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EFFICIENT NUMERICAL SOLVING OF DIFFICULT MULTIMODAL PROBLEMS

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ЕФЕКТИВНЕ ЧИСЕЛЬНЕ РОЗВ'ЯЗУВАННЯ СКЛАДНИХ МУЛЬТИМОДАЛЬНИХ ЗАДАЧ

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Abstract. Most mathematical optimization models of the applied problems are multimodal. Many methods and algorithms have been developed and are being developed for their solution. To verify the effectiveness of such methods, many test functions and problems have been developed. But most of such test functions are simple. They are symmetric, of low dimension, and have known solutions. This complicates the verification of the effectiveness of existing and new methods of global optimization. The paper proposes modifications of known test functions that satisfy the efficiency conditions. The minima of these functions are found by the method of exact quadratic regularization. The results obtained are significantly better than the solutions obtained by other methods.
Keywords: global optimization, test functions, exact quadratic regularization method, coordinate descent method, computational experiments.

Анотація. Більшість математичних оптимізаційних моделей прикладних задач є мультимодальними. Для їх розв'язування розроблено та розробляється багато методів та алгоритмів. Для перевірки ефективності таких методів розроблено багато тестових функцій та задач. Але більшість таких тестових функцій є простими. Вони симетричні, низької розмірності та мають відомі розв'язки. Це ускладнює перевірку ефективності існуючих та нових методів глобальної оптимізації. У статті запропоновано модифікації відомих тестових функцій, які задовольняють умовам ефективності. Мінімуми цих функцій знаходяться методом точної квадратичної регуляризації. Отримані результати значно кращі за розв'язки, отримані іншими методами.

Ключові слова: глобальна оптимізація, тестові функції, метод точної квадратичної регуляризації, метод координатного спуску, обчислювальні експерименти.

1. Introduction

In every sphere of human activity, it is desirable to make the best optimal decisions. This allows you to create reliable systems, and save resources and time. Over the past 50 years, many optimization models have been built. Most of these models are multimodal, that is, they contain many local extrema. Such problems are very difficult to solve numerically. Classical optimization methods get stuck at the points of local extrema. Multimodal models can contain 2^n or $n!$ local extrema. Then optimization methods will not be able to get out of the starting point. It seemed that the problem could be solved by a series of starting points that cover the entire feasible set of the problem. However, this idea does not work in high-dimensional spaces. Choosing only one point from each orthant gives 2^n points. This is very a lot for today's and future computers. Then, many algorithms were developed that reduce the number of starting points. These algorithms take into account the behavior (evolution) of the functions and contain many tuning parameters. To check the effectiveness of such algorithms, test functions were constructed. For some test functions, evolutionary algorithms showed good results. This was achieved by tuning the algorithm parameters. But our computational experiments have shown that the coordinate descent method is no worse than evolutionary methods.

Most of the existing test functions are very simple. They have known solutions and low dimensionality and cannot provide a test of the effectiveness of the algorithms. It is necessary to develop new test functions of arbitrary dimension with unknown solutions (global minima). Such functions are proposed in this paper. The minima of these functions were found by evolutionary algorithms and the exact quadratic regularization method (EQR).

The results obtained show that evolutionary algorithms on average give 50% of the results obtained by the exact quadratic regularization method. These computational experiments show the high efficiency of the EQR, which is built on new ideas in global optimization [1].

2. Brief evolution of global optimization

The first publications on global optimization appeared only in the 70s of the last century. Then it was shown that global optimization problems are NP-hard. This reduced the interest of optimization researchers in developing efficient global optimization methods.

However, in the 90s, many optimization multimodal models were developed in various fields of human activity, which stimulated the development of new methods of global optimization. These methods have two unsolved problems: the dimension of the problem and getting out of the local minimum point. These problems are solved by the exact quadratic regularization method. A detailed review of papers on global optimization can be found in [2, 3].

