $F'(x)$ keeps a permanent sign inwardly vidrizka $[a; b]$, equalization of $F(x) = 0$ on this segment has a root, thus unique.

In accordance with theorems 1 and 2 algorithms of separation of roots of equalization (5.1) can be formulated so:

1. To find the range of definition of equalization.
2. To find the critical points of function of $F(x)$.
3. To write down the intervals of monotony of function of $F(x)$.
4. To define the sign of function of $F(x)$ on the ends of intervals of monotony.
5. To define segments on the ends of which the function of $F(x)$ acquires the values of opposite signs.
6. If necessary to narrow the found segments of isolation of roots.

Example 1. To separate the scolded equalizations of $x^3-x-1=0$.

Function of $f(x)=x^3-x-1$ and its derivative, $f'(x)=3x^2-1$, continuous on all numerical wasp. Will define the intervals of monotony of function of $f(x)$. For this purpose will decide equalization of $f'(x)=3x^2-1=0$.

His roots

$$x_1 = -\frac{\sqrt{3}}{3} \text{ i } x_2 = \frac{\sqrt{3}}{3} .$$

Consequently, the intervals of monotony of function of $f(x)$ are intervals

$$(-\infty ; -\frac{\sqrt{3}}{3}) \quad (-\frac{\sqrt{3}}{3} ; \frac{\sqrt{3}}{3}) \quad (\frac{\sqrt{3}}{3} ; \infty)$$

Thus

$$\begin{aligned} \lim_{x \rightarrow -\infty} f(x) &= \lim_{x \rightarrow -\infty} x^3-x-1 = -\infty \\ f(-\frac{\sqrt{3}}{3}) &< 0, \quad f(\frac{\sqrt{3}}{3}) < 0 \\ \lim_{x \rightarrow +\infty} f(x) &= \lim_{x \rightarrow +\infty} x^3-x-1 = +\infty \end{aligned}$$

Consequently, intervals of monotony

$$(-\infty ; -\frac{\sqrt{3}}{3}) \quad (-\frac{\sqrt{3}}{3} ; \frac{\sqrt{3}}{3})$$

does not contain the roots of this equalization, because function of $f(x)=x^3-x-1$ does not change a sign on these intervals, on an interval $(\frac{\sqrt{3}}{3} ; \infty)$ located it

unique.

From the found endless interval will select a segment which contains the unique root of equalization now. For this purpose it is enough directly to check up the sign of function of $f(x)=x^3-x-1$ in belongings $(\frac{\sqrt{3}}{3} ; \infty)$ celochislennikh points.

$$\text{Have } f(\frac{\sqrt{3}}{3}) < 0, f(1) = 1-1-1 < 0, f(2) = 8-2-1 > 0$$

Consequently, the unique actual root of this equalization lies on a segment [1, 2]. Set the problem it is decided. Subsequent narrowing of granic' of the found interval - it already is a task about clarification of root.

5.2 Clarification of root by method of division of vidrizka in half

The method of division of vidrizka is in half (or method of dichotomy) applicable for clarification of root of equalization of $F(x)=0$ with the beforehand set exactness, possible for this Electronic calculable machine, if the function of $F(x)$ satisfies the terms of theorem 2.

Will designate through x is the exact meaning of root of equalization (5.1) on a segment $[a;b]$, and ε — it maximum absolute error. Essence of method is in that

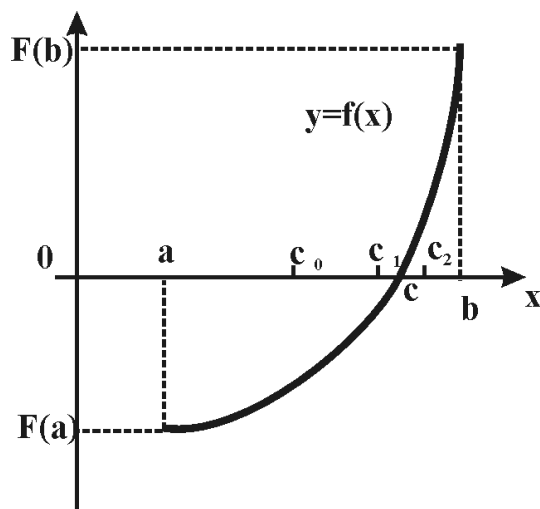


Fig. 5.2

a segment $[a;b]$ is gone fifty-fifty the point of $c_0=(a+b)/2$ and calculate $F(c_0)$. If $F(c_0)=0$, $x=c_0$ is the exact meaning of root. If $F(c_0) \neq 0$, but $b-a < 2\varepsilon$, $|x^*-c_0| < \varepsilon$ and a value of $x=c_0$ will be the sought after close root. If $F(c_0) \neq 0$ and $b-a > 2\varepsilon$, then examine that of two cuttings-off $[a;c_0]$ and $[c_0;b]$. On ends $[c_0;b]$ the function of $F(x)$ acquires the values of opposite signs, will designate this segment $[a;b]$ (7.2). On a segment $[a;b]$

the function of $F(x)$ satisfies the terms of

theorem 2. Farther segment $[a;b] / 2$ go the point of $c_1=(a+b)$ fifty-fifty and meditate similarly, as well as before.

Thus, after each the iteration a segment which the located root is on diminishes twice, that after n iterations it grows short in $2n$ times. Does an iteration process proceed until the value of function after a n iteration will not become less for the modules of some set number ε . Does not the absolute error of the found root exceed thus ε . Methods of dichotomy easily realized on Electronic calculable machine, but needs considerable volume of calculations, to attain high exactness of close root.

The program of method has cyclic character. In the program at every passing of cycle the series of commands

$$c=(a+b)/2 \quad (5.2)$$

If $F(a)F(b) < 0$ $b:=c$ differently $a:=c$ all. Reiteration of commands of cycle is continued until one of terms of $F(x)$ will not be executed $F(c) = 0$ or $b-a < 2 \epsilon$.

Example 1. In half to specify the root of equalization of $x^3-x-1=0$ the method of division of interval, separated on a segment $[1, 2]$.

$$\begin{aligned} f(x) &= x^3 - x - 1, \quad a=1, b=2, \\ c_0 &= (a+b)/2 = (1+2)/2 = 1.5. \\ f(1) &= -1 < 0, f(1.5) = 0.875 > 0, f(2) = 5 > 0. \end{aligned}$$

Because the sign of function of $f(x)$ changes on a segment $[1; 1.5]$ $a=1$, $b=c_0=1.5$.

$$\begin{aligned} c_1 &= (a+b)/2 = (1+1.5)/2 = 1.25. \\ f(1.25) &= 1.25^3 - 1.25 - 1 = -0.296875 \end{aligned}$$

If $f(c_1) \neq 0$ and $1.5-1 > 2\epsilon$, then examine that of two cuttings-off $[1; 1.25]$ and $[1.25; 1.5]$, on the ends of which the function of $f(x)$ acquires the values of opposite signs. Will designate this segment $[1.25; 1.5]$.

$$\begin{aligned} c_2 &= (a+b)/2 = (1.25+1.5)/2 = 1.375. \\ f(1.375) &= 1.375^3 - 1.375 - 1 = 0.224609375 \end{aligned}$$

Then will consider a segment $[1.25; 1.375]$:

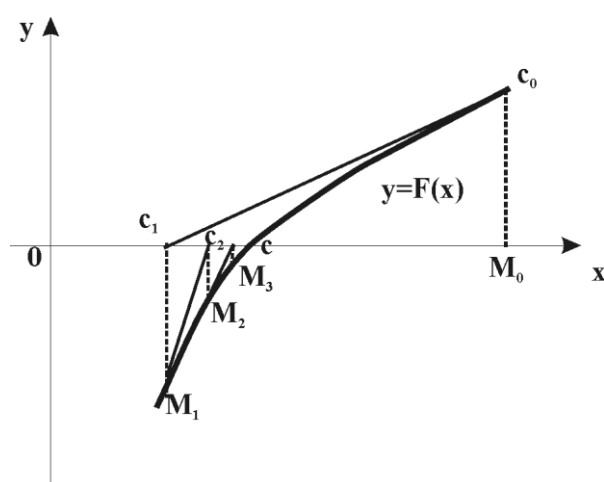
$$\begin{aligned} c_3 &= (a+b)/2 = (1.25+1.375)/2 = 1.3125 \\ f(1.3125) &= 1.3125^3 - 1.3125 - 1 = -0.051513671875 \end{aligned}$$

An iteration process proceeds until $|f(c_k)| < \epsilon$

In the method of division of interval in half position of point of s_k is determined regardless of properties of function of $f(x)$ of -left part of the set equalization. Naturally to expect that the account of properties of this function must improve the got approaching.

5.3 Method of Newton (method of tangents)

The idea of method consists in that a tangent is conducted to the curve $y = F(x)$ at $x = c$ and an intersection tangent is searched with abscise axis. Thus not necessarily to set a segment $[a, b]$ which contains the root of equalization (5.1), but it is enough only to find some initial approaching of root of $x = c_0$, in which



$$F(c_0)F''(c_0) > 0$$

Equalization of tangent, conducted to the curve of Fig. 5.3 $y = F(x)$ in a point M_0 with co-ordinates c_0 i $F(c_0)$, looks like:

$$y - F(c_0) = F'(c_0) \cdot (x - c_0).$$

From here will find the following approaching of root of c_1 as abscissa intersection tangent with the axis of Ox ($y = 0$): $c_1 = c_0 - F(c_0)/F'(c_0)$

Like there can be the found and next approaching as intersections tangents with abscise axis, conducted in the points of M_1 , M_2 , and so further (7.3). A formula looks like for the $n+1$ -first approaching

$$c_{n+1} = c_n - F(c_n)/F'(c_n). \quad (5.3)$$

The sufficient terms of convergence of method of Newton are given by such theorem.

Theorem. Let on a segment $[a; b]$ the function of $F(x)$ has continuous with permanent signs derivatives

$$F'(x) \neq 0, F''(x) \neq 0 \text{ i } F(a)F(b) < 0.$$

Then there is such okil $R \subset [a; b]$ root x^* equalization $F(x) = 0$ that for any sequence $\{c_k\}$, calculated on a formula (5.3), coincides to x^* .

Will estimate speed of convergence of method of Newton.

It is possible to prove that for the method of Newton just estimation

$$|c_k - x^*| \leq \frac{M_2}{2m_1} |c_k - c_{k-1}|^2,$$

$$\text{where } M_2 = \max_{x \in [a; b]} |f''(x)|, \quad m_1 = \min_{x \in [a; b]} |f'(x)|$$

From this estimation evidently, that for achievement of the set exactness ε an iteration process needs to be continued until for two progressive approximations of c_k and c_{k-1} will not be executed inequality

$$|c_k - c_{k-1}| \leq \sqrt{\frac{2m_1}{M_2}} \varepsilon$$

If on a segment $[a; b]$ just inequality of $M_2 < 2m_1$ it can make off an iteration process, when a condition is executed $|c_k - c_{k-1}| \leq \varepsilon$.

Advantage of method of Newton is before the method of iterations in that it has higher speed of convergence. Yes, a root of $x^3 - 2x - 5 = 0$ with exactness $\varepsilon = 10^{-6}$ and $\varepsilon = 10^{-9}$ by the method of Newton was calculated after five and six iterations accordingly, while it was calculated the method of iteration no less than for six and ten iterations accordingly.

From a formula (5.3) evidently, that than greater value $|f(x)|$ at an okoli root, the a less amendment is added to the previous approaching. Therefore comfortably to apply the method of Newton then, when at the okoli root of graphic arts of function $y = f(x)$ has a considerable steepness. It is in addition, possible to find the method of Newton not only actual roots equalizations but also complex. The method of Newton easily spreads and on rozv'yazuvannya systems of nonlinear equalizations with many unknown.

The lack of method of Newton is that on every iteration it is needed to calculate not only the value of function of $f(x)$ but also value of its derivative. A calculation of derivative of $f'(x)$ can be considerably more difficult from the calculation of $f(x)$.

Example 2. By the method of tangents to specify the root of equalization of $x^3 - x - 1 = 0$, viddileniy on a segment $[1, 2]$.

Have $f(x) = x^3 - x - 1$, $f'(x) = 3x^2 - 1$, $f''(x) = 6x$.

Because on the segment $[1, 2]$ of $f''(x) > 0$, a tangent needs to be taken in the right end of interval (that $x = b = 2$, where $f(2) = 5 > 0$). Yet not calculating c , maybe, that a point of c will be the right end of new segment $[a_1, b_1]$ ($a < x_0 < c$, $a_1 = a$, $b_1 = c$). Thinking $c = 2$, obsessed $f'(2) = 11$ and farther on a formula $c_{n+1} = c_n -$

$$f(c_n)/f'(c_n): c = 2 - \frac{5}{11} = 1.6$$

The close value of c is taken with surplus, because $c > x_0$. A new segment is guilty to be $[1; 1,6]$ ($a_1=a=1, b_1=c=1,6$).

We specified the root of equalization, substituted for one of ends of weekend the vidrizka $[a, b]$ point of c , more near to root. Obviously, a greater effect can be will attain at approaching to root simultaneously c of two sides. It is arrived at application of the combined methods.

5.4 A method of chords

Method of chords — one of widespread iteration methods. It is yet named the method of linear interpolation, method of proportional parts. Let equalization of $f(x)$ is set= 0, where $f(x)$ on a segment $[a;b]$ has continuous derivatives of the first and second orders, which keep permanent signs on this segment, and $f(a)f(b) < 0$, that the root of x^* equalization is separated on $[a;b]$.

An idea of method of chords is in that on a small enough segment the arc of curve of $y=f(x)$ is replaced a chord and abscissa of intersection chord with an axis Oh is

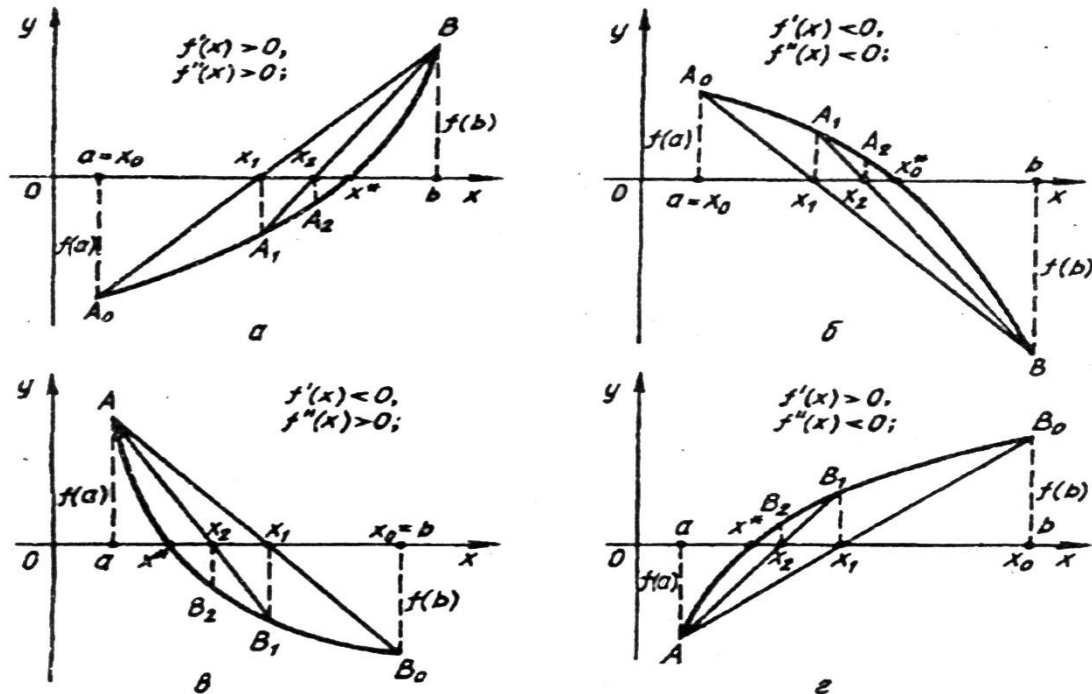


Figure 5.4

by the close value of root.

Let for definiteness $f(x) > 0$. $f'(x) > 0$, $f(a) < 0$. $f(b) > 0$ (7.4, a).

Will take for the initial approaching of the sought after root the x^* value of $x_0 = a$. Through the points of A_0 and B will conduct a chord

$$\frac{x-a}{b-a} = \frac{y-f(a)}{f(b)-f(a)}$$

and for the first approaching of root of x^* will take the abscissa of x_1 intersection chord with an axis Ox . Putting $y=0$, $x=x_1$ we will get

$$x_1 = a - \frac{f(a)(b-a)}{f(b)-f(a)} \quad \text{or} \quad x_1 = b - \frac{f(b)(b-a)}{f(b)-f(a)} \quad (5.4)$$

A new segment which separates a root can be defined, comparing the signs of $f(a)$, $f(x_1)$ and $f(b)$. Obviously, that point of x_1 nearer to the point of x^* , what and, if $y'y'' > 0$ (see rice. 7.4,a), and a segment which separates a root will be $[x_1, b]$, to the opposite case, if $y'y'' < 0$ (see ris.7.4, in), a segment which separates a root will be $[a, x_1]$.

An abscissa of x_2 intersection chord of A_1B will be the second approaching of root. Continuing this process without restriction, will get the sequence of $x_0, x_1, x_2, \dots, x_n, \dots$ close values of root of x^* of this equalization.

For x_{k+1} , if $y'(x)y''(x) > 0$ have:

$$x_{k+1} = x_k - \frac{f(x_k)(b-x_k)}{f(b)-f(x_k)} \quad \kappa=0,1,2,\dots \quad (5.5)$$

If $y'(x)y''(x) < 0$, then for x_{k+1} it is possible to write down a formula

$$x_{k+1} = x_k - \frac{f(x_k)(x_k-a)}{f(x_k)-f(a)}, \quad \kappa=0,1,2,\dots \quad (5.6)$$

The sufficient terms of convergence of method of chords are given by such theorem.

