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Improve-and-Branch Algorithm for the Global Optimization of Nonconvex NLP Problems

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Abstract. A new algorithm to solve nonconvex NLP problems is presented. It is based on the solution of two problems. The reformulated problem RP is a suitable reformulation of the original problem and involves convex terms and concave univariate terms. The main problem MP is a nonconvex NLP that outer-approximates the feasible region and underestimate the objective function. MP involves convex terms and terms which are the products of concave univariate functions and new variables. Fixing the variables in the concave terms, a convex NLP that overestimates the feasible region and underestimates the objective function is obtained from the MP. Like most of the deterministic global optimization algorithms, bounds on all the variables in the nonconvex terms must be provided. MP forces the objective value to improve and minimizes the difference of upper and lower bound of all the variables either to zero or to a positive value. In the first case, a feasible solution of the original problem is reached and the objective function is improved. In general terms, the second case corresponds to an infeasible solution of the original problem due to the existence of gaps in some variables. A branching procedure is performed in order to either prove that there is no better solution or reduce the domain, eliminating the local solution of MP that was found. The MP solution indicates a key point to do the branching. A bound reduction technique is implemented to accelerate the convergence speed. Computational results demonstrate that the algorithm compares very favorably to other approaches when applied to test problems and process design problems. It is typically faster and it produces very accurate results.

Key words: concave terms, convex hull, underestimating problem

1. Introduction

The problem of determining a global optimal solution of a nonconvex NLP or MINLP problem is in general a very difficult task. A great effort has been focused on studying theoretical and algorithmic aspects of global optimization in the last decades. This is because there are practical problems where local optimization is not satisfactory.

The applicability of some deterministic methods of global optimization is restricted to specific classes of problems. For bilinear programming problems, Sherali and Alameddine (1992) developed an algorithm that implements a *reformulation-linearization technique* embedded in a branch-and-bound procedure. Quesada and Grossmann (1995) proposed a branch-and-bound algorithm for linear fractional and bilinear programs.

Floudas and Visweswaran (1993) proposed a *primal–dual global optimization* algorithm. Later on they proposed a branch-and-bound framework for the GOP algorithm (Visweswaran and Floudas, 1996). The *branch and reduce* algorithm by Ryoo and Sahinidis (1996) implements reduction tests within a branch-and-bound framework. The αBB algorithm by Androulakis et al. (1995) addresses general continuous optimization problems with twice-differentiable constraints and objective function. It involves a parameter α for underestimating general nonconvex terms. The convergence rate of this algorithm depends on the accurate estimation of each parameter α.

Zamora and Grossmann (1999) presented a *branch and contract* algorithm for problems with concave univariate, bilinear and linear fractional terms.

The *extended cutting plane* algorithm by Westerlund and Pettersson (1995) solves pseudoconvex MINLP problems to global optimality. Adjiman et al. (2000) proposed two global optimization approaches for solving nonconvex MINLP problems. The first approach is for separable continuous and integer domains, while the second approach addresses general mixed integer nonlinear problems. For general problems, Smith and Pantelides (1999) propose a *reformulation/spatial branch-and-bound* algorithm.

A reference to the tunneling method developed by Levy and co-workers should be made (see Levy and Gomez, 1985). This method consists of two phases: the minimization phase and the tunneling phase. The former is designed to decrease the value of the objective function, starting from a good initial point. The tunneling phase attempts to obtain a good initial point for the next minimization phase.

The purpose of this paper is to present a new deterministic algorithm for solving nonconvex problems to attain global optimality, exploiting ideas of tunneling approach and convex hull of nonconvex regions. In the following section, the definition of the kind of problems we are interested in is addressed. Techniques to reformulate the problem are presented in Section 3, and a relaxed problem is constructed in Section 4. Section 5 presents the main problem as well as theoretical results relating this problem with the original one. Some branching strategies are discussed in Sections 6 and 7 exposes the proposed algorithm. Range reduction strategies based on feasibility and some implementations details are discussed in Sections 8 and 9. Finally, the performance of the algorithm is illustrated in Section 10 with the solution of 6 examples.

2. Problem Definition and Grounds

The problem analyzed in this work presents the general form:

$$\begin{aligned} &\min\ f(\bar{x}) \\ &\text{s.t.}\ \ \bar{h}(\bar{x}) = \bar{0} \\ &\qquad \bar{g}(\bar{x}) \leqslant \bar{0} \\ &\qquad \bar{x}^{LO} \leqslant \bar{x} \leqslant \bar{x}^{UP}, \end{aligned} \qquad \mathbf{P}$$

where $\bar{x} \in \Re^n$ is a vector of bounded continuous variables, $\bar{g} : \Re^n \rightarrow \Re^m$ is a set of inequality constraints, $\bar{h} : \Re^n \rightarrow \Re^q$ is a set of equality constraints and $f : \Re^n \rightarrow \Re$ is the objective function to be minimized. The pursued goal is to develop an algorithm of wide applicability in the area of chemical engineering problems. The only requirement for the functions involved in P is differentiability. However, problems that do not satisfy this requirement can be properly modeled in order to suit for the algorithm. Then, the proposed algorithm can be applied to any nonconvex problem in order to obtain the global optimum, including problems having discontinuous functions and/or integer variables. In Section 10, a problem including integer variables and discontinuous functions is solved as an illustration of the capability of the algorithm.

Tight convex relaxations have been proposed for several special algebraic forms. The convex envelope of bilinear functions was introduced by McCormick (1976). Convex underestimators for linear fractional terms were proposed in the works by Quesada and Grossmann (1995) and Zamora and Grossmann (1999); and Tawarmalani and Sahinidis (2001) constructed the convex envelope for this class of terms. The convex envelope of a concave function over a simplex is an affine function that can be uniquely determined by a system of linear equations. The convex envelope of products of univariate functions has been studied in Maranas and Floudas (1995). For general twice-differentiable terms, Androulakis et al. (1995) proposed the addition of a quadratic term with a parameter α. The tightness of these underestimators strongly depends on the precise estimation of α.

All these estimations share the property of an exact approximation on the boundary of the box $\bar{x}^{LO} \leqslant \bar{x} \leqslant \bar{x}^{UP}$. Therefore, most of the global algorithms are based on branch-and-bound techniques.

The methodology proposed here is focused on finding feasible points with improved objective value. This is the idea underlying in the tunneling algorithm (Levy and Gomez, 1985). The approach attempts to find a better solution in each step or to eliminate regions where the objective value cannot be improved.

It is easily shown that any algebraic expression is made up of binary operators (addition, subtraction, multiplication, division, and exponentiation) and unary operators corresponding to transcendental univariate function (logarithms, exponentials, exponentiation and trigonometric functions). Consequently, any problem having only arithmetic expressions can be transformed into a completely equivalent problem where nonconvexities correspond to bilinear terms, linear fractional terms, and concave univariate functions. Since the reformulation procedure is exact, any convex relaxation of the reformulated problem is also a valid relaxation for the original one. Smith and Pantelides (1999) automate this symbolic reformulation procedure and embed it in a spatial-branch and bound algorithm.

In this work we also reformulate the bilinear and linear fractional terms using only concave and convex expressions. As it is pointed by Ryoo and Sahinidis (1995), the separable reformulation of a nonlinear problem was first proposed by (McCormick, 1972).

It is well known that any point in a convex polyhedron can be represented as a convex combination of the extreme points and extreme directions. In general, the convex combination of the extreme points of certain region plus the nonnegative linear combination of extreme directions gives rise to the convex hull of that region. If the extreme points and extreme directions of a particular set are at hand, the convex hull is obtained with a straightforward formulation.

The mathematical formulation for the convex hull of Q is

$$\mathrm{conv}(Q) = \{x : x = \lambda x_1 + (1-\lambda)x_2;\ 0 \leqslant \lambda \leqslant 1,\ x_1, x_2 \in Q\}$$

Note that when $\lambda = 0$ or 1, or when $x_1 = x_2$, then $x \in Q$. Thus, if two points in Q are known (generally two extreme points), an interior point in Q can be calculated from the previous formulation, forcing $|x_2 - x_1| \to 0$. In Section 4, these ideas are used to construct the main problem.

3. Reformulated Problem: RP

As it was mentioned before, the problem P is reformulated. The symbolic reformulation is carried out adding new variables in order to simplify the expressions in the constraints. The reformulation procedure leads to a problem where nonconvexities are due to the presence of bilinear, linear fractional and concave univariate terms. However, without much more effort, it is possible to express each nonconvex term through concave univariate functions.

For linear fractional terms, a new variable z_{ij} is added representing the term x_i/x_j. The new variable z_{ij} replaces every occurrence of the fractional term, and the bilinear constraint $x_j z_{ij} = x_i$ is added to the model.

The manipulation of each bilinear term in order to express it using concave and convex terms requires three new variables: z, α and β. Variable

z replaces each occurrence of the product $x_1 x_2$. Variables α and β are restricted by $\alpha = x_1 + x_2$ and $\beta = x_1 - x_2$. Then, $x_1 x_2 = (\alpha^2 - \beta^2)/4$. This relation between the new variables is represented by the inequalities: $-4z + \alpha^2 - \beta^2 \leqslant 0$ and $4z + \beta^2 - \alpha^2 \leqslant 0$. There is a concave term in each inequality: $-\beta^2$ and $-\alpha^2$, respectively. This separable reformulation of the bilinear terms was also used by Ryoo and Sahinidis (1995).

Using the previous ideas any problem can be reformulated in the required form (except for the problems involving trigonometric functions. A problem of this type is analyzed in Section 10).

Therefore, the new problem is completely equivalent to the original one and has three kinds of constraints: linear equality constraints, convex inequality constraints and nonconvex inequality constraints. In addition, each nonconvex inequality constraint has only one nonconvex term being a concave univariate function.

