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THE PROBLEM OF HIGHLY ACCURATE DETETMINATION OF GLOBAL MINIMA OF SMOOTH FUNCTIONS OF SEVERAL VARIABLES

ABSTRACT

of the thesis for the degree of Doctor of Philosophy (PhD) in the specialty 6D060100 – Mathematics

Structure and scope of the thesis. The thesis consists of an introduction, 3 chapters (the first chapter consists of 7 sections, the second chapter consists of 3 sections, the third chapter consists of 4 sections), conclusion and list of references.

he number of illustrations, tables and references. The work used 7 tables, 15 illustrations and 142 sources.

Keywords. Auxiliary function, global extremum, global minimum, deterministic methods, global optimization methods, multiextremal optimization, properties of the auxiliary function, multidimensional optimization.

The actuality of the dissertation is due to the recent increased need for solving global optimization problems in various fields of science, technology, economics, the lack of universal methods of global optimization, as well as the rapid development of computer technology. The problem of global optimization is one of the most important problems in applied and computational mathematics today. Today, a lot is known and published about methods and problems of global optimization. However, global optimization problems constantly arise in various fields of science in connection with the solution and study of various practical problems. Since there are no universal algorithms, there is a constant need to create new methods.

Currently, all known global optimization methods can be divided into two categories: deterministic methods and stochastic methods. Deterministic optimization methods are a group of methods that theoretically guarantee that the resulting global minimum value is indeed the best result. The dissertation examines a deterministic method.

There are many difficulties in calculating the global minimum of a function. The main difficulties arise due to the fact that the target function is multi-extremal, multi-dimensional, non-convex and that existing methods do not provide precise guarantees about the approach to the global minimum. Many scientists are working on these difficulties.

The thesis examines an effective and economical method for searching for the global minimum of the multidimensional function F(x). To solve this problem, a new special function was built and called the “auxiliary function”. An algorithm based on the idea of an “auxiliary function” is constructed.

The main object of study is not the target function F(x) itself, but an auxiliary function with one variable, created by transforming the original target function using a multiple integral:

$$g_m(F,\alpha) = \int_E [|F(x) - \alpha| - F(x) + \alpha]^m dx,\ \ m \in N, m > 1, \qquad (0.1)$$

where: $F(x)$ is the objective function, $E \subset R^n$ is the admissible set of the objective function. Function (0.1) contains a multiple integral, which depends on the number of variables of the auxiliary function. To calculate the multiple integral by numerical methods, the cubic formulas of S.L. Sobolev[1] with a limited boundary layer were used. M. D. Ramazanov[2] assessed the accuracy of Sobolev cubic formulas for continuous functions and created an integration algorithm over a domain of arbitrary shape using Sobolev lattice cubic formulas.

To calculate the approximate value of the integral

$$I(\varphi) = \int_{\Omega} \varphi(x)dx$$

function $\varphi(x)$, defined in the set Ω, depending on n real variables, cubature formulas by S.L. Sobolev "with a constant boundary layer". In this case, the approximate value of the integral $I(\varphi)$ is defined as a linear combination of the values of the function $\varphi(x)$ at points $x^{(1)}, x^{(2)}, \dots, x^{(N)}$:

$$K_N\big(\varphi(x)\big) = h^n \sum_{s=1}^{N} C_s \varphi\big(x^{(s)}\big),$$

where N is the number of intervals dividing the integration domain for each component of the vector x. Here: $x^{(s)}$ are the nodes of the Sobolev cubature formula. C_s – boundary layer coefficients.

The main problem is to find the coefficients $\{C_s\}$ so that the integral $I(\varphi)$ quickly approaches the value $K_N(\varphi(x))$ as N tends to infinity.

Using the found coefficients, the cubature formula can be rewritten as follows:

$$\int_\Omega \varphi(x)dx \approx h^n \sum_{s=1}^{N} C_s \varphi(x^{(s)}), N = 1,2, \dots . \qquad (0.2)$$

Here h^n is a scaling factor that determines the size of the unit cell.

1. Соболев С.Л. Васкевич В.Л. Кубатурные формулы. Новосибирск: Математический университет Соболева, 1996. – 484 с.

