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DETERMINATION OF UNKNOWN PARAMETERS OF MATHEMATICAL MODEL USING THE EXPERIMENTAL DESIGN THEORY

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ABSTRACT

The range of problems that can be solved with the help of mathematical modeling is constantly increasing, which creates new theoretical problems. One of them is connected with identification of unknown parameters of models. The problem of parameters determination belongs to the class of inverse problems. They are usually considered within the optimization theory. In the present paper, we propose a fundamentally new approach. The method is based on the theory of planning and processing of experiments developed by American scientists Box and Wilson. To evaluate the adequacy of model, a numerical criterion W is formulated depending only on the model parameters a_1, a_2,... a_k. It is shown that the maximum adequacy is achieved for the minimum value of W. Therefore, solving the problem of calculating the parameters is reduced to determination of such values of a_1, a_2,... a_k that provide the minimum value of the criteria W. This problem is solved by the steep ascent method due to Box and Wilson.

Keywords: *Mathematical Modeling, Inverse Problems, Regression Equation, Algorithm Of Calculations.*

1. INTRODUCTION

A mathematical model represents real objects using mathematical methods. Mathematical modeling has come to us from the distant past. At the first stage it was restricted mainly to the range of problems of mechanics. The twentieth century was marked by widespread use of mathematics in the study of physical phenomena. It suffices to mention the classical studies due to L.D. Landau, N.N. Bogolyubov, A.N. Tikhonov, M.V. Keldysh and many other scientists [36]. Along with the applications in physics, mathematical models have become a powerful tool in all areas of scientific research. The literary sources testify to high effectiveness of using mathematical models in the study of chemical processes, technical objects [23], in considering the environmental [12], sociological [15] and economic [13] processes, in medicine [2] [22] biology and biophysics [1] [33], in the analysis of complex systems [17]; Gerashchenko, et al., 2006). The type of mathematical model depends on the nature of real object, the purpose of study and the required accuracy of solving the formulated problem. Any mathematical model describes the real object with a certain degree of approximation; therefore, the inaccuracy of forecasting with the help of mathematical modeling is inherent in the very method of investigation. A great contribution to the development of methods of constructing mathematical models and the methods of identifying their parameters has been made by A.S. Adalev, A.V. Bondarenko, S.A. Bukashkin, P.A. Butyrin, L.V. Danilov, K.S. Demirchyan, V.N. Ilyin, D. Kalakhan, A.M. Kostrominov, A.A. Lanne, L.G. Lerner, V.G. Mironov, A.G. Nakonechnyi, I.P. Norenkov Yu V. Rakitsky, A.V. Sidelnikov, L.A. Sinitsky, M.A. Shakirov and many other scientists.

The majority of the problems of mathematical modeling can be divided into two groups. The first group consists of the direct problems, the second group, the inverse problems [35]. Formulation of a direct problem includes solving equations with the known parameters, as well as the known initial and boundary conditions. Among the examples of models which are classified as direct problems, there are the classical equations of mathematical physics. Inverse problems involve unknown constants or unknown functions, which are used in the mathematical model [4]. To determine the unknown parameters, one has to engage the experimental data or additional conditions [27]. In

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many cases, an inverse problem is reduced to finding the coefficients of algebraic equations, polynomials, splines, differential or integral equations, or systems of equations, which form a mathematical model of a real process. These coefficients are determined by the properties of the environment. There is one requirement which is put before all inverse problems: the parameters to be determined must provide the maximum adequacy of the mathematical model. In this regard, inverse problems are similar to one-dimensional [31] and multi-dimensional [37] optimization problems.

We can classify as inverse problems the construction of response functions and the finding of the regression equations which are chosen by the experimenter to describe the process under study. As the regression equation there are often used the segments of the Taylor series, Chebyshev polynomials, Fourier series, and so on. [16]. Interpolation of functions with the help of polynomials and splines [37], the construction of surfaces [6][7]and geometric figures in accordance with the specified conditions [20] are also similar to inverse problems.

