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Strengthening of lower bounds in the global optimization of Bilinear and Concave Generalized Disjunctive Programs

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ABSTRACT

This paper is concerned with global optimization of Bilinear and Concave Generalized Disjunctive Programs. A major objective is to propose a procedure to find relaxations that yield strong lower bounds. We first present a general framework for obtaining a hierarchy of linear relaxations for nonconvex Generalized Disjunctive Programs (GDP). This framework combines linear relaxation strategies proposed in the literature for nonconvex MINLPs with the results of the work by Sawaya and Grossmann (2009) for Linear GDPs. We further exploit the theory behind Disjunctive Programming by proposing several rules to guide more efficiently the generation of relaxations by considering the particular structure of the problems. Finally, we show through a set of numerical examples that these new relaxations can substantially strengthen the lower bounds for the global optimum, often leading to a significant reduction of the number of nodes when used within a spatial branch and bound framework.

1. Introduction

Generalized Disjunctive Programming (GDP), developed by Raman and Grossmann (1994), has been proposed as a framework that facilitates the modeling of discrete-continuous optimization problems by allowing the use of algebraic and logical equations through disjunctions and logic propositions that are expressed in terms of Boolean and continuous variables. In order to take advantage of existing solvers (Bonami et al., 2008; Kesavan, Allgor, Gatzke, & Barton, 2004; Leyffer, 2001; Sahinidis, 1996; Viswanathan & Grossmann, 1990; Westerlund & Pettersson, 1995), GDPs are often reformulated as MILP/MINLP problems by using either the Big-M (BM) (Nemhauser & Wolsey, 1988), or the Convex Hull (CH) (Lee & Grossmann, 2000) reformulation. It is important to note that GDP problems can always be reformulated as an MINLP. However, these reformulations are not unique and may have associated relaxations that are not very tight, consequently having an adverse effect on the efficiency of the algorithm that is used. In general, the tighter the relaxation of the reformulation and the fewer the number of variables and constraints, the smaller the computational effort is.

In the particular case of nonconvex GDP problems the direct application of traditional algorithms to solve the reformulated MINLPs such as Generalized Benders Decomposition (GBD) (Benders, 1962; Geoffrion, 1972) or Outer Approximation (OA) (Duran & Grossmann, 1986), may fail to find the global optimum since the solution of the NLP subproblem may correspond to a local optimum and the cuts in the master problem may not be valid. Therefore, specialized algorithms should be used in order to find the global optimum (Floudas, 2000; Horst & Tuy, 1996, Tawarmalani & Sahinidis, 2002). Nonconvex GDP problems with bilinear constraints are of particular interest since these arise in many applications, for instance, in the design of pooling problems (Meyer & Floudas, 2006), in the synthesis of integrated water treatment networks (Karuppiah & Grossmann, 2006), or generally, in the synthesis of process networks with multicomponent flows (Quesada & Grossmann, 1995b). In addition, nonconvex GDP problems with concave constraints frequently arise when nonlinear investment cost functions are considered (Turkay & Grossmann, 1996). To tackle this problem, Lee and Grossmann (2003) proposed a global optimization method that first relaxes the bilinear terms by using the convex envelopes of McCormick (1976) and the concave terms by using linear under-estimators. The convex hull (Balas, 1985) is then applied to each disjunction. This formulation is then used within a spatial branch and bound technique in which the branching is first performed on the Boolean variables followed by the continuous variables. While the method proved to be effective in solving several problems, a major question is whether one might be able to obtain stronger lower bounds to enhance the efficiency for globally optimizing GDP problems.

Sawaya and Grossmann (2009) have recently established new connections between Linear GDP and the Disjunctive Programming theory by Balas (1979). As a result, a family of tighter reformulations has been identified. These are obtained by performing a sequence

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of basic steps on the original disjunctive set (i.e. each basic step is characterized by generating a new set of disjunctions by intersecting the former), bringing it to a form closer to the Disjunctive Normal Form (DNF), and hence tightening its discrete relaxation (Balas, 1985). It is important to note that each intersection usually creates new variables and constraints. Therefore, it is important to recognize when it may be useful to make these intersections. Some general rules are described in this work.

In this work we build on the work by Sawaya and Grossmann (2009) exploiting the newly discovered hierarchy of relaxations in order to solve more efficiently nonconvex GDP problems, particularly, with bilinearities and concave functions in their constraints, namely Bilinear GDP and Concave GDP.

This paper is organized as follows. In Section 2 we present the general structure and particular properties of the problems for which we aim at finding stronger relaxations (i.e. Bilinear GDP and Concave GDP). In Sections 3 and 4, a general theoretical framework is proposed for obtaining tighter linear relaxations efficiently for nonconvex GDPs. The implementation of this framework is then illustrated in Section 5 by finding a relaxation for two small examples, one of them formulated as a Bilinear GDP and the other as a Concave GDP. Section 6 outlines the implementation of the tighter reformulation within a spatial branch and bound procedure whose performance is compared with current methodologies (i.e. Lee & Grossmann, 2003) in Section 7.

