

MINISTRY EDUCATION AND SCIENCE OF UKRAINE
Kyiv National University of Construction and Architecture

MATHEMATICAL METHODS IN ECOLOGY

Methodical instructions
to practical work
for students majoring in 101 «Ecology»,
183 «Technologies of environmental defense»
educational - qualification Master's level

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They contain methodical instructions for performing practical works and necessary for their implementation concise theoretical material on the basic methods of equations approximate solution, with the help of which ecological systems and processes models can be presented.

Intended for students majoring in 101 «Ecology», 183 «Technologies of environmental defense» educational – qualification Master's level.

Математичні методи в екології: методичні вказівки до виконання практичних робіт / уклад.: О. А. Котовенко, О.Ю. Мірошніченко. –

Містять методичні вказівки до виконання практичних робіт та необхідний для їх виконання стислий теоретичний матеріал з основних методів наближеного вирішення рівнянь, за допомогою яких можуть бути подані моделі екологічних систем та процесів

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General provisions

Nowadays, mathematical modeling is a powerful tool in ecological research. But mathematical modeling and forecasting without mathematical methods of solving equations, which can be used to provide mathematical models environmental objects, processes and phenomena, is impossible. Therefore, mastering the basic approaches and methods of solving equations is one of the most necessary requirements for the training a modern specialist in ecology and environmental protection, which provides the opportunity to carry out both numerical modeling and forecasting the development ecological systems, processes and phenomena in the surrounding natural environment.

These methodological instructions are intended to help student's specialties 101 "Ecology" and 183 "Environmental Protection Technologies" in performing practical work from the course "Mathematical Methods in Ecology".

The practical work purpose is for students to acquire practical skills in the application of solving equations approximate methods and various types equations systems, in the form of which various objects and processes models that take place in ecosystems can be presented (that is, they provide the opportunity to use numerical modeling).

Methodical instructions contain the most necessary and most common methods for performing the necessary calculations, theoretical information that is necessary for performing practical works, examples of the use of methods, recommendations for their application, as well as control questions for each practical work.

Practical work № 1

Solving nonlinear equations

Work purpose: Familiarizing students and providing them with the skills to apply methods of solving nonlinear equations.

Tasks for the work: Data for the work is provided by the teacher according to the options.

Theoretical information

An important task applied analysis in ecology and environmental technology is the solution of functional equations

$$f(x)=0 \quad (1.1)$$

Depending on the form of the function, $f(x)$ equation (1.1) can be transcendental (which includes exponential, logarithmic, or trigonometric functions) or algebraic.

The solution of equation (1.1) consists in finding the roots, that is, those values of x that turn the equation into an identity. The exact solution of (1.1) is not always possible. In practice, there is often no need for the exact solution of (1.1). It is sufficient to find the roots of the equation with a given degree of accuracy.

The process of finding the approximate roots of equation (1.1) consists of two stages:

- 1) *separation of roots*, i.e. division of the domain of function definition $f(x)$ into segments, in each of which there is only one root of equation (1.1);
- 2) *refinement of approximate roots*, that is, bringing them to a certain degree of accuracy.

To clarify the roots of equation (1.1), the following numerical methods are used:

- sample method (a special case is the halving method);
- chord method;
- Newton's method (tangent method);
- combined method of chords and tangents;
- simple iteration method (method of successive approximations).

Separation of roots can be carried out in two ways - graphically and analytically.

Graphic method. The graph of the function is constructed $y = f(x)$. The abscissa of the points of its intersection with the Ox axis will be the approximate values of the roots. As the interval in which the root is located, you can take some segment on the Ox axis, which includes this point. In order to make sure that the

found segment really has only one root, check the signs at the ends of the segment. At the same time, a well-known property of continuous functions is used: if the function $f(x)$ is continuous and monotonic on the segment $[a, b]$, and at its ends takes values different signs, then within the segment $[a, b]$ there is one and only one root.

It is often convenient to replace equation (1.1) with an equivalent equation form $\varphi_1(x) = \varphi_2(x)$, where $\varphi_1(x)$ and $\varphi_2(x)$ are functions simpler than $f(x)$ and they easy to plot graphically. After constructing the graphs $y = \varphi_1(x)$, $y = \varphi_2(x)$ we obtain the approximate roots values, as the abscissas the points of intersection these graphs.

The analytical method is based on the property of monotonicity the function $f(x)$. As a sign of monotonicity the function, $f(x)$ the condition constancy of sign of the derivative is used $f'(x)$ (the function $f(x)$ is monotonically increasing if $f'(x) > 0$, and monotonically decreasing if $f'(x) < 0$). Thus, the segments separating the roots of equation (1) should be searched for on the interval where the derivative $f'(x)$ keeps a constant sign. If $f'(x) = 0$, or does not exist, then, accordingly, the function $f(x)$ reaches an extremum at point x . Hence, to separate the roots analytically, the following procedure is performed:

1. find the first derivative $f'(x)$;
2. the equation is solved $f'(x) = 0$;
3. a table of signs of the function is drawn up at the boundary points the domain its existence and at the points zero values its derivative (or points close to it).
4. it is necessary to allocate intervals at the ends of which the function $f(x)$ takes values of opposite signs. In the middle of these intervals there is one and only one root, which is the required root of the equation.

Roots refinement. Each specifying roots methods has its advantages and disadvantages, therefore, when choosing a method, it is necessary to take into account the specific form $f(x)$, the fulfillment of each method application conditions, and the convergence speed.

The method of samples is algorithmically simple, but the volume calculations will be greater, the more precisely the root needs to be found. It can be used for rough finding of roots or in combination with other methods.

Other methods are united by the fact that they are iterative, i.e. in each of them, the previous rough approximation is successively refined. The general property of these methods is that the rounding error does not accumulate, because any

approximation can be considered as a new initial approximation and the error assumed when calculating any approximation will not affect the result (in the worst case, it will lead to an increase in the amount of calculations). The total rounding error is equal to the error that occurred in the last iteration.

Let's consider one of the methods sequential refinement roots - *the method of iterations*. Let it be necessary to find the root of the equation (1.1). We can present this equation in the form:

$$x = \varphi(x) \tag{1.2}$$

As a rough approximate value of the sought root, we will take any point $x_0 \in [a, b]$ and substitute its value in the right-hand side equation (1.2); we denote the found value by x_1 , i.e

$$x_1 = \varphi(x_0);$$

Next we find:

$$\begin{aligned} x_2 &= \varphi(x_1); \\ x_3 &= \varphi(x_2); \\ &\dots \\ x_n &= \varphi(x_{n-1}). \end{aligned}$$

In this way, we will get a sequence of numbers $x_0, x_1, x_2, \dots, x_n$ that can converge, that is, have a limit that will be the root of equation (1.1), or diverge, then the method of iterations does not achieve its goal.

