39

A Global Optimization Algorithm for Linear Fractional and Bilinear Programs

IGNACIO QUESADA and IGNACIO E. GROSSMANN*
Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, U.S.A.

Abstract. In this paper a deterministic method is proposed for the global optimization of mathematical programs that involve the sum of linear fractional and/or bilinear terms. Linear and nonlinear convex estimator functions are developed for the linear fractional and bilinear terms. Conditions under which these functions are nonredundant are established. It is shown that additional estimators can be obtained through projections of the feasible region that can also be incorporated in a convex nonlinear underestimator problem for predicting lower bounds for the global optimum. The proposed algorithm consists of a spatial branch and bound search for which several branching rules are discussed. Illustrative examples and computational results are presented to demonstrate the efficiency of the proposed algorithm.

Key words: Nonconvex optimization, bilinear programming, fractional programming, convex underestimators.

1. Introduction

Many problems in engineering design, economics and managment can be formulated through nonlinear programming models. These models, however, often involve nonconvex functions and therefore when conventional techniques are used they can get trapped in local solutions. Recently there has been a significant effort in the area of global optimization. Stochastic and deterministic methods have been developed; for recent extensive reviews, see Schoen (1991) and Horst (1990). Deterministic methods have the advantage that they can provide rigorous guarantee of global optimality of the solution but require some assumptions about the mathematical structure of the model. Since many nonlinear optimization models do exhibit a special structure, there is a clear incentive to consider the solution of these problems with deterministic methods.

An important class of nonconvex optimization problems with special structure correspond to nonlinear programming problems with bilinear or linear fractional terms. These commonly arise for instance in engineering design problems (e.g., see Reklaitis and Ravindran, 1983; Papalambros and Wilde, 1988; Grossmann, 1990; Floudas and Pardalos, 1990). Al-Khayyal (1992) presented a review of models and applications of bilinear programming. The bilinear and linear fractional terms are factorable functions for which McCormick (1976) has presented a general

---

approach for deriving underestimator functions that can be incorporated in global optimization algorithms. Al-Khayyal and Falk (1983) proposed an algorithm for bilinear programs with linear constraints in which linear estimators over the bilinear terms are used. Swaney (1993) addressed the asymptotic behavior that can occur in this type of algorithm when a solution does not lie at an extreme point. Algorithms for bilinear programming models have also recently been developed by Sherali and Alameddine (1992). These authors presented a linearization reformulation technique that embeds the method proposed by Al-Khayyal and Falk (1983) and predicts stronger bounds for the global optimum. However, the main limitation is that the size of the linear programming underestimator problems grows exponentially with the number of constraints in the original problem.

Falk and Palocsay (1992) proposed an algorithm for optimizing the sum of linear fractional functions subject to linear constraints. The algorithm consists of a sequence of linear programming problems in which bounds on feasible subsets are added. These bounds are tightened iteratively to reduce the search space. These authors also developed convergence properties for this algorithm by extending the approach presented by Dinkelbach (1967). However, the rate of convergence of this method can be slow. Konno *et al.* (1991) addressed the minimization of the sum of two linear fractional functions over a polytope for which they applied parametric linear programming algorithms. Floudas and Visweswaran (1990) presented an algorithm based on a Benders based decomposition approach that can be used to solve bilinear and/or fractional programming problems. In this method a sequence of subproblems and relaxed dual subproblems are solved. Although the advantage of this method is that there is freedom for choosing the structure of the subproblems (e.g., they can correspond to linear programs or some special type of problem), one potential difficulty is that the number of relaxed dual subproblems that have to be solved at each iteration may grow exponentially with the number of variables interacting in different nonconvex terms. Among other more general methods, Horst and Tuy (1990) proposed a global optimization algorithm that makes use of quadratic outer approximation cuts to represent the feasible region.

In this paper a new deterministic method is proposed for the global optimization of mathematical programs that involve the sum of linear fractions and/or bilinear terms. The proposed method is a generalization of the algorithm presented by Quesada and Grossmann (1993) for minimizing the sum of linear fractional functions that arises in the global optimal design of Heat Exchanger Networks. The unique feature of the proposed method is that bilinear and linear fractional terms are substituted by both linear and nonlinear convex estimator functions that can be derived using the approach presented by McCormick (1976). Conditions under which the estimator functions for different types of terms are nonredundant are determined. A convex nonlinear underestimator problem is then proposed that predicts lower bounds for the global optimum. These bounds can be further strengthened by the inclusion of additional estimators that are obtained through projections of the feasible space. For the particular case of bilinear terms, the additional estimators

are equivalent to the reformulation technique of Sherali and Alameddine (1992). To find the global optimum, a spatial branch and bound search is conducted in which the lower bounds are obtained from the nonlinear underestimator problem. Modifications to the branching rules proposed by Sherali and Alameddine (1992) are used in this search.

The paper is organized as follows. Firstly, the case of a nonconvex objective function and a convex feasible region is considered. Here the properties of the different estimators functions, the formulation of the convex NLP underestimator problem and the basic algorithm are presented. Also, the performance of the algorithm is illustrated through a small example. The algorithm is then extended to the case of nonconvex feasible regions for which the necessary modifications are described. Finally, numerical results are given for a variety of problems that have been reported in the literature.

2. The Problem

2.1. MATHEMATICAL MODEL

The following mathematical programming problem that is considered in this paper involves a nonconvex objective function with linear fractional, bilinear and convex terms, and is defined over a bounded convex feasible region,

$$\min f = \sum_{i \in I} \sum_{j \in J} c_{ij} \frac{p_i}{q_j} - \sum_{i \in I'} \sum_{j \in J'} c_{ij} p_i q_j + h(p, q, z)$$

$$\text{s.t. } g(p, q, z) \le 0$$
$$z \in Z \subset R^n$$
$$p^L \le p \le p^u \tag{P0}$$
$$q^L \le q \le q^u,$$
$$p \in R_+^{|I|+|I'|}, \quad q \in R_+^{|J|+|J'|}$$

The functions $h, h : R^{|I|+|I'|+|J|+|J'|} \to R^1$, and $g, g : R^{|I|+|I'|+|J|+|J'|} \to R^m$, are assumed to be convex and differentiable. The set Z is bounded; c_{ij} are real coefficients of the linear fractional terms or bilinear terms. The variables p_i and q_j are bounded and without loss of generality it is assumed that $p^L \ge 0$ and $q^L > 0$. For simplicity in the presentation the sets I and I', and J and J' are assumed to be disjoint. This condition can be relaxed or it can easily be satisfied by defining additional variables and identities in problem (P0).

2.2. REFORMULATION

To provide a compact and uniform representation for the bounding functions of the linear fractional and bilinear terms, problem (P0) will be reformulated in the space (x, y, z, r) by relabeling the variables p and q and by defining the fractions and bilinear products as follows:

(a) Fractional terms

$$p_i = x_{i0} \quad q_j = y_j \quad \frac{p_i}{q_j} = r_{ij} \quad i \in I, \quad j \in J \tag{1}$$

b) Bilinear terms

$$p_i = r_{i0} \quad q_j = y_j \quad p_i q_j = x_{ij} \quad i \in I', \quad j \in J' \tag{2}$$

Also the following sets are defined to relate the variables (x, y, r) with the corresponding positive (P) and negative (N) fractions and bilinear terms in the objective of (P0):

$$P_R = \{(i,j,k,m) \mid i \in I, j \in J, c_{ij} > 0, k = j, \ m = 0\}$$
$$P_B = \{(i,j,k,m) \mid i \in I', j \in J', c_{ij} > 0, k = 0, \ m = j\}$$
$$N_R = \{(i,j,k,m) \mid i \in I, j \in J, c_{ij} < 0, k = j, \ m = 0\}$$
$$N_B = \{(i,j,k,m) \mid i \in I', j \in J', c_{ij} < 0, k = 0, \ m = j\}$$

with $P = P_R \cup P_B$ and $N = N_R \cup N_B$.

By using (1) and (2) and the above definition of sets, problem (P0) can be written in the following compact form:

$$\min f = \sum_{i \in I} \sum_{j \in J} c_{ij} r_{ij} - \sum_{i \in I'} \sum_{j \in J'} c_{ij} x_{ij} + h(x_0, y, r_0, z)$$
$$\text{s.t. } y_j r_{ik} \geq x_{im} \quad (i,j,k,m) \in P$$
$$y_j r_{ik} \leq x_{im} \quad (i,j,k,m) \in N$$
$$g(x_0, y, r_0, z) \leq 0 \tag{P1}$$
$$x^L \leq x \leq x^u$$
$$y^L \leq y \leq y^u$$
$$r^L \leq r \leq r^u$$
$$z \in Z$$

where the new inequalities have been relaxed according to the sign of the cost coefficient ($c_{ij} > 0$ for $(i,j,k,m) \in P$ and $c_{ij} < 0$ for $(i,j,k,m) \in N$). Also, $x_0 = [x_{i0}]$ and $r_0 = [r_{i0}]$ are the subsets of x and r variables that are involved in the functions $h(.)$ and $g(.)$. The bounds for x, y and r are obtained from (1) and (2) using the bounds for p and q in (P0). Problems (P1) and (P0) are equivalent and the algorithm is presented based on formulation (P1). The reader is encouraged to read Appendix A which presents a small problem that is reformulated to the form of (P1).

2.3. VARIABLE BOUNDS

It is important to have tight lower and upper bounds for the variables x, y and r involved in the nonconvex terms in (P1) since these bounds will determine the

quality of the approximation that will be developed later in the paper. These bounds determine the size of the search space for the global optimum, but also as shown later in the paper, from the value of these bounds it is possible to determine in advance whether some of the estimator functions will be redundant.

In the initialization step of the algorithm, lower and upper bounds for the variables x_{i0} and y_j in the fractional terms ($i \in I, j \in J$) and for the variables r_{i0} and y_j in the bilinear terms ($i \in I', j \in J'$) are calculated. This is accomplished by solving the corresponding minimization and maximization subproblems for each variable:

$$y_j^L = \{\min y_j \mid g(x, y, r, z) \leq 0\} \quad j \in J \cup J' \tag{3a}$$

$$y_j^u = \{\max y_j \mid g(x, y, r, z) \leq 0\} \quad j \in J \cup J' \tag{3b}$$

$$x_{i0}^L = \{\min x_{im} \mid g(x, y, r, z) \leq 0\} \quad i \in I \tag{3c}$$

$$x_{i0}^u = \{\max x_{im} \mid g(x, y, r, z) \leq 0\} \quad i \in I \tag{3d}$$

$$r_{i0}^L = \{\min r_{ik} \mid g(x, y, r, z) \leq 0\} \quad i \in I' \tag{3e}$$

$$r_{i0}^u = \{\max r_{ik} \mid g(x, y, r, z) \leq 0\} \quad i \in I' \tag{3f}$$

where the bounds in (P1) are used for the variables x, y, r and z in the above subproblems. These subproblems have a unique solution since the feasible region is convex. Also, since they have the same feasible region and are independent, they can be solved in parallel. In some particular instances, it is possible to generate these variable bounds through simple evaluations (Quesada and Grossmann, 1995).

Furthermore, for the fractional terms it is possible to calculate lower and upper bounds for each individual term $r_{ij}, i \in I, j \in J$ by solving the subproblems,

$$r_{ij}^L = \{\min \frac{x_{i0}}{y_j} \mid g(x, y, r, z) \leq 0, z \in Z\} \quad i \in I, j \in J \tag{4a}$$

$$r_{ij}^u = \{\max \frac{x_{i0}}{y_j} \mid g(x, y, r, z) \leq 0, z \in Z\} \quad i \in I, j \in J \tag{4b}$$

The subproblems in (4) have a unique solution (Bazaara and Shetty, 1979) and in the case that the feasible region is given by linear constraints they can be reformulated as LP problems through the transformation proposed by Charnes and Cooper (1962). Note that for the bilinear terms, it is not possible to obtain valid bounds for the variables $x_{ij}, i \in I', j \in J'$, since the resulting subproblems are nonconvex.