Theorem. Let on a segment $[a;b]$ the function of $f(x)$ is continuous together with the derivatives to the second order inclusive, thus $f(a)f(b) < 0$, and the derivatives of $f'(x)$ i $f''(x)$ keep permanent signs on $[a;b]$, then there is such okil root of x^* equalization of $f(x) = 0$, that for any initial approaching of x_0 from it an okolu sequence $[x_k]$, calculated on a formula (5.5) or (5.6), will coincide to Cornu of x^* .

For the estimation of error it is possible to take advantage of formula

$$|x_k - x^*| \leq \frac{M_1 - m_1}{m_1} |x_k - x_{k-1}|,$$

$$\text{де } \mathbf{M}_2 = \max_{x \in [a; b]} |f''(x)|, \quad \mathbf{m}_1 = \min_{x \in [a; b]} |f'(x)|$$

Consequently, root of x^* equalization of $f(x)=0$ it will be found the method of chords with the beforehand set exactness is, if for two progressive approximations of x_k, x_{k-1} will be carried out inequality

$$|x_k - x_{k-1}| \leq \frac{m_1}{M_1 - m_1} \varepsilon.$$

Example 3. By the method of chords to specify the root of equalization of $x^3 - x - 1 = 0$, viddileniy on a segment $[1, 2]$.

$$f(x) = x^3 - x - 1, f'(x) = 3x^2 - 1, f''(x) = 6.$$

Because on a segment $[1, 2]$ have $f''(x) > 0$, $f(1) < 0$, $f(2) > 0$, point x_1 , it is on a formula (5.4)

$$x_1 = 1 - \frac{f(1)(2-1)}{f(2)-f(1)} = 1 - \frac{2-1}{5-(-1)}(-1) = 1.1,$$

it will be the left end of new segment $[a_1, b_1]$ ($x_1 < x^* < b$, $a_1 = x_1$, $b_1 = b$).

Will notice that the close value of s is taken with failing, because $x_1 < x^*$, and at rounding off with surplus there is a danger to «step» over through a root. As it costs now to take a segment $[a_1, b_1]$ segment $[1.1; 2]$.

5.5 Combined method of tangents and chords

Characteristic feature of methods tangent and chords and, that the sequences of their approaching are monotonous. Thus, if for this equalization the sequence of approaching of method of chords droningly descending, sequence of approaching of method of tangents — monotonous growing, and vice versa. Simultaneous application of these methods enables to approach root, equalization from two sides, reaching approaching with a shortage and surplus

Will consider equalization $f(x)=0$, root of which $x^* \in [a;b]$. Let, for example, $f(x) > 0$, $f'(x) > 0$, $f(a) < 0$, $f(b) > 0$ (рис. 7.5). In this

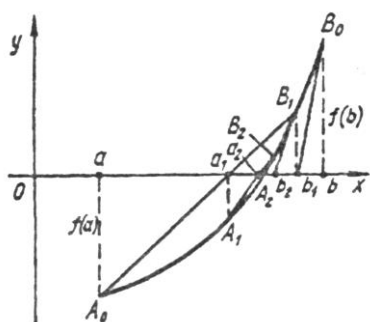


Fig. 5.5

case for the initial approaching in the method of chords choose the point of $x = a$, and in the method of tangents — point of b . On a segment $[a;b]$ apply the method of tangents and chords (at first tangents, and then chords). In the total reach the new approaching of a_1, b_1 and the initial segment of isolation of root narrowed. For finding of the new approaching apply the method of tangents and chords already on a segment $[a_1;b_1]$. In the total does

reach approaching of a_2 and b_2 accordingly, thus $[a_2;b_2] \subset [a_1; b_1] \subset [a;b]$. Is such process continued until length of vidrizka $[a_k;b_k]$ will become less or will equal a size 2ε , where ε it is the beforehand set exactness of root.

For the sought after value of root \bar{x} take the half-sadness of approaching a_k and b_k , that $\bar{x} = 0,5(a_k + b_k)$, and their half-difference will give the module maximum absolute error of close root, that

$$|x^* - \bar{x}| \leq 0,5|a_k - b_k|$$

Will mark that the at every step combined method for the immobile end of s in the formula of method of chords it is needed to take approaching, calculated thereon step after a formula, tangents.

The formulas of the combined method of tangents and chords look like

$$b_{k+1} = b_k - F(b_k)/F'(b_k), \quad k=0,1,2... \quad (5.7)$$

$$a_{k+1} = a_k - \frac{f(a_k)(a_k - b_k)}{f(a_k) - f(b_{k+1})}, \quad k=0,1,2... \quad (5.8)$$

For the initial approaching of b_0 in the formula (5.7) of method of tangents take that of ends of segment $a [a;b]$ in which value of function of $f(x)$ and it flexon have identical signs, then the opposite end of segment $[a;b]$ is taken for the initial approaching of a_0 in the formula (5.8) of method of chords.

Due to original combination of methods tangent and chords the combined method has higher speed of convergence, than methods of chords and tangents are separately taken. Yes, for equalization of $x^3 - 2x - 5 = 0$ his root of $x^* \in [2;3]$ within 10^{-6} and 10^{-9} it is calculated the combined method for two and three

iterations accordingly, while for the method of tangents it is needed it was five and six iterations accordingly, and for the method of chords — twelve and nineteenth iterations accordingly.

Example 4. By the method of chords and tangents to specify the root of equalization of $x^3 - x - 1 = 0$, separated on a segment $[1, 2]$.

On a segment $[1, 2]$ have

$$f(x) = x^3 - x - 1, \quad f(1) = -1 < 0, \quad f(2) = 5 > 0;$$

$$f'(x) = 3x^2 - 1, \quad f'(x) = 6 > 0.$$

Consequently, a_1 it is needed to calculate on a formula

$$a_1 = a - \frac{f(a)(b-a)}{f(b)-f(a)} \text{ — method of chords, } b_1 \text{ — on a formula } b_1 = b - F(b)/F'(b) \text{ — method of tangents.}$$

Taking the results of calculations for to the formulas from examples 3 and 4, observed, that segment $[a_1, b_1]$ there must be a segment $[1, 1; 1, 6]$.

Remark. In this case combination of method of chords with the method of division of segment in half would give more narrow segment $[1, 1; 1, 5]$. But in general case of combining these two methods can not be specified terms which provide approaching to root from two sides. It is investigation of that, as specified already, method of distributing of segment in half not decide with the conduct of function of $f(x)$ of -left part of the set equalization.

Chapter 6 SOLVING SYSTEMS OF LINEAR ALGEBRAIC EQUATIONS STATEMENT OF THE PROBLEM

6.1 Let the system of n linear equations in n variables

$$\sum_{j=1}^n a_{ij} x_j = b_i \quad (i = 1, 2, \dots, n). \quad (6.1)$$

System (6.1) can be written as a matrix equation

$$AX=B, \quad (6.2)$$

Ordered set of n numbers c_1, c_2, \dots, c_n , which, when substituted in (6.1) instead of x_1, x_2, \dots, x_n , converts all equations in the correct numerical equality, called the solution of system (6.1). If the determinant of the system (6.1) $\Delta = \det A \neq 0$ it has a unique solution, it will be calculated by Kramer

$$x_k = \frac{\det A_k}{\det A} \quad (k=1, \dots, n) \quad (6.3)$$

where the matrix A_k take out from the matrix A , replacing it with the k -th column column terms. Cramer formulas are of great theoretical significance, but because of the large amount of computational work was effective in the numerical solution of linear systems. These formulas should calculate the value of $(n + 1)$ th determinants of order n , for which perform a significant number of arithmetic operations. Methods for solving systems of linear equations can be divided into two groups: precise and iterative Exactly call these methods allow you to find the exact solution of system (6.1) by executing finite number of arithmetic operations on the assumption that all calculations are performed exactly (without rounding), and the coefficients of the system and free members - the exact number. In practice, all calculations are performed with a limited number of decimal places, and irrational coefficients and free terms, if any, are replaced by rational numbers. Therefore, in the calculations resorted to rounding, which means that decisions which are calculated using exact methods actually are approximate numbers of certain errors (rounding errors). To include accurate method Gauss method of square roots, etc. Cramer rule. Iterative call these methods allow to find an approximate solution of system (6.1) with the specified accuracy in advance by performing finite number of arithmetic operations, although most computations can be carried out without rounding and rates and terms of the system to be accurate numbers. The exact solution of system (6.1) using iterative methods can be found only in theory as border convergent infinite process. Solving the system of equations iterative methods, in addition to rounding errors, we must also take into account the level of

accuracy of the method. By the iterative method include iteration method Seidel and others. In exploring the various issues of economy, science, technology, etc. have to solve a system of linear algebraic equations. In particular, such systems reduces the numerical solution of differential and integral equations. In such systems, the coefficients and free terms equations - approximate number. This leads to additional (so-called fatal) errors that must be considered in the process of calculation and rounding the final result. The coefficients of linear systems that arise during the processing of the experimental results misspelled observations. If the coefficients of system performance formulas, the calculation of their results in rounding errors. If the system of equations in the machine memory even add exactly is in the process of solving computer must have rounding errors that can not affect the accuracy of the solution. However, if the matrix A of the system (6.2) almost degenerate, we can expect that small changes in the coefficients and (or) free states also lead to significant changes in its interpretation. If small perturbations of coefficients and (or) the terms of the system (6.1) is very disturbing its solution, the following system of equations called poorly determined. Conversely, if a small perturbation coefficients and (or) the terms of the system (6.1) was disturbing its solution, then a system called well conditioned. An indication of poor conditioning system of linear equations is its almost vyrodzhenist. In other words, if the value of the determinant of a rather small compared to its coefficients, the system is close to degenerate (special). Then only considered such a system of linear equations that are not degenerate (special), that their determinant is not zero, is a well-defined, ie the determinant of the system is of no lower order than its coefficients and coefficients and terms of the system - the exact number.

6.2 Method of successive exclusion of variables (Gauss method)

The simplest method for solving systems of linear algebraic equations method is consistent exclusion of variables or method of Gauss. There are several versions of this method. Consider the scheme of a single division for which the system solved in two stages. In the first stage the original system of equations is equivalent to deceive her system triangular shape. This conversion process is called direct way. In the second stage, called reverse course, find the solution of linear systems of equations triangular shape. Confine ourselves to a system of three equations with three variables

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2 \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3 \end{cases} \quad (6.4)$$

Δ key which is not zero. Let deeds $a_{11} \neq 0$ (this can always be achieved permutation equations system for $\Delta \neq 0$, so there is always this equation, which $a_{11} \neq 0$). Divide the coefficients of the first equation of system (6.4), including the free term, the coefficient a_{11} recieve new equation

$$x_1 + a_{12}^{(1)}x_2 + a_{13}^{(1)}x_3 = b_1^{(1)} \quad (6.5)$$

$$a_{1j}^{(1)} = a_{1j} / a_{11} \quad (j=2,3,4). \quad (6.6)$$

Exclude now variable x_1 of the second and third equations of system (6.4). For the equation (6.5), multiply by a factor consistently first a_{21} and subtract it from the second equation of (6.4), and then the a_{31} and subtract the third equation of (6.4). Remove the system of two equations with two variables x_2 and x_3

$$\begin{cases} a_{22}^{(1)}x_2 + a_{23}^{(1)}x_3 = b_2^{(1)} \\ a_{32}^{(1)}x_2 + a_{33}^{(1)}x_3 = b_3^{(1)} \end{cases} \quad (6.7)$$

where the coefficients $a_{ij}^{(1)}$ calculated by the formulas

$$a_{ij}^{(1)} = a_{ij} - a_{i1}a_{1j}^{(1)} \quad (i = 2,3; j = 2,3,4). \quad (6.8)$$

Superscript (1) indicates that the coefficients of system (6.4) completed the first conversion.

Then divide the coefficients of the first equation of (6.7) $a_{22}^{(1)}$ in (if $a_{22}^{(1)} = 0$, the equation permuted places). Remove the equation

$$x_2 + a_{23}^{(2)}x_3 = b_2^{(2)} \quad (6.9)$$

where

$$a_{2j}^{(2)} = a_{2j}^{(1)} / a_{22}^{(1)} \quad (j=3,4). \quad (6.10)$$

From the system (6.7) exclude variable x_2 is the same as x_1 , system (6.4). Remove the equation

$$a_{33}^{(2)} x_3 = b_3^{(2)} \quad (6.11)$$

where

$$a_{3j}^{(2)} = a_{3j}^{(1)} - a_{32}^{(1)} a_{2j}^{(2)} \quad (j=3,4). \quad (6.12)$$

From equation (6.11) we have

$$x_3 = b_3^{(3)} \quad (6.13)$$

where

$$b_3^{(3)} = b_3^{(2)} / a_{33}^{(2)} \quad (6.14)$$

After a three-step transformation we obtain the system of equations triangular shape

$$\begin{cases} x_1 + a_{12}^{(1)} x_2 + a_{13}^{(1)} x_3 = b_1^{(1)} \\ x_2 + a_{23}^{(2)} x_3 = b_2^{(2)} \\ x_3 = b_3^{(3)} \end{cases} \quad (6.15)$$

which is equivalent to the system (6.4).

This direct method of Gauss course completed. The described process transformation system (6.4) is equivalent to her system (6.15) can be done if the conditions $a_{11} \neq 0$, $a_{22}^{(1)} \neq 0$, $a_{33}^{(2)} \neq 0$.

Proximity diagonal coefficients of system (6.4) to zero can lead to significant loss of accuracy.

Since the system (6.4) and (6.15) are equivalent, then the solution of system (6.4) is a solution of system (6.15), which can be written formulas

$$\begin{cases} x_1 = b_1^{(1)} - a_{12}^{(1)} x_2 - a_{13}^{(1)} x_3 \\ x_2 = b_2^{(2)} - a_{23}^{(2)} x_3 \\ x_3 = b_3^{(3)} \end{cases} \quad (6.16)$$

This complete reversal method Gauss.

Since the transformation of equations is actually turning them coefficients of the variables and absolute terms, for the implementation of reforms do not need to write the system. Enough to write only the matrix of coefficients and free terms upon them to fulfill the above transformation.

6.3 Simple Iteration Method

Application of Gauss for solving systems of linear equations with many unknowns rather cumbersome. In addition, the number of unknowns can be so great that the coefficients of the system is not always possible to place in memory computers. Then apply it to solving method Gauss did not. In these cases, solve the system of iterative methods. Consider the simple iteration method. Let the given system of linear equations

[illegible]

or in matrix form •

$$Ax=b, \quad (6.18)$$

where

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}.$$

Let diagonal elements a_{ii} ($i = 1, 2, \dots, n$) matrix A nonzero. Then, solving the first equation of system (6.17) with respect to x_1 , and the second - a relatively x_2 , etc., we obtain a system

[illegible]

where

$$\alpha_{ij} = \begin{cases} -\frac{a_{ij}}{a_{ii}}, i \neq j \\ 0, i = j \end{cases} \quad \beta_i = \frac{b_i}{a_{ii}}$$

It solve the method of successive approximations. For the initial approximation we take, for example, column free members, that is $x^{(0)} = \beta$. Then consistently find

$$x_i^{(k+1)} = \sum_{j=1}^n \alpha_{ij} x_j^{(k)} + \beta_i \quad i=1,2,\dots,n; \quad k=0,1,2,\dots \quad (6.20)$$

If the sequence of approximations $x^{(0)}, x^{(1)}, \dots, x^{(k)}, \dots$ a border $x^* = \lim_{k \rightarrow \infty} x^{(k)}$, then the border will be a solution of system (6.19).

The method of successive approximations determined by formulas (6.20) is called by a simple iteration method or iteration. The method is simple iteration should end by becoming fair inequality

$$\max_{1 \leq i \leq n} |x_i^{(k)} - x_i^{(k-1)}| \leq \frac{1-l_1}{l_1} \varepsilon$$

where ε - pre-specified accuracy approximations. Theorem. If the elements of the matrix A satisfying one of the conditions

$$\sum_{i=1}^n \frac{1}{a_{ii}^2} \sum_{\substack{j=1 \\ i \neq j}}^n a_{ij}^2 < 1, \quad \sum_{\substack{j=1 \\ i \neq j}}^n |a_{ij}| < |a_{ii}| \quad i=1,2,\dots,n;$$

or

$$\max_{1 \leq j \leq n} \sum_{\substack{i=1 \\ i \neq j}}^n \left| \frac{a_{ij}}{a_{ji}} \right| < 1$$

the system of equations (8.18) has a unique solution $x^* = (x_1^*, x_2^*, \dots, x_n^*)$, which can be obtained as a limit of the sequence $\{x^{(k)}\}$, constructed by the formula

$$x_i^{(k)} = \frac{1}{a_{ii}} (b_i - \sum_{j=1}^n a_{ij} x_j^{(k-1)}) \quad i=1,2,\dots,n; \quad k=1,2,\dots \quad (6.21)$$

starting from an arbitrary initial approximation $x^{(0)} = (x_1^{(0)}, x_2^{(0)}, \dots, x_n^{(0)})$.

