№ 2 (4), 2022 ISSN: 2682 – 9517 (print) ISSN: 2683 – 0930 (online)

INSTITUTE OF INFORMATICS AND INNOVATIVE TECHNOLOGIES

AN HEURISTIC ALGORITHM FOR SEARCHING A GLOBAL OPTIMUM, BASED ON GROUP ANALYSIS

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Abstract. **A new heuristic optimization algorithm with accelerated convergence is proposed for search a global optimum of multy-dimensional, multimodal objective functions. The new optimization algorithm is based on the idea proposed by W. Price for grouping and analyzing cluster of points. In the new method, as in the Price method, the values of the worst result are constantly improving and thus the points begin to condense around the global maximum. A comparative analysis has been made with classic Price method and its effectiveness and accelerated convergence have been demonstrated. The method and proposed algorithm is suitable and efficient for complicated multimodal objective functions and for parameters estimation in mathematical models.**

Keywords: ***global optimum, multimodal objective function, heuristic algorithm, accelerated convergence, cluster analysis***

I. INTRODUCTION

In many optimization problems in engineering research, and especially when estimating parameters in nonlinear mathematical models, it is necessary to search for a global maximum or minimum, since the objective function has more than one optimum. A lot of methods have been proposed for global optimization. Many of them have mathematically proven convergence, but so far, no effective numerical algorithm has been proposed to ensure that the global optimum is found with a reasonable number of iterations. The gradient-free methods are mostly used for global search. The main advantage of them is the wider possible field of study, avoiding false global "optimums", such as saddle points, reduced number of objective function calculations, etc. It is not always known whether the objective function Q(**x**) is unimodal or multimodal in the feasible region of control parameters $\mathbf{x} \in [\mathbf{x}_{\min}, \mathbf{x}_{\max}]$. In such cases, it is necessary to use optimization algorithms which will ensure maximum probability of finding the global maximum or minimum.

Price proposed an algorithm [1] in which are generated M randomly distributed initial points (cluster) in the feasible region of control parameters **x** and the objective function is calculated in each point ($Q_j(\mathbf{x}^{(j)})$, j = 1,2, …, M). The results are analyzed and new points are calculated, which replace these with the worst values of the objective function. The disadvantage of Price's algorithm is the unreasonable mode of choice of the number of points in the sub-cluster groups, with which the search continues after the rejection of the points with the worst results for the objective function. A detailed study of the Price method given in [1, 2, 3, 4] show that Price's algorithm found the largest number of global optimum (22 tasks) of a total of 23 multimodal objective functions in a comparative analysis of 21 methods for global optimum searching, but with a significant average number of 3795 calculations of the objective functions.

The present article proposes a new optimization algorithm that borrows only the idea proposed by Price for grouping and analyzing groups of points. The new proposed method creates groups of point pairs, based on which new points are calculated to replace the worst ones. With the new method presented, as with the Price method, the values of the worst result are constantly improving and thus the points begin to condense around the global maximum.

According to Price's idea, M points are generated randomly in the feasible region $\mathbf{x} \in [\mathbf{x}_{min}, \mathbf{x}_{max}]$ and the objective function Q(**x**) is calculated in each one. Randomly are selected n + 1 points (where n is the number of control parameters) from all M points and after this, randomly is determining the so-called pole point ($\mathbf{x}^{(p)}$), the center of gravity of the remaining n points ($\mathbf{x}^{(c)}$) is calculated and with a help of $\mathbf{x}^{(p)}$ and $\mathbf{x}^{(c)}$, the new point is calculated:

$$x_i^{(N)} = 2x_i^{(c)} - x_i^{(p)}, \ i = 1, 2, \ldots, n \quad (1)$$

Price suggests that the value of the objective function, calculated in $\mathbf{x}_i^{(N)}$, to be compared with the "worst" objective function value of all M points. If the value of $Q^{(N)}$ is better than the value of the objective function at the "worst" point, the point $\mathbf{x}_i^{(N)}$ replaces the "worst" point, otherwise a new midpoint ($\mathbf{x}^{(G)}$) between $\mathbf{x}^{(c)}$ and $\mathbf{x}^{(N)}$ is calculated.

$$x_i^{(G)} = \frac{1}{2}\left(x_i^{(c)} - x_i^{(N)}\right), \ i = 1, 2, \ldots, n \quad (2)$$

The calculated point replaces the "worst" point.

