Alternative Bounding Approximations for the Global Optimization of Various Engineering Design Problems

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ALTERNATIVE BOUNDING APPROXIMATIONS FOR THE GLOBAL OPTIMIZATION OF VARIOUS ENGINEERING DESIGN PROBLEMS

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Abstract

This paper presents a general overview of the global optimization algorithm by Quesada and Grossmann (1993a) for solving NLP problems involving linear fractional and bilinear terms, and it explores the use of alternative bounding approximations. These are applied in the global optimization of problems arising in different engineering areas and for which different relaxations are proposed depending on the mathematical structure of the models. These relaxations include linear and nonlinear underestimator problems. Reformulations that generate additional estimator functions are also employed. Examples from structural design, batch processes, portfolio investment and layout design are presented.

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Introduction

One of the difficulties in the application of continuous nonlinear optimization techniques to engineering design problems is that one is often confronted with the following dilemma. One can either apply fairly efficient gradient based techniques (e.g. SQP or reduced gradient algorithms) or else one can apply direct or random heuristic search procedures (e.g. complex method or simulated annealing). The problem is that the former methods may only produce rigorous results when certain convexity conditions hold, while the latter may in principle produce improved solutions but at a computational expense that is unacceptably high. Also, if the nonlinear programming (NLP) problem at hand is known to be nonconvex the first alternative is generally inconsistent with the goal of finding **a global** optimum. **While** the second alternative may offer greater hope to globally optimize a design, the heuristic nature of these methods may produce results that are in fact worse than the ones obtained by a local search technique. Despite these difficulties, rigorous deterministic methods for nonconvex NLP models have been developed, especially over the last five years (see Horst (1990) for a recent review). In this way it Is increasingly possible to find global optimum solutions with reasonable computational expense . The specific structure of design problems is also being identified and better understood given the increased trend towards the use of equation based modeling systems.

The objective of this paper is to first present an overview of the global optimization algorithm proposed by Quesada and Grossmann (1993a) for solving nonconvex NLP problems that have the special structure that they involve linear fractional and bilinear terms. These problems can be represented in general as follows:

$$\begin{aligned} &\min g_0 \\ &\text{st } g_l \le 0 \qquad l = 1,\ldots,L \qquad \text{(NLP)} \end{aligned}$$

where $g_l = \sum_{i\in I}\sum_{j\in J} c_{ij}\frac{x_i}{y_j} - \sum_{i\in I^*}\sum_{j\in J'} c'_{ij}\, x_i y_j + h_l(x,y,z)$, $\quad l = 0,1,\ldots,L$

$$\begin{aligned} &x^L \le x \le x^U \\ &y^L \le y \le y^U \\ &z \in Z \end{aligned}$$

As shown above, the objective function and the constraints generally involve linear fractional and bilinear terms corresponding to the two summation terms, while the last term htfx, y, z) is assumed to correspond to a convex function. These type of problems arise very often in engineering and management applications (see Floudas and Pardalos, 1990). The difficulty involved in solving these NLP optimization problems is that a straightforward application of common local search methods is generally not rigorous. Not only can a conventional NLP algorithm produce local solutions that are suboptimal, but the method may even fail to converge to a feasible solution due to the nonconvexities of the constraints.

A major objective of this paper is to explore the possibility of using alternative bounding approximations for deriving valid relaxations. Different relaxations are **proposed** depending **on the mathematical** structure of **the model to** be solved. Linear and/or nonlinear estimators functions as the ones **considered** in Qucsada and Grossmann (1993a, 1993b) are included. In some cases, additional approximating functions are obtained through reformulating and linearizing **the** original models. These constraints, that are redundant for the original nonconvex problem, can often help to obtain a tight convex relaxation.

Another objective of **this paper** is **to consider the application** of **the** proposed **methods to** problems from a **variety of areas. The** first **includes a** layout design model. In this model a fixed layout configuration is given and **the** dimensions of the different units are to be optimized. A portfolio investment model is also considered and in this case, the percentage to be invested in each security is optimized to minimize the total variance. Also, a model for the design of truss structures is presented. The objective in this case is to minimize the total weight of the structure. Finally, two models for batch process design are considered where the size of the equipment has to be selected. Numerical results are reported for all these problems.

Algorithm Outline

The major steps in the global optimization algorithm by guesada and Grossmann (1993a) for NLP problems involving linear fractional and bilinear terms are as follows:

Step 0. *Initialization step.*

(a) Set the upper bound to f* = «, the tolerances e and y are selected.

(b) Bounds over the variables involved in the nonconvex terms are obtained. For this purpose specific subproblems can be solved or a relaxation of the original problem is used. Update the upper bound f*

(c) Define space fto as a valid relaxation of the feasible region in the space of the nonconvex variables. The branch and bound search will be conducted over HQ. The list F is initially defined as the region QQ.

