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Continuous Optimization

A solution algorithm for non-convex mixed integer optimization problems with only few continuous variables

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ABSTRACT

Geometric branch-and-bound techniques are well-known solution algorithms for non-convex continuous global optimization problems with box constraints. Several approaches can be found in the literature differing mainly in the bounds used.

The aim of this paper is to extend geometric branch-and-bound methods to mixed *integer* optimization problems, i.e. to objective functions with some continuous and some integer variables. Mixed-integer non-linear and non-convex optimization problems are extremely hard, containing several classes of NP-hard problems as special cases. We identify for which type of mixed integer non-linear problems our method can be applied efficiently, derive several bounding operations and analyze their rates of convergence theoretically. Moreover, we show that the accuracy of any algorithm for solving the problem with fixed integer variables can be transferred to the mixed integer case.

Our results are demonstrated theoretically and experimentally using the truncated Weber problem and the *p*-median problem. For both problems we succeed in finding exact optimal solutions.

1. Introduction

Geometric branch-and-bound methods are popular solution algorithms for continuous and non-convex optimization problems with a small number of variables, see e.g. Horst, Pardalos, and Thoai (2000) or Tuy (1998). These techniques find applications for example in facility location problems, see Plastria (1992), Drezner and Suzuki (2004), Blanquero and Carrizosa (2009), and Schöbel and Scholz (2010a) for general geometric branch-and-bound solution approaches in location theory and, e.g. Drezner and Drezner (2007), Fernández, Pelegrín, Plastria, and Tóth (2007), Blanquero, Carrizosa, and Hansen (2009), and Blanquero, Carrizosa, Schöbel, and Scholz (2011) among plenty of other references for some specific location problems solved by these techniques.

The most important task throughout any branch-and-bound algorithm is the calculation of lower bounds on the objective function for some smaller rectangles or boxes. Different techniques to do so are collected in Schöbel and Scholz (2010b), Scholz (2012b), and Scholz (2012a). Therein, the ***rate of convergence*** is introduced that allows to evaluate the quality of some well-known bounding operations.

All the above mentioned techniques deal with pure continuous objective functions. The contribution of this paper is to extend the method to mixed-integer non-linear (MINLP) optimization problems, see Hemmecke, Köppe, Lee, and Weismantel (2010, chap. 15) for a recent survey about methods in this field. Problems of this type are extremely hard to solve, containing several classes of NP-hard problems as special cases, among them, e.g.:

- the class of integer linear problems which is well known to be NP-hard, see Garey and Johnson (1979),
- the class of continuous quadratic programs with box constraints which is NP-hard if the problem is non-convex, see Pardalos and Vavasis (1991), or
- the problem of minimizing a polynomial function of degree 4 over $\mathbb{Z}^n$, which is NP-hard due to Lasserre (2001).

In contrast to the *classical* discrete branch-and-bound approach for mixed-integer (linear) optimization we propose a *geometric* branch-and-bound approach for solving mixed-integer non-linear problems. The idea is the following: In every step we branch along the *continuous* variables (as done in geometric methods such as, e.g., the big square small square method, see Plastria (1992)) and solve the discrete problem in any node to get a lower bound. Note that this is contrary to the usual discrete branch and bound approaches in which branching is done along the discrete variables and the continuous relaxation is solved in each node in order to obtain a bound.

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Although the algorithm we propose can theoretically be applied to any (MINLP), it only works efficiently if the (MINLP) admits some special properties. These are a small number of continuous variables admitting some box-constraints, and that fixing the continuous variables results in a discrete problem which can be efficiently solved, or at least bounded. Such problems appear in many fields (e.g. location theory or robust statistics), many of them being NP-hard, see Section 5 for more examples and references.

In order to apply geometric branch-and-bound techniques to mixed integer non-linear problems we derive some general bounding operations and we present theoretical results about the rate of convergence similar to Schöbel and Scholz (2010b). Moreover, we discuss an extension of the method which leads to exact optimal solutions under certain conditions given below. We implemented the approach and applied it to some facility location problems. The numerical results show that we succeeded in finding exact optimal solutions and that our method outperforms standard solution approaches.

The remainder of the paper is organized as follows. In the next section we will summarize notations and basic concepts which we use throughout the paper. Section 3 presents the geometric branch-and-bound prototype algorithm for mixed integer optimization problems before we prove the convergence of our algorithm in Section 4. In Section 5 we discuss some general bounding operations and results concerning their rates of convergence. Next, in Section 6 we suggest an extension of the algorithm which leads to exact optimal solutions under certain conditions. In the following two sections (Sections 7 and 8) we apply the proposed techniques to some facility location problems and report on some numerical results. Finally, a brief conclusion and aspects of further research can be found in Section 9.

2. Notations and basic concepts

Throughout the paper, we will use the following notations.