The new method proposes to distribute all M points into three separate groups, based on descending sorting. Two (group of the best points (Group BST) and intermediate group (Group MID) of the groups are used and the third group with the worst results of the objective function is abandoning. The points in the two working groups are grouped in pairs and new points are calculated:

$$x_i^{(N)} = 2x_i^{(Group\ 1)} - X_i^{(Group\ 2)}, \ i = 1, 2, \ldots, n \quad (3)$$

The value of the objective function calculated in $\mathbf{x}_i^{(N)}$ is compared with the objective function at the point in "Group 2". Depending on the value of $Q^{(N)}$, this point is included in the points of the two groups or a new random point is calculated, evenly distributed between $\mathbf{x}^{(Group\ 1)}$ and $\mathbf{x}^{(Group\ 2)}$:

$$x_i^{(N)} = x_i^{(Group\ 2)} + \alpha_i\left(x_i^{(Group\ 1)} - x_i^{(Group\ 2)}\right), \ i = 1, 2, \ldots, n \quad (4)$$

The value of the objective function at the point is calculated and the point is added to the points of the two groups.

All M points are sorted in descending order by objective function, with removing the points in the group of points with the worst values for the objective function. Thus, after each iteration there will be M number of points remaining, after 1/3 of the points with the "worst" results are eliminated.

In Price's algorithm, the parameters of the "best" and "worst" point of all M points and / or the values of the objective functions in them can be used as a stopping criterion. The newly developed algorithm uses the "best" point of Group 1 and the "worst" point of Group 2 and / or the values of the objective functions in them.

Four variants of the new method have been proposed and analyzed, which show an accelerated convergence for finding the global optimum of multimodal objective functions.

II. ALGORITHM OF THE PROPOSED METHOD

1. Setting the required input information: number of control parameters (n); the objective function Q(**x**) and the kind of searching optimum - global maximum or global minimum; the feasible region of control parameters $\mathbf{x} \in [\mathbf{x}_{min}, \mathbf{x}_{max}]$ and the criteria for stopping the search by riches the precision of control parameters ε_X, and / or by objective function ε_Q. An emergency stop criterion is also set according to a given maximum number of calculations of the objective function (for example 30,000 or another sufficiently large value).

2. The total number of points M is set, including the coordinates of all centroid points of all subspaces of the space "n", the point center of gravity of the feasible region and number K evenly distributed points $\mathbf{x}^{(j)}$. The number M is a positive integer number multiple of 3, for example 99, 105, 123 or another larger value.

3. The number of L points in the groups (Group BST, Group WST, Group MID, Group 1 and Group 2) is calculated, L = M / 3.

4. The coordinates of all centroid points of all subspaces of the space "n" are calculated.

5. The values of the objective function in the centroid points from item (4) are calculated.

6. Add the center of the feasible region

$$x_i^{(0)} = \frac{1}{2}\left(x_{max\ i} + x_{min\ i}\right), \ i = 1, 2, \ldots, n \quad (5)$$

7. The value of the objective function at the center of gravity of the feasible region is calculated.

8. The number of points K, supplementing the specified number of points M is calculated.

9. K number random points $\mathbf{x}^{(j)}$ are generated in the feasible region $\mathbf{x} \in [\mathbf{x}_{min}, \mathbf{x}_{max}]$ according to the formula:

$$x_i^{(j)} = x_{min\,i} + \alpha_i^{(j)} (x_{max\,i} - x_{min\,i}), \; i = 1, 2, \ldots, n,$$
$$j = 1, 2, \ldots, K \quad (6)$$

α_i – evenly distributed random numbers within the boundaries [0, +1]

10.The value of the objective function at each of the generated K points is calculated.

11.The values of the objective function of all M points are sorted in descending order.

12.The sorted points are divided into three groups with the same number of points (L) in each group: group of the best points (Group BST), group of the worst points (Group WST) and intermediate group (Group MID).

13.Based on the points sorted in the three groups, two main groups are created: Group 1 and Group 2 by the following two methods:

13.1. The points from Group BST with the best results for the target function form Group 1, and the points from Group WST with the worst results for the target function form Group 2.

13.2. The points of Group BST form Group 1, and the points of the intermediate group Group MID form Group 2.

14.Pairs from the points in Group 1 and Group 2 are formed in one of the following two ways:

14.1. **Method 1:** The first pair is formed by the point with the best result from Group 1 ($\mathbf{x}_1^{(Group\,1)}$) and the point with the worst result from Group 2 ($\mathbf{x}_L^{(Group\,2)}$). The second pair is formed by the points $\mathbf{x}_2^{(Group\,1)}$ and $\mathbf{x}_{L\text{-}1}^{(Group\,2)}$. The last pair will be formed from the point with the worst result from Group 1 ($\mathbf{x}_L^{(Group\,1)}$) and the point with the best result from Group 2 ($\mathbf{x}_1^{(Group\,2)}$).

14.2. **Method 2:** The first pair is formed by the point with the best result from Group 1 ($\mathbf{x}_1^{(Group\,1)}$) and the point with the best result from Group 2 ($\mathbf{x}_1^{(Group\,2)}$). The second pair is formed by the points $\mathbf{x}_2^{(Group\,1)}$ and $\mathbf{x}_2^{(Group\,2)}$. The last pair will be formed from the point with the worst result from Group 1 ($\mathbf{x}_L^{(Group\,1)}$) and the point with the worst result from Group 2 ($\mathbf{x}_L^{(Group\,2)}$).