(d) Construct a convex underestimator problem (CUJ by replacing the nonconvex terms in the original problem with additional variables and introducing valid convex approximations of these nonconvex terms. Constraints that are valid but were not present in the original problem because they were redundant can be included to tighten the convex relaxation.

Step 1. Convex underestimator problem.

(a) Solve problem CU_L over the relaxed feasible region Cl_0. The solution corresponds to a valid lower bound (P-) of the global optimum. The actual objective function is evaluated if this is a feasible solution; otherwise the original problem is solved using the convex solution as the initial point Update the upper bound.

(b) If (f* - fH .< £ f* stop and the global solution correspond to f\

Step 2. Partition.

From the list F consider a subregion ft, (generally the region with the smallest f* is selected) and divide it into two new subregions ftj+i and Qj+2 which are added to the list F and subregion Qj is deleted from F.

Step 3. Bounding.

(a) Solve problem CU_L for the two new subregions.

(b) If the solutions are feasible evaluate the actual objective function. Otherwise the original nonconvex problem can be solved according to a given criterion.

Step 4. Convergence.

Delete from list F any subregion with (f* - fH £ e f* . If list F is empty then stop and the global optimum is f*; otherwise go to step 2.

Remarks

The global optimization algorithm described in the previous section uses a spatial branch and bound procedure (steps 2 to 4). As many of the branch and bound methods, the algorithm consists of a set of branching rules, and upper bounding and lower bounding procedures.

The branching rules include the node selection rule, the branching variable selection and the level at which the variable is branched on. A simple branching strategy has been followed in this work. The node with the smallest lower bound is the node selected to branch on and two new nodes are generated using constraints of the type,

$$x_i \geq x_i^* \text{ and } x_i \leq x_i^* \qquad (1)$$

Different strategies can be used to do the branching. These include generating more than two nodes from a parent node, using different type of branching constraints or different node selection rules. For the latter, some type of degradation function similar to the one used in branch and bound for MILP problems can be used.

Additional criteria used in branch and bound algorithms for MILP problems can be extrapolated to the global optimization case. These include the fixing of variables, tightening of bounds, range reduction, etc. (see Sahinidis, 1993). One main difference between the branch and bound for binary variables and the spatial branch and bound search used here, is the fact that it might be necessaiy to branch more than once on the same variable. When in the selection rule there is more than one variable within a small range it is often useful to branch on a variable that has not been used previously even though it may not be the first candidate.

Information of the convex underestimator problem can be employed to select the branching variables. At this point only the difference between the convex solution and the actual value of the functions is used. It is also possible to consider dual information, second order information or to generate small selection subproblems (Swaney, 1990).

With respect to the upper bound there are two cases. The first one is when the feasible region of the original problem is convex. In this case the evaluation of the original objective function at the solution of the convex underestimator problem often provides a good upper bound. For the case of a nonconvex feasible region it is sometimes necessaiy to obtain an upper bound through a different procedure since the solution of the convex underestimator problems might be infeasible for the original problem. In some particular cases it may be better to use a specialized heuristic to obtain a good upper bound. In general, however, it may be necessary to solve the original nonconvex problem to generate an upper bound. As pointed out in Quesada and

Grossmann (1993a, 1993b) the solution of the convex underestimator problem provides a good initial point to the nonconvex problem.

Our previous work has mainly concentrated on the generation of tight convex relaxations that allow for an efficient lower bounding of the global optimum. The major motivation has been to reduce the effort in the spatial branch and bound search. The use of additional convex relaxations that are somewhat different from the ones used in Quesada and Grossmann (1993a) is explored for the models presented in this paper.

To be able to obtain a tight convex relaxation it is necessary to obtain a good approximation of the convex envelope of the nonconvex function. The linear and nonlinear estimators functions used in Quesada and Grossmann (1993a) correspond to the convex envelope over the boundaries defined by lower and upper bounds of the nonconvex variables. These bounds are a relaxation of the actual feasible region. It is often the case, however, that they do not yield a tight convex relaxation of the feasible region (see Fig. 1). The use of projections such as the ones described in Quesada and Grossmann (1993a, 1993b) help to obtain tighter relaxations of the feasible region. Moreover, reformulation and generation of additional constraints can also improve the approximation of the convex envelope over a tighter feasible region. To illustrate these points consider the linear constrained feasible region in Figure 1.