Non-degenerate system of linear equations identical transformations can always be reduced to a system for which operated sufficient conditions for the convergence of the method of iterations. For example, let us have a system

$$\begin{cases} 5x_1 - x_2 + 2x_3 = 8 \\ 3x_1 - 2x_2 + 9x_3 = 18 \\ 6x_1 - 5x_2 + 2x_3 = 10 \end{cases}$$

that does not have the conditions of Theorem 2. Transform the system to the form in which the main diagonal elements modules would be greater than the sum of modules corresponding lines of other elements. Construct a new system in which the first and third equations are respectively first and second equation of the system whose coefficients satisfy the condition

$$\sum_{\substack{j=1 \\ i \neq j}}^n |a_{ij}| < |a_{ii}| \quad i=1,3.$$

The second equation we obtain a new system, if the third equation of system subtract first. As a result, the system will have

$$\begin{cases} 5x_1 - x_2 + 2x_3 = 8 \\ x_1 - 4x_2 = 2 \\ 3x_1 - 2x_2 + 9x_3 = 18 \end{cases}$$

coefficients which satisfy the conditions of the theorem. This system is easily reduced to normal form

$$\begin{cases} x_1 = \frac{1}{5}x_2 - \frac{2}{5}x_3 + \frac{8}{5} \\ x_2 = \frac{1}{4}4x_1 - \frac{1}{2} \\ x_3 = -\frac{1}{3}x_1 + \frac{2}{9}x_2 + 2 \end{cases} \quad (6.22)$$

performed for which sufficient conditions for the convergence of the method of iterations.

Method of iterations easily implemented on a computer. The algorithm of solution of the form (6.19) provides:

1. Calculate the value $l = \max_{1 \leq j \leq n} \sum_{\substack{i=1 \\ i \neq j}}^n |a_{ij}|$.
2. Test conditions $l < 1$. If this condition is not met, then the calculation process ends and a message is displayed that the method can not be applied.
3. Calculation of acceptable error $\varepsilon_1 = \frac{1-l}{l} \varepsilon$
4. The choice of initial approximation $x_i^{(0)} = \beta_i$ ($i = 1, 2, \dots, n$).
5. Calculate the following approximation y_i ($i = 1, 2, \dots, n$) because previous x_i ($i = 1, 2, \dots, n$).
6. The test condition $\max |y_i - x_i| < \varepsilon$. If this condition is satisfied, $1 < i < n$ the process of iteration is completed, otherwise proceed to perform p.5.

Example 1 iteration method to find a solution of the system

$$\begin{aligned} X_1 &= 0,0092X_1 - 0,0061X_2 + 0,0701X_3 + 0,6636 \\ X_2 &= -0,0643X_1 + 0,0755X_2 - 0,0324X_3 - 0,8172 \\ X_3 &= -0,0210X_1 - 0,0130X_2 + 0,0817X_3 - 1,6411 \end{aligned}$$

assuming that the absolute error coefficient terms of the system do not exceed 0.00005.

By approaching zero solution accept terms of the system:

$$X_1^{(0)} = 0,6636, X_2^{(0)} = -0,8172, X_3^{(0)} = -1,6411.$$

The following approximation is calculated by the formula

$$\begin{aligned} X_1^{(1)} &= 0,0092X_1^{(0)} - 0,0061X_2^{(0)} + 0,0701X_3^{(0)} + 0,6636 \\ X_2^{(1)} &= -0,0643X_1^{(0)} + 0,0755X_2^{(0)} - 0,0324X_3^{(0)} - 0,8172 \\ X_3^{(1)} &= -0,0210X_1^{(0)} - 0,0130X_2^{(0)} + 0,0817X_3^{(0)} - 1,6411 \end{aligned}$$

or

$$X_1^{(1)} = 0,0092 \cdot 0,6636 - 0,0061 \cdot (-0,8172) + 0,0701 \cdot (-1,6411) + 0,6636 = 0,55974$$

$$X_2^{(1)} = -0,0643 \cdot 0,6636 + 0,0755 \cdot (-0,8172) - 0,0324 \cdot (-1,6411) - 0,8172 = -0,86838$$

$$X_3^{(1)} = -0,0210 \cdot 0,6636 - 0,0130 \cdot (-0,8172) + 0,0817 \cdot (-1,6411) - 1,6411 = -1,7784$$

Similarly compute $X_1^{(2)}$, $X_2^{(2)}$, $X_3^{(2)}$, etc. The results of calculations record in the table

Table 6.1

Approximate y of	Odds systems			Free members
	X_1	X_2	X_3	
	0,0092	-0,0061	0,0701	0,6636
	-	0,0755	-0,0324	-0,8172
	0,0643	-0,0130	0,0817	-1,6411
$X_i^{(0)}$	0,6636	-0,8172	-1,6411	
$X_i^{(1)}$	0,5597	-0,86838	-1,77849	
$X_i^{(2)}$	0,5493	-0,86119	-1,78657	
$X_i^{(3)}$	0,5486	-0,85966	-1,78740	
$X_i^{(4)}$	0,5485	-0,85948	-1,78747	
$X_i^{(5)}$	0,5485	-0,85945	-1,78749	
$X_i^{(6)}$	0,5485	-0,85945	-1,78749	

In this case, the fifth and sixth approximation solution of the same with five decimal places. Alternate rounding mark finally have
 $X_1 = 0,5486$, $X_2 = -0,8594$, $X_3 = -1,7875$.

6.4 Method seidel

Seidel method - some modification of the method of simple iteration. In the method of simple iteration of the calculation components $x_1^{(K+1)}, x_2^{(K+1)}, \dots, x_n^{(K+1)}$ vector-column $x^{(K+1)}$ to $(k + 1)$ th step the values $x_1^{(K)}, x_2^{(K)}, \dots, x_n^{(K)}$ вектора-столбца $x^{(K)}$, calculated in the previous step. Seidel method differs from the method of simple iteration only that the calculation $(k + 1)$ th approximation components x_i captured values x_1, x_2, \dots, x_{i-1} , calculated on the same step. Formula for finding successive approximations are of the form

$$x_1^{(k+1)} = \sum_{j=1}^n \alpha_{1j} x_j^{(k)} + \beta_1$$

.....

$$x_i^{(k+1)} = \sum_{j=1}^{i-1} \alpha_{ij} x_j^{(k+1)} + \sum_{j=i}^n \alpha_{ij} x_j^{(k)} + \beta_i \quad (6.23)$$

.....

$$x_i^{(k+1)} = \sum_{j=1}^{n-1} \alpha_{ij} x_j^{(k+1)} + a_{in} x_n^{(k)} + \beta_i \quad k=0,1,2,\dots$$

Note that the sufficient conditions of convergence for the method of simple iteration method for the Gauss and Seidel. The program Seidel method differs from the method of simple iteration program only a fragment of calculating these approximations. The program includes a simple iteration method must simultaneously maintain all previous $x_i^{(K)}$ and next $x_i^{(K+1)}$ approximation, because the greatest difference $|x_i^{(K+1)} - x_i^{(K)}|$ can be found only after iteration step. Using Seidel method, there is no need to store all found approaching $x_i^{(K)}$ ($i = 1, 2, \dots, n$), just as they are used for. Because the program Seidel method $x_i^{(K+1)}$ variable denoted in variable y that stores the calculated value by the time $x_i^{(K+1)}$ until it prysvoyitsya variable $x_i^{(K)}$ (in the program it is labeled X (I)).

Seidel method often coincides rather than simple iteration method. For example, the solution $x_1 = 0.052980$, $-0.486755 = x_2$, $x_3 = 2.874172$ system (8.22) with accuracy $\varepsilon = 10^{-6}$ by simple iteration found in 20 steps, while it is calculated by Seidel in 15 steps. But this is not always the case. There is a system of linear equations for which a simple iteration method coincides rather than Seidel method. For example, the system

$$\begin{cases} x_1 = -0,5x_1 + 0,6x_2 + 1 \\ x_2 = -0,6x_1 - 0,5x_2 + 2 \end{cases} \quad (6.24)$$

iterative method matches and its solution $x_1 = 1.034483$, $0.919540 = x_2$ with accuracy $\varepsilon = 10^{-6}$ found by 68 steps, and Seidel method were scattered; for the system

$$\begin{cases} x_1 = 0,5x_1 + x_2 + 1 \\ x_2 = -x_1 + 0,5x_2 + 2 \end{cases}, \quad (6.25)$$

method of iteration diverges, and Seidel method matches, and its solution $x_1 = 2$, $x_2 = 0$ calculated for 23 iterations.

Example 2: Solve using the method Haussa- Seidel following system of equations:

$$\begin{aligned} 4X_1 - X_2 &= 4, \\ 2X_1 + 6X_2 - X_3 &= 7 \\ X_1 + 2X_2 - 3X_3 &= 0. \end{aligned}$$

It is easy to verify that the solution to the following system:

$$X_1=1, 2X_2=1, X_3=1.$$

Decision. Express the unknown x_1 , x_2 and x_3 respectively the first, second and third equations:

$$\begin{aligned} X_1 &= \frac{1}{4}(4 + X_2 - X_3) \\ X_2 &= \frac{1}{6}(7 - 2X_1 + X_3) \\ X_3 &= \frac{1}{3}(X_1 + 2X_2) \end{aligned}$$

As an initial approximation (as is common) will take $x_1^{(0)}=0$, $x_2^{(0)}=0$, $x_3^{(0)}=0$.

Find the new approach of the unknown:

$$\begin{aligned} X_1^{(1)} &= \frac{1}{4}(4 + X_2^{(0)} - X_3^{(0)}) = \frac{1}{4}(4 + 0 - 0) = 1 \\ X_2^{(1)} &= \frac{1}{6}(7 - 2X_1^{(1)} + X_3^{(0)}) = \frac{1}{6}(7 - 2*1 + 0) = \frac{5}{6} \\ X_3^{(1)} &= \frac{1}{3}(X_1^{(0)} + 2X_2^{(0)}) = \frac{1}{3}(1 + 2*\frac{5}{6}) = \frac{8}{9} \end{aligned}$$

Similarly, calculate the following approximation;

$$\begin{aligned} X_1^{(2)} &= \frac{1}{4}(4 + X_2^{(1)} - X_3^{(1)}) = \frac{1}{4}(4 + \frac{5}{6} - \frac{8}{9}) = \frac{71}{72} \\ X_2^{(2)} &= \frac{1}{6}(7 - 2X_1^{(2)} + X_3^{(1)}) = \frac{1}{6}(7 - 2*\frac{71}{72} + \frac{8}{9}) = \frac{71}{72} \\ X_3^{(2)} &= \frac{1}{3}(X_1^{(1)} + 2X_2^{(1)}) = \frac{1}{3}(\frac{71}{72} + 2*\frac{71}{72}) = \frac{71}{72} \end{aligned}$$

Iterative process can continue until a small difference between the values of unknowns in two consecutive iterations.

The advantage of iterative methods to accurate method of Gauss that the computer time required for computation by Gauss proportional to n^3 , and iterative methods it is proportional to n per iteration. Therefore, if for solving linear systems of equations with n variables n iterative methods require less n^3 iterations, these methods have the advantage over the method of Gauss. Practical problems often lead to systems of linear equations, which contain many zero coefficients. In such cases, iterative methods produce big savings computing time. For triangular matrix by using the Gauss-reaching, no longer will have zero elements.

Besides rounding error when using Gauss may lead to false results, while minor errors made in the calculation iterative methods do not affect the final result. It should be noted that iterative methods make it possible to significantly reduce the amount of computer memory needed to store the coefficients of the system as approximation for calculating the coefficients x_i used only i th equation. This is particularly important for solving systems of equations whose coefficients do not fit in memory computers.

Chapter 7 COMPUTER METHODS SOLUTIONS OF ORDINARY DIFFERENTIAL EQUATIONS

7.1 Statement of the problem

Often the problem of technology and science mathematically reduced to finding the solution of a certain differential equation (or system of equations) that satisfies certain initial conditions (Cauchy problem). Integrate this equation in a finite unable rare. At the same time obtain the following expression for the most part to which the desired function is implicit, and therefore use it uncomfortable.

In practice, used mostly approximate integration of differential equations. It allows you to find the approximate solution of the Cauchy problem or a certain analytical expression (eg, Taylor series), or as some table values. Consider some numerical methods for solving the Cauchy problem for ordinary differential equations of the first order derivative with respect unleashed. Approximate solution of the Cauchy problem written in the form of a table of values. The Cauchy problem is to find the solution $y(x)$ of the differential equation

$$y' = f(x, y), \quad (7.1)$$

which satisfies the initial condition

$$y(x_0) = y_0 \quad (7.2)$$

Geometric means that we must find the integral curve $y(x)$ of (7.1), which passes through the point (x_0, y_0) .

Cauchy problem (7.1) - (7.2) has a unique solution, such as the conditions of this theorem.

Theorem (Picard). If the function $f(x, y)$ of two variables x and y are continuous closed box

$$\bar{\Delta} = \{(x, y): |x - x_0| \leq l, |y - y_0| \leq l\}$$

centered at (x_0, Y_0) and satisfies the condition it Lipnytsya the variable y , that is, there is a number $K > 0$ independent of x and y such that

$$|f(x_1, y_1) - f(x_2, y_2)| \leq K|y_1 - y_2| \quad (7.3)$$

for all points $(x_1, y_1) \in \bar{\Delta}$ and are $(x_2, y_2) \in \bar{\Delta}$ are, then there exists a unique differentiable function in $y = \varphi(x)$, which is a solution of the differential equation (7.1) satisfying the initial condition (7.2). This solution is defined and continuously differentiated at least in the interval $[x_0 - h; x_0 + h]$,

where

$$h = \min \left\{ l, \frac{b}{M} \right\}, \quad M = \max_{(x,y) \in \bar{\Delta}} |f(x,y)| \quad (7.4)$$

Consider the so-called one-step numerical methods for solving the Cauchy problem (7.1) - (7.2) where to find the approximate solution at the point $x_{k+1} = x_k + h$, enough to know the solution at the point x_k . And because the solution of the problem at the point x_0 with known initial conditions, these methods allow to calculate the value of the solution successively the following points $x_1 = x_0 + h$, $x_2 = x_1 + h$, With one-step numerical methods consider only Explicit Runge-Kutta. Some representatives of these methods are the methods of Euler type, which chronologically preceded Runge-Kutta. Further assume that the function $f(x, y)$ of (7.1) satisfies the conditions of Theorem Picard.

Euler method. Let the interval $[x_0; x_0 + l]$ need to find a numerical solution of the Cauchy problem (7.1) - (7.2). For this segment $[x_0; x_0 + l]$ of divide by n (for simplicity) points equal parts $x_0, x_1, x_2, \dots, x_n = x_0 + l$, where

$$x_k = x_0 + kh \quad (k = 0, 1, 2, \dots, n), \quad h = \frac{l}{n}.$$

The value of h is called step numerical integration of the differential equation (7.1).

To solve the problem (7.1) - (7.2) numerically - it means for a given sequence $x_0, x_1, x_2, \dots, x_n = x_0 + l$, independent variable x and the number N_0 find a numerical sequence y_1, y_2, \dots, y_n for a given sequence of values of the independent variable $x_k = x_0 + kh$ ($k = 0, 1, \dots, n$) to build a table of approximate values of the solution 'communication Cauchy problem.

If the approximate solution of problem (7.1) - (7.2) at x_k known, then After integration equation (7.1) in the range from x_k to $x_k + 1$, we find its solution at the point of $x_k + 1$ by the formula

$$y(x_{k+1}) = y(x_k) + \int_{x_k}^{x_{k+1}} f(x, y(x)) dx. \quad (7.5)$$

It is this formula is starting to build many numerical methods for solving the problem (7.1) - (7.2). Euler method. If the integral on the right side of (7.5) calculated by the formula left rectangles, we find

$$y(x_{k+1}) = y(x_k) + hf(x_k, y(x_k)) + O(h^2). \quad (7.6)$$

Rejecting the term equality in this order 0 (h^2), we obtain the estimated formula

$$y(x_{k+1}) = y(x_k) + hf(x_k, y_k) \quad (k = 0, 1, 2, \dots, n-1), \quad h = x_{k+1} - x_k, \quad (7.7)$$

called Euler's formula. Hereinafter everywhere y_k and $y(x_k)$ - respectively approximate and the exact value of the desired solution of the problem (7.1) - (7.2) at the point x_k . The difference $y_k - y(x_k)$ is called the error of the approximate value y_k at the point x . Since the tangent to the graph of $y(x)$ at the point (x_k, y_k) has slope k , which is equal to the original $y'_k = f(x_k, y_k)$, then the equation of the tangent to the integral curve $y(x)$ of problem (7.1) - (7.2) at the point (x_k, y_k) will have the form

$$y - y_k = y'_k(x - x_k) \quad \text{or} \\ y - y_k = f(x_k, y_k)(x - x_k).$$

This ordinates for $y_k + 1$ point of intersection of the tangent with direct $x = x_k + 1$ we obtain the formula (7.7).

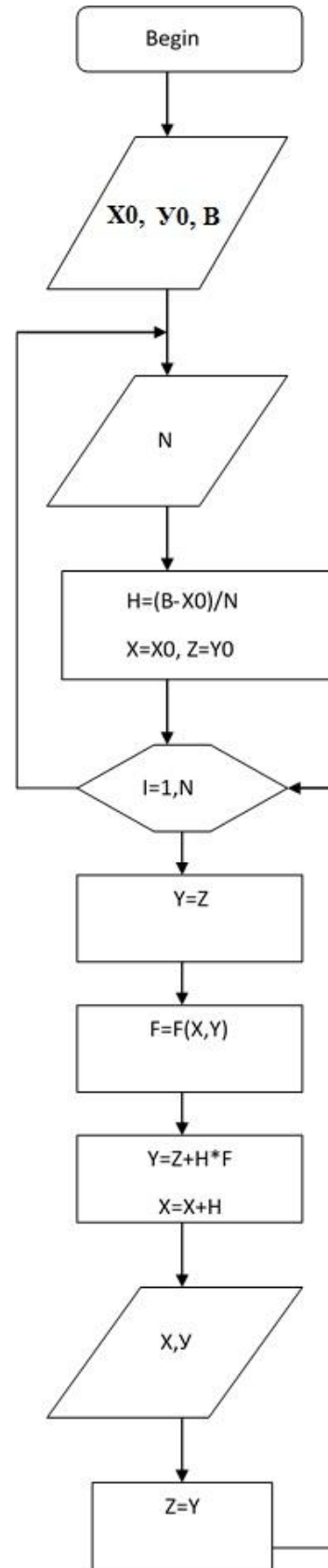


Figure 7.1.