To test the effectiveness of global optimization algorithms, test problems have been used for a long time [4, 5, 6]. Initially, these were constrained optimization problems. However, it is more efficient to evaluate algorithms on classes of test functions. Such functions can be found in [7, 8, 9]. Today, these functions cannot provide an objective evaluation of the effectiveness of new global optimization methods. Most of these functions are very simple, small in dimension, and have known trivial solutions.

This encourages authors to develop new functions [10, 11], but they have the same disadvantages.

3. Test functions for global optimization

Let us list the requirements that test functions for global optimization must satisfy:

1. Such functions must be multimodal.
2. Functions must have arbitrary dimensions.
3. Functions must be asymmetric.
4. The global minimum of such functions must be unknown.

Verification of these conditions is not a difficult problem. A function is multimodal if, at different starting points, we will obtain different values of their minimum by a local solver. The functions have arbitrary dimensions if this dimension is equal to n. A function is asymmetric if the minimum points have different coordinates. The test function must be difficult and non-separable so that their minimum point is unknown. If the solutions of the test functions are unknown, then we get a simple criterion for the best method or solver. The best method is the one that gives more minimum values of the test functions. Other criteria for evaluating the effectiveness of algorithms have been proposed, including the time to solve problems. However, this criterion is difficult to verify.

The paper [9] presents 315 test functions and provides 25 test functions that are most frequently used to test the effectiveness of new methods.

We will show that these functions do not satisfy the listed requirements.

All of the given functions have trivial solutions, most of them have dimension 2, some of them are separable (Alpine, Michalewicz, Rastrigin, Schwefel, Sphere) and several functions are even unimodal (Dixon Price, Rosenbrock, Sphere). Thus such functions cannot provide an objective evaluation of the effectiveness of new methods.

We believe that the dimensionality of text functions should be no less than one hundred variables. Among the 315 test functions, only two satisfy the specified requirements. This is the Egg holder function

$$f(x) = \sum_{i=1}^{n-1} \Big(-(x_{i+1} + 47) \sin\Big(\sqrt{|x_{i+1} + x_i/2 + 47|}\Big) - \\ - x_i \sin\Big(\sqrt{|x_i - x_{i+1} - 47|}\Big)\Big), \quad x \in [-512, 512], \quad (1)$$

and Rana function

$$f(x) = \sum_{i=1}^{n-1} \Big((x_{i+1}+1)\sin(\sqrt{|x_{i+1}+x_i+1|})\cos(\sqrt{|x_{i+1}-x_i+1|}) +$$
$$+ x_i \sin(\sqrt{|x_{i+1}-x_i+1|})\cos(\sqrt{|x_{i+1}+x_i+1|}) \Big), \quad x \in [-500, 500]. \quad (2)$$

The solutions for these functions for $n > 2$ are unknown.

Thus, the list of test functions for global optimization problems needs to be urgently updated.

4. New test functions for global optimization

Many well-known test functions of two variables can be generalized to functions of n variables. Separable functions can be transformed into non-separable ones. The asymmetry of functions will be ensured by introducing a summation index into the functions.

We generalize the functions Ackley 3, Adjman, Bird, Liang's, Mishra 5, Mishra 6, Siam, Trefethen to arbitrary dimensions. Accordingly, we have

$$f(x) = -\sum_{i=1}^{n-1} [200e^{-0.02\sqrt{x_i^2+x_{i+1}^2}} + 5e^{\cos(3x_i)+\sin(3x_{i+1})}], \quad x \in [-32, 32]; \quad (3)$$

$$f(x) = \sum_{i=1}^{n-1} [\cos(x_i)\sin(x_{i+1}) - \frac{x_i}{(x_{i+1}^2+1)}], \quad x \in [-1, 1]; \quad (4)$$

$$f(x) = \sum_{i=1}^{n-1} [\sin(x_i)e^{(1-\cos(x_{i+1}))^2} + \cos(x_{i+1})e^{(1-\sin(x_i))^2} +$$
$$+ (x_i - x_{i+1})^2], \quad x \in [-2\pi, 2\pi]; \quad (5)$$

