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A Branch and Contract Algorithm for Problems with Concave Univariate, Bilinear and Linear Fractional Terms

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Abstract. A new deterministic branch and bound algorithm is presented in this paper for the global optimization of continuous problems that involve concave univariate, bilinear and linear fractional terms. The proposed algorithm, the *branch and contract algorithm*, relies on the use of a *bounds-contraction subproblem* that aims at reducing the size of the search region by eliminating portions of the domain in which the objective function takes only values above a known upper bound. The solution of contraction subproblems at selected branch and bound nodes is performed within a *finite contraction operation* that helps reducing the total number of nodes in the branch and bound solution tree. The use of the proposed algorithm is illustrated with several numerical examples.

Key words: Bilinear terms, Bounds contraction, Branch and contract, Concave separable functions, Continuous global optimization, Linear fractional terms

1. Introduction

This paper deals with the development of a new deterministic algorithm for the global optimization of nonlinear programs involving concave univariate, bilinear and linear fractional terms in the objective function and constraints. For reviews on methods that address problems with these classes of functions see for instance: Benson (1995), Al-Khayyal (1990), and Schaible (1994, 1995). The extension of the proposed approach of this paper to the mixed-integer case can be found in Zamora (1997). The specific problem under consideration is the following:

$$\operatorname*{Min}_{x}\ f(x) = \sum_{(i,j)\in BL_0} a_{ij}x_ix_j + \sum_{(i,j)\in LF_0} b_{ij}\frac{x_i}{x_j} + \sum_{i\in C_0} g_i(x_i) + h(x)$$

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subject to (1)

$$f_k(x) = \sum_{(i,j)\in BL_k} a_{ijk} x_i x_j + \sum_{(i,j)\in LF_k} b_{ijk} \frac{x_i}{x_j}$$
$$+ \sum_{i\in C_k} g_{i,k}(x_i) + h_k(x) \le 0 \quad k \in K$$
$$x \in S \cap \Omega_0 \subset R^n$$

where $a_{ij}, a_{ijk}, b_{ij}, b_{ijk}$, are scalars with $i \in I = \{1, 2, \ldots, n\}$, $j \in J = \{1, 2, \ldots, n\}$, and $k \in K = \{1, 2, \ldots, m\}$. BL_0, BL_k, LF_0, LF_k are (i, j)-index sets, with $i \neq j$, that define the bilinear and linear fractional terms present in the problem. The functions $h(x), h_k(x)$ are convex, and twice continuously differentiable. C_0 and C_k are index sets for the univariate twice continuously differentiable concave functions $g_i(x_i), g_{i,k}(x_i)$. The set $S \subset R^n$ is convex, and $\Omega_0 \subset R^n$ is an n-dimensional hyperrectangle defined in terms of the initial variable bounds $x^{L,in}$ and $x^{U,in}$:

$$\Omega_0 = \{x \in R^n : 0 \le x^{L,in} \le x \le x^{U,in}, \quad x_j^{L,in} > 0 \text{ if } (i, j) \in LF_0 \cup LF_k,$$
$$i \in I, j \in J, k \in K\}$$

For future reference, the feasible region of problem (1) is denoted by D. Note that a nonlinear equality constraint of the form $f_k(x) = 0$ can be accommodated in (1) through the representation by the inequalities $f_k(x) \le 0$ and $-f_k(x) \le 0$, provided $h_k(x)$ is separable.

Given a positive relative tolerance ε_t, a deterministic global optimization algorithm that belongs to the class of branch and bound algorithms (Horst and Tuy, 1993) is presented in this paper to determine a point $x^* \in D$ such that,

$$\varepsilon(x) \le \varepsilon_t \quad \forall x \in D \tag{2}$$

where

$$\varepsilon(x) = \begin{cases} \dfrac{f(x^*) - f(x)}{|f(x^*)|} & \text{if } f(x^*) \neq 0 \\ -f(x) & \text{if } f(x^*) = 0 \end{cases}$$

The basic ideas in the proposed paper rely on the use of tight underestimating functions, and the solution of a *contraction subproblem* for variable bounds in order to reduce the number of nodes in the branch and bound tree. Previous methods reported in the literature that can solve (1) or particular instances of it include the algorithms by Al-Khayyal and Falk (1983), Al-Khayyal et al. (1995), Androulakis et al. (1995), Cambrini et al. (1989), Epperly and Swaney (1996), Falk and Palocsay (1992, 1994), Falk and Soland (1969), Konno et al. (1991), Pardalos and Phillips (1991), Phillips and Rosen (1990), Quesada and Grossmann (1995), Rosen (1983), Ryoo and Sahinidis (1996), Sherali and Alameddine (1992), Sherali and Tuncbilek (1995), Smith and Pantelides (1996), and Soland (1971); see also Horst and Pardalos (1995).

The remainder of the paper is organized as follows. A convex underestimating program for problem (1) is presented in the next section. In Section 3 we describe a convex *bounds-contraction subproblem* that can be used at a branch and bound node to eliminate portions of the feasible region in which the objective function will only take values above a known upper bound. A finite strategy for sequencing the solution of contraction subproblems is proposed in Section 4, and a branch and contract algorithm for continuous global optimization is presented in Section 5. Section 6 contains five examples that illustrate the use of this algorithm.

2. A convex underestimating problem

In this section we present the proposed convex underestimating problem for the global optimum solution of problem (1) that relies on the use of linear and nonlinear underestimators, and that predicts valid lower bounds.

To obtain a lower bound, $LB(\Omega)$, for the global minimum of problem (1) over $D \cap \Omega$, where $\Omega = \{x \in R^n : x^L \leq x \leq x^U\} \subseteq \Omega_0$, the following problem is proposed:

$$\begin{aligned}
&\underset{(x,y,z)}{\text{Min}}\ \hat{f}(x,y,z) = \sum_{(i,j)\in BL_0} a_{ij}y_{ij} + \sum_{(i,j)\in LF_0} b_{ij}z_{ij} + \sum_{i\in C_0} \hat{g}_i(x_i) + h(x)\\
&\text{subject to}\\
&\hat{f}_k(x,y,z) = \sum_{(i,j)\in BL_k} a_{ijk}y_{ij} + \sum_{(i,j)\in LF_k} b_{ijk}z_{ij}\\
&\qquad\qquad + \sum_{i\in C_k} \hat{g}_{i,k}(x_i) + h_k(x) \leq 0 \quad k \in K \qquad (3)\\
&(x,y,z) \in T(\Omega) \subset R^n \times R^{n_1} \times R^{n_2}\\
&x \in S \cap \Omega \subset R^n, \quad y \in R_+^{n_1}, \quad z \in R_+^{n_2},
\end{aligned}$$

where the functions and sets are defined as follows:

(a) $\hat{g}_i(x_i)$ and $\hat{g}_{i,k}(x_i)$ are the convex envelopes for the univariate functions over the domain $x_i \in [x_i^L, x_i^U]$ (Falk and Soland, 1969):

$$\hat{g}_i(x_i) = g_i(x_i^L) + \left(\frac{g_i(x_i^U) - g_i(x_i^L)}{x_i^U - x_i^L}\right)(x_i - x_i^L) \leq g_i(x_i) \qquad (4)$$

$$\hat{g}_{i,k}(x_i) = g_{i,k}(x_i^L) + \left(\frac{g_{i,k}(x_i^U) - g_{i,k}(x_i^L)}{x_i^U - x_i^L}\right)(x_i - x_i^L) \leq g_{i,k}(x_i) \qquad (5)$$

where $\hat{g}_i(x_i) = g_i(x_i)$ at $x_i = x_i^L$, and $x_i = x_i^U$; likewise, $\hat{g}_{i,k}(x_i) = g_{i,k}(x_i)$ at $x_i = x_i^L$, and $x_i = x_i^U$.

(b) $y = \{y_{ij}\}$ is a vector of additional variables for relaxing the bilinear terms in (1), and are used in the following inequalities which determine the convex and concave envelopes of bilinear terms:

$$\begin{aligned} y_{ij} &\geq x_j^L x_i + x_i^L x_j - x_i^L x_j^L \quad (i, j) \in BL^+ \\ y_{ij} &\geq x_j^U x_i + x_i^U x_j - x_i^U x_j^U \quad (i, j) \in BL^+ \end{aligned} \tag{6}$$

$$\begin{aligned} y_{ij} &\leq x_j^L x_i + x_i^U x_j - x_i^U x_j^L \quad (i, j) \in BL^- \\ y_{ij} &\leq x_j^U x_i + x_i^L x_j - x_i^L x_j^U \quad (i, j) \in BL^- \end{aligned} \tag{7}$$

where

$$BL^+ = \{(i, j) : (i, j) \in BL_0 \cup BL_k, a_{ij} > 0 \text{ or } a_{ijk} > 0,\ k \in K\}$$
$$BL^- = \{(i, j) : (i, j) \in BL_0 \cup BL_k, a_{ij} < 0 \text{ or } a_{ijk} < 0,\ k \in K\}$$

Note that the inequalities in (6) were first derived by McCormick (1976), and along with the inequalities in (7) theoretically characterized by Al-Khayyal and Falk (1983) and Al-Khayyal (1990).