15.New points are calculated on base of the generated pairs according to the following formula:

$$x_{k,i}^{(N)} = 2x_{j,i}^{(Group\,1)} - x_{j,i}^{(Group\,2)}, \; j = 1, 2, \ldots, L;$$
$$k = 1, 2, \ldots, L; \; i = 1, 2, \ldots, n \quad (7)$$

16.The limits $\mathbf{x} \in [\mathbf{x}_{min}, \mathbf{x}_{max}]$ of the feasible region are checked. If any of the points violates any of the limits, the calculated value in (7) accept the corresponding limit value $\mathbf{x}_{min,i}$ or $\mathbf{x}_{max,i}$ of the feasible region.

17.The objective function at each of the new points is calculated:

$$Q_k^{(N)} = Q\left(x_{i,k}^{(N)}\right), \; k = 1, 2, \ldots, L; \; i = 1, 2, \ldots, n \quad (8)$$

18. If $Q_k^{(N)} \le Q_j^{(Group\,2)}$, the point is omitted and a new point random evenly distributed between the pair $\mathbf{x}_{j,i}^{(Group\,1)}$ and $\mathbf{x}_{j,i}^{(Group\,2)}$ is calculated.

$$x_i^{(N)} = x_i^{(Group\,2)} + \alpha_i \left(x_i^{(Group\,1)} - x_i^{(Group\,2)}\right),$$
$$i = 1, 2, \ldots, N \quad (9)$$

α_i – evenly distributed random numbers within the boundaries [0, +1]

19.The objective function $Q^{(N)}$ at a point $\mathbf{x}^{(N)}$ is calculated. The point is included in all points of Group 1 and Group 2. The algorithm continues from item (21).

20.If the value of objection function, calculated in item (17) is greater than $Q^{(Group\,2)}$ ($Q_k^{(N)} > Q_j^{(Group\,2)}$), the calculated point in item (15) is included in all points of Group 1 and Group 2. The algorithm continues from item (21).

21.The values of the objective function from all M points (points from Group 1, Group 2 and the new calculated points) are sorted in descending order. The sorted points are separated into three groups Group BST, Group MID and Group WST.

22.Points from the Group WST are rejected.

23.The best point and the value of its target function in it from Group BST are saved as the best point ($x_i^{(B)}$ and $Q^{(B)}$). The worst point and the value of its target function in it from Group MID are saved as the worst point ($x_i^{(W)}$ and $Q^{(W)}$).

24.The stopping criteria are checked.

25.If the stopping criteria are satisfied, the search is terminated and the value for the objective function ($Q^{(B)}$) and the parameters of the best point ($x_i^{(B)}$) are displayed / printed. If the stopping criteria are not satisfied, the points from Group BST are stored in Group 1, and the points from Group MID are stored in Group 2. The algorithm continues from an item (14).

As a stopping criteria can be used the criteria regarding to the given accuracy of control variables ε_X , or desired accuracy of objective parameters ε_Q, or combined criteria of both of them, as well according to the criterion for emergency stopping the algorithm by the set in item (1) the maximum number of calculations of the objective function [2, 3, 4].

Based on the algorithm presented above, four variants of the new method were created, named as follows M 1, M 2, M 3 and M 4:

M 1 - For the creation of the two groups Group 1 and Group 2, an item 13.1 is used, and the formation of the separate pairs is carried out according to item 14.1.

M 2 - For the creation of the two groups Group 1 and Group 2, an item 13.2 is used, and the formation of the separate pairs is carried out according to item 14.1.

M 3 - For the creation of the two groups Group 1 and Group 2 an item 13.1 is used, and the formation of the separate pairs is carried out according to item 14.2.

M 4 - For the creation of the two groups Group 1 and Group 2 an item 13.2 is used, and the formation of the separate pairs is carried out according to item 14.2.

III. Analysis of the Results of the Studied Target Functions

(a) Study with a test objective function

$f(x_1,x_2)=x_1x_2.\sin x_1.\sin x_2$, $6,00 \le x_i \le 16,00$, i = 1, 2

The global maximum of the test function is:
$F_{max}(x_1^*, x_2^*)$ = 200,856; x_1^* = 14,2074 and
x_2^* = 14,2074
The results are shown in Table 1.

(b) Study with a test objective function

$$f(x_1,x_2)=\prod_{i=1}^{2}\sqrt{x_i}\sin x_i,\ 3,00 \le x_i \le 10,00,\ i = 1, 2$$

The global maximum of the test function is:
$F_{max}(x_1^*, x_2^*)$ = 7,8856; x_1^* = 7,91705 and
x_2^* = 7,91705
The results are shown in Table 2.

