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APPLICATION OF THE METHOD OF DIVIDING A SEGMENT IN HALF IN GLOBAL OPTIMIZATION BASED ON AN AUXILIARY FUNCTION

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Abstract

In this paper, the problem of global optimization of a smooth function of several variables given on a cuboid is considered. The search for a solution is carried out using an auxiliary function obtained by a special transformation of the objective function. An auxiliary function is a function of one variable, the zero of which coincides with the value of the global minimum of the objective function. Therefore, to solve the problem, the method of dividing the segment in half was used. The results of this work were revealed on the basis of a large number of computational experiments conducted on test functions using the proposed method. These results are formulated in the form of three theorems and theoretically proved. In the first theorem, conditions are defined that indicate the interval in which the value of the global minimum is located. The second theorem expresses the convergence of the iterative sequence to the value of the global minimum. In the third theorem, the linear convergence rate of the iterative procedure is established. As an example, the multiextremal Eckley function of two variables defined in a square centered at the origin is considered.

Keywords: global optimization, optimization methods, global optimization algorithms, global search, horizontal cross-section method, convergence of the global optimization method, auxiliary function.

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КӨМЕКШІ ФУНКЦИЯ НЕГІЗІНДЕ ГЛОБАЛЬДЫ ОҢТАЙЛАНДЫРУҒА КЕСІНДІНІ ҚАҚ БӨЛУ ӘДІСІН ҚОЛДАНУ

Бұл жұмыс кубоидта берілген бірнеше айнымалысы бар тегіс функцияның глобальды оңтайландыру есебін қарастырады. Шешімді іздеу берілген мақсатты функцияны арнайы түрлендіру арқылы алынған көмекші функцияны қолданумен жүзеге асады. Көмекші функция бір айнымалыға тәуелді. Оның нөлі мақсатты функцияның глобальды минимумының мәніне сәйкес келеді. Минимумды табу үшін кесіндіні қақ бөлу әдісін қолданылды. Есептеу тәжірибелері әдістің дұрыстығын көрсетті. Әр түрлі тесттік функциялардың глобальды минимумы анықталды. Бұл нәтижелер үш теорема түрінде тұжырымдалған және теориялықтұрғыдан дәлелденген. Бірінші теорема глобальды минимумның мәні жатқан аралықты көрсететің шарттарды анықтайды. Екінші теорема итерациялық тізбектің глобальды минимум мәніне жинақталатының көрсетеді. Үшінші теоремада итерациялық үрдістің жинақтылығының сызықтық жылдамдығы есептелді. Мысал ретінде екі айнымалыдан тәуелді көп экстремалды квадратта анықталған функция қаралды.

Түйін сөздер: глобальды оңтайландыру, оңтайландыру әдістері, глобальды оңтайландыру алгоритмдері, глобальды минимумды іздеу, көлденең қима әдісі, глобальды оңтайландыру әдісінің жинақтылығы, көмекші функция.

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ПРИМЕНЕНИЕ МЕТОДА ДЕЛЕНИЯ ОТРЕЗКА ПОПОЛАМ В ГЛОБАЛЬНОЙ ОПТИМИЗАЦИИ НА ОСНОВЕ ВСПОМОГАТЕЛЬНОЙ ФУНКЦИИ

Аннотация

В работе рассматривается задача глобальной оптимизации гладкой функции нескольких переменных, заданной на кубоиде. Поиск решения осуществляется с помощью вспомогательной функции, полученной путем особого преобразования целевой функции. Вспомогательная функция является функцией одной переменной, ноль которой совпадает со значением глобального минимума целевой функции. Поэтому для решения поставленной задачи применялся метод деления отрезка пополам. Результаты настоящей работы были выявлены на основе большого числа вычислительных экспериментов, проведенных на тестовых функциях с помощью предложенного метода. Эти результаты сформулированы в виде трех теорем и теоретически доказаны. В первой теореме определены условия, которые указывают на промежуток в котором находится значение глобального минимума. Вторая теорема выражает сходимость итерационной последовательности к значению глобального минимума. В третьей теореме установлена линейная скорость сходимости итерационной процедуры. В качестве примера рассмотрена многоэкстремальная функция Экли двух переменных, определенная в квадрате с центром в начале координат.

