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DMITRI KVASOV

Abstract. – *This paper briefly describes some results of the author's PhD thesis*[1], *which has been specially mentioned by the Italian INdAM–SIMAI Committee for the Competition "The Best PhD Thesis in Applied Mathematics defended in 2004–2006". In this work, a global optimization problem is considered where the objective function is a multidimensional black-box function satisfying the Lipschitz condition over a hyperinterval and hard to evaluate. Such functions are frequently encountered in practice that explains a great interest of researchers to the stated problem. A new diagonal scheme which is aimed for developing fast global optimization algorithms is presented, and several such algorithms are introduced and examined. Theoretical and experimental studies performed confirm the benefit of the new approach over traditionally used diagonal global optimization methods.*

1. – Introduction and problem statement.

The PhD thesis research, briefly described in this paper, is dedicated to *global optimization*—a field studying theory, numerical methods, and implementation of models and strategies for solving multiextremal optimization problems. The rapidly growing interest in this field is explained by both the raising number of applied decision-making problems, that are modelled by multiextremal objective functions and constraints, and the significant development of the advanced computer facilities during the last decades.

The attention to the field of global optimization is due to advantages that can be obtained in practice by applying globally optimal solutions instead of local ones provided by local optimization techniques. In fact, very often in real-life applications both the objective function and constraints can be black-box, multiextremal, non-differentiable, and hard to evaluate (see, e.g., [5, 8, 18-20, 33, 34]. An example

(*) Comunicazione tenuta a Bari il 26 settembre 2007 in occasione del XVIII Congresso dell'Unione Matematica Italiana.

([1]) The thesis "Multidimensional Lipschitz Global Optimization Based on Efficient Diagonal Partitions", supervised by Prof. Ya.D. Sergeyev, has been defended by the author on May 5, 2006, at the University of Rome "La Sapienza".

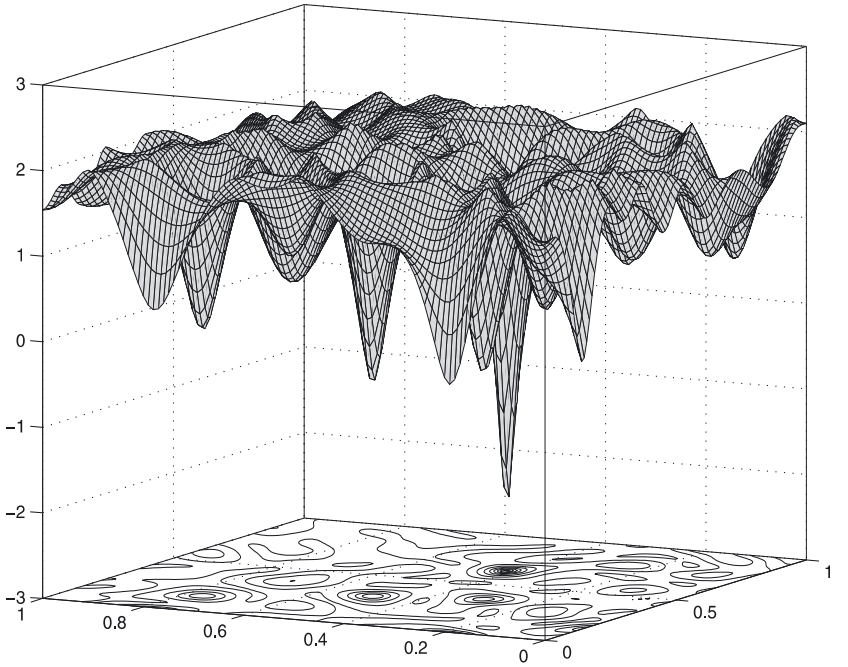

Fig. 1. – A multiextremal two-dimensional objective function.

of a two-dimensional multiextremal objective function (from the class of functions considered in [33]) is given in Fig. 1; this type of objective functions is encountered, for instance, when the maximal working stress over the thin elastic plate under some lumped transverse loads are estimated (see [33]). Nonlinear local optimization methods and theory (described in a vast literature, see, e.g., [1, 2, 17, 21] and the references given therein) are not very successful in solving these problems.

