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Global Simplex Optimization—A simple and efficient metaheuristic for continuous optimization

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ABSTRACT

A new hybrid optimization algorithm is proposed for minimization of continuous multi-modal functions. The algorithm called Global Simplex Optimization (GSO) is a population set based Evolutionary Algorithm (EA) incorporating a special multi-stage, stochastic and weighted version of the reflection operator of the classical simplex method. An optional mutation operator has also been tested and then removed from the structure of the final algorithm in favor of simplicity and because of insignificant effect on performance. The promising performance achieved by GSO is demonstrated by comparisons made to some other state-of-the-art global optimization algorithms over a set of conventional benchmark problems.

1. Introduction

Unconstrained global optimization of a continuous function f aims at finding its global optimum without being trapped into one of its local minima, where function f depends on a set of continuous decision variables or design parameters $y=(y_1,y_2,\ldots,y_n)$ and is assumed to be subject to only box type constraints, i.e. each variable is limited only by a lower and upper bound. Among the mathematical algorithms in the literature dedicated to the subject, one might see a special interest in Evolutionary Algorithms (EAs) and their main branches, including Genetic Algorithms (GAs), Genetic Programming (GP), Evolution Strategies (ESs), and Evolutionary Programming (EP). Their principal mode of operation is based on the same genetic concepts, a population of competing candidate solutions, random combinations and alterations of potentially useful structures to generate new solutions and a selection mechanism to increase the proportion of better solutions. The different approaches are distinguished by the genetic structures that are adopted and the genetic operators that are utilized in generating new candidate solutions.

Many 'hybrid' algorithms have been proposed in the literature combining a global optimization algorithm with a classical 'hill-climbing' algorithm in order to gain performance improvements. A subset of these works, dealing with the integration of EAs with the classical Nelder–Mead simplex method (Nelder and Mead, 1965), has drawn interest in recent years. Simplex method is a robust, easy to be programmed and fast local search algorithm, which also shows the feature of making no use of the derivatives of the objective function at hand. These characteristics have made the classical simplex method and its modifications an interesting choice for cooperation with EAs in developing hybrid global optimization schemes.

Many attempts have been made to hybridize GAs with the classical simplex methods, some of them have been published by Chelouah and Siarry (2003), Hedar and Fukushima (2003), Musil et al. (1999), Yen et al. (1998), Yang and Douglas (1998), and Renders and Bersini (1994). The remarkable features underlying these hybrid methods are global exploration and parallelism performed with GA, and local exploitation with a classical or modified simplex method. A multi-parent recombination operator for real-coded genetic algorithms, called simplex crossover (SPX), has also been proposed and investigated (Higuchi et al., 2000; Tsutsi et al., 1999).

Beside these GA–Simplex hybrids, there exist few works dealing with the hybridization of the simplex method with other branches of EAs. We are only aware of the works published by Malaek and Karimi (2008, 2006), Luo and Yu (in press), and Sotiropoulos et al. (2002), which are shortly described in subsequent paragraphs. However, it should be noted that, here, only the algorithms incorporating elements from two (or more) methods into a single unified scheme are considered; and as a consequence, a common practice in which a local search method, like simplex method, is employed to refine a preliminary solution obtained by an EA is naturally excluded from our consideration.

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Sotiropoulos et al. (2002) proposed an EA called Simplex Evolution (SE) based on a deterministic evolution operator, called Simplex Operator that is actually equivalent to one cycle of the classical Nelder–Mead simplex method. An iteration of SE starts by setting the first individual from the current population as the base point, randomly selecting $n+1$ other individuals from the current population to form a simplex, and performing Simplex Operator on the selected simplex to generate a new individual and put it into the new generation. The iteration continues by selecting the next individual as the base point and so forth. Once the new generation grows to a fixed population size, the algorithm proceeds to the next iteration by setting the new generation as the current population.

Malaek and Karimi (2008, 2006) proposed an EA, called Global Simplex Search (GSS), based on the stochastic modifications of the reflection and expansion operators of the simplex method. The method has been independently developed to efficiently find accurate solutions for the constrained optimization problem arising from a typical MDM (Mass Distribution Management) problem (Malaek and Karimi, 2008), following the failure of the appropriately modified versions of the algorithms CGA and CHA (Chelouah and Siarry, 2003, 2000) in delivering such capabilities. The reflection and expansion operators of the classical simplex method with random reflection and expansion factors have been employed as the recombination operators of GSS, together with a low mutation rate. The authors have recognized the impact of the lower and upper reflection factor limits on the performance of the algorithm and used them as control parameters. The concept of generation does not exist in GSS; this allows for smooth decrease of the population from an initial size to a final one; which also proves to have an impact on the performance of the algorithm, at least against the specific MDM problem for which it was designed.