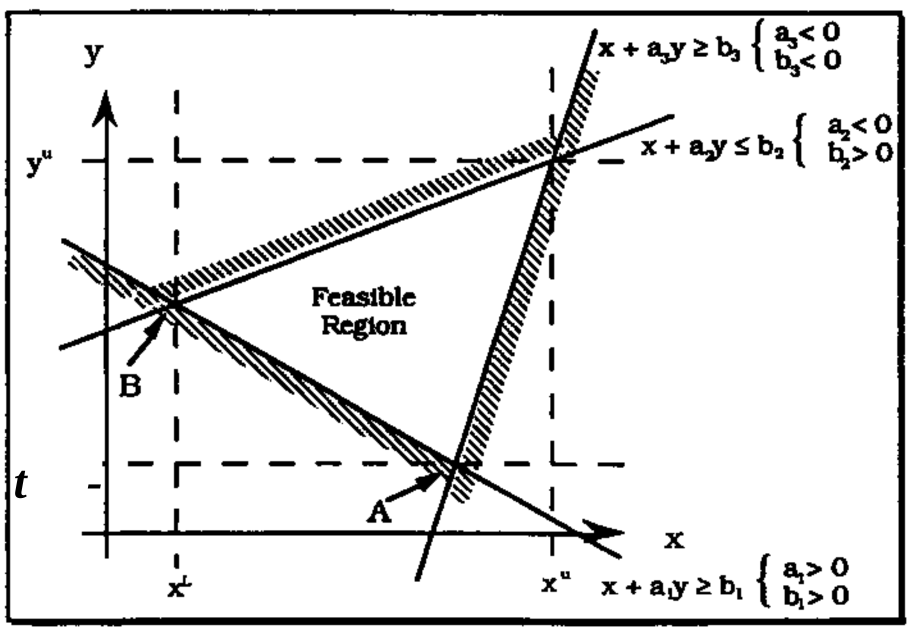

Figure 1. Linear constrained feasible region and relaxations.

Lower and upper bounds over the variables x and y can be obtained through heuristics or the solution of LP subproblems. In this particular case, the best possible bounds are given by x^L, x^u, y^{L*} and y". Now, consider the linear under and over estimators for the bilinear term, xy, used in Quesada and Grossmann (1993a 1993b),

$$x\,y \geq \max\,[x^L y + y^L x - x^L y^L,\; x^u y + y^u x - x^u y^u] \qquad (2)$$

$$x\,y \leq \min\,[x^L y + y^u x - x^L y^u,\; x^u y + y^L x - x^u y^L] \qquad (3)$$

Equations (2) and (3) correspond to the convex and concave envelopes of the bilinear tenn over the relaxation of the feasible region defined by the lower and upper bounds of the variables. As pointed out in Quesada and Grossmann (1993a, 1993b) these estimators have the property of matching the actual function at the boundaries. However, these equations do not always provide tight bounds since the relaxation of the actual feasible region can be very loose. Consider, the value of the bilinear term over the boundary defined by the first constraint x + aiy = b_{1t} that is given by;

xysfoi-atfjysbiy-a^2 (4)

This is a concave term and better approximations of it can be obtained by reformulating the problem. Take that particular inequality, bi -x - aiy £ 0, and multiply it by the valid bound constraint x - x^L £ 0, obtaining.

$$b_1(x - x^L) + x^L x - x^2 + a_1 x^L y \geq a_1\, xy \qquad (5)$$

The above is a concave overestimator and therefore a valid convex constraint that can be included in the formulation. It is also tighter since it provides an exact approximation of the bilinear term over the linear constraint. In the case that the valid bound constraint x^u - x £ 0, is used to generate additional constraints, the following equation is obtained

$$-b_1(x^u-x)-x^2 + x^{L*}x + a_1 x^{il} y \leq aixjr \qquad (6)$$

This is a concave underestimator and the concave term, $-x^2$, has to be linearized over the bounds, x^L and x^u. This corresponds to the approach followed by Sherali and Alameddine (1992). With this reformulation-linearization a linear underestimation of the bilinear term over that particular boundary is obtained. In fact this is the best approximation of the bilinear term in this boundary since it projects in a concave form (4) and the approximation is a linear estimator that matches the actual function at the extreme points A and B. Equation (6) corresponds to the convex underestimator envelope of the bilinear term in that boundary and helps to generate a tighter convex approximation.

In the case of constraints like the second one in Fig. 1, $x + a_2y \le b_2$, the bilinear term behaves in a convex form. Convex quadratic underestimators that match the function in the boundary and tighter linear overestimators can be obtained.

The introduction of these additional constraints yields a tighter convex underestimator problem. However, there is a trade-off since the size of the underestimator problems can become substantially large. Nevertheless, the use of projections or some particular mathematical structures can be employed to identify the most relevant additional constraints so as to avoid generating a large number of constraints. In the following applications different types of relaxations are used which include linear and/or nonlinear constraints.

Layout Design

In this example a floor layout is given in which the distribution of the rooms is known. The dimensions of the rooms are to be optimized to minimize the total cost that is a function of the area of the rooms.