It should be stressed that the possibility to outperform the item-by-item examination techniques in solving multiextremal problems is fundamentally based on the availability of some realistic a priori assumptions characterizing the objective function and constraints (see, e.g., [8, 18, 19, 33]). They serve as mathematical tools for obtaining estimates of the global solution related to a finite number of function evaluations and, therefore, play a crucial role in the construction of any efficient global search algorithm.

One of the natural and powerful (from both the theoretical and the applied points of view) assumptions on the global optimization problem is that the objective function and constraints have bounded slopes. In other words, any limited change in the object parameters yields some limited changes in the character-

istics of the objective performance. This assumption can be justified by the fact that in technical systems the energy of change is always limited (see the related discussion in [32, 33]). One of the most popular mathematical formulations of this property is the Lipschitz continuity condition, which assumes that the difference (in the sense of a chosen norm) of any two function values is majorized by the difference of the corresponding function arguments, multiplied by a positive factor L. In this case, the function is said to be *Lipschitz* and the corresponding factor L is said to be *Lipschitz constant*. The problem involving Lipschitz functions (the objective function and constraints) is said to be *Lipschitz global optimization problem*.

The Lipschitz continuity assumption, being quite realistic for many practical problems (see, e.g., [8, 9, 19, 33] and the references given therein), is also an effective tool for constructing global optimum estimates with a finite number of function evaluations, which allows one to construct numerical global optimization algorithms and to prove their convergence and stability.

The PhD thesis deals (see [11, 12] for the abstracts of the thesis) with approaches to solving numerically multidimensional Lipschitz global optimization problems, in which the objective function is defined over a hyperinterval D of the multidimensional Euclidean space $\mathbb{R}^N$ (the so-called *box-constrained optimization*). This particular case of the general global optimization problem can be formulated as follows

$$f^* = f(x^*) = \min f(x), \qquad x \in D, \tag{1}$$

where

$$D = [a, b] = \{x \in \mathbb{R}^N : a(j) \le x(j) \le b(j),\ 1 \le j \le N\}, \qquad a, b \in \mathbb{R}^N, \tag{2}$$

the objective function $f(x)$ satisfies the Lipschitz condition

$$|f(x') - f(x'')| \le L\|x' - x''\|, \quad x', x'' \in D, \quad 0 < L < \infty, \tag{3}$$

and $\|\cdot\|$ denotes the Euclidean norm.

The function $f(x)$ is supposed to be multiextremal, black-box, and it can be also non-differentiable. Thus, global optimization methods using derivatives cannot be taken for solving the problem (1)-(3). It is also assumed that evaluation of the objective function at a point (hereafter, this operation will be referred to as a *trial*) is a time-consuming operation.

This kind of problem is very frequent in practice. Let us refer only to the following examples: general (Lipschitz) nonlinear approximation; solution of nonlinear equations and inequalities; calibration of complex nonlinear system models; black-box systems optimization; optimization of complex hierarchical systems (related, for example, to facility location, mass-service systems); etc. (see, e.g., [4, 8, 19, 20, 33] and the references given therein).

In the next two sections, some known approaches to solving the stated pro-

blem are briefly described. The diagonal approach from [19] is particularly studied, especially from the viewpoint of the strategies for partitioning the search hyperinterval (see section 3). It is shown that traditionally used diagonal partition strategies execute many redundant evaluations of the objective function, independently of the rule for selecting hyperintervals for subdivision. This slows down the algorithm because of the time needed for the function evaluations. A new diagonal partition strategy, proposed in [26], is described in section 4. It allows one to avoid the computational redundancy of traditional diagonal strategies and to considerably speed up the search. By using this efficient partition strategy, a new diagonal scheme for creating fast Lipschitz global optimization algorithms is introduced (see [15, 30, 31]). In the framework of this new scheme, several powerful global optimization methods are presented (see section 5). The problem of testing global optimization algorithms systematically (see [7, 30]) is also considered in section 5.

2. – State of the art.