The methods of solving inverse problems are quite diverse. In the first half of the twentieth century, there were most widely used the methods of optimization [32], the least squares method [5], the gradient methods, the analytical methods which are developed for the partial differential equations [35]. Each of them has its user and has its own advantages. The purpose of the present study is to develop a new method for solving inverse problems based on the ideology of the theory of experimental design [9].

2. METHODS:

Inverse problems, which include finding the regression equations, interpolation [11], approximation [28], the construction of geometric figures [6][7] and surfaces [20] have been widely used to solve many technical problems. In particular, the construction of a surface that meets given criteria is one of topical problems in the theory of geometric modeling [24].

Suppose that a mathematical model with the variables $x_1, x_2,... x_n$ defines a function $Y(a_1,... a_k, x_1, x_2,... x_n)$ of the variables $(x_1, x_2,... x_n)$ with k unknowns numerical parameters $a_1, a_2,... a_k$. This function can be viewed as an equation of a surface with k unknown numerical parameters $a_1, a_2,... a_k$ in the (n + 1)-dimensional Cartesian space. In what follows, this equation will be called an original. Suppose that for m points in the n+1-dimensional space with the known coordinates $x_{1i}, x_{2i},... x_{ni}$, where i = 1,2 ... m, there are known the approximate or exact values of the original. We denote the corresponding values as Y_i:

$Y_i \approx Y_i(a_1, a_2,... a_k, x_{1i}, x_{2i},... x_{ni})$, i=1, 2… m (1)

The nature of the genesis of information about Y_i is not relevant in this case. It can be obtained from experimental data or calculated using a mathematical model for selected values of $a_1, a_2,... a_k$. It is required to construct a model of the original surface of the same kind $Y(a^*_1, a^*_2,... a^*_k, x_1, x_2,... x_n)$ with the parameters a^*_i, which are different, in general, from a_i. Due to fuzziness of setting up the points, between which the surface is "stretched", this formulation allows for the possibility of deviation between the points of original and its model. As a criterion of smallness of such deviation, we choose a residual function in the form of the squared deviations between the values of the obtained function at given points and the approximate values at these points:

$V(a_1, a_2,... a_k)=\sum(Y(a_1, a_2,... a_k, x_{1i}, x_{2i},... x_{ni}) - Y_i)^2$,(2)

where the summation is over all indices i = 1, 2, ... m.

For the fixed values $x_{1i}, x_{2i},... x_{ni}$ the function (2) is defined in the space of variables $a_1, a_2,... a_k$. The problem comes down to determining such values of the unknown $a^*_1, a^*_2,... a^*_k$ that provide the minimum of (2). The resulting solution, if it exists, has a simple geometric interpretation: in the (n + 1)-dimensional space there is found the equation of a geometric model of a surface which at the points with the coordinates $(x_{1i}, x_{2i},... x_{ni})$, where i = 1, 2, .. m, coincides with the original $Y(a_0, a_1,... a_k, x_1, x_2,... x_n)$ with the precision given by the expression (2). In general, the domain of the variables in the (k + 1)-space may be bounded or unbounded, whereas the function (2) itself may or may not have an extremum. The condition for the extremum is the requirement:

$$\frac{\partial V(a_1, a_2,...a_k)}{\partial a_j} = 0, j = 1,2...k \qquad (3)$$

Thus, the general formulation of the inverse problem is reduced to finding the unknown $a_1, a_2,... a_k$ that provide the minimum value of the function (2). Its solution depends on the particular model. It can be given in the form of partial differential equations, in the form of a multidimensional regression equation, etc. Thus, our further consideration will be based on particular cases.