This means that each of the segments $[x_k, x_{k+1}]$, $(k=0,1,\dots,n-1)$ integral curve segment replaced approximately tangent to it at the point (x_k, y_k) . If the plane Oxy point mark $M_k (x_k; y_k)$, $k = 0,1,2, \dots, n$ and combine them in order segments, it will get broken (it is called Euler Lohman), which represents approximately schedule desired solution ' connection problem (7.1) - (7.2). This is the geometric meaning of the Euler method (Fig. 5.1). Note that the error of Euler's method at each step is of the order $O(h^2)$. The accuracy of the method is fairly small and the transition from point x_k to point x_{k+1} its systematic error increases. A flow chart of the algorithm Euler method is presented in Figure 7.2.

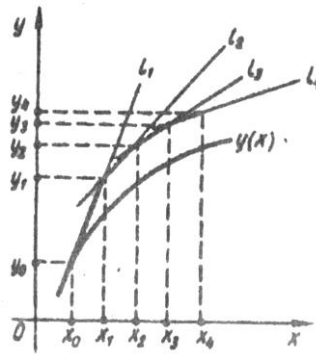


Figure 7.2

Improved Euler method. If the integral on the right side of (7.5) calculated by the formula medium rectangles, that is the value of the integrand function $f(x, y(x))$ calculate the point $x_{k+\frac{1}{2}} = x_k + h/2$ we find

$$y(x_{k+1}) = y(x_k) + hf(x_{k+\frac{1}{2}}, y(x_{k+\frac{1}{2}})) + O(h^3). \quad (7.8)$$

The value of an unknown value function $y(x_{k+\frac{1}{2}})$ calculate the formula (7.6) with step $h/2$ will have

$$y(x_{k+\frac{1}{2}}) = y(x_k) + \frac{1}{2} hf(x_k, y(x_k)) + O(h^2)$$

Substituting this value $y(x_{k+\frac{1}{2}})$ in (7.8), we obtain

$$y(x_{k+1}) = y(x_k) + hf(x_{k+\frac{1}{2}}, y(x_{k+\frac{1}{2}})) + \frac{1}{2} hf(x_k, y(x_k)) + O(h^2) + O(h^3) =$$

$$= y(x_k) + hf(x_{k+\frac{1}{2}}, y(x_k)) + \frac{1}{2} hf(x_{k+\frac{1}{2}}, y(x_k)) + O(h^3)$$

Dropping this term is proportional to h^3 , will have

$$y_{k+1} = y_k + hf(x_{k+\frac{1}{2}}, y_k) + \frac{1}{2} hf(x_k, y_k)$$

Formulas improved Euler method can be written as

$$y_{k+\frac{1}{2}} = y_k + \frac{1}{2} hf(x_k, y_k) \quad (7.9)$$

$$y_{k+1} = y_k + hf(x_{k+\frac{1}{2}}, y_{k+\frac{1}{2}}) \quad (7.10)$$

Thus, the improved Euler method initially by Euler (equation (7.9)) compute an approximate solution $y_{k+\frac{1}{2}}$ problem (7.1) - (7.2) at $x_{k+\frac{1}{2}} = x_k + \frac{h}{2}$, then the formula (7.10) - approximate solution y_{k+1} at the point of x_{k+1} ; at every step of integrating the right side of the equation (7.1) is calculated twice (at the points x_k, y_k) and $(x_{k+\frac{1}{2}}, y_{k+\frac{1}{2}})$).

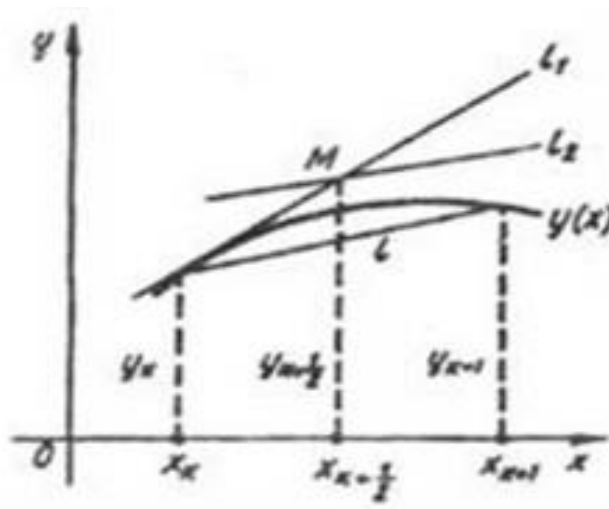


Figure 7.3 – The function plot.

Geometric means that the interval $[x_k, x_{k+1}]$ schedule integral curve of the problem (7.1) - (7.2) is replaced by the line segment that passes through the

point (x_k, y_k) and has a slope $k = f(x_{k+\frac{1}{2}}, y_{k+\frac{1}{2}})$. In other words, the straight line (Fig. 5.3) forms with the positive direction of the axis Ox angle $\varphi = \arctg f(x_{k+\frac{1}{2}}, y_{k+\frac{1}{2}})$. As for the point $(x_{k+\frac{1}{2}}, y_{k+\frac{1}{2}})$, it is the point of intersection of the tangent to the integral curve of the problem (7.1) - (7.2) at the point (x_k, y_k) with direct $x = x_k + h$. Accuracy improved Euler method at every step of the order of $O(h^3)$.

7.2 Runge-Kutta

With the advent of computers and the development of numerical integration of ordinary differential equations rapid development are the method of Runge-Kutta type. Such methods are built up to the 10th order of accuracy inclusive. In practice, their computer is widely used because. they:

- one-step, is to calculate the solution of the problem (7.1) - (7.2) at x_{k+1} should know the solution only at the point x_k
- allow you to perform numerical integration with variable step;
- especially useful for computer programming, because calculating them is cyclical.

In addition to these methods have advantages and disadvantages. Yes, it is very difficult to estimate the error of the approximate solution of problem (7.1) - (7.2) for guaranteed well-known local estimation error is largely overstated, but because of their practical value is negligible. The disadvantages include the fact that it is necessary to calculate the number of points in the right part of equation (7.1) (the function $f(x, y)$) at every step of integration. In an improved method for each step of the integration value of the function $f(x, y)$ calculated at two points, and Runge-Kutta third and fourth order accuracy of the calculated according to three or four points. As for Runge - Kutta, order accuracy which is greater than four, the right-hand side of equation (7.1) at every step of integration always calculated in points, whose number greater than the order of accuracy of the method. The idea of giving this tab. 6.1.

Table 7.1.

s	2	3	4	5	6	7	8	9	10
n	2	3	4,5	6	7,8	9	11	14	18

Here s - order accuracy Runge-Kutta, n - number of points at which the function is computed $f(x, y)$ at every step of integration.

Then the Cauchy problem (7.1) - (7.2) rozv'yazuvatymemo numerically by the Runge-Kutta, order accuracy does not exceed four. Assume that the function $f(x, y)$ in the rectangle $\bar{\Delta}$ has continuous partial derivatives up to some order n . Then the solution $y(x)$ have continuous derivatives up to the $(n + 1)$ th order and for sufficiently small values of h at the point $x_{k+1} = x_k + h$, $h > 0$ can be represented as the schedule

$$y(x_{k+1}) = y(x_k) + hy'(x_k) + \frac{h^2}{2!} y''(x_k) + \dots + \frac{h^n}{n!} y^{(n)}(x_k) + O(h^{n+1}). \quad (7.11)$$

Derivative $y^{(i)}(x_k)$ ($i = 1, 2, \dots, n$) $y^{(i)}(x_k)$ ($i = 1, 2, \dots, n$) on the right side of (7.11) can be expressed in terms of the value of the function f and its partial derivatives at the point (x_k, y_k) .

We have

$$y'(x_k) = f(x_k, y_k) = f_k \quad (7.12)$$

$$y''(x_k) = f'_{x_k}(x_k, y_k) + y'_k f'_{y_k}(x_k, y_k) = (f'_{x_k} + y'_k f'_{y_k})_k, \quad (7.13)$$

where the index k hereinafter means that the corresponding function is calculated at the point (x_k, y_k) .

Similarly calculate higher order derivatives and, being expressions with increasing order much more complicated. Therefore, direct use to calculate their approximate value solution $Y(x_{k+1}) = y(x_k + h)$ at the point x_{k+1} formula (7.11) is unlikely to be appropriate.

It should be noted that computer programs developed systems that enable the machine to perform independently formal differentiation functions unless asked the program to compute the function $f(x, y)$. Thus, there is no need to create a program evaluation of derivatives of the function $f(x, y)$.

However, the cost of computer time to implement these algorithms can often be so great that better use numerical methods of integration of ordinary differential equations, Runge-Kutta particular. Instead derivatives $y^{(i)}_k$ ($i = 1, 2, \dots, n+1$), k (and $i = 1, 2, \dots, n+1$). within the right of (7.11), Runge suggested values approximate solution y_{k+1} at the point of x_{k+1} calculated by formulas like:

$$y_{k+1} = y_k + \sum_{i=1}^r w_i k_i \quad (7.14)$$

where function $k_i = hf(c_i, d_i)$ ($i=1, 2, \dots, n$), $c_i = x_k + a_i h$, $d_i = y_k + \sum_{j=1}^{i-1} \beta_{ji} k_j$, but $w_i, a_i, (\alpha_1=0)$ and β_{ij} some steel that nazvyvatymemo parameters Runge-Kutta formulas.

The unknown parameters w_i, a_i, β_{ij} determined such that expansion in powers of h right-hand side of formula (7.14) coincides with the schedule (7.11) to as high degrees h for an arbitrary function $f(x, y)$ and the random integration step h .

Before building design formulas Runge-Kutta introduce the concept of order of accuracy of these methods. Let $y(x_{k+1}) = y(x_k + h)$ and y_{k+1} and - according exact and approximate solutions of the problem (7.1) - (7.2) at x_{k+1} , and the exact solution calculated by the formula (7.11) and close - by formula (7.14), which after expansion in powers of h can be written as:

$$y_{k+1} = y_k + h a_1 + \frac{h^2}{2!} a_2 + \frac{h^3}{3!} a_3 + \dots + \frac{h^{n+1}}{(n+1)!} a_{n+1} \quad (7.15)$$

where a_i ($i=1, 2, \dots$) — some numerical coefficients.

The greatest of the exponents h , at which expansion coefficients (7.11) and (7.15) are equal, called the order of accuracy of the approximate method. So, if the order of accuracy of the approximate method is s , then it means that the decomposition (7.11) and (7.15) coefficients

$$a_1 = y'_k, a_2 = y''_k, a_3 = y'''_k, \dots \text{ but } a_{s+1} \neq y^{(s+1)}_k$$

Note that error method one step integration procedure is always one greater than the order of accuracy of the method. Therefore, the order of accuracy of the method is Euler unit for error method in one step is of order h^2 , and order accuracy improved Euler method is two, because the order of the error of these methods in one step h^3 .

Runge-Kutta formulas of first-order accuracy. Let the function $f(x, y)$ in the neighborhood of the point (x_k, y_k) has continuous partial derivatives of the first order. Then the solution $y(x)$ of the Cauchy problem in the neighborhood of x_k have continuous derivatives up to second order inclusive. Therefore, for sufficiently small values of h at the point $x_k = x_k + h$ can be represented as powers of h , taking into account (7.12), as follows:

$$y(x_{k+1}) = y(x_k) + hf(x_k, y_k) + O(h^2). \quad (7.11)$$

Runge-Kutta formulas of first order accuracy build as follows:

$$y_{k+1} = y_k + w_1 k_1 \quad (7.16)$$

where $k_1 = hf(x_k, y_k)$, and w_i unknown parameter. Expanding the powers of h on right side of (7.16), we obtain

$$y_{k+1} = y_k + hf(x_k, y_k) w_1 \quad (7.17)$$

Equating coefficients at each other h in formulas (7.11) and (7.17), we find $w_1 = 1$. Substituting this value w_1 in equation (7.16), we see that formula Runge-Kutta first order accuracy ($s = 1$) is Euler's formula. The error of this method $y_{k+1} - y_k$ every step is of order h^2 . Formula Runge-Kutta second order accuracy Let a function $f(x, y)$ in a neighborhood of (x_k, y_k) has continuous partial derivatives up to second order inclusive. Then the solution $y(x)$ of the Cauchy problem (7.1) - (7.2) in a neighborhood of x_k have continuous derivatives up to third order inclusive. Therefore, for sufficiently small values of h at the point $x_{k+1} = x_k + h$ can be represented in the form of the expansion in powers of h

$$y(x_{k+1}) = y(x_k) + hy'(x_k) + \frac{h^2}{2!} y''(x_k) + O(h^3). \quad (7.18)$$

Formula Runge-Kutta second order accuracy ($s = 2$) will look like this:

$$y_{k+1} = y_k + w_1 k_1 + w_2 k_2 \quad (7.19)$$

where

$$k_1 = hf(x_k, y_k). \quad (7.20)$$

$$k_2 = hf(x_k + a_2 h, y_k + \beta_{21} k_1). \quad (7.21)$$

where $w_1, w_2, a_2, \beta_{21}$ unknown parameters that define so that (7.19) was the formula of the second order of accuracy ($s = 2$), that is the coefficients in the expansion (7.18) and (7.19) in a series of h are equal to each other at h and h^2 . Features k_1 and k_2 are laid in a series of h as follows:

$$k_1 = hf(x_k, y_k)$$

$$k_2 = hf(x_k + a_2 h, y_k + \beta_{21} k_1) = hf(x_k) + a_2 h^2 (f'_x)_k + h^2 \beta_{21} (ff'_y)_k + O(h^3).$$

Substituting these expansions k_1 and k_2 in (7.19), we obtain expansion in powers of h (leave only members proportional to h^2) of the form:

$$y_{k+1} = y_k + h(w_1 + w_2)fk + h^2(w_2a_2(f'_x)_k + w_2\beta_{21}(ff'_y)_k) + O(h^3). \quad (7.22)$$

Equating the coefficients of hfk , $h^2(f'_x)_k$, $h^2(ff'_y)_k$

in formulas (7.18) and (7.22) to determine the four unknown parameters w_1 , w_2 , a_2 and β_{21} we obtain the algebraic system of three equations like

$$\begin{cases} w_1 + w_2 = 1 \\ w_2a_2 = \frac{1}{2} \\ w_2\beta_{21} = \frac{1}{2} \end{cases} \quad (7.23)$$

Since the system (7.23) shows that $w_2 \neq 0$, $a_2 \neq 0$, $\beta_{21} \neq 0$ and $a_2 = \beta_{21}$. It has an infinite set of solutions, depending on one parameter, each formula gives the solution of Runge-Kutta second order accuracy.

If you put $w_2 = \frac{3}{4}$, тоді $w_1 = \frac{1}{4}$, $a_2 = \beta_{21} = \frac{2}{3}$ and formulas (7.19) - (7.21) takes the form

$$y_{k+1} = y_k + \frac{1}{4}(k_1 + 3k_2),$$

$$k_1 = hf(x_k, y_k), \quad k_2 = hf(x_k + \frac{2}{3}h, y_k + \frac{2}{3}k_1).$$

Runge-Kutta fourth order accuracy ($s = 4$) can be constructed similarly to the previous ones, though this will require biggest calculations and solving a nonlinear system of algebraic equations and complex structure. Accuracy of these methods at each step of integration is of the order of h^5 . Most formulas are of the form

$$y_{k+1} = y_k + \sum_{i=1}^4 w_i k_i \quad (7.24)$$

where

$$k_1 = hf(x_k, y_k),$$

$$\begin{aligned}
k_2 &= hf(x_k + a_2 h, y_k + \beta_{21} k_1), \\
k_3 &= hf(x_k + a_3 h, y_k + \beta_{31} k_1 + \beta_{32} k_2), \\
k_4 &= hf(x_k + a_4 h, y_k + \beta_{41} k_1 + \beta_{42} k_2 + \beta_{43} k_3).
\end{aligned} \tag{7.25}$$

These formulas are 13 unknown parameters w_i , a_i , β_{ij} . It is proved that there is an infinite set of formulas of the form (7.24), (7.25), which depends on two arbitrary real parameters and a fourth order accuracy. We confine ourselves to the following specific examples of formulas that belong to this set:

$$\begin{aligned}
y_{k+1} &= y_k + \frac{1}{6} (k_1 + 2k_2 + 2k_3 + k_4) \quad . \\
k_1 &= hf(x_k, y_k). \\
k_2 &= hf(x_k + \frac{1}{2} h, y_k + \frac{1}{2} k_1). \\
k_3 &= hf(x_k + \frac{1}{2} h, y_k + \frac{1}{2} k_2). \\
k_4 &= hf(x_k + h, y_k + k_3) \quad .
\end{aligned} \tag{7.26}$$

This formula is most often used in computational practice. From the geometric point of view of formula (7.26) the integral curve of the problem (7.1) - (7.2) on the interval $[x_k, x_{k+1}]$ replacing line segment that passes through the point (x_k, y_k) and forms a positive direction of the axis Ox angle

$$\varphi = \text{artg} \frac{k_1 + 2k_2 + 2k_3 + k_4}{6h}.$$

Finally, we note that discussed above Runge-Kutta method is also used to normal systems of differential equations of the first order. German mathematician R. Tsurmyul generalized Runge-Kutta method to the case of differential equations of second, third and higher orders.

7.3 About error estimates for approximate cauchy problem solving

For Runge-Kutta used a number of a priori estimates of the error of the approximate solution of the Cauchy problem (7.1) - (7.2). These estimates is

largely overestimated. Because hardly appropriate to recommend them for control in practical calculations. Their importance is not so much practical as theoretical, because of which directly follows the conclusion of the convergence of these methods. In addition, a priori estimates include a number of constants to find that often need to perform fairly complex calculations.

