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New quadratic lower bound for multivariate functions in global optimization

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Abstract

The method investigated in this paper is concerned with the multivariate global optimization with box constraints. A new quadratic lower bound in a branch and bound framework is proposed. For a continuous, twice differentiable function f, the new lower bound is given by a difference of the linear interpolant of f and a quadratic concave function. The proposed BB algorithm using this new lower bound is easy to implement and often provides high quality bounds. The performances of the proposed algorithm are compared with those of two others branch and bound algorithms, the first uses a linear lower bound and the second a quadratic lower bound. Computational results conducted on several test problems show the efficiency of the proposed algorithm.

Keywords: Global optimization; Branch and bound; Linear and quadratic underestimation

1. Introduction

We consider the following problem

$$(P)\begin{cases}\alpha := \min f(x)\\ x \in B\end{cases}$$

where B is a box in $\mathbb{R}^n$ and $f : O \subset \mathbb{R}^n \to \mathbb{R}$ is twice continuously differentiable on an open convex set O containing B. Although the constraints are simple, the problem is still very hard in view of the need to find a *global* solution. Several methods in the literature have been investigated for solving this problem. They can be divided into two approaches: heuristic and deterministic approaches [11,15,16]. The most popular deterministic approaches are interval analysis [13,14], and exact algorithms as the adaptation of branch and bound proposed in [4].

Deterministic branch and bound methods for the solution of general nonlinear programs have become increasingly popular during the last decade or two, with increasing computer speed, algorithmic improvements, and multiprocessors. These methods are mostly based on the construction of a convex underestimating problem which allows the generation of two converging sequences of upper and lower bounds.

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The computation of a good convex lower bound function is very important in global optimization, since the tightness of the lower bound of nonconvex functions has a strong influence on the amount of computation. Constant and affine lower bound functions are extensively used in global optimization because of their simplicity and ease of computation [12,23]. In [1,4], the authors developed the αBB algorithm that uses a convex relaxation strategy to determine rigorous lower bounds on the global minimum solution. The algorithm implements a branch and bound strategy that utilizes convex NLPs for bounding. Convex envelopes and tight convexifications are obtained for specially structured nonconvex terms, and α-convex underestimations for twice continuously differentiable functions. The latter are determined by adding a non-positive convex function to the original nonconvex function such that the Hessian of the sum is guaranteed to be positive semi-definite [2]. In [20], a new spline is introduced to refine the convex underestimation approach used in the αBB. In [9], the authors introduced a new method for computing tight affine lower bound functions for a polynomial in Bézier form, by using a linear least squares approximation of the control points. Unfortunately, this method needs the translation of the polynomial from the power to the Bernstein basis. In [21], the authors compute the range of values of real functions using B-splines form. A survey of recent advances in global optimization may be found in [8]. In [18], the authors exploit the structure of f and the fact that a non convex function can be described by the difference of convex functions. The DC (difference of convex functions) programming and related DCA algorithms have been applied successfully to global optimization of non convex functions. In [19], the authors proposed a branch and bound DC algorithm combined with an ellipsoid technique, for solving box constrained non convex quadratic problems. In [17], the authors proposed an efficient algorithm for the univariate case, based on branch and bound techniques and a quadratic lower underestimation. It was shown in that work that the quadratic lower underestimation is easy to build and gives much improvement than the widely used linear underestimation. Motivated by these benefits, in this work we extend the algorithm to the multivariate case. The organization of this paper is as follows. In Section 2, we present the main results of the paper concerning the lower bounding procedure. The case of quadratic programming is discussed in Section 3. The algorithm and its convergence are studied in Section 4, while numerical results are reported in Section 5. The conclusions of the work are given in Section 6.

2. Main results

Let $S := [p, q]$ be a bounded closed interval in $\mathbb{R}$. Let f be a continuously twice differentiable function S, such that $|f''(x)| \leq K$ for all x in $[p, q]$. Let x^0 and x^1 be two real numbers in $[p, q]$ such that $x^0 \leq x^1$. Let w_0 and w_1 be real valued functions defined by

$$w_0(x) = \frac{x^1 - x}{x^1 - x^0} \quad \text{if } x^0 \leq x \leq x^1, \qquad w_1(x) = \frac{x - x^0}{x^1 - x^0} \quad \text{if } x^0 \leq x \leq x^1. \tag{1}$$

Clearly, w_0 and w_1 are positives and verifies the partition of unity properties: for all x in the interval $[x^0, x^1]$, we have $w_0(x) + w_1(x) = 1$. We have also $w_i(x^j)$ is equal to 0 if $i \neq j$, and 1 otherwise.

Let $h = x^1 - x^0$ and $L_h f$ be the piecewise linear interpolant to f at points x^0, x^1 [5,7]

$$L_h f(x) = \sum_{i=0}^{1} f(x_i)\, w_i(x). \tag{2}$$

In [17], the authors proposed a quadratic underestimation $LB(f)$ of f on the interval $[x^0, x^1]$ as a difference of a piecewise linear interpolant and a concave quadratic perturbation. It is given by

$$LB(x) = L_h f(x) - \frac{1}{2}K\left(x - x^0\right)\left(x^1 - x\right), \quad h = x^1 - x^0 \tag{3}$$

where K is a positive number such that $\left|f''(x)\right| \leq K$, for all x in the interval $[p, q]$. We can generalize the result in Eq. (3), to multivariate global optimization problem (P). In this case, problem (P) can be written in the form

$$(P)\begin{cases} \min f(x_1, \ldots, x_n) \\ (x_1, \ldots, x_n) \in B. \end{cases}$$

Let B be the box $\Pi_{i=1}^{n}\left[x_i^0, x_i^1\right]$ and $V(B)$ the set of vertices of B. An element in $V(B)$ is denoted as $(x_1^{i_1}, \ldots, x_n^{i_n})$ with $i_k = 0$ or 1, for $k = 1, \ldots, n$. Let $h_i = x_i^1 - x_i^0$, the piecewise linear interpolant of f at $x_0, x_1, \ldots, x_n$ is