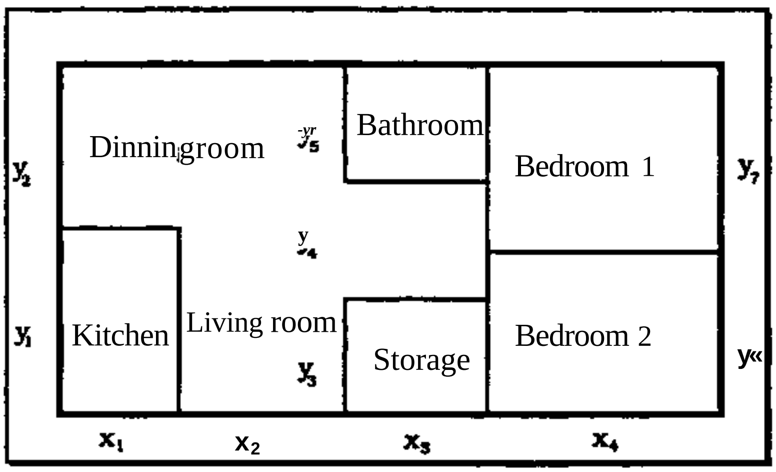

Figure 2. Layout for **example 1.**

Example 1

Consider the layout given in Fig. 2. Here the two bedrooms have the same length. The storage room and the bathroom have also the same length. The complete formulation is given by;

min f = 2 (x ^ + x&J + ^{x}iY2 + *2yt + *ay4 + X4jr$_6$ + X4y_7 + 0.5 (x_3y_3)

$y_T = y_1 + y_2$

$y_T = y_3 + y_4 + y_5$

$y_T = y_6 + y_7$

X_T= X! + X_2 4- X_3 + X4 (NLP$_{LAY1}$)

$y_7 - y_5 \geq 1$

$y_6 - y_3 \geq 1$

$x_1 + x_2 \geq 8$

$3 \leq x_1 \leq 5,\ 4 \leq x_2 \leq 6,\ 2 \leq x_3 \leq 4,\ 4 \leq x_4 \leq 6$

$5 \leq y_1 \leq 7,\ 2 \leq y_2 \leq 5,\ 2 \leq y_3 \leq 5,\ 2 \leq y_4 \leq 4,\ 3 \leq y_5 \leq 5,\ 3 \leq y_6 \leq 6,\ 4 \leq y_7 \leq 6$

$13 \leq x_T \leq 21,\ 8 \leq y_T \leq 12$

The objective function consists of minimizing the total cost as a function of the area of the rooms. The fifth and sixth constraints ensure that some hall space is left for the doors. Bounds over the dimensions of the rooms are given. The feasible region is linear and the nonconvexities are involved in the objective function. The bilinear terms can be linearized (w,j = xy,) and the linear underestimators used in (2) and (3) are included.

$w_{ij} = x_iy_j \geq x_i^L$yj + $y_J^L x_4$ - *xf-yf* (7)

w_r xty £ x^yj + $y_J^u x_i$ - x^y/* (8)

Only underestimators are considered because the bilinear terms are only present in the objective function with a positive coefficient. The nonlinear estimators are not used since there are no bounds over the individual bilinear terms (see Quesada and Grossmann, 1993a). The linear underestimates problem is solved and a solution of f- =130 is obtained. The approximations are exact and this solution corresponds to the global solution with Xi=3, x_2=5, x_3=2, X4=4, yi=5, y_2=3, y3=3, y_4=2, y_5=3, y_6=4 and y7=4.

Example 2

A second layout example is considered using a similar configuration (see Fig. 3). In this case the dimensions of the bathroom are allowed to change independently. Constraints over the aspect ratio and the size of the rooms are included. The objective function contains an additional term that accounts for the perimeter of the layout. The complete formulation is the following.

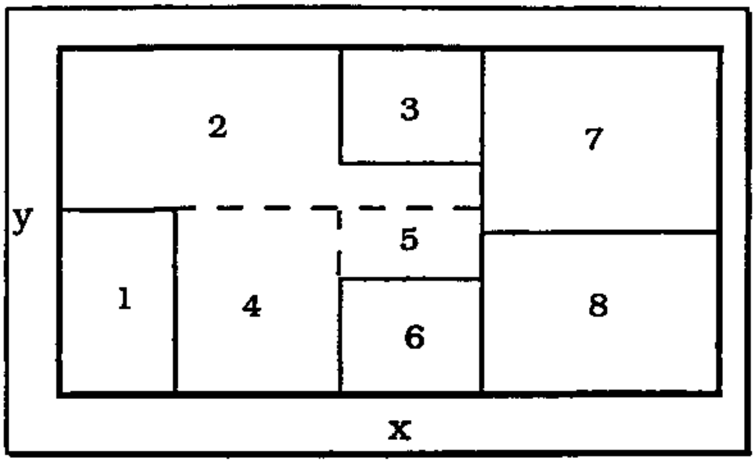

Figure 5. Layout for example 2.