3. Estimator Functions

3.1. DEFINITION AND PROPERTIES

Following the treatment of McCormick (1976) (see Appendix B), the bilinear terms that appear in the constraints of (P1) can be replaced by linear convex estimator

functions (B.11 and B.12) yielding the following constraints:

$$x_{im} \leq y_j^u r_{ik} + r_{ik}^L y_j - y_j^u r_{ik}^L \quad (i,j,k,m) \in P \tag{5a}$$

$$x_{im} \leq y_j^L r_{ik} + r_{ik}^u y_j - y_j^L r_{ik}^u \quad (i,j,k,m) \in P \tag{5b}$$

$$x_{im} \geq y_j^L r_{ik} + r_{ik}^L y_j - y_j^L r_{ik}^L \quad (i,j,k,m) \in N \tag{6a}$$

$$x_{im} \geq y_j^u r_{ik} + r_{ik}^u y_j - y_j^u r_{ik}^u \quad (i,j,k,m) \in N \tag{6b}$$

Note from the above that it is only necessary to include over or underestimators depending of the sign of the cost coefficient, c_{ij}.

Additionally, as shown in Appendix B, it is possible to develop nonlinear convex underestimator functions according to (B.15) for the constraints with $(i, j, k, m) \in P$ which yields:

$$r_{ij} \geq \frac{x_{im}}{y_j^u} + x_{im}^L \left(\frac{1}{y_j} - \frac{1}{y_j^u} \right) \quad (i,j,k,m) \in P \tag{7a}$$

$$r_{ij} \geq \frac{x_{im}}{y_j^L} + x_{im}^u \left(\frac{1}{y_j} - \frac{1}{y_j^L} \right) \quad (i,j,k,m) \in P \tag{7b}$$

The following properties can be established for the linear and nonlinear estimator functions in (5) and (7) for the linear fractional terms in (P0) with positive cost coefficients, c_{ij}.

PROPERTY 1. *When* $r_{ik}^L = \frac{x_{im}^L}{y_j^u}$ (*or* $r_{ik}^u = \frac{x_{im}^u}{y_j^L}$), $(i, j, k, m) \in P_R$, *the linear overestimator* (5a) (*or* (5b)) *is a linearization of the nonlinear underestimator* (7a) (*or* (7b)).

Proof. See Appendix C.

COROLLARY 1. *The nonlinear underestimator* (7a) (*or* (7b)) *is stronger than the linear overestimator* (5a) (*or* (5b)) *when* $r_{ik}^L = \frac{x_{im}^L}{y_j^u}$ (*or* $r_{ik}^u = \frac{x_{im}^u}{y_j^L}$), $(i, j, k, m) \in P_R$.

Proof. See Appendix C.

The following property, however, establishes that the linear overestimators in (5) are not necessarily redundant.

PROPERTY 2. *When* $r_{ik}^L > \frac{x_{im}^L}{y_j^u}$ (*or* $r_{ik}^u < \frac{x_{im}^u}{y_j^L}$), $(i, j, k, m) \in P_R$, *the linear overestimator* (5a) (*or* 5b) *is nonredundant.*

Proof. See Appendix C.

For the bilinear terms in (P0) with positive cost coefficients, c_{ij}, the following properties can be established.
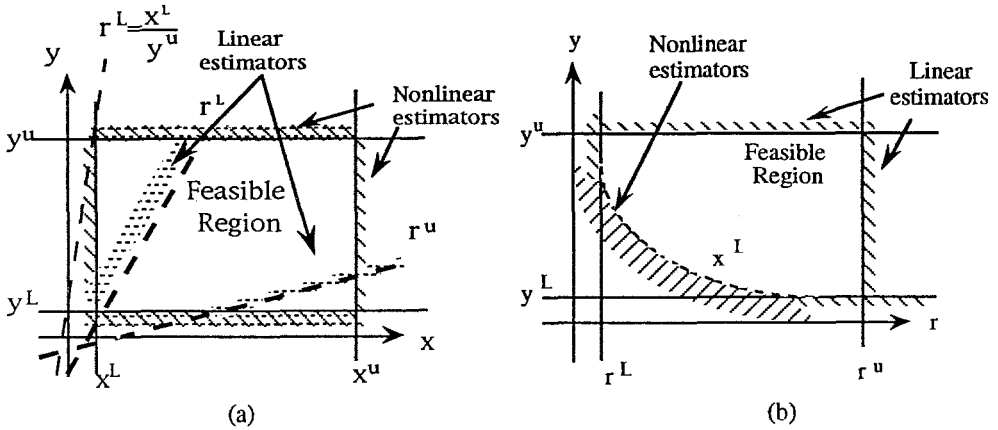
Fig. 1. Projected feasible region for (a) fractional term and (b) bilinear term.

PROPERTY 3. When $x_{im}^L = r_{ik}^L y_j^L$ (or $x_{im}^u = r_{ik}^u y_j^u$), $(i,j,k,m) \in P_B$, the linear overestimator (5a) (or (5b)) is a secant of the nonlinear underestimator (7a) (or (7b)).

Proof. See Appendix C.

COROLLARY 2. The linear overestimator (5a) (or (5b)) is stronger than the nonlinear underestimator (7a) (or (7b)) over the feasible region when $x_{im}^L = r_{ik}^L y_j^L$ (or $x_{im}^u = r_{ik}^u y_j^u$), $(i,j,k,m) \in P_B$.

Proof. See Appendix C.

PROPERTY 4. When $x_{im}^L > r_{ik}^L y_j^L$ (or $x_{im}^u < r_{ik}^u y_j^u$), $(i,j,k,m) \in P_B$, the nonlinear underestimator (7a) (or (7b)) is nonredundant.

Proof. See Appendix C.

3.2. GEOMETRICAL INTERPRETATION

The estimator functions (5), (7) have the property of yielding an exact approximation at the boundary defined by the lower or upper bounds of x, y, r (see Appendix B). A geometrical interpretation of Properties 1 to 4 is as follows. Consider the case of a fractional term $((i,j,k,m) \in P_R$, Property 1 and 2) and the projection of the feasible region into the space of the variables involved in the nonconvex term (variables x and y, Figure 1a). Note that the contours of the fractional term $(r = \frac{x}{y})$ correspond to the straight lines that pass through the origin (dashed lines in Figure 1a). The nonlinear estimators (7) provide the exact function value of the fractional term at the bounds of the variables x and y as can be easily verified from (7) by substituting the corresponding bounds. As shown in Corollary 1, when the bound over the individual nonconvex term is redundant (e.g. $r^L = \frac{x^L}{y^u}$) there is no

part of the feasible region in which the linear estimator (5) is stronger. However, when this bound is not redundant (e.g. $r^L > \frac{x^L}{y^u}$ in Figure 1a) the linear estimator provides an exact approximation at points in which the nonlinear cannot.

For the case of a bilinear term $((i, j, k, m) \in P_B$, Property 3 and 4), the linear estimators (5) are the ones that are expressed in terms of the variables involved in the nonconvex term, y and r and therefore they provide an exact approximation at the bounds of these variables as seen in Figure 1b. This can also be easily verified from (5). Also, according to Property 4, the nonlinear estimator in (7) will only be nonredundant if there is a strong bound over the individual bilinear term (e.g. $x^L > r^L y^L$ in Figure 1b).

3.3. PROJECTIONS

The linear and nonlinear estimator functions in (5), (6) and (7) presented in the previous section use fixed lower and upper bounds of the variables over which the approximation is obtained. Additional estimators that tighten the convex representation can be generated by considering bounds corresponding to hyperplanes of the boundary of the feasible region and which are projected in the space of the variables involved in the estimator function. In particular, from the solution of the subproblems (3), (4) solved in the initialization step in which bounds for the individual variables are determined, the following inequalities projected in the space (y_j, x_{im}) can be obtained:

$$0 \geq \sum_\ell \lambda_\ell g_\ell^{lin}(y_j, x_{im}, \zeta^*) \tag{8}$$

where λ_ℓ are the Lagrange multipliers and $g_\ell^{lin}(y_j, x_{im}, \zeta^*)$ is a linearization of the constraint g_ℓ given in terms of y_j and x_{im} with the remaining variables ζ fixed at their optimal value ζ^*:

$$g_\ell^{lin}(y_j, x_{im}, \zeta^*) = g_\ell(y_j^*, x_{im}^*, \zeta^*) + \nabla_{y_j, x_{im}} g_\ell(y_j^*, x_{im}^*, \zeta^*) \begin{bmatrix} y_j - y_j^* \\ x_{im} - x_{im}^* \end{bmatrix} \tag{9}$$

The projections in (8) give rise to linear inequalities of the following form:

$$y_j \leq a + b x_{im} \tag{10a}$$
$$y_j \geq a' + b' x_{im} \tag{10b}$$

from which the following nonlinear underestimators that are similar to (7) can be generated:

$$r_{ik} \geq \frac{x_{im}}{y_j} \geq \frac{x_{im}}{a + b x_{im}} + x_{im}^L \left(\frac{1}{y_j} - \frac{1}{a + b x_{im}} \right) \quad (i, j, k, m) \in P_R \tag{11a}$$

$$r_{ik} \geq \frac{x_{im}}{y_j} \geq \frac{x_{im}}{a' + b' x_{im}} + x_{im}^u \left(\frac{1}{y_j} - \frac{1}{a' + b' x_{im}} \right) \quad (i, j, k, m) \in P_R \tag{11b}$$

The following property can be established for these estimators:

PROPERTY 5. *The nonlinear inequality* (11a) *(or* (11b)) *is a valid convex underestimator when* $b < 0$ *(or* $b' < 0$), *and is nonredundant with respect to the nonlinear underestimator in* (7a) *(or* (7b)).

Proof. See Appendix C.

It can happen that when the projected inequalities in (10) are obtained using the solution of the bounding subproblem, only a simple bound over the variable is obtained (e.g. $b = 0; a = y_j^u$) instead of a linear inequality. In this case, one might try to obtain an inequality by solving an additional problem fixing the projection variable at a given value within the bounds (i.e. $x_{im} = x'_{im}$ with $x_{im}^L < x'_{im} < x_{im}^u$).

The inequalities in (8) can also be projected in the space $(y_j, r_{i0}), i \in I', j \in J'$ for the bilinear terms in (P0) The projections for the case of r_{io} as a function of y_j have the following form (the case of y_j as a function of r_{i0} can also be considered (see example 1))

$$r_{i0} \geq a + by_j \tag{12a}$$
$$r_{i0} \leq a' + b'y_j \tag{12b}$$

These can also be used to generate additional estimator functions through the linear estimators (5) and (6). In the bilinear case the estimators have the following form:

$$x_{im} \leq y_j r_{ik} \leq y_j^L r_{ik} + (a+by_j)y_j - y_j^L(a+by_j) \quad (i,j,k,m) \in P_B \tag{13a}$$
$$x_{im} \leq y_j r_{ik} \leq y_j^u r_{ik} + (a'+b'y_j)y_j - y_j^u(a'+b'y_j) \quad (i,j,k,m) \in P_B \tag{13b}$$

$$x_{im} \geq y_j r_{ik} \geq y_j^L r_{ik} + (a+by_j)y_j - y_j^L(a+by_j) \quad (i,j,k,m) \in N_B \tag{14a}$$
$$x_{im} \geq y_j r_{ik} \geq y_j^u r_{ik} + (a'+b'y_j)y_j - y_j^u(a'+b'y_j) \quad (i,j,k,m) \in N_B \tag{14b}$$

where $b < 0$ and $b' < 0$ yield convex estimators in (13) and $b > 0, b' > 0$ for (14). These type of inequalities are in fact equivalent to the ones proposed by Sherali and Alameddine (1992). The difference is that (13) and (14) are only generated when quadratic convex terms are obtained and here only the bilinear term is linearized. With the approach presented in this paper, only a small number of this type of constraints are generated since it is possible to identify nonredundant linear functions in an explicit form.

The bilinear terms in the constraints of problem (P1) can arise from bilinear or fractional terms in the objective function of problem (P0). When the original term was a fractional one, projections of the type of equation (13) are not possible to be generated since the variable $r_{ij}, i \in I, j \in J$, does not exist in the constraint set $g(x, y, r, z) \leq 0$. Hence, it is not possible to project the bounds of y_j over r_{ij}.