In order to illustrate such reformulation, let us consider the following reactor network design problem (this problem is solved in Section 10, example 4):

$$\begin{aligned}
\min \quad & f(x) = -x_4,\\
\text{s.t.} \quad & x_1 - 1 + k_1 x_1 V_1 = 0,\\
& x_2 - x_1 + k_2 x_2 V_2 = 0,\\
& x_3 + x_1 - 1 + k_3 x_3 V_1 = 0,\\
& x_4 - x_3 + x_2 - x_1 + k_4 x_4 V_2 = 0,\\
& V_1^{0.5} + V_2^{0.5} \leqslant 4,\\
& 0 \leqslant x_i \leqslant 1 \quad i = 1, \ldots, 4,\\
& 0 \leqslant V_i \leqslant 16 \quad i = 1, 2,\\
& k_1 = 0.09755988 \quad k_2 = 0.99 k_1 \quad k_3 = 0.0391908 \quad k_4 = 0.9 k_3.
\end{aligned}$$

It has 4 bilinear terms and two concave terms. To reformulate it, new variables are added, simplifying the terms and restrictions, to obtain an equivalent problem in a higher dimensional space, having at the most one nonconvex (concave univariate) term in each inequality constraint. The resulting problem is:

$$\begin{aligned}
\min \quad & f(x) = -x_4,\\
\text{s.t.} \quad & x_1 - 1 + k_1 z_1 = 0,\\
& x_2 - x_1 + k_2 z_2 = 0,\\
& x_3 + x_1 - 1 + k_3 z_3 = 0,\\
& x_4 - x_3 + x_2 - x_1 + k_4 z_4 = 0,\\
& z_5 + z_6 \leqslant 4
\end{aligned}$$

$$\begin{array}{lll}
\alpha_i = x_i + V_1 & \beta_i = x_i - V_1 & i = 1, 3 \\
\alpha_i = x_i + V_2 & \beta_i = x_i - V_2 & i = 2, 4 \\
\alpha_i^2 - \beta_i^2 \leqslant 4z_i & \beta_i^2 - \alpha_i^2 \leqslant -4z_i & i = 1, \ldots, 4 \\
V_1^{0.5} \leqslant z_5, & & \\
V_2^{0.5} \leqslant z_6, & & \\
0 \leqslant \alpha_i \leqslant 17 & -16 \leqslant \beta_i \leqslant 1 & i = 1, \ldots, 4 \\
0 \leqslant z_i \leqslant 16 & i = 1, \ldots, 4 & \\
0 \leqslant z_i \leqslant 4 & i = 5, 6 & \\
0 \leqslant x_i \leqslant 1 & i = 1, \ldots, 4 & \\
0 \leqslant V_i \leqslant 16 & i = 1, 2 &
\end{array}$$

The bounds for the variables z's, α's, and β's, are calculated from the x's and V's ones. In the previous problem, each constraint is either linear or has only one concave univariate term.

In general, given any problem P (except for problems involving trigonometric functions), a reformulated problem RP can be generated, taking the form:

$$\begin{array}{ll}
\min & f^c(\bar{x}, \bar{z}), \\
\text{s.t.} & \bar{h}^l\left(\bar{x}, \bar{z}, \bar{\alpha}, \bar{\beta}\right) = \bar{0}, \\
& \bar{g}^c\left(\bar{x}, \bar{z}, \bar{\alpha}, \bar{\beta}\right) \leqslant \bar{0}, \\
& \overline{tcu} + \bar{k}^c\left(\bar{x}, \bar{z}, \bar{\alpha}, \bar{\beta}\right) \leqslant \bar{0}, \\
& \bar{x}^{LO} \leqslant \bar{x} \leqslant \bar{x}^{UP} \qquad \bar{z}^{LO} \leqslant \bar{z} \leqslant \bar{z}^{UP}, \\
& \bar{\alpha}^{LO} \leqslant \bar{\alpha} \leqslant \bar{\alpha}^{UP} \qquad \bar{\beta}^{LO} \leqslant \bar{\beta} \leqslant \bar{\beta}^{UP},
\end{array} \qquad \textbf{RP}$$

where $\bar{h}^{\mathrm{l}}$ are linear functions, f^{c}, $\bar{g}^{\mathrm{c}}$ and $\bar{k}^{\mathrm{c}}$ are convex functions, and each term *tcu* is a concave univariate function. Although RP is defined in a space of higher dimension, P and RP are completely equivalent in the sense that there exists a biunivoque correspondence between the feasible points of both problems and the values of the objective function in the correspondent points. Note that variables z are auxiliary variables included for reformulating and convexifying P. In general, $\bar{z} = \bar{z}(\bar{x})$. Thus, $f^c(\bar{x}, \bar{z}(\bar{x})) = f(\bar{x})$.

4. The Convex Relaxation

According to Section 3, it is just necessary to consider the concave univariate terms. Consider the following restriction (r):

$$tcu(w) + k^c\left(\bar{x}, \bar{z}, \bar{\alpha}, \bar{\beta}\right) \leqslant 0, \qquad \textbf{(r)}$$

where k^c is a convex function and *tcu* is a concave univariate function of w. Note that w is one of variables in $\bar{x}$, $\bar{z}$, $\bar{\alpha}$ or $\bar{\beta}$.

The set R of points defined by (r) is nonconvex. The convex hull of R can be mathematically described through the convex combination of the two extreme points $\left(w^{LO}, tcu\left(w^{LO}\right)\right)$ and $\left(w^{UP}, tcu\left(w^{UP}\right)\right)$, where w^{LO} and w^{UP} are the bounds for w, in the following way:

$$\begin{aligned}
&\lambda\, tcu\left(w^{LO}\right)+(1-\lambda)\, tcu\left(w^{\mathrm{UP}}\right) \leqslant -k^{\mathrm{c}}\left(\bar{x}, \bar{z}, \bar{\alpha}, \bar{\beta}\right)\\
&w=\lambda w^{LO}+(1-\lambda)\, w^{UP}\\
&0 \leqslant \lambda \leqslant 1\\
&w^{LO} \leqslant w \leqslant w^{UP}
\end{aligned} \qquad \textbf{(r')}$$

It is clear that the feasible set defined by (r') is a convex set and contains the feasible set defined by (r).

It should be noted that, although we have constructed the convex hull in a high dimensional space, the projection onto the space of original variables x does not correspond to the convex hull of the original feasible region but to a valid convex relaxation of it.

Figure 1 shows in solid line the concave boundary for the feasible set defined by constraint $x_1 x_2 \leqslant 3.5$ in the domain D=$[1,4] \times [1,4]$. The relaxation of the proposed separable reformulation of the constraint was constructed in the $(x_1, x_2, z, \alpha, \beta)$-space and its projection onto the (x_1, x_2)-space is depicted in dark line.

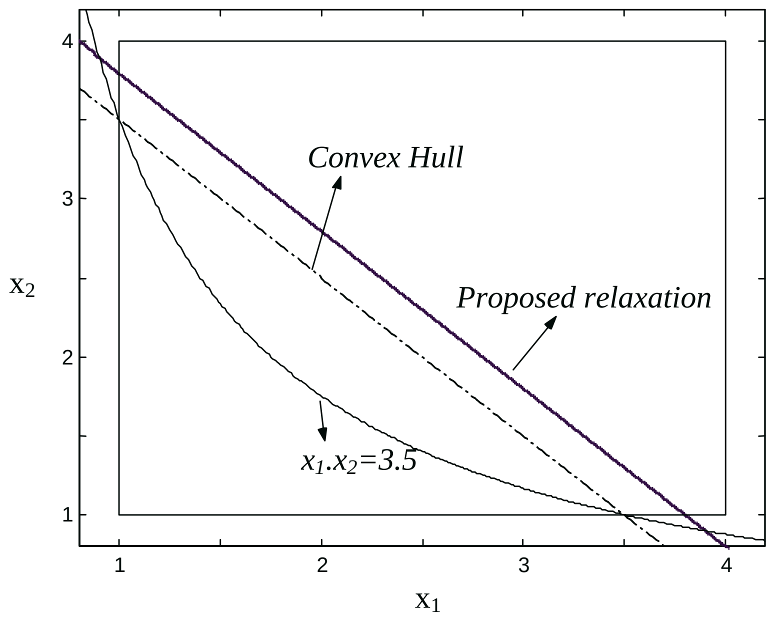

Figure 1. Relaxation of bilinear constraint.

The boundary of the convex hull of the set $\{(x_1, x_2) : x_1 x_2 \leqslant 3.5, 1 \leqslant x_1 \leqslant 4, 1 \leqslant x_2 \leqslant 4\}$ is also shown in dashed line in Figure 1. Note that the projection of the relaxation constructed in the higher dimensional space is less tight than the convex hull in the (x_1, x_2)-space and there exists a relaxation gap in the extreme points. This is due to the methodology that overestimates the feasible region on a different space. Although tighter relaxations can be used, the proposed underestimation methodology entails some advantages.

If the first two constraints in (r') are changed replacing the bounds w^{LO} and w^{UP} by new variables w_L and w_U, a valid underestimation for the concave univariate function is also obtained. The new variables are bounded by the same bounds as w. Also, w_L is constrained to be lower than or equal to w_U. The new relaxation is:

$$\begin{aligned}
&\lambda\, tcu\,(w_L) + (1-\lambda)\, tcu\,(w_U) \leqslant -k^c\left(\bar{x}, \bar{z}, \bar{\alpha}, \bar{\beta}\right), \\
&w = \lambda w_L + (1-\lambda)\, w_U, \\
&w_L \leqslant w_U, \\
&0 \leqslant \lambda \leqslant 1, \\
&w^{LO} \leqslant w_L \leqslant w^{UP}, \\
&w^{LO} \leqslant w_U \leqslant w^{UP}.
\end{aligned} \qquad (\mathbf{r}^{\mathbf{nc}})$$

The last three constraints are simply bounds for the variables and the third constraint is a linear inequality. However, the first two inequalities in (r^{nc}) are nonconvex, regardless of the form of the concave function *tcu*.