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The purpose of this work is to develop an algorithm of identification of the mathematical model parameters using a mathematical theory of experiment [16]. To achieve this goal it is necessary to solve the **following problems**:
- to carry out an analysis of research methods for solving inverse problems,
- to choose the type of residual function for assessing the adequacy of the mathematical model,
- on the basis on the experiment planning theory, to formulate an algorithm for calculating the unknown parameters of the mathematical model,
- to assess the model error,
- to compare the efficiency of the proposed method with the known gradient methods of finding extremum.

A hypothesis of the study is that the obtained results can be used for solving inverse problems, in particular, for identifying unknown parameters in the known mathematical models.

3. Results. In one of the first works on the analysis of inverse problems, there is considered a mathematical model in the form of the partial differential equation of parabolic type [35]:

$$\frac{\partial T(t,x)}{\partial t} = a\frac{\partial^2 T(t,x)}{\partial x^2} \quad (4)$$

where T is the temperature, it is time, whereas a is the thermal conduction coefficient.

A.N. Tikhonov showed that equation (4) uniquely defines the parameter "a" if the exact temperature distribution T (t, x) is known and the initial and boundary conditions are given. A.N. Tikhonov's method was further developed in the works of Russian [27] and Ukrainian [8] scientists.

Consider yet another example of solving the inverse problem in the case of mathematical processing of a single-factor experiment. Suppose that, on the basis of experimental data on the dependence of the response function Y (x), a conclusion was made about the possibility of presenting the results in the form of a polynomial:

$$Y(x) = b_0 + b_1 x + b_2 x^2 + \ldots + b_k x^k \quad (5)$$

To determine the unknown parameters in the regression equation (5), one should have information in m>k experiments. Let us denote the values Y at the points with coordinates $x_1, x_2, \ldots x_m$ by $Y_1, Y_2, \ldots Y_m$. Substitute these values into the formula (2) and obtain the expression, using which we can determine the unknown parameters $b_0, b_1, \ldots b_k$ with the help of the least squares method. In the simplest case of linear dependence, the regression equation $Y(x)=b_0 + b_1x$ contains two parameters, which are determined by the formulas [16]:

$$b_0 = \frac{y_s \sum_{i=1}^{m} (x_i)^2 - x_s \sum_{i=1}^{m} x_i y_i}{\sum_{i=1}^{m} (x_i - x_s)^2},$$

$$b_1 = \frac{\sum_{i=1}^{m} x_i y_i - m x_s y_s}{m s_x^2}, \quad (6)$$

where x_s is the average value of the variable x, y_s is the average value of the variable y, s_x is the root-mean-square deviation of x.

The formulas for calculating the coefficients b_i in the regression equation (5) for k> 2 are presented in the work [29]. Similar problems can be solved using the method of least squares and gradient methods. In the opinion of J. Bernal, the effectiveness of this processing is about 2%. The situation changed in the 20-s of XX century, when the English statistician R. Fisher first proposed to carry out an experiment while varying all parameters at once [26]. This method laid the foundation of mathematical planning of multifactorial experiment. In the 50-s, the American scientists Box and Wilson took another step in the development of the experiment planning theory. The essence of the method proposed by them is as follows. On the first stage, for some local multifactorial domain D of existence of the studied object, the regularities of its behavior are examined. After carrying out an analysis, the direction of change of the input factors towards the optimum is determined. Then another experiment is conducted in a new domain of existence of the object, etc. until the optimum conditions are reached [9].

The method of Box–Wilson or the so-called steepest ascent method combines the best features of the gradient methods and the Gauss–Seidel method. In it, the movement along the gradient vector is borrowed from the gradient method, whereas the principle of advancing by more than one working step is taken from the Gauss–Seidel method. The trial experiments to determine the direction of movement are performed in a special way: by the method of complete factorial experiment or fractional factorial experiment [18]. From this it is clear that the mathematical theory of experiment and the theory of optimization in the case of two or more variables solve one and the same problem: the determination of extremum in a multifactorial space. The problem of identification of unknown parameters ($a_1, a_2, \ldots a_k$) of a known

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mathematical model is reduced to the determination of such values of these parameters that provide the maximum adequacy of the model. If an appropriate criterion is chosen for the adequacy of the model, for example, in the form $V(a_1, a_2,... a_k)$, the function (2), then solving the identification problem is reduced to finding the minimum value of this criterion, that is, to determining an extremum.

