Parallel Global Optimization for Non-Convex Mixed-Integer Problems

Konstantin Barkalov (⋈) and Ilya Lebedev {konstantin.barkalov,ilya.lebedev}@itmm.unn.ru

Lobachevsky State University of Nizhni Novgorod, Nizhni Novgorod, Russia

Abstract. The paper considers the mixed-integer global optimization problems. A novel parallel algorithm for solving the problems of this class based on the index algorithm for solving the continuous global optimization problems has been proposed. The comparison of this algorithm with known analogs demonstrates the efficiency of the developed approach. The proposed algorithm allows an efficient parallelization including the employment of the graphics accelerators. The results of performed numerical experiments (solving a series of 100 multiextremal mixed-integer problems) confirm a good speedup of the algorithm with the use of GPU.

Keywords: Global optimization \cdot Non-convex constraints \cdot Mixed-integer problems \cdot Parallel algorithms

1 Introduction

In this paper the global optimization problems and the method of their solving are considered. The global optimization problems are the time-consuming ones since the global optimum is an integral characteristic of the problem being solved and requires the investigation of the whole search domain. As a result, the search of the global optimum is reduced to the construction of a coverage (in general, a nonuniform one) of the space of parameters; such problems are common in applications [1–3]. The problems, in which some parameters can take the discrete or integer values only (mixed-integer global optimization problems) are of special interest because for these problems it is more difficult to build the estimates of the optimum as compared to the continuous ones.

The situation when some parameters are featured by the discreteness or integerness is frequent in applied problems. As a rule, the integer parameters take a small number of values and may denote, for example, the trademarks of the materials used, the variant of typical layouts of components, etc.

A lot of publication have been devoted to the methods of solving the mixed-integer problems (see, for example, the reviews [4,5]). The well known deterministic methods of solving the problems of this class are based, as a rule, on the Branch-and-Bound [6] or on the Branch-and-Reduce approach [7]. Also, a number of the metaheuristic and genetic algorithms are known, which are based one way or another on the random search concept [8,9].

In the present study, we proposed a novel parallel method for solving the mixed-integer problems based on the index approach to solving the constrained global optimization problems [10, 11]. Within the framework of this approach:

- the solving of the multidimensional problems is reduced to solving the equivalent one-dimensional problems; the corresponding reduction is based on the use of the space-filling curves;
- when solving the constrained optimization problems, each constraint is taken into account and processed separately, the penalty functions are not used;
- the parallelization of the search process is performed by means of the simultaneous computing of several objective function values at different points of the search domain within every iteration.

The paper text reflecting the results of the performed study is organized in the following way. In Section 2, a brief description of the dimensionality reduction scheme using the space-filling curves is given. Also, the index scheme of accounting for the constraints is described. Here the formulation of the parallel index algorithm for solving the continuous global optimization problems is given as well. In Section 3, the approach to the generalization of the parallel index algorithm with the purpose of solving the mixed-integer problems is presented. A method that allows to reduce solving of mixed-integer problem to solving a set of the continuous optimization problems, which can be performed in parallel, is given. Section 4 contains the results of numerical experiments. The comparison of the sequential version of the algorithm with the known analogs is conducted here. Also, the efficiency of the parallel CPU- and GPU-versions of the algorithm for solving a series of the multiextremal mixed-integer problem is demonstrated. Section 5 concludes the paper.

2 Global optimization algorithm and dimension reduction

A constrained global optimization problem can be formulated as follows

$$\varphi(y^*) = \min \{ \varphi(y) : y \in D, \ g_i(y) \le 0, \ 1 \le i \le m \}, \tag{1}$$

$$D = \{ y \in R^N : a_j \le y_j \le b_j, 1 \le j \le N \}.$$
 (2)

The objective function $\varphi(y)$ (hereafter denoted by $g_{m+1}(y)$) and the left-hand sides $g_i(y)$, $1 \le i \le m$, of the constraints satisfy the Lipschitz condition

$$|g_i(y_1) - g_i(y_2)| \le L_i ||y_1 - y_2||, \ 1 \le i \le m+1, \ y_1, y_2 \in D,$$

with a priori unknown constants L_i , $1 \le i \le m+1$, and may be multiextremal. It is assumed that the functions $g_i(y)$ are defined and computable only at the points $y \in D$ satisfying the conditions

$$g_k(y) \le 0, \ 1 \le k < i.$$
 (3)