(c) $z = \{z_{ij}\}$ is a vector of additional variables for relaxing the linear fractional terms in (1); these variables are used in the following inequalities:

$$\begin{aligned} z_{ij} &\geq \frac{x_i}{x_j^L} + x_i^U \left(\frac{1}{x_j} - \frac{1}{x_j^L} \right) \quad (i, j) \in LF^+ \\ z_{ij} &\geq \frac{x_i}{x_j^U} + x_i^L \left(\frac{1}{x_j} - \frac{1}{x_j^U} \right) \quad (i, j) \in LF^+ \end{aligned} \tag{8}$$

$$z_{ij} \geq \frac{1}{x_j} \left(\frac{x_i + \sqrt{x_i^L x_i^U}}{\sqrt{x_i^L} + \sqrt{x_i^U}} \right)^2 \quad (i, j) \in LF^+ \tag{9}$$

$$\begin{aligned} z_{ij} &\leq \frac{1}{x_j^L x_j^U} (x_j^U x_i - x_i^L x_j + x_i^L x_j^L) \quad (i, j) \in LF^- \\ z_{ij} &\leq \frac{1}{x_j^L x_j^U} (x_j^L x_i - x_i^U x_j + x_i^U x_j^U) \quad (i, j) \in LF^- \end{aligned} \tag{10}$$

where

$$LF^+ = \{(i, j) : (i, j) \in LF_0 \cup LF_k, b_{ij} > 0 \text{ or } b_{ijk} > 0,\ k \in K\}$$
$$LF^- = \{(i, j) : (i, j) \in LF_0 \cup LF_k, b_{ij} < 0 \text{ or } b_{ijk} < 0,\ k \in K\}$$

The inequalities in (8) and (9) are convex underestimators due to Quesada and Grossmann (1993, 1995), and Zamora and Grossmann (1997, 1998), respectively. The inequalities in (10) are proposed in this work, and have the properties given below in Theorem 1.

(d) $T(\Omega) = \{x, y, z) \in R^n \times R^{n_1} \times R^{n_2}$: (6)–(10) are satisfied with x^L, x^U as in $\Omega\}$. The feasible region, and the solution of problem (3) are denoted by $M(\Omega)$, and $(\hat{x}, \hat{y}, \hat{z})_\Omega$, respectively. We define *the approximation gap* $\varepsilon(\Omega)$ at a branch and bound node as

$$\varepsilon(\Omega) = \begin{cases} \infty & \text{if } OUB = \infty \\ -LB(\Omega) & \text{if } OUB = 0 \\ \dfrac{(OUB - LB(\Omega))}{|OUB|} & \text{otherwise} \end{cases}$$

where the *overall upper bound*, *OUB*, is the value of $f(x)$ at the best available feasible point $x \in D$; if no feasible point is available, then $OUB = \infty$.

THEOREM 1. *The function*

$$\gamma_{ij}^{lf}(x_i, x_j) = \text{Min}\left[\frac{1}{x_j^L x_j^U}(x_j^U x_i - x_i^L x_j + x_i^L x_j^L), \frac{1}{x_j^L x_j^U}(x_j^L x_i - x_i^U x_j + x_i^U x_j^U)\right]$$

is the concave envelope of the linear fractional term x_i/x_j *over the rectangle* $\Omega_{ij} = \{(x_i, x_j) : 0 \le x_i^L \le x_i \le x_i^U, 0 < x_j^L \le x_j \le x_j^U\}$. *Furthermore,* $\gamma_{ij}^{lf}(x_i, x_j) = x_i/x_j$ *at* $x_j = x_j^L$, *and* $x_j = x_j^U$

Proof. See the Appendix.

THEOREM 2. *The program in (3) is a convex underestimating problem for problem (1) over* $D \cap \Omega$.

Proof. Convexity of the program in (3) follows from the convexity properties of its objective function and constraints. The solution of problem (3) underestimates the solution of problem (1) since, by construction, $\hat{f}(x, y, z) \le f(x)$, and $D \cap \Omega \subset M(\Omega)$. □

REMARKS

1. The underestimating problem in (3) is a linear program if $LF^+ = \emptyset$.
2. During the execution of the branch and bound algorithm that is proposed in Section 5, problem (3) is solved initially over $M(\Omega_0)$ (root node of the branch and bound tree). If a better approximation is required, $M(\Omega_0)$ is refined by partitioning Ω_0 into two smaller hyperrectangles, Ω_{01} and Ω_{02}, and two children nodes are created with relaxed feasible regions given by $M(\Omega_{01})$ and $M(\Omega_{02})$.

3. The problem given in (3) might be regarded as a basic underestimating program for the general problem in (1). In some cases, however, it is possible to develop additional convex estimators that might strengthen the underestimating problem. See for instance the projections proposed by Quesada and Grossmann (1995), the reformulation-linearization technique by Sherali and Alameddine (1992), and the reformulation-convexification approach by Sherali and Tuncbilek (1995).

THE SET OF BRANCHING VARIABLES

A set of branching variables, characterized by the index set $BV(\Omega)$ defined below, is determined by considering the optimal solution $(\hat{x}, \hat{y}, \hat{z})_\Omega$ of the underestimating problem:

$$\begin{aligned} BV(\Omega) = \{i, j : {} & |\hat{y}_{ij} - \hat{x}_i\hat{x}_j| = \xi_\ell \text{ or } |\hat{z}_{ij} - \hat{x}_i/\hat{x}_j| = \xi_\ell \text{ or} \\ & g_i(\hat{x}_i) - \hat{g}_i(\hat{x}_i) = \xi_\ell \text{ or } g_{i,k}(\hat{x}_i) - \hat{g}_{i,k}(\hat{x}_i) = \xi_\ell, \\ & \text{for } i \in I, j \in J, k \in K, \ell \in L\} \end{aligned}$$

where, for a pre-specified number ℓ_n, $L = \{1, 2, \dots, \ell_n\}$, and ξ_1 is the magnitude of the largest approximation error for a nonconvex term in problem (1) evaluated at $(\hat{x}, \hat{y}, \hat{z})_\Omega$:

$$\xi_1 = \operatorname*{Max}_{i \in I, j \in J, k \in K} [|\hat{y}_{ij} - \hat{x}_i\hat{x}_j|, |\hat{z}_{ij} - \hat{x}_i/\hat{x}_j|, g_i(\hat{x}_i) - \hat{g}_i(\hat{x}_i), g_{i,k}(\hat{x}_i) - \hat{g}_{i,k}(\hat{x}_i)]$$

Similarly, we define $\xi_\ell < \xi_{\ell-1}$, with $\ell \in L\backslash\{1\}$, as the ℓ-th largest magnitude for an approximation error; for instance, $\xi_2 < \xi_1$ is the second largest magnitude for an approximation error. Note that in some cases it might be convenient to introduce weights in the determination of $BV(\Omega)$ in order to scale differences in the approximation errors, or to induce preferential branching schemes. This might be particularly useful in applications where specific information can be exploited by imposing an order of precedence to the set of complicating variables.

3. A contraction subproblem for the reduction of the search region

We define the *set of nonconvex or complicating variables* as the subset of variables that appear in the nonconvex functions or terms in problem (1). The complicating variables are characterized by the index set *CV* defined as follows:

$$\begin{aligned} CV = \{i, j : {} & i \in C_0 \cup C_k \text{ or } (i, j) \in BL_0 \cup BL_k \text{ or} \\ & (i, j) \in LF_0 \cup LF_k, i \in I, j \in J, k \in K\} \end{aligned}$$

To reduce the size of a hyperrectangle $\Omega = \{x : x^L \leq x \leq x^U\} \subset \Omega_0$, and therefore to improve the quality of the convex relaxation at the corresponding branch and bound node, we consider the following convex LP/NLP *contraction subproblem* for the complicating variables, $x_i, i \in CV$ (Maranas and Floudas 1997; Sourlas and Manousiouthakis 1995; Sourlas et al. 1992; Zamora and Grossmann 1996):

$$\begin{aligned}
&\operatorname*{Min\ or\ Max}_{(x,y,z)}\ x_i\\
&\text{subject to}\\
&\hat{f}(x,y,z) \le OUB \qquad\qquad (11)\\
&(x,y,z) \in M(\Omega) \subset R^n \times R^{n_1} \times R^{n_2}
\end{aligned}$$

The inequality $\hat{f}(x,y,z) \le OUB$ will be called *the OUB constraint*, and a solution to problem (11) will be denoted as $(\tilde{x},\tilde{y},\tilde{z})_\Omega$. The *optimization direction*, Min or Max, is selected depending upon which of the bounds, x_i^L or x_i^U, is to be contracted. We define a *contraction step* as the process of computing and updating a bound, x_i^L or x_i^U, through the solution of problem (11). The *performance* of a contraction step is quantified by the parameter SP defined as the fraction of the x_i-domain that can be discarded because the objective function can only take values above the current *OUB*:

$$\mathrm{SP} = \begin{cases} \left(\dfrac{\tilde{x}_i - x_i^L}{x_i^U - x_i^L}\right) & \text{if the } \textit{optimization direction} = \text{Min}\\[2ex] \left(\dfrac{x_i^U - \tilde{x}_i}{x_i^U - x_i^L}\right) & \text{if the } \textit{optimization direction} = \text{Max}\end{cases}$$

where $\tilde{x}_i$ is the minimum (maximum) value of the variable x_i, obtained by solving (11) with a Min (Max) direction. A contraction step is said to be *successful* if the step performance parameter takes a value higher than or equal to a minimum prespecified value $\mathrm{SP_{min}}$. The contraction step is *unsuccessful* otherwise.

REMARKS

1. The value of *OUB* is set to a large positive number in problem (11) if no feasible point for problem (1) is available when performing a contraction step. Also note that, according to the problem statement given in Section 1, it suffices to set the r.h.s. of the *OUB* constraint equal to $OUB - \varepsilon_t|OUB|$ (if $OUB \neq 0$), or $-\varepsilon_t$ (if $OUB = 0$). To keep the presentation simple, this is left as shown in (11).
2. The size of the relaxed feasible region $M(\Omega)$ is reduced after a contraction step if $\mathrm{SP} > 0$ is obtained. Hence, the iterative solution of problem (11), with contraction performed for different variables and directions, may significantly reduce the size of the search region, and improve the quality of the underestimating problems decreasing, and in some cases eliminating, the need for branching.
3. Infeasibility of problem (11) indicates that the feasible region of the convex underestimating problem has become empty, or that the relaxed objective function can not take values below the current *OUB*. In either case, the branch and

bound node can be safely discarded, since there is no feasible point for problem (1) over $D \cap \Omega$ with an objective function value below OUB.

4. Although the contraction subproblem is used in this work to contract only the bounds of the complicating variables, it can also be used to contract the bounds of any of the other x_i, y_{ij}, or z_{ij} variables by applying the objective function in (11) to these variables.

