Optimal Approximation for Multidimensional Nonlinear Point Data Sets

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***Abstract*—The mathematical modelling of complex physical processes (objects) is based on the approximation of their experimental output variables (point data sets). It is well known that the respective mathematical models are multidimensional and significantly nonlinear, thus various mathematical methods were developed to approximate the experimental point data, each having its own inherent approximation advantages and disadvantages. However, these methods did not take into account the data structural and parametric characteristics. and thus motivated this research to develop a more universal approximation methodology to this kind of problem. The applied approximation method, named Cut-Glue Approximation, takes into account any data order and/or any nonlinear dependency based on 3 principles: fragmentation of the initial data approximated by known methods; high-precision analytical approximation of local fragments; multiplicative analytic fragmentation of local functions isolated in the factor space. This paper considers the second stage of the Cut-Glue Approximation - analytical approximation of local fragments. The direct advantage of this approximation is the resulting mathematical model differentiability, which enables their analytical investigation, appropriate for modelling complex dynamical systems.**

Keywords-experimental data; fragments; math modeling; approximation; error; evolutionary-genetic algorithm; optimization; heuristic algorithms

I. INTRODUCTION

In the process of scientific and technological progress for the majority of real technical and technological objects, the experimental construction of Mathematical Models (MM) and their study by computer simulation methods are the only effective methods for solving problems.

This is because, due to the lack of a priori knowledge, theoretical research methods are not available for such objects. In addition, in the presence of significant nonlinearities of the internal relationships of the input and output data, the dependences for these objects are not always amenable for manipulation by known numerical methods.

For example, when modelling the aerodynamic characteristics of aeronautical vehicles, researchers often encounter significant nonlinearity and ambiguity of the aerodynamic laws of their own movement and interaction with the environment. For example, mechanical production processes, apparatuses of the chemical industry and land vehicles, have substantially nonlinear characteristics.

The experimental MM construction of such objects is the mathematical data processing task. The complexity of the approximation of such nonlinear dependences is obvious and can be the source of the significant errors. The errors reduction is achieved through the use of effective approaches based on the original array fragmentation of Experimental Data (ED). The effective approaches are the following: piecewise approximation [1][2], methods of spline functions [3][4], and also radial basis functions [5][6]. These approaches significantly increase the approximation accuracy when compared to the ED array methods as a whole (polynomial expansions [5]–[8], regression analysis [9], etc.). However, this excludes or makes it difficult for using them for the analytical MM transformation due to their conditional logical form.

One of the effective means of expanding the possibilities and increasing the effectiveness of experimental methods for constructing MM was a method oriented to a highly formalized approach by constructing MM for essentially nonlinear objects based on the ED conducted in active experiments. In a number of papers, starting from 2012, the Cut-Glue Approximation method (CGA) was developed [10][11][12][13]. It is based on the special multiplicative processing of individual MM dependency sections, fairly accurately approximated by analytical functions. The result of such processing is a function that describes only isolated (at each site) areas of their definition. With similar properties of these functions, subjected to multiplicative processing, it is admissible to additively combine them into a single function that has the MM object properties [3][8].

The CGA method includes the sequential execution of a number of stages: fragmentation of ED - partitioning an array into separate sections - fragments (FED), local approximation of each of the FED by a certain function and the multiplicative processing that follows it and the additive combination of these functions of the MM object under study [12][13]. In this case, the phase of local FED approximation [10][12], for the constructed MM, is decisive for the overall final quantitative accuracy.

However, despite the rather large number of publications on the topic [8][13] the absence of fundamental restrictions on the dimensionality of the simulated nonlinear

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dependencies is missing, and they were mainly illustrated by examples applying the CGA method for objects not higher than the second order. This was partly due to the need to illustrate the transformations and simulation results. Within the framework of this problem (approximation), there are mathematical and technological difficulties. Therefore, a detailed analysis of the solution for the 3-dimensional problem and its influence on the model dimension and methods applied with the obtained results seem relevant. This paper is dedicated to this topic.

It is necessary to develop an algorithm for the mathematical modelling of ED fragments with fairly simple analytical functions in structure that allow variation of their structural complexity and supplement it with a search algorithm for supporting structural parametric optimization. The aggregate (hybrid) algorithm finds a mathematical model of minimal complexity for any ED fragment being of any dimension ensuring the specified fragment approximation accuracy.