2. Nonconvex Generalized Disjunctive Programs

The general structure of a nonconvex GDP can be represented as follows (Lee & Grossmann, 2000; Raman & Grossmann, 1994; Turkay & Grossmann, 1996):

$$\mathit{Min}\ Z = f(x) + \sum_{k\in K} c_k$$

$$s.t.\ g^l(x) \le 0, \quad l \in L$$

$$\bigvee_{i\in D_k} \begin{bmatrix} Y_{ik} \\ r^j_{ik}(x) \le 0 \quad j \in J_{ik} \\ c_k = \gamma_{ik}(x) \end{bmatrix} \quad k \in K \quad (GDP_{NC})$$

$$\Omega(Y) = True$$

$$x^{lo} \le x \le x^{up}$$

$$x \in R^n,\ c_k \in R^1,\ Y_{ik} \in \{True, False\}$$

where f: $R^n \to R^1$ is a function of the continuous variables x in the objective function, g^l: $R^n \to R^1$, $l \in L$, belongs to the set of global constraints, the disjunctions $k \in K$, may be composed of a number of terms $i \in D_k$, that are connected by the OR operator. In each term there is a Boolean variable Y_{ik}, a set of inequalities $r^j_{ik}(x) \le 0$, $r^j_{ik} : R^n \to R^1$, and a cost variable c_k. If Y_{ik} is true, then $r^j_{ik}(x) \le 0$ and $c_k = \gamma_{ik}(x)$ are enforced; otherwise they are ignored. Also, $\Omega(Y) = True$ are logic propositions for the Boolean variables. As indicated in Sawaya and Grossmann (2009), we assume that the logic constraints $\underset{i\in D_k}{\vee} Y_{ik}$ are contained in $\Omega(Y) = True$. In a nonconvex GDP, f, r_{ik}, γ_{ik} and/or g^l are nonconvex functions.

Bilinear GDPs (BGDP) are the first class of nonconvex GDP problems that we address in this paper. A BGDP is a nonconvex GDP where the functions in the constraints only contain bilinear and linear terms. In general we can represent a BGDP as:

$$\mathit{Min}\, Z = d^T x + \sum_{k\in K} c_k$$

$$s.t.\, x^T Q^l x + a^l x \le b^l, \quad l \in L$$

$$\bigvee_{i\in D_k} \begin{bmatrix} Y_{ik} \\ x^T Q^j_{ik} x + a^j_{ik} x \le b^j_{ik} \quad j \in J_{ik} \\ c_k = \gamma_{ik} \end{bmatrix} \quad k \in K \quad (GDP_B)$$

$$\Omega(Y) = True$$

$$x^{lo} \le x \le x^{up}$$

$$x \in R^n,\ c_k \in R^1,\ Y_{ik} \in \{True, False\}$$

where some of the matrices Q^l, Q^j_{ik} are indefinite

Remark 1. Note that if all matrices Q^l, Q^j_{ik} are positive semidefinite then the continuous relaxation of the problem is convex and no global optimization methods are required to find the optimal solution. Without loss of generality we consider the diagonal of the matrices to be 0.

Remark 2. To make the notation clearer, we assume γ_{ik} to be constant in (GDP_B).

In order to solve (GDP_B) with a spatial branch and bound method, a *convex GDP relaxation* is required. A valid *Linear GDP relaxation* (see Proposition 1) can be obtained by finding suitable under- and over-estimating functions of the nonconvex constraints. Although this set of estimators is not unique, we propose to use the convex envelopes proposed by McCormick (1976) for bilinear terms (see also Al-Khayyal & Falk, 1983).

Defining $X = xx^T$ we can find a relaxation for each term $X_{ij} = x_i x_j$ as:

$$\begin{aligned} X_{ij} &\le x_i x_j^{up} + x_j x_i^{lo} - x_j^{up} x_i^{lo} \\ X_{ij} &\le x_i x_j^{lo} + x_j x_i^{up} - x_j^{lo} x_i^{up} \\ X_{ij} &\ge x_i x_j^{lo} + x_j x_i^{lo} - x_j^{lo} x_i^{lo} \\ X_{ij} &\ge x_i x_j^{up} + x_j x_i^{up} - x_j^{up} x_i^{up} \end{aligned} \qquad i = 1, 2, \ldots, n, \quad i < j < n+1$$

This leads to the following Linear GDP,

$$\mathit{Min}\, Z^L = d^T x + \sum_{k\in K} c_k$$

$$s.t.\, Q^l \cdot X + a^l x \le b^l, \quad l \in L$$

$$\bigvee_{i\in D_k} \begin{bmatrix} Y_{ik} \\ Q^j_{ik} \cdot X + a^j_{ik} x \le b^j_{ik} \quad j \in J_{ik} \\ c_k = \gamma_{ik} \end{bmatrix} \quad k \in K \quad (GDP_{RB})$$

$$\begin{aligned} X_{ij} &\le x_i x_j^{up} + x_j x_i^{lo} - x_j^{up} x_i^{lo} \\ X_{ij} &\le x_i x_j^{lo} + x_j x_i^{up} - x_j^{lo} x_i^{up} \\ X_{ij} &\ge x_i x_j^{lo} + x_j x_i^{lo} - x_j^{lo} x_i^{lo} \\ X_{ij} &\ge x_i x_j^{up} + x_j x_i^{up} - x_j^{up} x_i^{up} \end{aligned} \qquad i = 1, 2, \ldots, n, \quad i < j < n+1$$

$$\Omega(Y) = True$$