A LOWER BOUND ESTIMATE OVER THE REDUCED FEASIBLE REGION

A lower bound $LB(\Omega)$ for the global optimum solution of problem (1) over $D \cap \Omega$ can be computed by solving the lower bounding problem (3). If a successful reduction of the hyperrectangle Ω is achieved through the performance of a contraction step for a variable x_i, then the convex underestimating problem can be resolved over the, now smaller, region $M(\Omega)$ to compute a potentially tighter value for $LB(\Omega)$. A drawback of this strategy is that it demands extra computational effort without necessarily providing additional useful information. Therefore, we propose to make use of Theorems 3 and 4 given below to try to determine an improved lower bound without additional computational cost.

THEOREM 3. *Consider the following alternative formulation of problem (11) for the contraction of the lower bound x_i^L:*

$$\underset{(x,y,z)}{\text{Min}}\ x_i$$

subject to

$$\begin{aligned} & G_1(x, y, z) = \hat{f}(x, y, z) - OUB \leq 0 \\ & G_k(x, y, z) \leq 0 \quad k = 2, 3, \ldots, p_c \\ & (x, y, z) \in R^n \times R^{n_1} \times R^{n_2} \end{aligned} \tag{12}$$

in which the constraints that define $M(\Omega)$ in (11) have been arranged to have:

$$M(\Omega) = \{(x, y, z) \in R^n \times R^{n_1} \times R^{n_2} : G_k(x, y, z) \leq 0, \quad k = 2, 3, \ldots, p_c\}$$

Assume that problem (12) has a solution $(\tilde{x}, \tilde{y}, \tilde{z})_\Omega$ that satisfies the Karush–Kuhn–Tucker conditions with optimal Lagrange multipliers given by $\tilde{\lambda} = (\tilde{\lambda}_1, \tilde{\lambda}_2, \tilde{\lambda}_3, \ldots, \tilde{\lambda}_{p_c})^T$. Let $\tilde{\lambda}_1$ be the Lagrange multiplier associated with the OUB constraint, $G_1(x, y, z)$. Then, the following lower bound for $\hat{f}(x, y, z)$ is valid if $\tilde{\lambda}_1 > 0$:

$$\hat{f}(x, y, z) \geq OUB - (x_i^U - \tilde{x}_i)/\tilde{\lambda}_1 \tag{13}$$

Proof. See the Appendix.

COROLLARY 1. *Assume that a contraction step is performed, and the value of a variable x_i, $i \in CV$, is minimized by solving problem (12). Then, the corresponding* *branch and bound node can be discarded if a solution* $(\tilde{x}, \tilde{y}, \tilde{z})_\Omega$ *with* $\tilde{x}_i = x_i^U$*, and a strictly positive Lagrange multiplier for the contraction constraint are obtained.*

Proof. This result is a direct consequence of Theorem 3.

THEOREM 4. *Consider the following alternative formulation of problem (11) for the contraction of the upper bound* x_i^U*:*

$$\min_{(x,y,z)} -x_i$$

subject to

$$\begin{aligned} &G_1(x, y, z) = \hat{f}(x, y, z) - OUB \leq 0 \\ &G_k(x, y, z) \leq 0 \quad k = 2, 3, \ldots, p_c \\ &(x, y, z) \in R^n \times R^{n_1} \times R^{n_2} \end{aligned} \tag{14}$$

in which the constraints that define $M(\Omega)$ *in (11) have been arranged to have:*

$$M(\Omega) = \{(x, y, z) \in R^n \times R^{n_1} \times R^{n_2} : G_k(x, y, z) \leq 0, \quad k = 2, 3, \ldots, p_c\}$$

Assume that problem (14) has a solution $(\tilde{x}, \tilde{y}, \tilde{z})_\Omega$ *that satisfies the Karush–Kuhn–Tucker conditions with optimal Lagrange multipliers given by* $\tilde{\lambda} = (\tilde{\lambda}_1, \tilde{\lambda}_2, \tilde{\lambda}_3, \ldots, \tilde{\lambda}_{p_c})^T$*. Let* $\tilde{\lambda}_1$ *be the Lagrange multiplier associated with the OUB constraint,* $G_1(x, y, z)$*. Then, the following lower bound for* $\hat{f}(x, y, z)$ *is valid if* $\tilde{\lambda}_1 > 0$*:*

$$\hat{f}(x, y, z) = OUB - (\tilde{x}_i - x_i^L)/\tilde{\lambda}_1 \tag{15}$$

Proof. Similar to the proof of Theorem 3.

COROLLARY 2. *Assume that a contraction step is performed, and the value of a variable* x_i*,* $i \in CV$ *is maximized by solving problem (14). Then, the corresponding branch and bound node can be discarded if a solution* $(\tilde{x}, \tilde{y}, \tilde{z})_\Omega$ *with* $\tilde{x}_i = x_i^L$*, and a strictly positive Lagrange multiplier for the contraction constraint are obtained.*

Proof. This result is a direct consequence of Theorem 4.

ADDITIONAL MULTIPLIER BASED BOUNDING INEQUALITIES

The following bounding inequalities for the variables involved in problem (1) can also be obtained from the solution of contraction subproblems for a variable x_i.

$$x_j \leq x_j^L + (x_i^U - x_i^L)/\tilde{\lambda}_j \tag{16}$$

for the case when the constraint $x_j^L - x_j \leq 0,\ j \in J$, is active at the solution of the contraction step, and

$$x_j \geq x_j^U - (x_i^U - x_i^L)/\tilde{\lambda}_j \tag{17}$$

for the case when the constraint $x_j - x_j^U \leq 0,\ j \in J$, is active. In both cases, a Lagrange multiplier $\tilde{\lambda}_j > 0$ is required for the application of the bounding inequalities.

REMARK. The inequalities in (16) and (17) are analogous to some of the inequalities presented by Ryoo and Sahinidis (1995, 1996). Note, however, that the inequalities developed by Ryoo and Sahinidis involve the solution of the convex underestimating program for the nonconvex problem as opposed to the solution of the contraction subproblem that is utilized in this paper.

4. The contraction operation

As mentioned before, the solution of the contraction subproblem, for different variables and directions, may significantly reduce the size of the search region, and improve the quality of the underestimating problems decreasing, and in some cases, eliminating the need for branching. A strategy for sequencing the contraction steps at a given branch and bound node is presented in this section within a *contraction operation* that has finite termination.

THE FOCAL POINT

We define the *focal point* at a branch and bound node as the point $x^b \in R^n$ that provides the best known upper bound for problem (1) over the corresponding subset, $D \cap \Omega$, of the feasible region. If no such point is available, then the focal point is given by the x component of the solution $(\hat{x}, \hat{y}, \hat{z})_\Omega$ of the convex underestimating problem over $M(\Omega)$.

Given a positive parameter ε_x, a focal point is said to be ε_x-close to the boundary at $x_i^L > 0$ if $x_i^b \leq x_i^L(1+\varepsilon_x)$; it is ε_x-close to $x_i^L = 0$ if $x_i^b \leq \varepsilon_x$. Similarly, a focal point is said to be ε_x-close to the boundary at $x_i^U > 0$ if $x_i^b \geq x_i^U(1-\varepsilon_x)$; it is ε_x-close to $x_i^U = 0$ if $x_i^b = 0$.

The *lower focal distance*, $\Delta_i^{f,L}(\Omega),\ i \in CV$, is the relative distance from the focal point to the boundary at x_i^L defined as follows:

$$\Delta_i^{f,L}(\Omega) = \frac{x_i^b - x_i^L}{x_i^{U,in} - x_i^{L,in}}$$

Likewise, we define the *upper focal distance*, $\Delta_i^{f,U}(\Omega),\ i \in CV$, as

$$\Delta_i^{f,U}(\Omega) = \frac{x_i^U - x_i^b}{x_i^{U,in} - x_i^{L,in}}$$

In this way, $\Delta_i^{f,L}(\Omega)$ ($\Delta_i^{f,U}(\Omega)$) represents the fraction of the initial x_i-domain that remains on the left (right) of the focal point at the current node. Depending on the position of the focal point or the outcome of a contraction step, a focal distance can be labeled either as *marked* or *unmarked*.

Contraction operation

Step C1. Specify the minimum value, $SP_{\min}$, for a successful contraction step. Specify the minimum value, SP_r, for the application of *feasibility based reduction techniques* (Step C8).
Specify the parameter ε_x, which determines the ε_x-closeness property.
Specify the maximum number of contraction steps to be performed, $NC_{\max}$.
Specify the maximum number for unsuccessful contraction steps, $NUC_{\max}$.
Specify the index set $BLUE_0 \subseteq CV$ that determines the subset of complicating variables over which contraction is to be performed (*contraction variables*).
Initialize the control sets $BLUE := BLUE_0$, and $RED := \emptyset$.
Specify the maximum fraction of *contraction variables*, F_{CV}, allowed in the *RED* set.
Initialize counters NC = 0, NUC = 0.

Step C2. For $i \in BLUE$, Compute $\Delta_i^{f,L}(\Omega)$, and $\Delta_i^{f,U}(\Omega)$. Label all these focal distances as unmarked.
If x^b is ε_x-close to x_i^L, then mark $\Delta_i^{f,L}(\Omega)$. If x^b is ε_x-close to x_i^U, then mark $\Delta_i^{f,U}(\Omega)$.

