A Combined Penalty Function and Outer-Approximation Method for MINLP Optimization

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OUTER-APPROXIMATION METHOD

FOR MINLP OPTIMIZATION

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ABSTRACT

An improved outer-approximation algorithm for MINLP optimization is proposed in this paper which is aimed at the solution of problems where convexity conditions may not hold. The proposed algorithm starts by solving the NLP relaxation. If an integer solution is not found, a sequence of iterations consisting of NLP subproblems and MILP master problems is solved. The proposed MILP master problem is based on the outer-approximation/equality-relaxation algorithm and features an exact penalty function that allows violations of linearizations of nonconvex constraints. The search proceeds until no improvement is found in the NLP subproblems. Computational experience is presented on a set of 18 test problems The results show that the proposed method has a high degree of reliability for finding the global optimum in nonconvex problems.

Introduction

There has been recently an increased interest in the development and application of nonlinear optimization algorithms that can handle both continuous and integer variables, especially of the 0-1 type. These problems, which **are** commonly referred to as mixed-integer nonlinear programming (MINLP) problems, have many applications in engineering design, planning, scheduling and marketing. Often the corresponding MINLP models exhibit special structures (e.g. graphs, networks, separable functions) that can be effectively exploited for developing specialized solution procedures. However, it is also very often the case, particularly in engineering design, that nonlinearities in the continuous variables do not exhibit any special form since they result from complex engineering models. Thus, there is clearly a strong motivation to develop MINLP algorithms that that are not overly restrictive in the assumptions of the form and properties of the functions that are involved.

Among the general purpose algorithms for MINLP, we can cite branch and bound (Beale,1977; Gupta, 1980), Generalized Benders Decomposition, GBD, (Benders, 1962; Geoffrion, 1972), the Outer-Approximation/Equality-Relaxation Method, OA/ER (Duran and Grossmann, 1986; Kocis and Grossmann, 1987), and the Feasibility Technique (Murtagh and Mawengkang, 1986; Mawengkang, 1988). The branch and bound method has the drawback that it can require the solution of a large number of NLP subproblems in the search tree, unless the NLP relaxation is very tight. GBD has the advantage that one can exploit more readily special structures in the NLP subproblems, but has the drawback that it may require a significant number of major iterations where NLP subproblems and MILP master problems must be solved successively. The OA/ER algorithm has the advantage that it typically requires only few major iterations, but has the drawback that the size of its MILP master problem is considerably larger than in GBD. Finally, the Feasibility Technique requires the least computational expense since it is based on the idea of finding a feasible integer point that has the smallest local degradation with respect to the relaxed NLP solution. However, it has the drawback that it does not guarantee optimality. Other related procedures for MINLP have been reported by Yuan et al. (1987) who extended the OA algorithm for convex nonlinear 0-1 variables, and by Floudas et al. (1988) who applied partitioning of variables in GBD to induce convex NLP subproblems.

The branch and bound, GBD and OA/ER algorithms require that some form of convexity assumption be satisfied in order to guarantee that they can find the global optimum of the MINLP. On the other hand, the OA/ER algorithm, which tends to be the most efficient method when the NLP subproblems are expensive or difficult to solve, is the most stringent in terms of convexity requirements. In particular, the OA/ER algorithm relies on assumptions of convexity of the functions f and g and also the quasi-convexity (resp. quasi-concavity) of nonlinear equality constraints, h (Kocis and Grossmann, 1987). When these conditions are met, the algorithm will determine the global optimum. Otherwise, the linearizations of the master problem can cut into the feasible region of candidate integer points which may result in sub-optimal solutions (Kocis and Grossmann, 1988a).

To overcome this problem, a two-phase strategy was proposed by Kocis and Grossmann (1988a) where in the first phase the OA/ER was applied. In the second phase, linearizations of nonconvex functions are identified by local and global tests so as to relax the master problem. This scheme proved successful in locating the global optimum in about 80 % of test problems. The implementation of the local and global tests is, however, somewhat difficult and they are not guaranteed to identify all the nonconvexities.