A great number of algorithms for solving the problem (1)-(3) have been proposed in the literature (see, e.g., [3, 4, 8, 9, 19, 32, 33] and the references given therein). These algorithms can be distinguished, for example, by the mode in which information about the Lipschitz constant from (3) is obtained and by the strategy of exploration of the search domain D from (2).

There are at least four approaches to specifying the Lipschitz constant L. First of all, it can be given a priori (see the references in [8, 9]). This case is very important from the theoretical viewpoint but is not very frequent in applications. The most practical approaches are based on an adaptive estimation of L in the course of the search for the global optimum. In such a way, algorithms can use either a global estimate of the Lipschitz constant (see, e.g., [9, 15, 19, 32, 33]) valid for the whole search region, or local estimates valid only for some subregions of the search domain (see, e.g., [14, 16, 23, 24, 33]). Finally, estimates of the Lipschitz constant can be chosen from a certain set of possible values (see, e.g., [6, 10, 30]).

It is important to note that global optimization algorithms using in their work a global estimate of the Lipschitz constant L (or some value of L given a priori) do not take into account local information about behavior of $f(x)$ over every small subregion of the search domain D. As has been shown in [23, 24, 33], estimating local Lipschitz constants allows one to accelerate significantly the global search.

In exploring the multidimensional search domain D, various adaptive partition strategies have been proposed in the literature. For example, partitions of D into hyperintervals based on evaluating the objective function at central points of hyperintervals (the so-called center-sampling partition

strategies—see, e.g., [4, 6, 10]) or at two vertices corresponding to the main diagonal of hyperintervals (the so-called *diagonal partition strategies*—see, e.g., [9, 16, 19, 26]) have been used in Lipschitz global optimization. Various multisection techniques for partitions of hyperintervals have been studied in the framework of interval analysis (see the references in [4, 8, 19]). More complex partitions based on simplices (see, e.g., the references in [9]) and auxiliary functions of various nature have also been introduced (see, e.g., the references in [19, 33]). Moreover, several attempts to generalize various partition schemes in a unique theoretical framework have been made (see, e.g., [9, 19, 25]).

Another possible approach to solving multidimensional Lipschitz global optimization problems consists of extending some efficient one-dimensional algorithms to the multidimensional case. There exist at least three extensions of these algorithms to the multidimensional case: diagonal approach (see [19]), which is a special case of the scheme of adaptive partition algorithms (or a more general scheme of the 'divide-the-best' algorithms [25]), reduction of the dimension by using Peano curves (see [32, 33]), and nested global optimization scheme (see [8, 28, 32, 33]).

In the diagonal approach to solving Lipschitz global optimization problems, the initial hyperinterval D from (2) is partitioned into a set of smaller hyperintervals D_i, the objective function is evaluated only at two vertices corresponding to the main diagonal of hyperintervals of the current partition of D, and the results of these evaluations are used to select a hyperinterval for the further subdivision. In the approach of the dimension reduction, a certain space-filling curve is used in numerical algorithms to approximate the Peano curve with a prescribed partition order (which depends on the desired search accuracy), which is then used to reduce the original multidimensional problem to a one-dimensional one by considering the objective function along this one-dimensional curve. Finally, in the nested optimization scheme, the multidimensional problem is reduced to the nested family of one-dimensional subproblems.

3. – Diagonal approach.

Our main attention is focused on the diagonal approach (see [19]). First, because the extension of one-dimensional global optimization algorithms to the multidimensional case can be performed naturally by means of the diagonal scheme (see, e.g., [16, 19, 26]). Second, because the diagonal approach is close from the computational point of view to one of the simplest strategies—center-sampling technique—but at the same time, the objective function is evaluated at two points of each hyperinterval of the current partition of the search domain, providing in this way more information about the function than center-sampling methods.