As it can be seen in Figure 2, there exist several ways to represent a value w as a convex combination of variables w_L and w_U, and each of them leads to different values for the variable λ. From Figure 2, $tcu(w) \geqslant \lambda^j\, tcu(w_L^j) + (1-\lambda^j) tcu(w_U^j)$ for both j=1 and j=2, where $\lambda^j = (w_U^j - w)/(w_U^j - w_L^j)$. This degree of freedom allows the proposed

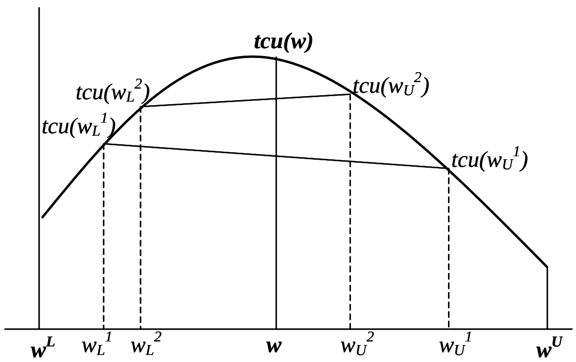

Figure 2. Convex combination of *tcu(w)*.

algorithm to look for those values of w_L and w_U representing w that have the smallest difference $w_U - w_L$.

5. Main Problem

The main problem to be solved in the proposed algorithm is formulated. The solution of this problem indicates if a new better point has been found or provides a key point to do a branching.

Given a general problem in the P form, it is transformed as it was explained before, in order to put it in the equivalent RP form. Then, the relaxation is constructed replacing the concave univariate terms like (r) with the formulation (r^{nc}). Let J be the cardinality of the set of concave terms in RP. Then, there are J new variables w_L, denoted by w_{Li}, $i = 1, \ldots, J$. In the same way, the J new variables w_U are denoted by w_{Ui}, $i = 1, \ldots, J$. Finally, the J new variables λ are denoted by λ_i, $i = 1, \ldots, J$.

Let us assume that an upper bound $f^{UP}$for the global minimal objective value is known (it may be given from the best solution point found at the moment). The main problem MP is formulated as follows,

$$
\begin{aligned}
\min \quad & \sum_{\mathrm{i}=1}^{\mathrm{J}} (w_{U\mathrm{i}} - w_{L\mathrm{i}}), \\
\text{s.t.} \quad & f^{\mathrm{c}}(\bar{x}, \bar{z}) \leqslant f^{UP} - \varepsilon, \\
& \bar{h}^{\mathrm{l}}(\bar{x}, \bar{z}, \bar{\alpha}, \bar{\beta}) = \bar{0}, \qquad\qquad\qquad\qquad \mathbf{MP} \\
& \bar{g}^{\mathrm{c}}(\bar{x}, \bar{z}, \bar{\alpha}, \bar{\beta}) \leqslant \bar{0}, \\
& \left.\begin{array}{l}
\lambda_i tcu_i\,(w_{Li}) + (1-\lambda_i)\, tcu_i\,(w_{Ui}) \leqslant -k_i^{\mathrm{c}}\left(\bar{x}, \bar{z}, \bar{\alpha}, \bar{\beta}\right) \\
w_i = \lambda_i w_{Li} + (1-\lambda_i)\, w_{Ui}, \\
w_{Li} \leqslant w_{Ui},
\end{array}\right\} \quad i = 1, \ldots, J \\
& \bar{x}^{LO} \leqslant \bar{x} \leqslant \bar{x}^{UP} \qquad \bar{z}^{LO} \leqslant \bar{z} \leqslant \bar{z}^{UP} \\
& \bar{\alpha}^{LO} \leqslant \bar{\alpha} \leqslant \bar{\alpha}^{UP} \qquad \bar{\beta}^{LO} \leqslant \bar{\beta} \leqslant \bar{\beta}^{UP} \\
& w_i^{LO} \leqslant w_{Li} \leqslant w_i^{UP} \quad w_i^{LO} \leqslant w_{Ui} \leqslant w_i^{UP} \\
& 0 \leqslant \lambda_i \leqslant 1 \quad i = 1, \ldots, J
\end{aligned}
$$

The objective function in MP minimizes the difference between the variable bounds. The constraint $f^c(\bar{x}, \bar{z}) \leqslant f^{UP} - \varepsilon$ acts as a reduction constraint. It forces the original objective function to improve when solving MP. It also reduces the feasible region to be considered in each iteration, eliminating regions, where f^c is worse than the best known upper bound. The presence of this restriction in MP makes avoidable the generation of sequences of increasing lower bounds and decreasing upper bounds.

MP is clearly nonconvex. However, the nonconvex part consists of those constraints where the variables λ_i appear.

It is important to note that the variables involved in the nonconvex terms $(w_{Li}, w_{Ui}, \lambda_i, i = 1, \ldots, J)$ appear in three constraints at the most: two nonconvex constraints representing convex combinations, and a constraint requiring that w_{Li} shall be lower than or equal to w_{Ui}. Remember that w_i is one of the variable in $\bar{x}, \bar{z}, \bar{\alpha}$ or $\bar{\beta}$ and not a new variable. These are qualities that could be exploited. As it will be shown, if the MP problem could be solved for global optimality easily, conclusions would be strong.

Note that when variables w_{Li} and w_{Ui} are fixed, the MP is a convex problem. Let CP be the problem obtained from MP by fixing these variables at the bound values and changing the objective function by f^c. Thus, CP generates a convex overestimation of the original feasible region, and its solution provides a lower bound to the global optimal objective.

$$
\begin{array}{ll}
\min & f^{\mathrm{c}}(\bar{x}, \bar{z}), \\
\text{s.t.} & f^{\mathrm{c}}(\bar{x}, \bar{z}) \leqslant f^{\mathrm{UP}} - \varepsilon, \\
& \bar{h}^{\mathrm{l}}(\bar{x}, \bar{z}, \bar{\alpha}, \bar{\beta}) = \bar{0}, \\
& \bar{g}^{\mathrm{c}}(\bar{x}, \bar{z}, \bar{\alpha}, \bar{\beta}) \leqslant \bar{0}, \qquad\qquad\qquad\qquad\qquad\qquad \textbf{CP} \\
& \left.\begin{array}{l} \lambda_i tcu_i\left(w_i^{LO}\right) + (1-\lambda_i)\, tcu_i\left(w_i^{UP}\right) \leqslant -k_i^c\left(\bar{x}, \bar{z}, \bar{\alpha}, \bar{\beta}\right) \\ w_i = \lambda_i w_i^{LO} + (1-\lambda_i)\, w_i^{UP} \end{array}\right\} i = 1, \ldots, J \\
& \bar{x}^{LO} \leqslant \bar{x} \leqslant \bar{x}^{UP} \quad \bar{z}^{LO} \leqslant \bar{z} \leqslant \bar{z}^{UP}, \\
& \bar{\alpha}^{LO} \leqslant \bar{\alpha} \leqslant \bar{\alpha}^{UP} \quad \bar{\beta}^{LO} \leqslant \bar{\beta} \leqslant \bar{\beta}^{UP}, \\
& 0 \leqslant \lambda_i \leqslant 1 \qquad i = 1, \ldots, J.
\end{array}
$$

The following properties analyze possible solutions for MP.

Properties:

(P1) If the feasible point in MP $\bar{p}^* = \left(\bar{x}^*, \bar{z}^*, \bar{\alpha}^*, \bar{\beta}^*, \bar{w}_L^*, \bar{w}_U^*, \bar{\lambda}^*\right)$ has an objective value equal to 0, it is a global optimal of MP. Moreover, this solution represents a feasible solution of P with an objective value better than the upper bound f^{UP}.

(P2) If the feasible point in MP $\bar{p}^* = \left(\bar{x}^*, \bar{z}^*, \bar{\alpha}^*, \bar{\beta}^*, \bar{w}_L^*, \bar{w}_U^*, \bar{\lambda}^*\right)$ has an objective value greater than 0, but $\lambda_i^* = 0$ or 1, for those i so that $0 < w_{Ui}^* - w_{Li}^*$, it corresponds to a feasible point of P with an objective value better than the upper bound f^{UP}.

(P3) If the global optimum of MP $\bar{p}^* = \left(\bar{x}^*, \bar{z}^*, \bar{\alpha}^*, \bar{\beta}^*, \bar{w}_L^*, \bar{w}_U^*, \bar{\lambda}^*\right)$ has an objective value greater than 0, there does not exist any solution of P with an objective value smaller than $(f^{UP} - \varepsilon)$.

(P4) If MP is infeasible, there does not exist any solution of P with an objective value smaller than $(f^{UP} - \varepsilon)$.

THEOREM 1.
(a) *CP is feasible if and only if MP is feasible.*
(b) *If CP is infeasible, there does not exist any solution of P with an objective value smaller than $f^{UP} - \varepsilon$.*

Proof. (a) Let $\bar{p}_0 = (\bar{x}_0, \bar{z}_0, \bar{\alpha}_0, \bar{\beta}_0, \bar{\lambda}_0)$ be a feasible point in CP. Let $\bar{w}_{L_0} = \bar{w}^{LO}$ and $\bar{w}_{U_0} = \bar{w}^{UP}$. Clearly, the point $(\bar{x}_0, \bar{z}_0, \bar{\alpha}_0, \bar{\beta}_0, \bar{w}_{L_0}, \bar{w}_{U_0}, \bar{\lambda}_0)$ is feasible in MP.

Conversely, let $(\bar{x}_0, \bar{z}_0, \bar{\alpha}_0, \bar{\beta}_0, \bar{w}_{L_0}, \bar{w}_{U_0}, \bar{\lambda}_0)$ be a feasible point in MP. Let us define $\lambda_i = (w_i^{UP} - w_{0i})/(w_i^{UP} - w_i^{LO})$ for all $i = 1, \dots, J$. Then, the constraint $w_i = \lambda_i w_i^{LO} + (1 - \lambda_i)\, w_i^{UP}$ is satisfied.

In order to check constraint $\lambda_i\, tcu_i\left(w_i^{LO}\right) + (1 - \lambda_i)\, tcu_i\left(w_i^{UP}\right) \leqslant -k_i^c\left(\bar{x}, \bar{z}, \bar{\alpha}, \bar{\beta}\right)$ in CP, the two possible cases for each i are analyzed.