Therefore, for the practical use of the iteration method, it is necessary to know the sufficient conditions for the convergence of the iterative process, which are expressed by the following theorem.

Theorem. Let there be a single root of the equation $x = \varphi(x)$ on the segment $[a, b]$ and at all points of this segment the derivative $\varphi'(x)$ satisfies the inequalities

$$|\varphi'(x)| \leq q < 1. \tag{1.3}$$

If at the same time all values $\varphi(x)$ belong to $[a, b]$, then the iterative process coincides, and any number on the segment $[a, b]$ can be taken as the zero approximation.

The convergence of the iteration process will be faster, the smaller the number q , which satisfies inequality (1.3) (can be accepted $q = \max_{[a, b]} |\varphi'(x)|$).

From all of the above, it is possible to formulate the following practical rule for using the iteration method:

- 1) convert equation (1.1) to form (1.2) in such a way that $|\varphi'(x)|$ it satisfies condition (1.3). For example, you can search for a function $\varphi(x)$ from a ratio

$$\varphi(x) = x - \frac{f(x)}{-k} \quad (1.4)$$

moreover k , it is necessary to choose in such a way that $|k| \geq \frac{Q}{2}$, where $Q = \max_{[a,b]} |f'(x)|$ and the sign k would coincide with the sign $f'(x)$ on $[a, b]$;

2) any number from the interval $[a, b]$ as an initial approximation x_0 ;

3) we calculate successive approximations according to the formula

$$x_n = \varphi(x_{n-1}) \quad (n=1,2,\dots) \quad (1.5)$$

until inequality (1.4) holds for two successive approximations.

Newton's method (tangent method) using an example.

Let it be necessary to specify the root of the equation with precision

$$\varepsilon = 0,001$$

$$x^3 - 2,002x^2 + 1,277x - 0,240 = 0, \quad (1.6)$$

located on the segment $[0,3; 0.4]$.

Solution. Let's determine which of the ends of the segment $[0,3; 0.4]$ to choose as an initial approximation:

$$f''(x) = 6x - 4,004 < 0 \text{ on the segment } [0,3; 0.4];$$

$$f(a) = -0,0101 < 0; f(a), f''(x) > 0.$$

That is,

$$x_0 = a = 0,3; f''(x) = 3x^2 - 4,004x + 1,277.$$

We summarize all calculations in Table 1.1

The table shows that $|x_3 - x_2| < 0,001$ because $x = \xi = 0,332$

Table 1.1

Results of solving equation (1.6) by Newton's method

n	x_n	x_n^3	$2,002x_n^2$	$f(x_n)$	$3x_n^2$	$4,004x_n$	$f''(x_n)$	$-\frac{f(x_n)}{f'(x_n)}$
0	0.3000	0.027	0.1802	-0.0101	0.2700	1,2012	0.3458	0.0292

1	0.3292	0.0357	0.2170	-0.0009	0.3251	1.3181	0.2840	0.0032
2	0.3324	0.0367	0.2212	0.0000	0.3315	1.3309	0.2776	0.0000
3	0.3324	–	–	–	–	–	–	–

Control questions

1. Which the considered methods of approximate solution nonlinear equations converge the fastest?
2. What is the convergence of iterative methods?
3. What features of the iteration method make it convenient to use?
4. What determines the accuracy of iterative processes?
5. How are convergence and accuracy of iterative methods related?

Practical work №2

Solving systems of linear algebraic equations

Work purpose: Familiarizing students and providing them with the skills to apply methods of solving systems of linear equations.

Tasks for the work: Data for the work is provided by the teacher according to the options.

Solve the system of linear algebraic equations:

- 1) using the single division scheme (Gauss method);
- 2) by the iterative Gauss-Seidel method.

Theoretical information

"Matrix models", which are often encountered when describing ecological processes, can be represented by systems of linear equations. Methods for solving systems of linear equations are mainly divided into two groups: direct (exact), such as Kramer's rule, the Gauss method, and iterative (approximate), which include the method of iterations, the Gauss-Seidel method. The Gaussian method is one of the most widespread methods for solving systems of linear equations, based on the idea sequential elimination unknowns. The calculation schemes in which this method can be implemented are different, one of them is the single division scheme.

Iterative methods make it possible to obtain the solution of the system with a given accuracy by means of convergent infinite processes. Consider the iterative Gauss-Seidel method.

Iterative Gauss-Seidel method

We will consider the essence of the Gauss-Seidel method on the system example

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1, \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2, \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3. \end{cases} \quad (2.1)$$

Suppose that $a_{11} \neq 0, a_{22} \neq 0, a_{33} \neq 0$, we rewrite the system (2.1) in the form

$$x_1 = \frac{1}{a_{11}}(b_1 - a_{12}x_2 - a_{13}x_3); \quad (2.2)$$

$$x_2 = \frac{1}{a_{22}}(b_2 - a_{21}x_1 - a_{23}x_3); \quad (2.3)$$

$$x_3 = \frac{1}{a_{33}}(b_3 - a_{31}x_1 - a_{32}x_2). \quad (2.4)$$

Let $(x_1^{(0)}, x_2^{(0)}, x_3^{(0)})$ – some rough approximation of the system solution. Let's call this set of numbers an initial approximation. Zero values of variables or values free members can be taken as an initial approximation

$$x_1, x_2, x_3 \left(x_1^{(0)} = x_2^{(0)} = x_3^{(0)} = 0 \right)$$

$$x_1^{(0)} = \frac{b_1}{a_{11}}, x_2^{(0)} = \frac{b_2}{a_{22}}, x_3^{(0)} = \frac{b_3}{a_{33}}.$$

