Geometric modeling of multifactor processes and phenomena by the multidimensional parabolic interpolation method

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Abstract. The paper presents the results of multidimensional parabolic interpolation studies, (one of the special cases of the multidimensional interpolation method), applied to solve problems of modelling multifactor processes and phenomena using geometric objects of multidimensional affine space. The authors describe the technique of geometric model tree forming of the process under study and its analytical description based on computational point algorithms with subsequent implementation on a computer. Such an approach makes it possible to effectively use multidimensional interpolation instead of multidimensional approximation (based on the least squares method) for solving problems of mathematical and computer modelling of multifactor 3-level processes and phenomena of animate and inanimate nature, technology, economy, construction, and architecture The study gives an example of multidimensional parabolic interpolation application to simulate the dependence of the fine-grained tar-polymer concrete compressive strength on 4 factors: tar viscosity, polyvinyl chloride dropout concentration in coal tar, activator concentration on the mineral powder surface and temperature, followed by optimization of the composition and operating conditions road pavement.

Keywords: geometric modelling, multifactor processes, multidimensional parabolic interpolation, influence factors, response function, parabolic arc, point equation, computational algorithm, experimental and statistical information.

1. Introduction

One of the most effective and common methods of exploring and learning the world by humanity is an experiment. At the same time, simulation of experimental statistical data (which can be analytical, computer, imitational, etc.) is no less popular tool in the arsenal of scientists. Usually, modeling types do not contradict, but complement each other. The experimental data replacing with a model allows limiting the number of experiments, which saves material, technical, human, financial, and other resources. On the other hand, it is necessary to remember that the model is always an approximate representation of the actual process (or phenomenon) course. Model is a scientific hypothesis, confirmed by the initial experimental and statistical data only to a certain extent. Therefore, the development of tools that increase models accuracy (reliability) obtained from the experiment will always be a pressing scientific task.

Today, one of the most popular methods of mathematical modeling based on the initial experimental statistical information is regression analysis [1-3], which is based on the least squares method [4]. In this case, the least squares method relates to approximation modeling methods. However, due to the high cost of conducting experimental studies in the process of their planning, the
most widespread are 2-level (coded factors values «-1» and «+1») and 3-level (coded factors values «-1», «0» and «+1») regression models. In most cases, interpolation modeling methods give better results, given the large amount of experimental data. Then, a 3-level mathematical model (for a one-factor experiment) can be represented as a parabolic dependence. Analytical description of multifactor experiments, using existing methods of multidimensional interpolation, poses considerable difficulties. The reason for this is the lack of a universal approach to the mathematical model structure formation. In addition, each individual method is more focused on solving a particular practical problem. For example, the research [5] describes a comparison of various multidimensional interpolation methods which include: interpolation by the Lagrange polynomial, polynomial recursive interpolation and rational interpolation. The work [6] studies the several variables periodic function interpolation, which is given in the generalized parallelepiped mesh nodes of an integer lattice. The problem of a function interpolation defined on a regular grid is given in the study [7] for the case of variables large number. The work [8] is devoted to solving the problem of multidimensional spline interpolation on chaotic grids with a huge number of interpolation points. In addition, the problems of multidimensional interpolation and approximation can be solved on the basis of the random functions theory [9]. Most of the considered methods require significant refinement, and in some cases are not suitable for the analytical description of multifactor 3-level models.

To solve the problem (creating an analytical description and computational algorithms for modeling multifactor 3-level processes and phenomena based on the original experimental statistical information), the authors use geometric multifactor processes and phenomena modeling [10-12]. At the same time, the geometrical model of the studied multifactor process is represented by some multi-parametric geometrical multidimensional affine space object. A parabolic arc passing through 3 predetermined points is the basis for the desired geometric object construction.