For each i such that $w_{L_{0i}} = w_{U_{0i}} (= w_{0i})$, $-k_i^c\left(\bar{x}_0, \bar{z}_0, \bar{\alpha}_0, \bar{\beta}_0\right) \geqslant tcu_i\,(w_{0^i}) \geqslant \lambda_i\, tcu_i\left(w_i^{LO}\right) + (1 - \lambda_i)\, tcu_i\left(w_i^{UP}\right)$, since tcu is a concave univariate function.

For each i such that $w_{L_0 i} < w_{U_0 i}$, $\lambda_{0i} = (w_{U_0 i} - w_{0i})/(w_{U_0 i} - w_{L_0 i})$. Moreover, $w_{L_0 i}$ and $w_{U_0 i}$ can be represented by a convex combination of w_i^{LO} and w_i^{UP}, using $\lambda_{Li} = \left(w_i^{UP} - w_{L_0 i}\right) / \left(w_i^{UP} - w_i^{LO}\right)$ and $\lambda_{Ui} = \left(w_i^{UP} - w_{U_0 i}\right) / \left(w_i^{UP} - w_i^{LO}\right)$, respectively. Since tcu is a concave univariate function, $tcu_i\left(w_{L_0 i}\right) \geqslant \lambda_{Li} tcu_i\left(w_i^{LO}\right) + \left(1 - \lambda_{Li}\right) tcu_i\left(w_i^{UP}\right)$ and $tcu_i\left(w_{U_0 i}\right) \geqslant \lambda_{Ui} tcu_i\left(w_i^{LO}\right) + (1 - \lambda_{Ui})\, tcu_i\left(w_i^{UP}\right)$. Then, using these inequalities in $-k_i^c\left(\bar{x}_0, \bar{z}_0, \bar{\alpha}_0, \bar{\beta}_0\right) \geqslant \lambda_{0i} tcu_i\left(w_{L_0 i}\right) + \left(1 - \lambda_{0i}\right) tcu_i\left(w_{U_0 i}\right)$ and the values of λ_{0i}, λ_{Li}, λ_{Ui} and λ_i, the inequality $-k_i^c\left(\bar{x}_0, \bar{z}_0, \bar{\alpha}_0, \bar{\beta}_0\right) \geqslant tcu_i\left(w_{0i}\right) \geqslant \lambda_i tcu_i\left(w_i^{LO}\right) + \left(1 - \lambda_i\right) tcu_i\left(w_i^{UP}\right)$ is satisfied.

Then, the point $(\bar{x}_0, \bar{z}_0, \bar{\alpha}_0, \bar{\beta}_0, \bar{\lambda}_0)$ is feasible in CP.

(b) It is a consequence of part (a) and property (P4).

This theorem will be used in step 2 of the new algorithm to check infeasibility of MP.

6. Branching

Let $\bar{p} = \left(\bar{x}, \bar{z}, \bar{\alpha}, \bar{\beta}, \bar{w}_L, \bar{w}_U, \bar{\lambda}\right)$ be a feasible solution in MP, having $\sum_{i=1}^{J} (w_{Ui} - w_{Li}) > 0$. This positive value is called *gap*. Also, a variable w_i is involved in the gap if $w_{Li} < w_{Ui}$.

Four possible cases may arise when MP is solved in Region D.

Case 1. A feasible point with an objective value equal to 0 is obtained. It represents a new feasible point of the original problem with an objective value lower than the upper bound f^{UP}. Then, the upper bound to the global optimal objective can be updated.

Case 2. A feasible point with an objective value greater than 0 is obtained and all the values of λ_i are equal to 0 or 1 for those i so that w_i is involved in the gap. In this case, although the variable bounds are not equal, the solution represents a new feasible point of P.
Case 3. The problem is infeasible in the current region D and therefore there is no solution of P in D with an objective value lower than $f^{UP}-\varepsilon$. The region can be discarded for further considerations.
Case 4. A feasible point with an objective value greater than 0 is obtained and at least one variable λ_i is not 0 or 1 for some i so that w_i is involved in the gap. This point may be a local optimal of MP and therefore it is not possible to obtain any conclusion about the original problem. The point is feasible in MP but infeasible in RP. Then, the local optimum has to be eliminated, and this is accomplished by subdividing D into smaller regions. MP is solved again in each subdomain, in order to obtain a better solution of P or discard the region.

The following theorem is applied to the previous fourth case.

THEOREM 2. *Let us assume* $\bar{p}^* = \left(\bar{x}^*, \bar{z}^*, \bar{\alpha}^*, \bar{\beta}^*, \bar{w}_L^*, \bar{w}_U^*, \bar{\lambda}^*\right)$ *be an optimal solution for* MP, *with* $\sum_{i=1}^{J}\left(w_{Ui}^* - w_{Li}^*\right) > 0$. *And assume* $G^0 = \left\{i : w_{Li}^* < w_{Ui}^* \wedge 0 < \lambda_i^* < 1, i = 1, \ldots, J\right\}$. *Then, the constraint* $\lambda_i\ tcu_i\left(w_{Li}\right) + \left(1-\lambda_i\right) tcu_i\left(w_{Ui}\right) \leqslant -k_i^c\left(\bar{x}, \bar{z}, \bar{\alpha}, \bar{\beta}\right)$ *is active in* MP *for* $i \in G^0$.

Proof. Let $i \in G^0$. The KKT conditions for $\bar{p}^*$ that correspond to variables λ_i, w_{Li} and w_{Ui} are

$$\mu_1\left(tcu(w_{Li}^*) - tcu(w_{Ui}^*)\right) + \gamma\left(w_{Li}^* - w_{Ui}^*\right) - \mu_\lambda^1 + \mu_\lambda^2 = 0, \qquad (1)$$
$$-1 + \mu_1\left(\lambda_i^* tcu'(w_{Li}^*)\right) + \gamma\left(\lambda_i^*\right) + \mu_2 - \mu_{w_L}^1 + \mu_{w_L}^2 = 0, \qquad (2)$$
$$1 + \mu_1\left((1-\lambda_i^*) tcu'(w_{Ui}^*)\right) + \gamma\left(1-\lambda_i^*\right) - \mu_2 - \mu_{w_U}^1 + \mu_{w_U}^2 = 0, \qquad (3)$$
$$\mu_1\left(\lambda_i^* tcu_i\left(w_{Li}^*\right) + \left(1-\lambda_i^*\right) tcu_i\left(w_{Ui}^*\right) + k_i^c\left(\bar{x}^*, \bar{z}^*, \bar{\alpha}^*, \bar{\beta}^*\right)\right) = 0,$$
$$\mu_2\left(w_{Li}^* - w_{Ui}^*\right) = 0,$$

$$\mu_\lambda^1\left(0 - \lambda_i^*\right) = 0,$$
$$\mu_\lambda^2\left(\lambda_i^* - 1\right) = 0,$$
$$\mu_{w_L}^1\left(w_i^{LO} - w_{Li}^*\right) = 0,$$
$$\mu_{w_L}^2\left(w_{Li}^* - w_i^{UP}\right) = 0,$$
$$\mu_{w_U}^1\left(w_i^{LO} - w_{Ui}^*\right) = 0,$$
$$\mu_{w_U}^2\left(w_{Ui}^* - w_i^{UP}\right) = 0,$$
$$\mu_1, \mu_2, \mu_\lambda^1, \mu_\lambda^2, \mu_{w_L}^1, \mu_{w_L}^2, \mu_{w_U}^1, \mu_{w_U}^2 \geqslant 0.$$

By hypothesis: $0 < \lambda_i^* < 1$. Then, $\mu_\lambda^1 = \mu_\lambda^2 = 0$. Moreover, $w_{Li}^* < w_{Ui}^*$, so $\mu_2 = 0$. Also $\mu_{w_L}^2 = \mu_{w_U}^1 = 0$, since, $w_{Li}^* < w_{Ui}^* \leqslant w_i^{UP}$ and $w_i^{LO} \leqslant w_{Li}^* < w_{Ui}^*$. Suppose the constraint is not active, then $\mu_1 = 0$. From (1), since $w_{Li}^* < w_{Ui}^*$, it must be $\gamma = 0$. Thus, from (2) and (3): $\mu_{w_L}^1 = -1$ and $\mu_{w_U}^2 = -1$. This is absurd due to the nonnegativity of multipliers. Therefore, the constraint must be active.

Therefore, if MP is solved and Case 4 takes place, the set G^0 defined in Theorem 2 is not empty. Also, each $i \in G^0$ satisfies:

$$\lambda_i^* \, tcu_i\left(w_{Li}^*\right) + \left(1 - \lambda_i^*\right) tcu_i\left(w_{Ui}^*\right) = -k_i^c\left(\bar{x}^*, \bar{z}^*, \bar{\alpha}^*, \bar{\beta}^*\right),$$
$$w_i^* = \lambda_i^* w_{Li}^* + \left(1 - \lambda_i^*\right) w_{Ui}^*,$$
$$0 < \lambda_i^* < 1 \quad w_{Li}^* < w_i^* < w_{Ui}^* \quad w_i^{LO} \leqslant w_{Li}^* < w_i^{UP} \quad w_i^{LO} < w_{Ui}^* \leqslant w_i^{UP}.$$

Then, the local optimum of MP satisfies all constraints in RP, except for $tcu_i(w_i) \leqslant -k_i^c\left(\bar{x}, \bar{z}, \bar{\alpha}, \bar{\beta}\right)$ for $i \in G^0$. Then, it is desirable to eliminate this local optimal point from the feasible set of MP.

A suitable way to eliminate it is by partitioning the range for variable w_{i_0}, for some $i_0 \in G^0$. The current Region D is divided into two subregions, D_1 and D_2, both having the same bounds as Region D for every variable, except for w_{i_0}. The range for this variable in $D_1$is $[w_{i_0}^{LO}, w_{i_0}^*]$, and the range in D_2 is $[w_{i_0}^*, w_{i_0}^{UP}]$. Now, the previous local optimal point is infeasible in both new regions.