2. Рамазанов М. Д. Теория решетчатых кубатурных формул с ограниченным пограничным слоем. – Уфа: ДизайнПолиграфСервис, 2009. – 178 с.

Formula (0.2) is the main tool for calculating the values of the integral auxiliary function $g_m(F,\alpha)$ with high accuracy. If in this cubature formula instead of $\varphi(x)$ we take the integrand expression of the function $g_m(F,\alpha)$, then we obtain:

$$g_m(F,\alpha) = \int_Q [|F(x) - \alpha| - (F(x) - \alpha)]^m dx \approx$$

$$\approx h^n \sum_{s=1}^{N} C_s \, [|F(h \cdot s) - \alpha| - (F(h \cdot s) - \alpha)]^m.$$

The new method discussed in the dissertation work is implemented using the theory of cubic formulas developed by S.L. Sobolev, M.D. Ramazanov and other scientists.

During the study, the corresponding properties of the auxiliary function (0.1) were determined and proven: uniform continuity, differentiability, strict convexity, monotonicity, non-negativity.

Theorem 0.1. *The auxiliary function* $g_m\left(F,\alpha\right)$, $m \in N$, $m > 1$, *is uniformly continuous on any bounded interval* $[\alpha_0, \alpha_0 + h)$, $\alpha_0 \geq \hat{\alpha}$, $h > 0$.

To prove the theorem, the values α_1 and α_2 were taken from the interval $(\alpha_0, \alpha_0 + h)$ and the modulus of the difference of the auxiliary functions in these values was studied.

Theorem 0.2. *The auxiliary function* $g_m(F,\alpha)$ *is differentiable at each point* α, $\alpha > \hat{\alpha}$, *where* $\hat{\alpha} = min_E F(x)$.

To prove the theorem, the increment of the auxiliary function was considered. The order of differentiation of the auxiliary function depends on the exponent m. m – affects the smoothness of the auxiliary function.

Corollary 0.1. *For any* $m \in N$, $m > 1$*derivative of the* m *- th order auxiliary function*

$$\frac{d^m g_m}{d\alpha^m} = (2)^m m! \, \mu(E(F,\alpha)).$$

Convexity is an important property of a function in optimization theory. The theory of convex optimization is well studied. Therefore, reducing a multiextremal function to a convex function means that a solution to the problem can be found.

Theorem 0.3. *The function* $g_m\left(F,\alpha\right)$, $\in N, m > 1$, *is strictly convex in the interval* $\alpha \geq \alpha_0$, *where* $\alpha_0 > \hat{\alpha}$.

To prove the theorem:

$$g_m\left(F, \frac{\alpha_1 + \alpha_2}{2}\right) < \frac{1}{2}\left(g_m(F,\alpha_1) + g_m(F,\alpha_2)\right)$$

it is necessary to prove the correctness of the inequality. The left side of the inequality was revealed by the definition of the auxiliary function and proved using Cauchy's inequality.

The following two theorems about the order of modification of the auxiliary function also provide important information:

Theorem 0.4. *The function* $g_m(F,\alpha)$ *increases by* $(\hat{\alpha},+\infty)$.

Theorem 0.5. *Let* $r > s,\ r,s \in N, r > 1,\ \ s > 1$. *Then*

1) if $\alpha-\hat{\alpha} \leq 0$, *then* $g_r(F,\alpha)=0$ *and* $g_s(F,\alpha)=0$;

2) if $0 < \alpha-\hat{\alpha} \leq \hat{\alpha}+\frac{1}{2}$, *then* $g_r(F,\alpha) \leq g_s(F,\alpha)$.

Regardless of the number of local minima of the objective function, the number of variables, the resulting auxiliary function depends only on one parameter α and it is uniformly continuous, has derivatives, is convex, non-negative and monotonically increasing.

Necessary and sufficiently optimal conditions for the global minimum of a multidimensional multiextremal function are derived and proven. The obtained conditions led to the transition from the search for the global minimum of the objective function to the problem of searching for the "largest zero" of the auxiliary function.

