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# Test problem generator for unconstrained global optimization ☆

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ABSTRACT

We develop in this paper a high performance test problem generator for generating analytic and highly multimodal test problems for benchmarking unconstrained global optimization algorithms. More specifically, we propose in this research a novel and computationally efficient procedure for generating nonlinear nonconvex not separable unconstrained test problems with (i) analytic test functions, (ii) known local minimizers that are distributed uniformly in the interior of a compact box, among which only one is the global solution, and (iii) controllable difficulty levels. A standard set of test problems with different sizes and different difficulty levels is produced for both MATLAB and GAMS and is available for downloading. Numerical experiments have demonstrated the stability of the generating process and the difficulty of solving the standard test problems.



## 1. Introduction

Optimization, as a powerful search engine in decision-making, finds wide applications in almost all fields of engineering, finance, and management as well as social science. The existence of multiple local minima of a general nonconvex objective function makes global optimization a great challenge. Since the publication of the two-volume books entitled "Towards Global Optimization" in 1975 [9] and 1978 [10], the study of global optimization has grown by leaps and bounds. The last four decades have witnessed rapid development in both theory and numerical techniques for global optimization. Nevertheless, it is difficult to compare the efficiencies of different solution algorithms directly. Thus, empirical computational testing is always necessary.

Construction of test problems for benchmarking global optimization algorithms is a challenging task. There are three main types of test problems in the literature: problems modeling a variety of real-world applications, problem instances with certain designated characteristics, and randomly generated test problems with known solutions. Excellent collections of test problems of the first two types can be found in [12,13,20,29,33], for example. For the third type, some test problem generators have been proposed for constrained global optimization (see, e.g., [5,11,27,31,32]. However, the generation of nontrivial test problems for unconstrained global optimization algorithms seems to be difficult as evidenced by the fact that very few papers have addressed this subject.

Unconstrained global optimization is an important subject within the optimization community. It not only forms the foundation of global optimization, but also has many applications in the real world. Various practical problems can be modeled by or be transformed into unconstrained global optimization problems. Examples include seismic analysis in earthquake and exploration seismologies; protein folding problems in biomedical sciences; solution to polynomial equations that arise frequently in symbolic computation, algebraic geometry and computer algebra; and satisfiability problems that arise frequently in computer vision, VLSI design and computer-aided design. Numerous papers in the literature have been devoted to the development of theories and/or algorithms for unconstrained global optimization, including tunneling algorithms (see, e.g., [3,6,24]), filled function methods (see, e.g., [17,18,39]), multistart algorithms (see, e.g., [2,21,28]), simulated annealing algorithms (see, e.g., [7,19]), DIRECT algorithm (see, e.g., [14,22]), methods using Peano curves (see, e.g., [35,36]), and global descent method (see [30]). Benchmarking unconstrained global optimization algorithms is thus an important and interesting subject both from the theoretical and practical points of view.

In 1993, Schoen [34] proposed, probably, the first test problem generator for benchmarking unconstrained global optimization algorithms. Denote the usual Euclidean norm of a vector by $\|\cdot\|$. Suppose that $k$ distinct points, $z_i \in (0,1)^n$, $i = 1, \ldots, k$, and their values, $f_i \in \Re$, $i = 1, \ldots, k$, are given. Assume further that $k$ parameters, $a_i > 1$, $i = 1, \ldots, k$, are also given. Schoen's generator generates the following family of functions:

$$f(x) = \frac{\sum_{i=1}^{k} f_i \prod_{j \neq i} \|x - z_j\|^{a_j}}{\sum_{i=1}^{k} \prod_{j \neq i} \|x - z_j\|^{a_j}} \quad \text{where } x \in [0,1]^n.$$

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It can be proved that the $k$ points, $z_i$, $i=1,\ldots,k$, are stationary points, and $\min_i f_i \le f(x) \le \max_i f_i$, $\forall x \in [0,1]^n$. Moreover, if $a_i \ge 2 \in \mathbf{Z}$, $\forall i \in \{1,\ldots,k\}$, then $f \in C^\infty$. Note, however, that there is no prior knowledge or ways to control the properties of the stationary points, in general.

In 1998, Gaviano and Lera [16] introduced a family of functions that included a class of $C^1$ and a class of $C^2$ test functions with a priori known local minimizers and their regions of attraction (also known as basins) (see, e.g., [8,17] for the definition of the region of attraction of a minimizer). They, with other coworkers, further extended the family to include a class of $C^0$ test functions in [15] in 2003. The idea of their method is to dig some deep holes in the hillside of a convex quadratic function. The width of a hole is actually the region of attraction of its minimum. For the class of $C^0$ test functions, they used quadratic polynomials to maintain the continuity of the resulting class of composite functions. For the class of $C^1$ test functions, they used cubic polynomials to maintain the first-order continuous differentiability. While for the class of $C^2$ test functions, they used quintic polynomials to maintain both the first- and second-order continuous differentiabilities. Denote the box-constrained admissible region of $x$ by $X$. Suppose that $k$ distinct points, $z_i \in \text{int}(X)$, $i=1,\ldots,k$, and their values, $f_i \in \Re$, $i=1,\ldots,k$, are given. Let $S_i = \{x \in \Re^n : \|x-z_i\| \le \rho_i,\ \rho_i > 0\}$, $i=2,\ldots,k$, where $\rho_i$, $i=2,\ldots,k$, are chosen such that $S_i \cap S_j = \varnothing$, $\forall i \ne j$. Their generator produces the following family of functions:

$$f(x) = \begin{cases} g_i(x), & x \in S_i \ (i \in \{2,\ldots,k\}), \\ \|x-z_1\|^2 + f_1, & x \notin S_2 \cup \cdots \cup S_k, \end{cases}$$

where $g_i$, $i=2,\ldots,k$, are suitable quadratic, cubic or quintic polynomials for $C^0$, $C^1$ or $C^2$-class test functions, respectively. Interested readers can find the details of these polynomials in [15]. As mentioned in their papers, all three classes have many parameters to be coordinated. The correlations of the parameters indeed do not allow simple and fast generation. The parameter coordination problem was finally relaxed by their test problem generator presented in [15]. Since they provided a complete mechanism for tuning the parameters, from our point of view, their generator is so far the most controllable one that is capable of generating numerous test problems. Nevertheless, their generator has two obvious weaknesses. First, the region of attraction of $z_1$ is not well defined since the hillside of the convex quadratic function, $\|x-z_1\|^2 + f_1$, has been destroyed by the holes $S_2,\ldots,S_k$. Moreover, it is well known within the global optimization community that just the value, and the first- and second-order derivatives of a function, in general, do not provide sufficient information for finding a global minimizer of the function. Since the functions in Gaviano et al. are composite functions with at most second-order continuous differentiability, it can be seen from the definition of $f$ that no information about the function $g_i$, $i=2,\ldots,k$, is available at any $x \notin S_2 \cup \cdots \cup S_k$. It can thus never provide sufficient information for locating the minimizers $z_2,\ldots,z_k$. Without doubt, this property makes their test functions hard to be minimized globally and thus excellent for competitive testing. However, due to the same reason, only a few papers in the literature have actually adopted it for a comparison purpose of global optimization algorithms. We thus believe that analytic functions are better choices of test problems for benchmarking global optimization algorithms.

In 2007, Addis and Locatelli [1] proposed a test problem generator for generating a class of functions that are analogous with the molecular conformation problems. They first defined two types of one-dimensional component with multiple local minimizers obtained through some oscillation terms based on cosine functions. By addition and linear transformation of several one-dimensional components with different parameters, they obtained a class of not separable $n$-dimensional component, namely basic component function. Through their combination operations on two instances of the basic component function, they finally obtained a basic test function. In fact, by using basic component functions or the result of previous combination operations as parameters of their combination operations, more test functions can be obtained. As their functions contain numerous components and each component contains several parameters, interested readers should refer to [1] for more details. Essentially, one of the two types of one-dimensional component in [1] is

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

where $p$, $K$, $c_1$, $c_2$, and $H$ are parameters, $O^{K,H}_{c_1,c_2}(x)$ is an oscillation term based on a cosine function, and $\xi_p(x)$ is a composite function with continuous first derivative. Therefore, their generator produces at most $C^1$ test problems. It is evident that some significant difficulties still exist to block the generation of analytic functions for benchmarking unconstrained global optimization algorithms, notwithstanding the above-mentioned promising progress.

The main purpose of this research is to develop a high performance test problem generator for generating analytic and highly multimodal test problems for benchmarking unconstrained global optimization algorithms. Unlike Schoen's functions in [34], the proposed test problems have a priori known minimizers, a maximizer and saddle points as well as their values. Unlike Gaviano et al.'s functions in [15,16] and Addis and Locatelli's function in [1], the proposed test problems are analytic polynomial-type functions; the parameters of the proposed test problems can be generated directly without any coordination problem. This paper indeed describes a novel and computationally efficient procedure for generating nonlinear nonconvex not separable unconstrained test problems with (i) analytic test functions, (ii) known minimizers that are distributed uniformly in the interior of a compact box, and (iii) controllable difficulty levels.

This paper is organized as follows. In Section 2, we first construct $n$ univariate nonlinear nonconvex unconstrained minimization problems with known optimal solutions. Combining the $n$ univariate problems, we produce a separable nonlinear nonconvex unconstrained $n$-variable problem. In Section 3, we disguise the separability of the problem and introduce randomness by adopting a technique from Calamai et al. [5] to obtain a not separable function by linear transformations of variables of a separable function. Since many algorithms for solving unconstrained global minimization problems require that all local minimizers of the objective function be contained in the interior of a compact box, we pay special attentions to this issue in Section 4. We devote Section 5 to discuss the realization of the generator and the developed software packages, while generation of random numbers, control of the difficulty levels of the test problems, description of the software packages, and summary of the parameters are the topics of this section. In Section 6, we report the results of the stability tests on the standard test problems. We also report the results of some test experiments with a multistart algorithm and with a deterministic global optimization solver, namely GAMS/BARON. Finally, we draw some conclusions in Section 7.

## 2. Generation of separable nonlinear nonconvex unconstrained test problems

### 2.1. Construction of separable problems

Consider a general class of separable problems for unconstrained global minimization which takes the following form:

$$(P) \quad \min_{x \in \Re^n} f(x),$$