By employing the continuous single-valued Peano-Hilbert curve y(x) mapping the unit interval [0,1] on the x-axis onto the N-dimensional domain (2), it is possible to find the minimum in (1) by solving the one-dimensional problem

$$\varphi(y(x^*)) = \min \{ \varphi(y(x)) : x \in [0, 1], \ g_i(y(x)) \le 0, \ 1 \le i \le m \}.$$

Algorithms for numerical construction of Peano-Hilbert curve approximation (evolvent) are considered in [10,11]. These evolvents are fractals generated by an iterative process, that fill in the hypercube D with accuracy 2^{-m} , where integer m>0 is the evolvent construction parameter. Examples of the evolvent with different m in two dimensions are given in Fig. 1.

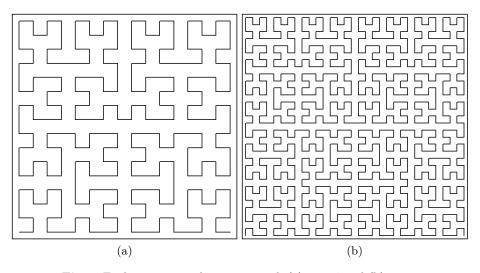


Fig. 1. Evolvents in two dimensions with (a) m = 4 and (b) m = 5

Due to (3) the functions $g_i(y(x))$ are defined and computable in the subranges

$$Q_1 = [0,1], \ Q_{i+1} = \{x \in Q_i : g_i(y(x)) \le 0\}, \ 1 \le i \le m.$$

These conditions allows us to introduce a classification of the points $x \in [0,1]$ according to the number $\nu(x)$ of the constraints computed at this point. The index $\nu(x)$ can also be defined by the conditions

$$g_i(y(x)) \le 0, \ 1 \le i < \nu, \ g_{\nu}(y(x)) > 0,$$
 (4)

where the last inequality is inessential if $\nu = m + 1$.

In the dimensionality reduction scheme considered here, a multidimensional problem with Lipschitzian functions is juxtaposed with a one-dimensional problem, where the corresponding functions satisfy uniform Hölder condition (see [11]), i.e.,

$$|g_i(y(x_1)) - g_i(y(x_2))| \le H_i |x_1 - x_2|^{1/N}, \ x_1, x_2 \in [0, 1], \ 1 \le i \le m + 1.$$

Here, N is the dimensionality of the initial multidimensional problem and the coefficients H_i are related to the Lipschitz constant L_i of the initial problem as $H_i \leq 2L_i\sqrt{N+3}$.

Thus, a trial at a point $x^k \in [0,1]$ executed at the k-th iteration of the algorithm will consist of the following sequence of operations:

- Determine the image $y^k = y(x^k)$ in accordance with the mapping y(x);
- Compute the values $g_1(y^k), ..., g_{\nu}(y^k)$, where $\nu = \nu(x^k)$ is from (4).

The dyad

$$\{\nu = \nu(x^k), \ z^k = g_{\nu}(y(x^k))\}$$
 (5)

will be referred to as the *trial outcome*.

An efficient parallel index algorithm (PIA) for solving the constrained global optimization problem (1) has been developed at University of Nizhni Novgorod. The scheme of the algorithm is as follows.

Suppose we have $p \geq 1$ computational elements (e.g., processor cores), which can be used to run p trials simultaneously. In the first iteration of the method, p trials are run in parallel at various random points $x^i \in (0,1)$, $1 \leq i \leq p$. Suppose $n \geq 1$ iterations of the method have been completed, and as a result of which, trials were carried out in k = k(n) points $x^i, 1 \leq i \leq k$. Then the points $x^{k+1}, ..., x^{k+p}$ of the search trials in the next (n+1)-th iteration will be determined according to the rules below.