Substituting the zero approximation into (2.2), we get $x_1^{(1)}$:

$$x_1^{(1)} = \frac{1}{a_{11}}(b_1 - a_{12}x_2^{(0)} - a_{13}x_3^{(0)})$$

initial $x_1^{(0)}$ value for the calculated value in (2.3). $x_1^{(1)}$ we find $x_2^{(1)}$:

$$x_2^{(1)} = \frac{1}{a_{22}}(b_2 - a_{21}x_1^{(1)} - a_{23}x_3^{(0)})$$

Then, substituting the calculated values $x_1^{(1)}$ into $x_2^{(1)}$ (2.3), we find $x_3^{(1)}$:

$$x_3^{(1)} = \frac{1}{a_{33}}(b_3 - a_{31}x_1^{(1)} - a_{32}x_2^{(1)})$$

Thus, we got the first approximation - $(x_1^{(1)}, x_2^{(1)}, x_3^{(1)})$. This ends the first iteration. Similarly, we find the second, third and subsequent approximations. In the general case, k – that approximation is determined by the formulas:

$$\begin{cases} x_1^{(k)} = \frac{1}{a_{11}}(b_1 - a_{12}x_2^{(k-1)} - a_{13}x_3^{(k-1)}) \\ x_2^{(k)} = \frac{1}{a_{22}}(b_2 - a_{21}x_1^{(k)} - a_{23}x_3^{(k-1)}) \\ x_3^{(k)} = \frac{1}{a_{33}}(b_3 - a_{31}x_1^{(k)} - a_{32}x_2^{(k)}) \end{cases} \quad (2.5)$$

The iterative process continues until the inequalities are satisfied

$$|x_i^{(k)} - x_i^{(k-1)}| \leq \varepsilon (i=1,2,3), \quad (2.6)$$

where $x_i^{(k)}, x_i^{(k-1)}$ – two successive approximations; ε – specified precision.

Without proof, we will state sufficient conditions for the convergence the iterative Gauss-Seidel method: if for system (2.1) the diagonal coefficients modules each equation are greater than the modules sum of all other coefficients (not including free terms), that is, if the inequalities are satisfied

$$|a_{ii}| > \sum_{j \neq i} |a_{ij}| (i, j = 1, 2, 3), \quad (2.7)$$

then the iterative process converges to a system single solution, regardless of the initial approximation choice.

Control questions

1. Which mathematical models of environmental objects or processes known to you are described using linear equations systems?
2. By what features are the methods of solving linear systems divided equations?
3. In what cases is it necessary to apply approximate methods of solving linear equations systems?

Practical work № 3

Solving systems of nonlinear equations

Work purpose: Familiarizing students and providing them with the skills to apply methods of approximate solution nonlinear equations systems

Task of the work: Solve the nonlinear equations system (the view of the system is provided by the teacher) using iteration and Newton methods with an accuracy 0.001.

Theoretical information

Models some processes and objects natural environment can be represented using nonlinear equations systems ("predator-prey" models, hydro-ecological, and others).

Let the model be presented as a system of two nonlinear equations with two unknowns:

$$\begin{cases} F_1(x, y) = 0 \\ F_2(x, y) = 0 \end{cases} \tag{3.1}$$

Let's find real roots with the required degree of accuracy. The method of iterations and Newton's method can be used to solve this problem.

Method of iterations

The system (3.1) can be presented in the form

$$\begin{cases} x = \varphi_1(x, y) \\ y = \varphi_2(x, y) \end{cases} \tag{3.2}$$

If x_0 and y_0 are the initial approximations of the roots obtained graphically, then by substituting them to the right-hand side of the system, we obtain

$$\begin{cases} x_1 = \varphi_1(x_0, y_0) \\ y_1 = \varphi_2(x_0, y_0) \end{cases} \tag{3.3}$$

Similarly, we will construct successive approximations

$$\begin{aligned} x_2 &= \varphi_1(x_1, y_1); y_2 = \varphi_2(x_1, y_1); \\ x_3 &= \varphi_1(x_2, y_2); y_3 = \varphi_2(x_2, y_2); \\ &\dots\dots\dots \\ x_n &= \varphi_1(x_{n-1}, y_{n-1}); y_n = \varphi_2(x_{n-1}, y_{n-1}); \end{aligned} \tag{3.4}$$

If the iterative process converges, that is, there are limits

$$x^* = \lim_{n \rightarrow \infty} x_n; y^* = \lim_{n \rightarrow \infty} y_n, \text{ then the limit values } x^*, y^* \text{ are the roots of}$$

system (3.2) and, accordingly, of system (3.1).

We present the theorem on the convergence condition the iterative process without proof.

Theorem. Let there be one and only one solution of system (3.2)

$x = x^*, y = y^*$ in some closed neighborhood $R(a \leq x \leq A, b \leq y \leq B)$. Then, if

- 1) functions $\varphi_1(x, y)$ are both $\varphi_2(x, y)$ defined and continuously differentiable in R ;

- 2) initial approximations x_0 i y_0 and all subsequent approximations of x_n i y_n ($n = 1, 2, \dots$) belong to R ;
 3) in the R region inequalities are fulfilled

$$\left| \frac{\partial \phi_1}{\partial x} \right| + \left| \frac{\partial \phi_2}{\partial x} \right| \leq q_1 < 1$$

$$\left| \frac{\partial \phi_1}{\partial y} \right| + \left| \frac{\partial \phi_2}{\partial y} \right| \leq q_2 < 1$$
(3.5)

or inequalities

$$\left| \frac{\partial \phi_1}{\partial x} \right| + \left| \frac{\partial \phi_1}{\partial y} \right| \leq q_1 < 1$$

$$\left| \frac{\partial \phi_2}{\partial x} \right| + \left| \frac{\partial \phi_2}{\partial y} \right| \leq q_2 < 1$$
(3.6)

then the process of successive approximations (3.4) converges to the solution $x = x^*, y = y^*$.

The error estimate of the n -th approximation is determined by the inequality

$$|x^* - x_n| + |y^* - y_n| \leq \frac{M}{1 - M} (|x_n - x_{n-1}| + |y_n - y_{n-1}|) \quad (3.7)$$

where M is the largest of the numbers q_1 i q_2 included in inequality (3.5) or (3.6). When $M < 0,5$ the convergence of the iteration method is considered good. At the same time $\frac{M}{1 - M} < 1$, so that if in two consecutive approximations, for example, the first three decimal places after the decimal point match, then the error of the last approximation does not exceed 0.001.

Newton's method for a two equations system

Let the model be presented as a two nonlinear equations system with two unknowns:

$$\begin{cases} f(x, y) = 0 \\ \phi(x, y) = 0 \end{cases} \quad (3.8)$$

where $f(x, y)$ and $\phi(x, y)$ are continuously differentiable functions.