Theorem 0.6. If $glob\ min_E F = \hat{\alpha}$, then

$$g_m(F,\hat{\alpha}) = 0. \tag{0.3}$$

Corollary 0.2. *The global minimum of the objective function* F *is the zero of the auxiliary function* $g_m(F,\alpha)$.

Theorem 0.7. If $max_\alpha\{\alpha \in \mathbb{R}: g_m(F,\alpha)=0\} = \hat{\alpha}$, then it is sufficient that $glob\ min_E F = \hat{\alpha}$.

Corollary 0.3. The required zero $\hat{\alpha}$ of the auxiliary function $g_m(F,\alpha)$ is the exact value of the global minimum of the objective function F.

The main result of the thesis is that the desired global minimum value of a given continuous multidimensional function is equal to the "largest zero" of the auxiliary function proved in Theorems 0.6, 0.7.

The task now is to determine the "largest zero" of the auxiliary function. In the thesis, the "largest zero" of the function $g_m(F,\alpha)$ was considered by adapting various numerical methods: dichotomy, golden section, gradient descent, tangent method, modified chord method. The research examined the speeds of numerical methods and carried out computational experiments. At this stage of research, symmetric methods are more economical.

The main advantage of the method is that it reduces the problem of finding the global minimum of a multidimensional and multiextremal objective function to determining the largest zero of a one-dimensional uniformly continuous, convex function. Its meaning is that the maximum value of the argument at which the auxiliary function and its derivatives are equal to zero is equal to the global minimum of the target function.

The thesis defines and proves the main properties of the auxiliary function $g_m\left(F,\alpha\right)$, creates an algorithm for calculating the global minimum, and calculates the global minima of multimodal functions with several variables in the C++ programming environment.

Practical and theoretical significance of the results obtained. The results obtained in the dissertation are theoretical and practical in nature: the creation of a new method using an auxiliary function for finding the global minimum of a multidimensional continuous objective function; proof of convergence of the proposed method; studying the important properties of the auxiliary function (non-negativity, strict convexity, monotonicity, uniform continuity, differentiability, etc.); obtaining the necessary and sufficient condition for the global minimum of a multidimensional multiextremal objective function. In addition, it is used as a tool for solving inverse problems, solving systems of differential equations, etc.

It is possible that the proposed method and algorithm will make a positive contribution to expanding the scope as an important application to optimization theory and numerical methods. The results of the dissertation work can contribute to the further development of this theory and can be used to develop elective courses for students, master's and doctoral students in physics and mathematics, engineering, computer technology and software, etc.

The aim of the thesis research. Develop a new effective method for finding the global minimum of a continuous multiextremal and multidimensional function with high accuracy.

The research problems:

a) creation of a global optimization method using a new “auxiliary function” to find the global minimum of a continuous objective function of many variables and proof of its convergence;

b) study the important properties of the “auxiliary function” (non-negativity, strict convexity, monotonicity, uniform continuity, differentiability, etc.);

c) obtaining necessary and sufficient conditions for the global minimum of the objective function;

d) study of changes in the behavior of an auxiliary function in relation to its degree;

e) calculation of global minima of multidimensional multiextremal objective functions in the C++ programming environment using the proposed new method;

f) application of known numerical methods to calculate the largest zero of the auxiliary function, comparative analysis of the optimality of their application.

The research methods. The dissertation work applies the basic principles of the theory of multidimensional mathematical analysis, Sobolev’s cubature formulas “with a constant boundary layer”; Numerical methods were used to determine the roots of transcendental equations and find the minimum of a convex function.

The objects of research are a continuous objective function; an auxiliary function of one variable, expressed as a multiple integral, obtained by transforming the objective function; a method built on the basis of an auxiliary function.

