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A new class of test functions for global optimization

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Abstract In this paper we propose a new class of test functions for unconstrained global optimization problems. The class depends on some parameters through which the difficulty of the test problems can be controlled. As a basis for future comparison, we propose a selected set of these functions, with increasing difficulty, and some computational experiments with two simple global optimization algorithms.

Keywords Global optimization · Test problems · Multilevel structure · Molecular conformation problems

1 Introduction

In the field of optimization the definition of test problems is an important and non-trivial task. Test problems should reflect the wide variety of difficulties encountered when solving practical problems and are essential in validating algorithms. In the field of Global Optimization (GO in what follows) there exists an old class of test functions, the Dixon–Szegö test set (see Dixon and Szegö 1978). Unfortunately, these problems are of limited dimension and of mild difficulty (they usually have only few local minimizers). Therefore, testing *only* on them is not an appropriate way to validate GO algorithms. The test functions presented in Hock-Schittkowski (1981) and Schittkowski (1987) are widely employed for constrained local optimization but many of these test problems have several local minimizers with different function values and are thus also appropriate tests for GO methods. More multimodal functions are also included in Moré et al. (1981). In Schoen (1993) a class of test functions is proposed

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whose global minimizer is a priori known, whose smoothness is controllable by means of a set of parameters, and for which the number and location of stationary points are controllable by the user. In Mathar and Žilinskas (1994) a method in multidimensional scaling is employed to define multimodal test functions. There also exist test sets for specific GO problems (see, e.g., Kalantari and Rosen 1986 for concave optimization problems, Pardalos 1987 for quadratic problems). The interest for new and widely recognized GO test problems emerged in a number of recent publications. Here we recall a book (Floudas et al. 1999), some papers (Gaviano et al. 2003, Lavor and Maculan 2004, Neumaier et al. 2005, Pinter 2002), and the global optimization web site (GO-site 2005). In this paper, we will focus our attention on unconstrained GO problems for which it can be guaranteed that the global minimizer lies within a limited region and for which efficient local search procedures exist. We will propose a new class of test functions depending on a limited number of user-specified parameters, through which it is possible to control a relevant source of difficulty of these unconstrained problems related to the positions of local minimizers. In particular, the proposed test functions will be able to mimic situations which have been observed in some practical GO applications, namely molecular conformation problems.

The paper is structured as follows. In Sect. 2, we recall some features on which the difficulty of GO problems depend. In particular, we will discuss the role played by the number and positions of local minimizers. In Sect. 3, we introduce some basic one-dimensional and multidimensional component functions, and we generate GO test functions with the required properties by iterative procedures starting from the basic components. For any generated test function the objective function value of the global minimizer will be known, but its position will not. In Sect. 4, we summarize the (user-defined and randomly assigned) parameters employed to define the test functions. In Sect. 5, we present the results of two simple GO algorithms on some selected test functions, which can be employed as a basis for future comparison, and we give some information about the web site (GOL 2006) where a C++ library of our test functions can be downloaded.

2 Features making a GO problem difficult

The difficulty of a GO problem depends on many factors. Among the most relevant ones we recall: the *size of the basin of attraction* of the global minimizer (which can be explicitly controlled in, e.g., the test functions proposed in Gaviano et al. 2003); the *shape* of the function around the global minimizer, the classical example being the Rosenbrock function, where the minimum point is inside a long, narrow and paraboloic-shaped flat valley, which makes convergence difficult; *dimension* (many existing test functions depend on a dimension parameter); *high multimodality*.

In this paper, we will focus our attention on the last source of difficulty. In Locatelli (2005) it is observed that the difficulty of highly multimodal GO problems is not merely connected to the number of local (and not global) minimizers. An important factor is how "chaotic" is the position of these local minimizers. This observation was stimulated by the analysis of some practical GO problems, namely molecular conformation problems such as the Lennard-Jones, Morse, Dzugutov, binary Lennard-Jones cluster optimization (see, e.g., Doye 2006), where one aims at predicting the most stable structure of a cluster of N atoms by globally minimizing a potential energy function. The number of local minimizers for such problems has been experimentally

observed to increase exponentially with the number N of atoms within the cluster, but the introduction of the notions of *funnel* and *funnel bottom* (see, e.g., Wales and Doye 1997) considerably simplified the solution of these problems. These notions lead to the definition of local minimizers at different levels in Locatelli (2005) which will be discussed in the following subsection.

2.1 Local minimizers at different levels

The notion of local minimizer is strictly connected to that of neighborhood: a local minimizer is a point with the lowest function value among all those in its neighborhood. By changing the neighborhood we also change the set of local minimizers. A standard local minimizer is a point with lowest function value within a d-dimensional sphere centered at it and with positive radius (d denotes the number of variables on which the function depends). According to the terminology in Locatelli (2005), a standard local minimizer is called a local minimizer at level 1. If we define a directed graph whose nodes are the local minimizer at level 1 and arcs are defined by a suitable neighborhood structure, then the local minimizers over this graph are called local minimizers at level 2. The definition of a suitable neighborhood structure is an important and nontrivial task. One possibility is to define arcs through transition points of first order (stationary points with a single negative eigenvalue) as done in Floudas and Jongen (2005). In this paper, we employ the following definition of an arc.

Definition 1 Given a threshold distance r_1 and two local minimizers X and Y at level 1, then the directed arc (X, Y) exists if the following two conditions are satisfied:

(1) $\exists\, Z \neq X : \|X - Z\| \leq r_1$ and $f(X) \geq f(Z)$, where f denotes the objective function;
(2) there exists a nonascending continuous path starting at Z and ending at Y, i.e., more formally $\exists\, W(\lambda)$, $\lambda \in [0, 1]$ such that
   (a) $W(0) = Z$;
   (b) $W(1) = Y$;
   (c) $g(\lambda) = f(W(\lambda))$ is a nonincreasing function for $\lambda \in [0, 1]$.

In particular, note that it must hold $f(Y) \leq f(X)$.

Given the above definition, a local minimizer at level 2 is a node/local minimizer at level 1 for which we have an ingoing arc from each of its neighbors. It also holds that a local minimizer at level 2 is a local minimizer at level 1 for which there exists no point at distance not larger than the threshold distance r_1 with a better function value.

Local minimizers at level 2 are the equivalent of funnel bottoms in the terminology of the above mentioned molecular conformation problems.

Some remarks follow.

Remark 1 Definition 1 depends on the threshold distance r_1. The choice of r_1 determines the neighborhood of local minimizers at level 1 and, as for combinatorial problems,[1] this choice is fundamental. We should choose a neighborhood structure so that the number of local minimizers at level 2 is small but at the same time the size of the neighborhood of local minimizers at level 1 is also small so that it can be efficiently explored. The extreme choice $r_1 = 0$ makes the neighborhood of any local minimizer at level 1 empty and, thus, trivial to explore, but at the same time local minimizers

[1] Note that, under the assumption of a finite number of local minimizers at level 1, if we restrict the attention to them we are reducing our GO problem to a combinatorial one.

at level 2 coincide with local minimizers at level 1. At the other extreme, the choice $r_1 = +\infty$ reduces the number of local minimizers at level 2 to the number of global minimizers but the neighborhood of each local minimizer at level 1 contains all other local minimizers at level 1, making the neighborhood too large. The value r_1 should be chosen, when possible, in such a way that the number of local minimizers at level 2 is much smaller than the number of local minimizers at level 1, but at the same time the neighborhoods can still be efficiently explored.

This has been a key observation in solving the above mentioned molecular conformation problems. Indeed, in these problems it is usually possible to define neighborhoods of manageable size for which the number of local minimizers at level 2 (or funnel bottoms) is much lower than the (huge) number of local minimizers at level 1 (see, e.g., Leary 2000).

Remark 2 Efficient algorithms for the detection of local minimizers at level 2 exist in the literature (see, e.g., Leary 2000; Addis and Leyffer 2004,; Addis et al. 2005). These algorithms are based on local moves between neighbor local minimizers at level 1, i.e., local moves on the directed graph. One of these algorithms (Monotonic Basin Hopping) will be shortly presented in Sect. 5.

Remark 3 Detecting a local minimizer at level 2 is much more time consuming than detecting a local minimizer at level 1. Indeed, while the cost of the latter is that of a single call of a local search routine, algorithms aimed at detecting local minimizers at level 2 have to move within the graph of local minimizers at level 1 and, thus, have to start multiple local searches.