$$\min f = 10 x_1 y_1 + 11 x_3 y_3 + 1.5 x_7 y_7 + 1.5 x_8 y_8 + (x_2 y_2 - x_3 y_3) + x_4 y_4 + x_5 y_5 + 0.5\,(x_6 y_6) + 1.5\,(y_1 + y_2) + x_T$$

$$
\begin{aligned}
\text{st} \quad & y_T = y_1 + y_2 \\
& y_T = y_7 + y_8 \\
& y_1 = y_4 \\
& y_4 = y_5 + y_6 \\
& y_7 - y_3 \geq 1 \\
& y_8 - y_6 \geq 1 \\
& y_3 \leq y_2 \qquad\qquad (NLP_{LAY2}) \\
& x_T = x_2 + x_3 + x_7 \\
& x_7 = x_8 \\
& x_2 = x_1 + x_4 + x_5 \\
& x_6 = x_5 \\
& x_3 \leq x_2 \\
& x_3 \leq x_5 \\
& a_i x_i \leq y_i \\
& y_i \leq b_i x_i \\
& x_i y_i \geq d_i
\end{aligned}
$$

This new problem has a nonconvex objective function and nonlinear constraints. The data for the ratio constants (a_i, b_i) and the area lower bounds (d_i) are given in Table 1. The nonconvex terms in the objective function are linearized and linear estimators are introduced. The nonlinear constraints over the area can be written in a convex form as.

$$x_i \geq \frac{d_i}{y_i} \qquad (9)$$

Room	1	2	3	4	5	6	7	8
a.	1.25	1/3	1/1.5	1.25	1	1	1.25	1.25
b,	1.5	1/2	1/1.25	1.5	1.25	1.25	1.5	1.5
dk	16	40	10	20	4	4	20	20

Table. Datafor the second layout example.

Additional convex nonlinear approximations can be generated. These nonlinear constraints are obtained using the aspect ratio constraints. Consider equation

$$0 \leq b_i x_i - y_i \qquad (10)$$

multiplying by the constraint y_t £0 and linearizing, yields

$$y_i^2 - b_i w_i \leq 0 \qquad (11)$$

which is a convex constraint. In the same form the other ratio constraints can be multiplied by x, £ 0 to obtain the following constraints;

$$a_1 x_1^2 - w_1 \leq 0 \qquad (12)$$

In this form a convex nonlinear underestimator is obtained by introducing equations (7), (8), (9). (11) and (12) in model NLPuvrc and linearizing the bilinear terms. The convex nonlinear underestimator problems has a solution of i* = 440.6. This solution is feasible and has an actual objective function of f = 440.99. Since the difference is e = 0.07% it is considered as the global optimal solution.

Optimal Design of Structures

An application in civil engineering is the design of a truss structure (Grossmann et al.f 1992). It is assumed that a truss consists of a given number of bars, m, with a fixed location and that are subject to a number of different loading conditions (see Fig. 4). The objective is to determine the cross section areas of the bars to minimize the weight of the truss structure. The NLP formulation is the following,

a) Objective function, minimize the total weight

$$\min f = \sum_{i=1}^{m} \rho_i \lambda_i a_i \qquad (13)$$

b) Equilibrium equations

$$\sum_{i=1}^{m} b_{ik} s_{ij} = P_{jk} \qquad \text{for } j=1\ldots L, k=1\ldots n \qquad (14)$$

c) Compatibility equations

$$\sum_{k=1}^{n} b_{ik} d_{jk} = v_{ij} \qquad \text{for } i=1\ldots m\ j=1\ldots L \qquad (15)$$

d) Hooke's law

$$\frac{E_i}{\lambda_i} a_i v_{ij} = s_{ij} \qquad \text{for } i=1\ldots m\ J=1\ldots L \qquad (16)$$

e) Stress equations

$$\frac{E_i}{\lambda_i} v_{ij} = \sigma_{ij} \qquad \text{for } i=1\ldots m\ J=1\ldots L \qquad (17)$$

0 Bounds

$$d_{jk}^{L} \le d_{jk} \le d_{jk}^{u} \qquad (18)$$

$$\sigma_{ij}^{L} \le \sigma_{ij} \le \sigma_{ij}^{u} \qquad (19)$$

$$s_{ij}^{L} \le s_{ij} \le s_{ij}^{u} \qquad (20)$$

$$v_{ij}^{L} \le v_{ij} \le v_{ij}^{u} \qquad (21)$$

$$0 \le a_1^{L} \le a_1 \le a_1^{u} \qquad (22)$$

where n is the number of degrees of freedom. L the number of loading conditions. The parameters are the following; X_f is the length of bar i. E_t is the modulus of elasticity of bar i. p_t is the density of bar i, P_{Jk} is the kth component of load at condition j. b_{lk} is the direction cosine relating force in bar i with degree of freedom k. The variables are $a_{(J}$ the stress of bar i for condition j, at the cross section area of bar i, s_{tJ} the force in bar i for condition j, v_y the elongation of bar i for condition j and d_{Jk} the displacement at degree of freedom k for condition j.

