Available online at www.sciencedirect.com

ScienceDirect

Procedia Computer Science 119 (2017) 90–96

Procedia Computer Science

www.elsevier.com/locate/procedia

6th International Young Scientists Conference in HPC and Simulation, YSC 2017, 1-3 November 2017, Kotka, Finland

Multidimensional Global Optimization Method Using Numerically Calculated Derivatives

Alexey S. Goryachih*, Maria A. Rachinskaya

Lobachevsky State University of Nizhni Novgorod, Nizhni Novgorod, Russia

Abstract

In the present paper, an efficient method for solving complex computationally consuming multiextremal global optimization problems is considered. To organize the adaptive global search, both the objective function and its first partial derivatives are supposed to satisfy the Lipschitz condition. The proposed approach deals with numerical estimates of the derivatives, which makes it possible to essentially reduce the amount of required computations with a nested dimension reduction. The results of the performed experiments prove the prospects of the developed approach.

Peer-review under responsibility of the scientific committee of the 6th International Young Scientist conference in HPC and Simulation

Keywords: Multiextremal optimization; global search algorithms; Lipschitz condition; numerical estimates for derivatives values; dimension reduction; computational experiments

1. Introduction

The global (or multiextremal) optimization problems [5, 13, 14, 19, 20] are referred to be among the most complex optimization problems. An objective function in the multiextremal problems may have several local optima in the search domain, which makes it substantially more difficult to find a global minimum due to the necessity of examining the entire feasible search domain. The amount of computations required for solving the global optimization problem may grow exponentially while increasing the number of variable parameters.

The global optimization problem is a problem of searching the minimum value of the real function $\varphi(y)$, which can be formulated as

$$\varphi(y^*) = \min\{\varphi(y) \colon y \in D\}, \tag{1}$$

where

* Corresponding author. Tel.: +7-961-635-9206.
E-mail address: a_goryachih@mail.ru

1877-0509 © 2018 The Authors. Published by Elsevier B.V.
Peer-review under responsibility of the scientific committee of the 6th International Young Scientist conference in HPC and Simulation
10.1016/j.procs.2017.11.164

- $y = (y_1, y_2, \dots, y_N)$ is a vector of variable parameters;
- N is a dimension of the multiextremal optimization problem;
- D is a search domain which represents an N-dimensional hyperparallelepiped

$$D = \{y \in R^N \colon a_i \le x_i \le b_i, 1 \le i \le N\}$$

for the given boundary vectors a and b.

It is supposed that the objective function $\varphi(y)$ (minimized function) is a multiextremal function whose value evaluation may require a great amount of computations.

The guaranteed global minimum estimates can be obtained only if some assumptions about the behavior of the minimized function $\varphi(y)$ are made a priori. One of the most commonly used assumptions is the satisfaction of the Lipschitz condition, i.e.,

$$|\varphi(y_2) - \varphi(y_1)| \le L\|y_2 - y_1\|, \ y_1, y_2 \in D, \tag{2}$$

where $L > 0$ is the Lipschitz constant and $\|\cdot\|$ denotes the Euclidean norm in R^N.

The Lipschitz condition corresponds to an assumption that the function variation is bounded if the variations of its variables are bounded. Such condition allows one to construct evaluates of possible behavior of the function $\varphi(y)$ based on the finite set of its values calculated at some points within the search domain D.

In a number of works [1, 3, 7, 9, 16, 17], the Lipschitz condition (2) was also expanded to the partial derivatives $\varphi_i'(y)$, $1 \le i \le N$, of the objective function $\varphi(y)$, i.e.,

$$|\varphi_i'(y_2) - \varphi_i'(y_1)| \le L_i\|y_2 - y_1\|, \ y_1, y_2 \in D, \ 1 \le i \le N, \tag{3}$$

where $L_i > 0$, $1 \le i \le N$, are the corresponding Lipschitz constants for the partial derivatives $\varphi_i'(y)$, $1 \le i \le N$.

The satisfaction of the conditions (3) allows one to obtain more accurate estimates for the possible values of the function $\varphi(y)$. In turn, this provides an opportunity to essentially increase the efficiency of the developing algorithms. However, to use the partial derivatives, it is necessary to calculate their values, which leads to additional computations. Moreover, the amount of such computations increases while increasing the dimension of the problems (a number of partial derivatives matches the dimension). Besides, when solving many applied optimization problems, the calculation of the derivatives may be constrained or even unavailable. In this respect, the development of the global optimization methods using numerical computation of the necessary values of the derivatives may become helpful.

In the present paper, the global optimization algorithms that use numerical derivatives of the minimized function $\varphi(y)$ are developed. In Section 2, a basic one-dimensional algorithm that uses numerical derivatives is given. Section 3 introduces a nested dimension reduction scheme that allows one to generalize the proposed one-dimensional algorithm to solving multidimensional global optimization problems. In Section 4, the results of the performed computational experiments that approve the prospects of the developed approach are described.

2. One-dimensional Global Optimization Algorithm Using Numerical Derivatives

The multidimensional method proposed in the present paper is based on the Adaptive Global Method using Numerical Derivatives (AGMND) designed to solve one-dimensional global optimization problems of the form

$$\varphi(x^*) = \min\{\varphi(x), \ x \in [a, b]\}.$$

In turn, the AGMND algorithm is a certain modification of the Adaptive Global Method using Derivatives (AGMD) that supposes the values of the first derivative of the objective function are substituted with their numerical estimates [9].

The computational scheme of the AGMND algorithm consists in as follows.

The first two iterations are performed at the points a and b at the ends of the search domain $[a, b]$. One more additional iteration is performed at a certain point $x^2 \in (a, b)$[1]. Next, let k, $k > 2$, global search iterations be performed,

[1] This additional point x^2 may be given a priori as well as be computed with the help of some additional computational procedure.