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ϵ-OA for the solution of bi-objective generalized disjunctive programming problems in the synthesis of nonlinear process networks

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ABSTRACT

There has been an increasing interest in multicriteria optimization (MCO) of nonlinear process network problems in recent years. Several mathematical models have been developed and solved using MCO methodologies including ϵ-constraint, weighted sum, and minimum distance. In this paper, we investigate the bi-objective nonlinear network synthesis problem and propose an effective algorithm, ϵ-OA, based on augmented ϵ-constraint and logic-based outer approximation (OA). We provide theoretical characterization of the proposed algorithm and show that the solutions generated are efficient. We illustrate the effectiveness of our novel algorithm on two benchmark problems. The ϵ-OA is compared to the straightforward use of OA with augmented ϵ-constraint algorithm (ϵ-con + OA), the augmented ϵ-constraint without OA (ϵ-MINLP), and the traditional ϵ-constraint (T-ϵ-con). Based on the results, our novel algorithm is very effective in solving the bi-objective generalized disjunctive programming problems in the synthesis of process networks.

1. Introduction

The generalized disjunctive programming (GDP) framework for the representation of superstructures and its demonstration in linear systems was presented by Raman and Grossmann (1994). The discrete–continuous nature of the system was modeled using disjunctions and the logical interrelationships among the discrete decisions were represented with propositional logic expressions. The extension of GDP to nonlinear systems was investigated by Turkay and Grossmann (1996a). They presented efficient logic-based outer approximation (OA) and Benders decomposition algorithms to solve this challenging problem. The efficiency of the proposed algorithms was illustrated on nonlinear process networks with complex investment costs (Turkay and Grossmann, 1996b, 1998). The GDP uses Boolean variables (Y) to formulate nonlinear disjunctions for process units in the networks. If a process unit is present in the network, Y becomes "True" and a nonlinear convex inequality between flows holds, otherwise, the unit is absent, Y is "False" and the associated flows are zero. The GDP also incorporates propositional logics that are redundant and do not eliminate optimal solutions; however, they are very useful in reducing the search space so that the solution time decreases (Turkay and Grossmann, 1996a). The algebraic representation of nonlinear disjunctions and the propositional logics are investigated in the literature (Raman and Grossmann, 1994; Turkay and Grossmann, 1996a, 1998; Grossmann and Trespalacios, 2013; Sawaya and Grossmann, 2007; Lee and Grossmann, 2005; Grossmann and Lee, 2003).

As the decision making in optimization of real world problems usually involves multiple criteria, e.g. cost, social issues, environmental impacts, and profit, MCO has gained increasing interest in various applications in recent decades. In most cases, the MCO problems can be formulated as mathematical programs where the efficient solutions can be obtained from solving these problems. Van Veldhuizen and Lamont (2000), Marler and Arora (2004), and Figueira et al. (2005) provide a comprehensive literature review on MCO. Several researchers used Multi-Objective Mixed Integer Nonlinear Programming (MOMINLP) to solve MCO problems in different applications. Martinez and Eliceche (2008, 2011) studied minimization of environmental impacts and cost in operation of steam and power plant and formulated the problem as MOMINLP. They solved the resulting MCO problem using minimum distance to the utopia point, ϵ-constraint, weighted sum and global criterion. Cucek et al. (2012) developed a MI(N)LP model for regional biomass energy supply chains and used ϵ-constraint method to find the

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efficient solutions to this problem. Cucek et al. (2012) reduced the dimensionality of the criteria in MOMINLP of biomass energy supply chains based on similar behavior among criteria. Chakraborty and Linninger (2002) presented combinatorial process synthesis for developing plant-wide recovery and treatment policies with conflicting objectives cost and environmental impact. A common issue in all of the previous work is the straightforward use of existing methods, specially the traditional ϵ-constraint (T-ϵ-con), to solve the MCO problems. In T-ϵ-con, one of the objectives optimized while the values of other criteria are bounded by a parameter, ϵ. Then, a set of efficient solutions are found by systematic variation of ϵ (Haimes et al., 1971; Hwang and Masud, 1979). Several methods for selecting ϵ-values are studied (Goicoechea et al., 1976; Stadler, 1988). The drawback of T-ϵ-con is, however, the possibility of generating weekly efficient solutions. The augmented ϵ-constraint method overcomes this impediment by including the slacks of the constraints that are added due to the other criteria to the objective function, weighted by a parameter μ, to eliminate the possibility of generating weekly dominated solutions (Mavrotas, 2009; Mavrotas and Florios, 2013). In this paper, we investigate bi-objective nonlinear networks where two objective functions are simultaneously minimized (without loss of generality), and develop an efficient algorithm (ϵ-OA), using augmented ϵ-constraint and OA, to find efficient solutions in a very short CPU time.