1. Renumber the points $x^1, ..., x^k$ from previous iterations with lower indices, lowest to highest coordinate values, i.e.

$$0 = x_0 < x_1 < \dots < x_i < \dots < x_k < x_{k+1} = 1, \tag{6}$$

and match them with the values $z_i = g_{\nu}(y(x_i))$, $\nu = \nu(x_i)$, $1 \le i \le k$, from (5), calculated at these points; points $x_0 = 0$ and $x_{k+1} = 1$ are introduced additionally, the values z_0 and z_{k+1} are indeterminate.

2. Classify the numbers $i, 1 \le i \le k$, of the trial points from (6) by the number of problem constraints fulfilled at these points, by building the sets

$$I_{\nu} = \{i : 1 \le i \le k, \ \nu = \nu(x_i)\}, \ 1 \le \nu \le m+1,$$
 (7)

containing the numbers of all points $x_i, 1 \le i \le k$, with the same values of ν . The end points $x_0 = 0$ and $x_{k+1} = 1$ are interpreted as those with zero indices, and they are matched to an additional set $I_0 = \{0, k+1\}$. Identify the maximum current value of the index

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$$M = \max \{ \nu = \nu(x_i), \ 1 \le i \le k \}.$$
 (8)

3. For all values of ν , $1 \le \nu \le m+1$, calculate the values

$$\mu_{\nu} = \max \left\{ \frac{|z_i - z_j|}{(x_i - x_j)^{1/N}} : i, j \in I_{\nu}, j < i \right\}.$$
 (9)

If the set I_{ν} contains less than two elements or μ_{ν} from (9) equals zero, then assume $\mu_{\nu} = 1$.

4. For all non-empty sets I_{ν} , $1 \leq \nu \leq m+1$, determine the values

$$z_{\nu}^{*} = \begin{cases} -\epsilon_{\nu}, \nu < M, \\ \min\{g_{\nu}(x_{i}) : i \in I_{\nu}\}, \nu = M, \end{cases}$$
 (10)

where M is the maximum current value of the index, and the vector $\epsilon_R = (\epsilon_1, ..., \epsilon_m)$ with positive coordinates is called the *reserve vector* and is used as a parameter in the algorithm.

5. For each interval $(x_{i-1}, x_i), 1 \le i \le k+1$, calculate the *characteristic* R(i):

$$R(i) = \Delta_i + \frac{(z_i - z_{i-1})^2}{(r_\nu \mu_\nu)^2 \Delta_i} - 2 \frac{z_i + z_{i-1} - 2z_\nu^*}{r_\nu \mu_\nu}, \quad \nu = \nu(x_{i-1}) = \nu(x_i),$$

$$R(i) = 2\Delta_i - 4 \frac{z_i - z_\nu^*}{r_\nu \mu_\nu}, \quad \nu(x_{i-1}) < \nu(x_i) = \nu,$$

$$R(i) = 2\Delta_i - 4 \frac{z_{i-1} - z_\nu^*}{r_\nu \mu_\nu}, \quad \nu = \nu(x_{i-1}) > \nu(x_i).$$

where $\Delta_i = (x_i - x_{i-1})^{1/N}$, and the values $r_{\nu} > 1, 1 \le \nu \le m+1$, are used as parameters in the algorithm.

6. Reorder the characteristics R(i), $1 \le i \le k+1$, from highest to lowest

$$R(t_1) \ge R(t_2) \ge \dots \ge R(t_k) \ge R(t_{k+1})$$
 (11)

and choose p largest characteristics with interval numbers $t_j, 1 \leq j \leq p$.

7. Carry out p new trials in parallel at the points x^{k+j} , $1 \le j \le p$, calculated by the formulae

$$x^{k+j} = \frac{x_{t_j} + x_{t_j-1}}{2}, \ \nu(x_{t_j-1}) \neq \nu(x_{t_j}),$$
$$x^{k+j} = \frac{x_{t_j} + x_{t_j-1}}{2} - \frac{\operatorname{sign}(z_{t_j} - z_{t_j-1})}{2r_{\nu}} \left[\frac{|z_{t_j} - z_{t_j-1}|}{\mu_{\nu}} \right]^N,$$
$$\nu(x_{t_j-1}) = \nu(x_{t_j}) = \nu.$$

The algorithm stops if the condition $\Delta_{t_j} \leq \epsilon$ becomes true for at least one number $t_j, 1 \leq j \leq p$; here $\epsilon > 0$ has an order of magnitude of the desired coordinate accuracy.