There is another way to branch. Instead of dividing Region D in two subregions, it can be divided in four subregions. All of them have the same bounds as Region D for every variable, again except for w_{i_0}. The ranges for variable w_{i_0} in the four generated subregions are $[w_{i_0}^{LO}, w_{Li_0}^*]$, $[w_{Li_0}^*, w_{i_0}^*]$, $[w_{i_0}^*, w_{Ui_0}^*]$ and $[w_{Ui_0}^*, w_{i_0}^{UP}]$, considering of course only the intervals that has nonempty interior. This alternative creates many more nodes, but it has particular advantages. It is highly probable that the first and the last subregions give rise to infeasible MP problems. This can be expected from the solution obtained in Region R. (The solver could not find a local solution in these ranges). In such a case, the region might be reduced faster than carrying out partition in two subregions.

The branching is performed in one variable in the gap. A selection rule has to be applied when there are more than one variable in the gap. The variable is chosen obeying one of the rules:

Rule 1. choose the variable which has the greatest gap $i_0 = \arg\max\limits_{i \in G^0} \left\{w_{Ui}^* - w_{Li}^*\right\}$.

Rule 2. select the variable with the greatest weighted gap: $i_0 = \arg\max_{i \in G^0} \left\{(w^*_{Ui} - w^*_{Li})/(w_i^{UP} - w_i^{LO})\right\}$.

Rule 3. select the variable with the greatest approximation error: $i_0 = \arg\max_{i \in G^0} \left\{tcu_i\left(w_i^*\right) - \left(\lambda_i^* tcu_i\left(w^*_{Li}\right) + \left(1-\lambda_i^*\right) tcu_i\left(w^*_{Ui}\right)\right)\right\}$.

Rule 4. select the variable with the greatest minimal approximation $i_0 = \arg\max_{i \in G^0} \left\{\min\{w_i^* - w^*_{Li}, w^*_{Ui} - w_i^*\}\right\}$

Rule 5. weighted version of Rule 4.

Rule 6. choose the variable in a sort of priority order.

Alternatively, the branching can be performed on all the variables in G^0. In this case, all combinations between the subdomains of the variables should be considered. If bisection is used for each variable, then the number of generated subregions is $2^{|G^0|}$. If the branching is performed subdividing the range of each variable in four intervals, then the number of generated subregions is $4^{|G^0|}$ (supposing that no interval is empty). Clearly, the number of subregions grows fast. Therefore, this option is just suitable for small problems, that is, for problems having a few variables.

7. The Improve-and-Branch algorithm

Given a problem in the P form, the algorithm involves the following steps:

Step 1. Initialization:
Select a value for improvement parameter ε. Reformulate the problem in order to put it in the RP form and formulate the main problem MP. Let $P = \{\text{Ro}\}$ be the set of regions to be explored, where Ro is the hyperectangle defined by the bounds in RP. Solve the RP problem with a local solver. If a feasible solution is found, denote this solution by $\left(\bar{x}^{OPT}, \bar{z}^{OPT}, \bar{\alpha}^{OPT}, \bar{\beta}^{OPT}\right)$ and f^{UP} the objective value. If not, assign f^{UP} a value big enough. Set iter=1 and R_{iter}=Ro.

Step 2. Solution of the MP Problem:
Solve the MP problem in Region R_{iter} with a local solver.
If MP is infeasible in Region R_{iter}, set $P = P \setminus \{R_{\text{iter}}\}$. Go to Step 5.
Otherwise, let $\left(\bar{x}^*, \bar{z}^*, \bar{\alpha}^*, \bar{\beta}^*, \bar{w}^*_L, \bar{w}^*_U, \bar{\lambda}^*\right)$ be the optimum.
Define $G^0 = \left\{i : w^*_{Li} < w^*_{Ui} \wedge 0 < \lambda_i^* < 1, i = 1, \ldots, J\right\}$.
If $G^0 = \emptyset$, (the current solution is a feasible point of RP) go to Step 3, else go to Step 4.

Step 3. Solution of the RP Problem:
Solve the RP problem in Region R_{iter} starting from the feasible point $(\bar{x}^*, \bar{z}^*, \bar{\alpha}^*, \bar{\beta}^*)$ with a local solver adding constraint $f^c(\bar{x}, \bar{z}) \leqslant f^{UP} - \varepsilon$. Let $(\bar{x}^*, \bar{z}^*, \bar{\alpha}^*, \bar{\beta}^*)$ be the local solution and f^* the objective value. Update: $(\bar{x}^{OPT}, \bar{z}^{OPT}, \bar{\alpha}^{OPT}, \bar{\beta}^{OPT}) = (\bar{x}^*, \bar{z}^*, \bar{\alpha}^*, \bar{\beta}^*)$, $f^{UP} = f^*$. Go to Step 5.

Step 4. Branching:
Apply a branching rule to R_{iter} in one or more variables involved in the gap, generating new subregions $\{R_{\text{iter}_1}, R_{\text{iter}_2}, \ldots, R_{\text{iter}_q}\}$, place them on the list P and set $P = P \setminus \{R_{\text{iter}}\}$. Go to Step 5.

Step 5. Stop Criterion:
If P=Ø, stop: the current best solution is the global optimal. Otherwise, set iter = iter + 1 and choose R_{iter} from P. Return to Step 2 (See Figure 3).

8. Bound Reduction Strategies and Convergence

The proposed algorithm has the same structure than the branch-and-bound ones, but it does not look for bounds for the objective function. However, one region is discarded when it is infeasible, requiring that the objective function value shall be less than the best one at the moment, like in a branch-and-bound method. Thus, the finite convergence characteristics of the branch-and-bound algorithms are valid for the proposed algorithm.

Nevertheless, the critical importance of the tightness of variable bounds to reach reasonable convergence speed is widely known. The proposed algorithm finishes when all subregions have been discarded due to infeasibility. Success of many branch-and-bound methods relies on good procedures for tightening the bounds in the variables (Ryoo and Sahinidis, 1996; Zamora and Grossmann, 1999). The practice of solving 2n problems has been proposed to find the maximal and minimal values of each variable subject to the relaxation of the original constraints. This procedure may be too costly to be applied.

In the algorithm proposed in this paper, a feasibility-based range reduction is applied. The bound-tightening procedure used here is, in some sense, similar to the monotonicity and bounding tests proposed by Hansen et al. (1991) in their analytical approach to global optimization. It captures the relationship between the variables based on the original constraints.

9. Implementation Issues

Since MP is solved with a local optimization solver, there exists the possibility of declaring a subregion infeasible when actually it is not. An efficient strategy to overcome this difficulty is to solve the convex problem CP

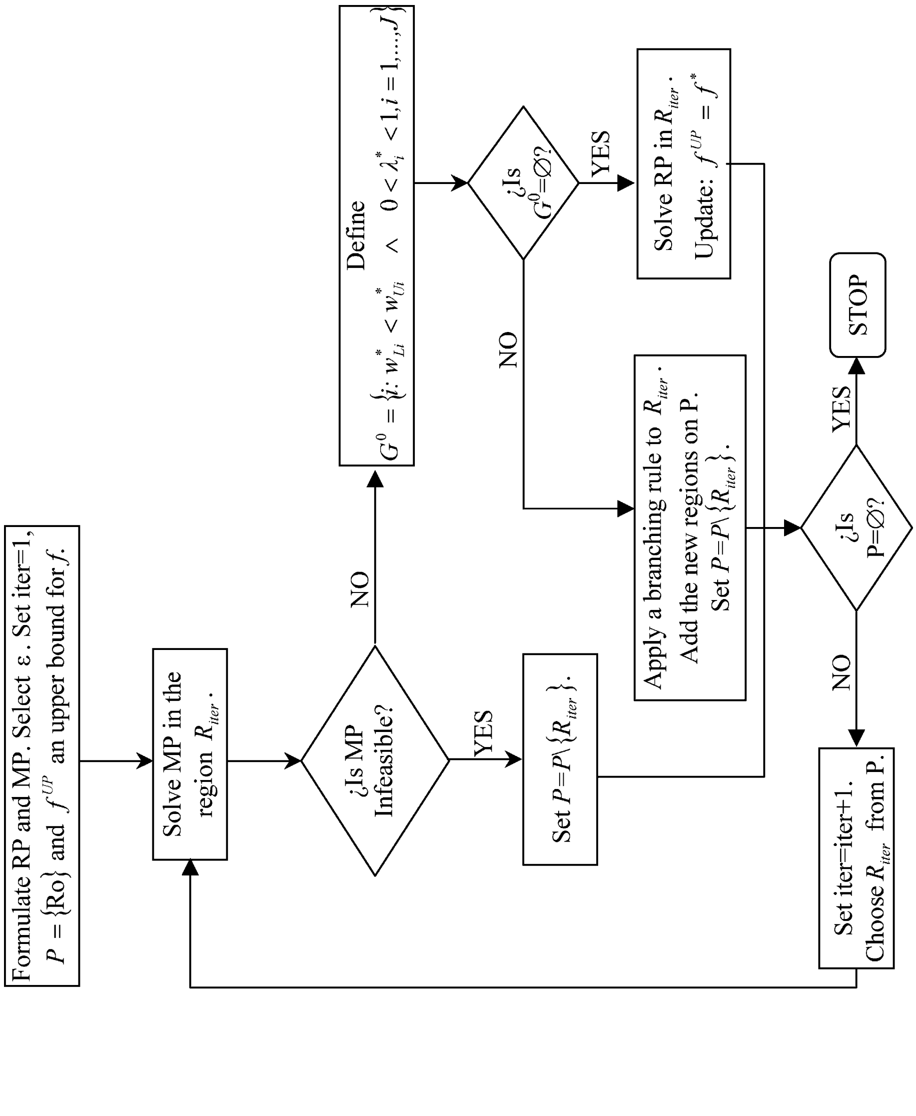

Figure 3. Algorithm scheme.

before discarding the current region. Note that solving CP provides a feasible point of MP or proves that MP is infeasible (Theorem 2.a). In the first case, the MP is solved with the solution of CP as starting point.

It should be noted that the initial (feasible) point for RP is provided by the solution of MP where the objective value is 0. Then, each time RP is solved, it is feasible and provides a new upper bound.