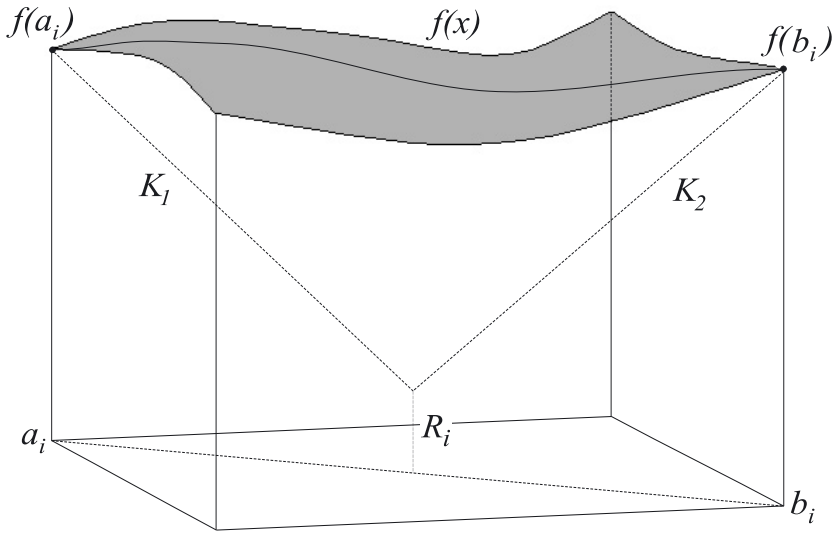

Fig. 2. – Estimation of the lower bound of a Lipschitz function over a hyperinterval D_i in diagonal algorithms.

In a sense, the diagonal approach can be viewed as an approach unifying ideas of adaptive partition algorithms and techniques of the problem dimension reduction. In order to decrease the computational efforts needed to describe the objective function $f(x)$ at every small hyperinterval $D_i \subset D$, $f(x)$ is evaluated only at the vertices a_i and b_i corresponding to the main diagonal of D_i (see Fig. 2). At every iteration the 'merit' of each hyperinterval so far generated is estimated. The higher 'merit' of a hyperinterval D_i corresponds to the higher possibility that the global minimizer x^* of $f(x)$ belongs to D_i. The 'merit' is measured by a real-valued function R_i called *characteristic* (see [33]). In order to calculate the characteristic R_i of a multidimensional hyperinterval D_i, some one-dimensional characteristics can be used as prototypes. After an appropriate transformation they can be applied to the one-dimensional segment being the main diagonal $[a_i, b_i]$ of the hyperinterval D_i. For example, in Fig. 2 the characteristic R_i is represented by the lower bound of $f(x)$ over the main diagonal of D_i, which can be (under some sufficiently general conditions) the lower bound of $f(x)$ over the whole hyperinterval D_i. It is found at the intersection of the lines K_1 and K_2, which are minorant linear (with the slopes $\pm\hat{L}$, $\hat{L} \geq L$ where L is from (3)) functions for $f(x)$ over this main diagonal.

A hyperinterval having the 'best' characteristic (e.g., the biggest one, as in the information approach (see, e.g., [32]), or the smallest one, as in the geometric approach, see, e.g., [24, 33]) is partitioned by means of a partition operator (diagonal partition strategy), and new trials are performed at two vertices corre-

sponding to the main diagonal of each generated hyperinterval. The concrete choice of the characteristic R_i and the partition strategy determines the particular diagonal method.

The diagonal approach is mainly analyzed from the viewpoint of the partition strategy. Traditionally, two diagonal strategies for hyperinterval partitioning are used in adaptive partition algorithms: 2^N-*Partition* (see, e.g., [9, 10, 14, 16, 19) and *Bisection* (see, e.g., [9, 14, 19]). In the former, a hyperinterval D_t to be partitioned is divided into 2^N new hyperintervals by N mutually orthogonal hyperplanes (where N is the problem dimension from (2)). In the latter, it is divided into two hyperintervals by only one hyperplane that is perpendicular to the edge of D_t having the largest length. After partitioning D_t, the function is evaluated only at the vertices of the main diagonals of the hyperintervals obtained.