An algorithm combining the Differential Evolution (DE) (Price et al., 2005; Storn and Price, 1997) and the classical Nelder–Mead simplex method called 'm-simplex evolution' has recently been proposed by Luo and Yu (in press). The method is a population set based EA incorporating stochastic reflection and contraction operators of the classical Nelder–Mead simplex method with an additional step, in which an individual not attaining at least the average fitness of the overall population will take a deterministic step toward the best individual or away from the worst one, in an attempt to increase its fitness or at least increase the population diversity. The main feature of this method is the use of so-called 'low dimensional' simplexes consisting of m individuals, where $2<m<n+1$. For cases where n is much larger than m, the method has been called Low-Dimensional Simplex Evolution (LDSE), which has been claimed to exhibit better performances, compared to Full-Dimensional Simplex Evolution (FDSE). The authors have also provided numerical results comparing a special case of m-simplex evolution, called Triangle Evolution (TE) (i.e. $m=3$), with an enhanced DE method.

This paper presents the results of recent research aimed at further enhancement of the original GSS algorithm and presenting it as a general continuous global optimization method. The resulting algorithm, renamed to Global Simplex Optimization (GSO), to reflect the distinctions it has with the original GSS, can be viewed as a generalization of the traditional Nelder–Mead Simplex method to global optimization. The paper is organized as follows. Section 2 is devoted to the detailed presentation of the algorithm. Section 3 presents the experimental setup used to compare the algorithm to other methods, and some words of conclusion make up Section 4.

2. Global Simplex Optimization

In this section a brief review of the Nelder–Mead simplex method is presented, followed by the detailed presentation of our new algorithm.

2.1. Nelder–Mead simplex method

The Nelder–Mead simplex algorithm is a very powerful classical local descent algorithm, making no use of the objective function derivatives. A 'simplex' is a geometrical figure consisting, in n dimensions, of $n+1$ points $x_0,\ldots,x_n$. If any point of a simplex is taken as the origin, the n other points define vector directions that span the n-dimensional vector space. Through a sequence of elementary geometric transformations (reflection, contraction, expansion and multi-contraction), the initial simplex moves, expands or contracts (see Fig. 1). To select the appropriate transformation, the method only uses the values of the function to be optimized at the vertices of the simplex considered. After each transformation, a better one replaces the current worst vertex. Trial moves shown in Fig. 1 are generated according to the following basic operations:

reflection: $x_r=(1+\alpha)\bar{x}-\alpha x_w$
expansion: $x_e=\gamma x_r+(1-\gamma)\bar{x}$
contraction: $x_c=\beta x_w+(1-\beta)\bar{x}$

where x_b and x_w denote the best and worst vertices of the current simplex, respectively; $\bar{x}$ is defined by $\bar{x}=(1/n)\sum_{i=1}^{n} x_i$ and α, γ

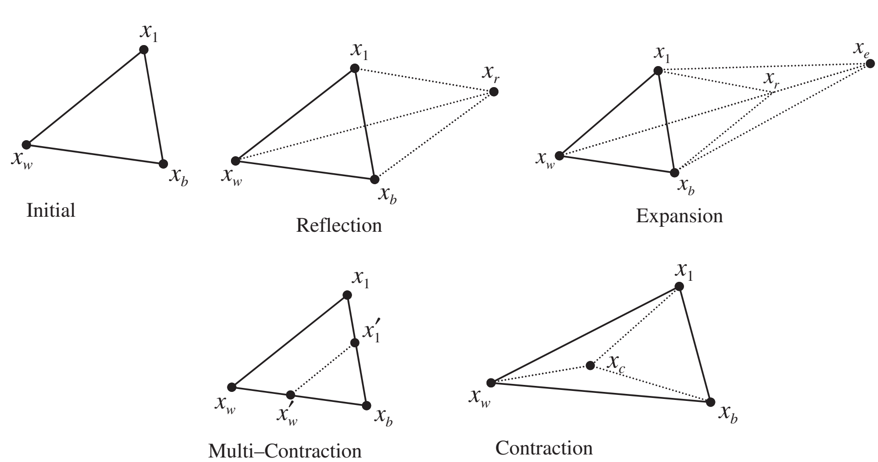

Fig. 1. Available moves in the Nelder–Mead simplex method.