Therefore, to estimate the error of the approximate solution of problem (7.1) - (7.2), try to use the information you obtain the numerical calculation process (such assessments called a posteriori).

The most effective evaluation of the double transfer. Spynymos more on the double conversion.

Consider the following three cases:

1. Given the integration step h and must identify the exact figures approximate solution at each nodal point x_k
2. Given a precision $\varepsilon > 0$, which must calculate an approximate solution of the problem, reaching out properly as the method and integration step h .
3. Evaluate the error $\varepsilon_k = y_k - y(x_k)$, where y_k and $y(x_k)$ - respectively approximate and exact solutions of the problem in each nodal point x_k . For this solution to the problem (7.1) - (7.2) in each nodal point x_k calculated twice: with step h and $h/2$. Denote them respectively in the y_k^* . Decimal digits approximations in y_k^* , which coincide with each other, find exact figures approximate solution at the point x_k .

For absolute error at the point of x_k are:

$$|\varepsilon_k^*| = |y_k^* - y(x_k)| = \frac{|y_k - y_k^*|}{2^s - 1}$$

where s - order of accuracy Runge-Kutta.

Example 1: Solve the Cauchy problem

$$dy/dx = 2(x^2 + Y), Y(0) = 1, 0 \leq x \leq 1, h = 0.1.$$

Decision. Formulated Cauchy problem can be solved with the known course of higher mathematics methods. Lowering the presentation, we write the final expression for the exact solution of the given initial conditions into account. It has the form

$$Y = 1.5e^{2x} - x^2 - x - 0.5$$

Draw now the solution of this problem numerically using the above methods.

1. Euler method to find the values in X by the following formulas:

$$Y_1 = y_0 + h * f(x_0, y_0) = 1 + 0.1 * [2 * (0^2 + 1)] = 1.2000$$

$$Y_2 = y_1 + h * f(x_1, y_1) = 1.2000 + 0.1 * [2 * (0.12 + 1.2000)] = 1.4420$$

$$Y_3 = y_2 + h * f(x_2, y_2) = 1.4420 + 0.1 * [2 * (0.22 + 1.4420)] = 1.7384 \text{ ect.}$$

Numerical results are given in Table. 7.2. The modified Euler method is initially calculated intermediate *znachennya*. Napryklad to stay Y_1 :

$$X_{1/2} = x_0 + h/2 = 0 + 0.05 = 0.05$$

$$Y_{1/2} = y_0 + h/2 * f_0 = 1 + 0.05 * [2 * (0^2 + 1)] = 1.10$$

$$f_{1/2} = f(X_{1/2}, Y_{1/2}) = 2 * (0.05^2 + 1.10) = 2.205$$

then

$$Y_1 = y_0 + h * f_{1/2} = 1 + 0.1 * 2.205 = 1.2205$$

Numerical results are given in Table. 7.2. For the Runge-Kutta method of calculating an approximate value U_1 in the next point X_1 produced by the formulas:

$$X_1 = x_0 + h = 0 + 0.1 = 0.1$$

$$K_1 = hf(x_0, y_0) = 0.1 * [2 * (0^2 + 1)] = 0.2$$

$$K_2 = hf(x_1 + h/2, y_0 + K_1/2) = hf(0.05, 1.1) = 0.1 [2 * (0.05^2 + 1.1)] = 0.2205$$

$$K_3 = hf(x_1 + h/2, y_0 + K_2/2) = hf(0 + 0.051 + 0.2205/2) = 0.1 [2 * (0.05^2 + 1.11025)] = 0.22255$$

$$K_4 = hf(x_1 + h, y_0 + K_3) = hf(0.1, 1 + 0.22255) = 0.1 [2 * (0.1^2 + 1.22255)] = 0.24651$$

$$\Delta Y_1 = 1/6 (K_1 + 2K_2 + 2K_3 + K_4) = 1/6 (0.2 + 2 * 0.2205 + 2 * 0.22255 + 0.24651) = 0.222$$

$$Y_1 = y_0 + \Delta Y_1 = 1 + 0.2221 = 1.2221$$

Then all calculations continue in the same manner, taking the starting point (X_1, Y_1) .

Numerical results are given in Table. 6.2. As can be seen from this table is the most accurate solution obtained by Runge - Kutta. Analysis of the solution using Euler method allows us to trace the growth of errors with increasing X_i . If $X_i = 1$ error is about 18%. Thus, when a large number of nodes Euler method can lead to significant errors in such cases is preferable enjoy numerous methods of higher order accuracy.

With decreasing step h local error Euler method will decrease, but it will increase the number of nodes that adversely affect the accuracy of the results.

Therefore Euler method is relatively rare in the small number of calculation points. The most common method is the one-step Runge - Kutta.

Table 7.2

X_i	Euler method	The modified Euler method	Runge-Kutta	Exact solution
0.1	1.2000	1.2205	1.2221	1.2221
0.2	1.4420	1.4923	1.4977	1.4977
0.3	1.7384	1.8284	1.8432	1.8432
0.4	2.1041	2.2466	2.2783	2.2783
0.5	2.5569	2.7680	2.8274	2.8274
0.6	3.1183	3.4176	3.5201	3.5202
0.7	3.8139	4.2257	4.3927	4.3928
0.8	4.6747	5.2288	5.4894	5.4895
0.9	5.7376	6.4004	6.8643	6.8645
1.0	7.0472	8.0032	8.5834	8.5836

With the implementation of the Runge-Kutta method of computer automatic selection step course in each point x_i make a double first in increments h , then with step $h / 2$. If the value obtained with the y_i vary within acceptable accuracy, then move to the next point $h (x_{i+1})$ double, otherwise take a half step. The methods can also be used to solve systems of differential equations.

Chapter 8 FINITE DIFFERENCE METHOD (METHOD OF GRIDS)

8.1 Method nets, or method of finite differences

Method nets, or method of finite differences is one of the most common methods for the numerical solution of partial differential equations. It is based on the introduction of some *riznychnoyi* grid in the given region. The value of derivatives, initial and boundary conditions are expressed in terms of value functions in the grid, resulting in a system of algebraic equations is obtained, called *riznychnoyu* scheme. Solving this system of equations can be found in the grid value grid functions that are considered approximately equal to the value desired functions. We will consider equations of the second order partial derivatives:

wave equation (hyperbolic)

$$\frac{\partial^2 u}{\partial t^2} = a^2 \frac{\partial^2 u}{\partial x^2} \quad (8.1)$$

heat equation or diffusion (parabolic)

$$\frac{\partial u}{\partial t} = a^2 \frac{\partial^2 u}{\partial x^2} \quad (8.2)$$

Laplace equation (elliptical)

$$\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \quad (8.3)$$

The reduced equation are called equations of mathematical physics. By their decision reduced many applications.

The basis of the method is the idea of replacing nets derivatives end-*riznychnymy* relations.

Let the plane xOy means a region G of Γ . We construct a boundary in the plane parallel direct two families:

$$x=x_0+ih, \quad i=0,\pm 1,\pm 2,\dots$$

$$y=y_0+kl, \quad k=0,\pm 1,\pm 2,\dots$$

The points of intersection of these direct host name. Similarly introduced for multidimensional grid areas containing more than two dimensions. The rectangular grid in the most convenient of the computational algorithm. However, some schemes use a grid of triangular and hexagonal cells even Two nodes are called neighbors if they are removed from each axis Ox or Oy a distance equal to the grid spacing h or l respectively. Units, in which all four neighboring nodes

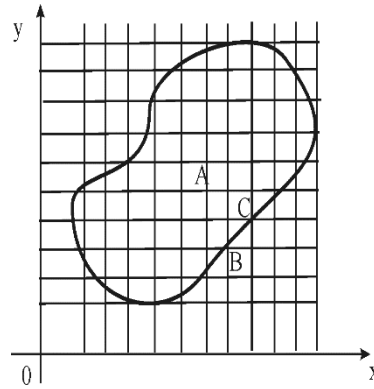


Figure 8.1

Units, in which all four neighboring nodes are region $G + \Gamma$, called internal (node A). Last of the selected nodes are called boundary (nodes B, C). The value of the unknown function $u = u(x, y)$ in the grid denoted through $u_{ik} = u(h_0 + ih, A_0 + kl)$. Each internal node $(h_0 + ih, A_0 + kl)$ replace the partial derivatives respects:

$$\left(\frac{\partial u}{\partial x}\right)_{ik} \approx \frac{u_{i+1,k} - u_{i-1,k}}{2h}, \quad (8.4)$$

$$\left(\frac{\partial u}{\partial y}\right)_{ik} \approx \frac{u_{i,k+1} - u_{i,k-1}}{2l} \quad (8.5)$$

at the boundary points we have to enjoy less accurate formulas of the form

$$\left(\frac{\partial u}{\partial x}\right)_{ik} \approx \frac{u_{i+1,k} - u_{i,k}}{h} \quad (8.6)$$

$$\left(\frac{\partial u}{\partial y}\right)_{ik} \approx \frac{u_{i,k+1} - u_{i,k}}{l} \quad (8.7)$$

Similarly, the second order derivatives are replaced, for example:

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{ik} \approx \frac{u_{i+1,k} - 2u_{i,k} + u_{i-1,k}}{h^2} \quad (8.8)$$

$$\left(\frac{\partial^2 u}{\partial y^2}\right)_{ik} \approx \frac{u_{i,k+1} - 2u_{i,k} + u_{i,k-1}}{l^2} \quad (8.9)$$

These replace the original in every grid node allows to reduce the solution of partial differential equations to the solution of difference equations.

8.2 Method grids for hyperbolic equation

Wave equation. One of the most common in engineering equations of the second order is the wave equation describing the different types of vibrations. Since fluctuations - transient process, then one of the independent variable is time t . In addition, the independent variables in the equation is also the spatial coordinates x, y, z . Depending on their number distinguish one-dimensional, two-dimensional and Three-dimensional wave equation. One-dimensional wave equation describing the transverse vibrations of a thin rod (string) and other tasks.

$$\frac{\partial^2 u}{\partial t^2} = a^2 \frac{\partial^2 u}{\partial x^2} \quad (8.10)$$

and initial conditions:

$$u(x, 0)=f(x) \quad \text{и} \quad \frac{\partial u}{\partial t}(x,0) = \Phi(x), \quad (0 \leq x \leq s) \quad (8.11)$$

and boundary conditions: and boundary conditions:

$$u(0,t)=\varphi(t), u(s,t)=\psi(t) \quad (8.12)$$

Because the input variable $\tau=a^2$ results in equation (8.10) to the form

$$\frac{\partial^2 u}{\partial \tau^2} = \frac{\partial^2 u}{\partial x^2} \quad (8.13)$$

then later we can take $a = 1$.

Constructing a napivsmuzi $t>0$, $0 \leq x \leq s$ two families of parallel straight:

$$x=ih \quad (i=0,1,2, \dots), \quad t=jl \quad (j=0,1,2, \dots).$$

Denote $x_i=ih$, $t_j=jl$, $u(x_i, t_j) = u_{ij}$ and replacing the derivatives in equation (8.13) riznychnymy relations. Using the formulas for symmetric derivative, we have

$$\frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{l^2} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} \quad (8.14)$$

Denoting $\alpha = l / h$, we obtain an equation that will be sustainable when $\alpha < 1$

$$u_{i,j+1} = 2u_{ij} - u_{i,j-1} + \alpha^2 (u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) \quad (8.15)$$

In particular, when $\alpha = 1$, equation (8.15) has the simple form:

$$u_{i,j+1} = u_{i+1,j} + u_{i-1,j} - u_{i,j-1} \quad (8.17)$$

Error of approximate solutions obtained from equations (8.15) in the band $0 \leq x \leq s$; $0 \leq t \leq T$, in accordance with the type

$$|u - \tilde{u}| \leq \frac{h^2}{12} [(M_4 h + 2M_3)T + T^2 M_4], \quad (8.18)$$

where u -exact solution of the problem

$$M_k = \max \left\{ \left| \frac{\partial^k u}{\partial t^k} \right|, \left| \frac{\partial^k u}{\partial x^k} \right| \right\} \quad (k=3,4)$$

Note that to obtain equation (8.15) has been used a clear diagram nodes that allows you to find the value function $u(x, t)$ on the layer $(i, j + 1)$, if we know the values of the two previous layers. To find the approximate solution of the problem, it is necessary to know the value of the solution at the previous two layers. They can be found from the initial conditions of the following ways.

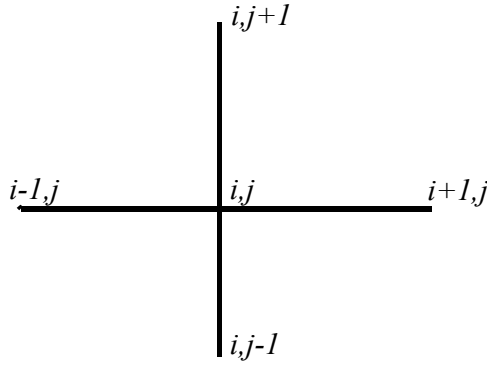


Figure 8.2

The first method. Replaces the initial condition (8.11) derivatives $u_t(x,0)$ ratio

$$\frac{u_{i1} - u_{i0}}{l} = \Phi(x_i) = \Phi_i ;$$

to determine the values of $u(x, t)$ on layers $j = 0, j = 1$, we obtain

$$u_{i0} = f_i, \quad u_{i1} = f_i + l\Phi_i. \quad (8.19)$$

Estimation error values u_{i1} in this case has the form

$$|\tilde{u}_{i1} - u_{i1}| \leq \frac{\alpha h}{2} M_2, \quad (8.20)$$

where $M_k = \max\{|\frac{\partial^k u}{\partial t^k}|, |\frac{\partial^k u}{\partial x^k}|\}$ ($k=2$)

The second method. Replaces original $u_t(x,0)$ ríznym ratio $\frac{u_{i1} - u_{i,-1}}{2l}$

where $u_{i,-1}$ - value function $u(x,t)$ in layer $j = -1$. Then the initial conditions (8.11) becomes

$$u_{i0} = f_i, \quad \frac{u_{i1} - u_{i,-1}}{2l} = \Phi_i. \quad (8.21)$$

We write equation (8.17) for layer $j = 0$:

$$u_{i1} = u_{i+1,0} + u_{i-1,0} - u_{i,-1} \quad (8.22)$$

Eliminating the equations (8.21), (8.22) values $u_{i,-1}$, we obtain

$$u_{i0}=f_i, \quad u_{il}=\frac{1}{2}(f_{i+l}+f_{i-l})+l\Phi_i \quad (8.23)$$

Estimation error values u_{il} has the form

$$|\tilde{u}_{il} - u_{il}| \leq \frac{h^4}{12} M_4 + \frac{h^3}{6} M_3,$$

where $M_k = \max\{|\frac{\partial^k u}{\partial t^k}|, |\frac{\partial^k u}{\partial x^k}|\}$ ($k=3,4$)

The third way. If the function $f(x)$ has a finite second derivative, the value u_{il} can be determined using Taylor's formula

$$u_{il} \approx u_{i0} + l \frac{\partial u_{i0}}{\partial t} + \frac{l^2}{2} \frac{\partial^2 u_{i0}}{\partial t^2} \quad (8.24)$$

Using equation (8.13) and the initial conditions (8.11), we can write

$$u_{i0}=f_i, \quad \frac{\partial u_{i0}}{\partial t} = \Phi_i, \quad \frac{\partial^2 u_{i0}}{\partial t^2} = \frac{\partial^2 u_{i0}}{\partial x^2} = f''_i$$

Then the formula (8.24) becomes

$$u_{il} \approx u_{i0} + l\Phi_i + \frac{l^2}{2} f''_i \quad (8.25)$$

Example 1. The method of mesh find solution to the problem.

$$\frac{\partial^2 u}{\partial t^2} = a^2 \frac{\partial^2 u}{\partial x^2}$$

$$u(x,0)=0, 2x(1-x) \sin \pi x,$$

$$\frac{\partial u}{\partial t}(x,0) = 0,$$

$$u(0,t)=u(1,t)=0$$

Decision. Take a square grid increments $h=l=0,05$.

Given the fact that $u(0,t)=u(1,t)=0$, will be $u_{0j}=0, u_{1j}=0$ ($j=0,1,2,\dots,10$)

The value of $u(x, t)$ on two primary layers find the second method:

$$u_{i0}=f_i, \quad u_{i1}=\frac{1}{2}(f_{i+1}+f_{i-1})+l\Phi_i$$

8.3 Completion of the table

1) Calculate the value $u_{i0}=f(x_i)=0,2x_i(1-x_i) \sin \pi x_i$ at $x_i=ih$ and write the first line (it corresponds to the value to $=0$) in the first column of Table 6.1 (it corresponds to the $x_0=0$) record thresholds.