This method of organizing parallel computing has the following justification. The characteristics of intervals R(i) used in the index algorithm can be considered as probability measures of the global minimum point location in these intervals. Inequalities (11) arrange intervals according to their characteristics, and trials are carried out in parallel in the first p intervals with the largest probabilities. A detailed description of the algorithm convergence theory is presented in [10]. The results of comparison of the algorithm with other sequential and parallel global optimization algorithms have been presented in [12].

3 Parallel algorithm for mixed-integer problems

Now let us consider the case when the argument of the problem functions consists of two components: the vector y from the hyperinterval D and the vector u taking a finite (and not too large) set of possible values, i.e.

$$\min \{ g_{m+1}(y, u) : y \in D, \ g_i(y, u) \le 0, \ 1 \le i \le m \},$$

$$D = \{ a_j \le y_j \le b_j, \ 1 \le j \le N \}.$$

$$(12)$$

Such finite sets can characterize, for example, the variant of material, which the object is made from, the geometric sizes, or other quantities, which can belong to a standard discrete series, etc.

Let us number by the integer values $s, 1 \leq s \leq S$, all possible values of the vector u, i.e. juxtapose each considered value s with the vector u_s . Then, the considered problem can be written in the form

$$\min_{s \in \{1, \dots, S\}} \left\{ \min \left\{ g_{m+1}(y, u_s) : y \in D, \ g_i(y, u_s) \le 0, \ 1 \le i \le m \right\} \right\},$$

$$D = \left\{ a_i \le y_i \le b_i, \ 1 \le j \le N \right\}.$$
(13)

Using the dimensionality reduction scheme with the evolvent $y(x), x \in [0, 1]$, one can superimpose each nested minimization problem with respect to y to a one-dimensional problem

$$\min\{g_{m+1}(y(x), u_s) : x \in [0, 1], g_i(y(x), u_s) \le 0, 1 \le i \le m\}, s \in \{1, ..., S\}.$$

Now let us consider the relation

$$Y(x) = y(x - E(x)), x \in [0, S],$$

mapping any point of the interval [0,S] onto the domain D (the notation E(x) corresponds to the integer part of the number x) and define the functions

$$g_i(x) = g_i(Y(x), u_{E(x)+1}), x \in [0, S],$$

having, in general, the jump discontinuities at the integer points $x_k = i, 1 \le i \le S - 1$. The values $z_k = g_{\nu}(y(x_k))$ from (5) at these points will be considered to be undefined, and the values of the indices – to equal to 0, i.e. $\nu(x_k) = 0$.

Using the introduced notations, one can reformulate the original problem as

$$\min \{ g_{m+1}(x) : x \in [0, S], \ g_i(x) \le 0, \ 1 \le i \le m \}.$$
(14)

As an illustration, Fig. 2 presents the plots of the functions corresponding to a problem $\,$

$$\min\left\{u^2(\sin(x)+\sin(10x/3):x\in[2.7,7.5],u\in\{1,2\}\right\}$$

with one continuous parameter x and one integer parameter u.

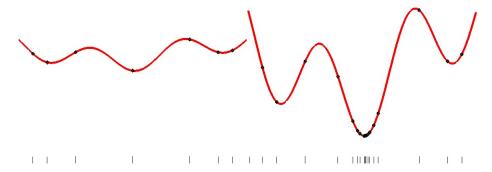


Fig. 2. Reduced mixed-integer global optimization problem

Applying the parallel index algorithm to solving the problem (14), we will find the solution of the problem (12). In this case the major part of trials will conducted in the subproblem, the solving of which corresponds to the solving of the initial problem (12). In the rest subproblems, only the minor part of trials will be performed since the solutions of these subproblems are the locally optimal ones. All the above is confirmed by Fig. 2, where the points of trials executed in the course of solving this problem are denoted by the dashes.