Section 2 explains the possible options for defining the applied polynomial approximation and the method to compute the related regression coefficients. Section 3 describes the importance of structural and parametric optimization of the proposed polynomial approximation, and section 4 describes the structural and parametric searches enabling to find the optimal fragment model of experimental data. The respective example is described in Section 5, where the optimal structural and parametric representation for the 3rd dimensional fragment is computed.

II. PERFORMANCE ALGORITHM FOR 3-DIMENSIONAL DATA FRACTURES IN CGA

The already published research results [10]-[13], performed during the development of the CGA method, as well as, numerous studies of the ED approximation problem [3][8], showed that to build Locally Approximating Functions (LAF), i.e. implementation of the phase of the FED approximation, it is appropriate to use a well-developed apparatus of classical regression analysis (CRA) [8][9]. In this case, the fragmentary nature of the approximation, which implies a not too large amount of experimental data included in the ED, makes it expedient to restrict oneself to methods of polynomial approximation. They guarantee both the analyticity of LAF and the regularity of its structure. The importance of the latter property will become clear from the further description of the problem.

The fragmentary nature of the approximation of the array of ED in the CGA method means that the number of components of its FED can be quite large, and the complexity of the LAF for each FED will depend both on its size by the amount of data and on the dimension of the ED. In other words, the complexity of the LAF in approximation on the basis of only an accuracy criterion can be very high. When combining a large number of complex LAF in a single MM, the complexity of the latter may be unacceptably high. This circumstance indicates the need to state and solve the problem of the structural-parametric optimization of each LAF, which, in turn, requires the regularity of their structure in order to be able to control its complexity.

The Power Polynomials (PP) have this property due to their regular structure, which allows to implement unambiguous algorithms for constructing joint ventures and their combinatorial variation. For the dependence of any dimension of PP has a canonical structure. The uniqueness of its complication relies on maintaining a clear sequence of the introduced members [13]. The following is an example of PP for a 3-dimensional fragment of experimental data:

$$Y(x) = b_0 + b_1x_1 + \cdots + b_nx_n + b_{11}x_1^2 + b_{12}x_1x_2 + b_{13}x_1x_3 + \cdots + b_{1n}x_1x_n + b_{22}x_2^2 + \\ + b_{23}x_2x_3 + \cdots + b_{2n}x_2x_n + \cdots + b_{(n-1)n}x_{n-1}x_n + b_{nn}x_n^2 + b_{111}x_1^3 + b_{112}x_1^2x_2 + \cdots \\ + b_{11n}x_1^2x_n + \cdots + b_{122}x_1x_2^2 + \cdots + b_{1nn}x_1x_n^2 + b_{222}x_2^3 + b_{223}x_2^2x_3 + \cdots + b_{22n}x_2^2x_n + \cdots \\ + b_{nnn}x_n^3 + b_{1111}x_1^4 + b_{1112}x_1^3x_2 + \cdots + b_{111n}x_1^3x_n + b_{1122}x_1^2x_2^2 + b_{1123}x_1^2x_2x_3 + \cdots, \quad (1)$$

where $b_{ijk\ldots}$ – coefficients of a polynomial of the 4th degree with the 3rd dimensionality of the simulated dependence. Their indices indicate the variables to be multiplied. For example, b_{1123} – product multiplier $(x_1x_1x_2x_3)$; x_i indexed independent variables of the experimental dependence under study.

The PP Universal Structure (PP US) applies 2 loops. The internal loop is used to explore different factors values, x_i of minimum to maximum index, as well as for the members of the same power order, and during their transition to a higher order. The outer loop ensures a consistent order increase to the next group of polynomial members starting from zero to the specified order, following after the exhaustion of combinatorial variants when multiplying factors.

This approach and the shape of PP simplify the formal evaluation and comparison of the PP complexity in respect to their structures. However, their use in the FED regression modelling complicates the finding of the optimal regression coefficients. One of the most simple and well-known simplification methods is the possibility of representing the nonlinear terms with PP arguments for the extended pseudo-linear factor space with a new vector modelling the conditionally independent variables of higher dimension:

$$q(\tilde{x}) = \sum_{i=0}^{\tilde{n}} \tilde{b}_i \cdot \tilde{x}_i = \sum_{i=0}^{n} b_i \cdot x_i + \sum_{i=n+1}^{\tilde{n}} \hat{b}_i \cdot \hat{x}_i \quad (2)$$

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where $\tilde{b}_i$ – pseudo-linear polynomial coefficients, $\tilde{n}$ -th dimensional, $\tilde{x}_i$ – generalized arguments of the dependency being investigated, including, as initial arguments x_i, so are the pseudo-arguments formed from them $\hat{x}_i = \prod_n x_i$ which are replaced by the multiplicative nonlinearities of the power polynomial.