Motivated by observations with our experience in solving MINLP problems, it is the purpose of this paper to develop a new variant of the OA/ER algorithm which does not require the explicit identification of nonconvexities. As will be shown, this can be accomplished with a new MILP master problem that incorporates an augmented penalty function for the violation of linearizations of the nonlinear functions. Furthermore, the proposed algorithm (AP/OA/ER) has the important feature of not requiring the specification of an initial set of 0-1 variables since the algorithm starts with the solution of the relaxed NLP problem. Also, if appropriate convexity conditions hold, the AP/OA/ER algorithm has embedded the OA/ER algorithm. Numerical results are reported for a set of 18 test problems which arise in engineering design. Although convergence to the global optimum cannot be guaranteed, the numerical results suggest that the proposed algorithm is not only computationally efficient, but also very robust for finding the global optimum solution.

Outline of the AP/OA/ER Algorithm

We consider here the MINLP (mixed-integer nonlinear program) of the form:

$$
\begin{aligned}
\text{Min} \quad & z = c^T y + f(x) \\
\text{s.t.} \quad & Ay + h(x) = 0 \\
& By + g(x) \leq 0 \\
& Cy + Dx \leq 0 \\
& x \in X = \{x \in R^n : x^L \leq x \leq x^U\} \\
& y \in Y = \{0,1\}^m
\end{aligned}
\qquad (P)
$$

Here, x denotes the vector of continuous variables and y denotes the vector of binary variables corresponding to logical decisions (e.g. the existence of units). The functions f, g and h are defined over appropriate domains and have continuous partial derivatives. The matrices A, B, C and D have compatible dimensions. For each fixed binary vector y^K, we assume that the corresponding NLP (nonlinear program):

$$
\begin{aligned}
\text{Min} \quad & z := c^T y^K + f(x) \\
\text{s.t.} \quad & Ay^K + h(x) = 0 \\
& By^K + g(x) \leq 0 \\
& Cy^K + Dx \leq 0 \\
& x \in X = \{x \in R^n : x^L \leq x \leq x^U\}
\end{aligned}
\qquad [P(y^K)]
$$

satisfies any of the constraint qualifications (Mangasarian, 1969) so that the solution vector is a KKT (Karush-Kuhn-Tucker) point.

The algorithm that we propose involves the following steps :

1. Solve the NLP relaxation of (P) with $y \in Y_r = \{ y \in R^m, 0 \leq y \leq e \}$, where e is the unity vector, to obtain the KKT point (x^0, y^0). If y^0 is integer, stop. Otherwise, go to step 2

2. Find an integer point y^1 with an MILP master problem that features an augmented penalty function to find the minimum over the convex hull determined by the half-spaces at the KKT point (x^0, y^0).

3. Solve the NLP $[P(y^K)]$ at y^1 to obtain the KKT point (x V) •

4. Find an integer point y^2 with the MILP master program that corresponds to the minimization over the intersection of the convex hulls determined by the half-spaces of the KKT points at y^0 and y^1.

5. Repeat steps 3 and 4 until there is an increase in the value of the NLP objective function. (Repeating step 4 means augmenting the set over which the minimization is performed with additional linearizations - i.e , half-spaces - at the new KKT point).

The above algorithm is in the spirit of earlier algorithms proposed by Duran and Grossmann (1986) and Kocis and Grossmann (1987), but there are some important differences.

In both the previously cited algorithms it was assumed that an initial integer point y was supplied so that steps 1 and 2 were absent. Also, the termination criterion used in these algorithms, viz:

5'. Repeat steps 3 and 4 until the objective function of the MILP was greater than or equal to the lowest value of the objective function among the previously solved NLP minima at fixed values of the integer vector y .

is different from the one proposed here.

While the OA/ER algorithm has proved to be quite successful in solving a variety of problems (Kocis and Grossmann, 1989), its major limitation has been that it relies on assumptions of convexity of the functions as discussed previously.