However, projections can be performed for the bounds of $r_{ij}, i \in I, j \in J$, when the following fractional bounding problems in (4) are solved:

$$
\begin{aligned}
&\min(\text{or max})\frac{x_{i0}}{y_j} = r_{ij} \\
&\text{s.t. } g(x_0, y, r_0, z) \leq 0 \\
&\quad 0 \leq x^L \leq x \leq x^u \\
&\quad 0 < y^L \leq y \leq y^u
\end{aligned}
\tag{PR}
$$

The nonlinear problem in (PR) has a unique solution. Moreover, as Charnes and Cooper (1962) have shown, if the constraints $g(x, y, r, z)$ are linear, (PR) can be transformed into a linear programming problem. To achieve this, the transformation variable $t_j = \frac{1}{y_j}$ is introduced yielding the formulation:

$$
\begin{aligned}
&\min(\text{or max})t_j x_{i0} \\
&\text{s.t. } g(x_0, y, r_0, z) \leq 0 \\
&\quad t_j y_j = 1 \\
&\quad 0 \leq x^L \leq x \leq x^u \\
&\quad 0 < y^L \leq y \leq y^u
\end{aligned}
\tag{PR1}
$$

The linear constraints and bounds in (PR1) are multiplied by t_j and the resulting products of variables are denoted as (x', y', r', z') which yields the LP problem:

$$
\begin{aligned}
&\min(\text{or max})x'_{i0} \\
&\text{s.t. } g'(x', y', r', z', t) \leq 0 \\
&\quad y'_j = 1 \\
&\quad x' \geq 0, y' > 0
\end{aligned}
\tag{PR2}
$$

Here g' includes the transformed original constraints and the additional linear constraints generated from the bounds. The solution of the LP problem (PR2) is used to generate projections of the variable x'_{i0} over t_j in a similar form as in (8),

$$
0 \geq \sum_{\ell} \lambda_\ell g_\ell(x'_{i0}, t_j, \zeta^*)
\tag{15}
$$

In this form the projection that is generated has the form:

$$
x'_{i0} \geq d + e\, t_j \quad (\text{or } x'_{i0} \leq d' + e't_j)
\tag{16}
$$

or expressing it in terms of the original variables,

$$
r_{ij} \geq d + \frac{e}{y_j} \quad (\text{or } r_{ij} \leq d' + \frac{e'}{y_j})
\tag{17}
$$

In this way, additional estimator functions can be obtained by using equation (17) in the linear underestimators (6),

$$
x_{im} \geq r_{ij}y_j \geq (dy_j + e) + y_j^L r_{ik} - (d + \frac{e}{y_j}y_j^L) \quad (i, j, k, m) \in N_R
\tag{18a}
$$

$$
x_{im} \geq r_{ij}y_j \geq (d'y_j + e') + y_j^u r_{ik} - (d' + \frac{e'}{y_j}y_U^L) \quad (i, j, k, m) \in N_R
\tag{18b}
$$

These estimators are convex when $e < 0(e' < 0)$.

PROPERTY 6. *The nonlinear estimators in (13), (14) and (18) provide an exact approximation at the boundary defined by the projected cut.*

Proof. See Appendix C.

The estimators in (11), (13), (14) and (18) are only a subset of all the projected estimators functions that can be generated. In this paper at most one projected estimator for each variable in the nonconvex term is used. The estimators (13) and (18) can be particularly relevant because when the cost coefficient, c_{ij}, is negative the nonlinear estimators (7) cannot be used. This is illustrated later in Example 3.

3.4. CONVEX NONLINEAR UNDERESTIMATOR PROBLEM

Having derived the linear and nonlinear bounding approximations (5), (6), (7), (11), (13), (14) and (18) for the nonconvex terms in (P1), a convex nonlinear underestimator problem (NLP$_L$) for problem (P1) can be defined as follows. Valid bounds over the variables are generated from (3) and (4) to define the set $\Omega = \{x, y, r : x^L \le x \le x^u, y^L \le y \le y^u, r^L \le r \le r^u\}$ and the nonconvex terms in problem (P1) are substituted by the convex approximating functions. This then leads to the following convex nonlinear programming problem:

$$\min f_L = \sum_{i \in I} \sum_{j \in J} c_{ij} r_{ij} - \sum_{i \in I'} \sum_{j \in J'} c_{ij} x_{ij} + h(x_0, y, r_0, z)$$

$$\text{s.t. } x_{im} \ge y_j^L r_{ik} + r_{ik}^L y_j - y_j^L r_{ik}^L \quad (i, j, k, m) \in N$$

$$x_{im} \ge y_j^u r_{ik} + r_{ik}^u y_j - y_j^u r_{ik}^u \quad (i, j, k, m) \in N$$

$$x_{im} \le y_j^L r_{ik} + r_{ik}^u y_j - y_j^L r_{ij}^u \quad (i, j, k, m) \in P \quad \text{According to}$$

$$x_{im} \le y_j^u r_{ik} + r_{ik}^L y_j - y_j^u r_{ik}^L \quad (i, j, k, m) \in P \quad \text{Properties 1 to 4.}$$

$$r_{ik} \ge \frac{x_{im}}{y_j^L} + x_{im}^u \left(\frac{1}{y_j} - \frac{1}{y_j^L}\right) \quad (i, j, k, m) \in P$$

$$r_{ik} \ge \frac{x_{im}}{y_j^u} + x_{im}^L \left(\frac{1}{y_j} - \frac{1}{y_j^u}\right) \quad (i, j, k, m) \in P$$

$$r_{ik} \ge \frac{x_{im}}{a + b x_{im}} + x_{im}^L \left(\frac{1}{y_j} - \frac{1}{a + b x_{im}}\right) \quad (i, j, k, m) \in P_R$$

$$r_{ik} \ge \frac{x_{im}}{a' + b' x_{im}} + x_{im}^u \left(\frac{1}{y_j} - \frac{1}{a' + b' x_{im}}\right) \quad (i, j, k, m) \in P_R \quad \text{(NLP}_L\text{)}$$

$$x_{im} \le y_j^L r_{ik} + (a + b y_j) y_j - y_j^L (a + b y_j) \quad (i, j, k, m) \in P_B$$

$$x_{im} \le y_j^u r_{ik} + (a' + b' y_j) y_j - y_j^u (a' + b' y_j) \quad (i, j, k, m) \in P_B$$

$$x_{im} \ge y_j^L r_{ik} + (a + b y_j) y_j - y_j^L (a + b y_j) \quad (i, j, k, m) \in N_B$$

$$x_{im} \ge y_j^u r_{ik} + (a' + b' y_j) y_j - y_j^u (a' + b' y_j) \quad (i, j, k, m) \in N_B$$

$$x_{im} \ge (d y_k + e) + y_j^L r_{ik} - (d + \frac{e}{y_j}) y_j^L \quad (i, j, k, m) \in N_R$$

$$x_{im} \ge (d' y_k + e') + y_j^u r_{ik} - (d' + \frac{e'}{y_j}) y_j^u \quad (i, j, k, m) \in N_R$$

$$g(x_0, y, r_0, z) \le 0$$

$$(x, y, r) \in \Omega, z \in Z$$

where for the sake of simplicity the indices in the parameters a, a', b, b', d, d', e and e' have been omitted.

PROPERTY 7. *The optimal solution f'_L of (NLP$_L$) provides a valid lower bound to the global optimum (f^*) of problem (P1).*
   Proof. See Appendix C.

COROLLARY 3. *If the value of the objective function from (P1) evaluated at the optimal solution of NLP$_L$ is f'_L then this solution corresponds to the global optimum of (P1).*
   Proof. See Appendix C.

4. A Branch and Bound Algorithm

4.1. PARTITIONING SCHEME

An optimal solution of problem NLP$_L$ provides a valid lower bound to the global optimum of problem (P1) (Property 7). At the same time this solution is a feasible solution to the problem (P1) since problem NLP$_L$ includes all the original constraints. Hence, only an evaluation of the original objective function is required to obtain a valid upper bound. Also, the solutions of the bounding subproblems (3) and (4) provide a feasible solution that can be used to generate an upper bound of the global solution. When the lower and upper bound are equal, the global solution has been obtained (Corollary 3). If there is a gap between these bounds, a partition of the feasible region must be performed. The estimator functions can then be updated in each subregion to yield tighter lower bounds over each subregion. A spatial branch and bound search is performed to successively partition the feasible region along the coordinate directions of the variables. When the lower bound for a particular subregion is greater or equal than the best upper bound available, the subregion is discarded. Also during this search procedure feasible solutions are obtained with which the best upper bound can be updated.

   For partitioning the feasible region, it is necessary to select a variable over which the division of the space will be performed and its corresponding value. The first rule considered here is the same as the one used by Sherali and Alameddine (1992), only that now bilinear and fractional terms are present in the objective function.

Rule 1: $(v, w, v', v'') \in \arg\max_{(i,j,k,m)} \{c_{ij}(r_{ik} - \frac{x_{im}}{y_j})\}$

$$\text{if } v' = 0 \quad \beta_v = \sum_j \text{Abs}\{c_{vj}(r_{v0} - \frac{x_{v,j}}{y_j})\}$$

$$\beta_w = \sum_i \text{Abs}\{c_{iw}(r_{i0} - \frac{x_{iw}}{y_w})\}$$

   if $\beta_v > \beta_w$ select r_{v0} else select y_w

$$\text{if } v'' = 0 \quad \beta_v = \sum_j \text{Abs } \{c_{vj}(r_{vj} - \frac{x_{v0}}{y_j})\}$$

$$\beta_w = \sum_i \text{Abs } \{c_{iw}(r_{iw} - \frac{x_{i0}}{y_w})\}$$

if $\beta_v > \beta_w$ select x_{v0} else select y_w.

In this way the nonconvex term for which the approximation differs the most is selected, and the variable that is involved in this term and can affect the most the other approximations is selected. A second rule that can also be used is as follows:

Rule 2: $(v1, w1, v1', v1'') \in \text{arg max}_{(i,j,k,m)}\{c_{ij}(r_{ik} - \frac{x_{im}}{y_j})\}$

$$\omega = \alpha \text{ Abs } \{c_{v1\ w1}(r_{v1\ v1'} - \frac{x_{v1\ v1''}}{y_{w1}})\}$$

select a (v, w, v', v'') for which Abs $(r_{vv'} - \frac{x_{vv''}}{y_w}) > \omega$

proceed as in Rule 1.

where $1 \geq \alpha > 0$. This rule reduces to the first one when $\alpha = 1$. There is a tradeoff between the two rules. Rule 1 may be attractive when the size of $\mid I \mid, \mid I' \mid, \mid J \mid$ or $\mid J' \mid$ is small because the variables that are present in more terms are selected and a smaller number of partition variables are used. In practice rule 2 can be more useful since there are cases in which there are more than one term for which the difference in the approximation can be large. In this situation it may be useful to select a variable on which partitioning has not been performed previously because this allows for the tightening of its bounds.

4.2. ALGORITHM

Step 0. Initialization
  (a) Set $f^* = \infty, F = \emptyset$, select tolerances ε and γ
  (b) For each variable $x_{i0}, i \in I, y_j, j \in J$, and $r_{i0}, i \in I', y_j, j \in J'$, and the terms $\frac{x_{i0}}{y_j}, i \in I, j \in J$, determine:
   · lower and upper bounds by solving the bounding programs in (3) and (4).
   · Optional: obtain projections of the variables (as in (10), (12) and (16)) using either the solutions of the previous bounding problems or problems at a fixed level for the projection variable.
   · Evaluate the original objective function for each of these feasible solutions. If $f < f^*$ set $f^* = f$ and store the solution as the incumbent solution (*).
  (c) Store the bounds in Ω^0, and set $F = F \cup \{0\}$.

Step 1. Convex Underestimator Problem
  (a) Solve problem NLP_L for Ω^0 to obtain f_L^0.
  (b) Evaluate the original objective function f^0. If $f^0 < f^*$ set $f^* = f^0$ and store the solution as the incumbent solution (*).

Step 2. Convergence

  (a) For the subregions j in F, if $f^* - f_L^j \leq \varepsilon f^*$ delete subregion j from $F(F = F \backslash \{j\})$.
  (b) If $F = \emptyset$ the ε-global solution is given by the incumbent solution.

Step 3. Partition

  (a) Take the last region k in F (Ω^k) and apply the selection rule (Rule 1 or Rule 2).
  (b) Subdivide subregion Ω^k in subregions Ω^{k+1} and Ω^{k+2} by adding the respective bound or inequality. Delete subregion Ω^k from F and store subregions Ω^{k+1} and Ω^{k+2} in $F(F = (F \backslash \{k\}) \cup \{k+1, k+2\})$.

     Optional: Update the bounds in subregions $k+1$ and $k+2$ for the variables involved in the nonconvex term with the partition variable.

Step 4. Convex Underestimator Problems

  (a) Solve problem NLP$_L$ for Ω^{k+1} and Ω^{k+2} to obtain f_L^{k+1} and f_L^{k+2}.
  (b) Evaluate the original objective function for each of these feasible solutions. If $f < f^*$, set $f^* = f$ and store the solution as the incumbent solution (*).