In this connection, two new diagonal algorithms are proposed (see [14]). They extend the one-dimensional geometric method [24], which uses the local tuning on the behavior of the objective function, to the multidimensional case by means of the diagonal approach. The two proposed methods differ in the usage of the partition strategies they apply to subdivide the search hyperinterval $D \subset \mathbb{R}^N$: the first method uses the 2^N-Partition strategy, while the second one uses the Bisection strategy. Convergence analysis of both methods is performed and the results of numerical experiments with the new methods are reported in [14]. The goal of these numerical experiments is dual: first, to compare the local tuning technique with the traditional approach using adaptive estimates of the global Lipschitz constant in the case of diagonal methods; second, to establish which of two traditionally used diagonal partition strategies, i.e., 2^N-Partition or Bisection, works better. As shown, the new diagonal methods with local tuning outperform the methods using adaptive estimates of the global Lipschitz constant on the considered set of test problems from the literature. In its turn, the Bisection strategy seems to work better than the 2^N-Partition strategy.

Both the 2^N-Partition and Bisection appear to be quite efficient when applied at a separate iteration of a diagonal algorithm. However, as shown in [14, 26], both strategies generate too many trial points in the course of the algorithm execution, independently of the form of the characteristic that determines which hyperinterval is to be divided at each particular iteration. In fact, high performance is ensured in both strategies by evaluating the function only at two vertices corresponding to the main diagonal of each newly generated hyperinterval. Unfortunately, it turns out that each hyperinterval contains more than two trial points in both strategies. Another, more serious, difficulty arising when these strategies are used is the loss of information about proximity of the vertices of hyperintervals generated at different iterations, which leads to unnecessary evaluation of $f(x)$ at close points. In the worst case, the vertices of different

hyperintervals coincide, in which case $f(x)$ is evaluated twice at the same point (see [15, 26]).

Thus, it is demonstrated that the traditional diagonal partition strategies do not fulfill the requirements of computational efficiency because of the execution of many redundant evaluations of the objective function.

4. – New diagonal partition strategy.

A new diagonal adaptive partition strategy, originally proposed in [26] (see also [27]), that allows one to avoid the computational redundancy in diagonal algorithms is described. The properties of the introduced diagonal partition strategy are examined and its advantages with respect to traditional diagonal partition schemes are discussed (see [15, 26]). In contrast to the traditional diagonal partition strategies which execute a great number of redundant function evaluations and, thus, can slow down the global search, the proposed partition strategy produces regular meshes of the function evaluation points and significantly outperforms the traditional strategies in terms of the number of function evaluations. It is also demonstrated that the advantages of the new partition strategy become more pronounced when the problem dimension increases (see, e.g., [15, 30]).

Let us illustrate the new diagonal strategy by an example without going into describing its computational scheme formally. This example (see Fig. 3) represents partitions of the admissible hyperinterval $D = [a, b]$ from (2) after twelve iterations of a diagonal algorithm using the new strategy. Trial points of $f(x)$ are represented by black dots. The numbers around these dots indicate iterations at which the objective function is evaluated at the corresponding points. Hyperintervals to be subdivided at each iteration are shown in grey. In Fig. 3*(a)*, the situation after the first two iterations is presented. At the first, initial, iteration, the objective function $f(x)$ is evaluated at the vertices a and b of the search hyperinterval $D = [a, b]$. At the next iteration, the hyperinterval D is subdivided into three equal hyperintervals. This subdivision is performed by two hyperplanes orthogonal to the longest edge (in this case, orthogonally to the vertical axis) of D and passing through points ξ and ζ, selected in such a way that the longest edge is subdivided into three equal segments (see Fig. 3(a)). Two trials are performed at both the points ξ and ζ.