2. Simulation of a parabolic arc passing through 3 forward set points

The authors propose a technique for modeling arcs of algebraic curves passing through predetermined points described in [13], for geometric modeling and analytical description of a parabolic arc. The peculiarity of this approach is as follows: when defining a parabolic arc equation, there is no need to re-solve the system of linear algebraic equations every time to determine the square polynomial coefficients, which excludes the possibility of using the movable simplex method [14-15] to construct geometric objects in advance of the specified conditions. The algebraic curves modeling arcs method passing through the given points on the parabolic arc was considered as a case. In this work, the mathematical apparatus of the BN-calculus (Baliuba-Naidysh point calculus [16–18]) is used for the analytical description and parametrization of all geometric objects.

The following task was set. A parabolic arc (also known as a second-order Bezier curve) is specified in the simplex (Fig. 1) and determined by the following point equation:

\[ M_A = A\pi^2 + 2C\pi u + Bu^2, \]

where \( M_A \) is the current arc curve point;
- \( A \) is starting point of a parabolic arc;
- \( B \) is the end point of a parabolic arc;
- \( C \) is tangent intersection point of \( AC \) and \( BC \);
- \( u \) is current parameter, that changes from 0 to 1;
- \( \pi = 1 - u \) is parameter addition \( u \) to 1.
It is necessary to redefine the points $A$, $B$ and $C$ so, that the parabolic arc passes through the preset points $A_I$, $A_4$ and $A_5$, instead of the original points.

To solve the problem, the current parameter $u$ changes as the parabolic arc passes through the given points $A_1$, $A_4$ and $A_5$ were analyzed. Figure 1 shows that the points $A_1$ and $A_4$ coincide with the beginning and end of the desired curve arc. Thus, when $u = 0$ there is a point $A_1$, and when $u = 1$ - a point $A_5$. To sum it up, parabolic arc it passes through a point $A_4$ when $u = 0.5$. When the fixed current parameter values and the original parabolic arc point equation were substituted, the following system of linear equations was:

$$\begin{align*}
A &= A_1; \\
A + 2C + B &= 4A_4; \\
B &= A_5.
\end{align*}$$

In accordance with the BN-calculus, the points were used as arithmetic numbers. Based on this, it is possible to redefine the point $C$ through the points $A_1$, $A_4$ and $A_5$ by the Kramer’s method (the other two points have already been redefined):

$$C = -0.5A_1 + 2A_4 - 0.5A_5.$$

The authors have obtained the following equation after substituting points $A$, $B$ and $C$ into the original parabolic arc point equation:

$$M_\lambda = A_1\bar{u}(1 - 2u) + 4A_4\bar{u}u + A_5u(2u - 1).$$

To perform computational operations on points, the point equations, which are only symbolic representations have been changed into a system of parametric equations. It results in the system for 3-dimensional space:

$$\begin{align*}
x_{M_\lambda} &= x_{A_1}\bar{u}(1 - 2u) + 4x_{A_4}\bar{u}u + x_{A_5}u(2u - 1); \\
y_{M_\lambda} &= y_{A_1}\bar{u}(1 - 2u) + 4y_{A_4}\bar{u}u + y_{A_5}u(2u - 1); \\
z_{M_\lambda} &= z_{A_1}\bar{u}(1 - 2u) + 4z_{A_4}\bar{u}u + z_{A_5}u(2u - 1).
\end{align*}$$

Such an operation was called the coordinate calculation in the BN-calculus. Its geometric meaning is in the fact that each of the system parametric equations represents an analytical description of the simulated geometric object projection (in this case, a parabolic arc) on one of the global Cartesian coordinate system axes. Similarly, one can get the required number of parametric equations. Thus, the dimension of space is provided which is necessary to solve a specific problem.

It should be noted, that the resulting equation is the basis of multifactor processes and phenomena geometric modeling through the method of multidimensional parabolic interpolation. At the same time, in comparison with experimental-statistical models, one of the parabolic arc three points can be put into correspondence with one of the regression model levels. Only coding is performed using geometric points. So, the point $A_1$ corresponds to the level «-1», the point $A_4$ – to «0», and the point $A_5$ – to «+1».
Now, regardless of the original three-point position in multidimensional space, it is always possible to uniquely determine the parabolic arc point equation passing through these predetermined points. To do this, it is enough to substitute the corresponding coordinates in the resulting parabolic arc equation instead of the base points. An important feature is that the source points can be not only fixed (constant coordinate values), but also current (variable coordinate values).