Once local minimizers at level 2 were defined, in Locatelli (2005) also local minimizers at level 3 were defined in a similar way: they are the local minimizers over a directed graph where nodes are all the local minimizers at level 2 and arcs are defined as follows.

Definition 2 Given a threshold distance r_2 and two local minimizers $\mathcal{X}$ and $\mathcal{Y}$ at level 2, then the directed arc $(\mathcal{X}, \mathcal{Y})$ exists if the following two conditions are satisfied:

(1) $\exists$ a local minimizer $\mathcal{Z} \neq \mathcal{X}$ at level 1 such that $\| \mathcal{X} - \mathcal{Z} \| \leq r_2$ and $f(\mathcal{X}) \geq f(\mathcal{Z})$;
(2) there exists a nonascending path within the graph of the local minimizers at level 1 starting at $\mathcal{Z}$ and ending at $\mathcal{Y}$.

Remarks 1 and 3 immediately extend to local minimizers at level 2, pointing out the relevance of the choice of the parameter r_2 and the higher cost of detecting local minimizers at level 3 with respect to local minimizers at level 2. It is possible to define algorithms aimed at detecting local minimizers at level 3 which are based on local moves within the directed graph whose nodes are the local minimizers at level 2 (see Locatelli 2005) but more research in this direction is expected for the future. We also make the following remark.

Remark 4 The global minimizer is always a local minimizer at any level.

Note that we could also define higher levels but level 3 is already enough to define very challenging GO problems.

Figure 1 offers an example where we move from local minimizers at level 1 up to local minimizers at level 3. In Fig. 1a the white squares represent the local minimizers at level 1 of some objective function. In Fig. 1b a neighborhood structure is imposed

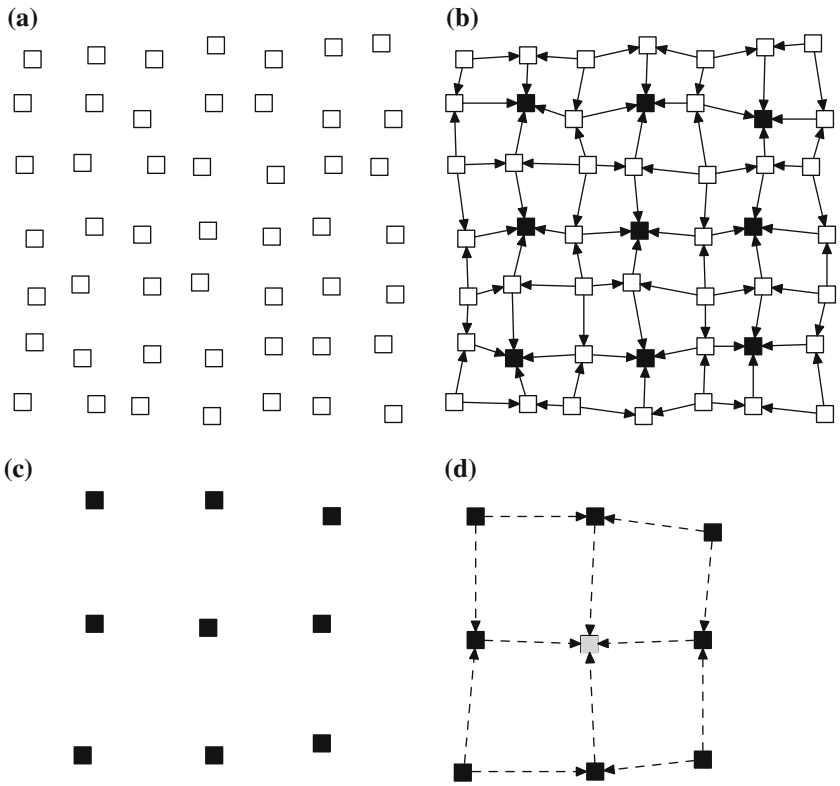

Fig. 1 **(a)** local minimizer at level 1, **(b)** neighborhood structure between local minimizer at level 1, **(c)** local minimizers at level 2, and **(d)** neighborhood structure between local minimizers at level 2: the grey square is the unique local minimizer at level 3

over the set of local minimizers at level 1 and local minimizers at level 2 (black squares) emerge. These correspond to nodes with only ingoing arcs. The local minimizers at level 2 are isolated in Fig. 1c. Finally, in Fig. 1d we impose a neighborhood structure over the set of local minimizers at level 2 and a single local minimizer at level 3 (the grey square) appears. This must also be the global minimizer.

2.2 Existing highly multimodal test functions

Once minimizers at different levels have been introduced, we can define different degrees of difficulty based on the first level at which only one or few local minimizers exist. The easiest GO problems are those with one or few local minimizers at level 1. In these cases a single or few runs of a local search procedure started at random initial points are able to reach the global minimizer, unless its region of attraction is particularly narrow (the so called golf-hole situation).

Highly multimodal problems are usually more difficult to solve. As pointed out in the previous subsection, in this case an essential feature to establish the difficulty of the problem is not only the number of local minimizers but also their positions. If many local minimizers (at level 1) exist but they are placed in a regular way in the search space, in particular in such a way that a single or few local minimizers at level 2 exist,

then this case can be efficiently solved by a run or few runs of algorithms aimed at detecting local minimizers at level 2. If not only many local minimizers at level 1 exist, but also many local minimizers at level 2, then the problem becomes more difficult and the difficulty further increases with the number of local minimizers at level 3.

Many highly multimodal test functions exist in the literature with a number of local minimizers (at level 1) which increases exponentially with the dimension. Most of these functions have (under suitable choices of the neighborhood of local minimizers at level 1) a single local minimizer at level 2 coinciding with the global minimizer. These include Rastrigin function (see Törn and Žilinskas 1989), Ackley function (see Ackley 1987), Levy functions (Levy and Montalvo 1985), Lavor and Maculan function (see Lavor and Maculan 2004). For all these functions an algorithm to detect local minimizers at level 2 is often quite efficient in detecting their global minimizers (see, e.g., the experiments in Addis et al. 2005). An exception is represented by the Schwefel function (see Schwefel 1981). The n-dimensional version of this function has 2^n local minimizers at level 2 but (again under suitable choices of the neighborhood of local minimizers at level 2) a single local minimizer at level 3 (see the experiments in Locatelli 2005).

With respect to the existing test functions, our aim is to introduce a set of test functions where the choice of the number of local minimizers at levels 2 and 3 (which affect the difficulty of a GO problem) is more flexible and, as we will see in the following section, is given by two parameters which are under the control of the user. These test functions allow to mimic the behavior of the previously mentioned molecular conformation problems for which the number of local minimizers at level 2 (funnel bottoms) is quite variable with the number N of atoms (see, e.g., the experiments in Leary 2000 for Lennard-Jones clusters). This fact makes the proposed test functions different from those presented in Lavor and Maculan (2004), which are also thought as test functions for molecular conformation problems but only have a single local minimizer at level 2.

3 Building the test functions

The aim of this section is to build progressively test functions with the required number of local minimizers at levels 2 and 3. Note that, following Definitions 1 and 2, in order to define local minimizers at levels 2 and 3 we need to specify values r_1 and r_2. For our test functions reasonable choices (i.e., as pointed out in Remark 1, choices which are able to considerably reduce the number of local minimizers when moving from one level to the upper one and at the same to keep the size of neighborhoods manageable) will be specified in what follows.

The proposed test functions will depend on some parameters. A complete summary of all the introduced parameters, the ranges within which they can be chosen, a short description of their meaning, and the indication if they have to be specified by the user or if they are randomly chosen will be given in Sect. 4.

3.1 The one-dimensional components

The first step toward the definition of the test functions is the introduction of some basic one-dimensional components with multiple minimizers at level 1. Following a common practice in the definition of test functions with many local minimizers at

level 1 (see, e.g., the definition of the Rastrigin test function in Törn and Žilinskas 1989), multiple minimizers are obtained through an *oscillation* term based on the cosine function

$$O^{K,H}_{c_1,c_2}(x) = -H\cos\left[2\pi\left\lceil\frac{K(c_2-c_1)}{10}\right\rceil\frac{(x-c_1)}{c_2-c_1}\right]+H. \tag{1}$$

Here c_1, c_2, K, and H are parameters, where c_1 is constrained to belong to the interval $[-3.5,-2]$, c_2 to the interval $[2,3.5]$, H to the interval $[10,30]$, K to the interval $[10,20]$. This oscillation term has (approximately) K local minimizers at level 1 (all with function value equal to 0) in the interval $[-5,5]$, two of which are in c_1 and c_2.