Ключевые слова: глобальная оптимизация, методы оптимизации, алгоритмы глобальной оптимизации, глобальный поиск, метод горизонтальных сечении, сходимость метода глобальной оптимизации, вспомогательная функция.

Materials and methods

The convergence of the global optimization method for multidimensional and multiextremal smooth functions is considered in the article. Gradient optimization methods require gradient calculation and in the case of minimum search, the starting point moves along the anti-gradient. Such actions lead us to a stationary point, not to a global minimum. The gradient cannot overcome the maximum point. The search for the global minimum by the gradient method is carried out by selecting a set of starting points and performing the above actions. But this will not guarantee that the found point is a global minimum. Since the global minimum may be in a narrow range. In the iteration method, the allowable set is divided into a grid. The value of the objective function is calculated at the nodes. The point where the objective function takes the minimum value will be defined as the global minimum. This algorithm is suitable if the grid step is very small. But reducing the step increases the number of calculations of the objective function and you have to remember a lot of values. Computational costs increase significantly if the dimension of the objective function increases.

In recent years, new improved versions of the methods described above have appeared. Zero-order optimization methods use information only about the function itself. For example, the method of simulated annealing [1, 2], randomized descent [3], evolutionary method [4], genetic algorithm [5], Hook-Jeeves method [6], dichotomy method [7] and others.

First-order optimization methods use information about the function itself and information about first-order derivatives. Such algorithms include: the parabola method, the conjugate gradient method [8], the steepest descent method [9], the gradient method with step splitting [10] and others.

As we can see, the multidimensionality and multiextremality of the objective function is an obstacle for numerical methods [11]. The optimization methods described above do not guarantee convergence to the global minimum.

In [12], a new algorithm is described, which is very different from the methods described above. The search begins with the value of the global minimum, and not with the definition of coordinates. This gives great savings. The idea of the method is based on the search for a horizontal section of the objective function that passes close (to the desired accuracy) with the global minimum of the objective function. The following is a theorem and the convergence of this algorithm is proved.

Problem statement

We give a mathematical formulation in the form of an objective function f to problems from different fields of application where it is necessary to find the smallest or largest value. So, we need to find the global optimum of the objective function. For certainty, the problem of finding a global minimum is considered. The task of finding the global maximum is performed similarly for an objective function with a minus sign. Let $f\colon Q \to R$ be a smooth objective function

$$f(x) = f(x_1, \dots, x_n) \tag{1}$$

from n – variables. It can be multi-extreme and multidimensional. The set of valid solutions is a $Q\ - n$ dimensional cube:

$$x \in Q = \left\{x \in R^n \middle| a_j \le x_j \le b_j, 1 \le j \le n\right\}$$

It is required to find the value and coordinates of the global minimum point $(\hat{x}; \hat{y})$. We will denote them:

$$\hat{y}\ = globminf(x) \tag{2}$$

$$\hat{x} = argglobmin_{x \in Q} f(x) = arg\hat{y} \tag{3}$$

The algorithm for finding the global minimum point consists of two parts. The first part of the task is to find the value of the global minimum point (2), and the second part is to find the coordinates of the global minimum (3).

Let's explain some notation: $f(x_1,...,x_n)$– objective function, minimized function; Q – search area for solutions; $x(x_1, x_2, ... x_n)$ vector of variables; $\hat{x} \in Q$ – the point of the global minimum of the function f on the set Q.

The results of the study

The idea of the new algorithm is radically different from the existing methods. We need to find a horizontal hyperplane $y = \alpha$ that intersects the graph of the objective function $y = f(x_1,...,x_n)$ near the global minimum. Such an approximation to the global minimum can be performed to the desired accuracy. To determine the global minimum, an auxiliary function is constructed. If the objective function $f(x_1,...,x_n)$ depends on n – variables, the auxiliary function will contain an n – fold integral:

$$g(\alpha) = \int_{a_1}^{b_1} ... \int_{a_n}^{b_n} [|f(x_1,...,x_n) - \alpha| - (f(x_1,...,x_n) - \alpha)]^m dx_1...dx_n. \quad (4)$$

Here $y = f(x_1,...,x_n)$ – is the objective function, $Q = \{x \in R^n | a_j \leq x_j \leq b_j, 1 \leq j \leq n\}$ – is a valid set, $y = \alpha$ is the equation of the horizontal hyperplane m – is the smoothness of the auxiliary function $g(\alpha) \in W_2^m$ from Hilbert space.