The calculation of the regression coefficients for the considered polynomial variant in the matrix equation is the CRA linear variant:

$$\tilde{b} = (X^T X)^{-1} X^T y, \quad (3)$$

giving only suboptimal solution. In (3) $y - N_k$ - vector of values of the k-th FED; X –input matrix $\tilde{x}_{ij}; j \in [1, N_k]$ and i - numbers of experiments that coincide with the numbers of pseudo-variables. Interdependence part $\tilde{x}_i$ determines the calculated sub-optimal coefficients $\tilde{b}_i$ with respect to the criterion used in CRA: in the Least Squares Method (LSM) - this critera is only heuristic. Therefore, the non-quadratic criterion solves the problem successfully with a combinatorial approach.

It should be noted that the CRA apparatus is used in its standard form without any modification, since the obtained best approximation variant is performed with the structural-parametric optimization (STR), as explained in this paper follow up. The parametric sub-optimization of polynomial coefficients is solved by CRA for each structural variant of PP.

The developed software supports the first CGA method stage when approximating a fragmented ED with the approximating PP optimal or suboptimal variant. The low problem complexity is solved (the approximating PP dimension and order) applying the direct variants search. If the complexity of the problem results in an unacceptable computing time, then the heuristic search optimization algorithms is applied, as already proven themselves in such cases. Therefore, the developed EGA modifications are subject-oriented for the FED approximation.

III. STRUCTURAL-PARAMETRIC OPTIMIZATION OF FED MATHEMATICAL MODEL

The need for not only parametric search, requires in addition the optimal structural variant search, due to the fact that all included components cannot provide the required accuracy, since the properties of some nonlinear functions contradict the nature of the experimental dependences. Such specific functions that approximate well the curvature of the FED hyper-surface are unknown in advance for each individual fragment. The universal structure definition of the approximation function, with sufficient variety of elementary functions and their forms becomes a problem. A full PP meets this requirement. Within the search, first of all, it is necessary to identify its order m, which sets the data approximation accuracy, which is decreased when compared to the full polynomial of order m-1. In addition, the effective FP members search increases the approximation accuracy.

The advantage of using the regression PP resolves this problem, as its structure can be implemented by a regular mathematical record of the "mask" type, which represents the PP structure of the n^{th} dimension and the m^{th} degree (special digital code). This code is convenient for the FP structure, which has a similar dimension and degree. The initial arrangement of the FP elements corresponds to the combinatorial rules for increasing the indexes of coefficients described above. This corresponds to a structural and parametric increasing series of the polynomial coefficients, where the prime numbers 0, 1, 2 ... indicate the number of the multiplicative factor in the polynomial member. Their combination specifies all the factors constituting a member, and the number of nonzero numbers determines the order of PP. The code description example for the 4^{th} order FP structure of the 3^{rd} dimension follows:

$$\begin{gathered} 0,1,2,3,11,12,13,22, \\ 23,33,111,112,113,122,123,133, \\ 222,223,\ 233,333, \\ 1111,1112,1122,1123,1133, \\ 1222,1223,1233,1333,2222,2223,\ 2233,2333,3333 \end{gathered} \quad (4)$$

In (4) it is an enumeration of the terms of a fourth order polynomial of 3 dimensions, where "1" - corresponds to x1, "2" - corresponds to x2, "3" - corresponds to x3, "4" - corresponds to x4.

It should be noted, when approximating a fragment consisting of q elements by CRA methods, it is possible to describe it by a polynomial of the same order. The number of polynomial members is less than the number of members of the fragment $p < q$. Thus, the maximum possible order for the FED approximation is its structure order.