For the algorithm proposed here, no assumptions concerning convexity of the functions in the MINLP are made. The main idea relies on the definition of a new MILP master problem the uses a linear approximation to an exact penalty function (Zhang, Kim and Lasdon, 1985), and therefore allows violations in the linearizations of the nonlinear functions. The algorithm is also based on extensive computational experience that has confirmed the desirability of starting with the solution of the relaxed NLP and the use of termination criterion 5 instead of 5 . The algorithm embeds the OA/ER algorithm in the case the assumptions concerning convexity of the latter are fulfilled. Although the proposed method has no theoretical guarantee of finding the global optimum, it was able to locate global optima in virtually all test problems despite the presence of nonconvexities in the MINLP problem. Our experience includes solving some challenging problems in distillation column design

The following sections describe the three major items of the proposed algorithm: starting point, MILP master problem and the termination criterion. Implementation of the algorithm is discussed and numerical results are also presented.

Starting point

Both Generalized Benders Decomposition (Geoffrion, 1972) and the OA/ER algorithm (Duran and Grossmann, 1986; Kocis and Grossmann, 1987) assume that an initial integer value y^1 is supplied. On the other hand, the branch and bound method (Gupta, 1980) and the feasibility technique of Mawengkang (1988) start the calculations by solving the relaxed MINLP problem. This means that :

1. The user need not provide an initial integer vector.

2. If the relaxed MINLP provides an integer solution, further calculations are not necessary.

It is also reasonable to expect that the solution of the relaxed MINLP will provide very good estimates of the continuous variables and, hence, the linear approximation to the MINLP at this point is often of good quality.

Thus, we begin computations by solving the relaxed MINLP:

$$\begin{aligned} \text{Min} \quad & z := c^T y + f(x) \\ \text{s.t.} \quad & Ay + h(x) = 0 \\ & By + g(x) \leq 0 \\ & Cy + Dx \leq 0 \\ & x \in X = \{x \in R^n : x^L \leq x \leq x^u\} \\ & y \in Y_r = \{y \in R^m, 0 \leq y \leq e\} \end{aligned} \quad (1)$$

The solution to this problem may be obtained by any NLP solver such as MINOS, SQP, etc .

Let the solution be (x^0, y^0). If y^0 is integer, we stop. Otherwise, we proceed for the search of an integer solution. Note that if problem (1) is infeasible or unbounded, the same is true of the original problem (P). As may be expected, the solution of the relaxed MINLP generally takes longer time to solve than the time required for the case of a NLP with fixed binary vector. Also, it should be noted that the NLP solution in (1) is only guaranteed to correspond to a global optimum if appropriate convexity conditions are satisfied (see Bazaraa and Shetty, 1979).

Master Problem

If y^0 is not integer, we wish to find an integer vector y^1, whose corresponding NLP solution is a likely candidate to the global optimum of the program (P). For the case where the objective function is convex and the MINLP has only inequality constraints which are also convex, the "best" integer point lies in the convex hull determined by the half-spaces at (x^0, y^0) (see Duran and Grossmann, 1986). The motivation is to find an estimate of the KKT point but with integer coordinates.

That is, given

$$\begin{aligned} \text{Min } & z^0 := c^T y^0 + \alpha \\ \text{s.t. } & f(x) - \alpha \le 0 \\ & Ay^0 + h(x) = 0 \\ & By^0 + g(x) \le 0 \\ & Cy^0 + Dx \le 0 \\ & x \in X = \{ x \in R^n : x^L \le x \le x^U \} \end{aligned} \tag{2}$$

the convex hull $C(x,\alpha,y)$ determined by the half-spaces of the KKT point of (2) at y^0 is given by

$$\begin{aligned} & f(x^0) + \nabla f(x^0)^T (x - x^0) - \alpha \le 0 \\ & T^0 [Ay^0 + h(x^0) + \nabla h(x^0)^T (x - x^0) \le 0 \\ & B y^0 + g(x^0) + \nabla g(x^0)^T (x - x^0) \le 0 \\ & C y^0 + D x \le 0 \\ & x \in X = \{ x \in R^n : x^L \le x \le x^U \} \end{aligned} \tag{3}$$

where T^0 is the relaxation matrix of the equations $a_i^T y + h_i(x) = 0$, given by

$T^0 = \{ t_{ii}^0 \}$, $t_{ii}^0 = \text{sign}\{ \lambda_i^0 \}$, with λ_i^0 being the Lagrange multiplier of each equation i.