2) In the formula found $u_{i1}=\frac{1}{2}(f_{i+1}+f_{i-1})+l\Phi_i$, т.к. $\Phi_i=0$, то $u_{i1}=0,5(f_{i+1}+f_{i-1})$, ($i=0,1,2,\dots,10$), using the values u_{i0} from the first line. The results recorded in the second line tabl.8.1

Table 8.1

$x_i \quad t_j$	0	0,05	0,10	0,20	0,30	0,40	0,50
0	0	0.0015	0.0056	0.0188	0.0340	0.0457	0.0500
0.05	0	0.0028	0.0065	0.0190	0.0335	0.0447	0.0489
0.10	0	0.0050	0.0094	0.0198	0.0322	0.0419	0.0456
0.15	0	0.0066	0.0124	0.0209	0.0302	0.0377	0.0405
0.20	0	0.0074	0.0142	0.0228	0.0277	0.0321	0.0338
0.25	0	0.0076	0.0144	0.0236	0.0251	0.0260	0.0265
0.30	0	0.0070	0.0134	0.0221	0.0227	0.0196	0.0186
0.35	0	0.0058	0.0112	0.0186	0.0194	0.0139	0.0115
0.40	0	0.0042	0.0079	0.0133	0.0140	0.0092	0.0054
0.45	0	0.0021	0.0042	0.0070	0.0074	0.0042	0.0013
0.50	0	-0.0001	-0.0001	-0.0002	-0.0002	-0.0002	-0.0002
$\overline{u(x_i, 0,5)}$	0	0	0	0	0	0	0

3) Calculate the value u_{ij} on these shahah formula (8.17), because $\alpha = 1$. When $j = 2$ we obtain successively

$$u_{12}=u_{21} + u_{01}-u_{10}= 0,0065 + 0 - 0,0015 = 0,0050,$$

$$u_{22}=u_{31} + u_{11}-u_{20} = 0,0122 + 0,0028 - 0,0056 = 0,0094,$$

$$u_{10,2}= u_{11,1} + u_{91} - u_{19,0}=0,0478 + 0,0478 - 0,0500 = 0,0456.$$

Calculations with $j = 3, \dots, 10$ performed similarly. The last line (tabl.8.1) present values of the exact solution at $t = 0,5$.

8.4 Method for equation mesh parabolic type

Consider a mixed problem for the heat equation, namely a function $u(x, t)$, which satisfies the equation:

$$\frac{\partial u}{\partial t} = a^2 \frac{\partial^2 u}{\partial x^2} \quad (8.26)$$

$$\text{initial condition } u(x, 0) = f(x) \quad (0 \leq x \leq s) \quad (8.27)$$

$$\text{and boundary conditions: } u(0, t) = \varphi(t), \quad u(s, t) = \psi(t). \quad (8.28)$$

By introducing a new variable $\tau = a^2 t$ equation (8.26) is reduced to the form

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial x^2}$$

therefore continue to take $a = 1$

Construct a napivsmuzi $t > 0, 0 \leq x \leq s$ two families of parallel straight:

$$x = ih \quad (i=0, 1, 2, \dots), \quad t = jl \quad (j=0, 1, 2, \dots)$$

Denote $x_i = ih, t_j = jl, \quad u(x_i, t_j) = u_{ij}$ and make derivative approximate replacement

$$\frac{\partial^2 u}{\partial x^2} \text{ each internal node } (x_i, t_j) - \text{ratio}$$

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{ij} \approx \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} \quad (8.29)$$

$$\text{and derivative } \frac{\partial u}{\partial t}: \quad \left(\frac{\partial u}{\partial t}\right)_{ij} \approx \frac{u_{i,j+1} - u_{i,j}}{l} \quad (8.30)$$

Then for the equation (8.26) with $a = 1$ we obtain:

$$\frac{u_{i,j+1} - u_{i,j}}{l} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} \quad (8.31)$$

Marking $\sigma = l/h^2$, We result these equations to the form:

$$u_{i,j+1} = (1 - 2\sigma)u_{ij} + \sigma(u_{i+1,j} - u_{i-1,j}) \quad (8.32)$$

Note that for the preparation of (8.32) was used clear circuit nodes (rys.6.3). It is proved that equation (8.32) is stable at $0 \leq \sigma \leq 1/2$. The most convenient form of equation (8.32) has at $\sigma = 1/2$:

$$u_{i,j+1} = 1/2 * (u_{i+1,j} - u_{i-1,j}) \quad (8.33)$$

and at $\sigma = 1/6$:

$$u_{i,j+1} = 1/6 * (u_{i+1,j} + 4u_{ij} + u_{i-1,j}) \quad (8.34)$$

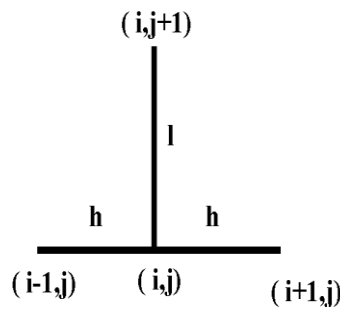


Figure 8.3

Estimates of the errors of approximate solutions obtained from equations (8.32), (8.33), (8.34) in the band $0 \leq x \leq s$; $0 \leq t \leq T$, in accordance with the type

$$|u - \tilde{u}| \leq \frac{T}{3} M_1 h^2, \quad (8.35)$$

$$|u - \tilde{u}| \leq \frac{T}{135} M_2 h^4, \quad (8.36)$$

$$|u - \tilde{u}| \leq T \left(\frac{l}{2} + \frac{h^2}{12} \right) M_1, \quad (8.37)$$

where u - true solution of the problem (8.26) - (8.28)

$$M_1 = \max \{ |f^{(4)}(x)|, |\varphi''(t)|, |\psi''(t)| \} \quad \text{at } 0 \leq t \leq T, \quad 0 \leq x \leq s,$$

$$M_2 = \max \{ |f^{(6)}(x)|, |\varphi^{(4)}(t)|, |\psi^{(4)}(t)| \} \quad \text{at } 0 \leq t \leq T, \quad 0 \leq x \leq s$$

With reduced estimates of errors shows that equation (8.34) gives higher accuracy than the solution to the equation (8.33).

8.5 Method grids for the Dirichlet problem

The first boundary-value problem, or Dirichlet problem for Poisson's equation

$$\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y) \quad (8.38)$$

placed as follows: find a function $u = u(x, y)$, satisfying some areas inside the G equation (8.38), and the border of Mr. condition: where $u|_{\Gamma} = \varphi(x, y)$, where $\varphi(x, y)$ — given continuous function. Choosing the steps h and l in x and y in accordance with, build grid.

$$x_i = x_0 + ih \quad (i=0, \pm 1, \pm 2, \dots), \quad y_k = y_0 + kl \quad (k=0, \pm 1, \pm 2, \dots)$$

and replaces each internal node (x_i, y_k) derivatives end-riznychnymy ratios (8.3):

$$\frac{u_{i+1,k} - 2u_{i,k} + u_{i-1,k}}{h^2} + \frac{u_{i,k+1} - 2u_{i,k} + u_{i,k-1}}{l^2} = f_{ik} \quad (8.39),$$

where $f_{ik} = f(x_i, y_k)$.

Equation (8.39), together with the values in u_{ik} boundary nodes form a system of linear algebraic equations on the function $u(x, y)$ in the nodes $((x_i, y_k))$. The most simple form, this system has to rectangular area for $l = h$. In this case, equation (8.39) is written in the following form:

$$u_{i+1,k} + u_{i-1,k} + u_{i,k+1} + u_{i,k-1} - 4u_{i,k} = h^2 f_{ik} \quad (8.40),$$

as mentioned in the boundary nodes is exactly equal to the marginal functions. If

$f(x,y)=0$ equation (8.38) is called the Laplace equation and the corresponding equations have the form

$$u_{i,k} = 1/4 * (u_{i+1,k} + u_{i-1,k} + u_{i,k+1} + u_{i,k-1}) \quad (8.41)$$

In the equations (8.40) and (8.41) was used circuit node symbol on rys.6.4.

Accuracy replacement differential equation riznychnym, ie the error term R_{ik} for the Laplace equation is estimated inequality

$$|R_{ik}| \leq 1/6 * h^2 M_4, \quad M_4 = \max \left\{ \left| \frac{\partial^4 u}{\partial x^4} \right|, \left| \frac{\partial^4 u}{\partial y^4} \right| \right\}$$

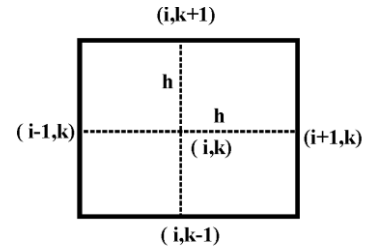


Figure 8.4

The error of the approximate solution obtained difference method consists of three errors: 1) error difference replacement differential equation; 2) approximation error boundary conditions; 3) error derived from the fact that the system of equations difference weighed close by.

8.6 Iterative methods decision of finite-difference equations

The direct solution of finite difference equations methods consistent with the exclusion of a large number of nodes is too cumbersome. Here are more convenient iterative solution methods that take into account special kind of systems and are convenient for implementation on a computer. We consider one of the simplest methods - the process of averaging Lybmana for the system (8.41).

According to the method of calculating Lybmana being so, choosing the initial approximation $u_{ij}^{(0)}$, successive approximation $u_{ij}^{(k+1)}$ for internal nodes of the grid area define the formula:

$$u_{i,j}^{(k+1)} = 1/4 * (u_{i+1,j}^{(k)} + u_{i-1,j}^{(k)} + u_{i,j+1}^{(k)} + u_{i,j-1}^{(k)}) \quad (k=0,1,2,3,...)$$

To obtain initial approximations can specify two ways:

- 1) value $u_{ij}^{(0)}$ in the internal nodes are obtained by interpolation using the known boundary values;
- 2) constitute a system of finite- difference equations for grid with a great step and solve it by process of elimination, and then interpolates the values at the

nodes of the mesh. It is proved that for any step process Lybmana h converges to the exact solution regardless of the choice of initial values. Iterative process matches faster if the calculation the following arithmetic using not only the value of the previous approach, but again found value. Of course iterations continue until two successive approximations do not coincide required number of decimal places. To estimate the error of the approximate solution of the Laplace equation can be used Runge principle according to which the error of the approximate solution u_h obtained from step h , given by the approximate formula:

$$\varepsilon_h \approx 1/3 * (u_h - u_{2h})$$

where u_{2h} -approximate solution obtained from step $2h$. Note that this method iterations results in a standardized averaging operations in each internal node, so it is very convenient for programming computers.

Example 2. Find the solution to Laplace's equation for the unit square with step $h = 1/8$ with boundary conditions:

$$u(0,y)=30y, u(1,y)=0, u(x,0)=0, u(x,1)=30(1-x^2).$$

8.7 Decision

1. Calculate the initial approximation. To calculate the initial approximation first build into the step $h = 1/8$, and we write the boundary conditions:

$$u_{0j}=30y_j, u_{8j}=0, u_{i,0}=0, u_{i8}=30(1-x_i^2).$$

Using these values, we find the value $u_{ij}^{(0)}$ other grid formulas:

$$u_{ij}(0) = \frac{\varphi_2 - \varphi_1}{n} * j + \varphi_1, \text{ де } \varphi_2=30(1-x_i^2), \varphi_1=0, n=8, j=1, \dots, 7$$

For example, the calculation $u_{1j}^{(0)}$ takes the formula:

$$u_{1j}(0) = \frac{29,5313 - 0}{8} * j + 0, j=1, \dots, 7$$

$$\text{Similarly, } u_{2j}(0) : u_{2j}(0) = \frac{28,125 - 0}{8} * j + 0, j=1, \dots, 7 \text{ etc.}$$

The results of calculation functions $u_{ij}^{(0)}$ are presented in tabl.6.2

Table 8.2

	i	0	1	2	3	4	6	7	8
j	y x	0,0000	0,1250	0,2500	0,3750	0,5000	0,7500	0,8750	1,0000
0	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000
1	0,1250	3,7500	3,6914	3,5156	3,2227	2,8125	1,6406	0,8789	0,0000
2	0,2500	7,5000	7,3828	7,0313	6,4453	5,6250	3,2813	1,7578	0,0000
3	0,3750	11,250	11,0742	10,5469	9,6680	8,4375	4,9219	2,6367	0,0000
4	0,5000	15,000	14,7656	14,0625	12,8906	11,2500	6,5625	3,5156	0,0000
5	0,6250	18,7500	18,4570	17,5781	16,1133	14,0625	8,2031	4,3945	0,0000
6	0,7500	22,5000	22,1484	21,0938	19,3359	16,8750	9,8438	5,2734	0,0000
7	0,8750	26,250	25,8398	24,6094	22,5586	19,6875	11,4844	6,1523	0,0000
8	1,0000	30,000	29,5313	28,1250	25,7813	22,5000	13,1250	7,0313	0,0000

Table 8.3

y	x	0,0000	0,1250	0,2500	0,3750	0,5000	0,6250	0,7500	0,8750	1,0000
0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000
0,1250	3,7500	3,6621	3,4863	3,1934	2,7832	2,2559	1,6113	0,8789	0,0000	0,0000
0,2500	7,5000	7,3242	6,9727	6,3867	5,5664	4,5117	3,2227	1,7578	0,0000	0,0000
0,3750	11,2500	10,9863	10,4590	9,5801	8,3496	6,7676	4,8340	2,6367	0,0000	0,0000
0,5000	15,0000	14,6484	13,9453	12,7734	11,1328	9,0234	6,4453	3,5156	0,0000	0,0000
0,6250	18,7500	18,3105	17,4316	15,9668	13,9160	11,2793	8,0566	4,3945	0,0000	0,0000
0,7500	22,5000	21,9727	20,9180	19,1602	16,6992	13,5352	9,6680	5,2734	0,0000	0,0000
0,8750	26,2500	25,6348	24,4043	22,3535	19,4824	15,7910	11,2793	6,1523	0,0000	0,0000
1,0000	30,0000	29,5313	28,1250	25,7813	22,5000	18,2813	13,1250	7,0313	0,0000	0,0000

Calculation of successive approximations perform the formula

$u_{i,j}^{(1)} = 1/4 * (u_{i+1,j}^{(0)} + u_{i-1,j}^{(0)} + u_{i,j+1}^{(0)} + u_{i,j-1}^{(0)})$, using data from the previous table.

For example, $u_{11}^{(1)} = 0,25 * (u_{10}^{(0)} + u_{12}^{(0)} + u_{01}^{(0)} + u_{21}^{(0)}) = 3,6621$;

$u_{21}^{(1)} = 0,25 * (u_{11}^{(0)} + u_{31}^{(0)} + u_{20}^{(0)} + u_{24}^{(0)}) = 3,75 + 7,3828 + 3,5156 + 0 = 3,4863$ etc.

Process iterations continue until two successive approximations results will differ by no more than 0, 1. All calculations are convenient to carry out the program MS EXCEL. At first calculates the boundary conditions $u_{0j} = 30y_j$.

To do this, you must enter the cell C2 formula: $=30*B4$

Similarly, to calculate the conditions $u(x,1) = 30(1-x^2)$ in cell D12 enter the formula:

$=30*(1-D3*D3)$

For a stay of values of functions $u_{ij}^{(0)}$ using the formula:

In cell D2 = $((\$ D \$ 12 - \$ D \$ 4) / 8) * A5 + \$ D \$ 4$

In cell E2 = $((\$ E \$ 12 - \$ E \$ 4) / 8) * A5 + \$ E \$$

In cell F2 = $((\$ F \$ 12 - \$ F \$ 4) / 8) * \$ A5 + \$ F \$ 4$ etc.

Then distribute these formulas using the manipulator required.

	A	B	C	D	E	F	G	H	I	J	K
1											
2		i	0	1	2	3	4	5	6	7	8
3	j	y	0,0000	0,1250	0,2500	0,3750	0,5000	0,6250	0,7500	0,8750	1,0000
4	0	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000
5	1	0,1250	3,7500	3,6914	3,5156	3,2227	2,8125	2,2852	1,6406	0,8789	0,0000
6	2	0,2500	7,5000	7,3828	7,0313	6,4453	5,6250	4,5703	3,2813	1,7578	0,0000
7	3	0,3750	11,2500	11,0742	10,5469	9,6680	8,4375	6,8555	4,9219	2,6367	0,0000
8	4	0,5000	15,0000	14,7656	14,0625	12,8906	11,2500	9,1406	6,5625	3,5156	0,0000
9	5	0,6250	18,7500	18,4570	17,5781	16,1133	14,0625	11,4258	8,2031	4,3945	0,0000
10	6	0,7500	22,5000	22,1484	21,0938	19,3359	16,8750	13,7109	9,8438	5,2734	0,0000
11	7	0,8750	26,2500	25,8398	24,6094	22,5586	19,6875	15,9961	11,4844	6,1523	0,0000
12	8	1,0000	30,0000	29,5313	28,1250	25,7813	22,5000	18,2813	13,1250	7,0313	0,0000
13											


The following table calculations are carried out with the data of the previous table. Therefore, enter in the appropriate sells the following formula:

In cell D2 = (D4 + C5 + D6 + E5) * 0,25

In E2 = (E4 + D5 + E6 + F5) * 0,25

In F2 = (F4 + E5 + F6 + G5) * 0,25 etc.