(c) Study with a test objective function

$$f(x_1,x_2)=-\sum_{i=1}^{2}\sin x_1\left(\sin\left(\frac{ix_i^2}{\pi}\right)\right)^{2m},\ 0,00 \le x_i \le 3,00,$$

i = 1, 2 = 1

The global minimum of the test function is:
$F_{min}(x_1^*, x_2^*)$ = -1,84093; x_1^* = 2,07169 and x_2^* = 1,570796
The results are shown in Table 3.

(d) Study with a test objective function

$$f(x_1,x_2)=\prod_{i=1}^{2}\sum_{j=1}^{5}\mathrm{j}\cos\left((\mathrm{j}+1)x_i+1\right),\ -5,12 \le x_i \le 5,12,$$

i = 1, 2

The global maximum of the test function is:
$F_{max}(x_1^*, x_2^*)$ = 210,4823 при x_1^* = -0,199679 and x_2^* = -0,199679
The results are shown in Table 4.

(e) Study with a test objective function

$$f(x_1,x_2)=\sum_{i=1}^{2}\sum_{j=1}^{5}\mathrm{j}\cos\left((\mathrm{j}+1)x_i+1\right),\ -3 \le x_i \le 2,\ i = 1, 2$$

The global maximum of the test function is:
$F_{max}(x_1^*, x_2^*)$ = 29,016 при x_1^* = -0,19968 and x_2^* = -0,19968

(f) Study with a test objective function

$$f(x_1,x_2)=\prod_{i=1}^{2}\sum_{j=1}^{5}\mathrm{j}\cos\left((\mathrm{j}+1)x_i+\mathrm{j}\right),$$

$-5,12 \le x_i \le 5,12$, i = 1, 2

The function is studied with the new methods in search of a global minimum. The function has four equivalent global minima: $F_{min}(x_1^*, x_2^*)$ = -186,73091.
The coordinates of the global equivalent minima are given in Table 6 and in Fig. 6 is presented the type of the function within the studied limits.

TABLE I. RESULTS FOR TEST FUNCTION (a)

ε_x	Accu-racy	Price		M 1		M 2		M 3		M 4	
		Q(X)	S	Q(X)	S	Q(X)	S	Q(X)	S	Q(X)	S
0,1	1	200,8387060	2379	200,853599	1176	200,8533312	1025	200,8362757	1055	200,8414252	950
0,01	2	200,8561735	3733	200,856071	1576	200,8561345	1539	200,8559677	1381	200,8556828	1276
0,001	3	200,8561837	4761	200,856185	1973	200,8561873	1862	200,8561879	1808	200,8561878	1691
0,0001	4	200,8561880	5820	200,856188	2414	200,8561880	2319	200,8561880	2227	200,8561880	2055
0,00001	5	200,8561880	6720	200,856188	2808	200,8561880	2711	200,8561880	2544	200,8561880	2435

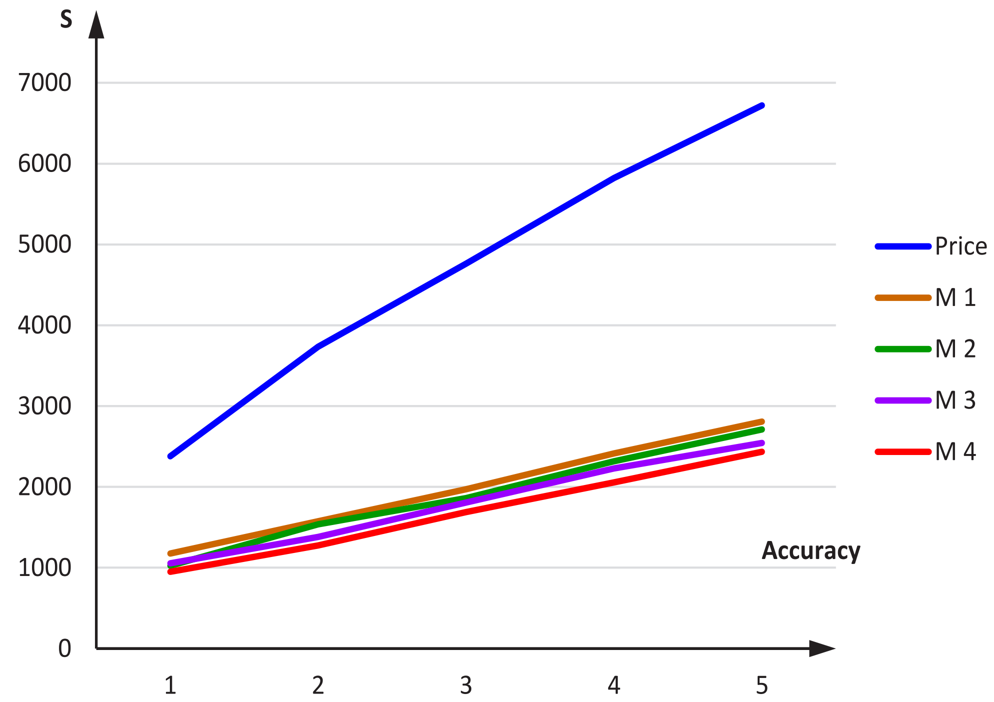

Fig. 1. Number of calculations (S) of the objective function (a) using accelerated global optimum search methods