The following proposition can then be established:

<u>Proposition 1</u>: If (x°, a) is a KKT point of (2) at y<>, then (x<>, a) is a KKT point of the problem

$$\text{Min} \quad z:=c^T y^\circ + a \qquad (4)$$

with (x°, a) satisfying (3).

Proof: The KKT conditions of (2) are given by :

$$1 - c = 0$$

$$\text{oVf (xO)} + X \text{ >-iVhj } (x^\circ) + X \text{ wVgj } (x^\circ) + £ \text{ Vjdj } + p^u - \rho^L = 0$$

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$$AyO + h(x^\circ) = 0$$
$$By^0 + g(x^\circ) \leq 0$$
$$Cy^\circ + D x^\circ \leq 0$$
$$x^L \leq x \leq x^u$$

$$[f(xO)-a]a = 0, \qquad a \geq 0$$
$$[b_j^T y^0 + g_j(x^0)]\, \mu_j = 0, \qquad \mu_j \geq 0$$
$$[c_j^T y^0 + d\, x_j^0 j] \Rightarrow v\, o, \qquad V J \geq 0$$
$$[-xp + xJ_i -]_{P_i}{}^L = 0, \quad {}_{P_i}{}^L \geq 0$$
$$[x\text{^}-XjO\ ]_{P_i}{}^u = 0, \quad {}_{P_i}{}^u \geq 0$$

These conditions are also identical for problem (4) at (x°, a) by setting

$$\text{afyo} + h_j(x^\circ) + \nabla h_j(x^\circ)^T (x - x^\circ) \leq 0 \qquad \text{if } A_j > 0$$
$$\text{ajV}^\circ + h_j(xO) + \nabla h_j(xO)^T (x - x^\circ) \geq 0 \qquad \text{if } X_j < 0$$

Q.E.D.

If f and g are convex and tjjhj is quasiconvex (see Bazaraa and Shetty, 1979), then the integer vector y^1 that has the "best" potential for yielding the lowest value for the objective function is given by the solution of the following MILP (see inequalities (3)) :

$$z l = \text{Min} \quad c^T y + a \qquad (5)$$

$$\text{s.t } (x.cc.y) \in C(x,a,y) \cap \{0,1\}^m$$

Furthermore, Z_L^{1} provides a valid lower bound to the solution of problem (P) (see Duran and Grossmann, 1986).

In the general case, where the assumptions concerning the convexity of f, g and h are not met, we cannot assert that problem (5) will provide a valid lower bound nor that it has a feasible integer solution even when problem (P) has. To circumvent this problem, we consider the following MILP with an augmented penalty function :

$$z_L^{1} := \text{Min} \quad c^T y + \alpha + w^{o} s^{o} + \sum_i w_i^p p_i + \sum_j w_j^q q_j$$

$$\begin{aligned} \text{s.t.} \quad & f(x^0) + \nabla f(x^0)^T (x - x^{o}) - \alpha \leq s^{o} \\ & T^{o}[\, Ay + h(x^0) + \nabla h(x^0)^T (x - x^{o}) \leq p \\ & By + g(x^{o}) + \nabla g(x^0)^T (x - x^0) \leq q \qquad (6) \\ & C y + D x \leq 0 \\ & x \in X = \{ x \in R^n : x^L \leq x \leq x^U \} \\ & y \in \{0,1\}^m, \; s^{o} \geq 0, p \geq 0, q \geq 0 \end{aligned}$$

where $w^{0} > |a|$, $w/Mx,|$, $w_j^q > ||ij|$ are the weights on the slack variables.