The objective function of this model is linear and the nonconvex terms in the form of bilinearities are involved in Hooke's law equations (16).

Example 3

This example consists of the truss illustrated in Fig. 4. The modulus of elasticity is 1×10^7 psi, the density is 0.1 lb/in^3 and the maximum stress is 20,000 psi in compression or tension. The remaining data is given in Table 2.

Bar	1	2	3	4	5
b«	-0.89443	-0.95783	-0.99504	-0.99504	-0.95783
b_Q	-0.44721	-0.28735	-0.0995	0.09950	0.28735
λ_1	111.8034	104.4031	100.4988	100.4988	104.4031

-2 £ d_{Jk} ≤, 2, -200,000 ≤ > Sy £ 200,000, -0.22 £ v,j £ 0.22,0 £ a_1 £ 10, -20,000 £ o,j £ 20,000

***Table 2. Datafor example* 3.**

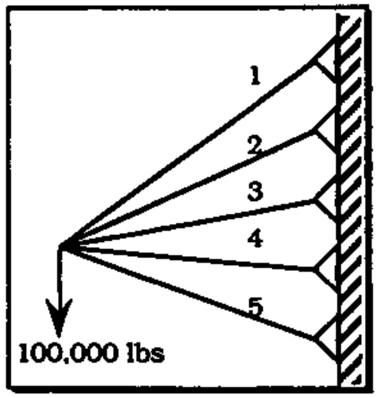

***Figure* 4. Structure/or *example* 3.**

The bilinear terms are linearized by Wy = Vy a_t and linear over and underestimators are included. In this case it is possible to exploit further the mathematical structure of this problem. Additional constraints are generated using the stress equations (17),

$$\frac{E_i}{\lambda_i} v_{ij} = \sigma_{ij} \qquad (17)$$

Multiplying by a_t £ 0 yields.

$$v_{ij}\, a_i = \sigma_{ij}\, a_i \qquad (23)$$

that can be linearized with Zy = c,j a, to obtain

$$\frac{E_i}{\lambda_i} w_{ij} = z_{ij} \qquad (24)$$

Linear over and underestimators are also included for zy » a_y 34. The resulting LP model includes the estimators for z^, w,j and the equations (24). The solution of this problem is P^* = 147.5 lb and the approximations are exact corresponding to the global solution with a= (7.102,0,0,0,6.525). If the additional equation (24) with the corresponding linear estimators is not generated the lower bound yields f^* = 144.0 lb which represents a 2.3 % gap from the global optimum. When the original nonconvex problem is solved with MINOS 5.2 providing zero values as an initial point no feasible solution is obtained.

Example 4

Consider the truss shown in Fig. 5. The modulus of elasticity is lxlO^7 psi, the density 0.1 lb/in^3 and the maximum stress is 25,000 psi in compression or tension. The remaining data are given in Table 3.

Bar	1	2 !	3	4	5	6	1◊	1*	9	10
b,,	1	-1	0	0	0	0	0	-.7071	-.7071	0
bQ	0	0	0	0	0	0	0	-.7071	.7071	0
b o	0	0	1	-1	0	0	.7071	0	0	-.7071
bM	0	0	0	0	-1	0	-.7071	0	0	-.7071
bfi	0	1	0	0	0	0	0	0	0	.7071
be	0	0	0	0	0	0	0	0	0	.7071
tv	0	0	0	1	0	0	0	0	.7071	0
b e	0	0	0	0	0	-1	0	0	-.7071	0
λ_1	360	360	360	360	360	360	509.1	509.1	509.1	509.1

-10 ≤ d$_{jk}$ ≤ 10, -250,000£Sij£250,000. -1.273SVyS 1.273, 0£a, £ 10, -25,000 £ a„ £ 25,000

***Table* 3. *Data for example* 4.**

The same reformulation than in example 3 is used. The LP solution is f^1- = 1,584 lb and it corresponds to the global solution with a = (8.0.8,4,0,0,5.657.5.657,5.657,0). It is important to notice that in both examples the reformulated LP converges in one iteration. The non reformulated LP has a solution of *f** = 1,373 lb that is still 15% under the global optimum.