TABLE II. RESULTS FOR TEST FUNCTION (b)

ε_x	Accu-racy	Price		M 1		M 2		M 3		M 4	
		Q(X)	S	Q(X)	S	Q(X)	S	Q(X)	S	Q(X)	S
0,1	1	7,8842788	2083	7,885481740	1175	7,885561123	945	7,884900684	1016	7,885392938	934
0,01	2	7,8855952	3071	7,885599927	1626	7,885599700	1401	7,885597817	1392	7,885600203	1307
0,001	3	7,8856006	4202	7,885600722	2037	7,885600700	1785	7,885600697	1698	7,885600721	1691
0,0001	4	7,8856007	5311	7,885600724	2467	7,885600724	2236	7,885600724	2075	7,885600724	2065
0,00001	5	7,8856007	6388	7,885600724	2858	7,885600724	2637	7,885600724	2460	7,885600724	2375

ISSN: 2682 – 9517 (print) ISSN: 2683 – 0930 (online)

TABLE III. RESULTS FOR TEST FUNCTION (c)

ε_x	Accu-racy	Price		M 1		M 2		M 3		M 4	
		Q(X)	S	Q(X)	S	Q(X)	Q(X)	S	Q(X)	S	Q(X)
0,1	1	-1,840577911	1327	-1,840683846	598	-1,840058908	679	-1,840897193	631	-1,840881505	585
0,01	2	-1,840923949	2329	-1,840929090	1052	-1,840928356	1081	-1,840929129	1054	-1,840929699	950
0,001	3	-1,840929770	3470	-1,840929761	1495	-1,840929829	1535	-1,840929807	1431	-1,840929823	1369
0,0001	4	-1,840929835	4638	-1,840929834	1884	-1,840929835	1862	-1,840929835	1805	-1,840929835	1697
0,00001	5	-1,840929835	5736	-1,840929835	2343	-1,840929835	2290	-1,840929835	2116	-1,840929835	1975

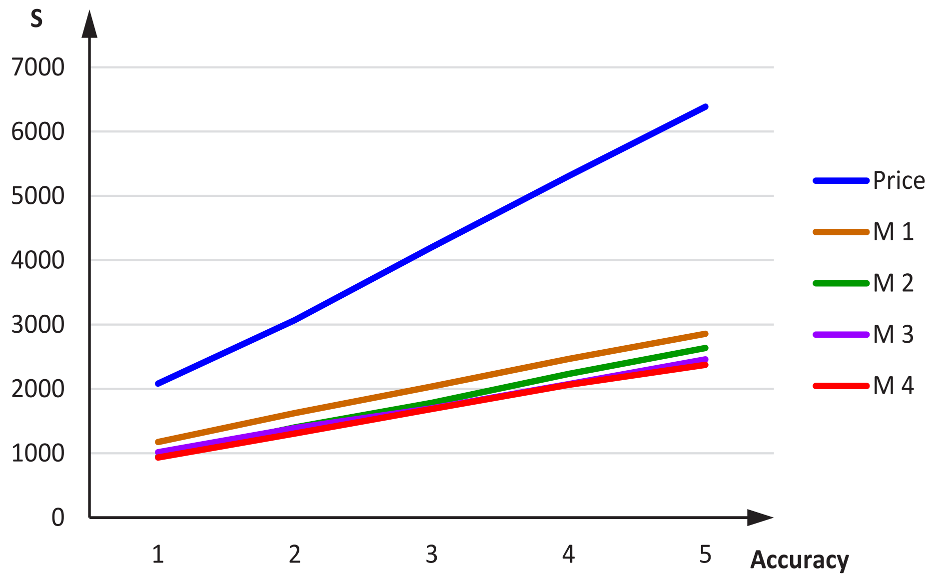

Fig. 2. Number of calculations (S) of the objective function (b) using accelerated global optimum search methods