Once the oscillation term has been introduced, we are ready to introduce the two types of one-dimensional components through which the test functions are built. The first type of one-dimensional component is defined as follows

$$s_{p,K}(x) = \gamma_p(x) + O^{K,H}_{c_1,c_2}(x), \tag{2}$$

where p is a binary parameter and:

$$\gamma_p(x) = \begin{cases} 0.5(x-c_2)^2+2, & \text{if } p=0,\\ 0.5(x-c_1)^2+2, & \text{if } p=1. \end{cases} \tag{3}$$

The global minimizer x^* of $s_{p,K}$ is

$$x^* = \begin{cases} c_1, & \text{if } p=1,\\ c_2, & \text{if } p=0 \end{cases}$$

and $s_{p,K}(x^*)=2$. A particular instance of function $s_{p,K}$ is reported in Fig. 2a.

The second type of one-dimensional component is obtained through the sum of a bimodal function, denoted by ξ, with two local minimizers at level 1 in $x=c_1$ and $x=c_2$, and the oscillation term O

$$d_{p,K}(x) = \xi_p(x) + O^{K,H}_{c_1,c_2}(x). \tag{4}$$

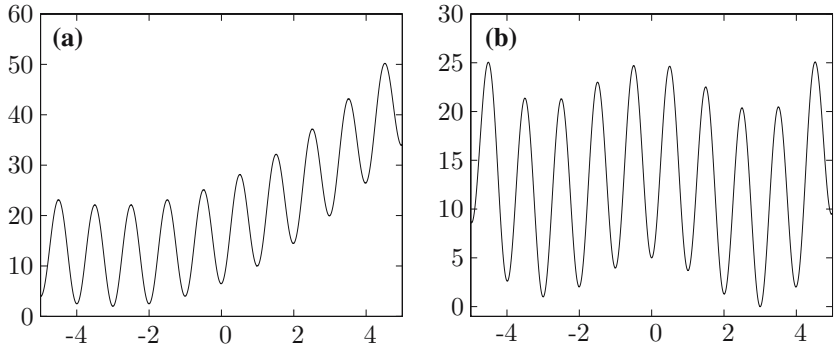

Fig. 2 One-dimensional component functions over the interval $[-5,5]$: **(a)** $s_{p,K}$ **(b)** $d_{p,K}$. In both cases the parameter values are $K=H=10$, $c_1=-3.0$, $c_2=3.0$, and $p=1$

The bimodal function ξ is defined as follows:

$$\xi_p(x) = \begin{cases} \xi^a(x) = \sum_{r=0}^{3} \alpha_r (x - c_1)^r, & \text{if } -5 \le x \le 0, \\ \xi^b(x) = \sum_{r=0}^{3} \beta_r (x - c_2)^r, & \text{if } 0 \le x \le 5. \end{cases}$$

The equations to find the parameters α_r and β_r, $r = 0, 1, 2, 3$ are

$$\begin{array}{llll} \frac{d\xi^a}{dx}(c_1) = 0 & \frac{d\xi^a}{dx}(0) = 0 & \xi^a(c_1) = p, & \xi^a(0) = 5, \\ \frac{d\xi^b}{dx}(c_2) = 0 & \frac{d\xi^b}{dx}(0) = 0 & \xi^b(c_2) = 1 - p, & \xi^b(0) = 5. \end{array}$$

Such equations guarantee that: ξ has continuous first derivative, has a minimizer in $x = c_1$ with value p, a minimizer in $x = c_2$ with value $1 - p$, and a maximum in $x = 0$ with value 5. Note that the constant 5 defining the value of ξ at $x = 0$ could be substituted by a further parameter (with value larger than 1), but we fixed this value in order to avoid the proliferation of parameters (the same observation applies to other constant values employed throughout the paper).

Function $d_{p,K}$ has, among others, two local minimizers at level 1 in $x = c_1$ with $d_{p,K}(c_1) = p$, and in $x = c_2$ with $d_{p,K}(c_2) = 1 - p$. The global minimizer is

$$x^* = \begin{cases} c_1, & \text{if } p = 0, \\ c_2, & \text{if } p = 1 \end{cases}$$

with $d_{p,K}(x^*) = 0$. A particular instance of function $d_{p,K}$ is reported in Fig. 2b.

Now we would like to find the local minimizers at level 2 for functions $s_{p,K}$ and $d_{p,K}$. A reasonable choice for the value r_1, needed to define local minimizers at level 2, is $r_1 = 1$. Indeed, we are going to prove that this choice allows to reduce the number of local minimizers at level 2 of functions $s_{p,K}$ to 1, and of functions $d_{p,K}$ to 2. We first prove the following lemma.

Lemma 1 *Any local minimizer at level* 1

(1) $\tilde{x} \neq c_1$ *of* $s_{1,K}$ *for any* $K \in [10, 20]$;
(2) $\tilde{x} \neq c_2$ *of* $s_{0,K}$ *for any* $K \in [10, 20]$;
(3) $\tilde{x} \neq c_1, c_2$ *of* $d_{p,K}$ *for any* $p \in \{0, 1\}$ *and any* $K \in [10, 20]$*;*

is not a local minimizer at level 2 for the corresponding function.

Proof We only give the proof for $s_{1,K}$. The proof for the other two cases is completely analogous. Following Definition 1 with $r_1 = 1$, it is enough to show that there exists a point y such that

$$| \tilde{x} - y | \le r_1 = 1 \quad \text{and} \quad s_{1,K}(y) < s_{1,K}(\tilde{x}).$$

We assume that $\tilde{x} < c_1$ (again, the proof for the case $\tilde{x} > c_1$ is completely analogous). Let us consider the difference between the argument of the cosine function in (1) at $\tilde{x} + 1$ and the same argument at $\tilde{x}$. Such difference is equal to

$$2\pi \left\lceil \frac{K(c_2 - c_1)}{10} \right\rceil \frac{1}{c_2 - c_1} \ge 2\pi \frac{K}{10} \ge 2\pi.$$

Therefore, the oscillation function certainly has a minimizer y in the interval $(\tilde{x}, \tilde{x}+1]$. Since $\tilde{x} < c_1$, we can choose $y \in (\tilde{x}, c_1]$. In view of the definiton (3) of γ_1, it holds that

$$\gamma_1(y) < \gamma_1(\tilde{x})$$

and, consequently,

$$s_{1,K}(y) < s_{1,K}(\tilde{x})$$

as we wanted to prove.

Observation 1 *Function $s_{1,K}$ has the unique local minimizer $x = c_1$ at level 2, while function $s_{0,K}$ has the unique local minimizer $x = c_2$ at level 2.*

Proof The point $x = c_1$ is the global minimizer of $s_{1,K}$ and, consequently, it is also a local minimizer at level 2 (see Remark 4). But, in view of Lemma 1, no other local minimizer at level 1 can be a local minimizer at level 2 for $s_{1,K}$. The proof for $s_{0,K}$ is completely analogous.

Observation 2 *Function $d_{p,K}$ has two local minimizers at level 2, namely $x = c_1$ and $x = c_2$.*

Proof We prove the result for $d_{0,K}$ (the proof for $d_{1,K}$ is completely analogous). The point $x = c_1$ is the global minimizer of $d_{0,K}$ and, thus, is also a local minimizer at level 2. But also point $x = c_2$ is a local minimizer at level 2. Indeed, this point turns out to be a global minimizer of $d_{0,K}$ over the interval $[0, +\infty)$. Since c_2 is constrained to belong to the interval $[2, 3.5]$, it holds that

$$[c_2 - 1, c_2 + 1] \subset [0, +\infty)$$

and, consequently, there is no point $y \neq c_2$ such that

$$|y - c_2| \leq 1 \quad \text{and} \quad d_{0,K}(y) \leq d_{0,K}(c_2)$$

from which we can conclude that $x = c_2$ is a local minimizer at level 2. Lemma 1 proves that there is no other local minimizer at level 2 for $d_{0,K}$.