     Optional: When the difference between the objective function of the convex underestimator problem NLP$_L$ and the incumbent solution f*is smaller than a given tolerance $((f^* - f_L)/f^* < \gamma)$, solve the original nonconvex problem (P) for Ω^{k+1} and/or Ω^{k+2} using its convex solution as the initial point. If $f < f^*$ set $f^* = f$ and store the solution as the incumbent solution (*).

  (c) If $f_L^{k+1} < f_L^{k+2}$ invert Ω^{k+1} and Ω^{k+2} in F. Go to step 2.

It should be noted that when there is a strong interdependence between the variables involved in the nonconvex terms, it can be useful to update the bounds of some of the variables when a partition is performed (Step 3 optional). In particular the bounds of the variables that are involved in nonconvex terms with the partition variables can be updated. Also, the original nonconvex problem (P1) can be solved over the corresponding subregion when the difference between the upper and lower bound are small to accelerate the convergence.

The proposed algorithm can be used for the global optimization of linear fractional programming problems, bilinear programming problems or problems that involve fractional and bilinear terms in the objective function and in which the feasible region is convex. When the feasible region is described by linear constraints the bounding problems solved in the initialization step 0.b are LP problems.

PROPERTY 8. *The branch and bound algorithm will either terminate in a finite number of partitions at a global optimal solution, or generate a sequence of bounds that converge to the global solution.*
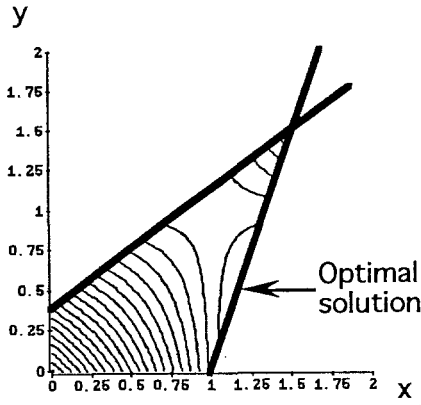
  Proof. See Appendix C.

Fig. 2. Feasible region and contours for example (ALK).

4.3. ILLUSTRATIVE EXAMPLE

EXAMPLE 1. *Bilinear objective.* The formulation of the NLP underestimator problem and the performance of the algorithm is illustrated by solving the following example given in Al-Khayyal and Falk (1983).

$$
\begin{aligned}
\min f &= -x + xy - y \\
\text{s.t.} \quad -6x + 8y &\leq 3 \\
3x - y &\leq 3 \\
0 \leq x, y &\leq 5
\end{aligned}
\tag{ALK}
$$

The feasible region with the original objective function is plotted in Figure 2. First, valid bounds are obtained for x and y by solving the corresponding LP's which yields:

$$
0 \leq x, y \leq 1.5.
\tag{19}
$$

From the solution of these LP problems the following two projected inequalities as in (12) can be obtained:

$$
x \leq \frac{3+y}{3}
\tag{20}
$$

$$
y \leq \frac{3+6x}{8}
\tag{21}
$$

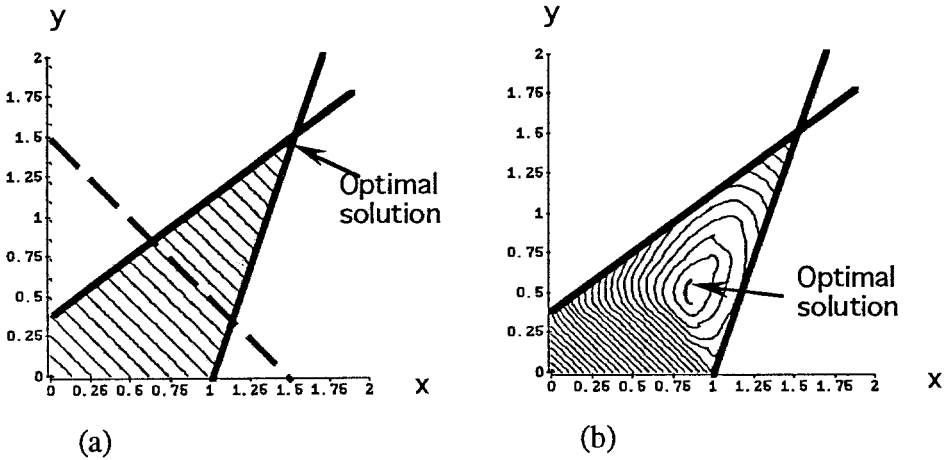(a)   (b)

Fig. 3.   Feasible region and contours for underestimators by (a) Al-Khayyal and Falk, (b) proposed method.

TABLE I. Computational results for Example 1 (or problem ALK)

Method	Size[a]	Initial f_L	Initial f^*	Subregions	Solution
Al-Khayyal	(3,4)	−3.000	−0.750	>103	−1.0833
Sherali	(5,23)	−1.500	−0.9375	11	−1.0833
Proposed	(3,6)	−1.2569	−0.892	5	−1.0833

[a](n, m) n= no. of variables, m = no. constraints.

The NLP underestimator problem is then given by:

$$\min f_L = -x + w - y$$
$$\text{s.t.} \quad -6x + 8y \leq 3$$
$$3x - y \leq 3$$
$$w \geq 0$$
$$w \geq 1.5y + 1.5x - 2.25 \qquad \text{(ALK}')$$
$$w \geq [\frac{3+y}{3}]y + 1.5x - 1.5[\frac{3+y}{3}]$$
$$w \geq 1.5y + [\frac{3+6x}{8}]x - 1.5[\frac{3+6x}{8}]$$
$$0 \leq x, y \leq 1.5$$

The solution of this initial NLP_L is f_L^0 = -1.2569 and the actual objective for this solution is f^* = -0.892 which is the incumbent solution. The initial underestimator problems for the Al-Khayyal and Falk method and the one proposed here are shown in Figure 3.

Since there is a gap between the lower bound and the incumbent solution a partition is made selecting the variable x. The solutions of problem NLP_L at the two subregions are $f_L^1 = -0.995(x \leq 0.803)$ and $f_L^2 = -1.1761(x \geq 0.803)$ and the incumbent solution is $f^* = -1.0048$. Therefore, the first subregion can be

eliminated. A new partition is performed in the second subregion with the variable y yielding $f_L^3 = -1.0833(y \leq 0.783)$ and $f_L^4 = -1.0807(y \geq 0.783)$ with the incumbent being $f^* = -1.0833$. Hence, the global solution is found at $x = 1.167$, $y = 0.5$, $f = -1.0833$. The computational results for this example are given in Table I. The results for the methods proposed by Al-Khayyal and Falk (1983) and Sherali and Alameddine (1992) are reported in Sherali and Alameddine (1992). It is worth mentioning that for the initial LP underestimator problem in the method by Sherali and Alameddine (1992) the same initial lower bound f_L is obtained using either the original bounds for the variables $(x, y \leq 5)$ or the tighter bounds $(x, y \leq 1.5)$.

The total time required to solve the problem with the proposed algorithm, including the time for the bounding problems, is 0.75CPU secs. on a IBM/R6000-530 using MINOS 5.2 for solving the LP and NLP problems.

This example has also been modified (Example 1a) to have an objective function that involves bilinear and fractional terms as in problem (P0):

$$
\begin{aligned}
\min f = &-x + xy - y + \frac{y}{x} \\
\text{s.t. } &-6x + 8y \leq 3 \\
&3x - y \leq 3 \\
&x + y \geq 1 \\
&0 \leq x, \quad y \leq 5
\end{aligned}
\qquad \text{(ALK1)}
$$

Applying the algorithm, the initial convex NLP_L problem has a solution of $f_L^0 = -1.00$ with $x = 1.00$ and $y = 0.00$, and the incumbent solution is $f^* = -1.00$. Hence, the global optimal solution is obtained in this case without having to perform a spatial branch and bound search.

5. Nonconvex Feasible Regions

5.1. MATHEMATICAL MODEL

The solution method presented for the nonconvex objective function defined over a convex feasible region in problem (P0) can be extended with some modifications to the case of nonconvex feasible regions. In this section an outline of the necessary modifications are given. Here the constraints that describe the feasible region can involve convex, linear fractional and bilinear terms in the same form than the nonconvex objective function in problem (P0). The problem considered is as follows (variable bounds are omitted):

$$
\begin{aligned}
&\min g_0 \\
&\text{s.t. } g_\ell \leq 0 \qquad \ell = 1, \ldots, L \\
&\text{where } g_\ell = \sum_{i \in I} \sum_{j \in J} c_{ij}^\ell \frac{p_i}{q_j} - \sum_{i \in I'} \sum_{j \in J'} c_{ij}^\ell p_i q_j + h(p, q, z), \\
&\ell = 0, 1, \ldots, L.
\end{aligned}
\qquad \text{(P2)}
$$

Problem (P2) can be reformulated in the same form as (P1) yielding,

$$\min g_0$$
$$\text{s.t. } g_\ell \leq 0 \qquad \ell = 1, \ldots, L$$
$$y_j r_{ik} \geq x_{im} \qquad (i, j, k, m) \in P$$
$$y_j r_{ik} \leq x_{im} \qquad (i, j, k, m) \in N$$

(P3)

$$\text{where } g_\ell = \sum_{i \in I} \sum_{j \in J} c_{ij}^\ell r_{ij} - \sum_{i \in I'} \sum_{j \in J'} c_{ij}^\ell x_{ij} + h^\ell(x, y, r, z),$$
$$\ell = 0, 1, \ldots, L.$$

The same type of transformations and estimator functions that were presented previously are used for every function $g_\ell(\ell = 0, \ldots, L)$.

5.2. MODIFICATIONS AND EXTENSIONS

Several modifications are required in the algorithm presented earlier to handle nonconvex feasible regions. Firstly, the solution of the nonlinear convex problems are not necessarily feasible solutions and they cannot always be used to update the upper bound. For this reason the original nonconvex problem (P2) can be solved to ensure that an upper bound is available during the search. In this work the solution of the first convex problem NLP_L is used as an initial point. To update the upper bound additional nonconvex problems can be solved during the search.

Secondly, to generate the lower and upper bounds of the variables there are different options. One is to simply consider the subset of convex constraints to generate these bounds. Alternatively, the nonconvex terms present in the constraints can be substituted by the linear estimator functions (5)–(6). This allows to consider the possible interactions between all the variables. The bounding subproblems can be solved in parallel since they are independent. In the case that they are solved in a sequential form the bounds that are obtained can be used in the subsequent subproblems if these variables are involved in estimator functions of nonconvex terms since better approximations will be obtained.

Finally, a modification of the branching rule is also necessary. The coefficients of the nonconvex terms in the constraints are not sufficient for comparing the approximations since the constraints can be scaled up or down by constant factors affecting in this form the selection of the term. This problem can be avoided by including the Lagrange multipliers of the constraints along with the coefficient of the nonconvex term in the selection rule. In this form the selection rule when nonconvex terms are present in the constraints and objective function is as follows:

Rule 3: $(v1, w1, v1', v1'') \in \arg \max_{(i,j,k,m)} \{ \lambda^\ell c_{ij}^\ell (r_{ik} - \frac{x_{im}}{y_j}) \}$ $\qquad \ell = 0, \ldots, L$
     proceed as in Rule 1 or Rule 2.

This rule has the advantage that when different expressions of the same constraint
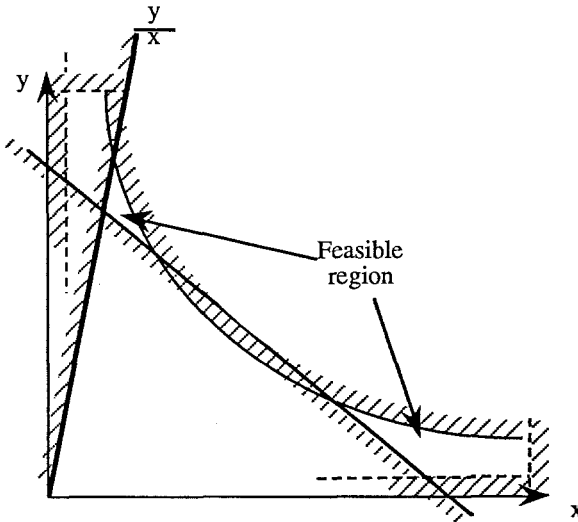
Fig. 4. Disjoint feasible region for Example 2.