By varying the PP terms, the optimal structure search is made for the FED PP under consideration. The use of the NP-complete exhaustive search taking into consideration all the possible combinations for an incomplete polynomial is found unacceptable for the high-dimensional FED. Thus the subject-oriented modification of EGA is used, and implemented as a tool for the variation search of terms included in the resulting polynomial. It should be noted that the use of the combinatorial exhaustive search for all the possible PP combinations is possible, and only applicable to small dependence dimensions with a small polynomial order.

IV. POLYNOMIALS APPROXIMATION FOR STRUCTURAL AND PARAMETRIC OPTIMIZATION

The structural optimization search to find the suboptimal structure variant is based on a criterion in respect to which its complexity is calculated. Therefore, to assess the PP complexity criterion, it is worth noting that this difficult task

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requires additional research. Intuitively, as in our case, the MM complexity depends on a discrete components number that determines the polynomial structure. The known approaches for the discrete complexity estimation use of the so-called "complexity scale" [13], and in the present research, the assessment of the structure complexity could be based on 2 types of scales:

1. Heuristic, in which the quantitative components of the overall polynomial complexity are associated with its parameters, such as the number of members of the "symbols", the order of the member, etc., and are set by the developer or expert;
2. Theoretical or experimental estimate of time resources for calculating the resulting value of each PP member.

According to them, and on the formula proposed below, the structure complexity of the polynomial variant is calculated as follows:

$$E(P) = \sum_{i=1}^{N} e_i \times x_i \quad (5)$$

where P – PP structure under consideration;

N – full PP member's number, which includes the maximum possible number of members to define the fragment;

e – estimate for the i^{th} member listed in table 2;

x – indicator of the occurrence or non-occurrence of the i^{th} member in the considered PP structure.

For the first approach, a scale was heuristically designed, see example given in Table 1 (2^{nd} line). This scale is constructed for the 4^{th} order FP having 2-dimensional dependency. In the second case, as shown in Table 1 (3^{rd} and 4^{th} line), the scale fixes the time resources for calculating each PP member. The calculation is performed on a large sample (> 100000) using the desktop computer (CPU Pentium (R) Dual-Core 2.10 GHz, RAM 3 GB).

The Microsoft Visual Studio (MVS) software development environment is used for the implementation in the C# programming language. This development environment enables measuring the computation time for each PP member operations.

In Table 1, the 2^{nd} column shows the 4^{th} order FP coefficients, in the 3^{rd} column the heuristic complexity estimates are shown for each FP member, in the 4^{th} and 5^{th} column the computing time (measured in MVS) respectively the corresponding estimates for the (*t-estimate*) computing time for the 4^{th} order FP members is shown.

TABLE I. POLYNOMIAL STRUCTURE HEURISTIC AND RESOURCE SCALES

№	Member structure	Heuristic *estimate*	Ms	t-*estimate*
1	0	0,5	310	3,1
2	1	1	310	3,1
3	2	1	310	3,1
4	3	1	310	3,1
5	11	2	375	3,75
6	12	2	375	3,75
7	13	2	375	3,75
8	22	2	375	3,75
9	23	2	375	3,75
10	33	2	375	3,75
11	111	3	415	4,15
12	112	3	415	4,15
13	113	3	415	4,15
14	122	3	415	4,15
15	123	3	415	4,15
16	133	3	415	4,15
17	222	3	415	4,15
18	223	3	415	4,15
19	233	3	415	4,15
20	333	3	415	4,15
21	1111	4	480	4,8
22	1112	4	480	4,8
23	1113	4	480	4,8
24	1122	4	480	4,8
25	1123	4	480	4,8
26	1133	4	480	4,8
27	1222	4	480	4,8
28	1223	4	480	4,8
29	1233	4	480	4,8
30	1333	4	480	4,8
31	2222	4	480	4,8
32	2223	4	480	4,8
33	2233	4	480	4,8
34	2333	4	480	4,8
35	3333	4	480	4,8

V. MATHEMATICAL MODEL EXAMPLE FOR STRUCTURAL AND PARAMETRIC OPTIMIZATION

As example for the proposed structural-parametric approximation of the ED array fragment, the complex balloon movement is considered. The balloon total air resistance force (its vertical component) is simulated with its ascending velocity v (m/s), angle α (angle), and height h(m), adopting the following notation: v ~ x1; α ~ x2; h ~ x3.