3.2 Basic function with 2^m local minima at level 2

Next step is the introduction of basic n-dimensional components with 2^m ($m = 0, 1, \ldots, n$) local minimizers at level 2. The easiest way to obtain these functions is by summing up one-dimensional components with one or two local minimizers at level 2. However, this way we would get separable functions. In order to avoid that explicit or implicit exploitation of the separability (e.g., by moves along single or few coordinates) leads to very good but misleading results, we remove separability. This is easily obtained, e.g., by a one-to-one linear transformation of the original variables (see also Whitley et al. 1995 for methods which allow to move from separable to non-separable test functions). In particular we consider the following distance-preserving transformation. Let $\mathbf{x} = \{x_1, \ldots, x_n\}$ and

$$\mathbf{w}(x_1, \ldots, x_n) = \mathbf{A}\mathbf{x}, \tag{5}$$

where $\mathbf{A}$ is a $n \times n$ orthonormal matrix obtained by randomly generating a nonsingular matrix $\mathbf{A}'$ and then orthonormalizing it through the Gram-Schmidt process. Next we

define the following n-dimensional function:

$$F_m(\mathbf{x}) = \sum_{i=1}^{m} d_{p_i,K_i}(w_i(\mathbf{x})) + \sum_{i=m+1}^{n} s_{p_i,K_i}(w_i(\mathbf{x})), \tag{6}$$

where p_i are binary parameters, K_i are parameters constrained to belong to the interval $[10, 20]$, and functions s_{p_i,K_i} and d_{p_i,K_i} are defined as in (2) and (4), respectively. The global minimizer of F_m is the point $\mathbf{x}^*$ which uniquely solves the following system of n linear equations

$$w_i(\mathbf{x}^*) = \begin{cases} c_1, & \text{if } (p_i = 0 \text{ and } i \le m) \text{ or } (p_i = 1 \text{ and } i > m), \\ c_2, & \text{otherwise} \end{cases} \tag{7}$$

and $F_m(\mathbf{x}^*) = 2(n - m)$.

If we denote by S_i the set of all local minimizers at level 1 of the one-dimensional function s_{p_i,K_i} for $i > m$, and by D_i the set of all local minimizers at level 1 of the one-dimensional function d_{p_i,K_i} for $1 \le i \le m$, then the set of all local minimizers at level 1 for F_m corresponds to the set of solutions of the following linear systems

$$w_i(\mathbf{x}) = \ell_i \quad \text{for } i \in \{1, \ldots, n\}, \tag{8}$$

where $\ell_i \in D_i$ for $i \le m$ and $\ell_i \in S_i$ for $i > m$. We prove the following observation.

Observation 3 *Function F_m has 2^m local minimizers at level 2 corresponding to the solutions of the 2^m linear systems (8) obtained by choosing*

$$\begin{array}{ll} \ell_i = c_1 \text{ or } c_2, & \text{if } i \le m, \\ \ell_i = c_1, & \text{if } i > m \text{ and } p_i = 1, \\ \ell_i = c_2, & \text{if } i > m \text{ and } p_i = 0. \end{array} \tag{9}$$

Proof First we prove that if for at least one index $i \in \{1, \ldots, n\}$ the value ℓ_i is not one of those specified in (9), then the solution $\bar{\mathbf{x}}$ of the corresponding linear system (8) is not a local minimizer at level 2 for F_m. We only give a proof for the case when there exists an index $j > m$ such that $p_j = 1$ and $\ell_j \ne c_1$. In a way completely analogous to the proof of Lemma 1 we can show that there exists a value $\eta_j \in [\ell_j - 1, \ell_j + 1]$ such that the solution $\tilde{\mathbf{x}}$ of the linear system

$$\begin{array}{ll} w_i(\mathbf{x}) = \ell_i & \text{for } i \ne j, \\ w_j(\mathbf{x}) = \eta_j, & \end{array}$$

satisfies

$$F_m(\tilde{\mathbf{x}}) - F_m(\bar{\mathbf{x}}) = s_{1,K_j}(\eta_j) - s_{1,K_j}(\ell_j) < 0.$$

Since

$$\|\tilde{\mathbf{x}} - \bar{\mathbf{x}}\| = \|\mathbf{w}(\tilde{\mathbf{x}}) - \mathbf{w}(\bar{\mathbf{x}})\| = |\ \eta_j - \ell_j\ | \le r_1 = 1,$$

we can immediately conclude from Definition 1 that $\bar{\mathbf{x}}$ is not a local minimizer at level 2 for F_m.

Next step will be the proof that all the solutions of the 2^m linear systems whose ℓ_i values are given in (9) are local minimizers at level 2 for F_m. Let $\bar{\mathbf{x}}$ be the solution of one of these systems. It holds that $\bar{\mathbf{x}}$ is a global minimizer of F_m over the set defined by the following m linear inequalities

$$\begin{array}{ll} w_i(\mathbf{x}) \ge 0 & \text{for } i \le m \text{ and } w_i(\bar{\mathbf{x}}) = c_2, \\ w_i(\mathbf{x}) \le 0 & \text{for } i \le m \text{ and } w_i(\bar{\mathbf{x}}) = c_1. \end{array}$$

Since all points outside this set have distance from $\bar{\mathbf{x}}$ larger than $r_1 = 1$, we can conclude, following Definition 1, that $\bar{\mathbf{x}}$ is a local minimizer at level 2 for F_m.

In order to define local minimizers at level 3, we need to specify a value for r_2. A reasonable choice for our test functions turns out to be

$$r_2 = \max\{5, c_2 - c_1\}. \tag{10}$$

Indeed, with this choice we prove in the following observation that F_m has a single local minimizer at level 3.

Observation 4 *If r_2 is defined as in (10), the unique local minimizer at level 3 for F_m is the global minimizer of F_m obtained by solving (7).*

Proof Obviously, the global minimizer of F_m is a local minimizer at level 3 for F_m (see Remark 4). Now, let us consider a local minimizer at level 2 different from the global minimizer. We remark that the global minimizer is a solution of (8) with the following ℓ_i values

$$\begin{array}{ll} \ell_i = c_1, & \text{if } i \le m \text{ and } p_i = 0, \\ \ell_i = c_2, & \text{if } i \le m \text{ and } p_i = 1, \\ \ell_i = c_1, & \text{if } i > m \text{ and } p_i = 1, \\ \ell_i = c_2, & \text{if } i > m \text{ and } p_i = 0. \end{array}$$

Consider a local minimizer $\bar{\mathbf{x}}$ at level 2 obtained by solving the linear system (8) where at least one index $j \le m$ is such that $\ell_j = c_2$ when $p_j = 0$ or $\ell_j = c_1$ when $p_j = 1$ (the unique local minimizer at level 2 for which such index does not exist is the global minimizer). Now consider the solution $\tilde{\mathbf{x}}$ of (8) with the same ℓ_i values returning the solution $\bar{\mathbf{x}}$ except ℓ_j which is substituted by c_1 if $p_j = 0$, or by c_2 if $p_j = 1$. Then, it holds that

$$F_m(\tilde{\mathbf{x}}) - F_m(\bar{\mathbf{x}}) = \left\{ \begin{array}{l} d_{0,K_j}(c_1) - d_{0,K_j}(c_2) \text{ if } p_j = 0 \\ d_{1,K_j}(c_2) - d_{1,K_j}(c_1) \text{ if } p_j = 1 \end{array} \right\} < 0$$

and that

$$\|\tilde{\mathbf{x}} - \bar{\mathbf{x}}\| = \|\mathbf{w}(\tilde{\mathbf{x}}) - \mathbf{w}(\bar{\mathbf{x}})\| = c_2 - c_1 \le r_2$$

from which we can conclude from Definition 2 that $\bar{\mathbf{x}}$ is not a local minimizer at level 3.

3.3 Combining basic components

Let F_{m_2} and F_{m_1} be two basic components with $m_2 > m_1$. We want to build a new function G_t, $t = 2^{m_1} + 2^{m_2}$, by combining F_{m_1} and F_{m_2}, with t local minimizers at level 2. The combination is defined in what follows.