3. Multifactor processes and phenomena geometric modelling through the method of multidimensional interpolation

According to the work [12], the main difference between geometric models and their mathematical analogues obtained by means of multidimensional interpolation is that the simulation result is not an abstract mathematical object, but a specific geometric parametrized object, that has predetermined geometric properties. The process of analytic description of certain phenomenon (or process) is an analytical definition of certain geometrical object possessing the following features:

1) The number of current (variable) parameters of geometric object corresponds to the number of studied factors.
2) Each of the global coordinate system axes, in which the desired geometric object is defined, corresponds to one of the factors under study. In addition, one of the global coordinate system axes corresponds to the response function. Thus, a number of the coordinate axes determining the space dimension where the desired geometric object is determined is always one unit more than the current parameters number.

The process of geometric object determining consists of two stages:

Stage 1. Geometric algorithm development for object constructing (the so-called tree of a geometric model).
Stage 2. Geometric algorithm analytical description using point equations and computational algorithms based on them.

Since a special case of a parabolic arc determining that passes through 3 predetermined points was given above, an example of constructing and analytically describing a parabolic response surface compartment corresponding to a two-factor process was considered.

Any surface compartment can be represented as a family of guides and a forming line. In this case, the forming line moves along the guide lines and fills the space, forming a continuous surface. Hence, a parabolic arc is used as a generator, passing through the 3 current points, belonging to the guide lines. This means that the family of guides will consist of 3 lines. Each of the guides will also be determined by a parabolic arc, and consist of 3 points. Thus, it results in a section of the response surface passing through 9 predetermined points (Fig. 2).

The analytical description of such a surface can be represented as a computational algorithm — a point equations sequence:

\[
\begin{align*}
M_A &= A_1 \bar{v}(1 - 2u) + 4A_2 \bar{u}u + A_3 u(2u - 1); \\
M_B &= B_1 \bar{v}(1 - 2u) + 4B_2 \bar{u}u + B_3 u(2u - 1); \\
M_C &= C_1 \bar{v}(1 - 2u) + 4C_2 \bar{u}u + C_3 u(2u - 1); \\
M_v &= M_1 \bar{v}(1 - 2v) + 4M_2 \bar{v}v + M_3 v(2v - 1),
\end{align*}
\]

where \( M_v \) is the current point of the parabolic surface compartment;
\( M_A, M_B, M_C \) are the current points of the guide parabolic arcs;
\( A_1, B_1, C_1 \) are the initial points, the coordinates of which correspond to the original experimental statistical information;
\( u \) and \( v \) are the current parameters of the parabolic surface compartment;
\( \bar{u} = 1 - u \) and \( \bar{v} = 1 - v \) are addition of the current parameters to 1.
Generalizing the considered example, the authors have obtained an analytical description of the three-parameter parabolic hypersurface of the response belonging to a 4-dimensional space, for the construction of which it is necessary to have 3 parabolic response surfaces combined by forming a hypersurface passing through 3 current points of 3 response surfaces.

Thus, a parabolic three-parameter response hypersurface corresponding to a three-factor 3-level process will be defined by 27 points, the coordinates of which correspond to the original experimental and statistical information:
\[
\begin{align*}
M_1 &= A_1 \bar{u} (1 - 2u) + 4A_2 \bar{u} u + A_3 u (2u - 1); \\
M_2 &= B_1 \bar{v} (1 - 2u) + 4B_2 \bar{v} u + B_3 u (2u - 1); \\
M_3 &= C_1 \bar{w} (1 - 2u) + 4C_2 \bar{w} u + C_3 u (2u - 1); \\
M_4 &= D_1 \bar{v} (1 - 2u) + 4D_2 \bar{v} u + D_3 u (2u - 1); \\
M_5 &= E_1 \bar{w} (1 - 2u) + 4E_2 \bar{w} u + E_3 u (2u - 1); \\
M_6 &= F_1 \bar{v} (1 - 2u) + 4F_2 \bar{v} u + F_3 u (2u - 1); \\
M_7 &= G_1 \bar{w} (1 - 2u) + 4G_2 \bar{w} u + G_3 u (2u - 1); \\
M_8 &= H_1 \bar{v} (1 - 2u) + 4H_2 \bar{v} u + H_3 u (2u - 1); \\
M_9 &= I_1 \bar{w} (1 - 2u) + 4I_2 \bar{w} u + I_3 u (2u - 1); \\
M_{v1} &= M_{v2} \bar{v} (1 - 2u) + 4M_{v3} \bar{v} u + M_{v4} v (2u - 1); \\
M_{w1} &= M_{w2} \bar{w} (1 - 2u) + 4M_{w3} \bar{w} u + M_{w4} w (2u - 1),
\end{align*}
\]