(as in 23 and 25) are included in the formulation, only the constraint that is active ($\lambda^\ell > 0$) is considered when selecting the partition variable.

An important difference between having the conconvex terms only in the objective function or in the constraint is that there are alternative representations of the nonconvex constraints. Depending of the individual bounds of each particular nonconvex term, different representations may be tighter or nonredundant.

Consider the following nonconvex constraint:

$$\sum_{j=1}^{n} z_j \leq x_1 x_2 \tag{22}$$

which can also be written as follows

$$\frac{z}{x_1} \leq x_2 \qquad (z \leq x_1 x_2) \tag{23}$$

$$z = \sum_{j=1}^{n} z_j. \tag{24}$$

With (23) and (24) it is possible to develop nonlinear overestimator functions over the fractional term, z/x_1. If the bounds are nonredundant, linear underestimators can also be obtained. These estimators give exact approximations at the lower and upper bounds of the variables involved in the estimators function (x_1, x_2 and z).

The constraint in (22), however, can also be expressed as,

$$\sum_{j=1}^{n} \frac{z_j}{x_1} \leq x_2 \tag{25}$$

TABLE II. Size and characteristics of example problems

Example	Total no. variables	Nonconvex var.	Nonconvex terms	Constraints	Feasible region	Terms
1	2	2	1	2	C	B
1a	2	2	2	3	C	B, F
2	4	4	4	6	N	B, F
3	6	4	2	5	C	F
4	7	4	2	9	C	F
5	6	4	2	6	C	F
6	4	4	4	6	C	B
7	4	3	2	3	C	B
8	2	2	1	1	N	B
9	4	4	2	4	N	B
10	9	6	2	6	N	B
11	10	7	5	7	N	B, F
12	20	14	7	16	C	F

C=convex, N=nonconvex; B=bilinear, F=fractional

and nonlinear underestimators can be generated over each fractional term, z_j/x_1. These estimators provide exact approximations at the lower and upper bounds of each variable z_j and which are nonredundant. There are points for which each variable z_j is at either of its bounds and $x_1^L < x_1 < x_1^u$, $x_2^L < x_2 < x_2^u$ and $z^L < z < z^u$. For this point, representation (23) cannot yield an exact approximation while the representation (25) is exact.

5.3. ILLUSTRATIVE EXAMPLE

EXAMPLE 2. *Nonconvex feasible region.* The following example has a feasible region that is disjoint (see Figure 4). The problem is given by:

$$\min f = -x_1 - 2x_2 - y_1 - 2y_2$$
$$\text{s.t. } x_1 y_1 \leq 10$$
$$x_2 y_2 \leq 10$$
$$2x_1 + 2y_1 \geq 13$$
$$15x_2 + 20y_2 \geq 87$$
$$\frac{y_1}{x_1} \leq 2x_2$$
$$\frac{y_2}{x_2} \leq 2x_1$$
$$0.5 \leq x_1 \leq 5$$
$$0.5 \leq x_2 \leq 4$$
$$0.5 \leq y_1 \leq 10$$
$$0.5 \leq y_2 \leq 3$$

TABLE III. Computational results for examples

Example	Initial lower bound	Initial upper bound	Global solution	Number of subregions
1	−1.2569	−0.892	−1.0833	5
1a	−1	−1	−1	1
2	−23.8	−23.06	−23.06	3
3	−5.053	−4.9919	−5.0	3
4	−2.47	−2.47	−2.47	1
5	1.5953	1.625	1.6231	3
6	−13	−13	−13	1
7	−6	−2	−4.5	3
8	−6.66	−6.66	−6.66	1
9	2.8284	2.966	2.966	5
10	−500	−400	−400	3
11	−2824	−1161	−1161	53[a]
12	126.91	131.87	127.01	3

[a] Not solved to optimality. Tolerance 5%.

The first convex underestimator problem has a solution of $f_L^0 = -23.8$. Using this solution as a starting point, the original nonconvex problem is solved to obtain an upper bound. This yields the incumbent solution with an objective function of $f^* = -23.06$. The variable y_1 is selected for partitioning ($y_1 = 8.944$) since it is over its terms that the approximations are not exact. The two new subregions have solutions that are greater or equal than the incumbent solution and the global solution is $x_1 = 1.118$, $x_2 = 4$, $y_1 = 8.944$ and $y_2 = 2.5$ with $f^* = -23.062$.

6. Computational Results

In this section the global optimization of linear fractional, bilinear and polynomial problems is considered with the proposed algorithm. Size and characteristics of these problems are given in Table II. Examples 3, 4 and 5 are fractional programs, Examples 6, 8, 9 and 10 correspond to bilinear problems, Example 7 is a polynomial problem that can be reformulated as a bilinear problem, Example 11 involves both bilinear and fractional terms and Example 12 is a larger fractional program. The computational results are given in Table III. As can be seen 4 out of the 12 examples only required the solution of one convex NLP underestimator problem. Except for Example 11, the computational requirements were very modest. The bounding subproblems, nonconvex subproblems and the convex NLP subproblems were solved using MINOS 5.2 through GAMS on a IBM/R6000-530. The total time requirements for the underestimator subproblems was less than 1 cpu sec. except for Problem 11 that required 10.3 sec. For the initialization step the total

time requirements were also less than 1 cpu sec. Details on the examples are given below.

Also, in some of these examples (Examples 9 and 10) it was not possible to generate nonlinear estimators and only the linear estimators were employed. Nevertheless, the algorithm presented here and the modifications to the branching rule (Rule 2 and 3) allowed fast convergence by using a different variable to partition on.

EXAMPLE 3. *Linear fractional objective.* The formulation for this example from Falk and Palocsay (1992) is given by:

$$\max f = \frac{37x_1 + 73x_2 + 13}{13x_1 + 13x_2 + 13} + \frac{63x_1 - 18x_2 + 39}{13x_1 + 26x_2 + 13}$$
$$\text{s.t. } 5x_1 - 3x_2 = 3$$
$$1.5 \leq x_1 \leq 3 \tag{FA1}$$

Introducing the additional variables, y_i and z_i, and constraints to express the objective function as a sum of linear fractions of single variables yields,

$$\min f = -\frac{y_1}{z_1} - \frac{y_2}{z_2}$$
$$\text{s.t. } y_1 = 37x_1 + 73x_2 + 13$$
$$z_1 = 13x_1 + 13x_2 + 13$$
$$y_2 = 63x_1 - 18x_2 + 39$$
$$z_2 = 13x_1 + 26x_2 + 13 \tag{FA1'}$$
$$5x_1 - 3x_2 = 3$$
$$1.5 \leq x_1 \leq 3$$
$$y, z \geq 0$$

Since this is a minimization problem and all the coefficients are negative, it is not possible to use the nonlinear underestimators (7) of the fractional terms. Bounds are generated for all the variables and it is possible to identify a projection for the first fractional term that can be used to generate an additional estimator

$$\frac{y_1}{z_1} = r_1 \leq \frac{-59.948}{z_1} + 4.5764. \tag{26}$$

The first convex underestimator problem has a solution of $f_L^0 = -5.053$ with the ratio terms $r = (-3.825, -1.228)$. The exact objective function is $f^* = -4.9919$ and it is the incumbent solution. The approximation for the first term is exact, so the second term $(r_2 = \frac{y_2}{z_2})$ is used for partitioning the feasible space and an update of the bounds for y_2 and z_2 is done. Two subregions are considered using the value of the incumbent solution to partition. The first one has a solution of $f_L^1 = -4.98$ $(r_2 \geq 1.1394)$ and it can be discarded, the second one has a solution of $f_L^2 = -5.0002$ $(r_2 \leq 1.1394)$. This subregion is 0.004% within global optimality. At this point the algorithm can stop or if an extra partition is done the

global solution with an objective function of $f^* = -5.0$ is found exactly with $x_1 = 3.0$ and $x_2 = 4.0$. It should be noted that Falk and Palocsay (1992) required 20 iterations to solve this problem. Also, the method proposed by Al-Khayyal and Falk (1983) can be used to solve this problem. The nonconvexites are formulated as bilinear terms and bounds are obtained for the variables r_i (e.g. $r_1^L = y_1^L/z_1^u$). The solution of the relaxed problem is -6.288 and the initial gap is 26%.

EXAMPLE 4. *Linear fractional objective.* For the next example taken from Falk and Palocsay (1992) a similar transformation is necessary. The problem is given by:

$$\min f = -\frac{y_1}{z_1} - \frac{y_2}{z_2}$$
$$\begin{aligned}
\text{s.t. } y_1 &= 3x_1 + x_2 - 2x_3 + 0.8 \\
z_1 &= 2x_1 - x_2 + x_3 \\
y_2 &= 4x_1 - 2x_2 + x_3 \\
z_2 &= 7x_1 + 3x_2 - x_3 \\
x_1 + x_2 - x_3 &\leq 1 \\
-x_1 + x_2 - x_3 &\leq -1 \\
12x_1 + 5x_2 + 12x_3 &\leq 34.8 \\
12x_1 + 12x_2 + 7x_3 &\leq 34.8 \\
-6x_1 + x_2 + x_3 &\leq -4.1 \\
x_1 \geq 0, \quad x_2 \geq 0, \quad x_3 &\geq 0
\end{aligned}$$
                                                                              (FA2)

The global optimal solution is $x_1 = 1$, $x_2 = 0$, $x_3 = 0$ and $f^* = -2.47$. Falk and Palocsay (1992) obtained the global solution in one iteration. In the case of the method by Al-Khayyal and Falk (1983), the relaxed solution is -3.179 with an initial gap of 38%.

EXAMPLE 5. *Linear fractional objective.* This problem is also taken from Falk and Palocsay (1992) and the formulation after the addition of extra variables is given by:

$$\min f = \frac{y_1}{z_1} + \frac{y_2}{z_2}$$
$$\begin{aligned}
\text{s.t. } y_1 &= -x_1 + 2x_2 + 2 \\
z_1 &= 3x_1 - 4x_2 + 5 \\
y_2 &= 4x_1 - 3x_2 + 4 \\
z_2 &= -2x_1 + x_2 + 3 \\
x_1 + x_2 &\leq 1.5 \\
x_1 &\leq x_2 \\
0 \leq x_1 &\leq 1 \\
0 \leq x_2 &\leq 1
\end{aligned}$$
                                                                              (FA3)

For this example a solution within $\varepsilon = 0.07\%$ of the global optimal $x_1 = 0, x_2 = 0.284$ and $f^* = 1.6231$ is obtained. Falk and Palocsay (1983) required more than
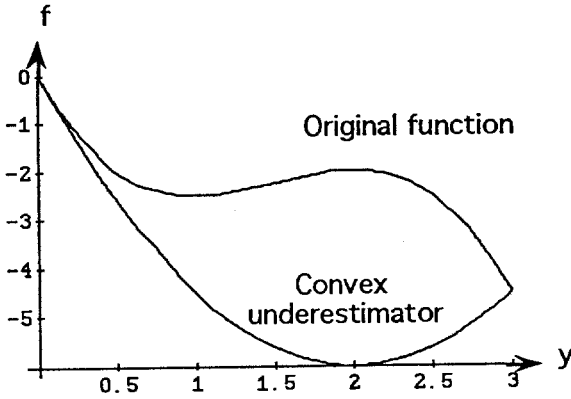
Fig. 5.   First underestimator for polynomial problem (example 7).

12 iterations and for the method by Al-Khayyal and Falk (1992) a relaxed solution of 1.385 with an initial gap of 46% is obtained.

EXAMPLE 6. *Bilinear objective.* The next example is a bilinear problem taken from Visweswaran and Floudas (1990) and the formulation is given by,

$$\min f = x_1 - x_2 - y_1 - x_1 y_1 + x_1 y_2 + x_2 y_1 - x_2 y_2$$

$$\text{s.t. } x_1 + 4x_2 \leq 8$$
$$4x_1 + x_2 \leq 12$$
$$3x_1 + 4x_2 \leq 12$$
$$2y_1 + y_2 \leq 8 \tag{FL1}$$
$$y_1 + 2y_2 \leq 8$$
$$y_1 + y_2 \leq 5$$
$$x_1, x_2, y_1, y_2 \geq 0$$

The global optimal solution corresponds to $x_1 = 3$, $x_2 = 0$, $y_1 = 4$, $y_2 = 0$ and $f^* = -13$. Visweswaran and Floudas (1990) required 3 iterations to obtain the global solution.