We find roughly (graphically or by approximation) initial approximations x_0, y_0 . The following approximations are calculated using the formulas:

$$\begin{aligned} x_{n+1} &= x_n + h_n; \\ y_{n+1} &= y_n + l_n \\ (n &= 0, 1, 2, \dots) \end{aligned} \quad (3.9)$$

where

$$h_n = \frac{\begin{vmatrix} -f(x_n, y_n); f'_y(x_n, y_n) \\ -\varphi(x_n, y_n); \varphi'_y(x_n, y_n) \end{vmatrix}}{\begin{vmatrix} f'_x(x_n, y_n); f'_y(x_n, y_n) \\ \varphi'_x(x_n, y_n); \varphi'_y(x_n, y_n) \end{vmatrix}} = \frac{\Delta_x^{(n)}}{\Delta_n};$$

$$l_n = \frac{\begin{vmatrix} f'_x(x_n, y_n); -f(x_n, y_n) \\ \varphi'_x(x_n, y_n); -\varphi(x_n, y_n) \end{vmatrix}}{\begin{vmatrix} f'_x(x_n, y_n); f'_y(x_n, y_n) \\ \varphi'_x(x_n, y_n); \varphi'_y(x_n, y_n) \end{vmatrix}} = \frac{\Delta_y^{(n)}}{\Delta_n},$$

and the determinant Δ_n must be different from zero. The process of calculations according to formulas (3.9) continues until the difference between two successive approximations by modulus is less than or equal to the specified accuracy.

Control questions

1. Which environmental models you know are described by nonlinear equations systems?
2. What methods of solving nonlinear equations systems do you know?
3. What are the necessary and sufficient conditions for the convergence of the process successive approximations?

Practical work № 4

Numerical solution of ordinary differential equations

Work purpose: To acquaint students with the basic numerical methods of solving ordinary differential equations

The task of the work: Numerically solve differential equations with defined initial conditions on the segment $[0; 1]$ and step by step $h \approx 0.001$ using:

- 1) Euler's method;
- 2) the improved Euler method;
- 3) the Runge-Kutta method.

All calculations are performed with accuracy up to 4 decimal places.

Theoretical information

Many problems that must be solved in ecological research lead to the need to construct and solve a differential equation that satisfies one or another initial conditions (this is one of the main approaches in modeling the dynamic systems processes, which are most inherent in the natural systems description).

If the model describing some ecological process has the form of a differential equation solved relative to the derivative

$$y' = f(x, y), \quad (4.1)$$

then solving a differential equation by a numerical method means compiling a table of approximate values differential equation integral that satisfies the given initial conditions.

Let $y(x)$ is the solution of equation (4.1) and $x = x_0$ is the initial value of the argument. The initial condition for solutions (4.1) is given in the form

$$y(x_0) = y_0, \quad (4.2)$$

where y_0 is the specified number.

It is obvious that the question finding approximate values integral $y(x)$ equation (4.1) can be asked if and only if a solution $y(x)$ satisfying condition (4.2) exists and is unique. For this, it is sufficient that the function $f(x, y)$ from the right-hand side of equation (4.1) is continuous in the domain under consideration by two arguments and has a bounded frequent derivative $\frac{\partial}{\partial y} f(x, y)$.

The simplest method of differential equations approximate integration is the Euler method, which consists in the fact that the integral curve is replaced by a straight (tangent) segment on a small segment of the change independent variable. That is, on the entire segment of integration, the integral curve is replaced by a broken one, which is called Euler's broken one.

These methods, depending on the form presentation solution, can be divided into three groups:

- 1) Analytical, giving an approximate solution in the form of an analytical expression;
- 2) Graphical, giving an approximate solution in the form of a graph;
- 3) Numerical, giving an approximate solution in the form of a table.

Problem formulation. Let an ordinary differential equation of the first order be given

$$y' = f(x, y) \quad (4.3)$$

It is necessary to find a solution $y=y(x)$ of this equation that satisfies the initial condition:

$$y(x_0) = y_0 \quad (4.4)$$

The geometric content of the problem consists in finding the integral curve $y=y(x)$ that passes through the given point $A_0(x_0, y_0)$.

The numerical solution of the Cauchy problem consists in finding the values y_1, \dots, y_n at the points $x_1 = x_0 + h, x_2 = x_0 + 2h, \dots, x_n = x_0 + nh$ at the segment $[a, b]$, where h is the integration step; $x_0 = a, x_n = b$.

1. Euler's method

Let's mark

$$\begin{aligned} \Delta y_i &= y_{i+1} - y_i; \Delta x_i = x_{i+1} - x_i = h \\ (i &= 1, \bar{n}) \end{aligned} \quad (4.5)$$

Replacing the derivative b (4.3) with the relation of finite differences, we obtain:

$$\frac{\Delta y}{\Delta x} = f(x, y) \quad (4.6)$$

from where $\Delta y = f(x, y)\Delta x$

When $x=x_0$ we get

$$\frac{\Delta y_0}{\Delta x} = f(x_0, y_0) \Rightarrow \Delta y_0 = f(x_0, y_0)\Delta x \quad (4.7)$$

When $x=x_1$, equation (4.6) has the form:

$$y_1 = y_0 + hf(x_0, y_0) \quad (4.8)$$

We find similarly

$$\begin{aligned} y_2 &= y_1 + hf(x_1, y_1) \\ y_{i+1} &= y_i + hf(x_{i+1}, y_{i+1}) \\ y_n &= y_{n-1} + hf(x_{n-1}, y_{n-1}) \end{aligned} \quad (4.9)$$

This is a simple and relatively rough numerical method; it is used for approximate calculations.

Euler's method can also be used to solve systems first order differential equations.

2. Modified Euler's method

1) We divide the segment $[a, b]$ into n equal parts by points

$$x_i = x_0 + ih, h = \frac{b-a}{n} \quad (4.10)$$

2) We find

$$x_i + \frac{1}{2} = x_i + \frac{h}{2} \quad (4.11)$$

3) We calculate the auxiliary value of the function we are looking for $y = y(x)$ in the points $x_i + \frac{1}{2}$:

$$y_{i+\frac{1}{2}} = y_i + \frac{h}{2} f(x_i, y_i) \quad (4.12)$$

4) We find

$$y_{i+\frac{1}{2}} = y_i + h y_{i+\frac{1}{2}} \quad (4.13)$$

5) We define

$$y_{i+1} = y_i + h y_{i+\frac{1}{2}} \quad (4.14)$$

Then the entire calculation process is repeated from point 2) until it is found y_i for all points x_i ($i = 1, \bar{n}$) segment $[a, b]$. This is a more accurate method.