Using a similar argument as before, the following proposition can then be easily proved:

<u>Proposition 2:</u> If (x^{o}, a) is a KKT point of (2), then it is also a KKT point of (6) at y^0.

Thus, problem (6) can be used to formulate a master problem which has the flexibilty of violating inequalities should this prove necessary when searching for a new integer vector y^1. We also note that in case the convexity assumptions are met and the weights are sufficiently large, problem (6) reduces to problem (5) Qualitatively, the convex hull described by (6) is an expansion of the convex hull determined by (3).

Assuming that the integer vector y^1 has been found and its corresponding NLP solved, we need to find a new integer vector y^2 where there is a further decrease in the objective function. Since an improved representation of the MILP master problem is required, we will consider the intersection of half-spaces at x^0 and x^1 following a similar reasoning as in the OA/ER algorithm, but the master problem will be defined with an augmented penalty function as in (6). More generally, if x^k ,k = 0,1,...K, with x^0 the solution of the relaxed

MINLP and x^k, k = 1....K, are the NLP solutions found at the previously determined integer vectors, the **MILP** for determining the integer vector y^{K+1} is :

$$z_L^K := \text{Min } c^T y + \alpha + \sum_k w_k^s s_k + \sum_{ik} w_{i,k}^p p_{i,k} + \sum_{ik} w_{i,k}^q q_{i,k}$$

subject to :

$$\left.\begin{aligned} f(x^k) + \nabla f(x^k)^T(x - x^k) - \alpha &\leq s_k \\ T^k [\, Ay + h(x^k) + \nabla h(x^k)^T(x - x^k) \,] &\leq p_k \\ By + g(x^k) + \nabla g(x^k)^T (x - x^k) &\leq q_k \end{aligned}\right\} \quad k = 0,1,\ldots K \qquad (7)$$

$$C y + D x \leq 0$$

$$\sum_{i \in B_k} y_{i,k} - \sum_{i \in N_k} y_{i,k} \leq |B_k| - 1 \qquad k = 1,\ldots K$$

$$x \in X = \{x \in R^n : x^L \leq x \leq x^U\}, \quad y \in \{0,1\}^m$$

$$s_k, p_{i,k}, q_{i,k} \geq 0 \quad k = 0,1,\ldots K$$

In the MILP (7) above, integer cuts have been introduced to eliminate the previously determined integer vectors $y^1, y^2, \ldots, y^K$ from further consideration. Note also that if convexity conditions hold, then for sufficiently large weights the above MILP reduces to the master problem of the OA/ER algorithm by Kocis and Grossmann (1987).

Infeasible NLP Subproblems

In the proposed algorithm it is possible that the MILP master problem in (7) may predict an integer vector y^{K+1} for which there is no feasible solution in the corresponding NLP subproblem. In this case there are two possible schemes to handle this problem. One is to simply disregard the associated infeasible continuous point x^{K+1} for the linearization, and just introduce an integer cut for y^{K+1} for the next master problem. The other option is to also add to the master problem the linearization at the infeasible continuous point. However, since in this case information on the Lagrange multipliers is required to relax the equations, it is desirable that the equations be satisfied at the infeasible NLP subproblem. This can be accomplished by reformulating the MINLP problem (P) as (Kocis and Grossmann, 1987):

$$
\begin{aligned}
\text{Min} \quad & z := c^T y + f(x) + r|u \\
\text{s.t.} \quad & Ay + h(x) = 0 \\
& By + g(x) <> u \\
& Cy + Dx \leq u \\
& x \in X = \{X \in R^n : x^L \leq x \leq x^u\} \\
& u \geq O, U \in R^1 \\
& y \in \{0,1\}^m
\end{aligned} \tag{8}
$$

where u is a scalar variable and ^ is a large positive constant. In this way the idea in (8) is that if the NLP subproblem has a feasible solution, the variable u is driven to a zero value. If it is infeasible for the given integer vector, it will determine a continuous point that satisfies the equations and minimizes the violation of the inequalities. It is clear that care must be excercised in this reformulation to ensure that these properties in fact hold.