4. Discussion.

4.1. Construction of the response function.

Let a function $Y(a_1, a_2,... a_k, x_1, x_2,... x_n)$ of a known type with unknown parameters $a_1, a_2,... a_k$ determine the original in the form of a surface. By the expression $Y(a_1, a_2,... a_k, x_1, x_2,... x_n)$ we mean a function which can be given, for example, in the form of an analytical expression, with the help of the regression equation (5) or by equation or system of equations. Let us restrict ourselves to the analysis of the case when $Y(a_1, a_2,... a_k, x_1, x_2,... x_n)$ is a continuous function in a given region with respect to all parameters and all variables and has no more than one extremum, as it is shown in Figure 1 on a particular example of function $Y(x_1, x_2)$.

Suppose that for m points with coordinates $x_{1i}, x_{2i},... x_{ni}$, where i=1, 2... m, this function has exact or inexact values (1). It is required to evaluate the unknown parameters $a_1, a_2,... a_k$ that provide the minimum of the criterion $V(a_1, a_2,... a_k)$, formula (2). In some cases the problem is to minimize not the quadratic form (2) but the residual function in the form of the integral:

$$W(a_1, a_2,... a_k) = \int_S [Y(a_1, a_2,... a_k, x_1, x_2,... x_n) - Y(a^*_1, a^*_2... a^*_k, x_1, x_2,... x_n)]^2 d x_1 d x_2... dx_n, \quad (7)$$

where integration is taken place over a given domain S.

Consider the basic idea of the method of solving the formulated problem for the criterion $W(a_1, a_2,... a_k)$, formula (7). In the domain of definition S we choose a subdomain D in the form of a multidimensional parallelepiped with sufficiently small length of edges $2d_i$ (i=1, 2... k) and the central point $a_{01}, a_{02},... a_{0k}$. Let us shift the coordinate origin to the point $a_{01}, a_{02},... a_{0k}$ and introduce normalized coordinates according to the formulas

$$z_i = (a_i - a_{0i})/d_i, \quad i = 1,2\ldots k. \quad (8)$$

In the new coordinate system, the values of z_i change from -1 to +1, as it is shown in Fig. 2 for the particular case k=2.

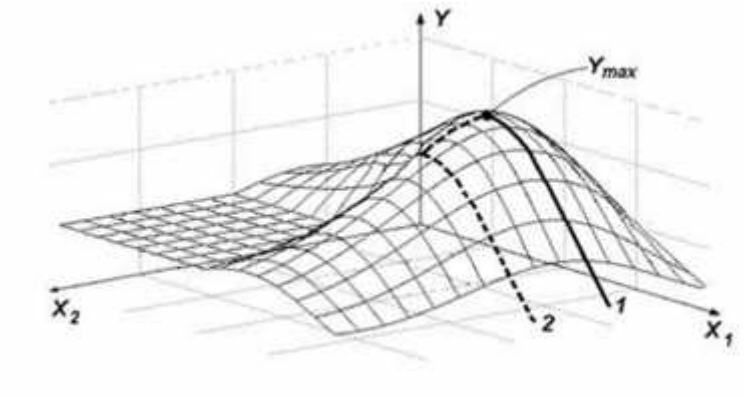

Figure 1. Surface In The Three-Dimensional Cartesian Space.