3. The Runge-Kutta's method

The Runge-Kutta's method is one of the methods of increased accuracy. According to the Runge-Kutta's method, successive values y_i of the desired function y are determined by the formula

$$y_{i+1} = y_i + \Delta y_i, \quad (4.15)$$

$$\Delta y_i = \frac{1}{6} (K_1^{(i)} + 2 \cdot K_2^{(i)} + 2 \cdot K_3^{(i)} + K_4^{(i)}), \quad (4.16)$$

where

$$K_1^{(i)} = h \cdot f(x_i, y_i)$$

$$K_2^{(i)} = h \cdot f\left(x_i + \frac{h}{2}, y_i + \frac{K_1^{(i)}}{2}\right)$$

$$K_3^{(i)} = h \cdot f\left(x_i + \frac{h}{2}, y_i + \frac{K_2^{(i)}}{2}\right)$$

$$K_4^{(i)} = h \cdot f\left(x_i + h, y_i + K_3^{(i)}\right). \quad (4.17)$$

This method geometric content can be easily traced from the sequence of formulas (4.17), from which it can be seen that each calculation step is a step according to Euler's method.

Calculations by the Runge-Kutta's method are conveniently arranged according to the scheme given in Table 5.1.

This table is filled in as follows.

Step 1. In columns 2 and 3 the current line, write the value x i y . If the line is the first, then the initial values x_0 and are recorded y_0 .

Step 2. Value of x and y the current row is substituted into the right-hand side the differential equation (1), determined $f(x,y)$ and recorded in column 4 the same row.

Step 3. The obtained value of column 4 is multiplied by the integration step h , calculated $K = h \cdot f(x,y)$ and recorded in column 5 the same row.

Step 4. The obtained value K is multiplied by the corresponding coefficient (by 1 if it is K_1 or K_4 , by 2 if it is K_2 or K_3), the result is recorded in column 6 of the current row.

Steps 1,2,3,4 are repeated to find each K in the i -th solution.

The results at the sixth column are added up, divided by 6, $\Delta y_i = \frac{1}{6} \sum$ and determined $y_{i+1} = y_i + \Delta y_i$.

Then all calculations are repeated, starting from step 1, until the entire segment $[a,b]$, on which the numerical solution of equation (4.1) needs to be found, is passed.

The Runge-Kutta's method has the order of accuracy h^4 on the entire segment $[a,b]$. Assessing the accuracy of the method is very complicated. A rough estimate of the error can be obtained by "double enumeration" according to the formula

$$\left| y_i^* - y(x_i) \right| \approx \frac{y_i^* - y_i}{15} \quad (4.18)$$

where $y(x_i)$ is the value the exact solution equation (4.1) at the point x_i , and y_i^* and y_i are approximate values with a step $\frac{h}{2}$ and h .

If ε is the specified accuracy of the solution, then the number n (number of divisions) for determining the integration step $h = \frac{b-a}{n}$ is chosen in such a way that $h^4 < \varepsilon$.

Table 4.1

Calculations by the Runge-Kutta's method

i	x	y	$y' = f(x, y)$	$K = h \cdot f(x, y)$	Δy
1	2	3	4	5	6
0	x_0	y_0	$f(x_0, y_0)$	$K_1^{(0)}$	$K_1^{(0)}$
	$x_0 + \frac{h}{2}$	$y_0 + \frac{K_1^{(0)}}{2}$	$f\left(x_0 + \frac{h}{2}, y_0 + \frac{K_1^{(0)}}{2}\right)$	$K_2^{(0)}$	$2 \cdot K_2^{(0)}$
	$x_0 + \frac{h}{2}$	$y_0 + \frac{K_2^{(0)}}{2}$	$f\left(x_0 + \frac{h}{2}, y_0 + \frac{K_2^{(0)}}{2}\right)$	$K_3^{(0)}$	$2 \cdot K_3^{(0)}$
	$x_0 + h$	$y_0 + K_3^{(0)}$	$f(x_0 + h, y_0 + K_3^{(0)})$	$K_4^{(0)}$	$K_4^{(0)}$
					$\frac{1}{6} \sum = \Delta y_0$
1	x_1	$y_1 = y_0 + \Delta y_0$	$f(x_1, y_1)$	$K_1^{(1)}$	$K_1^{(1)}$
	$x_1 + \frac{h}{2}$	$y_1 + \frac{K_1^{(1)}}{2}$	$f\left(x_1 + \frac{h}{2}, y_1 + \frac{K_1^{(1)}}{2}\right)$	$K_2^{(1)}$	$2 \cdot K_2^{(1)}$
	$x_1 + \frac{h}{2}$	$y_1 + \frac{K_2^{(1)}}{2}$	$f\left(x_1 + \frac{h}{2}, y_1 + \frac{K_2^{(1)}}{2}\right)$	$K_3^{(1)}$	$2 \cdot K_3^{(1)}$
	$x_1 + h$	$y_1 + K_3^{(1)}$	$f(x_1 + h, y_1 + K_3^{(1)})$	$K_4^{(1)}$	$K_4^{(1)}$
					$\frac{1}{6} \sum = \Delta y_1$
2	x_2	$y_2 = y_1 + \Delta y_1$

The calculation step can be changed when moving from one point to another. Equality is used to evaluate the correctness of step selection h

$$q = \frac{|K_2^i - K_3^i|}{|K_1^i - K_2^i|} \quad (4.19)$$

where q should be equal to several hundreds, otherwise the step is reduced.

Control questions

1. What is the Euler curve?
2. How is the accuracy of the Runge-Kutta's method evaluated?
3. How can you evaluate the correctness of step selection in the Runge-Kutta's method?
4. Which numerical methods for solving ordinary differential equations have the highest accuracy?

Practical work № 5

Numerical solution of a linear boundary value problem for an ordinary differential equation the second order

Work purpose: To acquaint students and provide them with the skills of applying the methods solving linear boundary value problems for an ordinary differential equation the second order.

The task of the work: On the segment $[a;b]$ to find the solution the differential equation $y'' + p(x)y' + g(x)y = f(x)$, which satisfies the boundary conditions

$$\begin{cases} \alpha y(a) + \alpha_1 y'(a) = A \\ \beta_0 y(t) + \beta_1 y'(t) = B \end{cases} \text{ according to the data provided by the teacher:}$$

- 1) by the finite difference's method, taking the step $h = 0,1$;
- 2) by the sweep method, taking the step $h = 0,06$.

Theoretical information

Let the model of some process taking place in the ecosystem be presented in the form of a linear differential equation the second order

$$y'' + p(x)y' + g(x)y = f(x) \quad (5.1)$$

where $p(x), q(x), f(x)$ – are known functions that are continuous on the segment $[a, b]$.

The linear boundary value problem for equation (5.1) consists in finding a function $y = f(x)$, that satisfies equation (5.1) inside the segment $[a, b]$, and linear boundary conditions at its ends

$$\begin{cases} \alpha_0 y(a) + \alpha_1 y'(a) = A \\ \beta_0 y(b) + \beta_1 y'(b) = B \end{cases} \quad (5.2)$$

where $\alpha_0, \alpha_1, \beta_0, \beta_1, A, B$ – are given constants, and $\alpha_0, \alpha_1, \beta_0, \beta_1$ are not equal to zero at the same time, i.e. $|\alpha_0| + |\alpha_1| \neq 0; |\beta_0| + |\beta_1| \neq 0$.