Thus, we have constructed the *Mixed-Integer Parallel Index Algorithm* (MIPIA) based on the reduction of the mixed-integer non-convex optimization problem to the non-convex optimization problem. The proposed computational scheme is based on the parallel index method for solving the continuous optimization problems and is not oriented onto any particular computational device. Here the parallel performing of several trials at different points of the search domain is one of key operations (see Step 7 of the algorithm), which can be implemented on CPU (with the use of OpenMP and/or MPI) as well as on GPU (with the use CUDA). The issues of the use of GPU for these purposes have been considered in details in [13, 14]. This approach to the use of GPU has been applied in the implementation of the MIPIA algorithm as well.

4 Results of experiments

The first series of experiments was conducted using the sequential version of the proposed algorithm in order to compare this one with well known methods of similar purpose.

Let us compare proposed MIPIA with a genetic algorithm for solving the mixed-integer global optimization problems implemented in Matlab Global Optimization Toolbox [15]. In Table 1, the numbers of trials required for solving the known test mixed-integer problems by these methods are presented. For both methods, the same accuracy of search 10^{-2} were used. These numerical experiments were conducted on a computer with Intel Core i5-7300 2.5 GHz processor and 8 Gb RAM under MS Windows 10. The results of experiments have demonstrated as the contract of the contract o

strated the advantage of MIPIA in the number of iterations as well as in the execution time.

Table 1. Comparison of MIPIA and GA

Test problem	GA		MIPIA	
1	k	t	\overline{k}	t
Problem 2 [16]	481	0.0601	417	0.04
Problem 3 [16]	1821	0.1130	3324	0.107
Problem 6 [16]	641	0.0510	118	0.001
Problem 1 [8]	481	0.1378	66	0.0007
Problem 2 [8]	481	0.0473	57	0.0006
Problem 7 [8]	841	0.0736	372	0.017

The next series of experiments were performed in order to evaluate the speedup of the parallel version of the proposed MIPIA algorithm with the use of CPU as well as GPU. In these experiments, a series of 100 mixed-integer test problems generated in a random way was solved. Computational experiments were carried out on Lobachevsky supercomputer. The node of supercomputer included two Intel Sandy Bridge E5-2660 2.2 GHz CPUs and 64 Gb RAM. The CPU had 8 cores, i.e. each node had a total of 16 cores and two NVIDIA Kepler K20X GPUs.

GKLS [17] is a well known generator of the test problems for the continuous multiextremal optimization. It allows generating the functions of arbitrary dimensionality with known properties (the number of local minima, the size of their domains of attraction, the global minimizer, etc.). This generator of multiextremal functions is often used for the investigations of the global optimization algorithms [18–22]. In Fig. 3 (a) and (b), the contour plots of two-dimensional GKLS functions are presented. Figures also shows the points of the trials performed by the method until the required accuracy $\epsilon = 10^{-2}$ was achieved.

In the performed experiments, the GKLS generator was used as a base for the construction the mixed-integer problems. The rules allowing generating the test problems of this type consist in the following.

- 1. A continuous multiextremal function $\varphi(y), y \in D = \{a_j \leq y_j \leq b_j, 1 \leq j \leq N\}$ is generated with the use of the GKLS generator. The global minimum of this function is achieved at the known point $y' = (y'_1, ..., y'_N)$ and equals $\varphi(y') = -1$.
- 2. A concave mixed-integer function

$$h(y,u) = -2 \left[\sum_{j=1}^{N} \left(\frac{y_j - y_j'}{b_j - a_j} \right)^2 + \sum_{j=1}^{M} \left(\frac{u_j - b_j}{b_j - a_j} \right)^2 \right],$$

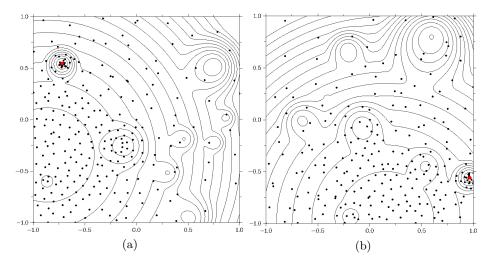


Fig. 3. Solving a two-dimensional problem using the index algorithm

is generated where

$$y \in D = \{a_j \le y_j \le b_j, 1 \le j \le N\} \subset \mathbb{R}^N,$$

 $u \in U = \{u_j \in \{a_j, ..., b_j\}, 1 \le j \le M\}.$

This function has N continuous and M discrete parameters and achieves its minimum value at the point (y',b).