Notation 1. A *box* or *hyperrectangle* with sides parallel to the axes is denoted by

$$X = [\underline{x}_1,\ \bar{x}_1] \times \ldots \times [\underline{x}_n,\ \bar{x}_n] \subset \mathbb{R}^n.$$

The *diameter* of a box $X \subset \mathbb{R}^n$ is

$$\delta(X) = \max\{\|x - x'\|_2 : x, x' \in X\} = \sqrt{(\bar{x}_1 - \underline{x}_1)^2 + \ldots + (\bar{x}_n - \underline{x}_n)^2}$$

and the *center* of a box $X \subset \mathbb{R}^n$ is defined by

$$c(X) = \left(\frac{1}{2}(\underline{x}_1 + \bar{x}_1), \ldots, \frac{1}{2}(\underline{x}_n + \bar{x}_n)\right).$$

Our goal is to minimize a mixed integer function

$$f : \mathbb{R}^n \times \mathbb{Z}^m \to \mathbb{R}$$

assuming a feasible region $X \times \Pi$ where $X \subset \mathbb{R}^n$ is a box with sides parallel to the axes and $\Pi \subset \mathbb{Z}^m$ with $|\Pi| < \infty$. In order to apply the algorithm presented in the next section, we further need the following definition which is an extension of the *bounding operation* defined in Schöbel and Scholz (2010b) to mixed integer functions.

Definition 2. Let $X \subset \mathbb{R}^n$ be a box, $\Pi \subset \mathbb{Z}^m$ with $|\Pi| < \infty$, and consider

$$f : X \times \Pi \to \mathbb{R}.$$

A *bounding operation* is a procedure to calculate for any subbox $Y \subset X$ a *lower bound* $LB(Y) \in \mathbb{R}$ with

$$LB(Y) \leqslant f(x, \pi) \quad \text{for all } x \in Y \text{ and } \pi \in \Pi$$

and to specify a point $r(Y) \in Y$ and a point $\kappa(Y) \in \Pi$.

3. The prototype algorithm

The algorithm suggested in this section is a generalization of the ***big cube small cube*** method presented in Schöbel and Scholz (2010a). Here, we extend the problem to mixed integer minimization problems, i.e. to problems which contain continuous *and* integer variables.

Given $X \subseteq \mathbb{R}^n$ and $\Pi \subseteq \mathbb{Z}^m$ the goal of our approach is to minimize

$$f : X \times \Pi \to \mathbb{R}.$$

This is done using the following algorithmic scheme with an absolute accuracy of $\varepsilon > 0$.

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(1) Let $\mathcal{X}$ be a list of boxes and initialize $\mathcal{X} := \{X\}$.
(2) Apply the bounding operation to X and set $UB := f(r(X), \kappa(X))$.
(3) If $\mathcal{X} = \emptyset$, the algorithm stops. Else set

$$\delta_{max} := \max\{\delta(Y) :\ Y \in \mathcal{X}\}.$$

(4) Select a box $Y \in \mathcal{X}$ with $\delta(Y) = \delta_{max}$ and split it into s subboxes Y_1 to Y_s such that $Y = Y_1 \cup \ldots \cup Y_s$.
(5) Set $\mathcal{X} = (\mathcal{X} \setminus Y) \cup \{Y_1, \ldots, Y_s\}$.
(6) Apply the bounding operation to Y_1 to Y_s and set

$$UB = \min\{UB,\ f(r(Y_1), \kappa(Y_1)), \ldots, f(r(Y_s), \kappa(Y_s))\}.$$

(7) For all $Z \in \mathcal{X}$, if $LB(Z) + \varepsilon \geqslant UB$ set $\mathcal{X} = \mathcal{X} \setminus Z$. If UB has not changed it is sufficient to check only the subboxes Y_1 to Y_s.
(8) Whenever possible, apply some further discarding test, see Section 6.
(9) Return to Step (3).

We remark that it is a non-trivial task to calculate the lower bound $LB(Y)$ as required throughout the algorithm. We will address this question in Section 5.

4. Theoretical results

In order to evaluate the quality of bounding operations, we first extend the definition for the rate of convergence given in Schöbel and Scholz (2010b).

Definition 3. Let $X \subset \mathbb{R}^n$ be a box, let $\Pi \subset \mathbb{Z}^m$ with $|\Pi| < \infty$, and $f : X \times \Pi \to \mathbb{R}$. Furthermore, consider the minimization problem

$$\min_{\substack{x \in X \\ \pi \in \Pi}} f(x, \pi).$$

We say a bounding operation has the *rate of convergence* $p \in \mathbb{N}$ if there exists a fixed constant $C > 0$ such that

$$f(r(Y), \kappa(Y)) - LB(Y) \leqslant C \cdot \delta(Y)^p \tag{1}$$

for all boxes $Y \subset X$.

As shown in Schöbel and Scholz (2010b) for pure continuous objective functions, the larger the rate of convergence the smaller the number of iterations needed throughout the algorithm.

The next theorem shows that the proposed algorithm terminates after a finite number of iterations if the bounding operation has a rate of convergence of at least one.

Theorem 1. *Let $X \subset \mathbb{R}^n$ be a box, let $\Pi \subset \mathbb{Z}^m$ with $|\Pi| < \infty$, and $f : X \times \Pi \to \mathbb{R}$. Furthermore, consider the minimization problem*

$$\min_{\substack{x \in X \\ \pi \in \Pi}} f(x, \pi)$$

and assume a bounding operation with a rate of convergence of $p \geqslant 1$.