If $A = B = 0$, the boundary conditions (5.2) are called *homogeneous*.

A linear boundary value problem is called *homogeneous* if the differential equation (5.1) ($f(x) = 0$) and the boundary conditions (5.2) are homogeneous.

Otherwise, the boundary value problem (5.1), (5.2) is called *inhomogeneous*. Since the conditions must be fulfilled at two points - at the ends of the interval $[a, b]$, they are called *two-point boundary conditions*, and the boundary value problem - *a two-point boundary value problem*.

An exact solution the boundary value problem is possible in rare cases. Therefore, in practice, approximate methods of solving the boundary value problem are often used, which can be divided into two groups: difference and analytical. Let's consider one of the difference methods - the finite difference method.

Finite difference method

This is one of the simplest methods solving the linear boundary value problem (5.1), (5.2), which consists in reducing it to a finite difference equations system.

Let's divide the segment $[a, b]$ into n equal parts of length h (step), where

$h = \frac{b-a}{n}$. Let us denote the points of division of the segment $[a, b]$ as

$x_0 = a, x_n = b, x_i = x_0 + ih (i = 1, 2, \dots, n-1); p_i = p(x_i), q_i = q(x_i), f_i = f(x_i); y(x_i) = y_i, y'(x_i) = y'_i; y''(x_i) = y''_i$.

derivatives $y'(x_i)$ and $y''(x_i)$ finite-difference relations at approximately every internal point x_i of the segment $[a, b]$:

$$y'_i = \frac{y_{i+1} - y_i}{h} \quad (5.3)$$

$$y''_i = \frac{y_{i+2} - 2y_{i+1} + y_i}{h^2} (i = 1, 2, \dots, n-1)$$

For the boundary points $x_0 = a$, $x_n = b$ we put

$$y'_0 = \frac{y_1 - y_0}{h}; \quad y'_n = \frac{y_n - y_{n-1}}{h} \quad (5.4)$$

Using formulas (5.3) and (5.4), we approximately replace equations (5.1) and boundary conditions (5.2) with a system of $n + 1$ linear algebraic equations with $n + 1$ unknowns $y_0, y_1, y_2, \dots, y_n$, representing the values of the sought function $y = y(x)$ at the points x_0, x_1, \dots, x_n :

$$\begin{cases} \frac{y_{i+2} - 2y_{i+1} + y_i}{h^2} + p_i \frac{y_{i+1} - y_i}{h} + q_i y_i = f_i \\ (i = 0, 1, 2, \dots, n-2) \\ \alpha_0 y_0 + \alpha_1 \frac{y_1 - y_0}{h} = A, \\ \beta_0 y_n + \beta_1 \frac{y_n - y_{n-1}}{h} = B \end{cases} \quad (5.5)$$

After solving this system, if it is possible, we will get a table approximate value of the desired function $y = y(x)$.

In practice, derivatives are often $y'(x_i)$ replaced $y''_1(x_i)$ by finite-difference relations at internal points x_i at the segment $[a, b]$

$$y'_1 = \frac{y_{i+1} - y_{i-1}}{2h}; \quad y''_1 = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} \quad (5.6)$$

and for the limit points $x_0 = a$ and $x_n = b$, as before, formulas (5.4) are valid.

Then the system equations for determination y_0, y_1, \dots, y_n takes the form

$$\begin{cases} \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + p_i \frac{y_{i+1} - y_{i-1}}{2h} + q_i y_i = f_i \\ (i = 0, 1, 2, \dots, n-1) \\ \alpha_0 y_0 + \alpha_1 \frac{y_1 - y_0}{h} = A, \\ \beta_0 y_n + \beta_1 \frac{y_n - y_{n-1}}{h} = B \end{cases} \quad (5.7)$$

To estimate the finite-difference method error, the following approximate inequality is usually used in practice

$$|y^*_i - y(x_i)| \approx \frac{1}{3} |y^*_i - y_i|$$

where $y(x_i)$ is the value the exact solution the boundary value problem at the point $x = x_i$; y_i – the value the approximate solution, calculated at a point $x = x_i$ with step h ; y_i^* – the value the approximate solution, calculated at a point $x = x_i$ with a step $h/2$.

To find an approximate solution the boundary value problem with a given accuracy ε , it is necessary to carry out calculations with a step h and $h/2$ and compare the obtained results. If $|y_i^* - y_i| < 3\varepsilon$, then, accordingly, $|y_i^* - y(x_i)| < \varepsilon$ and the value y_i^* ($i = 1, 2, \dots, n$) can be taken as the sought solution the boundary value problem.

Sweep method

When n is large, the direct solution of the system becomes quite cumbersome. Let's consider a method that was developed specifically for solving systems of this type - the sweep method.

Let the system (5.7) be solved. Consider the first $n - 1$ equations.

$$\frac{y_{i+2} - 2y_{i+1} + y_i}{h^2} + p_i \frac{y_{i+1} - y_i}{h} + q_i y_i = f_i$$

$$(i = 0, 1, 2, \dots, n - 2)$$

After the simplest transformations, we get:

$$y_{i+2} + (-2 + hp_i)y_{i+1} + (1 - hp_i + h^2q_i)y_i = h^2 f_i \quad (5.8)$$

Let's enter the notation

$$m_i = -2 + hp_i; \quad k_i = 1 - hp_i + h^2q_i$$

$$(i = 0, 1, 2, \dots, n - 2) \quad (5.9)$$

and write (5.8) in the form

$$y_{i+1} = \frac{h^2}{m_i} f_i - \frac{1}{m_i} y_{i+2} - \frac{k_i}{m_i} y_i \quad (5.10)$$

If we exclude y_i from equation (5.10) using the boundary conditions of system (5.7), we get this equation in the form:

$$y_{i+1} = c_i(d_i - y_{i+2}) \quad (i = 0, 1, 2, \dots, n - 2), \quad (5.11)$$

where c_i, d_i are some coefficients.