Termination **Criterion**

The MILP in (7) will not, in general, produce valid lower bounds for the objective function of problem (P) unlike the convex case (Duran and Grossmann, 1986; Kocis and Grossmann, 1987). Therefore, we resort to termination based on the progress of the objective function of the NLP sub-problems. For the case when no integer solution is found in the NLP relaxation problem, the search is stopped when at iteration $k \geq 2$, we have $z(y^k) > z(y^{k-1})$ assuming the corresponding NLP subproblems are feasible. When this is not the case, the termination criterion is applied between two successive feasible NLP subproblems. Interestingly, for the convex case, we have observed that if we use this criterion for all the test problems we have examined, the global solution is correctly found in all cases. Hence, this criterion has been adopted in this work. Note that if an integer solution y^0 is not obtained in the relaxed NLP, the proposed algorithm would examine at least two additional NLP sub-problems with fixed 0-1 variables.

Finally, it should also be noted that for the implementation it would always be possible to use a termination criterion based on the lower bound of the MILP master problem for those cases when it is known a-priori that the convexity conditions are satisfied.

Summary of Algorithm

The main steps in the proposed AP/OA/ER algorithm are as follows:

Step 1. Solve the relaxed NLP problem in (1) to determine a KKT point (x°, y°). If y° is integer, the solution is found, stop. Otherwise, set K=0, $zOLD = +\infty$ and go to step 2.

Step 2. Set up the MILP master problem in (7), and solve to find the integer vector y^{K+1}. Set K=K+1.

Step 3. Solve the NLP subproblem $[P(y^{K+1})]$ to determine the KKT point (x^{K+1}, y^{K+1}) with objective value z^{K+1}. If the NLP is infeasible set FLAG=0. If the NLP is feasible, set $z^{NEW} = z^{K+1} | FLAG=1$.

Step 4. (a)If FLAG=1, determine if $z^{NEW} > z^{OLD}$; if satisfied, stop. The optimal solution is z^{OLD}. Otherwise, set $z^{OLD} = z^{NEW}$ and return to step 2.
(b) If FLAG=0, return to step 2.

It should be noted that the above algorithm will terminate in one iteration if an integer solution is found in step 1, or else it will terminate after 3 or more iterations when the termination condition in step 4 (a) is satisfied. Note that in the latter case, N iterations implies the solution of N NLP subproblems, and N-1 MILP subproblems. Also, as was mentioned previously, if convexity of the MINLP can be established a-priori, the termination criterion in step 4 can be replaced by the use of the lower bound predicted by the MILP master problem as in the OA/ER algorithm.

Computer Implementation

The proposed AP/OA/ER algorithm has been implemented as the program DICOPT++ in the GAMS system (Brooke et al, 1988) for both IBM/CMS and VAX/VMS computers. The NLP solver used is MINOS (Murtagh and Saunders, 1985). On IBM, the MILP step is executed by MPSX/370 (IBM, 1979), and on VAX by ZOOM (Marsten, 1986).The authors may be contacted about the availability of this program.

Computational Results

The AP/OA/ER algorithm in DICOPT++ has been tested on the set of 18 MINLP problems that are shown in Table 1. Note that in terms of size, these problems involve up to 60 0-1 variables, 709 continuous variables and 719 constraints.