$$f(x) = -\sum_{i=1}^{n-1} [(x_i \sin(20x_{i+1}) + x_{i+1}\sin(20x_i))^2 \coth(\sin(10x_i)x_i) +$$
$$+ (x_i\cos(20x_{i+1}) - x_{i+1}\sin(10x_i))^2 \coth(\cos(10x_{i+1})x_{i+1})], \quad x \in [1, 4]; \quad (6)$$

$$f(x) = \sum_{i=1}^{n-1} [(f_1(x_i, x_{i+1}) + f_2(x_i, x_{i+1}) + x_i)^2 +$$
$$+ 0.01(x_i + x_{i+1})], \quad x \in [-10, 10], \quad (7)$$

where

$$f_1(x_i, x_{i+1}) = \sin^2(\cos(x_i) + \cos(x_{i+1}))^2,$$
$$f_2(x_i, x_{i+1}) = \cos^2(\sin(x_i) + \sin(x_{i+1}))^2;$$

$$f(x) = \sum_{i=1}^{n-1} [-\ln((f_1(x_i, x_{i+1}) + f_2(x_i, x_{i+1}) + x_i)^2) +$$
$$+ 0.01((x_i - 1)^2 + (x_{i+1} - 1)^2)], \quad x \in [-10, 10]; \quad (8)$$

$$f(x) = \sum_{i=1}^{n-1}[e^{\sin(x_i)} + \sin(60e^{x_{i+1}}) + \sin(70\sin(x_i)) + \\ + \sin(\sin(80x_{i+1})) - \sin(10(x_i - x_{i+1})) + \frac{1}{4}(x_i^2 - x_{i+1}^2)], \quad x \in [-1, 1]; \tag{9}$$

$$f(x) = \sum_{i=1}^{n-1}[e^{\sin(50x_i)} + \sin(60e^{x_{i+1}}) + \sin(70\sin(x_i)) + \sin(\sin(80x_{i+1})) - \\ - \sin(10(x_i - x_{i+1})) + \frac{1}{4}(x_i^2 - x_{i+1}^2)], \quad x \in [-10, 10]. \tag{10}$$

The solution to the problems (1)–(10) is unknown for dimensions $n \geq 100$. The problems (1)–(10) are difficult multimodal problems.

But only the problems (1)–(2) and (8)–(10) have asymmetric solutions.

Let us consider the following modifications of the test functions Adjman, Bird, Mishra 5, Mishra 6, Trefethen (4)–(11), which significantly complicate the search for the global minimum:

$$f(x) = \sum_{i=1}^{n-1}[\cos(x_i)\sin(ix_{i+1}) - \frac{x_i}{(x_{i+1}^2 + 1)}], \quad x \in [-1, 1]; \tag{11}$$

$$f(x) = \sum_{i=1}^{n-1}[\sin(ix_i)e^{(1-\cos(x_{i+1}))^2} + \\ + \cos((i+1)x_{i+1})e^{(1-\sin(x_i))^2} + \\ + (x_i - x_{i+1})^2], \quad x \in [-2\pi, 2\pi]; \tag{12}$$

$$f(x) = \sum_{i=1}^{n-1}[(f_3(x_i, x_{i+1}) + f_4(x_i, x_{i+1}) + x_i)^2 + \\ + 0.01(x_i + x_{i+1})], \quad x \in [-10, 10], \tag{13}$$

where

$$f_3(x_i, x_{i+1}) = \sin^2(\cos(ix_i) + \cos(x_{i+1}))^2,$$

$$f_4(x_i, x_{i+1}) = \cos^2(\sin(ix_i) + \sin(x_{i+1}))^2;$$

$$f(x) = \sum_{i=1}^{n-1}[-\ln((f_3(x_i, x_{i+1}) + f_4(x_i, x_{i+1}) + x_i)^2) + \\ + 0.1((x_i - 1)^2 + (x_{i+1} - 1)^2)], \quad x \in [-10, 10]. \tag{14}$$