3. The coefficient

$$h_{max} = 4 - \min_{y,u} h(y,u), \ y \in D, u \in U.$$

is computed. It is obvious, that the minimum of a concave function $\mu(y,u)$ is located at one of the corner points of the search domain. Therefore, if the problem dimensionality is of the order of 10 it can be found by the brute force method.

4. A multiextremal mixed-integer function

$$f(y,u) = \left(\varphi(y) + \sum_{j=1}^{M} u_j\right) \left(h_{max} + h(y,u)\right).$$

is formed. By construction, f(y,u) would take its minimum value at the point (y',b).

In the problems generated in our experiments, there were 5 discrete and 6 continuous parameters $\,$

$$y \in D = \{-1 \le y_j \le 1, 1 \le j \le 6\} \subset R^6,$$

 $u \in U = \{u_j \in \{-1, -1/3, 0, 1/3, 1\}, 1 \le j \le 5\}.$

A hundred 11-dimensional mixed-integer problems of this type were generated in total. For the purpose of simulation of the computational complexity inherent to applied optimization problems, calculation of the objective function in all performed experiments was made more complex by additional calculations without changing the type of function and arrangement of its minima (series summation from 80 thousand elements). The accuracy of the search was equal to 10^{-2} .

In Table 2, the results of experiments on CPU with the use of OpenMP are presented subject to the number of employed threads p. Total 1, 8, and 16 threads were used. The average number of iterations K_{av} required to solve the problem, the average time of solving T_{av} (in seconds), the time speedup S, and iteration speedup s (with respect to the sequential run, i.e. for p=1) are presented. In accordance with the parallelization scheme, the number of trials within a single iteration of the parallel algorithm was equal to the number of employed threads.

Table 2. The results of experiments on CPU

p	T_{av}	K_{av}	S	s
1 8		3221023 512314		 6 2
0	717	209237		0.0

As one can see from Table 2, almost linear speedup in iterations and an significant speedup in the problem solving time have been observed. At that, the sequential algorithm spent almost 1.5 hours in average to solve a problem.

In Table 3, the results of experiments on GPU with the use of CUDA are presented subject to the number of GPU threads employed. The average number of iterations K_{av} required to solve a problem, the average solving time T_{av} (in seconds), the time speedup S, and iteration speedup s (with respect to the full load of CPU on a cluster node) are presented.

Table 3. The results of experiments on GPU

p	T_{av}	K_{av}	S	s
256	33.6	1522	21.3	137
512	31.2	919	23.0	228
1024	30.2	412	23.7	508
2048	38.5	244	18.6	858

The results of experiments demonstrate almost the same time speedup and linear iteration speedup when using p=256,512, and 1024 threads. However, when using p=2048 threads, the algorithm worktime increased but the number of iterations continued to decrease. This effect was explained by the fact that for parallel running of p trials GPU is used but for processing the results of the trials (which implies the processing of the whole search information accumulated during the preceding iterations) CPU is uses. And when employing p=2048 GPU threads, the time, which is spent for the transfer and processing of the results of 2048 trials became comparable to the time of executing the trials that leads to the slowing down of the algorithm as a whole.

5 Conclusion

In the paper the results obtained in Lobachevsky State University of Nizhni Novgorod when developing and investigating the parallel global optimization algorithms for solving the multiextremal problems, in which some parameters are continuous and the others are the discrete ones are presented. An efficient parallel algorithm has been proposed for solving the problems of the specified class. In the sequential variant, this algorithm does not inferior to similar purpose algorithm implemented in Matlab Global Optimization Toolbox. In the parallel variant, the proposed algorithm allows the efficient implementations on CPU as well as on GPU. The numerical experiments on a series of 100 multiextremal mixed-integer test problems have been carried out convincingly demonstrating a good speedup of the algorithm with the use of GPU. Thus, the parallel algorithm with the use of GPU demonstrated the time speedup S=182 relative to the sequential one and S=23.7 relative to the algorithm fully employing two CPU on the cluster node.

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