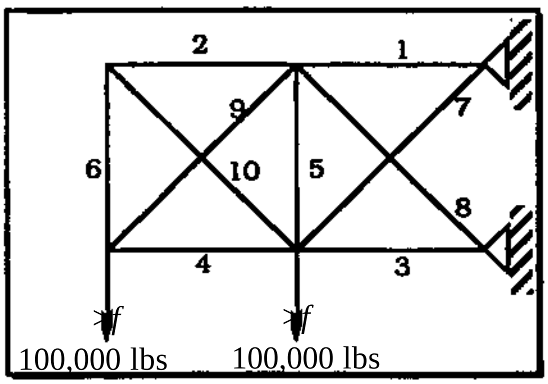

Figure 5. Structure for ***example* 4.**

Portfolio Investment

A set of securities, i, is available for investing. The investment has to be done achieving a target mean annual return according to the mean annual returns on the individual securities, ni|. The total variance of the investment has to be minimized. By defining Xi as the fraction to be invested for each security i, the optimization problem can be expressed as:

$$\min f = \sum_{i}\sum_{i'} x_i v_{ii'} x_{i'}$$
$$\text{s.t.} \sum_{i} x_i = 1$$
$$\sum_{i} m_i x_i = \text{target} \qquad (NPL,)$$
$$0 \le x_i \le 1$$

In this case the bilinear terms in the objective function are linearized introducing variables w_u and the linear estimators. The quadratic terms $X4^2$ remain in the convex underestimator problem when the variance coefficient, v_u, is positive. The upper bounds on the investment fractions, x_t, can in some cases be tightened according to the following equation

X4 £ min [1, target/mi] (25)

Example 5

The data for this example are given in Table 4. The initial lower bound is f^L= 5.22 and corresponds to an actual objective function of f = 5.429. Since the difference is greater than the tolerance, e, a branch and bound search is conducted. After 7 nodes the global optimal of f =5.429 is obtained with x=*(0.143,0.143, 0.714, 0.0).

	t 1	2	3	4
V,,	4	3	-1	0
VQ	3	6	1	0
V 0	-1	1	10	0
V*	0	0	0	0
m,	8	9	12	7

target = 11

Table 4. Data for example 5.

Batch ProcessDesign

Consider the design and production planning of a multiproduct batch plant with one unit per stage (see Fig. 6).

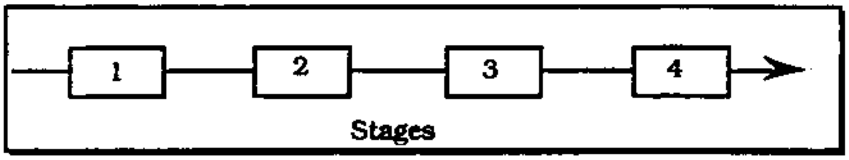

***Figure* 6. Multiple stages batch process.**

The objective is to maximize the profit given by the income from the sales of the products minus the investment cost Lower bounds are specified for the demands of the products and the investment cost is assumed to be given by a linear cost function. Since the sizes of the vessels and the number of batches are assumed to be continuous, this gives rise to the following NLP model:

$$\max P = \sum_i p_i n_i B_i - \sum_j \alpha_j V_j$$

$$\text{s.t} \quad V_j \geq S_{ij} B_i \qquad i=1...N,\ j=...N \qquad \text{(NLPp)}$$

$$\sum_i n_i T_i \leq H$$

$$\frac{Q_i^L}{n_i} - B_i \leq 0 \qquad i=1...N$$

$$V_j, B_i, n_i \geq 0$$

where n_i and B_i are the number and size of the batches for product i, and Vj is the size of the equipment at stage j. The first inequality is the capacity constraint in terms of the size factors Sy. the second is the horizon constraint in terms of the cycle times for each product Ti and the total time H, and the last inequality is the specification of lower bounds for the demands Qi^L. Note that the objective function is nonconvex as it involves bilinear terms, while the constraints are convex.

Example 6

The data for this example are given in Table 5. A maximum size of 5000 L is specified for the units in each stage.

Product	T_i (hrs)	P_i ($/Kg)	Q_i^L (Kg)	S_{ij} (L/kg) 1	2	3
A	16	15	80000	2	3	4
B	12	13	50000	4	6	3
C	13.6	14	50000	3	2	5
D	18.4	17	25000	4	3	4

$\alpha_1 = 50, \alpha_2 = 80, \alpha_3 = 60$ ($/L) ; H = 8,000hrs

Table 5. Data far Example 5

When a standard local search algorithm (MINOS 5.2) is used for solving this NLPp problem the predicted optimum profit is $8,043.800/yr and the corresponding batch sizes and their number are shown in Table 6.