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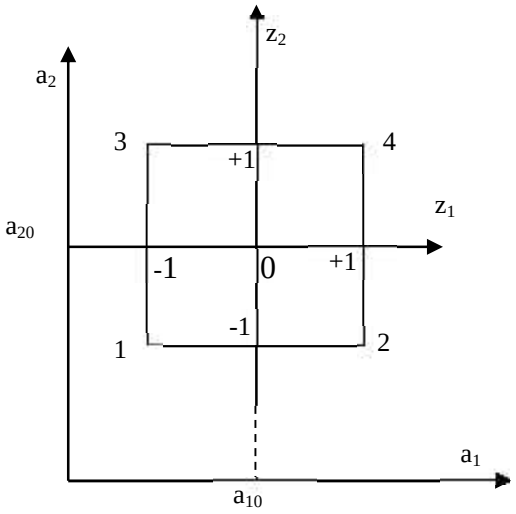

Figure 2. Systems Of Coordinates

According to (8), the old coordinates are expressed through the new ones according to the formulas:

$a_i = a_{0i}+d_i z_i$, i = 1,2… k. (9)

After the transition to the new system of coordinates by the formulas (9), the function $W(a_1, a_2,... a_k)$ will have the form $W(z_1, z_2…z_k)$. If the domain D and the edge lengths $2d_i$ are sufficiently small, the $W(z_1, z_2…z_k)$ in this domain can be represented approximately in the form of an equation of plane:

$W(z_1, z_2…z_k)= c_0+c_1z_1+ c_2z_2+…c_kz_k$ (10)

where c_0, c_1, $c_2…c_k$ are unknown parameters defining the equation of plane (10).

Let us require that the number m of the points, for which the values are defined with the help of the formulas (1), be equal to the number N of the vertices of the cube

$m = N = 2^k$, (11)

whereas the coordinates of the points coincide with these vertices.

The set of m points with coordinates $z_1, z_2,... z_k$ at the vertices of multidimensional cube, which satisfy the condition (11), is called a complete set for k-dimensional factorial space (CSFS). To determine the coefficients $c_0, c_1, c_2… c_k$ in the formula (10), we need information about the criterion $W(z_1, z_2… z_k)$, at least, at (k +1) points.

In the theory of CSFS it is suggested to use the values of this function at 2^k points. The coordinates of these points z_{ji} in the normalized coordinate system must be at the vertices of the selected cube. In this case z_{ji} will be equal to -1 or +1. Such requirement is represented as a matrix of study planning. An example of the planning matrix for k = 2 is given in Table 1, which is consistent with the notations in Figure 2.

Table 1. Matrix Of Coordinates Of The Vertices Of The Cubic Domain D For N=2.

Vertex number, i	z_{1i}	z_{2i}	W_i
1	-1	-1	W_1
2	+1	-1	W_2
3	-1	+1	W_3
4	+1	+1	W_4

It is easy to see that, in the case of CSFS and for the normalized coordinate system, the following equalities hold [16]:

$$\sum_{i=1}^{N} z_{ji} = 0 \quad \sum_{i=1}^{N} z_{ji}^2 = N \quad \sum_{i=1}^{N} z_{ji} z_{ki} = 0, \; k \neq j \quad (12)$$

The first of the formulas (12) reflects symmetry of the matrix of normalized coordinates $z_1, z_2,... z_k$ with respect to the center. The second formula is the condition of normalization of variables; the third formula represents the orthogonality condition. When the equalities (12) hold, the parameters $c_0, c_1,... c_k$ in the plane equation (10) can be calculated using the formulas [16]:

$$c_i = (\sum_{j=1}^{j=N} z_{ij} W_j) / N, i = 0,1,2,..k \quad (13)$$

4.2. Estimation of errors. It is assumed that the data about the function $W(z_1, z_2… z_k)$ at the vertices of the cubic domain D are known. The necessary information to determine $W(z_1, z_2…z_k)$ can be obtained by calculation if the mathematical model is built, or taken from the experiment. In the case of using the experimental data, the experiment results are usually duplicated in order to increase reliability of the conclusions. Denote the number of repetitions of experiments at the i-th vertex of the cube, i = 1, 2 ... N, by r, whereas the value in one of repetitions, by W_{is}, s = 1, 2, ... r. (Davis, 1979). Let us assume that the data for each of the vertices are subject to the normal distribution law. We will calculate the variance s_v^2 of reproducibility of experiments and the variance s_{ad}^2 of the model adequacy by the formulas:

$$s_v^2 = \sum_{i=1}^{N} \sum_{s=1}^{r} (W_{is} - W_i^0)^2 / N(r-1) \quad (14)$$

$$s_{ad}^2 = \sum_{i=1}^{N} (W_{ir} - W_i^0)^2 / (N-k), \quad (15)$$

where W_i^0 is the average value for W_{is}, s=1,2,… r, W_{ir} is the value calculated by the formula (10). The adequacy of the model (10) can be evaluated

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using Fisher's criterion with N-k and N(n-1) degrees of freedom:

$$F = s_{ad}^2 / s_v^2 \quad (16)$$

The variance of the error of calculation of the coefficients (13) equals

$$s^2_{aj} = s_v^2 / N \quad (17)$$

Finally, we estimate the integral (7). Substituting the equation of the plane and its approximate version (10) into the expression (7), represented in the normalized coordinate system, we obtain:

$$W = \int_{-1}^{+1} \dots \int_{-1}^{+1} (c_0 + c_1 z_1 \dots + c_k z_k - c_0^* - c_1^* \dots - c_k^* z_k)^2 dz_1 \dots dz_k \quad (18)$$

Since the variance for all the coefficients c_0, c_1,... c_k is the same and is equal to (17), then after substituting (17) into (18) we have the following estimate:

$$W < \int_{-1}^{+1} \dots \int_{-1}^{+1} (k+1)^2 (c_0 - c_0^*)^2 dz_1 \dots dz_k = 2^k (k+1)^2 s_v^2 / 2^k = (k+1)^2 s_v^2 \quad (19)$$

The absolute inaccuracy of the model ascribed to a single point is equal to

$$W / N = (k+1)^2 s_v^2 / 2^k \quad (20)$$

Formula (20) does not take into account the errors of calculations. When using the modern computational tools, this error is not large. Let us note that W is a random variable. For a particular multidimensional space, the value of k is a constant; thus, the improvement of accuracy can be achieved only through increasing the sample size r. In accordance with formula (10), the increasing of r will lead to diminishing of σ^2_v, decreasing of W and, respectively, to improving the accuracy of the model.

4.3. Movement in the direction of gradient. Let there be known a mathematical model $W(a_1,\dots a_k, x_1, x_2,\dots x_n)$ in the variables $(x_1, x_2,\dots x_n)$ with k unknown numerical parameters $a_1, a_2,\dots a_k$. The problem is to determine such values of $a_1^*, a_2^*,\dots a_k^*$ that provide a minimum for the function $W(a_1, a_2,\dots a_k)$, the integral (7). In rare cases, one of which was studied for the mathematical model (4), there exists a unique solution when $W(a_1^*, a_2^*,\dots a_k^*)$ equals 0 [35]. In most cases, the value of $W(a_1^*, a_2^*,\dots a_k^*)$ is not equal to 0. Moreover, the inverse problem can have several solutions. The using of the necessary condition (3) for an extremum at the point $a_1^*, a_2^*,\dots a_k^*$ greatly facilitates the search of optimal solution.

Suppose that in a certain domain S the function $W(a_1, a_2,\dots a_k)$ has no extremum or has one extremum, as shown in Figure 1 for the surface equation $Y(x_1, x_2)$. Suppose that in a certain region D in the form of a multidimensional cube with $N = 2^k$ vertices, $D \subset S$, the plane equation (10) is found. If the size of this region is small enough, then the points of the plane practically coincide with the points of the surface $W(z_1, z_2 \dots z_k)$ in this region (hereinafter, all the calculations are in the normalized coordinate system). Let us determine the projections of the gradient of the function (10) at the central point of the region D for the normalized coordinate system:

$$\nabla W(0,0,\dots 0) = \left(\frac{\partial W}{\partial z_1}, \frac{\partial W}{\partial z_2}, \dots \frac{\partial W}{\partial z_k}\right) \quad (21)$$