The scientific novelties:

a) a global optimization method was created using a new “auxiliary function” to find the global minimum of a continuous objective function of many variables and its convergence was proven;

b) a special algorithm for searching the coordinates of the global minimum was created;

c) the number of iterations required to find the global minimum using the constructed method is determined with a predetermined accuracy;

d) to calculate the value of the “auxiliary function”, Sobolev’s cubature formulas with a constant boundary layer and the calculation of their boundary coefficients were used;

e) important properties of the “auxiliary function” (non-negativity, strict convexity, uniform continuity, differentiability, etc.) have been studied and proven;

f) necessary and sufficient conditions for the global minimum of the objective function are determined and proven;

g) existing numerical methods for finding the largest zero of the auxiliary function were investigated and a comparative analysis was made of them from the point of view of optimality;

h) the dependence of changes in the behavior of the auxiliary function in relation to the indicator of its degree was studied.

The results of the thesis which are taken out on defense:

a) a new global optimization method for finding the global minimum of a continuous function of many variables and proof of its convergence;

b) an algorithm for determining the coordinates of the global minimum of a multidimensional continuous objective function;

c) calculating the values of auxiliary functions using the Sobolev cubature formulas with a constant boundary layer;

d) important properties of the “auxiliary function” (non-negativity, strict convexity, monotonicity, uniform continuity, differentiability, etc.);

e) a necessary condition for the global minimum of a continuous multivariable function;

f) necessary and sufficient conditions for the global minimum of a continuous multivariable function;

h) special test functions, solved on the basis of a new method, created to search for global minima of continuous functions of many variables in the C++ programming environment.

The personal contribution of the author. All results presented in the dissertation belong to the author himself. Co-authors and scientific consultants contributed to the formulation of the problem and discussion of the results.

Approbation of the received results. The main results of the work were presented and discussed at the following scientific events:

- traditional April international scientific conference, Institute of Mathematics and Mathematical Modeling of the Ministry of Education of the Republic of Kazakhstan (Almaty, Kazakhstan, April 5-8, 2021);

- IX International Scientific Conference “Differential Equations, Analysis and Problems of Algebra”, Aktobe Regional University named after. K. Zhubanova (Aktobe, Kazakhstan, May 24-28, 2022);

- traditional April international scientific conference, Institute of Mathematics and Mathematical Modeling of the Ministry of Education of the Republic of Kazakhstan (Almaty, Kazakhstan, April 4-8, 2022);

- scientific seminar “Qualitative and approximate methods for studying differential equations”, Institute of Mathematics and Mathematical Modeling of the Ministry of Education, Culture and Sports of the Republic of Kazakhstan, Almaty, Kazakhstan (seminar leader - Ph.D., Professor A.T. Asanova);

- scientific seminar “Modern problems of mathematics”, Department of Mathematics and Informatics, branch of Moscow State University named after M.V. Lomonosov in Kazakhstan, Astana, Kazakhstan (seminar leaders - Ph.D., Professor Nursultanov E.D., Associate Professor Bekmagabetov K.A.);

- “Mathematical problems of natural science. City scientific seminar “Inverse and incorrect calculations”, Al-Farabi State University, Almaty, Kazakhstan (seminar leaders - Professor of Abai KazNPU, Ph.D., Bektemesov M.A., Professor of MIIT, Ph.D. Rysbayuly B., Dean of the Faculty of Mechanics and Mathematics, Ph.D., Ph.D. Zhakebaev);

- scientific seminar “Problems of applied mathematics and computer science”, Department of Mathematics, Aktobe Regional University named after K. Zhubanov, Aktobe, Kazakhstan (seminar leader – Ph.D., Professor Sartabanov Zh.);

- scientific seminar “Seminar on computational mathematics and related issues”, Ufa, Russian Federation, 2024. (Seminar leader – Doctor of Physical and Mathematical Sciences, Professor Ya. Sh. Ilyasov);

- International Eurasian scientific conference “Inverse and ill-posed problems in natural science and artificial intelligence” (Almaty, Kazakhstan, April 17-20, 2024).

Publications. On the topic of the dissertation, 10 articles were published, including 2 publication in a ranking scientific journal indexed in the Scopus database, 4 publication in scientific journal included in the list recommended by the Committee for Quality Assurance in the Field of Science and Higher Education of the Ministry of Science and Higher Education of the Republic of Kazakhstan for publication of the main scientific results of scientific activities, 4 publications in the materials of the international scientific conferences.