Product	A	B	C	D
B_i	1250	833.33	1000	1250
n_i	79.15	60	50	289.87

Table 6. Suboptimal solution Cor example 5

Since the formulation in (NLP_p) is nonconvex there is no guarantee that this solution is the global optimum. This problem can be reformulated by replacing the nonconvex terms in the objective function by underestimator functions to generate a valid NLP underestimator problem with the following constraints;

$$q_i \leq n_i^L B_i + B_i^u n^i - n_i^L B_i^u \qquad (26)$$

$$q_i \leq n_i^u B_i + B_i^L n^i - n_i^u B_i^L \qquad (27)$$

The underestimator functions require the solution of LP subproblems to obtain tight bounds on the variables, and yield a convex NLP problem with 8 additional constraints.

The optimal profit predicted by the nonlinear underestimator problem is $8,128,100/yr with the variables given in Table 7. When the objective function of the original problem (NLPP) is evaluated for this feasible point the same value of the objective function is obtained proving that it corresponds to the global optimal solution. It is interesting to note that both the local and global solutions had the maximum equipment sizes. The only difference was in the number of batches produced for products A and D.

Product	A	B	C 1	D
Bi	1250	833.33	1000	1250
ni	389.5	60	50	20

Table *7.* **Global optimum solution for example** S

Alternative Model for Batch Process

The next example corresponds to an alternative formulation of the batch process design problem considered in the previous section. A process with one line per stage is also considered operating with single product campaigns. All the products require the same sequence of processing stages. The sizes of the **equipment** V_{Jt} and the output of the products, Qi, are optimized to minimize the cost Removing the number of batches n_4 as variables the NLP formulation becomes;

$$\min f = \sum_j \alpha_j V_j - \sum_i \beta_i Q_i$$

$$V_j \geq S_{ij} B_i \qquad \text{for } i=1...N,\ j=1...M$$

$$\sum_i T_{Li} \frac{Q_i}{B_i} \leq H$$

$$\sum_i d_i Q_i = F$$

$$V_j^L \leq V_j \leq V_j^u \qquad (NLP_B)$$

$$Q_i^L \leq Q_i \leq Q_i^u$$

$$B_i \geq 0$$

The first set of constraints corresponds to the volume requirements for each unit with respect to all the products. The second constraint states that the total time of production has to be smaller that the allocated time H. The third constraint represents a raw material limitation. Bounds over the volumes, V_{Jt} and the production levels. Qi, are given. Note that the nonconvexities appear in the time constraint in the form of a sum of linear fractions. Nonlinear underestimator of these terms are included and have the following form;

$$\frac{Q_i}{B_i} = R_i \geq \frac{Q_i}{B_i^L} + Q_i^u\left(\frac{1}{B_i} - \frac{1}{B_i^L}\right) \qquad \textbf{(28)}$$

$$\frac{Q_i}{B_i} = R_i \geq \frac{Q_i}{B_i^u} + Q_i^L\left(\frac{1}{B_i} - \frac{1}{B_i^u}\right) \qquad (29)$$

It is necessary to have bounds over the batch sizes B_t. These are given by the following valid relaxations of the original constraints in NLP_B,

$$\min_j \left[\frac{V_j^u}{S_{ij}}\right] = B_i^u \geq B_i \quad (30)$$

$$B_i \geq B_i^L \geq \frac{Q_i^L T_{Li}}{H} \quad (31)$$

Exflmple 7

This example involves 5 products and 6 stages, and the corresponding data are given in Table 8. The following additional linear constraints are imposed;

$$Q_B \geq Q_E \quad (32)$$

$$Q_C + Q_D \geq Q_E \quad (33)$$

Product	A	B	C	D	E
Q^L	200.000	120.000	180.000	130.000	100.000
Q^u	300.000	180.000	200.000	160.000	150.000
d,	0.8	0.7	0.6	0.4	0.5
P,	0.1	0.15	0.15	02	0.2
TLI	8.31	6.8	11.9	3.5	4.2

a, = 2,5: V_j^L = 3,000 It V_j^u - 6,000 It F=550,000

Tables. ***Datafor batch design example*** **6.**

The initial lower bound is $* = - 74,4480 and it corresponds to an infeasible solution of NLP_B. The original nonconvex problem is solved to generate an upper bound using the solution of the underestimator problems as the initial point. In this form an upper bound of f = -73,270 is generated. It is necessary to perform a branch and bound and after 7 nodes the initial upper bound is proven to be globally optimal with tolerance e= 0.01. The global solution has V = (5737, 3600, 3776, 4983, 4430, 4014).

Conclusions

This paper has presented a general overview of the global optimization algorithm by Quesada and Grossmann (1993a) and outlined several alternative bounding approximations which can be applied in layout design, truss structures, portfolio investment and batch process design. As has been shown the use of some of these alternatives approximations can sometimes tighten the relaxations so that the solution of only one convex programming problem is required.

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