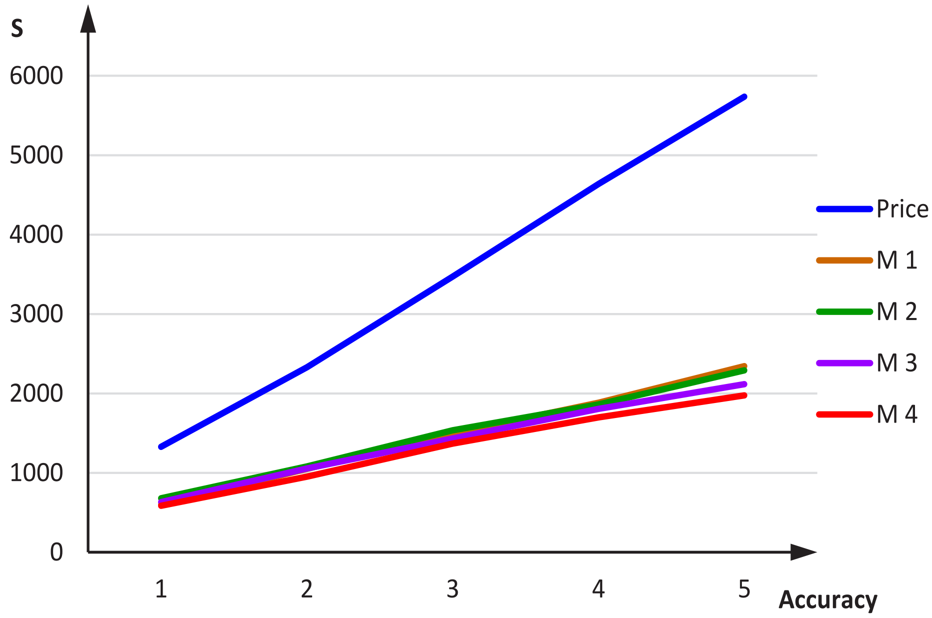

Fig. 3. Number of calculations (S) of the objective function (c) using accelerated global optimum search methods

TABLE IV. RESULTS FOR TEST FUNCTION (d)

εx	Accu-racy	Price		M 1		M 2		M 3		M 4	
		Q(X)	S	Q(X)	S	Q(X)	Q(X)	S	Q(X)	S	Q(X)
0,1	1	210,458697518	3014	210,280988753	1950	210,295171047	1629	210,396190837	1751	210,346325932	1720
0,01	2	210,472920323	4204	210,477601527	2399	210,476745123	2022	210,481202308	2074	210,481547958	2099
0,001	3	210,482271538	5378	210,482285522	2791	210,482283777	2466	210,482285828	2511	210,482290739	2475
0,0001	4	210,482293677	6462	210,482293862	3236	210,482293810	2921	210,482294013	2825	210,482293811	2827
0,00001	5	210,482294014	7594	210,482294012	3645	210,482294012	3318	210,482294015	3204	210,482294013	3135

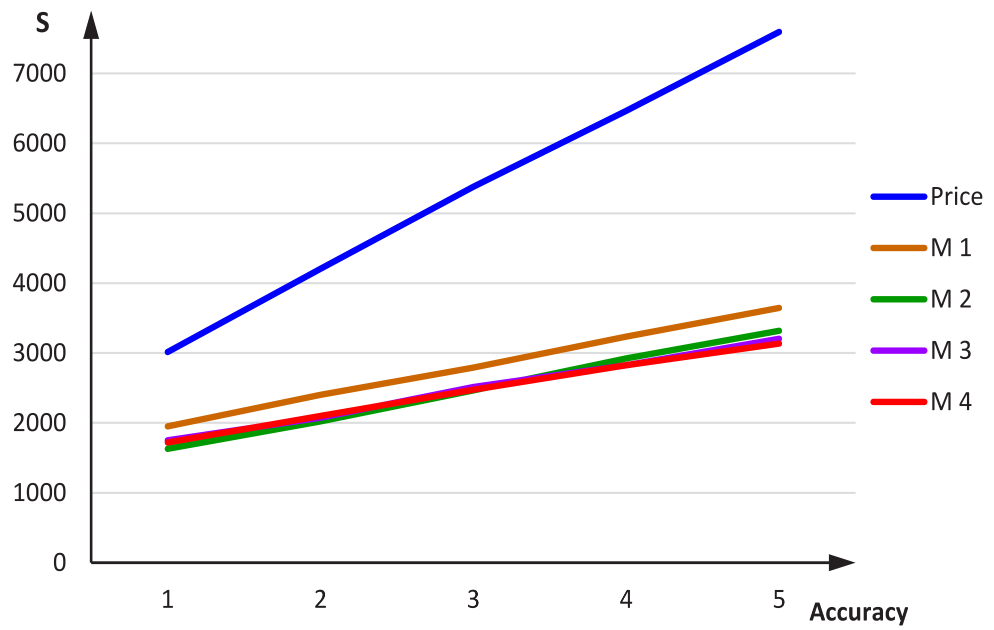

Fig. 4. Number of calculations (S) of the objective function (d) using accelerated global optimum search methods

TABLE V. RESULTS FOR TEST FUNCTION (e)

εx	Accu-racy	Price		M 1		M 2		M 3		M 4	
		Q(X)	S	Q(X)	S	Q(X)	Q(X)	S	Q(X)	S	Q(X)
0,1	1	28,996138678	2123	28,954682680	1379	29,008956454	1254	29,010304973	1294	29,012491880	1174
0,01	2	29,015781332	3160	29,016015799	1823	29,015999456	1699	29,015945867	1599	29,015848340	1541
0,001	3	29,016014966	4287	29,016015799	2151	29,016015223	2101	29,016015724	1967	29,016014505	1861
0,0001	4	29,016015846	5468	29,016015841	2604	29,016015839	2489	29,016015849	2331	29,016015849	2232
0,00001	5	29,016015854	6541	29,016015854	2980	29,016015854	2900	29,016015854	2596	29,016015854	2611

