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Tightening piecewise McCormick relaxations for bilinear problems

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ABSTRACT

We address nonconvex bilinear problems where the main objective is the computation of a tight lower bound for the objective function to be minimized. This can be obtained through a mixed-integer linear programming formulation relying on the concept of piecewise McCormick relaxation. It works by dividing the domain of one of the variables in each bilinear term into a given number of partitions, while considering global bounds for the other. We now propose using partition-dependent bounds for the latter so as to further improve the quality of the relaxation. While it involves solving hundreds or even thousands of linear bound contracting problems in a pre-processing step, the benefit from having a tighter formulation more than compensates the additional computational time. Results for a set of water network design problems show that the new algorithm can lead to orders of magnitude reduction in the optimality gap compared to commercial solvers.

1. Introduction

The simplest and perhaps most common type of constraint in Chemical Engineering is the blending equation, in which the property of a product resulting from a mix of materials is estimated as a weighted sum by flowrates of the properties of the components. The products of flowrates by properties form bilinear terms that are nonconvex and therefore give rise to multiple local solutions. Blending constraints arise in crude oil operations in refineries (Lee et al., 1996; Jia et al., 2003; Yadav and Shaik, 2012), in the blending of different distilled fractions such as gasoline and diesel (Moro et al., 1998; Jia and Ierapetritou, 2003; Kolodziej et al., 2013b), in the design of distributed wastewater treatment systems (Galan and Grossmann, 1998; Meyer and Floudas, 2006; Teles et al., 2012), integrated water (Karuppiah and Grossmann, 2006; Faria and Bagajewicz, 2012; Rubio-Castro et al., 2013) and mass and property integration networks (Nápoles-Rivera et al., 2010). Bilinear terms also arise in the trim loss problem in paper plants (Harjunkoski et al., 1998; Zorn and Sahinidis, 2013) and in the operation of hydro energy systems (Catalão et al., 2011; Castro and Grossmann, 2014).

In order to find rigorous global optimal solutions to bilinear problems, which can be of the nonlinear (NLP) or mixed-integer nonlinear (MINLP) type, alternative algorithms can be used that have in common the generation of linear (LP) or mixed-integer linear (MILP) relaxations of the original problem. Assuming that we are dealing with a minimization problem, a relaxation provides a lower bound, any feasible solution provides an upper bound and global convergence is achieved when bounds lie within a specified tolerance. It is thus critical to derive tight relaxations to improve the lower bound and also, indirectly, to provide initialization points leading to better solutions.

In the standard McCormick (1976) relaxation, each bilinear term is replaced by a new variable and four sets of linear inequality constraints are added to the formulation. In these, the new variable is related to the two variables forming the bilinear term and their lower and upper bounds. As the tighter the lower and upper bounds, the higher the quality of the relaxation, most global optimization solvers do variable bounding to reduce the search space of the relaxed problem. For instance, the new solver GloMIQO (Misener and Floudas, 2013b) uses different techniques such as interval arithmetic, reduced cost and optimality-based bound contraction. In the latter, which is the subject of this paper, a sequence of minimization and maximization problems are solved for each nonlinearly participating variable to find the tightest possible bounds. Faria and Bagajewicz (2011) proposed a global optimization algorithm based on a more thorough optimality-based bound contraction procedure for one of the variables of each bilinear term. It consists of successive contracting steps that first involve solving a relaxation problem to compute reference values for the bilinear participating variables and then on solving multiple auxiliary linear

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models to update the bounds. Note that direct discretization was used, which has the advantage of requiring two rather than four sets of inequality constraints per bilinear term and the disadvantage of leading to weaker relaxation problems.

Further reduction in the feasible space of the relaxed problem requires domain partitioning. It can be done sequentially as in spatial branch and bound (Tawarmalani and Sahinidis, 2005; Misener and Floudas, 2013b) by, for example, bisecting the domain of one of the variables belonging to the bilinear term that most violates the feasible region of the original problem (Ruiz and Grossmann, 2011); or simultaneously. For the simultaneous approach, one can rely on the piecewise McCormick envelopes, proposed by Grossmann and co-workers for the case of univariate and uniform partitioning (Bergamini et al., 2005; Karuppiah and Grossmann, 2006) and extensively studied by, among others, Floudas and co-workers (Gounaris et al., 2009; Misener et al., 2011), Karimi and co-workers (Wicaksono and Karimi, 2008; Hasan and Karimi, 2010), and Faria and Bagajewicz (2012); or on multiparametric disaggregation, a new concept developed by Castro and co-workers (Teles et al., 2013a,b; Kolodziej et al., 2013a). While piecewise McCormick and multiparametric disaggregation are conceptually standalone approaches, proving global optimality for a typically large number of partitions, they can naturally be integrated within spatial branch and bound frameworks as is the case with GloMIQO. In addition, they can replace the standard McCormick relaxation to provide stronger bounds when performing optimality-based bound contraction, at the expense of higher computational times resulting from the solution of multiple MILPs instead of LPs (Castro and Grossmann, 2014).