Step C3. Determine

$$\Delta_{\max}^{f}(\Omega) = \underset{i\in BLUE}{\mathrm{Max}}[\Delta_i^{f,L}(\Omega),\ \Delta_i^{f,U}(\Omega)]$$
$$\text{for } \Delta_i^{f,L}(\Omega),\ \Delta_i^{f,U}(\Omega),\ \text{unmarked}$$

Then, select a complicating variable x_t, with $t \in BLUE$, such that

$$\Delta_t^{f,L}(\Omega) \text{ is unmarked and } \Delta_t^{f,L}(\Omega) = \Delta_{\max}^{f}(\Omega)$$

or

$$\Delta_t^{f,U}(\Omega) \text{ is unmarked and } \Delta_t^{f,U}(\Omega) = \Delta_{\max}^{f}(\Omega)$$

Step C4. If $\Delta_t^{f,L}(\Omega)$ is unmarked and $\Delta_t^{f,L}(\Omega) = \Delta_{\max}^{f}(\Omega)$ perform a contraction step with a Min direction to contract x_t^L. Otherwise, perform a contraction step with a Max direction to contract x_t^U. Set $NC := NC + 1$.

Step C5. If the contraction subproblem in Step C4 is feasible, then:
Determine SP.
If x_t^L was contracted and $SP < SP_{\min}$, then mark $\Delta_t^{f,L}(\Omega)$, and set $NUC := NUC + 1$.
If x_t^L was contracted and $x_t^b < x_t^L$, then set $x_t^b := x_t^L$.
If x_t^U was contracted and $SP < SP_{\min}$, then mark $\Delta_t^{f,U}(\Omega)$, and set $NUC := NUC + 1$.
If x_t^U was contracted and $x_t^b > x_t^U$, then set $x_t^b := x_t^U$.
Use the inequality given in (13) or (15) to try to tighten the value of the lower bound $LB(\Omega)$.
Compute $\varepsilon(\Omega)$.

Step C6. If the contraction subproblem in Step C4 is infeasible or $\varepsilon(\Omega) \leq \varepsilon_t$, then terminate the *contraction operation*.

Step C7. If possible, use the inequalities in (16) and (17) to try to contract the bounds of the x variables.

Step C8. (Optional). If $SP \geq SP_r$, utilize *feasibility based reduction techniques* developed for problem (1) to try to contract the bounds of the x variables. If crossing of these bounds occurs at any point, then terminate the *contraction operation*.

Step C9. Let $MV^L \subseteq BLUE$ be the index subset that characterizes the variables whose lower bound were contracted during the execution of Steps C4, C7, or C8. Similarly, let $MV^U \subseteq BLUE$ be the index subset that characterizes the variables whose upper bound were contracted during the execution of Steps C4, C7, or C8.
For $i \in MV^L$, mark $\Delta_i^{f,L}(\Omega)$ if x^b is ε_x-close to x_i^L, else recompute $\Delta_i^{f,L}(\Omega)$.
For $i \in MV^U$, mark $\Delta_i^{f,U}(\Omega)$ if x^b is ε_x-close to x_i^U, else recompute $\Delta_i^{f,U}(\Omega)$.
For all $i \in MV^L \cup MV^U$, with $\Delta_i^{f,L}(\Omega)$ and $\Delta_i^{f,U}(\Omega)$ marked, set $BLUE = BLUE \backslash \{i\}$, and $RED = RED \cup \{i\}$.

Step C10. Terminate the *contraction operation* if any of the following conditions is met: (i) $|RED| \geq F_{CV}|BLUE_0|$; (ii) $NC = NC_{\max}$; (iii) $NUC = NUC_{\max}$. Otherwise, return to Step C3.

REMARK. By *feasibility based reduction techniques* (Step C8) we mean finite contraction techniques that manipulate, and reduce problem constraints deriving univariate bounding functions that can be used iteratively to eliminate portions of the domain in which the nonconvex problem is infeasible. These techniques exploit convexity, concavity, or monotonicity properties present in a problem, and frequently utilize monotonicity principles, or interval arithmetic (see e.g. Amarger et al. 1992; Hamed and McCormick 1993; Hansen et al. 1989 1991; Lodwick 1992;

Ryoo and Sahinidis 1995; Sherali and Tuncbilek 1995; Zamora and Grossmann 1998).

5. The branch and contract algorithm for continuous global optimization

Initialization

Set *OUB* $:= \infty$ and $x^b := (x^{L,in} + x^{U,in})/2$.

Phase 1 (Heuristic NLP search, optional)

Attempt to solve problem (1) starting from a small number of initial points. If feasible points are located, then use the best found local minimum to define the initial incumbent solution x^*, and update *OUB*. Set the focal point $x^b := x^*$.

Phase 2 (Global NLP search)

Step 1. Specify the parameter ℓ_n for the determination of the set of branching variables.
Specify, F_b, the minimum fraction of domain to be assigned to a children node.
Specify the maximum approximation gap, F_ε, under which *the contraction operation* is to be performed.
Set $LB(\Omega_0) := -\infty$.

Step 2. (Optional). Attempt to reduce Ω_0, and obtain a finite lower bound for $\hat{f}(x, y, z)$ with (13) or (15) by performing *the contraction operation* with $BLUE_0 := CV$ and $F_{CV} = 1$. If termination occurs at Step C10, then continue to Step 3. On the other hand, if termination occurs at Step C6 or C8, then Stop. If $OUB = \infty$, then problem (1) is infeasible. Otherwise, x^* is a global minimizer.

Step 3. Initialize the list of open nodes $\mathsf{ON} = \{0, LB(\Omega_0)\}$.

Step 4. If $\mathsf{ON} = \emptyset$, then stop. If $OUB = \infty$, then problem (1) is infeasible. Otherwise, x^* is a global minimizer.

Step 5. Determine the overall lower bound *OLB:*

$$OLB = \operatorname*{Min}_r [LB(\Omega_r)] \quad \text{for } (r, LB(\Omega_r)) \in \mathsf{ON}$$

Compute the *overall approximation gap* ε:

$$\varepsilon = \begin{cases} \infty & \text{if } OUB = \infty \\ -OLB & \text{if } OUB = 0 \\ \dfrac{(OUB - OLB)}{|OUB|} & \text{otherwise} \end{cases}$$

If $\varepsilon \leq \varepsilon_t$, then stop. In this case, x^* is a global minimizer of problem (1).

Step 6. Select a node s with $LB(\Omega_s) = OLB$ and $\Omega_s = \{x \in R^n : x^L \leq x \leq x^U\}$. Set ON := ON$\setminus\{s, LB(\Omega_s)\}$.

Step 7. (Optional). Apply *feasibility based reduction techniques* at the selected node to try to contract the bounds of the variables. If crossing of these bounds occurs at any point, then go to Step 4.

Step 8. Compute $LB(\Omega_s)$ by solving the lower bounding problem (3) over $M(\Omega_s)$. If the problem is infeasible, then go to Step 4. Else, calculate $\varepsilon(\Omega_s)$. If $\varepsilon(\Omega_s) \leq \varepsilon_t$, then go to Step 4. Else, determine the set of branching variables *BV*, and set $x^b := \hat{x}$.

Step 9. Set $UB(\Omega_s) := \infty$. Starting from $\hat{x}$, attempt to solve problem (1) over $D \cap \Omega_s$ with a local NLP optimizer. If no feasible point is found, then go to Step 11. Else, if a feasible solution x^s with an upper bound $UB(\Omega_s)$ is found, then set $x^b := x^s$.

Step 10. If $UB(\Omega_s) < OUB$, then (i) Set $x^* := x^s$; (ii) Update $OUB := UB(\Omega_s)$; (iii) Delete from ON all nodes r such that $LB(\Omega_r) \geq OUB$; (iv) Calculate $\varepsilon(\Omega_s)$, and (v) If $\varepsilon(\Omega_s) \leq \varepsilon_t$, then go to Step 4.

Step 11. If $\varepsilon(\Omega_s) \leq F_\varepsilon$, then execute the *contraction operation* at the current node. If the *contraction operation* terminates at Step C6 or C8, then go to Step 4.

Step 12. Select a variable x_b, with $b \in BV(\Omega)$, such that

$$\frac{x_b^U - x_b^L}{x_b^{U,in} - x_b^{L,in}} \geq \frac{x_i^U - x_i^L}{x_i^{U,in} - x_i^{L,in}} \quad \forall i \in BV(\Omega)$$

Create two new nodes, $s1$ and $s2$. Set $LB(\Omega_{s1}) := LB(\Omega_s)$, $LB(\Omega_{s2}) := LB(\Omega_s)$, and ON := ON $\cup \{(s1, LB(\Omega_{s1})), (s2, LB(\Omega_{s2}))\}$. Ω_{s1} and Ω_{s2} are defined as follows:

$$\text{If} \quad \text{Min}\left[\frac{x_b^b - x_b^L}{x_b^U - x_b^L}, \frac{x_b^U - x_b^b}{x_b^U - x_b^L}\right] \geq F_b$$

then $\Omega_{s1} := \Omega_s \cap \{x \in R^n : x_b \leq x_b^b\}$ and $\Omega_{s2} := \Omega_s \cap \{x \in R^n : x_b \geq x_b^b\}$. Otherwise $\Omega_{s1} := \Omega_s \cap \{x \in R^n : x_b \leq (x_b^L + x_b^U)/2\}$ and $\Omega_{s2} := \Omega_s \cap \{x \in R^n : x_b \geq (x_b^L + x_b^U)/2\}$. Go to Step 5.

REMARKS

1. Phase 1, and Steps 2 and 7 above are optional in the sense that their elimination does not compromise the convergence properties of the algorithm.
2. The *contraction operation* is only executed in Step 11 if the approximation gap at the branch and bound node takes a value less than or equal to the value of the control parameter F_ε. This measure prevents wasteful computations that may occur when contraction steps are performed under very poor convex relaxations. In other words, the algorithm will selectively perform the *contraction*

operation in branches of the branch and bound tree in which a relatively good convex approximation has already been obtained. The algorithm goes to a noncontraction mode in other sections of the tree allowing the execution of more branching to improve the quality of the approximation.