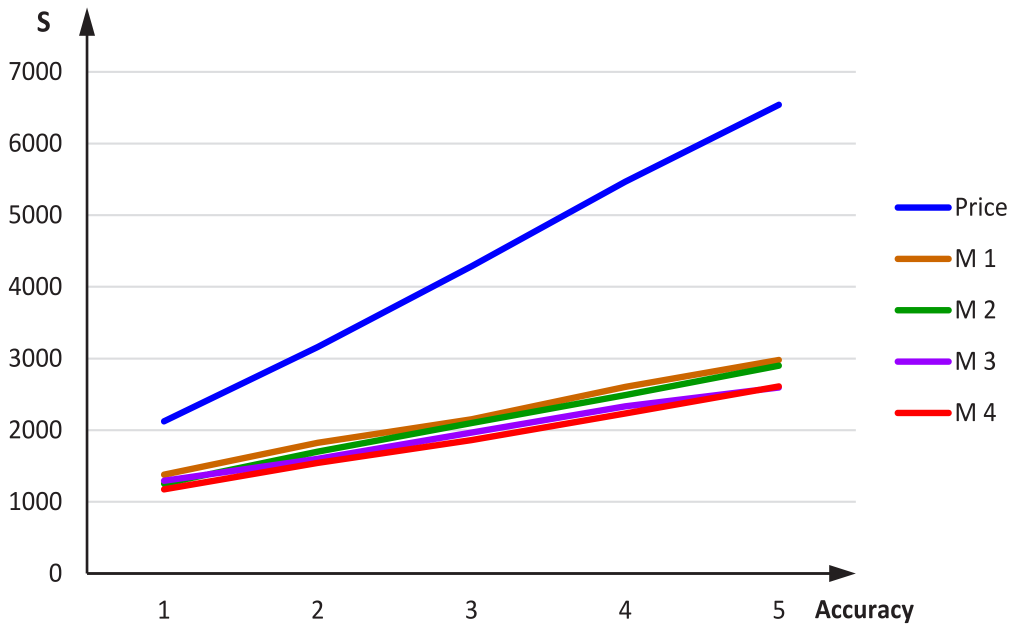

Fig. 5. Number of calculations (S) of the objective function (e) using accelerated global optimum search methods

TABLE VI. THE COORDINATES OF THE FOUR EQUIVALENT GLOBAL MINIMA

№	x_1^*	x_2^*	$F_{min}(x_1^*, x_2^*)$
1.	-0,80032	4,85806	-186,73091
2.	4,85806	-0,80032	-186,73091
3.	-1,42513	-0,80032	-186,73091
4.	-0,80032	-1,42513	-186,73091

In the present study, one of the global minima (№ 3 from TABLE VI) has been founded by the compared methods.

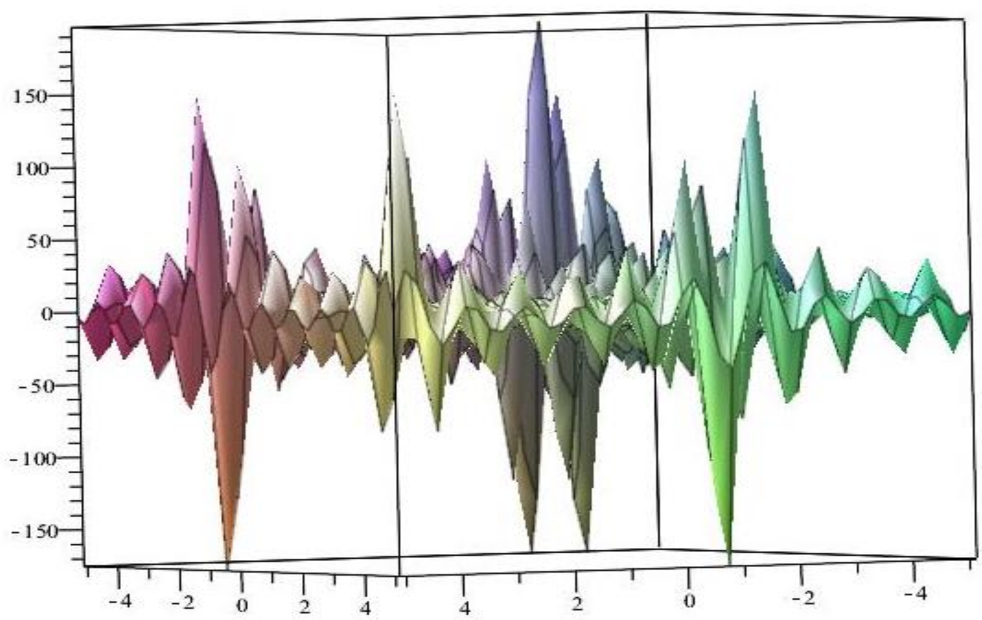

Fig. 6. Schubert function within the feasible region $-5,12 \leq x_i \leq 5,12$; $i = 1, 2$.