Similarly, these formulas distribute via filling manipulator and obtain $u_{ij}^{(1)}$:

	A	B	C	D	E	F	G	H	I	J	K
15											
16	j		0,0000	0,1250	0,2500	0,3750	0,5000	0,6250	0,7500	0,8750	1,0000
17	0	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000
18	1	0,1250	3,7500	3,6621	3,4863	3,1934	2,7832	2,2559	1,6113	0,8789	0,0000
19	2	0,2500	7,5000	7,3242	6,9727	6,3867	5,5664	4,5117	3,2227	1,7578	0,0000
20	3	0,3750	11,2500	10,9863	10,4590	9,5801	8,3496	6,7676	4,8340	2,6367	0,0000
21	4	0,5000	15,0000	14,6484	13,9453	12,7734	11,1328	9,0234	6,4453	3,5156	0,0000
22	5	0,6250	18,7500	18,3105	17,4316	15,9668	13,9160	11,2793	8,0566	4,3945	0,0000
23	6	0,7500	22,5000	21,9727	20,9180	19,1602	16,6992	13,5352	9,6680	5,2734	0,0000
24	7	0,8750	26,2500	25,6348	24,4043	22,3535	19,4824	15,7910	11,2793	6,1523	0,0000
25	8	1,0000	30,0000	29,5313	28,1250	25,7813	22,5000	18,2813	13,1250	7,0313	0,0000
26											

References

1. Bahvalov N S, Numerical methods. - M.: Science, 1977.
2. Berezin I S, Zhidkov N P, Methods for computing M.:Science,1972.
3. Turcha L I Fundamentals of numerical methods M.: Science,1987.
4. Marchuk G I, Methods of Computational Mathematics. - M.: Science, 1980.
5. Glushkov A.V., Relativistic Quantum Theory. Quantum, mechanics of Atomic Systems.-Odessa: Astroprint, 2008.
6. Glushkov A V, O Yu Khetselius, A A Svinarenko, A V Ignatenko, Computational Methods of Dynamics of Continuous media: Special Chapters.- Odessa: 2007.
7. Glushkov A V, O.Yu.Khetselius, A.A. Svinarenko, Computational Methods of Dynamics of Continuous media.- Odessa, 2008.
8. Glushkov A.V., Atom in electromagnetic field.-Kiev: KNT, 2005.
9. Glushkov A.V., Relativistic and correlation effects in spectra of atomic systems.-Odessa: Astroprint, 2006.
10. Glushkov A.V., Khetselius O.Yu., Gurnitskaya E.P., Loboda A.V., Florko T.A., Sukharev D.E., Lovett L., Gauge-Invariant QED Perturbation Theory Approach to Calculating Nuclear Electric Quadrupole Moments, Hyperfine Structure Constants for Heavy Atoms and Ions//Frontiers in Quantum Systems in Chemistry and Physics, Series: Progress in Theoretical Chemistry and Physics; Eds. S.Wilson, P.J.Grout, J. Maruani, G. Delgado-Barrio, P. Piecuch (Springer, Dordrecht), 2008.-Vol.18.-P.507-524.
11. Glushkov A.V., Khetselius O.Y., Malinovskaya S.V., New laser-electron nuclear effects in the nuclear γ transition spectra in atomic and molecular systems// Frontiers in Quantum Systems in Chemistry and Physics. Series: Progress in Theoretical Chemistry and Physics Eds. S.Wilson, P.J.Grout, J. Maruani, G. Delgado-Barrio, P. Piecuch (Springer, Dordrecht).-2008.-Vol.18.-525-541.
12. Glushkov A.V., Khetselius O.Yu., Loboda A.V., Svinarenko A.A., QED approach to atoms in a laser field: Multi-photon resonances and above threshold ionization//Frontiers in Quantum Systems in Chemistry and Physics, Series: Progress in Theoretical Chemistry and Physics; Eds. S.Wilson, P.J.Grout, J. Maruani, G. Delgado-Barrio, P. Piecuch (Springer, Dordrecht), 2008.-Vol.18.-P.543-560.

13. Glushkov A V, Rusov V D, Ambrosov S V, Loboda A V, Resonance states of compound super-heavy nucleus and EPP in heavy nucleus collisions // In: New projects and new lines of research in nuclear physics and differential geometry. Eds. G.Fazio, F.Hanape, Singapore : World Scientific, p. 126-152 (2003).
14. Nikiforov A SF., N.Y. Orlov, Uvarov V.B., The calculation of bremsstrahlung cross section based on the modified model of the Hartree-Fock - Slater. M., 1982 (Preprint of the Institute of Applied Mathematics Preprint they M. Keldysh Academy of Sciences of the USSR: 100).
15. Orlov N Y The influence of boundary conditions on the energy spectrum of the bound electrons. M, 1990 (Preprint of the Institute of Applied Mathematics Preprint them M. Keldysh Academy of Sciences of the USSR: 67).
16. Varentsova S A, A.G. Volkov, V.A. Trofimov, Conservative difference scheme for the problem of a femtosecond laser pulse in a cubic nonlinear medium // Zh. Mat. and Math. Physics -2003.-T. 43, №11.-P. 1709-1721.
17. Trofimov VA, A new approach to the modeling of nonlinear broadening of ultrashort laser pulses // Zh. Mat. and Math. Fiziki.-1998-T. 38, 5-P 835-839.
18. Trofimov V A, Nonlinear wave equation laser optics femtosecond pulses. // Differential equations.-1998-T.34, №7.-P. 1002-1004.
19. Popov V A, Solution Hartree-Fock equations for electrons in a crystal // J. Comput. Mat. and mat. physics. - 1998. - V. 38. - № 6. - P.978-991.
20. Hurinaga S., Gaussian-type functions for polyatomic systems // J. Chem.Phys. - 1965. - Vol. 42. - P. 1293-1302.
21. Clementi E, Roetti C. Atomic Data and Nuclear Data Tables. - 1974. - Vol. 14.-P. 177-278.
22. Zhogolev D A, V V Volkov, Methods, algorithms and programs for quantum-chemical calculations of molecules. - K .: Scientific Thought, 1976.
23. Glushkov A V, Ambrosov S V, Loboda A V, Gurnitskaya E P, Prepelitsa G P , Consistent QED approach to calculation of electron-collision excitation cross-sections and strengths: Ne-like ions // Int. Journ.Quant.Chem.-2005.-Vol.104, N4 .-P. 562-569 .
24. Belotserkovskii O M, Direct numerical simulation of fully developed turbulence // Zh. Mat. and Math. nat. 1985. T.№12. p 1856-1882.

25. Belotserkovskii O M, Gushchin V A, V.N. Konshin. The splitting method for the study of stratified fluid flows with free surface // Zh. Mat. and Math. nat. 1987.T. 27. № 4. p 594-609.
26. Kovenya V M, Yanenka N.N., The splitting method in problems of gas dynamics. Novosibirsk: Science, 1981.
27. Magomedov K M, A.S. Kholodov., Grid-characteristic numerical methods. M.:Science, 1988.
28. Oparin A M, Numerical modeling of the problems associated with the intensive development of hydrodynamic instabilities // New in number. simulation: algorithms calculated. experiment results. M.: Nauka, 2000.
29. Belotserkovskii O M, Davydov Y.M., Method of large particles in gas dynamics. M.: Science, 1982.
30. Grishin Yu A New schemes large particles method and their usage for optimization gas-air channels of engines // Mat. modeling. 2000. T. 14. № 8. p. 51-55
31. Booch G, Object-Oriented Design with application. M.: Concord, 1992.
32. Belotserkovsky O M, A M Oparin Numerical experiment in turbulence: from order to chaos. M.: Nauka, 2000.
33. Khetselius O.Yu., Hyperfine structure of atomic spectra.-Odessa: Astroprint, 2008.
34. Khetselius, O.Yu. Quantum structure of electroweak interaction in heavy finite Fermi-systems. Astroprint: Odessa, 2011.
35. Ivanova E.P., Ivanov L.N., Glushkov A.V., Kramida A.E., High Order Corrections in the Relativistic Perturbation Theory with the Model Zeroth Approximation, Mg-Like and Ne-Like Ions//Phys. Scripta.-1985.-Vol.32,N5.-P.513-522.
36. E.P.Ivanova, A.V.Glushkov, Theoretical investigation of spectra of multicharged ions of F-like and Ne-like isoelectronic sequences// Journal of Quantitative Spectroscopy and Radiative Transfer.-1986.-Vol.36(2).-P. 127-145.
37. Glushkov A.V., Ivanov L.N., Ivanova E.P., Radiation decay of atomic states. Generalized energy approach// Autoionization Phenomena in Atoms.- M.: Moscow State University.-1986. -P.58-160.
38. Glushkov A.V., Effective quasi-particle valence hamiltonian of molecules in the comprehensive semi-empirical theory// Sov. Journ. Struct. Chem.-1988.-Vol.29(4).-P.3-10.

39. Glushkov A V, Negative ions of inert gases// JETP Lett.-1992.-Vol.55, Issue 2.-P.97-100.
40. Glushkov A.V., Ivanov L.N., Radiation decay of atomic states: atomic residue polarization and gauge noninvariant contributions//Phys.Lett.A.-1992.-Vol. 170, N1.-P.33-36.
41. Glushkov A V, Ivanov L N, DC Strong Field Stark Effect for Non-hydrogenic Atoms: Consistent Quantum Mechanical Approach // Journal of Physics B: Atomic, Molecular and Optical Phys.-1993.-Vol.26,N14.-P.L379–386.
42. Glushkov A.V., Calculation of parameters of the interaction potential between excited alkali atoms and mercury atoms-the Cs-, Fr-Hg interaction//Optika i Spekt.-1994.-Vol.77 (1).-P.5-10.
43. AV Glushkov, SV Dan'kov, G Prepelitsa, VN Polischuk, AE Efimov, Qed theory of nonlinear interaction of the complex atomic systems with laser field multi-photon resonances//Journal of Techn.Physics.-1997.-Vol.38, Issue 2.-P.219-222.
44. Glushkov A.V., Malinovskaya S.V., Ambrosov S.V., Shpinareva I.M., Troitskaya O.V., Resonances in quantum systems in strong external fields consistent quantum approach//Journal of Techn.Physics.-1997.-Vol.38, Issue 2.-P.215-218.
45. Glushkov A.V., Malinovskaya S.V., New approach to the formation of model potential for valence-electrons//Zhurn. Fiz. Khimii.-1988.-Vol.62(1).-P.100-104.
46. AV Glushkov, AF Kivganov, VN Khokhlov, TV Buyadzhi, LA Vitavetskaya, VP Borovskaya, VN Polishchuk, Calculation of the spectroscopic characteristics of biatomic van der Waals molecules and ions: Inert gas atom—halogen-type inert gas ion in the ground state//Russian physics journal.-1998.-Vol.41(3).-p. 223-226
47. AV Glushkov, AV Malinovskii, VA Efimov, AF Kivganov, VN Khokhlov, LA Vitavetskaya, GA Borovskaya, Calculation of alkaline metal dimers in terms of model perturbation theory//Journal of structural chemistry.-1998.-Vol.39(2).-P. 179-185.
48. A V Glushkov, L A Vitavetskaya, Accurate QED perturbation theory calculation of the structure of heavy and superheavy element atoms and multicharged ions with the account of nuclear size effect and QED

- corrections// Herald of Uzhgorod Univ. Ser. Phys.-2000.-Vol.8(2).-P.321-324.
49. Glushkov, A.V.; Malinovskaya S.V. Co-operative laser nuclear processes: border lines effects In New Projects and New Lines of Research in Nuclear Physics. Fazio, G., Hanappe, F., Eds.; World Scientific: Singapore, 2003, 242-250.
 50. Turin A.V., Chernyakova Yu. G., Prepelitsa G.P., Characteristic features of the emission spectra of K plasma in a low inductive vacuum spark: Relativistic calculation// Phys. Aerodisp. Syst.-2003.-Vol.40.-P.327-332.
 51. Glushkov A V, Ambrosov S V, Loboda A V, Chernyakova Yu, Svinarenko A A , Khetselius O Yu, QED calculation of the superheavy elements ions: energy levels, radiative corrections, and hfs for different nuclear models//Journal Nucl.Phys. A.: nucl. and hadr. Phys.-2004.-Vol.734.-P.21
 52. AV Glushkov, SV Malinovskaya, YG Chernyakova, AA Svinarenko, Cooperative laser-electron-nuclear processes: QED calculation of electron satellites spectra for multi-charged ion in laser field// Int. Journal Quantum Chem.-2004.-Vol.99 (6).-P.889-893.
 53. Glushkov A.V., Ambrosov S.V., Ignatenko A.V., Korchevsky D.A., DC strong field Stark effect for nonhydrogenic atoms: Consistent quantum mechanical approach// Int.Journ.Quant.Chem.-2004.-Vol.99,N6.-P.936-939.
 54. V.D. Rusov, A.V. Glushkov, V.N. Vaschenko, D.A. Korchevsky, A.V. Ignatenko, Stochastic dynamics of the atomic systems in the crossed electric and magnetic field: the rubidium atom recurrence spectra//Bulletin of Kiev Nat. Univ.: Ser. Phys.-Math.-2004.-Issue 4.-P.433-438.
 55. Malinovskaya S V, Dubrovskaya Yu. V., Zelentzova T.N. The atomic chemical environment effect on the β decay probabilities: Relativistic calculation// Herald of Kiev Nat. Univ. Ser.: Phys.-Math., -2004.-Issue 4.-P.427-432
 56. Glushkov A.V., Energy Approach to Resonance states of compound super-heavy nucleus and EPPP in heavy nuclei collisions// Low Energy Antiproton Phys. AIP Conference Proceedings.-2005.-Vol.796 (1).-P.206-210.
 57. Glushkov A.V., Ambrosov S.V., Loboda A.V., Gurnitskaya E.P., Prepelitsa G.P., Consistent QED approach to calculation of electron-

- collision excitation cross sections and strengths: Ne-like ions// *Int. Journal Quantum Chem.*-2005.-Vol.104, Issue 4.-P.562–569.
58. S. Ambrosov, V. Ignatenko, D. Korchevsky, V. Kozlovskaya, Sensing stochasticity of atomic systems in crossed electric and magnetic fields by analysis of level statistics for continuous energy spectra// *Sensor Electronics and Microsyst. Techn.*-2005.-Issue 2.-P.19-23
 59. A.V. Glushkov, S.V. Malinovskaya, V.Dubrovskaya Yu, Sensing the atomic chemical composition effect on the β decay probabilities//*Sensor Electr. & Microsyst. Techn.*-2005.-N1.-P.16-20.
 60. AV Glushkov, SV Malinovskaya, AA Svinarenko, LA Vitavetskaya, Sensing spectral hierarchy, quantum chaos, chaotic diffusion and dynamical stabilisation effects in a multi-photon atomic dynamics with intense laser field// *Sensor Electronics and Microsystems Techn.*-2005.-Vol.2(2).-P. 29-36.
 61. Glushkov A.V., Malinovskaya S.V., Loboda A.V., Shpinareva I.M., Gurnitskaya E.P., Korchevsky D.A., Diagnostics of the collisionally pumped plasma and search of the optimal plasma parameters of x-ray lasing: Calculation of electron-collision strengths and rate coefficients for Ne-like plasma// *Journal of Physics: Conf.Ser.*-2005.-Vol.11.-P.188-198.
 62. A V Glushkov, S V Malinovskaya, G P Prepelitsa and V Ignatenko, Manifestation of the new laser-electron nuclear spectral effects in the thermalized plasma: QED theory of co-operative laser-electron-nuclear processes// *Journal of Physics: Conf.Ser.*-2005.-Vol.11.-P.199-206.
 63. Khetselius O.Yu., Hyperfine structure of radium// *Photoelectronics.*-2005.-Vol.14.-P.83-85.
 64. A-V Glushkov, S-V Ambrosov, A-V Loboda, E-P Gurnitskaya, O-Y Khetselius, QED calculation of heavy multicharged ions with account for correlation, radiative and nuclear effects// *Recent Advances in the Theory of Chemical and Physical Systems (Springer, Dordrecht)*-2006.-Vol.15.-P.285-299.
 65. Malinovskaya S.V., Glushkov A.V., Dubrovskaya Yu.V., Vitavetskaya L.A., Quantum calculation of cooperative muon-nuclear processes: discharge of metastable nuclei during negative muon capture// *Recent Advances in the Theory of Chemical and Physical Systems (Springer, Dordrecht)*.-2006.-Vol.15.-P.301-307.

66. Glushkov A.V., Malinovskaya S.V., Gurnitskaya E.P., Khetselius O.Yu., Dubrovskaya Yu.V., Consistent quantum theory of recoil induced excitation and ionization in atoms during capture of neutron// Journal of Physics: Conf. Series (IOP).-2006.- Vol.35(1).-P.425-430.
67. Glushkov A V, Malinovskaya S V, Loboda A V, Shpinareva I M and Prepelitsa G P, Consistent quantum approach to new laser-electron-nuclear effects in diatomic molecules // Journal of Physics: Conf. Series (IOP).- 2006.- Vol.35(1).-P.420-424.
68. Glushkov A.V., Khetselius O.Yu., Dubrovskaya Yu.V., Loboda A.V., Sensing the capture of negative muon by atoms: Energy approach// Sensor Electr. and Microsyst. Techn.-2006.-N4.-P.31-35.
69. Khetselius O.Y., Gurnitskaya E.P., Sensing the electric and magnetic moments of a nucleus in the N-like ion of Bi// Sensor Electr. and Microsyst. Techn.-2006.-N3.-P.35-39.
70. AV Glushkov, VN Khokhlov, Yu Bunyakova, AA Svinarenko, TV Solonko, Sensing the correlation between atmospheric teleconnection patterns and sea ice extent: micro technology “Geomath”//Sensor Electr. and Microsyst. Techn.-2006.-N2.-P.16-19.
71. Glushkov A.V., Khetselius O.Yu., Gurnitskaya E.P., Florko T.A., Sensing of nuclei available in little quantities by means of laser spectroscopy of hyperfine structure for isotopes: new theoretical scheme (U ,Hg) // Sensor Electr. and Microsyst. Techn.-2007.-N3.-P.8-12.
72. Glushkov A.V., Khetselius O.Yu., Malinovskaya S.V., Optics and spectroscopy of cooperative laser-electron nuclear processes in atomic and molecular systems - new trend in quantum optics// Europ.Phys.Journ. ST.- 2008.-Vol.160,N1.-P.195-204.
73. Glushkov A.V., Khetselius O.Yu., Malinovskaya S.V., Spectroscopy of cooperative laser-electron nuclear effects in multiatomic molecules// Molec. Physics (UK).-2008.-Vol.106.-N9-10.-P.1257-1260.
74. Khetselius O.Yu., Relativistic Calculating the Spectral Lines Hyperfine Structure Parameters for Heavy Ions // Spectral Line Shapes, AIP Conference Proceedings.-2008.-Vol.1058.-P.363-365.
75. S.V. Ambrosov, O.Y. Khetselius, A.V. Ignatenko, Wannier-Mott exciton and H, Rb atom in a DC electric field: Stark effect// Photoelectronics.- 2008.-Vol.17.-P.82-85.