$$f(x) = \sum_{i=1}^{n-1}[e^{\sin(50x_i)} + \sin(60e^{x_{i+1}}) + \sin(70\sin(ix_i)) + \\ + \sin(\sin(80x_{i+1})) - \sin(10(x_i - (i+1)x_{i+1})) + \\ + 0.01(x_i^2/i + x_{i+1}^2)], \quad x \in [-10, 10]; \tag{15}$$

and Chen's modified function

$$f(x) = \sum_{i=1}^{n-1} [\sin(x_i + i x_{i+1}) + \sin(2 x_i x_{i+1})/(3i))], \quad x \in [3, 13]. \tag{16}$$

The modifications include the summation index in the arguments of trigonometric functions, which significantly complicates such functions.

We obtained 16 test functions and propose to use them to test the effectiveness of global optimization methods and solvers for dimensions 100 and more. All test functions (1)–(16) satisfy by the conditions 1–4. Currently, the best solutions are known only for test functions Egg holder and Rana. We found the minima of 16 test functions using the exact quadratic regularization method and a Python solver that uses an evolutionary search algorithm. The results obtained can be a benchmark for testing the effectiveness of global optimization methods.

We give simple test for the best method. It is a method that gives more good results for problems with unknown solutions.

5. Exact quadratic regularization method

Consider the following global optimization problem

$$\min\{f(x) \,|\, x \in [a, b],\ x \in E^n\}, \tag{17}$$

where function $f(x)$ is twice continuously differentiable, x is a vector in n-dimensional Euclidean space E^n. Let the solution of the problem (17) exist and x^* is its global minimum point.

The problem (17) is transformed into the following equivalent problem

$$\min\{||x||^2 \,|\, f(x) + s \le ||x||^2,\ x \in [a, b]\}, \tag{18}$$

where $||x||^2 = x_1^2 + ... + x_n^2 + x_{n+1}^2$ and $s \ge ||x^*||^2 - f(x^*)$. After such a transformation, the point of the global minimum of the problem (18) will be closest to the origin of the coordinates. In addition, the transformation (18) allows using exact quadratic regularization to transform the problem (18) into the following

$$\min\{||x||^2 \,|\, f(x) + s + (r - 1)||x||^2 \le d,\ r||x||^2 = d,\ x \in [a, b]\}, \tag{19}$$

where the parameter $r > 0$ is chosen so that the feasible region

$$\{x \,|\, f(x) + s + (r - 1)||x||^2 \le d,\ x \in [a, b]\}$$

becomes convex.

The problem (19) is multimodal and very difficult, which is associated with the non-convex constraint $r||x||^2 = d$. Therefore, the second idea is to transform the problem (19) into the following one

$$\max\{||x||^2 \,|\, f(x) + s + (r - 1)||x||^2 \le d,\ x \in [a, b]\}, \tag{20}$$

and the condition $r||x||^2 = d$ should be considered separately. We call this condition the SP condition. In the problem (20), it is necessary to find the minimum value of the scalar variable d at which its solution will be satisfied by the condition $r||x||^2 = d$. This solution will also be the solution to the problem (17).

We will find the minimum value of d in several iterations. We will gradually increase the value of d until the solution of the problem (20) satisfies the condition $r||x||^2 = d$. For starters the iterations, it is necessary to find the minimum feasible value of d. This value d is easy to find from the solution of the following convex problem

$$\min\{d \,|\, f_0(x) + s + (r-1)||x||^2 \leq d, \; f_i(x) + r||x||^2 \leq 0, \; i = 1, ..., m\}. \quad (21)$$

We use only a local solver to solve the problems (20)–(21).

We can list the advantages of the exact quadratic regularization method:

1. The starting point for the problem (20) is always feasible.
2. The method can be applied to a wide class of multimodal problems.
3. The transformed multimodal problem (20) can become unimodal.
4. The method is easy to implement and uses only a local solver for unimodal problems.
5. This method allows us to solve large-scale multimodal problems.
6. The method has a simple geometric interpretation.