Following is a brief description of the test problems. LAZIMY is a bilinear MINLP reported by Lazimy (1982). HW74 is a small convex planning problem for the selection of 3 processes by Kocis and Grossmann (1987). NONCON is a small nonconvex MINLP and CAPITAL is a quadratic capital budgeting problem reported in Kocis and Grossmann (1988). YUAN is a convex MINLP problem by Yuan et al (1987). Since the problems LAZIMY, CAPITAL and YUAN exhibit nonlinearities in the 0-1 variables, these problems were reformulated with additional continuous variables in order to have linear 0-1 variables, (see Kocis and Grossmann, 1989). Problem FLEX is the MINLP formulation for the flexibility analysis of a heat exchanger network with uncertain flowrate by Grossmann and Floudas (1987). REL1 is a nonconvex reliability design problem considered by Kocis and Grossmann (1989). The three BATCH problems correspond to convexified formulations for the design of multiproduct batch plants described in Kocis and Grossmann (1988a), while TABATCH corresponds to a batch design with tasks assignments to be determined.

The last set of 5 MINLP problems correspond to various types of process applications. Problem UTILRED corresponds to the retrofit of a utility plant where the replacement of turbines by electric motors is considered (Kocis and Grossmann, 1989). TFYHEN corresponds to the retrofit of a small heat exchanger network that involves the aftercooler of a compressor and the reboiler of a column (Yee and Grossmann, 1988).

EX5FEED and EX5TRAY are distillation column design problems for optimal feed tray location and number of trays for the separation of toluene and benzene. Finally, HDASS corresponds to the MINLP model for the synthesis of the hydro-dealkylation of toluene process developed by Kocis and Grossmann (1988b).

The results in Table 1 were obtained on an IBM-3083 and IBM-3090 computers, using MINOS as the NLP solver and MPSX as the MILP solver. As can be seen in Table 1, the computational requirements with the AP/OA/ER are very reasonable. Note that the solution of 3 problems, NONCON, LAZIMY and EX5FEED, was achieved in one single major iteration since the integer solution was found in the relaxed NLP. All the other problems required only between 3 and 5 major iterations, which implied solving between 3NLP/2MILP and 5NLP/4MILP problems, respectively.

Perhaps, the more significant fact from the results shown in Table 1 is that the global optimum was found in all cases despite the fact that a significant number of these problems are in fact nonconvex (11 of 18). Thus, although the proposed algorithm has no guarantee of finding the global solution, it is clear that the AP/OA/ER algorithm has shown a remarkable degree of robustness. We feel that this is mainly due to a combination of two factors. First the initialization with the relaxed NLP which seems to provide very good linearization points. Secondly, the new MILP master problem which allows if needed the violation of any function linearization.

Conclusions

This paper has presented an augmented penalty version of the outer-approximation/equality-relaxation algorithm. The proposed algorithm has as main features that it starts with the solution of the NLP relaxation problem, and that it features an MILP master problem with an augmented penalty function that allows violations of linearizations of the nonlinear functions. This scheme provides a direct way of handling nonconvexities which are often present in engineering design problems. The proposed algorithm has been implemented in DICOPT++ as part of the modeling system GAMS. The numerical performance, which has been tested on a variety of applications, has shown that the computational requirements of this method are quite reasonable while providing a high degree of reliability for finding global optimum solutions.

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References

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

Beale, E.M.L. Integer Programming. (1977) The State of the Art in Numerical Analysis. (D. Jacobs, ed), Academic Press, London, pp.409-448

Benders, J,F, (1962). Partitioning Procedures for Solving Mixed-variables Programming Problems. *Numerische Mathematik 4,* 238-252.

Brooke, A., Kendrick, D. and Meeraus, (1988). A. GAMS A Users' Guide. Scientific Press. Palo Alto.

Duran, M.A. and Grossmann, I.E. (1986). An Outer-Approximation Algorithm for a Class of Mixed-Integer Nonlinear Programs. *Mathematical Programming* 36, 307-339.

Floudas, C.A., Aggarwal and Ciric, A.R. (1988) Global Optimum Search for Nonconvex NLP and MINLP Problems. Presented at Annual AIChE Meeting, Washington.

Geoffrion, A.M. (1972). Generalized Benders Decomposition. *Journal of Optimization Theory and Applications* 10, 237-260.

Grossmann, I.E. and Floudas, C.A. (1987). Active Constraint Strategy for Flexibility Analysis in Chemical Processes. *Computers and Chem. Eng.* 11, 675-693.