where \( M_{v1} \) is the current point of the compartment of the three-parameter parabolic response hypersurface;

\( M_A, M_B, M_C, M_D, M_E, M_F, M_G, M_H, M_I \) are the current points of the parabolic arcs guides;

\( M_{v1}, M_{v2}, M_{v3} \) are the current points of the parabolic surfaces guide compartments;

\( A_1, B_1, C_1, D_1, E_1, F_1, G_1, H_1, I_1 \) are the initial points, the coordinates of which correspond to the initial experimental statistical information;

\( u, v \) and \( w \) are current parameters of the parabolic hypersurface compartment;

\( \bar{u} = 1-u, \bar{v} = 1-v \) and \( \bar{w} = 1-w \) are addition of the current parameters to 1.

Similarly, it is possible to construct a geometric object belonging to a space of any dimension and analytically describe any 3-level processes and phenomena. The proposed method of parabolic multidimensional interpolation is completely universal, since the computational algorithm point equations for constructing geometric objects of multidimensional space are invariant with respect to the original experimental and statistical data. That is, the method of parabolic interpolation can be used in the simulation of absolutely any 3-level processes and phenomena. It is enough to change the coordinates of the initial points each time, corresponding to the initial experimental statistical information.

As can be seen from the above analogies, the number of multidimensional parabolic object points coincides with the requirements for the full-factor experiment planning matrix and for a 3-level model and is:

\[ y = 3^k, \]

where \( y \) is the number of initial experimental statistical data;

\( k \) is the number of factors of variation.

4. An example of multidimensional parabolic interpolation method using for simulate the fine-grained tar-polymer concrete ultimate compressive strength dependence from 4 factors.

As described above, multidimensional parabolic interpolation can be used to simulate a wide variety of nature processes and phenomena, technology, economy, construction and architecture. One example of its effective use is the ultimate strength dependence model in the compression of fine-grained tar-polymer concrete from 4 factors: tar viscosity \( C_{10}^{00} \), polyvinyl chloride dropout
concentration in coal road tar $- C_{\text{PVH}}^{\text{MT}}$ activator concentration on the mineral powder surface $- C_{\text{KM MT}}^{\text{C}}$ and temperature, which was described in [19]. The initial data for the simulation were the studies [20]. Also in the research [20], 3-level experimental-statistical models were constructed, the analysis of which showed that even with high values of the determination coefficient there are significant model values deviations from the original data [19]. In addition, in [20], models for each factor were obtained separately, which makes it impossible to assess the influence of a particular factor on the entire model as a whole. Based on this, it was decided to build a fine-grained tar-polymer concrete ultimate compressive strength dependence geometric model from 4 factors using parabolic interpolation.

The geometric representation of a 4-factor process is a 4-parameter parabolic response hypersurface belonging to a 5-dimensional space. According to equation (2), the initial data in the amount of 81 items are required. This means, that the desired 4-parametric parabolic hypersurface of the response must pass through the 81st pre-set point, the coordinates of which correspond to the initial information obtained in [19]. Analytically, the such response hypersurface description will consist of 3 sequences of point equations (1), combined with a generator passing through 3 predetermined points using the parameter $t$:

$$M_{i} = M_{w_1} T(1-2t) + 4M_{w_2} T + M_{w_3} T(2t-1),$$

where $M_i$ is the current point of the compartment of the three-parameter parabolic response hypersurface;

$M_{w_1}$, $M_{w_2}$, $M_{w_3}$ are the current points of the guiding compartments of the three-parameter parabolic response hypersurfaces;

$T = 1-t$ is addition of the parameter $t$ to 1.