3. The parameter F_b in the algorithm takes always a value greater than 0.05. As indicated in Step 12, branching occurs at the focal point if the smallest of the children nodes gets at least a fraction F_b of the x_b-domain of the father node. Otherwise the children nodes are created by bisection.
4. The convergence of the *branch and contract algorithm* is guaranteed by the following properties (see also Theorem IV.3 in Horst and Tuy 1993):
   (a) Any partition element in ON can be further refined at any point in the search.
   (b) When evaluated at the points determined by the bounds of the complicating variables, the bounding estimators in (4)–(10) are exact for each of the corresponding nonconvex terms in problem (1). Therefore, the lower bound predicted by problem (3) over the limit set of a decreasing sequence of partition sets, created by subdividing the subspace of complicating variables, is exactly the minimum of $f(x)$ over the limit set.
   (c) The node selection rule of the algorithm is bound improving.
   (d) The *contraction operation* and the *feasibility based reduction techniques* used in the algorithm are finite.
5. The extension of the proposed *branch and contract algorithm* for MINLP problems can be found in Zamora (1997).

6. Illustrative examples

Five global optimization problems are solved in this section to illustrate the performance of some of the algorithmic strategies embedded in the branch and contract algorithm presented in the previous section. Strategies S1 to S4 in Table 1 are determined by the inclusion or exclusion of each of the four optional features of the general algorithm. Note that *feasibility based reduction strategies* (Step 7, and Step C8) are only included in the strategies S2, and S4. The heuristic local search (Phase 1), and the initial contraction of the feasible region (Step 2) are only executed in the strategies S1 and S2. The strategy S5, introduced for comparison in Examples 1 and 5, excludes the four optional features of the branch and contract algorithm, as well as the *contraction operation* of Step 11. Therefore, S5 represents a simple version of a branch and bound algorithm which excludes both *contraction* and *feasibility based reduction techniques*.

For the sake of illustration, the solution strategies described above are applied to the Examples in the following manner:

(i) S1, S2 and S5 are applied to Example 1.
(ii) S1 is applied to Examples 2 and 3.
(iii) S3 and S4 are applied to Example 4.

Table 1. Algorithmic strategies applied to the illustrative examples.

Strategy	Phase 1	Step 2	Step 7	Step C8	Step 11
S1	*	*			*
S2	*	*	*	*	*
S3					*
S4			*	*	*
S5					

(iv) S1, S3, and S5 are applied to Example 5.

In all cases the solution is required to satisfy an $\varepsilon_t = 0.5 \times 10^{-6}$ and $BLUE_0 := CV$ is specified. Where needed, the following parameters are used: $\ell_n = 1$, $F_b = 0.20$, $F_\varepsilon = 5.0$, $F_{CV} = 0.50$, $SP_{\min} = 0.20$, $SP_r = 0.01$, $\varepsilon_x = 0.5e^{-8}$, $NC_{\max} = 1000$, and $NUC_{\max} = 1000$. Large values for $NC_{\max}$ and $NUC_{\max}$ are set to force termination with the criterion $|RED| \geq F_{CV}|BLUE|$ in Step C10 of the *contraction operation*. A summary of results is given later in Table 7. All computations were performed on an IBM RS-6000/530 workstation with a non-optimized GAMS/MINOS (Brooke et al. 1992) implementation of the algorithm.

EXAMPLE 1.

$$\underset{x}{\text{Minimize}} \;\; f(x) = x_1^2 + 2x_2^2 - 50x_1 - 80x_2 + 250$$

subject to

$$x_1x_2 + x_1 - 50 = 0 \tag{E1.1}$$

$$x \in \Omega_0$$

$$\Omega_0 = \{x \in R^2 : 0 \leq x_1 \leq 20, 0 \leq x_2 \leq 20\}$$

The convex underestimating problem is given by

$$\underset{x,y_{12}}{\text{Minimize}} \;\; \hat{f}(x) = x_1^2 + 2x_2^2 - 50x_1 - 80x_2 + 250$$

subject to

$$\begin{aligned}
&y_{12} + x_1 - 50 = 0\\
&y_{12} \geq x_2^L x_1 + x_1^L x_2 - x_1^L x_2^L\\
&y_{12} \geq x_2^U x_1 + x_1^U x_2 - x_1^U x_2^U\\
&y_{12} \leq x_2^L x_1 + x_1^U x_2 - x_1^U x_2^L\\
&y_{12} \leq x_2^U x_1 + x_1^L x_2 - x_1^L x_2^U\\
&x \in \Omega \subseteq \Omega_0, \quad \Omega = \{x \in R^2 : x^L \leq x \leq x^U\},\\
&y_{12} \in R_+^1
\end{aligned} \tag{E1.2}$$

Table 2. Computational results for Example 1, Strategy S1, Step 2.

Iter	Dir	Var	SP	$LB(\Omega_0)$	$\varepsilon(\Omega_0)$
1	min	x_2	0.26335	−1294.379	0.94021
2	max	x_1	0.60109	−1294.379	0.94021
3	min	x_2	0.47124	−793.5140	0.18944
4	min	x_2	0.30995	−782.7225	0.17326
5	max	x_1	0.59889	−782.7225	0.17326
6	min	x_2	0.49271	−678.4248	0.16927e^{-1}
7	min	x_1	0.77641	−678.4248	0.16927e^{-1}
8	max	x_2	0.43287	−669.2815	0.32221e^{-2}
9	min	x_2	0.85800	−668.0890	0.14346e^{-2}
10	max	x_1	0.86047	−667.7139	0.87235e^{-3}
11	min	x_2	0.46009	−667.2656	0.20033e^{-3}
12	max	x_2	0.52059	−667.1960	0.96043e^{-4}
13	max	x_2	0.28894	−667.1585	0.39809e^{-4}
14	min	x_2	0.26927	−667.1457	0.20619e^{-4}
15	min	x_1	0.72352	−667.1457	0.20619e^{-4}
16	min	x_2	0.34435	−667.1353	0.50298e^{-5}
17	max	x_2	0.60699	−667.1327	0.11226e^{-5}
18	max	x_1	0.84228	−667.1327	0.11226e^{-5}
19	min	x_2	0.51920	−667.1321	0.20781e^{-6}

The contraction subproblem in this case is

$$
\begin{aligned}
&\underset{x,y_{12}}{\text{Min or Max}}\ x_i\\
&\text{subject to}\\
&\hat{f}(x) = x_1^2 + 2x_2^2 - 50x_1 - 80x_2 + 250 \le OUB\\
&y_{12} + x_1 - 50 = 0\\
&y_{12} \ge x_2^L x_1 + x_1^L x_2 - x_1^L x_2^L\\
&y_{12} \ge x_2^U x_1 + x_1^U x_2 - x_1^U x_2^U\\
&y_{12} \le x_2^L x_1 + x_1^U x_2 - x_1^U x_2^L\\
&y_{12} \le x_2^U x_1 + x_1^L x_2 - x_1^L x_2^U\\
&x \in \Omega \subseteq \Omega_0, \quad \Omega = \{x \in R^2 : x^L \le x \le x^U\},\\
&y_{12} \in R_+^1, \quad i \in CV = \{1, 2\}
\end{aligned}
\tag{E1.3}
$$

Strategy S1

Phase 1

The following two solutions are found for the nonconvex problem in (E1.1): $x^1 = (2.56028691, 18.5290613)$ and $x^2 = (20.0000000, 1.50000000)$, with $f(x^1) = -667.131955$ and $f(x^2) = -465.500000$, respectively. Thus, we set $OUB := -667.131955$, and $x^* = x^b = (2.56028691, 18.5290613)$.

Phase 2

Table 2 shows the details of the execution of the *contraction operation* in Step 2 of the algorithm; each iteration represents the execution of a contraction step with the optimization direction, and objective function variable given on columns 2 and 3, respectively. As can be seen on the fourth column of Table 2, the fraction of the domain that is eliminated in this example after the execution of a contraction step ranges from 0.26335 to 0.86047. The lower bound obtained for $\hat{f}(x)$ by using the results presented in Theorems 3 and 4, is shown on the fifth column, and the respective approximation gap $\varepsilon(\Omega_0)$ is given on the last column. The execution of the *contraction operation* is terminated at Step C6 after 19 iterations, when the required precision ($\varepsilon_t = 0.5e^{-6}$) for the global optimum is achieved. Thus, $x^* = (2.56028691, 18.5290613)$ is proved to be a global minimizer with an optimal objective function value $f(x^*) = -667.131955$. Note that for the solution of this problem no underestimating problem is solved, and no branching is required.

EXAMPLE 1 (*continued*)

Strategy S2

The following four bounding inequalities for x_1 and x_2 can be easily developed from the only constraint in (E1.1):

$$\begin{aligned} x_1 &\geq \frac{50}{x_2^U + 1} \\ x_1 &\leq \frac{50}{x_2^L + 1} \\ x_2 &\geq \frac{50}{x_1^U} - 1 \\ x_2 &\leq \frac{50}{x_1^L} - 1 \end{aligned} \tag{E1.4}$$

These inequalities are used recursively in the optional step, Step C8, of the *contraction operation* to further tighten the bounds of the problem variables after a new contracted bound is obtained by the execution of a contraction step (Step C4).

Table 3. Computational results for Example 1, Strategy S2, Step 2.

Iter	Dir	Var	SP	$LB(\Omega_0)$	$\varepsilon(\Omega_0)$
1	min	x_2	0.26335	−1294.379	0.94021
2	min	x_2	0.47124	−793.5140	0.18944
3	min	x_2	0.55312	−688.0112	0.31297e^{-1}
4	min	x_2	0.36768	−673.1595	0.90350e^{-2}
5	max	x_2	0.46521	−669.0161	0.28243e^{-2}
6	min	x_2	0.41124	−667.7574	0.93752e^{-3}
7	max	x_2	0.43863	−667.3335	0.30204e^{-3}
8	min	x_2	0.42471	−667.1980	0.98962e^{-4}
9	max	x_2	0.43127	−667.1534	0.32143e^{-4}
10	min	x_2	0.42844	−667.1390	0.10488e^{-4}
11	max	x_2	0.42940	−667.1342	0.34142e^{-5}
12	min	x_2	0.42931	−667.1327	0.11126e^{-5}
13	max	x_2	0.42905	−667.1322	0.36244e^{-6}

This *feasibility based reduction* of Step C8 is stopped when the largest reduction of the bounds in the recursive strategy goes below a pre-specified small tolerance.