The algorithm is also applicable to MINLP problems. The approach is the same adopted by some researches (Ryoo and Sahinidis, 1995). Binary variables are modeled as continuous variables and integrality is forced at all feasible points by introducing integrality constraints. In particular, it has been suggested the integrality constraint: $x-x^2=0$, which forces x to a value of either 0 or 1. A valid convex relaxation of this constraint is obtained by replacing the quadratic term by a new variable z and formulating the convex envelope of this bilinear term: $z \leqslant x$, $z \geqslant 0$, $z \geqslant 2x-1$. As it was pointed out by Smith and Pantelides (1999), this inequalities combined with the original constraints $x-z=0$ are equivalent to $0 \leqslant x \leqslant 1$, which add no more information to the convex relaxation. In our approach, however, the noconvexities involved in the integrality constraints of the binary variables give rise to a new improvement direction. Integrality constraints can be expressed as two inequalities: $x^2-x \leqslant 0$ and $x-x^2 \leqslant 0$, the first one being convex and the second concave. Then, they are included in MP through the following formulation:

$$x^2-x \leqslant 0,$$
$$x-\left[\lambda(x_L)^2+(1-\lambda)(x_U)^2\right] \leqslant 0.$$

Then, x_U-x_L appears in the objective function.

It is worth noting that there exists a compromise between the magnitude of the improvement parameter ε and the algorithm performance. A large value might allow the algorithm to miss the global solution. On the other hand, a very small value of ε may slow down the region discarding speed.

10. Computational Results

The algorithm was implemented in GAMS (Brooke et al., 1997) and a large number of test problems were solved, six of which are presented here. GAMS/CONOPT solver was used to solve the NLP problems in a 1.5 GHz Pentium 4 PC.

It is difficult to compare the algorithm proposed here with other global optimization algorithms. That is because of several facts: the algorithms are tested in computers with different performances, each problem has several ways to deal with, improvements for the algorithms are made continuously, etc. Therefore, the examples in this section were taken from the literature

Table 1. Computational results for example 1

ε	With bound reduction techniques			Without bound reduction techniques		
	Total iterations	CPU time	n° iter. global sol.	Total iterations	CPU time	n° iter. global sol.
0.05	12	1.97	5	30	4.91	11
0.01	11	1.79	2	38	4.81	2
0.005	26	3.57	2	56	7.34	2
0.001	31	4.40	3	69	9.66	3

and the comparison with other algorithms was made taking as reference the computational results reported by other authors.

EXAMPLE 1. As a first example we consider the maximization of the Himmelblau's function (Himmelblau, 1972). The function is:

$$f_h(\bar{x}) = (x_1^2 + x_2 - 11)^2 + (x_1 + x_2^2 - 7)^2, \quad -4 \leqslant x_1 \leqslant 4, \quad -4 \leqslant x_2 \leqslant 4.$$

This is a classical test function. Inside the domain, it has four global minimums, 1 maximum, and four saddle points. However, the global maximum is a boundary point. The global solution is in point $\bar{x} = (0.3124484, -4)$.

The problem can be reformulated in the following way (minimization form):

$$\begin{aligned}
&\min f = -c_1 - c_2,\\
&\text{s.t.} - c_1 + w_1^2 \leqslant 0,\\
&\quad -c_2 + w_2^2 \leqslant 0,\\
&\quad -w_1 + x_1^2 + x_2 - 11 \leqslant 0,\\
&\quad -w_2 + x_2^2 + x_1 - 7 \leqslant 0,\\
&\quad -c_1 - w_1^2 \leqslant 0,\\
&\quad -c_2 - w_2^2 \leqslant 0,\\
&\quad -w_1 - x_1^2 - x_2 + 11 \leqslant 0,\\
&\quad -w_2 - x_2^2 - x_1 + 7 \leqslant 0.
\end{aligned}$$

There is a concave term in each last four constraints. The other constraints are convex. So, there are four variables involved in nonconvex terms.

The problem was solved with the proposed algorithm, applying the first rule of branching and employing bound reduction techniques.

The algorithm performance with different values of parameter ε was tested in order to study the importance of the parameter with and without bound reduction techniques. Table 1 shows the total number of iterations, the CPUs, and the number of iterations in which the global solutions was found.

It is interesting to stand out that in all the cases with bound reduction techniques, whenever there was a gap, it was in only one variable. Thus, any branching rule could be used. In the case without bound reduction techniques, there were two cases similar to the previous ones, and two cases in which a gap in two variables occurred.

EXAMPLE 2. The second example involves trigonometric functions. It was taken from Maranas and Floudas (1994). The problem studies the molecular conformation of pseudoethane, an ethane molecule in which all the hydrogen atoms have been replaced by C, N or O atoms. The objective is to minimize the potential energy of small molecules which is expressed in terms of a single dihedral angle (t):

$$
\begin{aligned}
\min f(t) = {} & \frac{588600}{\left(3r_0^2 - 4\cos(\theta)r_0^2 - 2\left(\sin^2(\theta)\cos\left(t - \frac{2\pi}{3}\right) - \cos^2(\theta)\right)\ r_0^2\right)^6} \\
& - \frac{1079.1}{\left(3r_0^2 - 4\cos(\theta)r_0^2 - 2\left(\sin^2(\theta)\cos\left(t - \frac{2\pi}{3}\right) - \cos^2(\theta)\right)\ r_0^2\right)^3} \\
& + \frac{600800}{\left(3r_0^2 - 4\cos(\theta)r_0^2 - 2\left(\sin^2(\theta)\cos(t) - \cos^2(\theta)\right)\ r_0^2\right)^6} \\
& - \frac{1071.5}{\left(3r_0^2 - 4\cos(\theta)r_0^2 - 2\left(\sin^2(\theta)\cos(t) - \cos^2(\theta)\right)\ r_0^2\right)^3} \\
& + \frac{481300}{\left(3r_0^2 - 4\cos(\theta)r_0^2 - 2\left(\sin^2(\theta)\cos\left(t + \frac{2\pi}{3}\right) - \cos^2(\theta)\right)\ r_0^2\right)^6} \\
& - \frac{1064.6}{\left(3r_0^2 - 4\cos(\theta)r_0^2 - 2\left(\sin^2(\theta)\cos\left(t + \frac{2\pi}{3}\right) - \cos^2(\theta)\right)\ r_0^2\right)^3} \\
& 0 \leqslant t \leqslant 2\pi,
\end{aligned}
$$

where r_0 is the covalent bond length (1.54Å) and θ is the covalent bond angle (109.5°).

Maranas and Floudas reported results on this problem applying their α-BB algorithm: the convergence to the global optimum solution within 10^{-6} tolerance is achieved in 21 iterations and 1.1 CPU seconds on an HP-9000/730.

The function f has three local minimums in the domain. Two local optimums appear at $t=1.0546$, $f=-0.7970$ and $t=5.1683$, $f=-1.0396$. The global minimum is at $t=3.2018$ and $f=-1.0709$.

The problem was solved in two different ways.

For the first approach the problem is reformulated in the following way:

$$
\begin{aligned}
&\textbf{RP1}: \min f = z_1+z_2+z_3+z_4+z_5+z_6,\\
&\text{s.t.}\quad z_1 \geqslant \frac{588600}{\left(A-B\cos\left(t-\frac{2\pi}{3}\right)\right)^6}=g_1(t) \quad z_2 \geqslant -\frac{1079.1}{\left(A-B\cos\left(t-\frac{2\pi}{3}\right)\right)^3}=g_2(t)\\
&\qquad z_3 \geqslant \frac{600800}{(A-B\cos(t))^6}=g_3(t) \qquad z_4 \geqslant -\frac{1071.5}{(A-B\cos(t))^3}=g_4(t)\\
&\qquad z_5 \geqslant \frac{481300}{\left(A-B\cos\left(t+\frac{2\pi}{3}\right)\right)^6}=g_5(t) \quad z_6 \geqslant -\frac{1064.6}{\left(A-B\cos\left(t+\frac{2\pi}{3}\right)\right)^3}=g_6(t)\\
&\qquad 0 \leqslant t \leqslant 2\pi,
\end{aligned}
$$

where $A=3r_0^2-4\cos(\theta)r_0^2+2\cos^2(\theta)r_0^2$, and $B=2\sin^2(\theta)r_0^2$. Since the algorithm is based on underestimating concave univariate functions, the intervals where functions $g_i(t)$ are concave or convex were determined. Each $g_i(t)$ has two inflection points in the domain. So, the interval $[0\leqslant t\leqslant 2\pi]$ was divided in thirteen subintervals, as it is shown in Figure 4a. Thus, the algorithm was applied in each interval. In each analyzed region, two or three $g_i(t)$ are concave, and the remaining ones are convex. The algorithm required a total of 45 iterations and 3.08 CPUs in order to guarantee globality within 10^{-6} tolerance.

The second approach reformulates the problem in the following way:

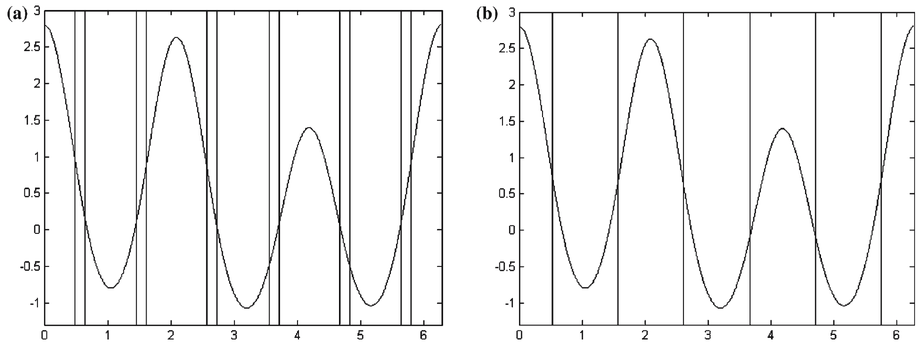

Figure 4. Subintervals defined by inflection points.