Definition 3 Given the combination operator $\times$, the combination operation is

$$G_t = F_{m_1} \times F_{m_2}$$

and its result is a function of the n-dimensional vector of basic variables $\mathbf{x} = (x_1, \ldots, x_n)$ and of the *auxiliary* variable y:

$$G_t(\mathbf{x}, y) = \left\{ \begin{array}{ll} G_t^a(\mathbf{x}, y) + O_{-2.5,2.5}^{\bar{K},F_{m_1}+F_{m_2}}(y), & \text{if } y \le 0, \\ G_t^b(\mathbf{x}, y) + O_{-2.5,2.5}^{\bar{K},F_{m_1}+F_{m_2}}(y), & \text{if } y > 0, \end{array} \right. \tag{11}$$

where

$$\bar{K} = \sum_{i=1}^{n} K_i/n, \tag{12}$$

the oscillation function O is defined as in (1), [2]

$$G_t^a(\mathbf{x}, y) = \sum_{r=0}^{3} \mu_r(\mathbf{x})(y + 2.5)^r$$

and

$$G_t^b(\mathbf{x}, y) = \sum_{r=0}^{3} \varphi_r(\mathbf{x})(y - 2.5)^r.$$

Parameters $\mu_r(\mathbf{x})$ and $\varphi_r(\mathbf{x})$, $r = 0, 1, 2, 3$, are functions of the basic variables $\mathbf{x}$ and their values can be obtained by solving, respectively, the following systems:

$$\begin{aligned} &\frac{dG_t^a}{dy}(\mathbf{x}, -2.5) = 0, \\ &\frac{dG_t^a}{dy}(\mathbf{x}, 0) = 0, \\ &G_t^a(\mathbf{x}, -2.5) = F_{m_1}(\mathbf{x}), \\ &G_t^a(\mathbf{x}, 0) = 2(F_{m_1}(\mathbf{x}) + F_{m_2}(\mathbf{x})) \end{aligned} \tag{13}$$

and

$$\begin{aligned} &\frac{dG_t^b}{dy}(\mathbf{x}, 2.5) = 0, \\ &\frac{dG_t^b}{dy}(\mathbf{x}, 0) = 0, \\ &G_t^b(\mathbf{x}, 2.5) = F_{m_2}(\mathbf{x}), \\ &G_t^b(\mathbf{x}, 0) = 2(F_{m_1}(\mathbf{x}) + F_{m_2}(\mathbf{x})). \end{aligned} \tag{14}$$

It follows from the above definition that function G_t is built in such a way that

$$G_t(\mathbf{x}, -2.5) = F_{m_1}(\mathbf{x}) \quad \text{and} \quad G_t(\mathbf{x}, 2.5) = F_{m_2}(\mathbf{x}) \quad \forall\, \mathbf{x}.$$

For each *fixed* $\mathbf{x}$, function G_t has, among others, two minimizers at level 1 in $y = -2.5$ and $y = 2.5$, the latter being also a global minimizer.

If we denote by $\mathbf{x}^*$ the global minimizer of F_{m_2}, then the global minimizer for G_t is $(\mathbf{x}^*, 2.5)$ and the global minimum value is

$$G_t(\mathbf{x}^*, 2.5) = F_{m_2}(\mathbf{x}^*) = 2(n - m_2).$$

Let us denote by $\mathcal{S}_1$ the set of 2^{m_1} local minimizers at level 2 for F_{m_1}, and by $\mathcal{S}_2$ the set of 2^{m_2} local minimizers at level 2 for F_{m_2}. Next observation proves that the number of local minimizers at level 2 for G_t is the sum of the number of local minimizers at level 2 for F_{m_1} and F_{m_2}.

[2] With a slight abuse of notation, parameter H in definition (1) of O has been substituted in (11) by the function $F_{m_1} + F_{m_2}$. A similar observation will apply to definition (17) of function Γ.

Observation 5 *The local minimizers at level* 2 *for* G_t *are the following*

$$\begin{array}{ll}(\overline{\mathbf{x}}_1, -2.5) & \forall\, \overline{\mathbf{x}}_1 \in \mathcal{S}_1,\\ (\overline{\mathbf{x}}_2, 2.5) & \forall\, \overline{\mathbf{x}}_2 \in \mathcal{S}_2.\end{array}$$

Proof Similarly to the proof of Observation 3, it is enough to observe that $(\overline{\mathbf{x}}_1, -2.5)$ is a global minimizer of G_t over the set defined by the following m_1+1 linear inequalities

$$\begin{array}{ll}w_i(\mathbf{x}) \geq 0 & \text{for } i \leq m_1 \text{ and } w_i(\overline{\mathbf{x}}_1) = c_2,\\ w_i(\mathbf{x}) \leq 0 & \text{for } i \leq m_1 \text{ and } w_i(\overline{\mathbf{x}}_1) = c_1,\\ y \leq 0. & \end{array}$$

Since points outside this set all have distance from $(\overline{\mathbf{x}}_1, -2.5)$ larger than $r_1 = 1$, this point is a local minimizer at level 2 for G_t. In a completely similar way we can prove that $(\overline{\mathbf{x}}_2, 2.5)$ is a local minimizer at level 2 for G_t for any $\overline{\mathbf{x}}_2 \in \mathcal{S}_2$.

What we still need to prove is that any local minimizer at level 1 $(\overline{\mathbf{x}}, \bar{y})$ for G_t with $\bar{y} \neq -2.5, 2.5$ is not a local minimizer at level 2 for G_t. Indeed, consider the one-dimensional function

$$u(y) = G_t(\overline{\mathbf{x}}, y).$$

We can follow proof of Lemma 1 to see that there exists at least one point $\tilde{y} \neq \bar{y}$ such that

$$\mid \bar{y} - \tilde{y} \mid \leq 1 \quad \text{and} \quad u(\tilde{y}) < u(\bar{y}).$$

It immediately follows that

$$\|(\overline{\mathbf{x}}, \bar{y}) - (\overline{\mathbf{x}}, \tilde{y})\| \leq r_1 = 1$$

and

$$G_t(\overline{\mathbf{x}}, \tilde{y}) < G_t(\overline{\mathbf{x}}, \bar{y}),$$

so that $(\overline{\mathbf{x}}, \bar{y})$ can not be a local minimizer at level 2.

We also prove that function G_t has a unique local minimizer at level 3.

Observation 6 *The unique local minimizer at level* 3 *for* G_t *is its global minimizer.*

Proof Note that in view of Observation 4 the unique candidates to be local minimizers at level 3 for G_t are the two points $(\mathbf{x}_1^*, -2.5)$, where $\mathbf{x}_1^*$ is the global minimizer of F_{m_1}, and $(\mathbf{x}_2^*, 2.5)$, where $\mathbf{x}_2^*$ is the global minimizer of F_{m_2}. The latter is the global minimizer for G_t and, consequently, it must also be a local minimizer at level 3. About the former it is enough to observe that $(\mathbf{x}_1^*, 2.5)$ is a local minimizer at level 2 for G_t for which it holds that

$$\|(\mathbf{x}_1^*, 2.5) - (\mathbf{x}_1^*, -2.5)\| = 5 \leq r_2,$$

where r_2 is defined as in (10), and

$$G_t(\mathbf{x}_1^*, 2.5) = F_{m_2}(\mathbf{x}_1^*) < F_{m_1}(\mathbf{x}_1^*) = G_t(\mathbf{x}_1^*, -2.5),$$

which proves that $(\mathbf{x}_1^*, -2.5)$ cannot be a local minimizer at level 3.

Once we have defined a procedure to combine two basic component functions F_{m_1} and F_{m_2}, we can generalize the combination operator $\times$ in such a way that each of its two arguments can either be one of the basic component functions F_m or the result of previous combination operations. The details of the generalization are analogous

to those for the combination of the two basic component functions F_{m_1} and F_{m_2} with just a slight difference. In order to describe this difference let us consider the case of the combination of a basic component function F_m with a function G obtained by previous combinations. We notice that function F_m only depends on the basic variables $\mathbf{x} = (x_1, \ldots, x_n)$, while function G depends on the basic variables *and* some auxiliary variables, say $y_1, \ldots, y_r$. In order to make both functions depending on the same set of variables, we modify as follows the basic component function:

$$\tilde{F}_m(\mathbf{x}, y_1, \ldots, y_r) = F_m(\mathbf{x}) + \sum_{j=1}^{r} \left[(y_j - 2.5)^2 + O^{\tilde{K},H}_{-2.5,2.5}(y_j) \right]. \tag{15}$$

Note that $\tilde{F}_m$ still has 2^m local minimizers at level 2, has the same global minimum value as F_m, and its global minimizer has the same $\mathbf{x}$ coordinates as the global minimizer of F_m while the y_j coordinates, $j = 1, \ldots, r$, are all equal to 2.5.

3.4 A function with L_2 local minimizers at level 2

We are finally ready to define a procedure returning a function with a given number L_2 ($1 \leq L_2 \leq 2^{n+1} - 1$) of local minimizers at level 2. Let $q_m q_{m-1} \ldots q_1 q_0$ be the binary code of L_2. Let

$$J = \{j : \ q_j = 1\} = \{j_0, \ldots, j_k\}, \quad j_0 < \cdots < j_k.$$

Then we can employ the following procedure.

