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Metaheuristic vs. deterministic global optimization algorithms: The univariate case

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ABSTRACT

Many practical problems involve the search for the global extremum in the space of the system parameters. The functions to be optimized are often highly multiextremal, black-box with unknown analytical representations, and hard to evaluate even in the case of one parameter to be adjusted in the presence of non-linear constraints. The interest of both the stochastic (in particular, metaheuristic) and mathematical programming (in particular, deterministic) communities to the comparison of metaheuristic and deterministic classes of methods is well recognized. Although both the communities have a huge number of journal and proceedings papers, a few of them are really dedicated to a systematic comparison of the methods belonging to these two classes. This paper meets the requirement of such a comparison between nature-inspired metaheuristic and deterministic algorithms (more than 125,000 launches of the methods have been performed) and presents an attempt (beneficial to practical fields including engineering design) to bring together two rather disjoint communities of metaheuristic and mathematical programming researchers and applied users.

1. Introduction

This work is dedicated to finite-dimensional global optimization – a field studying theory, methods, and implementation of models and strategies for solving multiextremal optimization problems. Our attention to the field of global optimization is explained by the advantages that can be obtained in practice by applying globally optimal solutions instead of local ones given by well studied local optimization methods. In many design problems (including mechanical, civil and environmental engineering problems), the multiextremal objective function (subject to some constraints) has no analytical representation and its evaluation (the operation of evaluating the objective function at an admissible point is often called "trial") is associated with performing computationally expensive numerical experiments. Since each trial is supposed to be a time-consuming operation, it is desirable to obtain the best solution (possibly together with a certificate of its quality) to the problem by evaluating the function at the less possible number of trial points within a given trials budget. Therefore, the usage of fast global optimization methods for solving such complex multiextremal problems is required in practice.

For example, one of the important applied fields of efficient finite-dimensional global optimization methods is the investigation of control systems under uncertain values of their parameters, in order to afford the desired safe functioning

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of a controllable object. A diversity of important problems of robust control can be reduced to the problem of establishing the positiveness of multiextremal functions. This problem can be successfully solved by global optimization methods: it is sufficient to establish that the global minimum of a function describing the system is positive over the set of parameters (see, e.g., [1]). Together with a solution to the problem, some "certificate" should also be provided by a method to guarantee the "quality" of the obtained solution (see, e.g., [2,3]).

In order to choose suitable methods for solving a global optimization problem, an applied user needs as more complete information on the comparison of the methods as possible, but often the available information is not sufficient. The user's choice is made even more difficult by the fact that numerical global optimization methods have different structures: for example, they can have a stochastic or deterministic nature (see, e.g., [4]). Stochastic methods offer a probabilistic guarantee of locating the global solution: their convergence theory usually states that the global minimum will be identified in an infinite time with probability one. Assuming exact computations and an arbitrarily long run time, deterministic methods ensure that after a finite time an approximation of a global minimizer will be found (within prescribed tolerances).

Adaptive stochastic search strategies are mainly based on random sampling in the search domain. Such techniques as adaptive random search, simulated annealing, evolution and genetic algorithms, tabu search, etc., can be cited here (see, e.g., [5–7] for details). Stochastic approaches can deal with black-box problems in a simpler manner than many deterministic algorithms. They are also suitable for the problems where the evaluations of the functions are corrupted by noise. However, there can be difficulties with these methods, as well. For example, solutions found by many stochastic algorithms (among them are popular heuristic nature-inspired methods like evolutionary algorithms, simulated annealing, etc.; see, e.g., [6,8–11]) can be only local solutions to the problems, located far from the global ones. Several restarts can also be involved, requiring even more expensive functions evaluations. This can preclude such methods from their usage in practice when an accurate and guaranteed estimate of the global solution is requested under some assumptions on the problem, while they can be useful to tackle some problems with a lack of a priori suppositions on the objective function.

Although there exist plenty of publications (see, e.g., the references in [5–7,12–14]) dedicated to numerical experimentations with various global optimization techniques (of either stochastic or deterministic types), not so many papers have appeared where results of a comparative analysis between metaheuristic and deterministic algorithms were reported, thus maintaining stochastic and deterministic research communities rather disjoint. The lack of such systematic results can be explained by both human factor (as, for example, professional/academic interests) and objective reasons (as, for example, the difficulty to perform a fair comparison, the lack of test classes suitable for both the communities and so on).

It is obviously, however, that the presence of results on deterministic methods within metaheuristic research environment, and vice versa, can bring significant benefits to applied users. That is why, in our opinion, it is important to increment research of this kind, in order to give the researchers/applied users the possibility to impartially choose a more appropriate method for tackling their applied problems. This paper[1] presents, therefore, an invitation for the stochastic and deterministic communities to participate in this important discussion with possibly more efficient methods and more interesting test/applied problems. It meets the requirement of a systematic comparison between metaheuristic and deterministic algorithms both for solving global optimization problems and for providing their solutions together with some guaranteed gaps.

The paper is organized as follows. Some aspects of testing optimization methods and benchmark problems from optimization literature and applied fields are briefly described in the following Section 2. Several popular black-box global optimization methods are discussed in the next two Sections: Section 3 is dedicated to metaheuristic algorithms, while deterministic Lipschitz-based methods are described in Section 4. Results of a numerical comparison between these methods on the benchmark set from Section 2 with respect to a given limited budget of trials are reported and commented on in Section 5. Section 6 concludes the paper.

2. Univariate constrained benchmark problems

It is well recognized that testing optimization software is a difficult problem; comparing different optimization methods is even more difficult (intuitive graphical tools for performing such a comparison can be useful; see, e.g., [16]). The usual practice is to solve a high number of tests (with respect to different solution criteria) with known solutions and, then, to proceed with practical problems (for which solutions are usually unknown and, therefore, it becomes more doubtful to get fair comparison results). In order to have more reliable results on the methods comparison, test functions should be first used (with the full information about their properties), as done in this paper. Since in real-life simulation-based applications the number of performed function evaluations is considered to be one of the important design requirements (see, e.g., [2,3,17]), this comparison criterion can be equally applied for test problems (to verify the methods performance) and for practical black-box formulations. The latter ones can be considered as a subsequent step of the methods comparison.

Test problems are often considered in their box-constrained versions, since the problems with general non-linear constraints can be reduced to the box-constrained ones either by penalty approaches or by some more advanced techniques as,

[1] The paper is based upon the work [15] and significantly extends the previous research in the experimental direction, by performing extensive numerical testing of metaheuristic nature-inspired and Lipschitz-based deterministic global optimization methods on benchmark and practical engineering univariate constrained problems.

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