Let, for example, $i = 0$. Then equation (5.10) takes the form

$$y_1 = \frac{h^2}{m_0} f_0 - \frac{1}{m_0} y_2 - \frac{k_0}{m_0} y_0 \quad (5.12)$$

Let's find from the boundary condition $\alpha_0 y_0 + \alpha_1 \frac{y_1 - y_0}{h} = A$

$$y_0 = \frac{Ah}{\alpha_0 h - \alpha_1} - \frac{\alpha_1}{\alpha_0 h - \alpha_1} y_1$$

and let's substitute this expression into (5.12). After the transformations, we will get

$$y_1 = \frac{\alpha_1 - \alpha_0 h}{m_0(\alpha_1 - \alpha_0 h) + k_0 \alpha_1} \left[\left(\frac{k_0 Ah}{\alpha_1 - \alpha_0 h} + h^2 f_0 \right) - y_2 \right].$$

Let's mark

$$\begin{aligned} c_0 &= \frac{\alpha_1 - \alpha_0 h}{m_0(\alpha_1 - \alpha_0 h) + k_0 \alpha_1} \\ d_0 &= \frac{k_0 Ah}{\alpha_1 - \alpha_0 h} + h^2 f_0 \end{aligned} \quad (5.13)$$

Based on (5.11), we obtain:

$$y_i = c_{i-1}(d_{i-1} - y_{i+1})$$

Substituting this expression into equation (5.10), we get

$$y_{i+2} + m_i y_{i+1} + k_i c_{i-1}(d_{i-1} - y_{i+1}) = h^2 f_i,$$

where

$$y_{i+1} = \frac{(h^2 f_i - k_i c_{i-1} d_{i-1}) - y_{i+2}}{m_i - k_i c_{i-1}} \quad (5.14)$$

Comparing (5.11) and (5.14), we obtain the following recursive formulas for determining c and d_i :

$$\begin{aligned} c_i &= \frac{1}{m_i - k_i c_{i-1}}; \quad d_i = h^2 f_i - k_i c_{i-1} d_{i-1} \\ (i &= 1, 2, \dots, n-2) \end{aligned} \quad (5.15)$$

On the basis of formulas (5.13), we determine the coefficients c_0, d_0, \dots , then, by successively applying the recurrent formulas (5.15), we obtain the value c_i, d_i ($i = 1, 2, \dots, n-2$) (direct flow).

The reverse course begins with the definition y_n . Using the second boundary condition of system (5.7) and formula (5.11) we $i = n-2$ write down the system of two equations:

$$\begin{aligned} \beta_0 y_n + \beta_1 \frac{y_n - y_{n-1}}{h} &= B; \\ y_{n-1} &= c_{n-2}(d_{n-2} - y_n) \end{aligned} \quad (5.16)$$

3. In what cases is it recommended to use the sweep method when solving a linear boundary value problem?

Practical work № 6

Numerical solution of partial differential equations

Work purpose: To acquaint students with the methods of solving linear partial differential equations.

The task of the work: According to the data provided by the teacher, using the grid method, find the solution $u(x,t)$ the mixed problem for the differential

equation the parabolic type $\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$ satisfying the initial condition $u(x,0) = f(x); (0 \leq x \leq 0,5)$ and the boundary conditions $u(0,t) = \varphi(t)$ and $u(0,5;t) = \psi(t) \quad 0 \leq t \leq 0,01$. Take $h = 0,1 \quad \sigma = \frac{1}{6}$;

Theoretical information

Partial differential equations are differential equations in which the unknown functions are functions of more than one independent variable.

A differential equation in partial derivatives the second order with two independent variables in the general case has the form

$$F(x, y, u, u_x, u_y, u_{xx}, u_{xy}, u_{yy}) = 0, \quad (6.1)$$

where are x, y – the independent variables; u – the desired function;

$u_x, u_y, u_{xx}, u_{xy}, u_{yy}$ – its first and second derivatives by arguments x, y (strokes are omitted for the convenience of writing derivatives).

The relation of equation (6.1) is called a function $u = u(x, y)$ that transforms this equation into an identity.

Equation (6.1) is called *linear* or *completely linear* if it is of the first degree with respect to the desired function and all its derivatives and does not contain their products. Such an equation can be written in the form

$$A \frac{\partial^2 u}{\partial x^2} + 2B \frac{\partial^2 u}{\partial x \partial y} + C \frac{\partial^2 u}{\partial y^2} + a \frac{\partial u}{\partial x} + b \frac{\partial u}{\partial y} + cu = F(x, y), \quad (6.2)$$

where the coefficients A, B, C, a, b, c can depend only on x and y . If the coefficients do not depend on x and y , then equation (6.2) is called *linear by a partial differential equation with constant coefficients*.

Equation (6.2) belongs to *the hyperbolic type* if the discriminant of the equation $D = AC - B^2 < 0$; belongs to *the parabolic type* if $D = 0$, and to *the elliptic type* if $D > 0$.

The problem finding a solution $u = u(x, y)$ to equation (6.2) that satisfies the initial conditions

$$u(x, y_0) = \varphi(x), u_y(x, y_0) = \varphi_1(x) \quad (6.3)$$

is called *the Cauchy problem*, and conditions (6.3) are called *the initial Cauchy data*.

One of the most widespread methods numerical solution partial differential equations is the *grids method*, or the *finite differences method*.

Grid method

The essence of the method is as follows:

1. The region G with the border Γ (Fig. 6.1), in which a solution needs to be found, is covered by a grid consisting of identical cells; the mesh area contour should be chosen so that they approximate the contour Γ the given area G as best as possible.

The grid area (Fig. 6.1), which approximates the given area G , was obtained by constructing two parallel lines on the xOy plane:

$$x = x_0 + ih \quad (i = 0, \pm 1, \pm 2, \dots)$$

$$y = y_0 + kl \quad (k = 0, \pm 1, \pm 2, \dots)$$

where h is the grid step in the direction of the Ox axis;

l is the grid step in the direction of the Oy axis.

These lines intersection points are called nodes. Two nodes are called adjacent if they are at a distance l or h . We denote by M the set of nodes that belong to the region $G + \Gamma$ and those that do not belong, but are located at a distance less than a step h or l , from the border of G . Then nodes are called *internal nodes*, all four neighboring nodes of which belong to the set M (node P , Fig. 6.1). Nodes of the set M that are not internal are called *boundary nodes* (nodes N, Q , Fig. 6.1).

2. The specified differential equation is replaced at the nodes of the constructed grid by the corresponding finite-difference equation.