Initialization Set $G = F_{j_0}$ and $h = 1$.
Step 1 If $h > k$, then STOP and return G, otherwise go to Step 2.
Step 2 Set

$$G = G \times \tilde{F}_{j_h}, \quad h = h + 1$$

(where $\tilde{F}_{j_h}$ is the modification of the basic component F_{j_h} as in (15) with the additional $y_1, \ldots, y_{h-1}$ auxiliary variables) and go back to Step 1.

Simple extensions of the previous proofs show that the resulting function has exactly L_2 local minimizers at level 2, the same global minimum value as F_{j_k} and a global minimizer whose $\mathbf{x}$ coordinates are the same as those of F_{j_k}, while the $y_1, \ldots, y_k$ coordinates are all equal to 2.5. Moreover, this function has a unique local minimizer at level 3.

3.5 A function with L_3 local minimizers at level 3

Next step is to define functions with a given number L_3 of local minimizers at level 3. In order to obtain this function, first we can build L_3 different components G^j, $j = 1, \ldots, L_3$, each one with L_2 local minimizers at level 2 and a single local minimizer at level 3. These functions are obtained by the procedure described in the previous subsection but the set of binary parameters used to define the basic multidimensional functions (6) is different for each component G^j, i.e., we introduce binary parameters p_i^j, $i = 1, \ldots, n$, $j = 1, \ldots, L_3$, for which we require that

$$\nexists\, j_1, j_2 \in \{1, \ldots, L_3\} : \ p_i^{j_1} = p_i^{j_2} \quad \forall i \in \{1, \ldots, n\}. \tag{16}$$

This way the position of the global minimizer (which is also the unique local minimizer at level 3) is different for each G^j component but they all have the same global mini-

mum value. Next we define a combination operator $\otimes$, similar to the one introduced in Sect. 3.3.

Definition 4 Given two components G^{j_1} and G^{j_2}, then

$$\Gamma = G^{j_1} \otimes G^{j_2}$$

is a function of the n basic variables $\mathbf{x} = (x_1, \ldots, x_n)$, of the *auxiliary* variables $\mathbf{y} = (y_1, \ldots, y_k)$ and of the further auxiliary variable z:

$$\Gamma(\mathbf{x}, \mathbf{y}, z) = \begin{cases} \Gamma^a(\mathbf{x}, \mathbf{y}, z) + O^{\bar{K}, G^{j_1}+G^{j_2}}_{-2.5,2.5}(z), & \text{if } z \le 0, \\ \Gamma^b(\mathbf{x}, \mathbf{y}, z) + O^{\bar{K}, G^{j_1}+G^{j_2}}_{-2.5,2.5}(z), & \text{if } z > 0, \end{cases} \tag{17}$$

where $\overline{K}$ is defined as in (12), O is the oscillation term defined in (1),

$$\Gamma^a(\mathbf{x}, \mathbf{y}, z) = \sum_{r=0}^{3} \eta_r(\mathbf{x}, \mathbf{y})(z + 2.5)^r,$$

and

$$\Gamma^b(\mathbf{x}, \mathbf{y}, z) = \sum_{r=0}^{3} \tau_r(\mathbf{x}, \mathbf{y})(z - 2.5)^r.$$

Parameters $\eta_r(\mathbf{x}, \mathbf{y})$ and $\tau_r(\mathbf{x}, \mathbf{y})$, $r = 0, 1, 2, 3$, are functions of the variables $\mathbf{x}$ and $\mathbf{y}$ and can be obtained by the following equations, similar to (13) and (14):

$$\begin{aligned} &\frac{d\Gamma^a}{dz}(\mathbf{x}, \mathbf{y}, -2.5) = 0, \\ &\frac{d\Gamma^a}{dz}(\mathbf{x}, \mathbf{y}, 0) = 0, \\ &\Gamma^a(\mathbf{x}, \mathbf{y}, -2.5) = G^{j_1}(\mathbf{x}, \mathbf{y}) + 1/L_3, \\ &\Gamma^a(\mathbf{x}, \mathbf{y}, 0) = 2(G^{j_1}(\mathbf{x}, \mathbf{y}) + G^{j_2}(\mathbf{x}, \mathbf{y})) + 2 \end{aligned}$$

and

$$\begin{aligned} &\frac{d\Gamma^b}{dz}(\mathbf{x}, \mathbf{y}, 2.5) = 0, \\ &\frac{d\Gamma^b}{dz}(\mathbf{x}, \mathbf{y}, 0) = 0, \\ &\Gamma^b(\mathbf{x}, \mathbf{y}, 2.5) = G^{j_2}(\mathbf{x}, \mathbf{y}), \\ &\Gamma^b(\mathbf{x}, \mathbf{y}, 0) = 2(G^{j_1}(\mathbf{x}, \mathbf{y}) + G^{j_2}(\mathbf{x}, \mathbf{y})) + 2. \end{aligned}$$

Function Γ is built in such a way that

$$\Gamma(\mathbf{x}, \mathbf{y}, -2.5) = G^{j_1}(\mathbf{x}, \mathbf{y}) + 1/L_3 \quad \forall\, (\mathbf{x}, \mathbf{y}),$$

and

$$\Gamma(\mathbf{x}, \mathbf{y}, 2.5) = G^{j_2}(\mathbf{x}, \mathbf{y}) \quad \forall\, (\mathbf{x}, \mathbf{y}),$$

Then, its global minimum value is the same as the one for G^{j_2}, while its global minimizer has the same $\mathbf{x}$ and $\mathbf{y}$ coordinates as the global minimizer of G^{j_2}, and $z = 2.5$. Let us denote by Δ_1 the set of local minimizers at level 2 for G^{j_1}, and by Δ_2 the set of local minimizers at level 2 for G^{j_2}.

Observation 7 *It holds that function* Γ *has*

(a) *the* $2L_2$ *local minimizers at level 2*

$$\begin{array}{ll}(\bar{\mathbf{x}}_1, \bar{\mathbf{y}}_1, -2.5) & \text{for any } (\bar{\mathbf{x}}_1, \bar{\mathbf{y}}_1) \in \Delta_1 \\ (\bar{\mathbf{x}}_2, \bar{\mathbf{y}}_2, 2.5) & \text{for any } (\bar{\mathbf{x}}_2, \bar{\mathbf{y}}_2) \in \Delta_2\end{array}$$

(b) *two local minimizers at level 3, namely* $(\mathbf{x}_1^*, \mathbf{y}_1^*, -2.5)$ *(where* $(\mathbf{x}_1^*, \mathbf{y}_1^*)$ *is the global minimizer for* G^{j_1}*) and* $(\mathbf{x}_2^*, \mathbf{y}_2^*, 2.5)$ *(where* $(\mathbf{x}_2^*, \mathbf{y}_2^*)$ *is the global minimizer for* G^{j_2}*).*

Proof The proof of (a) is completely analogous to the proof of Observation 5. In order to prove (b), we notice that, in view of Observation 6, the only possible local minimizers at level 3 for Γ are the two points $(\mathbf{x}_1^*, \mathbf{y}_1^*, -2.5)$ and $(\mathbf{x}_2^*, \mathbf{y}_2^*, 2.5)$. Point $(\mathbf{x}_2^*, \mathbf{y}_2^*, 2.5)$ is the global minimizer so it must be a local minimizer at level 3. About point $(\mathbf{x}_1^*, \mathbf{y}_1^*, -2.5)$ we note that

$$\Gamma(\mathbf{x}_1^*, \mathbf{y}_1^*, -2.5) = \Gamma(\mathbf{x}_2^*, \mathbf{y}_2^*, 2.5) + 1/L_3$$

and no local minimizer at level 2 for Γ different from $(\mathbf{x}_2^*, \mathbf{y}_2^*, 2.5)$ has a better function value (all other local minimizers at level 2 have a function value at least as large as the global minimum value plus one). Then, $(\mathbf{x}_1^*, \mathbf{y}_1^*, -2.5)$ is not a local minimizer at level 3 for Γ only if

$$\|(\mathbf{x}_1^*, \mathbf{y}_1^*, -2.5) - (\mathbf{x}_2^*, \mathbf{y}_2^*, 2.5)\| \leq r_2.$$

But, in view of (16), it holds that

$$\|(\mathbf{x}_1^*, \mathbf{y}_1^*, -2.5) - (\mathbf{x}_2^*, \mathbf{y}_2^*, 2.5)\| \geq \sqrt{(c_2 - c_1)^2 + 5^2} > r_2,$$

where r_2 is defined as in (10).