The execution of the Phase 1 of the algorithm is similar to the one shown for Strategy S1. Table 3 shows the results obtained for the global optimization of Example 1 when Step 2 in Strategy S2 is applied. The number of iterations required to prove that $x^* = (2.56028691, 18.5290613)$ is a global optimum decreases in this case from 19 (Strategy S1) to 13. A very interesting result is that the contraction steps are only performed for the variable x_2. Such a *reduced space search* is more effective, and arises here due to the combination of *contraction* and *feasibility based reduction*.

Strategy S5

To achieve the specified precision for the solution of Example 1, the solution strategy S5 requires the analysis of 39 branch and bound nodes. The upper bounding step of the algorithm is performed in 22 of these nodes.

Table 4. Computational results for Example 2, Strategy S1, Step 2.

Iter	Dir	Var	SP	$LB(\Omega_0)$	$\varepsilon(\Omega_0)$
1	max	x_3	0.27273	−800	1.00000
2	max	x_{10}	0.38889	−800	1.00000
3	max	x_3	1.00000	−400	0.00000

EXAMPLE 2 (Haverly 1978).

$$\underset{x}{\text{Minimize}}\ \ f(x) = 6x_1 + 16x_2 - 9x_5 + 10x_6 - 15x_9$$

subject to

$$\begin{aligned}
x_1 + x_2 - x_3 - x_4 &= 0\\
x_3 - x_5 + x_7 &= 0\\
x_4 + x_8 - x_9 &= 0\\
-x_6 + x_7 + x_8 &= 0\\
-2.5x_5 + 2x_7 + x_3x_{10} &\le 0\\
2x_8 - 1.5x_9 + x_4x_{10} &\le 0\\
3x_1 + x_2 - x_3x_{10} - x_4x_{10} &= 0\\
x \in \Omega_0 &
\end{aligned}$$

where

$$\begin{aligned}
\Omega_0 = \{x \in R^{10} : & 0 \le x_1 \le 300,\ 0 \le x_2 \le 300, 0 \le x_3 \le 100, 0 \le x_4 \le 200,\\
& 0 \le x_5 \le 100,\ 0 \le x_6 \le 300, 0 \le x_7 \le 100, 0 \le x_8 \le 200,\\
& 0 \le x_9 \le 200,\ 1 \le x_{10} \le 3\}
\end{aligned}$$

Strategy S1

Phase 1

The following solution is found: $x^1 = \{0, 100, 0, 100, 0, 100, 0, 100, 200, 1\}$, with $f(x^1) = -400$. Thus, we set $OUB := -400$ and $x^* = x^b = x^1$.

Phase 2

Table 4 shows the results obtained by executing the *contraction operation* in Step 2 of the algorithm, which only requires three iterations to prove that $x^* = \{0, 100, 0, 100, 0, 100, 0, 100, 200, 1\}$ is a global minimizer with an optimal objective function value $f(x^*) = -400$. Note that in the third iteration $SP = 1$ is obtained when

x_3^U is contracted to a value $x_3^U = x_3^L$ (see also the Corollary 2). Neither the solution of underestimating problems, nor branching are required to solve this problem.

EXAMPLE 3 (Stephanopoulos and Westerberg 1975).

$$
\begin{aligned}
&\underset{x}{\text{Minimize}}\ \ f(x) = x_1^{0.6} + x_2^{0.6} + x_3^{0.4} - 4x_3 + 2x_4 + 5x_5 - x_6 \\
&\text{subject to} \\
&\quad -3x_1 + x_2 - 3x_4 = 0 \\
&\quad -2x_2 + x_3 - 2x_5 = 0 \\
&\quad 4x_4 - x_6 = 0 \\
&\quad x_1 + 2x_4 \le 4 \\
&\quad x_2 + x_5 \le 4 \\
&\quad x_3 + x_6 \le 6 \\
&\quad x \in \Omega_0
\end{aligned}
\tag{E3.1}
$$

where

$$
\Omega_0 = \{x \in R^6 : 0 \le x_1 \le 3,\ 0 \le x_2 \le 4, 0 \le x_3 \le 4, 0 \le x_4 \le 2,\ 0 \le x_5 \le 2,\ 0 \le x_6 \le 6\}
$$

Strategy S1

Phase 1

The following solution is found for the problem in (E3.1): $x^1 = \{0.166666667, 2.00000000, 4.00000000, 0.500000000, 0.000000000, 2.00000000\}$, with $f(x^1) = -13.4019036$. Thus, we set $OUB := -13.4019036$ and $x^* = x^b = x^1$.

Phase 2

The execution of the *contraction operation* in Step 2 proves that the point x^1 is a global minimizer. Only 11 contraction steps are performed, and an average SP = 0.857 is obtained. In other words, the *contraction operation* discards in this case an average 85.7% of the box domain after the execution of each contraction step.

EXAMPLE 4 (Falk and Palocsay 1992)

$$
\begin{aligned}
&\underset{x}{\text{Maximize}}\ \ f_1(x) = \frac{37x_1 + 73x_2 + 13}{13x_1 + 13x_2 + 13} + \frac{63x_1 - 18x_2 + 39}{13x_1 + 26x_2 + 13} \\
&\text{subject to} \\
&\quad 5x_1 - 3x_2 = 3 \\
&\quad 1.5 \le x_1 \le 3
\end{aligned}
\tag{E4.1}
$$

Besides illustrating the application of Strategies S3 and S4, this example illustrates the effect of different formulations for the solution of a given problem. The problem reformulation 4A that is given below trades the two complicating variables problem in (E4.1) for a problem with four complicating variables, increasing the dimension of the branch and bound search space from 2 to 4. The reformulation 4A also changes the complicating variables of the original problem, (x_1, x_2), for a new group of complicating variables given by (x_3, x_4, x_5, x_6). On the other hand, the second problem reformulation that is presented, reformulation 4B, changes neither the group of complicating variables, nor the dimension of the search space. As will be seen, keeping the dimension of the search space small allows one to expedite the solution of the problem in (E4.1).

Problem reformulation 4A

Consider the solution of the following formulation to solve the problem in (E4.1):

$$
\begin{aligned}
&\underset{x}{\text{Minimize}} \;\; f(x) = -\frac{x_3}{x_4} - \frac{x_5}{x_6} \\
&\text{subject to} \\
&\qquad 5x_1 - 3x_2 - 3 = 0 \\
&\qquad x_3 - 37x_1 - 73x_2 - 13 = 0 \\
&\qquad x_4 - 13x_1 - 13x_2 - 13 = 0 \\
&\qquad x_5 - 63x_1 + 18x_2 - 39 = 0 \\
&\qquad x_6 - 13x_1 - 26x_2 - 13 = 0 \\
&\qquad x \in \Omega_0
\end{aligned}
\tag{E4.2}
$$

where

$$
\begin{aligned}
\Omega_0 = \{x \in R^6 :& 1.5 \le x_1 \le 3,\;\; 1.5 \le x_2 \le 4,\; 178 \le x_3 \le 416, \\
& 52 \le x_4 \le 104,\;\; 61.5 \le x_5 \le 201,\; 71.5 \le x_6 \le 156\}
\end{aligned}
$$

Note that the bounds that define Ω_0 are easily computed from the constraints in (E4.2).

Strategy S3

Tables 5, and 6 contain the results obtained for the solution of Example 4 by applying Strategy S3 to the problem formulation given in (E4.2). An iteration in Table 5 represents the analysis of a node of the branch and bound tree. Table 6 presents the node by node computational results for this problem. The value $LB(\Omega_f)$ on the third column of this Table corresponds to the tightest lower bound obtained while

Table 5. Overall computational results for the solution of Example 4 through the formulation in (E4.2), Strategy S3, Steps 3–12.

Iter	Node	*OLB*	*OUB*	ε(%)	|ON|
1	0	−6.45848	−5.00000	29.16958	2
2	1	−6.45848	−5.00000	29.16958	3
3	2	−5.36682	−5.00000	7.33631	4
4	3	−5.36682	−5.00000	7.33631	3
5	4	−5.30039	−5.00000	6.00776	2
6	5	−5.30039	−5.00000	6.00776	1
7	6	−5.03243	−5.00000	0.64856	2
8	7	−5.03243	−5.00000	0.64856	1
9	8	−5.00000	−5.00000	0.00000	0

Table 6. Node by node computational results for the solution of Example 4 through the formulation in (E4.2), Strategy S3, Steps 3–12.

Node	Father	$LB(\Omega_f)$	$LB(\Omega)$	$UB(\Omega)$	Contraction steps	Branching variable
0	–	–	−6.45848	−5.00000	6	x_4
1	0	−6.45848	−5.54017	−4.96284	8	x_3
2	0	−6.45848	−5.36956	−5.00000	7	x_4
3	1	−5.54017	−5.08686	−4.94463	4	–
4	1	−5.54017	−5.09959	−4.96027	4	–
5	2	−5.36956	−5.04811	−4.98487	5	–
6	2	−5.36956	−5.05032	−5.00000	9	x_4
7	6	−5.05032	−4.99765	infeasible	–	–
8	6	−5.05032	−5.00388	−5.00000	5	–

analyzing the father node. Therefore, $LB(\Omega_f)$ is the lower bound assigned to the children nodes when the branching step, Step 12, is performed, and the children nodes are created. Nine nodes are analyzed, and a total of 48 contraction steps are executed to prove that the point $x^* = \{3, 4, 416, 104, 156, 156\}$ is a global minimizer/maximizer for the problem in (E4.2)/(E4.1).