The ED fragment, see Figure 1, contains 36 elements. The full 4^{th} order polynomial for the 3-dimensional dependency modelling contains 35 terms. Therefore, the limit FP fragment order is 4. Thus, the fragment modelling with 36 elements that contains 35 polynomial members is not a statistically acceptable option, since it takes into account only one of the existing degrees of freedom, and this is not enough to evaluate the resulting model. However, it should

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be noted that often the PP variants, having a smaller number of members (but larger number of freedom degrees) are better modelling the approximation fragment than the full polynomial having the maximum possible order. Therefore, the maximum PP structure order is chosen, since it allows the search for the best approximation accuracy. This is enabled by varying its members, for example, using the combinatorial search algorithm, as described previously, and the search approach based on the modified EGA.

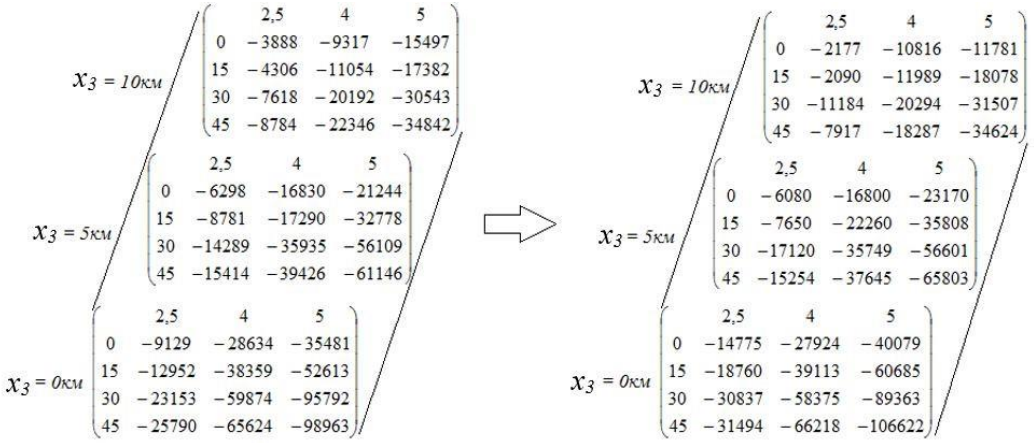

Figure 1: 3rd dimensional fragment results

To illustrate the 3-dimensional data source, we use a non-standard mathematical form writing. In the top rows and left columns of the ED matrices the fragments and the polynomial approximating it, see Figure 1, where the values x_1 and x_2 are shown. In the left part, the F_x (experimental data) matrix is shown, and in the right part, the analytically calculated values using STR are shown. The variation of the polynomial structure is carried out with the choice of PP variants satisfying the range of the ED relative error: 0.01–1% with a subsequent search in the resulting set of options for finding the minimal complexity structure.

Due to the fact that there is no universal and reliable theory of assessing the complexity of the joint, 2 types of criteria are proposed and validated: (1) Heuristic complexity scale, in which the polynomial members have assigned conditional estimate appropriate for their order and equal to it; (2) Considered to be more reasonable, since its complexity scale is based on the experimental estimates of the computational time for each PP member (see Table 1). By using them based on equation (5), the calculated structure complexity of the polynomial variant is shown.

The 4th order, PP members, with marks for their entry into the ranking of the 10 best structural-parametric polynomials indicators are shown in columns of Table 2. The best PP options with relative error within specified limits are considered. In each column, "1" indicates the inclusion of the corresponding term in the final PP structure (zi=1), and the sign "-", on the contrary, indicates its exclusion from the final PP structure (zi=0). The bottom lines below these columns show the estimates for each option.

In Table 2, in the last 6 lines, the following notation is used:

- "Absolute error" and "Relative error" characterize the values of absolute and relative approximation errors;
- "Sum. 4 "means the number of 4th order PP members is used as an additional criterion for assessing the complexity of the structure;
- "S1" denotes the total PP complexity based on the theoretical or experimental computational time estimates of the resulting value for each PP member;
- "S2" denotes the total PP complexity, based on the proposed heuristic scale;
- "SC" denotes the total PP complexity, based on 2 proposed scales.