The auxiliary function (4) is calculated using numerical methods, for example, using lattice cubature Sobolev formulas with a regular boundary layer [13, 14].

The calculation of the auxiliary function, a complete description of the algorithm and computational experiments are published in previous articles [12], [15]. Now we will prove the convergence of the new global optimization algorithm.

Formula (4) defines the relative position of the given objective function $y = f(x_1,...,x_n)$ and the horizontal plane $y = \alpha$. The auxiliary function is always positive or equal to zero, since the function contains the difference between the modulus of the function and the function itself.

To begin with, the interval $[c_0, d_0]$ is selected, where the value of the global minimum is located.

Theorem 1.

If for the auxiliary function (4) there is equality $g(c_0) = 0$ and inequality $g(d_0) > 0$, then the value of the global minimum of the function $\hat{\alpha} = f(\hat{x}_1, ..., \hat{x}_n)$ lies in the interval $\hat{\alpha} \in [c_0, d_0)$.

Proof of Theorem 1.

Consider the behavior of the auxiliary function (4). If $f\left(x_1,...,x_n\right) \geq \alpha$, then the module in (4) is expanded with a plus sign and the value of the auxiliary function $g(\alpha) = 0$.

On the other hand, this means that the graph of the objective function is above or touches the horizontal hyperplane $y = \alpha$ at the point of the global minimum. Therefore, the global minimum is located at least below the hyperplane $y = c_0$, that is, $\hat{\alpha} \geq c_0$.

Next, let's assume the opposite, that is, $\hat{\alpha} \geq d_0$. By the condition of the theorem $g(d_0) > 0$, hence the set множество $Q(d_0) = \{(\bar{x}_1, ..., \bar{x}_n) \in Q | f(\bar{x}_1, ..., \bar{x}_n) < d_0\}$ is not empty. Therefore, on the set $Q(d_0)$, by virtue of the assumption $\hat{\alpha} \geq d_0$, the inequality $f(\hat{x}_1, ..., \hat{x}_n) < \hat{\alpha}$. And this contradicts the fact that $\hat{\alpha}$ is the value of the global minimum, hence $\hat{\alpha} < d_0$. Thus, $\hat{\alpha} \in [c_0, d_0)$. Theorem 1 is proved.

Figure 1 shows an example of an objective function $y = x^2(x-2)^2(x+1)^2 - 0.8x$. As described above, the value of the global minimum is between the lines $y = c_0$ and $y = d_0$.

A full description of the method using the auxiliary function is described in the author's articles [12], [15]. The most important indicator of optimization methods is convergence. Consider the convergence of the algorithm and determine the convergence rate.

It is known from Theorem 1 that if $g(c_0) = 0$ and $g(d_0) > 0$, then the global minimum $\hat{\alpha}$ is in the segment $[c_0, d_0]$.

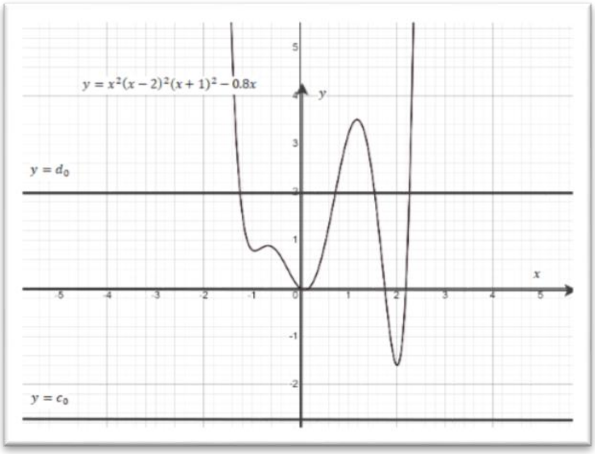

Figure 1. Graph of the function $y = x^2(x-2)^2(x+1)^2 - 0.8x$

We determine the middle $\alpha_0 = \dfrac{c_0 + d_0}{2}$ of the segment $[c_0, d_0]$ and calculate the value of the auxiliary function $g(\alpha_0)$. By the value of the auxiliary function, the location of the global minimum is determined:

A) If $g(\alpha_0) > 0$, then $\hat{\alpha} \in [c_0, \alpha_0]$. Then $c_0 = c_1$ and $\alpha_0 = d_1$. Then we work with the segment $[c_1, d_1]$, or

B) If $g(\alpha_0) = 0$, then $\hat{\alpha} \in [\alpha_0, d_0]$. Then $\alpha_0 = c_1$ and $d_0 = d_1$. Then we work with the segment $[c_1, d_1]$.