Moving along the direction opposite to the gradient $\nabla W(0,0,\dots 0)$ results in decreasing of $W(z_1, z_2 \dots z_k)$, and hence in improving the adequacy of the mathematical model. Denote the step of movement along each axis by Δz_i. The choice of the value of Δz_i is determined by the behavior of the function in the neighborhood of the starting point. In order to move strictly in the direction opposite to the gradient, it is necessary to require that the value of the steps along different axes are proportional to the projections of the vector (21) with the opposite sign. Denote the coordinates of points at each of the steps by z_{ij}, where the index j signifies the number of the step. Knowing z_{ij} and according to (9), we move on to the corresponding values of a_{ij} , and, by formula (7), we calculate the value of the integral $W(z_{1i}, z_{2i},\dots z_{ki})$ for all values of the parameters $z_{1j}, z_{2j},\dots z_{kj},\dots$, lying along the direction opposite to the gradient (21). The number of steps depends on the nature of changes in the function $W(z_{1j}, z_{2j},\dots z_{kj})$. Once this function ceases to decrease, the working of the movement procedure should be stopped. Our task is to find the coordinates $z_{1j}, z_{2j},\dots z_{kj}$ of such point, at which the function $W(z_{1j}, z_{2j},\dots z_{kj})$ attains a minimum. Let us denote these coordinates by $z_1^*, z_2^*,\dots z_k^*$. Perhaps they are the best, then the goal is reached. If it is necessary to modify the result, then it is recommended to select one more point as the starting one with the coordinates $z_1^*, z_2^*,\dots z_k^*$, to adopt a new normalized system of coordinates, to determine a new equation of the plane in the neighborhood of that point and repeat the movement in the direction opposite to the gradient.

As an alternative to carrying out the repeated procedure of movement against the gradient, we can indicate the following operation. A sufficiently small domain D is identified in the form of a cube with the central point $z_1^*, z_2^*,\dots z_k^*$ and, on its

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basis, a second order surface is constructed by the equation

$$M(z_1, z_2 \ldots z_k)=c_0+ c_1 z_1+..+ c_k z_k+ c_{11} z_1^2+..+ c_{kk} z_k^2+ c_{12} z_1 z_2+ c_{13} z_1 z_3+..+ c_{k-1,k} z_{k-1} z_k \quad (22)$$

As the base points, through which this surface passes, there are selected the points belonging to D. The recommendations concerning the selection of these points can be found in the literature [18]. Then the quadratic sum (2) or the integral (7) is calculated, and the coefficients of equation (22) are determined. In the paper [9], some recommendations are given allowing reducing the number of terms in (22). The multi-dimensional surface (22) is a sufficiently accurate model of residual function (formulas (2) and (7)). Finding the maximum (minimum) of the function (22) in the domain D is a simple problem. Let us denote its coordinates by $Z^{**} = (z_1^{**}, z_2^{**},... z_k^{**})$. In the first approximation, point Z^{**} coincides with the sought-for point. If it is necessary to refine the result, one needs to select Z^{**} as a starting point and repeat all operations, beginning from the movement in the direction opposite to the gradient.

5. CONCLUSION:

Determination of the parameters of mathematical models is a challenging problem in the theory of mathematical modeling, which belongs to the class of inverse problems [27]. The manifoldness of inverse problems does not allow uniting them by a single solution method. Here, as the additional means, there are used the results of experiments [30], analytical methods [36], optimization techniques [14], the gradient and other methods [33].

A special feature of the gradient methods is that the information about the maximum rate of increase or decrease of a function is obtained by processing the function in the small neighborhood of the starting point. This approach often leads to the effect of repeated passing past the extremum. The application of the method of steepest descent and the Gauss−Seidel method improves the situation, but does not guarantee the complete solving of the problem [38]. There arises a natural wish to find such path of moving towards the extremum that takes into account more precise behavior of the function in the neighborhood of the starting point and allows implementing the algorithm of finding the maximum (minimum) for a smaller number of iterations.