EXAMPLE 7. *Polynomial objective.* The next problem is a polynomial problem taken from Visweswaran and Floudas (1991) and the formulation is:

$$\min f = -6y + 4.5y^2 - y^3$$
$$0 \leq y \leq 3 \tag{FL3}$$

The feasible region is convex and the only nonconvex term is the one with the cubic term. The problem can be reformulated as:

$$\min f = -6y + 4.5y^2 - x_3$$
$$\text{s.t. } x_3 \leq x_2 y$$
$$x_2 \leq x_1 y \qquad \qquad \text{(FL3')}$$
$$x_1 = y$$
$$0 \leq x_1 \leq 3, \quad 0 \leq x_2 \leq 9, \quad 0 \leq x_3 \leq 27, \quad 0 \leq y \leq 3.$$

The original objective function and the approximation are plotted against the original variable in Fig. 5. The global optimal solution is at $y = 3$ with $f^* = -4.5$. The method by Visweswaran and Floudas (1991) required 4 iterations in this problem.

EXAMPLE 8. *Bilinear constraint.* Consider the small example presented by Sahinidis and Grossmann (1991) where the formulation includes a bilinear constraint,

$$\min f = -x - y$$
$$\text{s.t. } xy \leq 4$$
$$0 \leq x \leq 6 \qquad \qquad \text{(FL2)}$$
$$0 \leq y \leq 4$$

The global optimal solution is at $x = 6$, $y = 2/3$ and $f^* = -6.66$.

EXAMPLE 9. *Bilinear constraint.* The next small example is taken from Lo and Papalambros (1990). Here the model is given by:

$$\min f = 2x_1 + x_2$$
$$\text{s.t. } \frac{1}{x_2} - x_2 \leq 0$$
$$x_1 y_1 + x_2 y_2 \geq 0$$
$$x_1 = y_1$$
$$x_2 = y_2$$
$$0.1 \leq x, y \leq 2.5$$

The global solution is $x_1 = 0.517$, $x_2 = 1.932$ with $f^* = 2.966$.

EXAMPLE 10. *Bilinear constraint*. The following example is taken from Lasdon *et al.* (1979) and Swaney (1993),

$$\min f = 6x_1 + 16x_2 + 10x_4 - 9x_5 + 10x_7 - 15x_8$$
$$\text{s.t. } x_1 + x_2 - x_3 - x_6 = 0$$
$$0.03x_1 + 0.01x_2 - x_3x_9 - x_6x_9 = 0$$
$$x_3 + x_4 - x_5 = 0$$
$$x_6 + x_7 - x_8 = 0$$
$$x_3x_9 + 0.02x_4 - 0.025x_5 \leq 0$$
$$x_6x_9 + 0.02x_7 - 0.015x_8 \leq 0$$
$$x \geq 0, x_1 \leq 300, x_2 \leq 300, x_3 \leq 100, x_4 \leq 100,$$
$$x_5 \leq 100, x_6 \leq 200, x_7 \leq 200, x_8 \leq 200$$
$$0.01 \leq x_9 \leq 0.03$$

The global solution is located at $x_3 = 0$, $x_6 = 100$ and $x_9 = 0.01$ with $f^* = -400$. Swaney (1993) required the solution of 2 NLP's and 4 LP's to obtain the global solution.

EXAMPLE 11. *Bilinear and fractional constraints*. The last example is the mathematical model for an alkylation plant and is taken from Liebman *et al.* (1986). The model is:

$$\min f = 5.04x_1 + 0.035x_2 + 10x_3 + 3.36x_5 - 0.063x_4x_7$$
$$\text{s.t. } x_1 = 1.22x_4 - x_5$$
$$x_9 + 0.222x_{10} - 35.82 = 0$$
$$3x_7 - x_{10} - 133 = 0$$
$$x_7 \leq 86.35 + 1.098x_8 - 0.038x_8^2 + 0.325(x_6 - 89)$$
$$x_4x_9 + 1000x_3 - 9800\frac{x_3}{x_6} = 0;$$
$$x_2 + x_5 - x_1x_8 = 0$$
$$1.12 + 0.13167x_8 - 0.00667x_8^2 - \frac{x_4}{x_1} \geq 0$$
$$1 \leq x_1 \leq 2000, 1 \leq x_2 \leq 16000, 0 \leq x_3 \leq 120,$$
$$1 \leq x_4 \leq 5000, 0 \leq x_5 \leq 2000, 85 \leq x_6 \leq 93,$$
$$90 \leq x_7 \leq 95, 3 \leq x_8 \leq 12, 1.2 \leq x_9 \leq 4, 145 \leq x_{10} \leq 162.$$

Tighter bounds for the variables are obtained by solving the bounding subproblems. The nonconvex equality is substituted with two inequalities. In this formulation it is possible to rewrite some of the constraints. In particular, it proves to be useful to rewrite the sixth constraint in the following forms:

$$\frac{x_2}{x_1} + \frac{x_5}{x_1} - x_8 = 0$$
$$\frac{x_2}{x_8} + \frac{x_5}{x_8} - x_1 = 0$$

The first convex problem has a solution of $f_L^0 = -2824$ and using this solution as an initial point for solving a nonconvex problem an upper bound of $f^U = -1161$ with $x_5 = 2000$ is obtained and corresponds to the global solution. After 53 nodes the solution is proven optimal within a 5% tolerance.

EXAMPLE 12. *Linear fractional objective.* This formulation corresponds to a heat exchanger network in which the objective is to minimize the total area. The arithmetic mean is used for calculating the temperature driving force (see Quesada and Grossmann, 1992),

$$\min f = \frac{50Q_{11}}{\Delta T_{11}} + \frac{70Q_{11}}{\Delta T_{12}} + \frac{5Q_{21}}{\Delta T_{21}} + \frac{20Q_{22}}{\Delta T_{22}} + \frac{2Q_{H1}}{\Delta T_{H1}} + \frac{50Q_{C1}}{\Delta T_{C1}} + \frac{100Q_{C2}}{\Delta T_{C2}}$$

$$\text{s.t. } Q_{11} + Q_{12} = T_{C11} - 300$$
$$Q_{12} + Q_{22} = T_{C12} - T_{C11}$$
$$Q_{H1} = 400 - T_{C12}$$
$$Q_{C1} = 1.5(T_{H11} - 310)$$
$$Q_{11} = 1.5(T_{H12} - T_{H11})$$
$$Q_{12} = 1.5(410 - T_{H12})$$
$$Q_{C2} = 1.5(T_{H21} - 300)$$
$$Q_{21} = 1.5(T_{H22} - T_{H21})$$
$$Q_{22} = 1.5(420 - T_{H22})$$
$$\Delta T_{11} = \frac{T_{H12} - T_{C11} + T_{H11} - 300}{2}$$
$$\Delta T_{12} = \frac{410 - T_{C12} + T_{H12} - T_{C11}}{2}$$
$$\Delta T_{21} = \frac{T_{H22} - T_{C11} + T_{H21} - 300}{2}$$
$$\Delta T_{22} = \frac{420 - T_{C12} + T_{H22} - T_{C11}}{2}$$
$$\Delta T_{H1} = \frac{450 - 400 + 450 - T_{C12}}{2}$$
$$\Delta T_{C1} = \frac{310 - 285 + T_{H11} - 295}{2}$$
$$\Delta T_{C2} = \frac{300 - 285 + T_{H21} - 295}{2}$$
$$Q, \Delta T, T \geq 0.$$

The global optimal solution is $Q_{21} = 100$, $Q_{C1} = 150$ and $Q_{C2} = 80$ with $f = 127.01$.

7. Conclusions

An algorithm for the global optimization of linear fractional and bilinear programming problems has been proposed that relies on the solution of nonlinear convex underestimator problems which result from substituting the nonconvex terms by linear and nonlinear estimator functions. Conditions under which these functions

are nonredundant have been established. It has also been shown that additional valid estimator functions can be obtained through projections from subproblems for tightening the variable bounds. Thirteen examples have been solved using the proposed method, showing that strong lower bounds are obtained in most of the cases. This greatly reduces the enumeration of nodes in the spatial branch and bound search with which the computational requirements are kept small. To establish more definite trends, however, extensive numerical comparisons with other methods should be performed on larger test problems.

Appendix A. Example of Formulation (P1)

Consider the following example for problem (P0):

$$\min f = c_{11}\frac{p_1}{q_1} + c_{21}\frac{p_2}{q_1} - c_{22}p_2q_2 \qquad\qquad \text{(A.1)}$$
$$\text{s.t. } g = \alpha_1 p_1 + \alpha_2 p_2 + \beta_1 q_1 + \beta_2 q_2 + \gamma z + \delta \leq 0$$

in which the variables p_1, p_2, q_1, q_2 and z are specified with bounds and c_{11}, c_{21} and $c_{22} > 0$.

The estimator functions used in Section 3 can be applied directly to (A.1). However, for general presentation purposes problem (P0) will be transformed to (P1). The condition of disjoint variables between the linear fractional and bilinear terms can be achieved by introducing the new variable p_3, $p_3 = p_2$. The last term of the objective in (A.1) then becomes, $-c_{32}p_3\, q_2$ with $c_{32} = c_{22}$.

Defining the new variables for the fractional terms as in (1) yields:

$$x_{10} = p_1, \quad x_{20} = p_2, \quad y_1 = q_1, \quad r_{11} = \tfrac{p_1}{q_1}, r_{21} = \tfrac{p_2}{q_1}. \qquad \text{(A.2)}$$

Defining the new variables for the bilinear terms as in (2) yields:

$$x_{32} = p_3q_2, \quad y_2 = q_2, \quad r_{30} = p_3 \qquad\qquad \text{(A.3)}$$

Substituting (A.2) and (A.3) in (A.1) and adding the condition $p_3 = p_2$, the reformulation (P1) is given by;

$$\begin{aligned}
\min f &= c_{11}r_{11} + c_{21}r_{21} - c_{32}x_{32} \\
\text{s.t. } & y_1 r_{11} \geq x_{10} \\
& y_1 r_{21} \geq x_{20} \\
& y_2 r_{30} \geq x_{32} \\
& \alpha_1 x_{10} + \alpha_2 x_{20} + \beta_1 y_1 + \beta_2 y_2 + \gamma z + \delta \leq 0 \\
& r_{30} - x_{20} = 0
\end{aligned} \qquad\qquad \text{(A.4)}$$

Appendix B. Estimators for Factorable Functions

A concave overestimating function of a product of functions is given by (McCormick (1983)),

$$\begin{aligned}
f(x)g(y) \leq\ & \min[f^u C_g(y) + g^L C_f(x) - f^u g^L, f^L C_g(y) \\
& + g^u C_f(x) - f^L g^u]
\end{aligned} \qquad\qquad \text{(B.1)}$$

where f^u, g^u, f^L and g^L are positive bounds over the functions $f(x)$ and $g(y)$ such that:

$$0 \leq f^L \leq f(x) \leq f^u \tag{B.2}$$

$$0 \leq g^L \leq g(y) \leq g^u \tag{B.3}$$

and $C_f(x)$ and $C_g(y)$ are concave functions such that for all x and y in some convex set:

$$C_f(x) \geq f(x) \tag{B.4}$$

$$C_g(y) \geq g(y) \tag{B.5}$$

In a similar way as in (B.1), the convex underestimating function of a product of functions is given by:

$$f(x)g(y) \geq \max[f^u c_g(y) + g^u c_f(x) - f^u g^u, f^L c_g(y) + g^L c_f(x) - f^L g^L] \tag{B.6}$$

and $c_f(x)$ and $c_g(y)$ are convex functions such that for all x and y in some convex set:

$$c_f(x) \leq f(x) \tag{B.7}$$

$$c_g(y) \leq g(y). \tag{B.8}$$

In the case of bilinear functions ($f(x) = x$ and $g(y) = y$) the individual concave and convex bounding functions of each individual term are given by the function itself:

$$C_f(x) = x = c_f(x) \tag{B.9}$$

$$C_g(y) = y = c_g(y). \tag{B.10}$$

Thus, from (B.1) and (B.6) the following under and over estimator functions are obtained:

$$xy \geq \max[x^L y + y^L x - x^L y^L, x^u y + y^u x - x^u y^u] \tag{B.11}$$

$$xy \leq \min[x^L y + y^u x - x^L y^u, x^u y + y^L x - x^u y^L]. \tag{B.12}$$

For fractional linear terms ($f(x) = x$ and $g(y) = 1/y$), it is possible to generate a convex underestimator function because the individual convex bounding functions are given by

$$c_f(x) = x \tag{B.13}$$
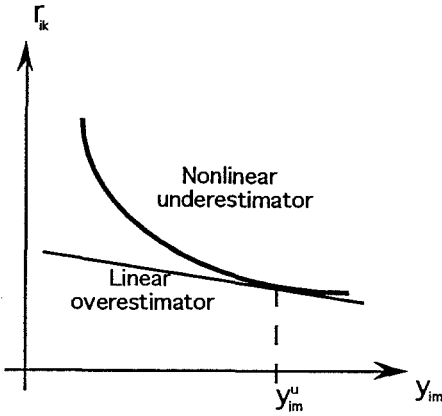
$$c_g(y) = 1/y. \tag{B.14}$$

Fig. 6.   Comparison between linear and nonlinear estimators (5a) and (7a) of the linear fractional terms in (P0).