Similarly, the following midpoints of the sub-sections are defined:

$$\alpha_1 = \frac{c_1 + d_1}{2},\ \alpha_2 = \frac{c_2 + d_2}{2},\ \ldots, \alpha_n = \frac{c_n + d_n}{2}. \tag{5}$$

Continuing the process of halving the selected segments, you can reach an arbitrarily small segment containing the value of the global minimum $\hat{\alpha}$. Since for each iteration the segment where the global minimum is located is halved, then after n iterations the interval will be equal $|d_n - c_n| = \dfrac{1}{2^n}|d_0 - c_0|$ at the same time $d_n \le \hat{\alpha} \le c_n$. The iteration with the determination of the middle of the resulting interval and with the selection of the desired segment will be repeated until we reach the accuracy we need:

$$\varepsilon_f \ge d_k - c_k$$

As a global minimum $\hat{\alpha}$, we take the right end of the segment d_n, that is $\hat{\alpha} = d_k \approx \hat{y}$, where $g(\hat{\alpha}) > 0$. Thus, the value of the global minimum (3) is found with sufficient accuracy ε_f. Next, we will consider the convergence of the method.

Theorem 2.

If Theorem 1 holds, then the iterative sequence (5) of global minimization using an auxiliary function (4) converges to the desired value of the global minimum $\hat{\alpha}$ with a given accuracy.

Proof of Theorem 2.

Consider a sequence of numbers α_i that are an approximation of the value of the global minimum at the i-th step.

$$\alpha_i = \frac{1}{2}(d_i + c_i), \qquad c_i \le \alpha_i \le d_i \qquad i = 0,1,\ldots \tag{6}$$

where c_i, d_i are the boundaries of the sub-segments in which $g(c_i) = 0$ and $g(d_i) > 0$.

Consider the differences:

$$|\alpha_1-\alpha_0|,\ |\alpha_2-\alpha_1|,...,|\alpha_n-\alpha_{n-1}| \tag{7}$$

We have

$$|\alpha_1-\alpha_0|=\frac{1}{2}|d_1+c_1-d_0-c_0|$$

Since we always have either $c_1=c_0$ and $d_1=\frac{1}{2}(d_0+c_0)$ or $c_1=\frac{1}{2}(d_0+c_0)$ and $d_1=d_0$.

Therefore, if $c_1=c_0$, then (7): $|\alpha_1-\alpha_0|=\frac{1}{2}(c_0+\frac{1}{2}(d_0-c_0)-d_0-c_0)=\frac{1}{4}|c_0-d_0|$, or if $d_1=d_0$, then (7):

$$|\alpha_1-\alpha_0|=\frac{1}{2}(d_0+\frac{1}{2}(d_0-c_0)-d_0-c_0)=\frac{1}{4}|d_0-c_0|.$$

Checking similar reasoning and considering that the relation either $c_i=c_{i-1}$ and $d_i=\frac{1}{2}(d_{i-1}+c_{i-1})$ or $d_i=d_{i-1}$ and $c_i=\frac{1}{2}(d_{i-1}+c_{i-1})$ is always fulfilled:

$$|\alpha_1-\alpha_0|=\frac{1}{4}|d_0-c_0|$$

$$|\alpha_2-\alpha_1|=\frac{1}{4}|d_1-c_1|=\frac{1}{8}|d_0-c_0|$$

$$|\alpha_3-\alpha_2|=\frac{1}{4}|d_2-c_2|=\frac{1}{8}|d_1-c_1|=\frac{1}{16}|d_0-c_0|$$

$$|\alpha_4-\alpha_3|=\frac{1}{4}|d_3-c_3|=\frac{1}{8}|d_2-c_2|=\frac{1}{16}|d_1-c_1|=\frac{1}{32}|d_0-c_0|$$

$$...|\alpha_n-\alpha_{n-1}|=\frac{1}{2^{n+1}}|d_0-c_0|$$

$|\alpha_n-\alpha_{n-1}|=\frac{1}{2^{n+1}}|d_0-c_0|$, it can be seen from here that no matter how small a number $\varepsilon_f>0$ we can find such n that $\frac{1}{2^{n+1}}|d_0-c_0|\le\varepsilon_f$. After 10 iterations, the initial segment will be $2^{10}=1024$ times shorter. Theorem 2 is proved.