TABLE VII. RESULTS FOR TEST FUNCTION (f)

εx	Accu-racy	Price		M 1		M 2		M 3		M 4	
		Q(X)	S	Q(X)	S	Q(X)	Q(X)	S	Q(X)	S	Q(X)
0,1	1	-186,586839	4424	-186,6620457	2201	-186,1285432	1826	-186,5307784	1722	-186,1301904	1561
0,01	2	-186,724532	6783	-186,7308967	2601	-186,7297277	2226	-186,7304766	2105	-186,7251743	2082
0,001	3	-186,730901	8907	-186,7308967	2999	-186,7308647	2617	-186,7309021	2513	-186,7309034	2519
0,0001	4	-186,730908	11019	-186,7309085	3445	-186,7309085	3015	-186,7309087	2837	-186,7309085	2934
0,00001	5	-186,730908	14005	-186,7309089	3839	-186,7309088	3513	-186,7309088	3225	-186,7309088	3303

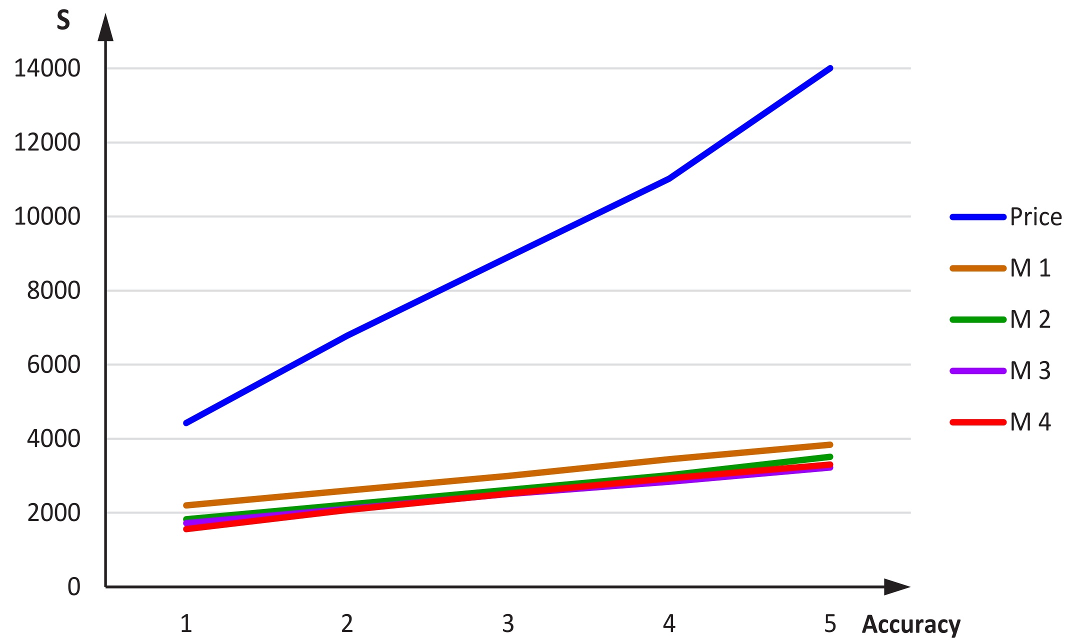

Fig. 7. Number of calculations (S) of the objective function (f) using accelerated global optimum search methods

From the performed comparative analysis and from the obtained results for the effectiveness of the proposed new method for searching the global optimum, tested with representative complex multi-modal test functions, confirm the faster convergence of the proposed four variants of the new method. The algorithms M 3 and M 4 showed the highest accelerated convergence in all test multimodal functions in comparison with M 1 and M 2. The proposed four variants of the new method significantly exceed the rate of convergence, expressed by the number of calculations of the objective function for finding the solution in comparison with Price's method.

The studies show that the proposed way of forming the pairs in the algorithm has a strong influence on the rate of convergence. The convergence rate is better when using the group of points with the best results for the values of the objective function (Group BST) and the group of points with intermediate results (Group MID) compared to the results obtained using the group BST and the group from points with the worst results (Group WST).

IV. CONCLUSION

(1) A new method with accelerated convergence in the search for a global optimum has been proposed. Four variants for realization of the new method are offered, based on cluster analysis of groups of points generated in the feasible region of the control variables.

(2) The comparative analysis of the proposed method and the four variants of the new algorithm using six test multimodal objective functions, show that the new method has a

significantly faster convergence, comparing with the method proposed by Price.

(3) The variants M 3 and M 4 of the proposed algorithm show the fastest convergence to the solution.

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