RP2: $\min f = z_1 + z_2 + z_3 + z_4 + z_5 + z_6$

$$\text{s.t.}\quad z_1 \geqslant \frac{588600}{(w_1)^6} = h_1(w_1), \qquad z_2 \geqslant \frac{600800}{(w_2)^6} = h_2(w_2),$$

$$z_3 \geqslant -\frac{481300}{(w_3)^3} = h_3(w_3), \qquad z_4 \geqslant -\frac{1079.1}{(w_1)^3} = h_4(w_1),$$

$$z_5 \geqslant -\frac{1071.5}{(w_2)^3} = h_5(w_2), \qquad z_6 \geqslant -\frac{1064.6}{(w_3)^3} = h_6(w_3),$$

$$(w_1 - A)/B \geqslant -\cos(t - \tfrac{2\pi}{3}) = h_7(t), \qquad (-w_1 + A)/B \geqslant \cos(t - \tfrac{2\pi}{3}) = h_8(t,)$$

$$(w_2 - A)/B \geqslant -\cos(t) = h_9(t) \qquad (-w_2 + A)/B \geqslant \cos(t) = h_{10}(t)$$

$$(w_3 - A)/B \geqslant -\cos(t + \tfrac{2\pi}{3}) = h_{11}(t) \qquad (-w_3 + A)/B \geqslant \cos(t + \tfrac{2\pi}{3}) = h_{12}(t)$$

Functions h_1, h_2 and h_3 are convex, and functions h_4, h_5 and h_6 are concave. However, each function h_i, i=7, ... ,12 has two inflection points in the domain. The inflection points are the same for the pairs $h_7 - h_8$, $h_9 - h_{10}$ and $h_{11} - h_{12}$. Thus, interval $[0 \leqslant t \leqslant 2\pi]$ was divided in seven subintervals, as it is shown in Figure 4b, and the algorithm was applied in them. In each analyzed region, six $h_i(t)$ are concave, and the remaining ones are convex. The algorithm took seven iterations and 1.02 CPUs, within 10^{-6} tolerance.

EXAMPLE 3. This example attempts to find the global minimum of the Hartman's function (Dixon and Szegö, 1978). The function is given by

$$f(x) = -\sum_{i=1}^{m} c_i \exp\left(\sum_{j=1}^{n} a_{ij}(x_j - p_{ij})^2\right)$$

for $0 \leqslant \bar{x} \leqslant 1$.

The minimization of f can be reformulated as the following problem RP:

$$\begin{aligned}
&\min f(x) = -\sum_{i=1}^{m} y_i,\\
\text{s.t.}\quad & y_i - c_i \exp(-z_i) \leqslant 0,\\
& -y_i + c_i \exp(-z_i) \leqslant 0 \qquad i = 1, \ldots, m,\\
& z_i = \sum_{j=1}^{n} a_{ij} w_j - 2a_{ij} x_j p_{ij} + a_{ij} p_{ij}^2,\\
& w_j - x_j^2 \leqslant 0 \qquad j = 1, \ldots, n,\\
& -w_j + x_j^2 \leqslant 0,\\
& x_j \leqslant 1 \qquad j = 1, \ldots, n,\\
& z_i, y_i, w_j, x_j \geqslant 0 \qquad i = 1, \ldots, m \;\; j = 1, \ldots, n.
\end{aligned}$$

Table 2. Data for instance 1 of example 3

i	a_{ij}			c_i	p_{ij}		
1	3.0	10	30	1.0	0.3689	0.1170	0.2673
2	0.1	10	35	1.2	0.4699	0.4387	0.7470
3	3.0	10	30	3	0.1091	0.8732	0.5547
4	0.1	10	35	3.2	0.03815	0.5743	0.8828

Table 3. Solution time for different values of improvement parameter ε

ε	With bound reduction		Without bound reduction	
	Iterations	CPU time	Iterations	CPU time
0.05	36	4.91	132	18.64
0.01	51	9.52	339	53
0.005	36	5.92	375	55.87
0.001	38	8.15	478	86.98

There are $m+n$ variables involved in nonconvex terms.

Two instances of this problem were solved with the proposed algorithm. The first instance of the problem has $m=4$ and $n=3$. In Table 2 the data for the problem are shown

The global solution is $f=-3.86278$, at $\bar{x}=(0.11464, 0.55565, 0.85255)$.

Again, a study about the importance of improvement parameter ε was made, assigning it several different values. Table 3 shows the number of iterations and computational time required in each case.

The second instance of the Hartman's problem that was implemented considers $m=4$ and $n=6$. The data are shown in Table 4 and Table 5.

Table 4. Data for instance 2 of example 3- parameters a and c

i	a_{ij}						c_i
1	10	3	17	3.5	1.7	8	1
2	0.05	10	17	0.1	8	14	1.2
3	3	3.5	1.7	10	17	8	3
4	17	8	0.05	10	0.1	14	3.2

Table 5. Data for instance 2 of example 3- parameters p

i	p_{ij}					
1	0.1312	0.1696	0.5569	0.0124	0.8283	0.5886
2	0.2329	0.4135	0.8307	0.3736	0.1004	0.9991
3	0.2348	0.1451	0.3522	0.2883	0.3047	0.6650
4	0.4047	0.8828	0.8732	0.5743	0.1091	0.0381

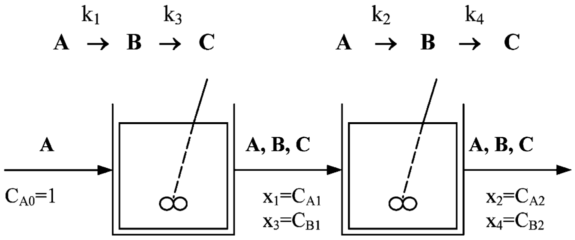

Figure 5. Reactor network design.

The global optimal solution is $f=-3.32314$ at $\bar{x}=(0.20165, 0.15021, 0.47737, 0.27531, 0.31163, 0.65740)$, and it was found in the first iteration. The algorithm requires 181 iterations to guarantee globality and takes 52.46 CPU sec. The value of improvement parameter ε was 0.01. Without bound reduction the problem could not be solved in less than 1000 iterations.

EXAMPLE 4. The next example is the simple reactor network design problem (see Figure 5), which was considered and reformulated in Section 3.

The global optimum is reached at the point $\bar{x}=(0.7715, 0.517, 0.2042, 0.3888, 3.0365, 5.0961)$ with objective value $f=-0.3888$. The problem also has two local minimums, at $\bar{x}=(0.390, 0.390, 0.375, 0.375, 16, 0)$ and at $\bar{x}=(1, 0.393, 0, 0.388, 0, 16)$. This example constitutes a very difficult test problem as it exhibits a local minimum with an objective function value that is very close to that of the global solution. Ryoo and Sahinidis (1995) solve this problem with a branch-and-reduce algorithm. Their algorithm finds the global solution in the first iteration and proves optimality after exploring more than 400 nodes, with a tolerance of $\varepsilon=10^{-6}$. Maranas and Floudas (1997) also solve this problem, using 299 iterations of the global optimization algorithm.

Introducing the separable formulation for the four bilinear terms leads to a problem with 10 nonconvex variables. Then, the main problem has 54 variables and 47 constraints. This problem is solved in 363 iterations with the proposed algorithm, taking 46.13 CPU s, using a tolerance $\varepsilon=10^{-4}$ and Rule 2 for variable branching selection.

However, note that nonconvex variables α and β are defined:

$$\alpha = x_i + V_j,$$
$$\beta = x_i - V_j,$$

where $0 \leqslant x_i \leqslant 1$ and $0 \leqslant V_j \leqslant 16$. The bounds for α and β are then: $0 \leqslant \alpha \leqslant 17$ and $-16 \leqslant \beta \leqslant 1$. A much tighter relaxation is obtained by scaling

Table 6. Computational results for example 4

Rule	Total Iterations	N° iter global solution	CPU Time	Epsilon
1	117	5	13.77	$\varepsilon = 10^{-4}$
2	151	5	15.72	$\varepsilon = 10^{-4}$
3	143	3	17.63	$\varepsilon = 10^{-4}$
4	147	3	17.68	$\varepsilon = 10^{-4}$
5	143	3	15.15	$\varepsilon = 10^{-4}$

variables V_1 and V_2 so that the range for these variables is $0 \leqslant V_j \leqslant 1$. The reaction constants are redefined so that they absorb the scale factor: $k_1 = 16^*0.09755988$, $k_2 = 0.99\,k_1$, $k_3 = 16^*0.0391908$, $k_4 = 0.9\,k_3$ and the last restriction is scaled: $V_1^{0.5} + V_2^{0.5} \leqslant 1$. In this way, the new ranges for α and β are: $0 \leqslant \alpha \leqslant 2$ and $-1 \leqslant \beta \leqslant 1$.

With this modification, the proposed algorithm finishes the search in 151 iterations taking 15.75 CPU s, with an improvement parameter value of $\varepsilon = 10^{-4}$ and Rule 2 for the branching variable selection. If a tolerance of $\varepsilon = 10^{-5}$ is used, the elimination of regions takes 209 iterations and if the tolerance is of $\varepsilon = 10^{-6}$, the number of required iterations is 225 (both with Rule 1).

Different branching variable selection rules were tested in this problem. Table 6 shows the number of total iterations for the application of each rule, improvement parameter and the iteration the global solution was found at.

Bound reduction plays a decisive role in this problem, since convergence could not be reached in less than 2000 iterations when bound reduction is not performed.

EXAMPLE 5. This example illustrates the applicability of the proposed algorithm to solve MINLP problems to global optimality.

The problem represents a heat exchanger network design, with a hot stream to be cooled and a cold stream to be heated. The network consists of one exchanger, one cooler and one heater. The cooler uses cooling water to reach the target temperature of the hot streams, and the heater uses high-pressure steam as heating utility. Data are given in Table 7.

The variables to be determined are heat loads, areas of the exchangers and temperatures T_1 and T_2. The objective function takes into account both utility and investment cost. The investment cost is defined over a set of subintervals for the areas of the exchangers, resulting in a discontinuous function. Türkay and Grossmann (1996) formulate the discontinuous cost with a disjunction.