Similarly to Sect. 3.3, we can generalize the combination operation in such a way that each of its two arguments can either be one of the basic component functions G^j (or even better its modification $\tilde{G}^j$ completely analogous to (15) with z variables in place of the y variables) or the result of previous combination operations.

Now, the following procedure, again similar to the one described in Sect. 3.3, returns a function with L_3 local minimizers at level 3.

Initialization Set $\Gamma = G^1$ and $h = 2$.
Step 1 If $h > L_3$, then STOP and return Γ, otherwise go to Step 2.
Step 2 Set

$$\Gamma = \Gamma \otimes \tilde{G}^h, \qquad h = h + 1$$

and go back to Step 1.

Proof of Observation 7 can now be extended in order to prove that function Γ has L_3 local minimizers at level 3 and $L_3 L_2$ local minimizers at level 2. Its global minimum value is the same as the one for G^{L_3} and its global minimizer has the same $\mathbf{x}$ and $\mathbf{y}$ coordinates as the global minimizer of G^{L_3}, while the $z_1, \ldots, z_{L_3 - 1}$ coordinates are all equal to 2.5.

4 A summary of the user-defined and random parameters

In this section, we summarize the parameters which have been employed to define the test functions. Some of them have to be specified by the user, some others are randomly chosen by the test generator.

4.1 User-defined parameters

(1) n: the *number of basic variables*. Basic variables are those on which the basic multidimensional functions F_m depend. Its lower bound is 1. Note that they are not the unique variables of the test functions, other variables have been introduced to combine different components of the test functions (the overall number d of variables on which the test functions depend will be specified in Observation (8)).
(2) L_2: it is the parameter which controls the number of local minimizers at level 2. It is constrained to belong to the interval $[1, 2^{n+1} - 1]$.
(3) L_3: the number of local minimizers at level 3. In view of the high difficulty introduced by local minimizers at level 3, we set the upper bound $\sqrt{n}$ for this value; then, L_3 is constrained to belong to the interval $[1, \sqrt{n}]$.
(4) $K_i, i = 1, \ldots, n$: the *oscillation frequencies*. They basically control the number of local minimizers at level 1 in the one-dimensional components by which the test functions are made up; they are constrained to belong to the interval $[10, 20]$. The user has the option of fixing them all equal to a given value $K \in [10, 20]$ or to let the value of each of them be randomly chosen in the above interval. In order to guarantee a high-enough variability among the K_i values, these are not uniformly sampled over the interval $[10, 20]$ but each of them is sampled with probability 0.5 in the interval $[10, 12.5]$ and with the same probability in the interval $[17.5, 20]$. We remark that the random choice of these values is a further source of difficulty because it introduces an anisotropic behavior of the function, i.e., a different behavior along distinct directions.
(5) H: the *oscillation width*. It controls the height of the barriers between neighbor local minimizers at level 1 in the one-dimensional components; it is constrained to belong to the interval $[10, 30]$.

4.2 Random parameters

(1) $c_1 \in [-3.5, -2.0]$ defines the position of the first local minimizer at level 2 in the one-dimensional components $d_{p,K}$ with two local minimizers at level 2 and of the unique local minimizer at level 2 in the one-dimensional components $s_{1,K}$ (see Sect. 3.1).
(2) $c_2 \in [2.0, 3.5]$ defines the position of the second local minimizer at level 2 in the one-dimensional components with two local minimizers at level 2 and of the unique local minimizer at level 2 in the one-dimensional components $s_{0,K}$ (see Sect. 3.1).
(3) $p_i^j \in \{0, 1\}, i = 1, \ldots, n, j = 1, \ldots, L_3$: for each i corresponding to a one-dimensional component of each function G^j introduced at the beginning of Sect. 3.5, p_i^j defines the position (c_1 or c_2) of the lowest local minimizer at level 2 if the one-dimensional component has two local minimizer at level 2, or of the unique local minimizer at level 2 if the one-dimensional component has a single local minimizer at level 2 (see Sect. 3.1).
(4) $\mathbf{A}'$: it is the nonsingular matrix from which, through orthonormalization, matrix $\mathbf{A}$ is generated (see Sect. 3.2). Matrix $\mathbf{A}$ defines the distance preserving transformation (5) from the n-dimensional vector $\mathbf{x}$ of the basic variables to the n-dimensional vector of variables $\mathbf{w}$.

The most important parameters from the point of view of the source of difficulty discussed in Sect. 2 are L_2 (controlling the number of local minimizers at level 2) and L_3 (controlling the number of local minimizers at level 3). But we remark that for fixed L_2 and L_3 we can also increase the difficulty of the test problems by increasing n (increase of the dimension d of the test functions), K (increase of the number of local minimizers at level 1), H (increase of the height of the barriers separating different local minimizers at level 1, thus making more difficult to jump over them).

The following observation returns the overall dimension d of the test functions as a function of the three user-defined parameters n, L_2 and L_3.

Observation 8 *The overall dimension d of the test functions is*

$$d = n + v(L_2) + L_3 - 2, \tag{18}$$

where $v(L_2)$ is the number of ones in the binary code of L_2.

Proof This immediately follows from the procedures to build functions G^j, $j = 1, \ldots, L_3$ in Sect. 3.4 and function Γ in Sect. 3.5.

Note that, according to (18) and recalling the bounds for the parameters, one-dimensional test functions ($d = 1$) must have $n = 1$, $L_2 \in \{1, 2\}$, $L_3 = 1$, and they correspond to the one-dimensional components described in Sect. 3.1 (two representatives of which are displayed in Fig. 2); two-dimensional test functions ($d = 2$) must have $n = 1$, $L_2 = 3$, $L_3 = 1$ (see the function displayed in Figs. 3 and 4) or $n = 2$, $L_2 \in \{1, 2, 4\}$, $L_3 = 1$.

Here, we also prove the following observation which allows to restrict the search region for the global minimizer.

Observation 9 *The global minimizer of the proposed test functions lies in the interior of a sphere centered at the origin and with radius $5\sqrt{d}$.*

Proof Let $(\mathbf{x}^*, \mathbf{y}^*, \mathbf{z}^*)$ be the d-dimensional vector corresponding to the global minimizer of our test function. Let $\mathbf{w}^* = \mathbf{A}\mathbf{x}^*$, where $\mathbf{A}$ is the distance-preserving transformation defined in (5). From the definition of the test functions it holds that all the

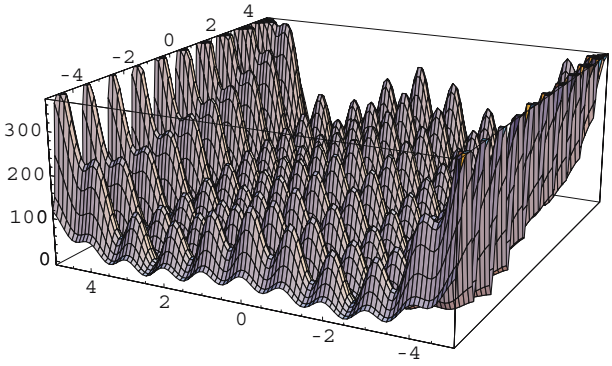

Fig. 3 A two-dimensional function with $n = 1$, $L_2 = 3$, $L_3 = 1$, $K = H = 10$, $p = 1$, $c_1 = -3$, and $c_2 = 3$, over the box $[-5, 5]^2$

components of the vectors $\mathbf{w}^*, \mathbf{y}^*$ and $\mathbf{z}^*$ lie in the interval $(-5, 5)$. Then,

$$\begin{aligned}\|(\mathbf{x}^*, \mathbf{y}^*, \mathbf{z}^*)\| &= \sqrt{\| \mathbf{x}^* \|^2 + \| \mathbf{y}^* \|^2 + \| \mathbf{z}^* \|^2} \\ &= \sqrt{\| \mathbf{w}^* \|^2 + \| \mathbf{y}^* \|^2 + \| \mathbf{z}^* \|^2} < 5\sqrt{d},\end{aligned}$$

where the last equality follows from the fact that the linear transformation $\mathbf{A}$ is distance-preserving.

In some cases, we also would like to define test functions of some *given* dimension d. For this reason the user is also allowed to specify d as a parameter in place of n. In these cases the user is first asked to introduce the values of the parameters L_2, L_3 (which, as explained above, control the source of difficulty discussed in Sect. 2), and the dimension d; then, the value of n is computed through (18); if n is not lower than 1 and both L_2 and L_3 are within their prescribed upper bounds with respect to n (respectively, $2^{n+1} - 1$ for L_2 and $\sqrt{n}$ for L_3) the user is finally asked to introduce the values of the K_i, $i = 1, \ldots, n$, and H parameters; otherwise, the assignment of the parameter values is declared unsuccessful (the user is also reported the minimal dimension d for which the given values of L_2 and L_3 are allowed) and the user is asked to insert the parameters again.