Theorem 3.

Let the conditions of Theorem 1 be fulfilled. Then the iterative sequence $\{\alpha_n\}$ obtained by dividing the segment in half (5) converges to the global minimum of the objective function $f(x_1,...x_n)$ with linear velocity $\beta=0.5$.

Proof of Theorem 3.

From the algorithm described above, it is clear that the smaller the segment $[c_i;d_i]$, the α_i is closer to the desired minimum value $\hat{\alpha}\approx\hat{y}$. In addition, after each iteration, the length of the segment is halved, so

$$\frac{|\alpha_{n+1}-\hat{\alpha}|}{|\alpha_n-\hat{\alpha}|}\le\frac{\frac{1}{2}|\alpha_n-\hat{\alpha}|}{|\alpha_n-\hat{\alpha}|}=0.5\Rightarrow|\alpha_{n+1}-\hat{\alpha}|\le0.5|\alpha_n-\hat{\alpha}|.$$

The latter inequality proves that the iterative sequence converges to the value of the global minimum of the objective function by linear velocity with a coefficient $\beta = 0.5$.

Example. Consider the multiextremal Eckley function [20] in three-dimensional space. Figure 2 shows a graph of the Eckley function, which has a large number of local minima.

$$f(x, y) = -20e^{-0.2\sqrt{0.5(x^2+y^2)}} - e^{0.5(\cos(2\pi x)+\cos(2\pi y))} + e + 20 \quad (10)$$

$$-5 \le x, y \le 5$$

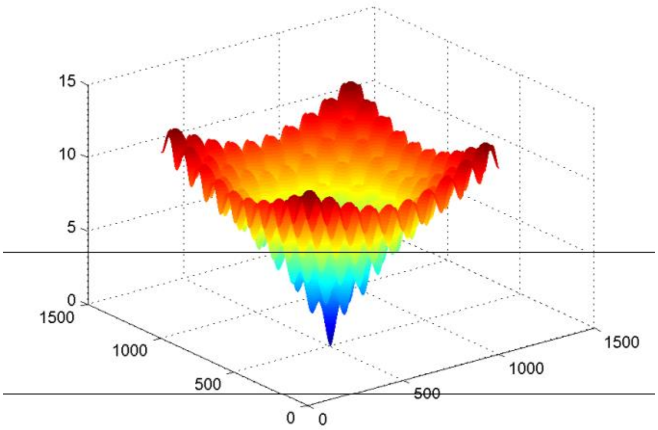

Figure 2. Graph of the Eckley function

Reference value of the global minimum point of the Eckley function $f(0; 0) = 0$. Computational experiments show the following results:

$$f(-10^{-10}, -10^{-10}) = 10^{-10}.$$

Error $\varepsilon_f = 10^{-10}$, $\varepsilon_{x,y} = 10^{-10}$.

Conclusions

The task of global optimization has a huge practical meaning. The algorithm described above is completely new. In other optimization methods, coordinates are first determined or set, then the values of the function at these nodes are compared and the smallest value of the function is selected. For gradient optimization methods, if the objective function is multiextremal, then convergence of the method means convergence to one of the local minimum points of the objective function.

In the proposed method, using horizontal sections, we determine the level where the global minimum is located. After that, we determine the coordinates of the minimum. The superiority of the new method is that the method converges immediately to the global minimum. In this algorithm, the middle is determined and one of the halves of the segment is selected. This provides greater savings than the brute force method.

Calculations of the global minimum by this method are performed in the C++ programming language. Computational experiments have been carried out for test smooth functions of two variables. The experimental results show that the proposed algorithm works correctly. The average accuracy of calculating the global minimum point $\varepsilon = 10^{-6}$ has been achieved.

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