Problem reformulation 4B

Consider now the solution of the following alternative formulation for Example 4:

$$\begin{aligned}
&\underset{x}{\text{Minimize}}\ \ f(x) = -z_{3,4} - z_{5,6}\\
&\text{subject to}\\
&5x_1 - 3x_2 - 3 = 0\\
&z_{3,4} \le \frac{37x_1 + 73x_2 + 13}{13x_1 + 13x_2 + 13}\\
&z_{5,6} \le \frac{63x_1 - 18x_2 + 39}{13x_1 + 26x_2 + 13}\\
&x \in \Omega_0
\end{aligned} \tag{E4.3}$$

where

$$\Omega_0 = \{x \in R^2 : 1.5 \le x_1 \le 3,\ 1.5 \le x_2 \le 4\}$$

Since the numerators and denominators in the linear fractional constraints in (E4.3) are all positive, and only upper bounding inequalities are required for $z_{3,4}$ and $z_{5,6}$, a special convex underestimator problem that needs the introduction of no extra problem variables can be developed in this case. Bounding inequalities for $z_{3,4}$ are obtained by using the inequalities given in (10) with

$$\begin{aligned}
x_i &= 37x_1 + 73x_2 + 13\\
x_j &= 13x_1 + 13x_2 + 13
\end{aligned}$$

and

$$\begin{aligned}
x_i^L &= 37x_1^L + 73x_2^L + 13; \qquad & x_i^U &= 37x_1^U + 73x_2^U + 13;\\
x_j^L &= 13x_1^L + 13x_2^L + 13; \qquad & x_j^U &= 13x_1^U + 13x_2^U + 13;
\end{aligned}$$

Similar bounding inequalities are obtained for $z_{5,6}$ by using

$$\begin{aligned}
x_i &= 63x_1 - 18x_2 + 39\\
x_j &= 13x_1 + 26x_2 + 13
\end{aligned}$$

and

$$\begin{aligned}
x_i^L &= 63x_1^L - 18x_2^U + 39; \qquad & x_j^L &= 63x_1^U - 18x_2^L + 39;\\
x_j^L &= 13x_1^L + 26x_2^L + 13; \qquad & x_j^U &= 13x_1^U + 26x_2^U + 13;
\end{aligned}$$

Table 7. Summary of results from the application of the branch and contract algorithm to the Illustrative Examples.

Illustrative example	Nodes	Contraction steps
Example 1		
S1	1	19
S2	1	13
S5	39	–
Example 2		
S1	1	3
Example 3		
S1	1	11
Example 4		
(E4.2), S3	9	48
(E4.3), S3	9	31
(E4.3), S4	7	15
Example 5		
S1	11	82
S3	11	61
S5	157	–

Strategy S3

The results for the solution of Example 4 by applying the Strategy S3 to the problem formulation given in (E4.3) are included in Table 7. Note that, although nine branch and bound nodes are analyzed, the number of contraction steps decreases from 48 (reformulation 4A) to 31.

Strategy S4

For the application of the *feasibility based reduction* steps of the algorithm (Steps 7 and C8), the following bounding inequalities are obtained from the linear equation in (E4.3):

$$x_1 \geq \frac{3x_2^L + 3}{5}$$

$$x_1 \leq \frac{3x_2^U + 3}{5}$$

$$x_2 \geq \frac{5x_1^L - 3}{3}$$

$$x_2 \leq \frac{5x_1^U - 3}{3}$$

Phase 2

The results obtained for the solution of Example 4 by applying Strategy S4 to the problem formulation given in (E4.3) are included in Table 7. In this case, 7 nodes are analyzed, and only 15 contraction steps are needed to achieve global optimality.

EXAMPLE 5.

$$\begin{aligned}
\underset{x}{\text{Minimize}}\ \ f(x) = {} & -71x_1 - 60x_2 + 65x_3 + 57x_4 - 30x_5 \\
& -65x_1x_4 - 56x_1x_3 - 85x_2x_3 - 87x_2x_5 + 142
\end{aligned}$$

subject to

$$\begin{aligned}
2.5x_1 - 1.8x_2 + 5x_4 - 5.6x_5 &\leq 296 \\
x_2 + 4.6x_4 - 5x_5 + 1.5x_3x_4 + 2x_1x_2 &\leq 250 \\
-3.5x_1 + 2.3x_2 + 4x_3 - 10x_5 - 6x_2x_4 + 2.2x_3x_5 &\leq 192.5 \\
1.9x_2 - 5x_3 + 1.4x_5 + 2.9x_2x_3 - 1.5x_3x_5 &\leq 134.5 \\
7.5x_1 + 5.8x_3 - 3x_5 + 1.5x_1x_2 - 3x_4x_5 &= 55 \\
-3.5x_2 - 10x_3 + 10.5x_5 - 3.5x_1x_2 &\leq 32 \\
3.7x_2 - 7x_3 + 3.8x_4 - 5x_5 + 3.5x_1x_2 - 6x_2x_4 &= 75 \\
-7x_2 + 2x_3 - 2x_4 + 4x_5 &\leq 20 \\
x_1 + x_3 - x_5 &\leq 61.5 \\
x_4 + 1.5x_5 &\leq 90 \\
2x_1 - x_2 + x_1x_3 &\leq 80
\end{aligned} \tag{E5.1}$$

$$x \in \Omega_0$$

where

$$\begin{aligned}
\Omega_0 = \{x \in R^5 : & 0 \leq x_1 \leq 53,\ 0 \leq x_2 \leq 85, 0 \leq x_3 \leq 40, \\
& 0 \leq x_4 \leq 64, 0 \leq x_5 \leq 68\}
\end{aligned}$$

This problem has at least the following five local minima:

$$x^1 = (7.43433668, 17.1613413, 11.0692684, 2.30008488, 25.8916639)$$
$$x^2 = (41.0031922, 2.00638433, 0.000000000, 23.6650756, 5.08041128)$$
$$x^3 = (3.42506894, 18.5362782, 6.35553388, 0.000000000, 34.2607198)$$
$$x^4 = (40.3427010, 0.685401961, 0.000000000, 41.7968590, 2.25130780)$$
$$x^5 = (2.95219726, 52.7658055, 0.000000000, 1.73641856, 24.4606926)$$

with $f(x^1) = -61, 865.6260$, $f(x^2) = -65, 652.2628$, $f(x^3) = -68, 311.5219$, $f(x^4) = -110, 185.701$ *and* $f(x^5) = -116, 491.474$, *respectively.*

Strategy S1

Phase 1

The heuristic local search is performed initializing the solution of problem (E5.1) from $x = \delta x^L + (1 - \delta)x^U$, with $\delta = 0, 0.25, 0.50, 0.75, 1$. In this case, the local solutions x^3, x^4, and x^5 are obtained. Thus, we set $OUB := -116, 491.474$ and $x^* = x^b = x^5$.

Phase 2

In Step 2 of the algorithm, 9 contraction step are executed. Due to the large initial relaxation gap, the performance parameter, SP, averages only a 4.974% in Step 2. Clearly, for the contraction strategy to be effective in this problem, some branching is required in order to tighten the convex representation. During the execution of Steps 3–12 of the global optimization algorithm, 11 nodes are analyzed, and 73 contraction steps are performed with an average SP = 33.965%. The point x^5 is proved to be a global minimizer.

Strategies S1, S3, and S5

Table 8 and Figures 1 and 2 show the results obtained for the solution of Example 5 with the Strategies S1, S3 and S5. Note that the simple branch and bound strategy (Strategy S5), is very successful in initially reducing the large approximation gap present in the problem. Nevertheless, this remarkable decrease in the approximation gap is paid with a rapid increase in the number of open nodes, which goes up to a maximum of 19. Strategies S1 and S3, on the other hand, seem to be very ineffective during the first few seconds of the computations, which are consumed mainly in the contraction of bounds; S1 and S3 outperform S5 at the end by keeping the number of open nodes low. The three strategies proved that the point x^5 is a global minimizer for Example 5. All computations were performed on an IBM RS-6000/530 workstation with a non-optimized GAMS/MINOS (Brooke et al. 1992) implementation of the algorithm.

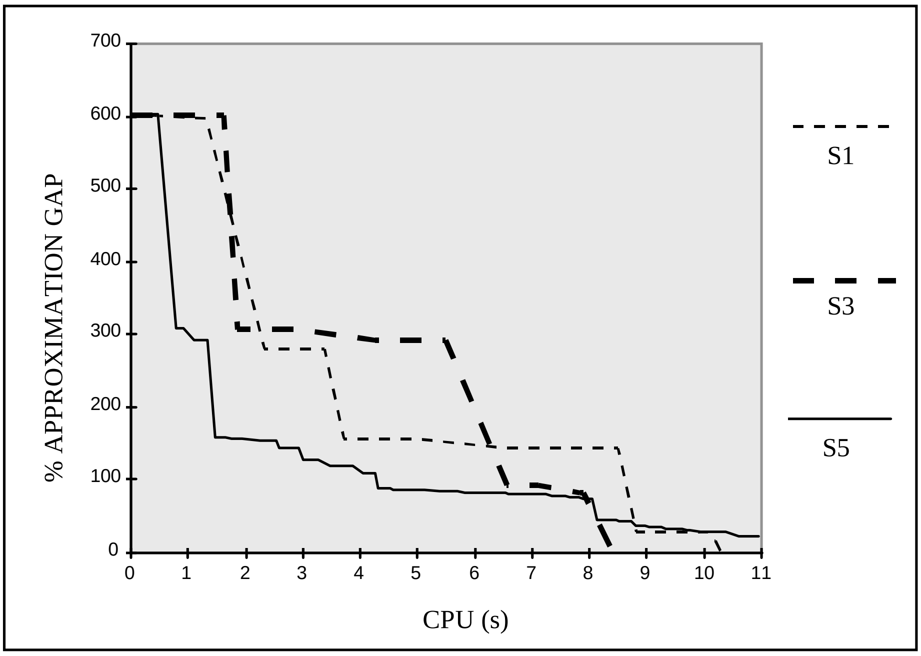

Figure 1. Computational results for Example 5.