The comparative study between uniform piecewise McCormick and multiparametric disaggregation has shown that the former is tighter when in the presence of quadratic terms but generates considerably larger MILPs for the same number of partitions (Kolodziej et al., 2013a). More precisely, the number of binary variables in piecewise McCormick grows linearly with the number of partitions, whereas for multiparametric disaggregation the growth is only logarithmic. In practice, this is translated into the ability to reach considerably lower optimality gaps due to a computational performance that is often orders of magnitude better, as can be seen for the design of water-using networks (Castro and Teles, 2013). Yet, piecewise McCormick allows for more freedom when choosing the number of partitions, which can be important when they are just a few, more likely to occur for larger problems or when integrated within a spatial branch-and bound solver. In this respect, the piecewise relaxation option in GloMIQO (Misener and Floudas, 2013b), although turned off by default since convergence is generally faster that way, increases the probability that the bilinear problem will solve to ε-global optimality within a given time limit. Experiments were conducted for 2, 4 and 8 partitions and for a maximum number of partitioned variables equal to 30 (Misener and Floudas, 2012).

The novelty of this work is to propose tighter constraints for the piecewise McCormick relaxation of a bilinear term that feature improved lower and upper bounds for the partitioned variable as well as for the non-partitioned variable. Partition-dependent bounds for the non-partitioned variable are determined through optimality-based bound contraction, which involves solving two linear problems per partition. Once the solution of the tightened relaxation approach is found, it is used as a starting point for the solution of the original problem so as to find a near optimal solution with a fast local solver and to compute a rigorous optimality gap. To illustrate the performance of the new algorithm, we will consider small test problems and larger water-using network design problems from the literature. While such problems are of the nonlinear type, it should be noted that mixed-integer bilinear problems can also be tackled by the proposed approach simply by solving MILPs rather than LPs when performing optimality-based bound contraction and by fixing the binary variables before using a local NLP solver to find a feasible solution (see Castro and Grossmann, 2014, who consider standard McCormick and multiparametric disaggregation relaxation approaches). Relaxation techniques for bilinear terms with binary variables and nonlinear integer problems with signomial terms can also be found in Rodriguez and Vecchietti (2013) and Tsai and Lin (2013).

2. Problem definition

We consider the class of nonconvex, nonlinear problems where all nonlinear terms are of the bilinear type $x_i x_j$ and all variables are continuous. In (**P**), x is an m-dimensional vector of non-negative variables that lie between given lower x^L and upper x^U bounds. Set Q includes all functions f_q, including the objective function f_0 and all the constraints. The function $h_q(x)$ is linear in x, BL is an (i,j)-index set that defines the bilinear terms $x_i x_j$ present in the problem and a_{ijq} is a scalar. Note that $i=j$ can be allowed to accommodate quadratic problems.

$$\min x = f_0(x) \tag{P}$$

subject to

$$f_q(x) \le 0 \quad \forall q \in Q \backslash \{0\}$$

$$f_q(x) = \sum_{(i,j) \in BL} a_{ijq} x_i x_j + h_q(x) \quad \forall q \in Q$$

$$x^L \le x \le x^U$$

$$x \in \mathbb{R}^m$$

3. Lower bounding formulation from piecewise McCormick envelopes

McCormick (1976) envelopes can be used to provide different types of relaxations to problems of type (**P**). In the standard approach, a linear programming (LP) relaxation is derived by replacing each bilinear term involving variables x_i and x_j with a new variable $w_{ij} = x_i x_j$ and adding four sets of constraints. A tighter mixed-integer linear programming (MILP) relaxation can be constructed by partitioning the domain of one of the variables (x_j) of the bilinear term into n disjoint regions, with new binary variables being added to the formulation to select the optimal partition for x_j. In the seminal work by Grossmann and co-workers (Bergamini et al., 2005; Karuppiah and Grossmann, 2006), partitions are generated uniformly and there is a linear increase in problem size with the number of partitions. This is the lower bounding approach considered in this work. A different uniform partitioning scheme featuring a logarithmic growth in the number of binary variables was proposed by Misener et al. (2011) but the results failed to show major benefits in their use. Other extensive studies involving a variety of piecewise under- and overestimators, some of them featuring non-identical segment lengths, have been performed by Wicaksono and Karimi (2008) and Gounaris et al. (2009). Hasan and Karimi (2010) report on the advantage of uniform placement of grid points.

Let x_{jn}^L and x_{jn}^U represent respectively the lower and upper bounds of variable x_j for partition n. If the value of x_j does belong to such partition, then binary variable $y_{jn} = 1$ and the McCormick envelopes hold. The piecewise McCormick relaxation (**PR-GDP**) can be formulated as a Generalized Disjunctive Program (Raman and Grossmann, 1994) and is tighter due to the use of the partition-dependent parameters x_{jn}^L and x_{jn}^U in the four constraints inside the disjunction, instead of the global bounds x_j^L and x_j^U.

$$\min z^R = f_0(x) = \sum_{(i,j) \in BL} a_{ij0} w_{ij} + h_0(x) \tag{PR-GDP}$$