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Globally convergent exact and inexact parametric algorithms for solving large-scale mixed-integer fractional programs and applications in process systems engineering

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ABSTRACT

This paper is concerned with the parametric algorithms for solving large-scale mixed-integer linear and nonlinear fractional programming problems, as well as their application in process systems engineering. By developing an equivalent parametric formulation of the general mixed-integer fractional program (MIFP), we propose four exact parametric algorithms based on the root-finding methods, including bisection method, Newton's method, secant method and false position method, respectively, for the global optimization of MIFPs. We also propose an inexact parametric algorithm that can potentially outperform the exact parametric algorithms for some types of MIFPs. Extensive computational studies are performed to demonstrate the efficiency of these parametric algorithms and to compare them with some general-purpose mixed-integer nonlinear programming methods. The applications of the proposed algorithms are illustrated through two case studies on process scheduling. Computational results show that the proposed exact and inexact parametric algorithms are more computationally efficient than several general-purpose solvers for solving MIFPs.

1. Introduction

A mixed-integer fractional programming (MIFP) problem has an objective as a ratio of two functions, and includes both discrete and continuous variables. A general form of MIFP can be stated as the following problem (P):

$$\max \left\{ Q(x) = \frac{N(x)}{D(x)} | x \in S \right\} \tag{P}$$

where the variables x contain both continuous and discrete variables, the feasible region S is nonempty, compact, bounded and the denominator function $D(x)$ is always positive in S, i.e. $D(x) > 0$ for $x \in S$ (Frenk & Schaible, 2009). The numerator function $N(x)$ and the denominator function $D(x)$ can be linear or nonlinear.

1.1. MIFP applications in process systems engineering

MIFP problems arise from a variety of real world applications (Schaible, 1981). Major MIFP applications in process systems engineering can be generally categorized into three types.

The first one is to optimize the productivity of a process system, which can usually be measured by the performance per unit of time or the process output per input. These include, but are not limited to overall cost or profit over the makespan, the resource generation or consumption rate, and the product yield per raw material or utility consumption. Production scheduling problems can be formulated as a mixed-integer linear fractional programming (MILFP) problem by optimizing the productivity subject to the mixed-integer linear constraints (Capón-García, Bojarski, Espuña, & Puigjaner, 2010; Shah, Pantelides, & Sargent, 1993). Cyclic process operations problems (Chu & You, 2012, 2013; Pinto & Grossmann, 1994) might involve the tradeoffs between inventory cost and fixed cost in the objective function that would lead to a mixed-integer quadratic fractional program (MIQFP).

Another important MIFP application is optimization for sustainability. Although overall environmental impact is usually used as the objective function for process optimization problems, environmental impact per functional unit could sometimes be a more appropriate objective function from the life cycle assessment perspective, especially for the problems focusing on the performance of products, rather than that of the entire process. Recent MIFP applications in this area include environmental-conscious sustainable scheduling of batch processes (Capón-García et al., 2010; Yue & You, 2013) and sustainable design of supply chains (Yue, Kim, & You, 2013).

The third MIFP application field is on the optimization for return rate, such as return on investment, return on cost and return on risk. The return rate is usually modeled by profit dividing the capital, revenue, asset or risk. One example is that capacity planning problems can be formulated as an MILFP problem to simultaneously

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optimize the decisions of capacity investment, inventory management, and production planning by maximizing the return over operating assets (Bradley & Arntzen, 1999). Portfolio selection problems can use financial return over risk as the objective function. Supply chain design problems can also be formulated as an MILFP by optimizing the total return over capital investment (Uddin & Sano, 2010) or market share capture per unit cost (Hua, Cheng, & Wang, 2011).

1.2. MIFP theory and algorithms

The nonlinear relaxation of an MIFP (by relaxing the integer variables to continuous variables with corresponding upper and lower bounds) is a continuous fractional program. Due to the ratio term in the objective function, fractional programs are in general non-convex nonlinear optimization problems (Bazaraa, Sherali, & Shetty, 2006). Various solution methods for continuous fractional programs have been proposed (Schaible, 1981). Charnes and Cooper (1962) proposed an exact linear programming reformulation of the continuous linear fractional program. An alternative approach is to solve the associated dual problem of the variable transformed fractional program that could be efficient for a class of quadratic fractional programs (Schaible, 1976). Another popular solution method was first introduced by Martos and Andrew Whinston (1964) and Jagannathan (1966) and they named it as the so-called "parametric" approach. The main idea of this parametric approach is to solve an equivalent parametric problem of the fractional program. Dinkelbach (1967) extended the parametric approach to solve the continuous, nonlinear fractional programs using the Newton's method. There are also several variants based on this parametric approach but using different methods for updating the parameters (Schaible & Ibaraki, 1983).