5 Computational experiments

If we are given a class of global optimization problems, our aim is to find algorithms which are able to solve them efficiently. If we want to propose a class of challenging test functions the situation is somehow reversed: we are given existing algorithms and we would like to find problems on which these algorithms are not efficient in order

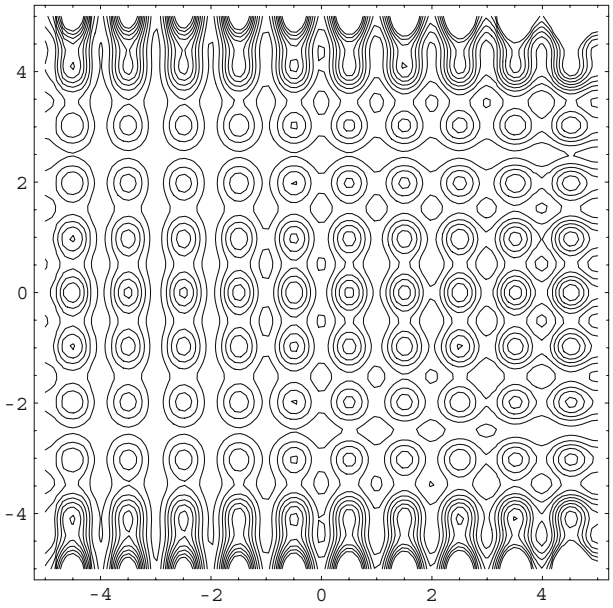

Fig. 4 Level curves for the function in Fig. 3

to stimulate the search of new techniques. Of course, it is impossible to test all the existing GO algorithms. Therefore, for those willing to test their GO algorithms on the proposed test functions, we make a C++ class available, downloadable at the web site (GOL 2006). In the same web site one can also find a link (RngStream 2004) to the pseudo random number generator RngStream which has been employed to generate the random parameters. Any feedback is more than welcome and at the same web site all updates based on the received feedbacks will be indicated.

Although we can not test all GO algorithms, we think it is a good idea to present at least some results as a basis for future comparison. Since the proposed test problems are highly multimodal ones, we think that testing methods based on multiple local searches is a good choice. Moreover, in the field of molecular conformation problems, which inspired the definition of this test set, since the observations made in Wales and Doye (1997) on the energy landscapes modified by local search procedures, it has become a common practice to define methods where only local minimizers are observed. We tested two simple GO algorithms, both based on multiple local searches, on some test functions of increasing difficulty from the class proposed in this paper. The first algorithm is the very simple Multistart algorithm. Following Observation 9, at each iteration a random point within the sphere centered at the origin and with radius $5\sqrt{d}$ (d is defined in (18)) is sampled and a local search is started from it. We tested the Multistart algorithm just to have an experimental confirm that for the proposed test functions the large number of local minimizers at level 1 does not allow to detect the global minimizer even when starting clever local search procedures (like the limited memory BFGS employed in this paper) from many random initial points. The second algorithm is Monotonic Basin Hopping (see Leary 2000), denoted by MBH in what follows:

Initialization Let `MaxNoImprove` be a fixed parameter and X_0 be a random initial local minimizer at level 1; set $h, k = 0$.

Step 1 Let Z_{k+1} be obtained by random sampling in the sphere $S(X_k, r)$, with center X_k and radius r, and Y_{k+1} be the local minimizer at level 1 reached by starting a local search from Z_{k+1};

Step 2 If $f(Y_{k+1}) < f(X_k)$, then set $X_{k+1} = Y_{k+1}$ and $h = 0$, otherwise set $X_{k+1} = X_k$ and $h = h + 1$;

Step 3 If $h \geq$ `MaxNoImprove`, then STOP, otherwise set $k = k + 1$ and go back to 1.

In spite of its simplicity, MBH turned out to be extremely efficient for very challenging global optimization problems, like molecular conformation problems (see Leary 2000, Doye et al. 2004 for results on Lennard-Jones and Morse clusters), and some highly multimodal test functions (see Locatelli 2005).

It can be viewed as a local search at level 2. In particular, Step 1 of MBH can be viewed as a random move within the set of local minimizers at level 1 belonging to the neighborhood of the current local minimizer X_k. We remark that the neighborhood explored by MBH is slightly different from that in Definition 1. Indeed, in MBH the neighborhood of a given local minimizer at level 1 is made up by all local minimizers at level 1 whose basin of attraction is within the threshold distance r from it.

Tuning r is not trivial (we refer to Locatelli 2005 for a simple adaptive scheme to tune it). In Table 1 we will always report the best results obtained with many different choices of r (ranging from $10/\bar{K}$ and $20/\bar{K}$, $\bar{K}$ defined as in (12)) just to show that for the most difficult test functions even *optimized* choices of r do not lead to high percentage of successes. The `MaxNoImprove` parameter has been set to a very large

Table 1 Results of MBH over the seven proposed test functions

Function	n	K_i	H	L_2	L_3	d	Successes	Average #LS
Test 1	50	$K_i = 10,\ i = 1,\ldots,n$	10	1	1	50	1000	1517
Test 2	50	$K_i = 20,\ i = 1,\ldots,n$	10	1	1	50	1000	2393
Test 3	50	K_i random in $[10, 20]$	10	1	1	50	1000	5271
Test 4	30	$K_i = 10,\ i = 1,\ldots,n$	10	10	1	31	82	1444
Test 5	30	$K_i = 10,\ i = 1,\ldots,n$	10	25	1	32	30	1810
Test 6	30	$K_i = 10,\ i = 1,\ldots,n$	10	25	4	35	15	1612
Test 7	30	$K_i = 10,\ i = 1,\ldots,n$	10	100	4	35	5	1867

value (10^5) in order to be reasonably sure that a local minimizer at level 2 has been reached.

Seven different test functions have been considered. The parameters defining these functions can be downloaded at the web site (GOL 2006) (in order to guarantee the possibility of repeating experiments, the software allows to save into a file all the user-defined and random parameters defining a test function, and to read them later from the same file). As expected, Multistart was unable to detect the global minimizer using twice as many local searches with respect to MBH even in the easiest (with respect to MBH) case (test function with $L_2 = L_3 = 1$, $H = K = 10$). Results for MBH are reported in Table 1. On each test function 1,000 runs have been performed. For each function we report the number of successes over the 1,000 runs and the average number of local searches per run (always excluding in each run those performed during the last 10^5 iteration where no improvement is observed). Testing has been performed on Pentium IV processors 2.4 GHz with 512 MB RAM running Linux.

Since MBH can be viewed as a procedure to detect local minimizers at level 2, we show that it is an appropriate method to solve problems with a low number of local minimizers at level 2 but often fails as the number of local minimizers at level 2 increases, thus pointing out the need for different strategies. MBH always solves the problems with $L_2 = L_3 = 1$. It can be seen that increasing the number of local minimizers at level 1 (i.e., increasing parameter K from 10 to 20) only slightly worsens the performance of MBH, while modifying the frequency of oscillations along different axes through the random selection (within the interval $[10, 20]$) of the K_i values, is a more serious source of difficulty (the average number of local searches increases). The reason for this is that the random generation of the point Z_{k+1} over a sphere centered at the current record X_k (Step 1 of MBH) does not take into account the anisotropic behavior of the function.

As the values L_2 and L_3 are increased, we observe a clear decrease of the performance of MBH (MBH often gets trapped at a local minimizer at level 2 and is unable to escape from it when this is not the global minimizer). Notice that in these cases MBH always reaches in a relatively fast time (i.e., within a number of local searches ranging from 1,500 to 2,000) a local minimizer at level 2 (it has been observed that MBH always stops at a local minimizer at level 2) but then is unable to escape from it.

6 Conclusion

In this paper, we have proposed a class of test functions for unconstrained global optimization problems. The difficulty of these problems can be controlled by an

appropriate choice of some parameters. A web site (GOL 2006) is maintained where users will be able to download a C++ class of the test functions, post their comments and get the parameters defining a set of seven test functions with increasing difficulty for which we also make available the results obtained by two simple GO algorithms as a basis of comparison.

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