76. Khetselius O.Yu., On possibility of sensing nuclei of the rare isotopes by means of laser spectroscopy of hyperfine structure//Sensor Electronics and Microsystem Technologies.-2008.-Vol.3.-P.28-33.
77. Glushkov A.V., Khetselius O.Yu., Loboda A.V., Ignatenko A., Svinarenko A., Korchevsky D., Lovett L., QED Approach to Modeling Spectra of the Multicharged Ions in a Plasma: Oscillator and Electron-ion Collision Strengths// Spectral Line Shapes. AIP Conference Proceedings.-2008.-Vol.1058.-P.175-177.
78. E P Gurnitskaya, O Yu Khetselius, A V Loboda, L A Vitavetskaya, Consistent quantum approach to quarkony energy spectrum and semiconductor superatom and in external electric field. Photoelectronics. 2008. Vol.17. P.127-130.
79. A V Glushkov, Ya I Lepikh, S V Ambrosov, O Yu Khetselius, Yu G Chernyakova, Computer modelling optimal schemes of the laser photoionization method for preparing the films of pure composition at atomic level// Photoelectronics. 2008. Vol.17. P.53-55.
80. Glushkov A.V., Loboda A.V., Gurnitskaya E.P., Svinarenko A.A., QED theory of radiation emission and absorption lines for atoms in a strong laser field//Physica Scripta.-2009.- Vol.T.135.-P. 014022.
81. Glushkov A.V., Khetselius O.Y., Lovett L., Electron- β -Nuclear Spectroscopy of Atoms and Molecules and Chemical Bond Effect on the β -Decay Parameters. In: Piecuch P., Maruani J., Delgado-Barrio G., Wilson S. (eds) Advances in the Theory of Atomic and Molecular Systems. Progress in Theoretical Chemistry and Physics, vol 20. Springer, Dordrecht.-2009.-Vol.20.-P. pp 125-152
82. Khetselius O.Yu., Relativistic perturbation theory calculation of the hyperfine structure parameters for some heavy-element isotopes// Int. Journal Quantum Chem.-2009.-Vol.109 (14).-P.3330-3335.
83. Khetselius O Yu, Relativistic calculation of the hyperfine structure parameters for heavy elements and laser detection of the heavy isotopes// Phys. Scripta.-2009.-Vol.T135.-P.014023
84. Malinovskaya S.V., Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Mischenko E.V., Florko T.A., Optimized perturbation theory scheme for calculating the interatomic potentials and hyperfine lines shift for heavy

- atoms in the buffer inert gas//Int. Journ. of Quantum Chemistry.-2009.- Vol.109,N14.-P.3325-3329.
85. AV Glushkov, SV Malinovskaya, OY Khetselius, AV Loboda, DE Sukharev, L Lovett, Green's function method in quantum chemistry: New numerical algorithm for the Dirac equation with complex energy and Fermi-model nuclear potential//Int. Journal Quant.Chem.-2009.- Vol.109 (8).-P.1717-1727.
 86. Glushkov A.V., Lovett L., Khetselius O.Yu., Gurnitskaya E.P., Dubrovskaya Yu.V., Loboda A.V., Generalized multiconfiguration model of decay of multipole giant resonances applied to analysis of reaction (μ -n) on the nucleus ^{40}Ca //International Journal of Modern Physics A.-2009.- Vol. 24, N.2-3.-P.611-615.
 87. AV Glushkov, O Khetselius, E Gurnitskaya, A Loboda, D Sukharev, Relativistic quantum chemistry of heavy ions and hadronic atomic systems: spectra and energy shifts//AIP Conference Proceedings 2009.-Vol.1102 (1).-P.168-171.
 88. Sukharev D.E., Khetselius O.Yu., Dubrovskaya Yu.V., Sensing strong interaction effects in spectroscopy of hadronic atoms// Sensor Electr. and Microsyst. Techn.-2009.-N3.-P.16-21.
 89. Glushkov A.V., Svinarenko A.A., Nuclear quantum optics: Energy approach to multi-photon resonances in nuclei // Sensor Electr. and Microsyst. Techn.-2010.-N2.-P.5-10.
 90. Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Prepelitsa G.P., Energy Approach to Atoms in a Laser Field and Quantum Dynamics with Laser Pulses of Different Shape//In: Coherence and Ultrashort Pulse Laser Emission (InTech).-2010.-P.159-186.
 91. Khetselius O. Yu., Lopatkin Yu. M., Dubrovskaya Yu. V., Svinarenko AA Sensing hyperfine-structure, electroweak interaction and parity non-conservation effect in heavy atoms and nuclei: New nuclear-QED approach// Sensor Electr. and Microsyst. Techn.-2010.-Vol.7(2).-P.11-19.
 92. Bunyakova Yu., Glushkov A., Analysis and forecast of the impact of anthropogenic factors on air basein of an industrial city. Odessa, Ecology, 2010.
 93. A.A. Svinarenko, A.V. Glushkov, A.V. Loboda, D.E. Sukharev, Y.V. Dubrovskaya, N.V. Mudraya, I.N. Serga, Green's Function of the Dirac

- Equation with Complex Energy and Non-singular Central Nuclear Potential//AIP Conference Proceedings.-2010.-Vol.1232(1).-P.259-266.
94. Khetselius O Yu, , TA Florko, LV Nikola, AA Svinarenko, IN Serga, TB Tkach, EV Mischenko, Hyperfine Structure, Scalar-pseudoscalar Interaction and Parity Non-Conservation Effect in Some Heavy Atoms and Ions//AIP Conference Proceedings.-2010.-Vol.1232(1).-P.243-250.
 95. A.S. Kvasikova, A.V. Ignatenko, T.A. Florko, D.E. Sukharev, Y.G. Chernyakova, Photoeffect and spectroscopy of the hydrogen atom in the crossed dc electric and magnetic field//Photoelectronics.-2011.-Vol.20.-P.71-75.
 96. Malinovskaya S.V., Glushkov A.V., Khetselius O.Yu., Lopatkin Yu.M., Loboda A.V., Svinarenko A.A. , Nikola L.V., Pereyagina T.B., Generalized energy approach to calculating electron collision cross-sections for multicharged ions in a plasma: Debye shielding model// International Journal of Quantum Chemistry.-2011.-Vol.111,N2.-P.288-296.
 97. A V Glushkov, A A Svinarenko, A V Ignatenko, Spectroscopy of autoionization resonances in spectra of the lanthanides atoms//Photoelectronics .-2011.-Vol.20.-P. 90-94.
 98. Glushkov, A.V. Methods of a Chaos Theory. OSENU: Odessa, 2012.
 99. Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Relativistic theory of cooperative muon- γ -nuclear processes: Negative muon capture and metastable nucleus discharge// Advances in the Theory of Quantum Systems in Chemistry and Physics. Series: Frontiers in Theoretical Chemistry and Physics, Eds. P.Hoggan, E.Brandas,J.Marvani, G. Delgado-Barrio, P.Piecuch (Springer, Dordrecht).-2012.-Vol.22.-P.51-68.
 100. Khetselius O.Yu., Relativistic energy approach to cooperative electron- γ -nuclear processes: NEET Effect// Quantum Systems in Chemistry and Physics: Progress in Methods and Applications. Ser.: Progress in Theoretical Chemistry and Physics, Eds. K.Nishikawa, J. Marvani, E. Brändas, G. Delgado-Barrio, P.Piecuch (Springer).-2012-Vol.26.-P.217-229.
 101. Glushkov, A.V. Advanced relativistic energy approach to radiative decay processes in multielectron atoms and multicharged ions. In Quantum Systems in Chemistry and Physics: Progress in Methods and Applications, Series: Progress in Theoretical Chemistry and Physics; Nishikawa, K.,

- Maruani, J., Brandas, E., Delgado-Barrio, G., Piecuch, P., Eds.; Springer: Dordrecht, 2012; Vol. 26, pp 231–252.
102. AV Glushkov, Spectroscopy of cooperative muon-gamma-nuclear processes: Energy and spectral parameters//J. Phys.: Conf. Series.-2012.-Vol.397(1).-P. 012011
 103. Khetselius O.Yu., Spectroscopy of cooperative electron-gamma-nuclear processes in heavy atoms: NEET effect// Journal of Physics: Conf. Series.-2012.-Vol.397(1).-P.012012
 104. Khetselius O.Yu., Quantum Geometry: New approach to quantization of the quasistationary states of Dirac equation for super heavy ion and calculating hyper fine structure parameters// Proceedings of International Geometry Center.-2012.-Vol.5, № 3-4.-P.39-45.
 - A. A. Kuznetsova, A. S. Kvasikova, A. N. Shakhman, L. A. Vitavetskaya Calculating the radiative vacuum polarization contribution to the energy shift of 2p-2s transition in mu-hydrogen// Photoelectronics. - 2012. – Vol. 21. – P.116-120.
 105. Glushkov, A.V. Operator Perturbation Theory for Atomic Systems in a Strong DC Electric Field. In Advances in Quantum Methods and Applications in Chemistry, Physics, and Biology, Series: Progress in Theoretical Chemistry and Physics; Hotokka, M., Brändas, E., Maruani, J., Delgado-Barrio, G., Eds.; Springer: Cham, 2013; Vol. 27, pp 161–177.
 106. Glushkov A.V., Khetselius O.Yu., Svinarenko A.A., Theoretical spectroscopy of autoionization resonances in spectra of lanthanide atoms// Physica Scripta.-2013.-Vol.T153.-P.014029.
 107. Khetselius O.Yu., Florko T.A., Svinarenko A.A., Tkach T.B., Radiative and collisional spectroscopy of hyperfine lines of the Li-like heavy ions and Tl atom in an atmosphere of inert gas//Physica Scripta (IOP).-2013.-Vol.T153-P.014037.
 108. Khetselius, O.Yu. Forecasting evolutionary dynamics of chaotic systems using advanced non-linear prediction method In Dynamical Systems Applications; Awrejcewicz, J., Kazmierczak, M., Olejnik, P., Mrozowski, J., Eds.; Wyd. Politech. Łódź.: Łódź, 2013; Vol T2, pp 145-152.
 109. Glushkov A.V., Kuzakon V., Ternovsky V.B., Buyadzhi V.V., Dynamics of laser systems with absorbing cell and backward-wave tubes with elements of a chaos// Dynamical Systems Theory, eds. J. Awrejcewicz, M.

- Kazmierczak, P. Olejnik, and J. Mrozowski (Lodz).-2013.-Vol.T1.-P.461-466
110. Glushkov, A.V.; Prepelitsa, G.P.; Svinarenko, A.A. ; Zaichko, P.A. Studying interaction dynamics of the non-linear vibrational systems within non-linear prediction method (application to quantum autogenerators) In Dynamical Systems Theory; Awrejcewicz, J., Kazmierczak, M., Olejnik, P., Mrozowski, J., Łódź, 2013; Vol T1, pp 467-477.
 111. Glushkov, A.V.; Buyadzhi, V.V.; Ternovsky V.B. Geometry of Chaos: Consistent combined approach to treating of chaotic self-oscillations in backward-wave tube. Proc. Intern. Geometry Center. 2013, 6(2), 6-12.
 112. Yu G Chernyakova, Yu V Dubrovskaya, TA Florko, A V Romanova, L A Vitavetskaya, An advanced approach quantization of the quasistationary states of Dirac-Slater equation// Proc.Intern. Geom. Center.-2013.-Vol.6(2).-P. 29-34.
 113. A V Glushkov, A A Svinarenko, V V Buyadzhi, P A Zaichko, V B Ternovsky, Chaos geometric attractor and quantum neural networks approach to simulation chaotic evolutionary dynamics during perception process In Advances in Neural Networks, Fuzzy Systems and Artificial Intelligence, Series: Recent Advances in Computer Engineering; Balicki, J., Ed.; WSEAS Press: Gdansk, 2014; Vol 21, pp 143-150
 114. Glushkov, A.V.; Khetselius, O.Yu.; Brusentseva, S.V.; Zaichko, P.A.; Ternovsky, V.B. Studying interaction dynamics of chaotic systems within a non-linear prediction method: Application to neurophysiology In Advances in Neural Networks, Fuzzy Systems and Artificial Intelligence, Series: Recent Advances in Computer Engineering; Balicki, J., Ed.; WSEAS Press: Gdansk, 2014; Vol 21, pp 69-75.
 115. Svinarenko A.A., Khetselius O.Yu., Buyadzhi V.V., Florko T.A., Zaichko P.A., Ponomarenko E.L., Spectroscopy of Rydberg atoms in a Black-body radiation field: Relativistic theory of excitation and ionization// Journal of Physics: Conf.Ser.-2014.-Vol.548.-P.012048.
 116. Svinarenko A.A., Study of spectra for lanthanides atoms with relativistic many- body perturbation theory: Rydberg resonances// Journal of Physics: Conf.Ser.-2014.-Vol.548.-P.012039.
 117. Glushkov A.V., Khetselius O.Yu., Lopatkin Yu.M., Florko T.A., Kovalenko O.A., Mansarliysky V.F., Collisional shift of hyperfine line for

- rubidium in an atmosphere of the buffer inert gas// Journal of Physics: Conf.Ser.-2014.-Vol.548.-P.012026.
118. Glushkov A.V., Spectroscopy of atom and nucleus in a strong laser field: Stark effect and multiphoton Resonances// Journal of Physics: Conf. Ser.-2014.-Vol.548.-P.012020.
 119. Glushkov A.V., Kondratenko P.A., Buyadzhi V.V., Kvasikova A.S., Shakhman A.S., SakunT.N., Spectroscopy of cooperative laser electron- γ -nuclear processes in polyatomic molecules// Journal of Physics: Conf. Ser.-2014.-Vol.548.-P.012025.
 120. V.V. Buyadzhi, A.V. Glushkov, L. Lovett, Spectroscopy of atom and nucleus in a strong laser field: stark effect and multiphoton resonances// Photoelectronics.-2014.-Vol.23.-P. 38-43
 121. Glushkov, A.V.; Buyadzhi, V.V.; Ponomarenko, E.L. Geometry of Chaos: Advanced approach to treating chaotic dynamics in some nature systems// Proc. Intern. Geom. Center. 2014 7(1),24-30.
 122. Prepelitsa, G.; Glushkov, A.V.; Lepikh, Ya.; Buyadzhi, V.; Ternovsky, V.; Zaichko, P. Chaotic dynamics of non-linear processes in atomic and molecular systems in electromagnetic field and semiconductor and fiber laser devices: new approaches, uniformity and charm of chaos. Sensor Electr. and Microsyst.Techn. 2014, 11, 43-57.
 123. Glushkov A.V., Khetselius O.Yu., Bunyakova Yu.Ya., Buyadzhi V.V., Brusentseva S.V., Zaichko P.A., Sensing interaction dynamics of chaotic systems within a chaos theory and microsystem technology geomath with application to neurophysiological systems// Sensor Electronics and Microsystems Technologies-2014.-Vol.11,N3.-P.62-69.
 124. Ternovsky V.B., Florko T.A., Ignatenko A.V., Svinarenko A.A., Tkach T.B., Advanced relativistic model potential approach to calculation of the radiation transition and ionization characteristics for rydberg atoms// Photoelectronics.-2014.-Vol.23.-P.91-95.
 125. Serga I.N., Relativistic theory of spectra of pionic atoms with account of the radiative corrections: hyperfine structure// Photoelectronics.-2014.-Vol.23.-P.171-175.
 126. Glushkov, A; Khetselius, O; Svinarenko, A.; Buyadzhi, V. Spectroscopy of autoionization states of heavy atoms and multiply charged ions. Odessa: TEC, 2015.

127. Glushkov A.V., Svinarenko A.A., Khetselius O.Y., Buyadzhi V.V., Florko T.A., Shakhman A.N. Relativistic Quantum Chemistry: An Advanced Approach to the Construction of the Green Function of the Dirac Equation with Complex Energy and Mean-Field Nuclear Potential. In: Nascimento M., Maruani J., Brändas E., Delgado-Barrio G. (eds) Frontiers in Quantum Methods and Applications in Chemistry and Physics. Progress in Theoretical Chemistry and Physics, vol 29. Springer, Cham.-2015.-P.197-217
128. Khetselius O.Yu., Optimized perturbation theory for calculating the hyperfine line shift and broadening of heavy atoms in a buffer gas// Frontiers in Quantum Methods and Applications in Chemistry and Physics. Series: Frontiers in Theoretical Chemistry and Physics, Eds. M.Nascimento, J.Maruani, E.Brändas, G.Delgado-Barrio (Springer, Cham).-2015-Vol.29.-P.55-76.
129. Buyadzhi V.V., Glushkov A.V., Mansarliysky V.F., Ignatenko A.V., Svinarenko A.A., Spectroscopy of atoms in a strong laser field: New method to sensing AC Stark effect, multiphoton resonances parameters and ionization cross-sections//Sensor Electr. and Microsyst. Techn.-2015.-Vol.12,N4.-P.27-36.
130. Ternovsky V.B., Glushkov A.V., Zaichko P.A., Khetselius O.Yu., Florko T.A., New relativistic model potential approach to sensing radiative transitions probabilities in spectra of heavy Rydberg atomic systems/ // Sensor Electr. and Microsyst. Techn.-2015.-Vol.12,N4.-P.19-26.
131. Buyadzhi V.V., Laser multiphoton spectroscopy of atom embedded in Debye plasmas: multiphoton resonances and transitions//Photoelectronics-2015.-Vol.24.-P.128-133.
132. Yu G Chernyakova, LA Vitavetskaya, PG Bashkaryov, IN Serga, AG Berestenko, The radiative vacuum polarization contribution to the energy shift of some levels of the pionic hydrogen// Photoelectronics.-2015.-Vol.24.-P.122-127.
133. Glushkov A.V., Safranov T.A., Khetselius O.Yu., Ignatenko A.V., Buyadzhi V.V., Svinarenko A.A., Analysis and forecast of the environmental radioactivity dynamics based on methods of chaos theory: General conceptions// Environmental Problems.-2016.-Vol.1(2).-P.115-120