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TABLE II. RESULTS OF STRUCTURAL-PARAMETRIC OPTIMIZATION BASED ON THE PROPOSED DIFFICULTY SCALES

№ СП (i)	1	2	3	4	5	6	7	8	9	10
0	1	1	1	1	1	1	1	1	1	1
1	--	1	--	1	1	1	--	1	--	1
2	--	--	--	1	--	1	--	1	--	1
3	1	1	1	1	1	--	--	--	--	--
11	--	--	--	--	--	1	--	--	--	--
12	1	1	1	--	--	--	--	--	1	--
13	--	--	--	--	--	--	1	1	--	1
22	1	--	--	1	1	--	1	--	1	--
23	--	1	1	--	--	1	1	1	--	1
33	1	1	1	1	1	1	1	1	1	1
111	1	--	--	1	1	1	--	1	1	1
112	1	1	1	--	1	--	1	1	1	--
113	1	1	1	--	--	--	1	1	1	--
122	--	1	1	--	1	1	--	--	--	--
123	1	--	--	1	--	1	1	1	1	1
133	1	1	1	--	1	1	--	--	1	1
222	--	1	1	1	1	--	1	1	--	1
223	1	--	--	--	1	1	--	--	1	--
233	--	--	--	--	--	--	--	--	--	--
333	1	1	1	1	1	1	1	1	1	1
1111	1	--	--	--	--	1	1	--	1	--
1112	--	--	--	--	--	--	--	--	--	--
1113	--	1	1	1	1	--	--	1	--	1
1122	1	1	1	1	1	--	1	1	1	1
1123	1	1	1	1	1	--	1	1	1	1
1133	1	1	1	1	1	--	1	1	1	1
1222	--	--	--	--	--	--	--	--	--	--
1223	1	--	--	--	--	1	1	--	1	--
1233	1	--	--	--	--	1	1	--	1	--
1333	1	1	1	1	1	1	1	1	1	1
2222	--	--	--	--	--	--	--	--	--	--
2223	1	1	1	1	1	--	1	1	1	1
2233	--	--	--	--	--	--	--	--	--	--
2333	--	--	--	--	--	--	--	--	--	--
3333	--	--	--	--	--	--	--	--	--	--
Absolute error	6062,9	6243,7	6465,4	6498,4	6791	6918,4	7187	7262,6	8078,7	8138,3
Relative error	0,063	0,065	0,067	0,068	0,071	0,072	0,075	0,076	0,084	0,085
Sum. 4	7	9	9	9	9	11	7	8	7	9
S1	84,905	74,25	71,15	65,305	74,655	64,65	77,255	74,25	81,805	70,1
S2	60,5	50,5	49,5	43,5	51,5	42,5	55,5	50,5	59,5	47,5
SC	145,405	124,75	120,65	108,805	126,155	107,15	132,755	124,75	141,305	117,6

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Rows S1, S2 and SC show the criteria values on the basis of which the PP structural complexity is estimated. In addition, the 4th order PP member's number is taken into account leading to a more complex structure.

The joint structure, which is shown in the 6th column for the accepted formulation, can be considered as an absolute structural-parametric optimum, since, with sufficient accuracy, it has the least structural complexity. It can be noted that PP, shown in the 1–5th columns, have an advantage over PP shown in the 6th column, in terms of the absolute and relative errors. However, PP in the 6th column is simpler than all the other 9 variations of the PP according to the 2 criteria formed in this work (S1, S2) and includes only 4th order members, which joint includes 6 members of the 4th order, as shown in the 4thcolumn.

VI. CONCLUSION

The proposed coding pattern for the polynomial approximation structure provides the unified and efficient approach for the formulation of the universal MM for describing 1-st, 2-nd, and 3-dimensional data fragments. Moreover, the possibility of using the applied algorithm to increase the order for their large values is outside the scope of this research. The proposed MM-s for estimating the PP structural complexity make possible to perform their structural optimizations by applying any discrete methods opening up new possibilities in finding optimal approximations methods. The combined heuristic search for parametric optimization and the combinatorial algorithm for the polynomial structural optimization enable solving the conditional optimization problem of the subject-based criteria. The heuristic polynomial optimization algorithm improves the approximation accuracy, based on the EGA modification, which makes possible to find a suboptimal mathematical description of the high-dimensional fragments for which the use of a combinatorial optimization method is not an effective approach in terms of time costs. However, the plans still have a lot of work to finalize the proposed approach to the approximation of fragments, for example, filtering descriptions of FED regarding their behavior between the FED points.

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