At the third iteration, three smaller hyperintervals are generated (see Fig. 3(b)). It seems that a trial point of the third iteration is redundant for the hyperinterval (in grey) selected for the next subdivision since only two points over it are used by a diagonal method. In reality, from Fig. 3(c) it can be seen that one of the two points of the fourth iteration (the iteration number around it is enclosed in brackets) coincides with the point 3 at which $f(x)$ has already been

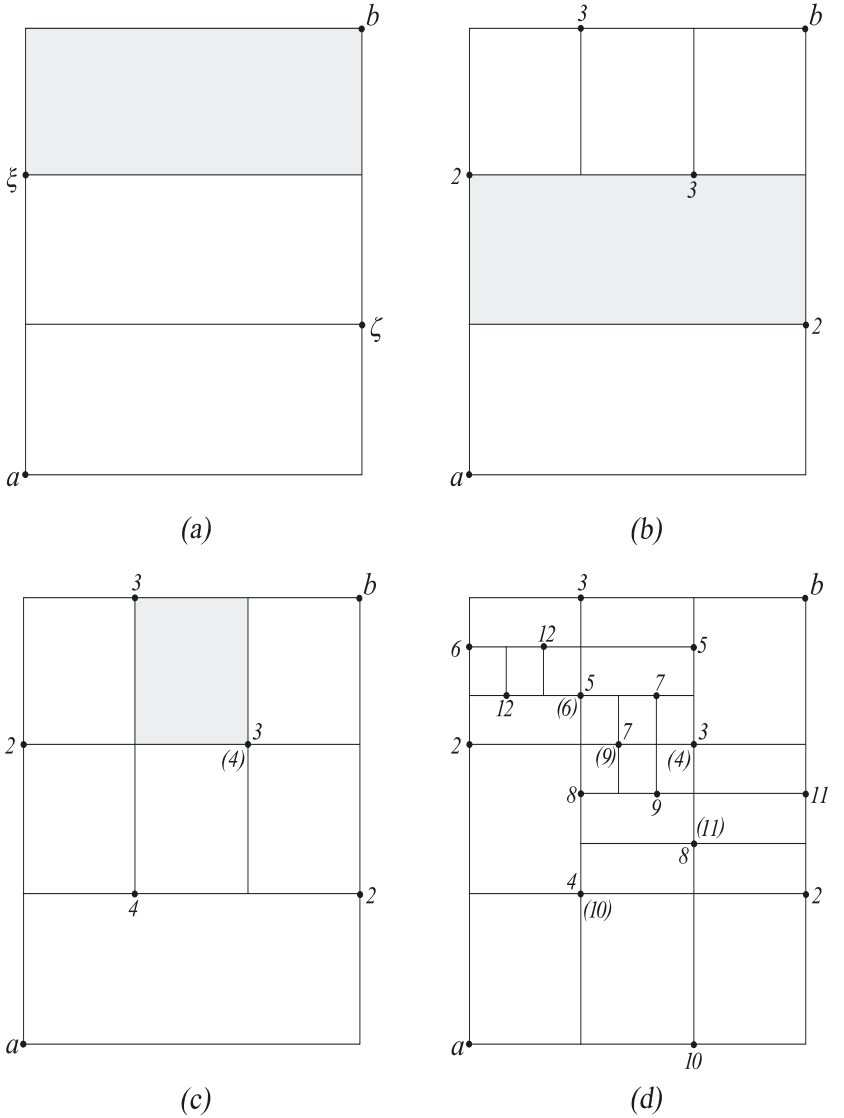

Fig. 3. – Subdivisions of a two-dimensional search hyperinterval by using the new diagonal partition strategy

evaluated. Thus, it is not necessary to evaluate the function at this point again: the function value obtained at previous iteration can be re-used. This value can be stored in a special vertex database (see [15, 29]) and is simply retrieved when necessary without performing a new trial. Fig. 3(*d*) demonstrates the situation

after 11 subdivisions. Among 24 points at which $f(x)$ is to be evaluated, there are 5 repeated points (the iteration numbers around these points are enclosed in brackets). That is, the objective function is evaluated 19 rather than 24 times. At the same time, the number of generated hyperintervals (equal to 23), which reflects the degree of a qualitative examination of the search domain D, is greater than the number of trial points (equal to 19). Such a difference becomes more significant in the course of further subdivisions, and the number of trial points with reused (not re-evaluated) function values increases.