We mark the value of the desired function $u = u(x, y)$ in the nodes of the grid:

$u_{ik} = u(x_0 + ih; y_0 + kl)$; in each internal node, $(x_0 + ih, y_0 + kl)$ we replace the partial derivatives with difference relations:

$$\left(\frac{\partial u}{\partial x}\right)_{ik} = \frac{u_{i+1,k} - u_{i-1,k}}{2h}; \quad \left(\frac{\partial u}{\partial y}\right)_{ik} = \frac{u_{i,k+1} - u_{i,k-1}}{2l} \quad (6.4)$$

at the limit points

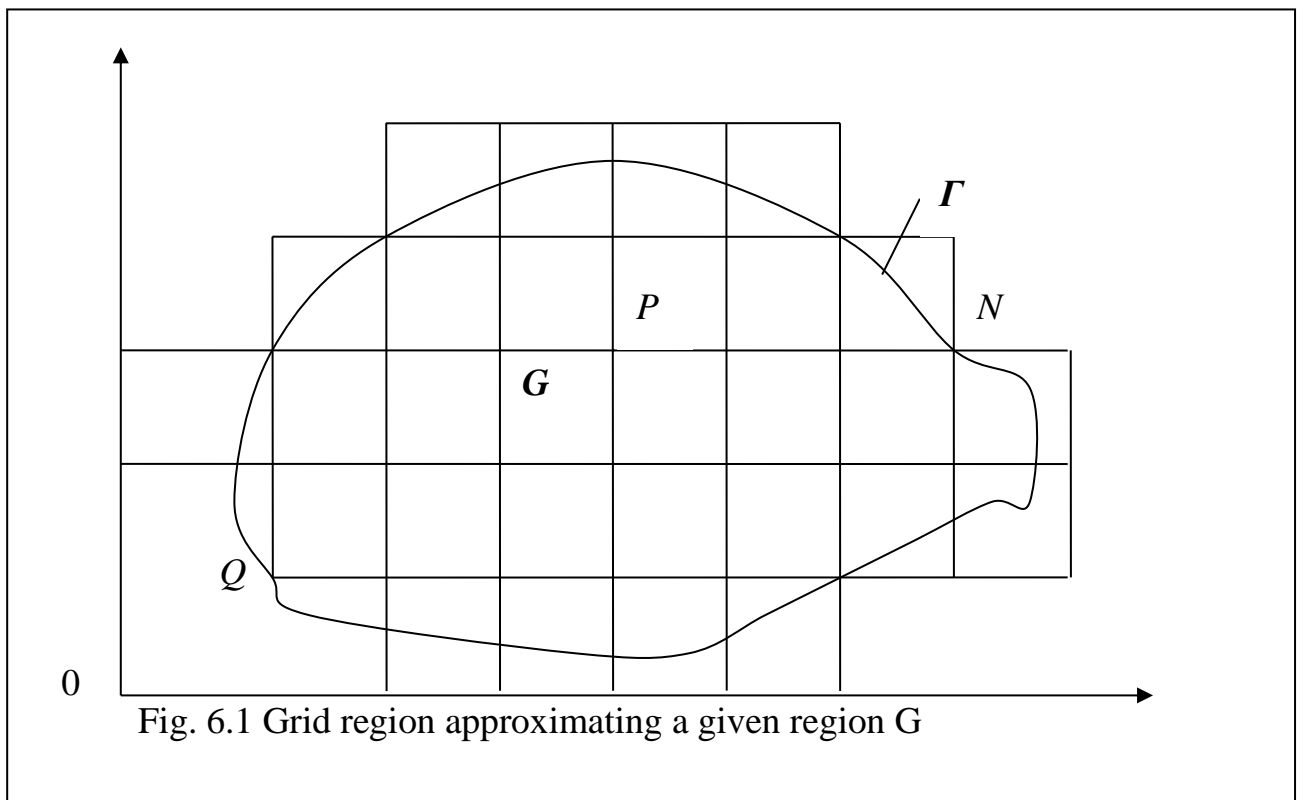
$$\left(\frac{\partial u}{\partial x}\right)_{ik} \approx \frac{u_{i+1,k} - u_{ik}}{h}; \quad \left(\frac{\partial u}{\partial y}\right)_{ik} \approx \frac{u_{i,k+1} - u_{ik}}{l} \quad (6.5)$$

Now let's replace the partial derivatives the second order

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{ik} \approx \frac{u_{i+1,k} - 2u_{ik} + u_{i-1,k}}{h^2} \quad (6.6)$$

$$\left(\frac{\partial^2 u}{\partial y^2}\right)_{ik} \approx \frac{u_{i,k+1} - 2u_{ik} + u_{i,k-1}}{l^2}$$

These formulas will make it possible to replace differential equations with a finite-difference equations system, that is, a system of linear algebraic equations. Having solved it, we will obtain the value the function in the grid nodes and thus obtain the numerical solution the given equation



Example:

Let it be necessary to solve the parabolic's type equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \quad (6.7)$$

where $u = u(x, t)$, $0 \leq x \leq s$

Find $u(x, t)$, what satisfies (6.7), the initial conditions

$$u(x, 0) = f(x) \quad (0 \leq x \leq s)$$

and boundary conditions

$$u(0, t) = \varphi(t), u(s, t) = \psi(t).$$

We denote $x_i = ih; t_j = jl; u_{ij} = u(x_i, t_j)$, where $h = \frac{s}{n}$, n - (integer) step along the Ox axis, $l = \sigma h^2$, σ - (constant) step along the Oy axis. In each internal node, (x_i, t_j) we approximately replace the derivative $\frac{\partial^2 u}{\partial x^2}$ with a difference relation

$$\left(\frac{\partial^2 u}{\partial x^2} \right)_{ij} \approx \frac{u_{i+1, j} - 2u_{ij} + u_{i-1, j}}{h^2} \quad (6.8)$$

derivative $\frac{\partial u}{\partial t}$ - one of two difference ratios

$$\left(\frac{\partial u}{\partial t} \right)_{ij} \approx \frac{u_{i, j+1} - u_{ij}}{l} \quad (6.9)$$

$$\left(\frac{\partial u}{\partial t} \right)_{ij} \approx \frac{u_{i, j} - u_{ij-1}}{l} \quad (6.10)$$

Then we replace equation (6.7) with a finite-difference equation

$$u_{i, j+1} = \sigma u_{i-1, j} + (1 - 2\sigma)u_{ij} + \sigma u_{i+1, j} \quad (6.11)$$

$$(1 + 2\sigma)u_{ij} - \sigma(u_{i+1, j} - u_{i-1, j}) - u_{i, j-1} = 0 \quad (6.12)$$

It is proved that equation (6.11) is constant for $0 < \sigma \leq 1/2$, and equation (6.12) for any σ .

Control questions:

1. What processes models that take place in ecosystems can be written in the form of a partial differential equation?
2. Name the methods known to you that can be used to solve partial differential equations?
3. What is the grid method?

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NOTES

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до виконання практичних робіт
для здобувачів спеціальностей 101 «Екологія»
183 «Технології захисту навколишнього середовища
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