From (B.6) the underestimator function can be expressed as:

$$\frac{x}{y} \geq \max[\frac{x}{y^L} + x^u(\frac{1}{y} - \frac{1}{y^L}), \frac{x}{y^u} + x^L(\frac{1}{y} - \frac{1}{y^u})] \tag{B.15}$$

The estimator functions (B.11), (B.12) and (B.15) have the property that they match the original function when one of the variables is at a bound. This is because the individual convex and concave bounding functions in (B.9), (B.10), (B.13) and (B.14) are the functions themselves.

Appendix C. Mathematical Properties and Proofs

PROPERTY 1. When $r_{ik}^L = \frac{x_{im}^L}{y_j^u}$ (or $r_{ik}^u = \frac{x_{im}^u}{y_j^L}$, $(i, j, k, m) \in P_R$, the linear overestimator (5a) (or (5b)) is a linearization of the nonlinear underestimator (7a) (or (7b)).

   Proof. Consider the linear overestimator (5a)

$$x_{im} \leq y_j^u r_{ik} + r_{ik}^L y_j - y_j^u r_{ik}^L. \tag{C.1}$$

Rearranging (C.1) leads to:

$$r_{ik} \geq \frac{x_{im}}{y_j^u} - \frac{r_{ik}^L y_i}{y_j^u} + r_{ik}^L. \tag{C.2}$$

Using the condition that $r_{ik}^L = \frac{x_{im}^L}{y_i^u}$, equation (C.2) yields

$$r_{ik} \geq \frac{x_{im}}{y_j^u} + x_{im}^L(\frac{1}{y_j^u} - \frac{y_j}{(y_j^u)^2}). \tag{C.3}$$

The nonlinear underestimator (7a) gives rise to the constraint

$$r_{ik} \geq \frac{x_{im}}{y_j^u} + x_{im}^L \left(\frac{1}{y_j} - \frac{1}{y_j^u} \right).$$ (C.4)

The first term of equations (C.3) and (C.4) is the same. Now compare the nonlinear term $NT(y_j) = \left(\frac{1}{y_j} - \frac{1}{y_j^u} \right)$ from (C.4) with the linear term $\left(\frac{1}{y_j^u} - \frac{y_j}{(y_j^u)^2} \right)$ from equation (C.3). Both terms are equal at y_j^u. Furthermore, a linearization of the nonlinear term at $y_j = y_j^u$ yields the linear term:

$$NT(y_j^u) + \nabla_{y_j} NT(y_j^u)(y_j - y_j^u) = -\frac{1}{(y_j^u)^2}(y_j - y_j^u) = \frac{1}{y_j^u} - \frac{y_j}{(y_j^u)^2}.$$ (C.5)

Thus, (5a) is a linearization of (7a) and in a similar form it can be proved that for $r_{ik}^u = \frac{x_{im}^u}{y_j^L}$, (5b) is a linearization of (7b). ∎

COROLLARY 1. *The nonlinear underestimator* (7a) *(or* (7b)) *is stronger than the linear overestimator* (5a) *(or* (5b)) *when* $r_{ik}^L = \frac{x_{im}^L}{y_j^u}$ *(or* $r_{ik}^u = \frac{x_{im}^u}{y_j^L}$), $(i, j, k, m) \in P_R$.

Proof. From Property 1 and the fact that the nonlinear underestimators in (7a) are convex in y_j, any linearization is a supporting hyperplane (see Figure 6). ∎

PROPERTY 2. *When* $r_{ik}^L > \frac{x_{im}^L}{y_j^u}$ *(or* $r_{ik}^u < \frac{x_{im}^u}{y_j^L}$), $(i, j, k, m) \in P_R$, *the linear overestimator* (5a) *(or* 5b) *is nonredundant.*

Proof. Consider a feasible point with x_{im}^+ and y_j^+ such that $\frac{x_{im}^+}{y_j^+} = r_{ik}^L$, with $x_{im}^+ > x_{im}^L$ and $y_j^+ < y_j^u$.

Evaluating the linear overestimator (5a) at (x_{im}^+, y_j^+) and rearranging it as in (C.2) yields:

$$r_{ik} \geq \frac{x_{im}^+}{y_j^u} - \frac{r_{ik}^L y_j^+}{y_j^u} + r_{ik}^L = \frac{r_{ik}^L y_j^+}{y_j^u} - \frac{r_{ik}^L y_j^+}{y_j^u} + r_{ik}^L.$$ (C.6)

The linear overestimator for that point then reduces to,

$$r_{ik} \geq r_{ik}^L.$$ (C.7)

The nonlinear underestimator (7a) for this point is,

$$r_{ik} \geq \frac{x_{im}^+}{y_j^u} + x_{im}^L \left(\frac{1}{y_j^+} - \frac{1}{y_j^u} \right).$$ (C.8)
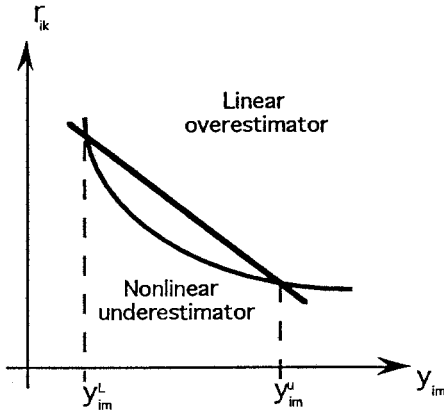
Fig. 7. Comparison between linear and nonlinear estimators (5a) and (7a) of the bilinear terms in (P0).

and using the relation $\frac{x_{im}^+}{y_j^+} = r_{ik}^L$, for expressing (C.8) in terms of r_{ik}^L yields

$$r_{ik} \geq \left(\frac{y_j^+}{y_j^u} + \frac{x_{im}^L}{x_{im}^+}\right) r_{ik}^L - \frac{x_{im}^L}{y_j^u}. \tag{C.9}$$

Defining $\alpha = $ and $\beta = \frac{x_{im}^L}{x_{im}^+}$, the equation (C.9) can be expressed as

$$r_{ik} \geq [\alpha + \beta] r_{ik}^L - \alpha\beta r_{ik}^L = r_{ik}^L[\alpha + \beta(1 - \alpha)] \tag{C.10}$$

Since $0 \leq \alpha < 1$ and $0 \leq \beta < 1$,

$$1 = \alpha + (1 - \alpha) > \alpha + \beta(1 - \alpha) = \phi \tag{C.11}$$

the nonlinear underestimator reduces to,

$$r_{ik} \geq \phi r_{ik}^L, \quad \phi < 1. \tag{C.12}$$

Comparing (C.7) and (C.12), it follows that the linear overestimator (5a) is stronger at the point (x_{im}^+, y_j^+) and therefore nonredundant. ∎

PROPERTY 3. *When $x_{im}^L = r_{ik}^L y_j^L$ (or $x_{im}^u = r_{ik}^u y_j^u$), $(i, j, k, m) \in P_B$, the linear overestimator (5a) (or (5b)) is a secant of the nonlinear underestimator (7a) (or (7b)).*

   Proof. The nonlinear underestimator (7a)

$$r_{ik} \geq \frac{x_{im}}{y_j^u} + x_{im}^L\left(\frac{1}{y_j} - \frac{1}{y_j^u}\right) \tag{C.13}$$

can be expressed as:

$$x_{im} - y_j^u r_{ik} - x_{im}^L + \frac{x_{im}^L y_j^u}{y_j} \leq 0. \tag{C.14}$$

Using $x_{im}^L = r_{ik}^L y_j^L$

$$x_{im} - y_j^u r_{ik} + r_{ik}^L \left(\frac{y_j^u y_j^L}{y_j} - y_j^L \right) \leq 0. \tag{C.15}$$

The linear overestimator (5a) is given by

$$x_{im} \leq y_j^u r_{ik} + r_{ik}^L y_j - y_j^u r_{ik}^L \tag{C.16}$$

that can be expressed as:

$$x_{im} - y_j^u r_{ik} + r_{ik}^L (y_j^u - y_j) \leq 0. \tag{C.17}$$

The difference between both equations (C.15) and (C.17) is in the last term $\left(\frac{y_j^u y_j^L}{y_j} - y_j^L \right)$ versus $(y_j^u - y_j)$. Both terms are equal at the extreme values $y_j = y_j^L$ and $y_j = y_j^u$. Since the nonlinear term is convex and the linear one matches its value at the extreme points the latter is a secant of the nonlinear estimator. ∎

COROLLARY 2. *The linear overestimator* (5a) *(or* (5b)) *is stronger than the nonlinear underestimator* (7a) *(or* (7b)) *over the feasible region when* $x_{im}^L = r_{ik}^L y_j^L$ *(or* $x_{im}^u = r_{ik}^u y_j^u$), $(i, j, k, m) \in P_B$.
    Proof. This follows trivially from Property 3 and the fact that the nonlinear underestimator (7a) is convex (see Fig. 7). ∎

PROPERTY 4. *When* $x_{im}^L > r_{ik}^L y_j^L$ *(or* $x_{im}^u < r_{ik}^u y_j^u$), $(i, j, k, m) \in P_B$, *the nonlinear underestimator* (7a) *(or* (7b)) *is nonredundant.*
    Proof. Consider a feasible point (r_{ik}^+, y_j^+) such that $r_{ik}^+ y_j^+ = x_{im}^L$, $r_{ik}^u > r_{ik}^+ > r_{ik}^L$ and $x_{im}^u > x_{im}^+ > x_{im}^L$. The nonlinear underestimator (7a) for this point gives:

$$r_{ik}^+ \geq \frac{x_{im}}{y_j^u} + x_{im}^L \left(\frac{1}{y_j^+} - \frac{1}{y_j^u} \right) \tag{C.18}$$

yielding

$$\frac{x_{im} - x_{im}^L}{y_j^u} \leq r_{ik}^+ - \frac{x_{im}^L}{y_j^+} = \frac{r_{ik}^+ y_j^+ - x_{im}^L}{y_j^+} = 0 \tag{C.19}$$

which in turn implies

$$x_{im} \leq x_{im}^L. \tag{C.20}$$

Now consider the linear overestimator (5a) for the same point:

$$x_{im} \le y_j^u r_{ik}^+ + r_{ik}^L y_j^+ - y_j^u r_{ik}^L = \frac{y_j^u x_{im}^L}{y_j^+} + \frac{r_{ik}^L x_{im}^L}{r_{ik}^+} - \frac{y_j^u r_{ik}^L r_{ik}^+}{r_{ik}^+} \qquad \text{(C.21)}$$

which yields,

$$x_{im} \le x_{im}^L \left(\frac{y_j^u}{y_j^+} + \frac{r_{ik}^L}{r_{ik}^+} - \frac{y_j^u r_{ik}^L}{y_j^+ r_{ik}^+} \right). \qquad \text{(C.22)}$$

Defining $\alpha = \frac{y_j^u}{y_j^+} > 1$ and $\beta = \frac{r_{ik}^L}{r_{ik}^+} < 1$, equation (C.22) reduces to:

$$\begin{aligned} x_{im} \le x_{im}^L (\beta + \alpha(1 - \beta)) &= x_{im}^L (1 - 1 + \beta - \alpha(\beta - 1)) \\ &= x_{im}^L (1 + (\beta - 1)(1 - \alpha)) \end{aligned} \qquad \text{(C.23)}$$

Since $(\beta - 1) < 0$ and $(1 - \alpha) < 0$, $x_{im} \le \Phi x_{im}^L$ with $\Phi > 1$. The comparison with the other linear overestimator (5b) is equivalent and also yields $x_{im} \le \Phi x_{im}^L$, which in turn implies that the nonlinear underestimator (7a) is stronger at (r_{ik}^+, y_j^+). ∎

PROPERTY 5. *The nonlinear inequality* (11a) (*or* (11b)) *is a valid convex underestimator when* $b < 0$ (*or* $b' < 0$), *and is nonredundant with respect to the nonlinear underestimator in* (7a) (*or* (7b)).