The new strategy produces regular meshes of the trial points in such a way that one vertex where $f(x)$ is evaluated can belong to several hyperintervals (up to 2^N). Thus, the time-consuming operation of performing a trial is replaced by a significantly faster operation of reading (up to 2^N times) the function values obtained at the previous iterations and saved in a special database. Hence, the new partition strategy considerably speeds up the search and also leads to saving computer memory. It should be highlighted that the advantages of the new strategy become more pronounced when the problem dimension N increases (see, e.g., [15, 30]).

The regular structure of subdivisions performed by the proposed partition strategy determines the existence (theoretically demonstrated in [26]) of a special indexation of hyperintervals establishing links between hyperintervals generated at different iterations. This indexation may avoid the necessity of storing the coordinates of vertices of hyperintervals at which the objective function is evaluated, since they can be calculated by knowing the indices of the corresponding hyperintervals. As it can be shown (see [15, 26, 29]), the indexation allows one to store information about vertices and the corresponding values of the objective function in a special database. In this case, the hyperintervals can have only pointers to the vertices and do not duplicate the coordinates and the related description information, thus avoiding redundant function evaluations. The objective function value at a vertex is calculated only once, stored in the database, and retrieved when required. An implementation of this database is not a simple task since both the operations of retrieving elements from the database and insertion of new elements into it are to be executed rapidly. A possible way for implementing these operations is suggested (see [29]), and a prototype of the system managing the database is presented (see also [31]). This prototype can be used to develop various diagonal methods based on the proposed efficient partition strategy.

5. – New methods based on efficient diagonal partitions and their numerical testing.

A new efficient scheme for creating fast Lipschitz global optimization algorithms is thus proposed (see [15, 30, 31]). It relies on the introduced diagonal

partition strategy and opens interesting perspectives for creating new global optimization methods. First, popular one-dimensional algorithms may be efficiently extended to the multidimensional case by using this scheme. Some new multidimensional diagonal methods for solving (1)-(3), based on the new strategy, are briefly described in this section. Second, the proposed partition strategy may be successfully parallelized by the technique from [28, 33], allowing one to obtain further speed up.

For example, a multidimensional diagonal information algorithm that uses an adaptive estimate of the global Lipschitz constant and extends the one-dimensional information method from [32, 33] to the multidimensional case is proposed in [15]. The choice of this particular one-dimensional method is motivated by good estimates of its convergence rate. Sufficient global convergence conditions of a new type are established for the algorithm. The results of extensive numerical experiments executed to test this new information algorithm and to compare it with diagonal global optimization methods that use traditional partition strategies (namely, the 2^N-Partition and Bisection strategies) are reported in [15]. The results of the experiments substantiate theoretical conclusions about the properties of the introduced partition strategy. They demonstrate that the proposed information algorithm has considerable advantages with respect to the traditional diagonal methods in terms of both the number of function trials and the qualitative analysis of the search domain. It is particularly important that the advantages of the new method increase with the growth of the problem dimension.

Another diagonal algorithm for solving Lipschitz global optimization problems (see [30]) can be characterized by using a new way to estimate the Lipschitz constant. In this method (which itself is constructed in the framework of the proposed diagonal scheme), in order to calculate the lower bounds of the objective function over hyperintervals, possible estimates of the Lipschitz constant varying from zero to infinity are considered at each iteration. The procedure of estimating the Lipschitz constant evolves the ideas of the popular method DIRECT from [10] (see also [4]) to the case of diagonal algorithms. A new technique balancing the usage of local and global information during the global search is also incorporated in the method. Convergence conditions of the algorithm are established. Extensive numerical experiments are performed (on more than 1600 functions) in order to compare the proposed method with the DIRECT algorithm [10] and its modification [6], widely used for solving industrial global optimization problems. The results of numerical experiments demonstrate (see [30]) that the new method has considerable advantage with respect to both the DIRECT-family algorithms in terms of the comparison criteria considered. It is especially important that advantages of the method become more pronounced when multidimensional multiextremal functions with a complex structure (like in many engineering applications) are considered.