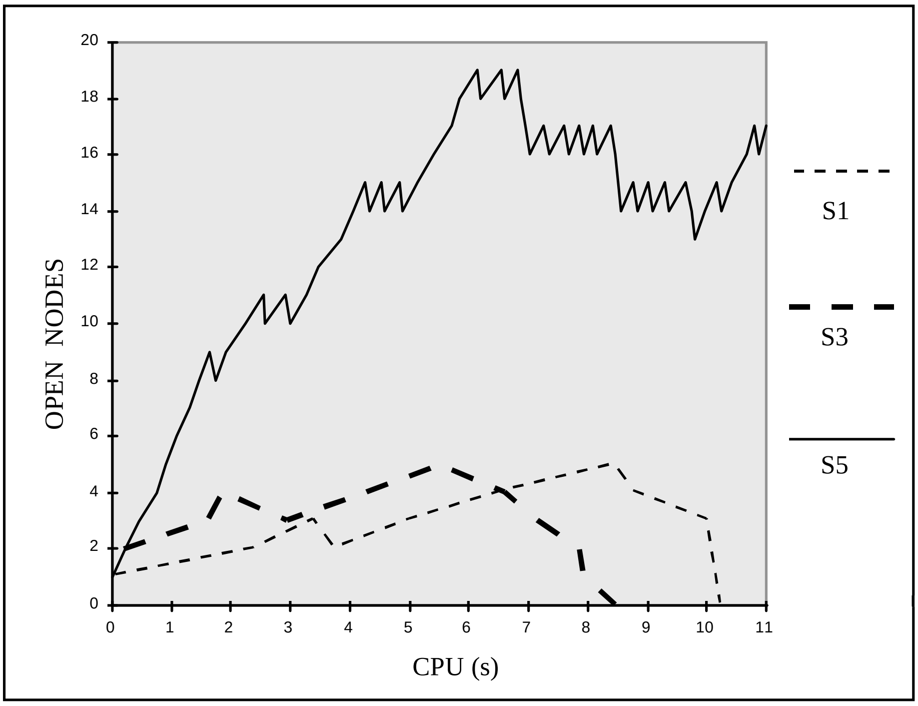

Figure 2. Computational results for Example 5.

Table 8. Computational results for the solution of Example 5 with Strategies S1, S3 and S5.

Feature	S1	S3	S5
No. of nodes	11	11	157
No. of upper bounding problems	13	10	78
No. of contraction steps	82	61	–
Average SP	30.787	47.224	–
CPU(s) convex underestimating problems	0.66 (6.4%)	0.78 (9.3%)	10.49 (51.1%)
CPU (s) upper bounding problems	1.5 (14.6%)	1.21 (14.4%)	10.03 (48.9%)
CPU (s) contraction subproblems	8.13 (79.0%)	6.42 (76.3%)	–
Total CPU time (s)	10.29 (100%)	8.41 (100%)	20.52 (100%)

7. Conclusions

In this paper we have addressed the global optimization of problems with concave univariate, bilinear, and linear fractional terms. A tight convex underestimating problem, and a *finite contraction operation* for variable bounds have been used to develop a *branch and contract* algorithm for the solution of NLP problems. A detailed description of the proposed algorithm has been presented, and tested on several example problems using different options. Although the computational experience is somewhat limited, the results suggest that the proposed approach is effective, keeps the size of the tree relatively small, and in some cases totally eliminates the need for branching.

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Appendix: Proofs of Theorems 1 and 3

Proof of Theorem 1

Let

$$l_1(x_i, x_j) = \frac{1}{x_j^L x_j^U}(x_j^U x_i - x_i^L x_j + x_i^L x_j^L) \tag{A.1}$$

and

$$l_2(x_i, x_j) = \frac{1}{x_j^L x_j^U}(x_j^L x_i - x_i^U x_j + x_i^U x_j^U) \tag{A.2}$$

The approximation error of $l_1(x_i, x_j)$ is given by

$$\Delta_{ij}^1 = l_1(x_i, x_j) - \frac{x_i}{x_j} = \left(\frac{x_j}{x_j^L} - 1\right)\left(\frac{x_i}{x_j} - \frac{x_i^L}{x_j^U}\right) \geq 0 \tag{A.3}$$

Similarly, the approximation error of $l_2(x_i, x_j)$ is

$$\Delta_{ij}^2 = l_2(x_i, x_j) - \frac{x_i}{x_j} = \left(1 - \frac{x_j}{x_j^U}\right)\left(\frac{x_i^U}{x_j^L} - \frac{x_i}{x_j}\right) \geq 0 \tag{A.4}$$

Since Δ_{ij}^1 and Δ_{ij}^2 are both nonnegative over Ω_{ij}, $\gamma_{ij}^{lf}(x_i, x_j) = \text{Min}[l_1(x_i, x_j), l_2(x_i, x_j)]$ overestimates the linear fractional term x_i/x_j over Ω_{ij}. Furthermore, it is easy to verify the following statements:

(i) $l_1(x_i, x_j) = x_i/x_j$ at $x_j = x_j^L$, and at the point (x_i^L, x_j^U).
(ii) $l_2(x_i, x_j) = x_i/x_j$ at $x_j = x_j^U$, and at the point (x_i^U, x_j^L).
(iii) Let T_{ij}^1 be the triangle determined by the vertices $v^1 = (x_i^L, x_j^L)$, $v^2 = (x_i^U, x_j^L)$ and $v^3 = (x_i^L, x_j^U)$, then $\gamma_{ij}^{lf}(x_i, x_j) = l_1(x_i x_j)$ over T_{ij}^1.
(iv) Let T_{ij}^2 be the triangle determined by the vertices v^2, v^3 and $v^4 = (x_i^U, x_j^U)$, then $\gamma_{ij}^{lf}(x_i, x_j) = l_2(x_i, x_j)$ over T_{ij}^2.
(v) $\Omega_{ij} = T_{ij}^1 \cup T_{ij}^2$.

If $\gamma_{ij}^{lf}(x_i, x_j)$ were not the concave envelope of x_i/x_j over Ω_{ij}, there would be a third overestimating affine function $l_3(x_i, x_j)$, such that

$$l_3(x_i, x_j) < \gamma_{ij}^{lf}(x_i, x_j) \text{ for some } (\bar{x}_i, \bar{x}_j) \in \Omega_{ij} \tag{A.5}$$

Assume that $(\bar{x}_i, \bar{x}_j) \in T_{ij}^1$, then there are unique coefficients $\lambda_1, \lambda_2, \lambda_3 \geq 0$, with $\sum_{i=1}^3 \lambda_i = 1$, such that $(\bar{x}_i, \bar{x}_j) = \sum_{i=1}^3 \lambda_i v^i$. Also, since $l_3(x_i, x_j)$ and $\gamma_{ij}^{lf}(x_i, x_j)$ are affine functions over T_{ij}^1, we obtain

$$\begin{aligned} l_3(\bar{x}_i, \bar{x}_j) &= l_3\left(\sum_{i=1}^3 \lambda_i v^i\right) = \sum_{i=1}^3 \lambda_i l_3(v^i) \\ \gamma_{ij}^{lf}(\bar{x}_i, \bar{x}_j) &= \gamma_{ij}^{lf}\left(\sum_{i=1}^3 \lambda_i v^i\right) = \sum_{i=1}^3 \lambda_i \gamma_{ij}^{lf}(v^i) \end{aligned} \tag{A.6}$$

But at the vertices of T_{ij}^1 we have $l_3(x_i, x_j) \geq x_i/x_j$, and $\gamma_{ij}^{lf}(x_i/x_j) = x_i/x_j$, therefore (A.6) implies that

$$l_3(\bar{x}_i, \bar{x}_j) \geq \gamma_{ij}^{lf}(\bar{x}_i, \bar{x}_j)$$

which is in contradiction with the assumption made in (A.5). A similar argument holds when $(\bar{x}_i, \bar{x}_j) \in T_{ij}^2$. The fact that $\gamma_{ij}^{lf}(x_i, x_j) = x_i/x_j$ at $x_j = x_j^L$, and $x_j = x_j^U$ can be easily verified by direct evaluation in the equation that defines $\gamma_{ij}^{lf}(x_i, x_j)$, or through (A.3) and (A.4). $\square$

Proof of Theorem 3

Since problem (12) is convex, its solution satisfies the saddle point conditions with the Lagrangian multiplier $\tilde{\lambda}$ serving as the multiplier in the saddle point criteria (see, e.g. Bazaraa et al. 1993). Consequently, $Z = \Phi(0) - \tilde{\lambda}q$, with $q \in R^p$, is a supporting hyperplane at $q = 0$ of the graph of the perturbation function $\Phi(q)$ defined as

$$\begin{aligned} &\Phi(q) \equiv \underset{(x,y,z)}{\text{Min}} \ x_i \\ &\text{subject to} \\ &G_k(x, y, z) \leq q_k \quad k = 1, 2, \ldots, p \\ &(x, y, z) \in R^n \times R^{n_1} \times R^{n_2} \end{aligned} \tag{A.7}$$

In other words,

$$\Phi(q) \geq \Phi(0) - \tilde{\lambda}q \quad \forall q \in R^p \tag{A.8}$$

(see, e.g. Minoux, 1986). Assuming that the *OUB* constraint is active at the solution $(\tilde{x}, \tilde{y}, \tilde{z})_\Omega$ of problem (12) with $\tilde{\lambda}_1 > 0$, and considering the perturbation vector $q = \{q_1, 0, 0, \ldots, 0\}$, with $q_1 \leq 0$, (A.8) reads

$$\Phi(q) \geq \Phi(0) - \tilde{\lambda}_1 q_1$$

from which it follows that

$$\Phi(q) \geq \tilde{x}_i - \tilde{\lambda}_1[\hat{f}(x, y, z) - OUB]$$

In particular, for $\Phi(q) \leq x_i^U$, we obtain

$$x_i^U \geq \tilde{x}_i - \tilde{\lambda}_1[\hat{f}(x, y, z) - OUB]$$

or

$$\hat{f}(x, y, z) \geq OUB - (x_i^U - \tilde{x}_i)/\tilde{\lambda}_1 \qquad \square$$

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