Proof. For the first part of the proof constraint (10) can be expressed as,

$$\frac{1}{y_j} - \frac{1}{a + b x_{im}} \ge 0 \qquad \text{(C.24)}$$

Multiplying by the lower bound constraint $(x_{im} - x_{im}^L \ge 0)$ yields the valid inequality,

$$(x_{im} - x_{im}^L)\left(\frac{1}{y_j} - \frac{1}{a + b x_{im}} \right) \ge 0 \qquad \text{(C.25)}$$

Rearranging yields:

$$\frac{x_{im}}{y_j} \ge \frac{x_{im}^L}{y_j} + (x_{im} - x_{im}^L)\left(\frac{1}{a + b x_{im}} \right) \qquad \text{(C.26)}$$

which corresponds to the nonlinear underestimator (11). The Hessian matrix of the underestimating function in (11) is given by

$$\begin{bmatrix} -\dfrac{2b(a + b x_{im}^L)}{(a + b x_{im})^3} & 0 \\ 0 & \dfrac{2 x_{im}^L}{y_j^3} \end{bmatrix} \qquad \text{(C.27)}$$

The term $(a + bx_{im})$ is positive over the feasible region since,

$$a + bx_{im} \geq y_j > 0 \tag{C.28}$$

and hence,

$$-\frac{2b(a + bx_{im}^L)}{(a + bx_{im})^3} > 0 \text{ if } b < 0. \tag{C.29}$$

Also for $x_{im}^L > 0$,

$$\frac{2x_{im}^L}{y_j^3} > 0. \tag{C.30}$$

If $x_{im}^L = 0$ equation (C.26) reduces to the convex inequality $(b < 0)$,

$$r_{ik} \geq \frac{x_{im}}{a + bx_{im}} \tag{C.31}$$

Therefore, if $b < 0$ the Hessian matrix (C.27) is positive definitive and the function is convex.

Now consider a feasible point (x_{im}^+, y_j^+) in the strict interior such that $y_j^+ = a + bx_{im}^+$ and $y_j^L < y_j^+ < y_j^u$ and $x_{im}^+ < x_{im}^+ < x_{im}^u$. Equation (11) for the nonlinear underestimator with projection reduces to,

$$\frac{x_{im}^+}{y_j^+} \geq \frac{x_{im}^+}{a + bx_{im}^+} + x_{im}^L\left(\frac{1}{y_j^+} - \frac{1}{a + bx_{im}^+}\right) = \frac{x_{im}^+}{y_j^+} + x_{im}^L\left(\frac{1}{y_j^+} - \frac{1}{y_j^+}\right)$$

$$= \frac{x_{im}}{y_j^+} \tag{C.32}$$

and is therefore an exact approximation of the linear fractional term. Since y_j^+ does not lie in the boundary defined by the bounds of the variables x_{im} and y_j the nonlinear underestimator (7a) yields,

$$\frac{x_{im}^L}{y_j^+} + \frac{x_{im}^+ - x_{im}^L}{y_j^u} < \frac{x_{im}^L}{y_j^+} + \frac{x_{im}^+ - x_{im}^L}{y_j^+} = \frac{x_{im}^+}{y_j^+} \tag{C.33}$$

which is a strict inequality. The other nolinear underestimator (7b) for this point yields,

$$\frac{x_{im}^+}{y_j^L} + x_{im}^u\left(\frac{1}{y_j^+} - \frac{1}{y_j^L}\right) < \frac{x_{im}^+}{y_j^L} + x_{im}^+\left(\frac{1}{y_j^+} - \frac{1}{y_j^L}\right) \leq \frac{x_{im}^+}{y_j^+} \tag{C.34}$$

which is a strict inequality. Hence, the projected nonlinear underestimator (11) is stronger than the nonlinear underestimators (7) for the point (x_{im}^+, y_j^+). ∎

PROPERTY 6. *The additional estimators in (13), (14) and (18) provide an exact approximation at the boundary defined by the projected cut.*

Proof. In the same spirit as the proof for Property 5, select a point for which the projected inequality is a strict inequality and for which the variables are not at their bounds. ■

Property 7. *The optimal solution f'_L of* (NLP$_L$) *provides a valid lower bound to the global optimum (f^*) of problem* (P1).

Proof. Any feasible point (x, y, r, z) for problem (NLP$_L$) is also a feasible solution to problem (P1) since the inequalities $g(x_0, y, r_0, z) \le 0$ are identical in both problems. Since the approximating functions in (NLP$_L$) represent a relaxation of the bilinear inequalities in (P1), they have the effect of underestimating the objective function C of problem (P1). Thus, it follows that at a given feasible point $f_L \le f$.

For the global optimum $(x*, y*, r*, z*)$ of problem (P1) it then follows that $f^* \ge f^*_L$ where f^*_L is the objective of NLP$_L$ evaluated at that point. Since f'_L, the optimal solution of NLP$_L$ is unique due to its convexity, $f^*_L \ge f'_L$, and thus $f^* \ge f'_L$. ■

COROLLARY 3. *If the value of the objective function from* (P1) *evaluated at the optimal solution of* NLP$_L$ *is f'_L then this solution corresponds to the global optimum of* (P1).

Proof. If f' is not the global optimal solution of problem (P) then there exists a global solution $f^* < f'$. But by Property 7, $f'_L \le f^*$ which contradicts the assumption that $f'_L = f'$ is a solution to NLP$_L$. ■

PROPERTY 8. *The branch and bound algorithm will either terminate in a finite number of partitions at a global optimal solution, or generate a sequence of bounds that converge to the global solution.*

Proof. Given the branch and bound procedure, there are two possibilities. In the first one, at a given node the lower bound f_L of the underestimator NLP$_L$ is identical to the original objective function in which case the algorithm terminates in a finite number of partitions.

In the second possibility an infinite sequence of partitions is generated. This in turn implies that there is a subregion that is being infinitely partitioned. Let the sequence of solutions be denoted by $(^{k'})$ and $\zeta = (x, y, r, z)$. By the termination criteria it is known that,

$$f^{u,k'} - f^{k'}_L > 0. \tag{C.35}$$

Since the upper bound is at least as strong as the evaluation of the actual objective function for the current solution ζ^k,

$$f(\zeta^{k'}) - f_L(\zeta^{k'}) \ge f^{u,k'} - f^{k'}_L > 0 \tag{C.36}$$

there must exist at least one nonconvex term, $+$, for which its feasible region is infinitely partitioned. By the partition rule 1,

$$\left(\frac{x_{im}}{y_j - r_{ik}}\right) \leq \left(\frac{x_{im}^+}{y_j^+ - r_{ik}^+}\right). \tag{C.37}$$

Summing up over all the nonconvex terms, t, it follows that

$$t\left(\frac{x_{im}^+}{y_j^+} - r_{ik}^+\right) \geq f(\zeta^{k'}) - f_L(\zeta^{k'}) \geq f^{u,k'} - f_L^{k'} > 0. \tag{C.38}$$

The variables for the nonconvex term $(+)$ have some bounds defining an interval. Since the partition is of the same nature as the one used by Al-Khayyal and Falk (1983), the variables in the sequence must converge to one of the bounds. Moreover, the series has to converge to a point. When one of the bounds of a variable are not changing, this variable is selected for the partition in the algorithm. When one of the variables is at its bounds the representation is exact, $\frac{x_{im}^+}{y_j^+} = r_{ik}^+$. Therefore,

$$0 \geq f(\zeta^{k'}) - f_L(\zeta^{k'}) \geq f^{u,k'} - f_L^{k'} > 0 \tag{C.39}$$

which means that equality between the lower bound f_L and the original function f must hold. Since by Property 7, $f_L^{k'}$ is a lower bound to the global optimal solution, it corresponds to the global solution. ∎

References

Al-Khayyal, F.A. (1992), Generalized bilinear programming: Part I. Models, applications and linear programming relaxation, *European Journal of Operational Research* **60**, 306–314.

Al-Khayyal, F.A. and Falk, J.E. (1983), Jointly constrained biconvex programming, *Mathematics of Operations Research* **8**, 273–286.

Bazaraa, M.S. and Shetty, C.M. (1979), *Nonlinear Programming Theory and Algorithms*, John Wiley & Sons, New York.

Charnes, A. and Cooper, W.W. (1962), Programming with linear fractional functionals, *Naval Research Logistics Quarterly* **9**, 181–186.

Dinkelbach, W. (1967), On nonlinear fractional programming, *Management Science* **13**, 492–498.

Falk, J.E. and Palocsay, S.W. (1992), Optimizing the sum of linear fractional functions, *Recent Advances in Global Optimization*, in Floudas, C.A and Pardalos, P.M. (eds.), 221–258.

Floudas, C.A. and Pardalos, P.M. (1990), *A Collection of Test Problems for Constrained Global Optimization Algorithms*, G. Goss and J. Hartmanis (eds.), Springer Velag.

Floudas, C.A. and Visweswaran, V. (1990), A global optimization algorithm (GOP) for certain classes of nonconvex NLPs-I Theory, *Computers Chem. Engng.* **14**, 1397–1417.

Grossmann, I.E. (1990), Mixed-Integer Non-Linear Programming Techniques for the Synthesis of Engineering System, *Res. Eng. Des.* **1**, 205–228.

Horst, R. (1990), Deterministic methods in constrained global optimization: Some recent advances and fields of application, *Naval Research Logistics* **37**, 433–471.

Horst, R. and Tuy, T. (1990), *Global Optimization: Deterministic Approaches*, Springer-Verlag, Berlin, New York.

Konno, H., Yajima, Y. and Matsui, T. (1991), Parametric Simplex Algorithms for Solving a Special Class of Nonconvex Minimization Problems. *Journal of Global Optimization* **1**, 65–81.

Lasdon, L.S., Waren, A.D., Sarkar, S., and Palacios, F. (1979), Solving the Pooling Problem Using Generalized Reduced Gradient and Successive Linear Programming Algorithms, *SIGMAP Bull* **77**, 9–15 .

Liebman, J., Lasdon, L., Schrage, L., and Waren, A. (1986), *Modelling and Optimization with GINO*, The Scientific Press, Palo Alto, CA.

Lo, C. and Papalambros, P.Y. (1990), A Deterministic Global Design Optimization Method for Nonconvex Generalized Polynomial Problems, *Advances in Design Automation*, New York.

McCormick, G.P. (1976), Computability of Global Solutions to Factorable Nonconvex Programs: Part I – Convex Underestimating Problems, *Mathematical Programming*, **10**, 146–175.

Papalambros, P. and Wilde, D.L. (1988), *Principles of Optimal Design: Modelling and Computation*, Cambridge University Press, Cambridge.

Quesada, I. and Grossmann, I.E. (1993), Global optimization algorithm for heat exchanger netwoks. *Ind. Eng. Chem. Res.*, **32**. 487–499.

Quesada, I. and Grossmann, I.E. (1995), Global optimization of process networks with multicomponent flows. To appear in *Computers and Chem. Eng.*

Reklaitis, G.V. and Ravindran, A. (1983), *Engineering Optimization: Methods and Applications*. Wiley, New York.

Sahinidis, N.V. and Grossmann, I.E. (1991), Convergence Properties of Generalized Benders Decomposition. *Computers and Chem. Eng.* **15**, 481–491.

Schoen, F. (1991), Stochastic Techniques for Global Optimization: A Survey of Recent Advances. *Journal of Global Optimization* **1**, 207–228

Sherali, H.D. and Alameddine, A. (1992), A new reformulation-linearization technique for bilinear programming problems, *Journal of Global Optimization* **2**, 379–410.

Swaney, R.E. (1993), Global solution of algebraic nonlinear programs. Paper MC36.3 presented at TIMS/ORSA meeting, Phoenix, AZ.

Visweswaran, V. and Floudas, C.A. (1990), A global optimization algorithm (GOP) for certain classes of nonconvex NLPs-II Application of theory and test problems, *Computers Chem. Engng.* **14**, 1419.

Visweswaran, V. and Floudas, C.A. (1991), Global optimization of problems with polynomial functions in one variable. *Recent Advances in Global Optimization*, in Floudas, C.A and Pardalos, P.M. (eds.), 165–199.