Other global optimization methods can also be proposed in the framework of the efficient diagonal scheme (see, e.g., [31]). They can be successfully applied for solving application problems. For example, the problem of global tuning of fuzzy power-system stabilizers, present in a multi-machine power system, in order to damp the power system oscillations (that plays an important role in enhancing overall system stability) is considered in [13]. The usage of the new global optimization techniques can provide a significant improvement on both the algorithm execution time and the quality (e.g., robustness) of the solution. In fact, the numerical results from [13] demonstrates that the new methods find a better global solution by spending a significantly fewer number of expensive function trials with respect to conventional genetic algorithms frequently used by engineers to solve this problem.

To conclude, it should be emphasized that a particular attention is also paid to the problem of testing global optimization algorithms. It is noted that despite the existence of test implementations and good literature studies describing benchmark databases and test sets (see, e.g., [3, 5, 22, 33, 34] and the references given therein), there still exist some difficulties during the work with tests. The lack of complete information (such as number of local optima, their locations, attraction regions, local and global values, etc.) describing global optimization tests taken from real-life applications creates additional difficulties in verifying validity of the algorithms.

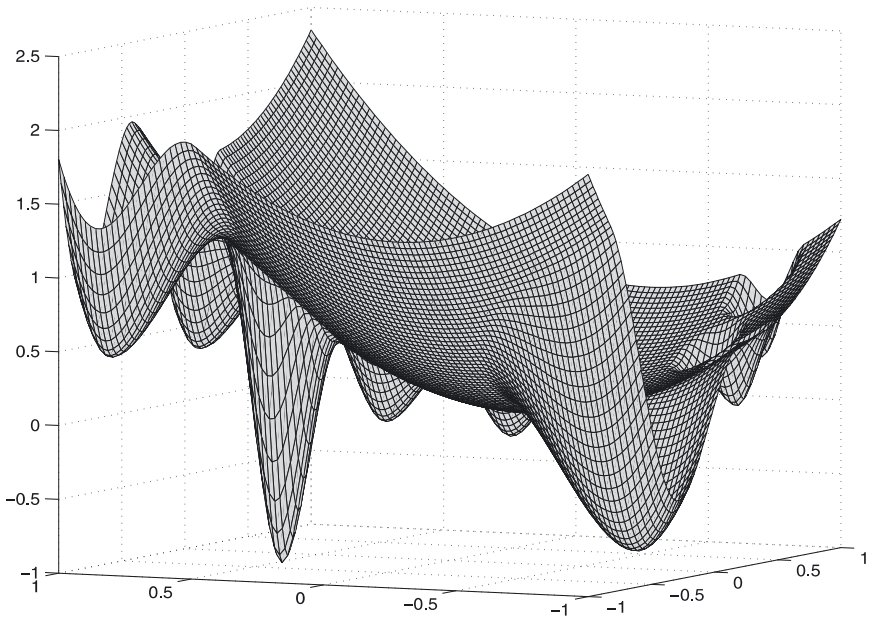

Fig. 4. – A two-dimensional differentiable GKLS test function with ten local minima.

A procedure (and the corresponding software, called *GKLS-generator*) for generating three types (non-differentiable, continuously differentiable, and twice continuously differentiable) of classes of multidimensional and multi-extremal test functions with known local and global minima is presented in [7] (an example of a test function from a differentiable class is given in Fig. 4). The procedure consists of defining a convex quadratic function systematically distorted by polynomials. Each test class provided by the generator consists of 100 functions and is defined only by the following five parameters: (i) problem dimension, (ii) number of local minima, (iii) global minimum value, (iv) radius of the attraction region of the global minimizer, (v) distance from the global minimizer to the quadratic function vertex. The other necessary parameters are chosen randomly by the generator for each test function of the class. It should be stressed that the generator produces always the same test classes for a given set of the user-defined parameters allowing one to perform repeatable numerical experiments. A set of criteria for comparison of different methods by using classes of test functions is also introduced (see, e.g., [30]).

The generator is available on the ACM Collected Algorithms (CALGO) database (the CALGO is part of a family of publications produced by the Association for Computing Machinery) and it is also downloadable for free from http://wwwinfo.deis.unical.it/~yaro/GKLS.html. It has already been downloaded by companies and research organizations from more than 20 countries of the world.

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