Gupta, O.K. (1980) Branch and Bound Experiments in Nonlinear Integer Programming. Ph.D. Thesis, Purdue University.

IBM Mathematical Programming System Extended/370 (MPSX/3709), Basic Reference Manual, White Plains (1979).

Kocis, G.R. and Grossmann, I.E. (1987). Relaxation Strategy for the Structural lOptimization of Process Flowsheets. *Ind.Eng.Chem. Research* 26, 1869-1880.

Kocis, G.R. and Grossmann, I.E. (1988). Global Optimization of Nonconvex MINLP problems in Process Synthesis. *Ind.Eng.Chem. Research* 27, 1421.

Kocis, G.R. and Grossmann, I.E. (1989). Computational Experience with DICOPT Solving MINLP Problems in Process Systems Engineering. *Computers and Chem. Eng.* 13, 307-315.

Kocis, G.R. and Grossmann, I.E. (1988b). A Modelling and Decomposition Strategy for the MINLP Optimization of Process Flowsheets. Paper 76a in Annual AIChE Meeting, Washington.

Lazimy, R. (1982). Mixed-Integer Quadratic Programming. *Mathematical Programming* 22, 332-349.

Mangasarian, O. L. (1969). Nonlinear Programming. McGraw Hill, New York..

Marsten, R. (1986). Users Manual for ZOOM/XMP. Department of Management Information Systems, University of Arizona

Mawengkang, H. (1988). Nonlinear Integer Programming. Ph.D. Thesis. The University of New South Wales, Australia.

Mawengkang, H. and Murtagh, B.A. (1986). Solving Nonlinear Integer Programs with Large Scale Optimization Software. *Annals of Operations Research* 5, 425-437

Murtagh, B.A. and Saunders, M.A. (1985). MINOS User's Guide. Systems Optimization Laboratory, Department of Operations Research, Stanford University.

Yee, T.F. and Grossmann, I.E. (1988). Screening and Optimization Approach for the Retrofit of Heat Exchanger Networks. Paper 81 d in Annual AIChE Meeting, Washington.

Yuan, X., Zhang, S., Piboleau, L. and Domenech, S. (1987). Une Methode d'optimisation non lineare en variables mixtes pour la conception de procedes. Partie I: Presentation de l'algorithme. Submitted for publication to *RAIRO Recherche Operationalle.*

Zhang, J., Kim, N.H. and Lasdon, L. (1985). An Improved Successive Linear Programming Algorithm. *Management Science* 31, 1312-1331.

Table 1

Computational Results with DICOPT++

(Augmented-Penalty/Outer-Approximation/Equality-Relaxation)

Problem	Size MINLP 0-1	Cont.V.	Const.	Iterations*	Time** (sec)	% NLP:MILP
LAZIMI	2	8	5	1	0.22	100:00
HW74	3	9	9	4	2.43	26:74
NONCON	3	3	6	1	0.1	100:00
YUAN	4	4	10	3	1.87	36:64
CAPITAL	10	3	7	4	2.32	22:78
FLEX	4	12	16	3	2.24	46:54
REL1	16	21	18	3	17.9	36:64
EX3	8	26	32	5	3.7	51:49
EX4	25	7	31	5	65.1	9:91
BATCH	24	23	74	3	7.9	70:30
BATCH8	40	33	142	4	24.4	63:37
BATCH12	60	41	218	4	38.5	45:55
TABATCH	24	71	129	3	53.6	53:47
UTILRED	28	118	168	3	41.9	14:86
TFYHEN	30	74	144	3	102.0	20:80
EX5FEED	10	238	239	1	19.2	100:00
EX5TRAY	30	338	467	4	103.6	39:61
HDASS	13	709	719	3	482.0	84:16

* N iterations require N NLP subproblems and N-1 MILP master problems

** Total time NLP:MINOS / MILP:MPSX. All problems on IBM-3083, except EX5TRAY on IBM-3090