MINLPs are categorized as the most difficult problems as they include both discrete and continuous variables and involve nonlinearity in objective function and constraints. Several methods have been proposed to solve MINLPs including NLP-based branch and bound (Nabar and Schrage, 1991), generalized Beneders decomposition (Geoffrion, 1972), and OA (Duran and Grossmann, 1986). The OA is suitable for convex MINLPs and its execution involves repeatedly solving the NLP subproblem, generated by fixing the values of discrete variables, and the Master problem, constructed by replacing the nonlinear functions by their linear approximations, until the bounds from these two problems converge. In this paper, we use logic-based OA to develop our ϵ-OA algorithm to solve bi-objective GDPs in the synthesis of nonlinear process networks. The ϵ-OA uses the results of the previously solved subproblems to eliminate the unnecessary operations in subsequent iterations. We conduct an experiment to compare the effectiveness of ϵ-OA with the straightforward use of OA to solve subproblems of the augmented ϵ-constraint method (ϵ-con + OA), the augmented ϵ-constraint with MINLP solvers (ϵ-MINLP), and T-ϵ-con. We illustrate these four algorithms on 3 and 8 process networks and show that ϵ-OA is very effective than others. Moreover, compared to T-ϵ-con, our novel algorithm ϵ-OA enhances the quality of the results as it guarantees the efficiency of the solutions.

The design of this paper goes as follows. Section 2 presents the bi-objective nonlinear process networks and illustrates on 3 and 8 process problems. The augmented ϵ-constraint model of this problem is given in Section 3. Section 4 outlines the foundation of logic-based OA with respect to the bi-objective nonlinear process networks problem. We propose the novel ϵ-OA algorithm in Section 5. A computational experiment is presented in Section 6 to illustrate the efficiency of ϵ-OA. This is followed by conclusion.

2. Bi-objective nonlinear process networks

The generalized disjunctive programming model of bi-objective nonlinear process networks (P) is represented as follows.

$$\min \quad Z = (z_1, z_2) = \left(\sum_i c_i + f_1(x), \sum_i p_i + f_2(x)\right) \tag{1}$$

$$\text{s.t.} \quad g(x) \le 0, \tag{2}$$

$$\begin{bmatrix} Y_i \\ h_i(x) \le 0 \\ c_i = \gamma_i \\ p_i = \eta_i \end{bmatrix} \vee \begin{bmatrix} \neg Y_i \\ B^i x = 0 \\ c_i = 0 \\ p_i = 0 \end{bmatrix} \quad \forall i \in D, \tag{3}$$

$$\Omega(Y) = True, \tag{4}$$

$$x \in \mathbb{R}^n,\ c \ge 0,\ p \ge 0,\ Y \in \{True, False\}^m. \tag{5}$$

The bi-objective optimization model involves continuous (x, c, and p) and Boolean (Y) decision variables. The Boolean variables are defined for process units in the network and show the existence of the corresponding unit. The objective function simultaneously minimizes two functions, z_1 and z_2. Eq. (2) represents global inequalities that always hold independent of the values of Boolean variables. Disjunctions (Eq. 3) are written for all processing units; if the corresponding Boolean variable is "True", then a particular relation among x's hold and the relevant fixed costs (c and p) are paid, otherwise the associated c, p, and x's become zero. Here, $B^i = [b_k^T]$, where $b_k^T = e_k^T$ if $x_k = 0$, and $b_k^T = 0^T$ if $x_k \neq 0$. Eq. (4) is the logic relations between Boolean variables based on the connections and interactions among units. In this model, $f_1(x)$, $f_2(x)$, $g(x)$, and $h_i(x)$ can be linear or nonlinear convex functions.

2.1. Example: 3-process network

In this section, we present the well-known 3-process network synthesis example (Kocis and Grossmann, 1989) to illustrate the bi-objective model given by Eqs. (1)–(5). This example consists of 3 processing units, as shown in Fig. 1. The raw material A should be processed in either units 2 or 3 to produce B. The material B can be also purchased from outside. Unit 1 processes B and produces C. The variables x_k, $k = 1, \ldots, 8$, are the amount of material flows.

The objective function of this problem is to simultaneously minimize z_1 and z_2. Note that we generate the second objective function, z_2, so that the solution corresponding to the best compromise between these objectives is found.

$$\begin{aligned} \min \quad & Z = (z_1, z_2) \\ & z_1 = c_1 + c_2 + c_3 + x_4 + 1.8x_1 + 1.2x_5 + 7x_6 - 11x_8 \\ & z_2 = p_1 + p_2 + p_3 \\ & \quad +1.8x_1 + 2x_2 + 3x_3 + x_4 + 1.2x_5 + 7x_6 - 5x_7 - 11x_8 \end{aligned} \tag{6}$$

The material balance equations at mixing/splitting points, and specifications on the flows are as follows. These relations are general and hold independent of the values of Boolean variables.

$$\begin{aligned} & x_1 - x_2 - x_3 = 0, \\ & x_7 - x_4 - x_5 - x_6 = 0, \\ & x_5 \le 5, \\ & x_8 \le 1 \end{aligned} \tag{7}$$

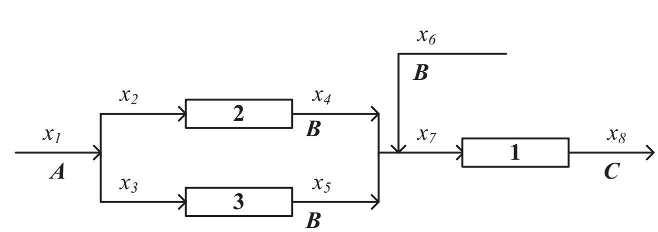

Fig. 1. Superstructure for the 3-process network synthesis.