Table 7. Data for example 5

Cost Coefficient			
Area of Exchanger (m^2)	Fixed charge (\$ /yr)	Variable cost (\$ /m^2 yr)	
$0 < A < 10$	$\beta_1 = 3000$	$\alpha_1 = 2750$	
$10 < A < 25$	$\beta_2 = 15000$	$\alpha_2 = 1500$	
$25 < A < 50$	$\beta_3 = 46500$	$\alpha_3 = 600$	
		$n = 0.6$	
Overall heat transfer coefficient U_j (kW/m^2 K)			
$U_1 = 1.5$	$U_2 = 0.5$	$U_3 = 1.0$	
Data of streams			
Stream	FC_p (kW/K)	Inlet temperature (K)	Outlet temperature (K)
Hot	10.0	500	340
Cold	7.5	350	560
Cooling water		300	320
Steam		600	600

The convex hull reformulation introduces 9 binary variables. The model, containing 21 continuous variables, 9 semicontinuous variables (partial areas), 9 binary variables and 43 constraints, is given as follows:

$$\min \quad c = 20Q_2 + 80Q_3 + \sum_{i=1}^{3}\sum_{j=1}^{3} c_{ji}$$

$$\text{s.t.} \quad c_{ji} = \alpha_i (A_{ji})^n + \beta_i y_{ji} \quad j = 1, 2, 3, \quad i = 1, 2, 3$$

$$A_j^{\text{tot}} = \sum_{i=1}^{3} A_{ji} \quad j = 1, 2, 3$$

$$\sum_{i=1}^{3} y_{ji} = 1 \quad j = 1, 2, 3$$

$$A_{lo\,i}\, y_{ji} \leqslant A_{ji} \leqslant A_{up\,i}\, y_{ji} \quad j = 1, 2, 3, \quad i = 1, 2, 3$$

$$Q_1 = Fcp^{\text{hot}}\left(T_{\text{in}}^{\text{hot}} - T_1\right)$$

$$Q_1 = Fcp^{\text{cold}}\left(T_2 - T_{\text{in}}^{\text{cold}}\right)$$

$$Q_1 = A_1^{\text{tot}} U_1 LMTD_1$$

$$LMTD_1 = \frac{\left((T_1 - T_{\text{in}}^{\text{cold}}) - (T_{\text{in}}^{\text{hot}} - T_2)\right)}{\ln\left((T_1 - T_{\text{in}}^{\text{cold}})/(T_{\text{in}}^{\text{hot}} - T_2)\right)}$$

$$Q_2 = Fcp^{\text{hot}}\left(T_1 - T_{\text{out}}^{\text{hot}}\right)$$

$$Q_2 = A_2^{\text{tot}} U_2 LMTD_2$$

$$LMTD_2 = \frac{\left((T_{\text{out}}^{\text{hot}} - T_{\text{in}}^{cw}) - (T_1 - T_{\text{out}}^{cw})\right)}{\ln\left((T_{\text{out}}^{\text{hot}} - T_{\text{in}}^{cw})/(T_1 - T_{\text{out}}^{cw})\right)}$$

$$Q_3 = Fcp^{\text{cold}}(T_{\text{out}}^{\text{cold}} - T_2)$$

$$Q_3 = A_3^{\text{tot}}\ U_3\ LMTD_3$$

$$LMTD_3 = \frac{\left((T^S - T_2) - (T^S - T_{\text{out}}^{\text{cold}})\right)}{\ln\left((T^S - T_2)/(T^S - T_{\text{out}}^{\text{cold}})\right)}$$

$$350 \leqslant T_1,\ \ T_2 \leqslant 500$$

$$c, c_{ij}, Q_j,\ \ A_j^{\text{tot}}, A_{ji} \geqslant 0$$

$$LMTD_j \in \Re \quad j = 1, 2, 3; \quad i = 1, 2, 3$$

$$A_{j1} \leqslant 10, \quad A_{j2} \leqslant 25, \quad A_{j3} \leqslant 50,$$

$$y_{ij} = 1, 0.$$

After reformulation, the problem has 19 variables appearing in convex terms, 21 variables in nonconvex terms (concave and bilinear), and 55 constraints; 29 of them are linear, 21 concave equalities and 5 bilinear equalities. When the bilinear terms are replaced by its separable formulation, the number of nonconvex variables increases to 31. The main problem involves 171 variables and 172 constraints.

The optimal values are shown in Table 9. The global solution corresponds to a cost of 117711$ /yr. The global solution was found in iteration 19. A total of 201 iterations were needed to check global optimality when Rule 1 for selection of branching variable and tolerance $\varepsilon = 100$ are used. The comparison of the number of total iterations and computational time required for different values of tolerance and branching selection rules are shown in Table 8. Bound reduction was critical for convergence in this example. It takes advantage of the semicontinuous and discrete nature of some variables (partial areas and binary variables y).

Table 8. Results for example 5

Rule	Total Iterations	N° iter global solution	CPU Time	Epsilon
1	201	19	72.69	$\varepsilon = 100$
1	204	21	91.29	$\varepsilon = 10$
2	270	17	105.47	$\varepsilon = 100$
2	552	27	225.28	$\varepsilon = 10$

Table 9. Optimal solution of example 5

Area of exchanger	Exchanger 1: 25 m^2 Exchanger 2: 20.33 m^2 Exchanger 3: 7.83 m^2
Temperature	T_1 = 397.76 K T_2 = 486.31 K
Heat loads	Q_1 = 1022.36 Q_2 = 577.64 Q_3 = 552.64

Although, this example was solved successfully; there exist some difficulties to solve general MINLP using the proposed algorithm. The binary nature of the variables is tackled using the integrality constraint $x - x^2 = 0$. Then, each binary variable adds one concave univariate term.

If the same approach is applied in order to deal with a general integer variable whose range is large enough, the problem size is enlarged considerably. Thus, the algorithm could require a high computational effort to solve the problem.

Therefore, the proposed strategy is efficient to solve MINLPs having few integer variables whose ranges are short enough. If the MINLP does not fit these characteristics, the common techniques used in general branch and bound algorithms can be applied, that is, considering integer variables as continuous and branching on fractional values.

EXAMPLE 6. This is a model of a heat exchanger network synthesis problem, taken from Floudas and Ciric (1989); Floudas et al. (1989). This is a stream superstructure of one cold stream and two hot streams for two heat exchangers. All possible flow configurations (splitting, mixing and bypassing) are considered. Variables f_i and t_i are thermal capacity flow rate and temperature of stream, respectively. H1 and H2 are heat streams whose heat loads are 800 kW and 1000 kW, inlet temperatures are 320 K and 340 K respectively, and outlet temperature is 300 K. C1 is cold stream with inlet temperature of 100 K and outlet temperature of 280 K. The problem is:

$$\min f = 1200\left[800/2.5\left(2/3\sqrt{(320-t_2)(300-t_1)} + \frac{(320-t_2)+(300-t_1)}{6}\right)\right]^{0.6}$$

$$+1200\left[1000/0.2\left(2/3\sqrt{(340-t_4)(300-t_3)} + \frac{(340-t_4)+(300-t_3)}{6}\right)\right]^{0.6},$$

$$
\begin{aligned}
\text{s.t.}\quad & f_1+f_2=10, \quad f_1+f_6=f_3, \quad f_2+f_5=f_4 \\
& f_5+f_7=f_3, \quad f_6+f_8=f_4 \\
& 100f_1+t_4f_6=t_1f_3, \quad 100f_2+t_2f_5=t_3f_4 \\
& f_3(t_2-t_1)=800, \quad f_4(t_4-t_3)=1000, \\
& 100\leqslant t_1\leqslant 290, \quad 100\leqslant t_2\leqslant 310, \\
& 100\leqslant t_3\leqslant 290, \quad 100\leqslant t_4\leqslant 330, \\
& 0\leqslant f_i\leqslant 10, \quad i=1,2,\dots,8.
\end{aligned}
$$

This problem has several local minimums, the global optimal solution is at $\bar{f}=(0,10,10,10,0,10,10,0)$, $\bar{t}=(200,280,100,200)$, with $f=12292.467132$.

Floudas and Ciric (1989) showed that the objective function is convex. Thus, the unique nonconvex terms are bilinear. The reformulated problem involves 12 variables in concave univariate terms (α_i and β_i) and 18 variables in convex terms. The proposed algorithm was applied using bound reduction techniques, within 10^{-6} tolerance. The global solution was determined in 1 iteration and 0.93 CPUs.

This example was used by Floudas et al. (1989) to test the decomposition global optimization approaches, and it took several iterations. Whereas, Ryoo and Sahinidis (1995) solved the problem using their branch-and-reduce algorithm. It took 1 iteration and 2.2 CPUs.

11. Conclusions

In this paper, a new global optimization method has been introduced to address nonlinear optimization problems, including nonconvexities both in the objective function and constraints. The proposed algorithm is deterministic and attains finite ε-convergence to the global optimal solution.

The algorithm is based on two problems, which are generated from the original problem. The first one is the reformulated problem, RP, and it is completely equivalent to the original problem. However, constraints of RP consist of linear equality constraints, convex inequality constraints and nonconvex inequality constraints. Also, each nonconvex inequality constraint has only one nonconvex term being a concave univariate function. The second one is the main problem, MP, and it is a nonconvex underestimation of the original problem. MP is formulated from RP, replacing each concave univariate term by its convex envelope, where the bound of the variables are variables. Thus, the objective function in MP minimizes the difference between variable bounds. In each iteration, MP forces the objective value to improve and minimizes the difference in upper and lower bounds. Then, there are two possibilities: a new better point is found, or a branch is performed over the current region. Moreover, the MP solution provides a key point to do the branching, a point that eliminates the local optimum of the current MP. The algorithm finishes when all the generated subregions have been analyzed and discarded. A bound reduction technique is performed in order to accelerate the convergence speed.

The algorithm is applicable to a large guide of optimization problems, as it was shown in the computational results. The examples include from general NLP to MINLP problems. All of them were solved efficiently.

The numerical performance of the proposed algorithm was tested with test problems and process design problems. Although reformulation introduces new variables and concave terms, the obtained results show that the algorithm compares very favorably to the ones reported in the literature. Moreover, several examples were solved in less time and iterations than the ones reported at the moment. Computational results and execution times indicate the algorithm is highly efficient.

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