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Comparison of global optimization algorithms for the design of water-using networks

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ABSTRACT

We address a special class of bilinear process network problems with global optimization algorithms iterating between a lower bound provided by a mixed-integer linear programming (MILP) formulation and an upper bound given by the solution of the original nonlinear problem (NLP) with a local solver. Two conceptually different relaxation approaches are tested, piecewise McCormick envelopes and multiparametric disaggregation, each considered in two variants according to the choice of variables to partition/parameterize. The four complete MILP formulations are derived from disjunctive programming models followed by convex hull reformulations. The results on a set of test problems from the literature show that the algorithm relying on multiparametric disaggregation with parameterization of the concentrations is the best performer, primarily due to a logarithmic as opposed to linear increase in problem size with the number of partitions. The algorithms are also compared to the commercial solvers BARON and GloMIQO through performance profiles.

1. Introduction

Water networks (Bagajewicz, 2000; Jezowski, 2010) are a special type of process network problems (Quesada & Grossmann, 1995) that can be formulated as non-convex bilinear programs. Another example is the pooling problem (Haverly, 1978), which has been receiving considerable attention in the literature (Faria & Bagajewicz, 2012b; Meyer & Floudas, 2006; Misener & Floudas, 2010; Misener, Thompson, and Floudas, 2011). The non-convex bilinear terms arise in the mixing of streams with different properties and are known to give rise to a multiplicity of local optima, which prevent gradient based solvers from certifying optimality of the nonlinear program (NLP). Further complexity will arise from binary decisions associated to alternative process units and/or connecting pipelines, leading to a mixed-integer nonlinear program (MINLP).

The most common global optimization algorithms are based on spatial branch and bound (Ryoo & Sahinidis, 1996) and involve multiple formulations of a lower bounding problem that is a relaxation of the original bilinear problem. The relaxations are frequently based on the standard McCormick (1976) envelopes, involving the variables domain still in consideration (full domain in the root node) and leading to a linear problem (LP), or on piecewise envelopes (Bergamini, Aguirre, & Grossmann, 2005; Karuppiah & Grossmann, 2006; Meyer & Floudas, 2006). In the latter, the domain of the variables is divided ab initio into a given number of partitions, with the purpose of generating multiple McCormick envelopes that will provide a tighter relaxation. The optimal set of partitions is identified through binary variables leading to a mixed-integer linear programming (MILP) problem.

Partitioning of the search space can be done with respect to one or both variables of the bilinear term. Wicaksono and Karimi (2008), Hasan and Karimi (2010), and Faria and Bagajewicz (2012a) have performed extensive computational tests for a variety of schemes, the former deriving the alternative MILP formulations from a disjunctive program (Balas, 1979). Between the two most common reformulation methods (Balas, 1985), the convex hull approach was found to be superior to its big-M counterpart. More importantly, these schemes require a number of binary variables proportional to the number of partitions, which given the fact that many partitions may be required to achieve a good relaxation, i.e. a low optimality gap, may result in a prohibitively large MILP. To overcome this limitation, Vielma, Ahmed, and Nemhauser (2010), Vielma and Nemhauser (2011), and Misener, Thompson, and Floudas (2011), have proposed MILP formulations that use a logarithmic number of binary variables.

An alternative global optimization approach called multiparametric disaggregation has recently been proposed by Teles, Castro, and Matos (2013) for polynomial problems, which shares the important property of using a logarithmic number of binary variables. Through the discretization of the domain of one of the variables of the bilinear term, the original problem can be

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