Although earlier work mainly focuses on fractional programming problems with only continuous variables, solution methods for MIFP problems drew significant attentions recently. MIFP problem is a special class of mixed-integer nonlinear programming (MINLP) problem. Thus, MIFP problems can be solved with the general-purpose MINLP algorithms (Floudas, 1999), such as the generalized Benders decomposition (Geoffrion, 1972), branch-and-bound method (Gupta & Ravindran, 1985), the outer-approximation method (Duran & Grossmann, 1986; Viswanathan & Grossmann, 1990), the branch-and-cut method (Quesada & Grossmann, 1992), the extended cutting plane method (Westerlund & Pettersson, 1995), the branch-and-reduce method (Tawarmalani & Sahinidis, 2005), the outer-approximation-based global optimization method (Kesavan & Barton, 2000a, 200b; Kesavan, Allgor, Gatzke, & Barton, 2004), just to name a few. However, due to the nature of nonconvexity and the presence of integer variables, solving large-scale MIFP problems directly using the general-purpose MINLP methods might be computationally intractable. Moreover, local MINLP solvers such as DICOPT (outer-approximation algorithm) and SBB (simple branch-and-bound algorithm) might not guarantee the global optimality of the solution and may lead to suboptimal solutions if they are used for solving the MIFP problems. As will be shown through the computational results in Sections 3 and 4, the global optimizer BARON 11.3 might not be able to return good feasible solutions of large-scale MIFP problems within reasonable computational time limit. Therefore, there is a need of developing efficient and tailored global optimization algorithms for solving large-scale, non-convex MIFP problems.

Most tailored MIFP solution algorithms in the literature focus on the special case of MILFP problems. Anzai (1973) investigated the properties of integer fractional programming problems. Granot and Granot (1977) developed valid cutting planes based on the Charnes-Cooper transformation for solving MILFP problems. A global optimization approach based on the branch-and-bound method and variable transformation to solve 0–1 fractional programs was proposed by Li (1994), which was extended by Wu (1997) to derive stronger cuts for the 0–1 fractional programs. Chang (2002) proposed an approximate approach to solving posynomial fractional programming problems by deriving the linear programming relaxation of the problem based on piecewise linearization techniques. Yue, Guillén-Gosálbez, and You (2013) proposed an exact mixed-integer linear programming (MILP) reformulation for MILFP problems, although it cannot be applied to mixed-integer nonlinear fractional programs. An algorithm based on the parametric approach was proposed to solve integer linear fractional programming problems by Ishii, Ibaraki, and Mine (1977). Pochet and Warichet (2008) and You, Castro, and Grossmann (2009) showed that the parametric approach is very efficient for solving MILFP models for cyclic scheduling, but their studies were not extended to the general mixed-integer nonlinear fractional programs that would be addressed in this paper.

1.3. Outline of this paper

The goal of this paper is to propose novel and efficient algorithms based on the parametric approach for solving MIFP problems, and to illustrate their effectiveness of solving process scheduling problems. We first show that the parametric approach for continuous fractional programs is applicable to the mixed-integer linear and nonlinear fractional programs. To solve the resulting parametric problem, which is equivalent to the original MIFP problem, we consider four one-dimension root-finding algorithms, including the bisection method, the Newton's method, the secant method and the false position method. These are all globally convergent exact methods with at least linear convergence rates. We further propose a novel, inexact parametric algorithm based on the Newton's method for solving the equivalent parametric problem. We show that this new algorithm has a linear convergence rate, but it could be much more computationally efficient in each iteration than the exact parametric algorithms. Thus, the inexact parametric algorithm can potentially require shorter total computational times than the exact parametric algorithms for some types of MIFPs.

We conduct extensive computational studies based on the randomly generated instances, in order to illustrate the efficiency of the proposed parametric algorithms for solving large-scale MILFP and MIQFP problems, and also to compare their performance with three general-purpose MINLP methods. Two applications of these algorithms in process operations are presented at the end of this paper.

The novel contributions of this paper are summarized below:

- Four efficient exact parametric algorithms for solving large-scale MIFP problems based on the application of existing root-finding algorithms;
- An inexact parametric algorithm based on the Newton's method for solving special structured MIFP problems, and the theoretical investigation of its convergence properties;
- Detailed comparison between the proposed parametric approaches and the general-purpose MINLP algorithms (DICOPT, SBB, BARON 11.3) for solving large-scale MILFP and MIQFP problems;

2. Parametric algorithms for solving MIFP problems

2.1. Equivalent parametric formulation and its properties

Considering the following parametric problem (P_q):

$$F(q) = \max \left\{ N(x) - q \cdot D(x) | x \in S \right\} \quad for \quad q \in \mathbb{R}^1 \tag{Pq}$$