After the substitution and transformations, the following equation was obtained depending on the compressive strength of fine-grained tar-polymer concrete from 4 parameters:

$$R = (((44w - 52,8w^2 + 22,4)u^2 + (-49,2w + 58,4w^2 - 24)u - 32,4w + 31,2w^2 + 9,2)v^2 + +((-83,6w + 72,8w^2 - 8)u^2 + (81,4w - 74w^2 + 10,8)u + 31,8w - 29,2w^2 - 9)v + + (7,6w - 2,4w^2 - 3,2)u^2 + (-11w + 7,6w^2 + 3,2)u - 4w^2 + 4,4w + 3,6)t^2 + +((-119,6w + 119,2w^2 - 23,2)u^2 + (148,6w - 149,2w^2 + 22)u + 15,4w - 12,4w^2 - 9,8)v^2 + + (179,4w - 158w^2 + 6)u^2 + (-196,7w + 179,4w^2 - 6,8)u - 21,9w + 16,2w^2 + 9,1)v + +(-8,6w + 1,2w^2 + 4,4)u^2 + (13,9w - 9,4w^2 - 5)u + 7,6w - 9,8w - 8)t + ((90,8w - 80,8w^2 - 0,8)u^2 + (-119,4w + 110w^2 + 4)u - 1 + 25,2w - 26,4w^2)v^2 + +((-115,8w + 104,4w^2 + 3,6)u + (141,7w - 131w^2 - 6)u + 1,7 - 19,4w + 22w^2)v + +(1,6w - 1)u^2 + (1,9 - 5,2w + 4,8w^2)u + 4,9 - 5,2w^2 + 7,4w, $$

where $R$ is the compressive strength of fine-grained tar-polymer concrete;

$u$, $v$, $w$ and $t$ are the current parameters, which vary from 0 to 1 and correspond to the viscosity of tar $- C_{\text{vis}}^{10}$, the polyvinyl chloride dropout concentration in coal tar $- C_{\text{m}}^{\text{PVBX}}$, the activator concentration on the mineral powder’s surface $- C_{\text{KM MT}}^{\text{C}}$ and temperature.

The resulting model allows optimizing the composition and performance characteristics of tar-polymer concrete to achieve maximum compressive strength. As a result, the maximum value of the compressive strength (12 MPa) was achieved at tar viscosity $- C_{\text{vis}}^{10} = 208$ s, polyvinyl chloride dropout concentration in coal tar $- C_{\text{m}}^{\text{PVBX}} = 2\%$, the concentration of activator on the mineral powder’s surface $- C_{\text{KM MT}}^{\text{C}} = 1\%$ and temperature $T = 0$ °C. However, road surfaces are not always operated at zero temperature, which is too high in the summer and low in the winter. Moreover, the greatest danger for road pavement is precisely the summer period, when there is a “softening” of tar-polymer concrete.
For this reason, a method for optimizing the composition of fine-grained tar-polymer concrete for different climatic zones depending on the average maximum temperature of the warmest month on the basis of the obtained model was proposed in [21]. In this case, the model itself remains unchanged, only the calculated temperature values are recorded.

5. Conclusion

Studies of multidimensional parabolic interpolation, as one of the special cases of multidimensional interpolation, proposed in the work in relation to the analytical description and optimization of multifactorial 3-level processes and phenomena can significantly expand the possible scope of its application. The example of modelling the dependence of the fine-grained tar-polymer concrete compressive strength on 4 factors given in the work (with subsequent optimization of the composition and operating conditions of pavement) confirms the effectiveness of the geometric modelling methods use based on multidimensional parabolic interpolation and the need for further research in this direction. It should be noted, that using 2nd order algebraic curves properties studies in various parametrization [22], it is possible to obtain and optimize models of multifactor processes and phenomena using not only parabolic, but also elliptic, hyperbolic and mixed interpolation without changing the geometric algorithms for constructing multiparameter geometric objects.

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