In this paper we propose a method for calculating the unknown parameters of a model on the basis of the theory of planning and processing of experiments due to American scientists Box and Wilson [9]. The calculation algorithm can be represented by the following stages:

Stage 1. There is formulated the criterion $W(a_1, a_2,... a_k)$, formula (7) (if necessary, the criterion $V(a_1, a_2,... a_k)$, formula (2)) and a procedure of its calculation is developed for the given values of the model parameters $a_1, a_2,... a_k$. Adequacy of the model increases with the decreasing of W, so further steps should be aimed at changing $a_1, a_2,... a_k$ in such direction that diminishes W.

Stage 2. A starting point is selected with the coordinates $a_{01}, a_{02},... a_{0k}$, there is defined a sufficiently small domain D in the form of a multidimensional cube, formulas (8) are used for the transition from the coordinate system $(a_1, a_2,... a_k)$ to the normalized system of coordinates $(z_1, z_2 \ldots z_k)$, and there is determined the equation of the plane (10) whose points differ little from the points of the surface $W(z_1, z_2 \ldots z_k)$ in the domain D.

Stage 3. Using formula (21), we compute the gradient of the function $W(z_1, z_2 \ldots z_k)$ at the center of the normalized coordinate system and realize the step-by-step movement of the point in the direction opposite to the gradient. Moving of the point is performed so long as the value of the criterion is diminishing. Once the value of $W(z_1, z_2 \ldots z_k)$ at some point $Z^* = (z_1^*, z_2^*,... z_k^*)$ begins to increase, the movement process stops. There an extremum is reached, which determines the sought-for point in the first approximation. If there is a need to improve the adequacy of the model, it is recommended to go to the next stage.

Stage 4. As a new starting point, we select the point Z^* which was defined on stage 3 and repeat all the operations of the stages 2 and 3. The number of repetitions depends on the function $W(z_1, z_2 \ldots z_k)$ and the required degree of accuracy of calculations. In many cases it is sufficient to restrict ourselves to the first or second approximations. An alternative to the second and subsequent refinements of the extreme point's location is the operations on the final stage.

Stage 5. In the neighborhood of the extremum point Z^* we construct a second order surface (22), which simulates the function $W(z_1, z_2 \ldots z_k)$ in this neighborhood. Finding the maximum (minimum) of the function (22) at the point Z^{**} for the domain D is a simpler problem. If one wants to refine the result, one needs to select Z^{**} as a starting point and repeat all the operations, beginning from the movement in the direction opposite to the gradient.

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The proposed algorithm of identification of unknown parameters of a mathematical model has been implemented in solving a number of problems. Our research has shown that if the criterion $W(z_1, z_2 \ldots z_k)$ has no more than one extremum, then this algorithm provides the optimal solution. When there are two or more extremums, the problem becomes more complicated. However, such difficulties in the case of multi-dimensional gradient optimization are characteristic of all gradient methods [34] [21]. Comparison of the proposed method with the known methods of determining the extremum leads to the following conclusions:

1. The total time of determining the extremum of a function of many variables while using the known methods (e.g., the steepest descent method) and this method is approximately the same. It is equal to the product of the number of iterations and the time of carrying out calculations in a single iteration.
2. The advantage of the proposed method is manifested in such problems where the calculation of the residual function (2) or (7) takes a long time. As an example we can refer to the complex mathematical models requiring large computation time.

In conclusion, we note that the search methods of finding the optimum involve some subjectively set parameters. Among them there are the coordinates of the starting point and the size of the step. They have a significant impact on the efficiency and the search time. Moreover, one and the same method can give different search trajectories. Therefore, the selection of method, especially in the case of several extrema, is crucial.

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