The numerical implementation of the EQR method uses the coordinate descent method. This simplifies solving difficult multimodal problems. The numerical implementation is presented in Algorithm 1.

Algorithm 1.

Step 1. Select the parameter values r, s, and the starting point, for example, $x^i = 1, i = 1, ..., n+1$.

Step 2. Solve the convex optimization problem (21) and find the minimum value d_0.

Step 3. Solve a sequence of problems (20) for increasing values of d ($d_1 = d_0 + \Delta d_0, ..., d_{k+1} = d_k + \Delta d_k, \Delta d_i > 0, i = 0, 1, ...$) until the SP condition is satisfied with a given accuracy. We obtain a sequence of solutions $x^1, ..., x^k$.

Step 4. Solve problem (17) by the method of coordinate descent with the starting point x^k. If we get a better solution, then move on to step 3. Otherwise, x^k is a solution to problem (17).

Table 1 shows the algorithm iterations for the Bird function when the parameters of problem (20) are equal to $s = 12000, r = 1500$.

Table 1. The algorithm iterations.

d_k	10857	20000	80000	120000	180000
$f_0(x^k)$	-1191.4	-2199.4	-4267.8	-5028.2	-5330.33

6. Computational experiments

For a computer implementation of EQR, it is sufficient to have a local solver. We use Open Solver for Excel.

Table 2 shows the results of solving 16 test problems with unknown solutions for $n = 100$. We see that the EQR method showed significantly better solutions for all test problems.

The Python solver found solutions in almost an hour, the EQR method takes up to 5 minutes. We have used other solvers, including Couenne. But this solver takes a lot of time. The problem (11) was not solved in 5 hours.

The starting point was usually chosen as $x = (1, 1, ..., 1)$. The solution to the problems sometimes depended on the choice of the parameter r and the step of changing d.

Table 2. Results of solving test problems.

Function name	EQR method best min	Best known min
Ackley 3	**-21766.8655**	-19494.03687(py)
Adjman	**-30.37418**	-23.30464(py)
Bird	**-5230.32938**	-4097.8487 (py)
Egg holder	**-89948.532**	-89938(web)
Liang‘s	**-85466.348**	-33162.8595(py)
Mishra 5	**-0.164278**	11.919746
Mishra 6	**-197.53142**	-154.07665(py)
Rana	**-50874.9533**	-47332(web)
siam	**-236.16287**	-51.496279(py)
Trefethen	**-200.37906**	17.0243597(py)
Adjman M.	**-124.147677**	-109,59992 (py)
Bird M.	**-5180.53596**	-1870.60098 (py)
Mishra 5 M.	**-0.857934**	4.87141(py)
Mishra 6 M.	**-1582.5753**	-239.6717(py)
Trefethen M.	**-312.11068**	34.201124 (py)
Chen M.	**-114.90839**	-68.527654 (py)

7. Conclusions

Existing libraries of test functions are not suitable for testing the effectiveness of global optimization methods. We propose requirements for text functions, as well as a set of test functions that satisfy these requirements. To minimize the test functions, we used the method EQR and other solvers. The EQR method showed the best results for all test functions, even for those functions (Egg holder, Rana) that have been solved by various methods in the last 30 years.

The author hopes that the list of new test functions will be continued in compliance with the specified requirements. The effectiveness of existing and new methods will be evaluated on these test functions.

We can solve multimodal problems with thousands of variables using the EQR method. But to check the effectiveness of modern global optimization methods, 100 variables are enough.

The paper does not consider test and applied problems of constrained optimization. For such problems, it is more difficult to determine the criteria for the effectiveness of the methods. This depends on the accuracy of the constraint's performance. Many such problems are in well-known libraries GlobalLib, MinlpLib, and PrincetonLib.

The author obtained better results using the EQR method for problems from these libraries. However, the analysis of the obtained results is beyond the scope of this article.

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