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Integer & Nonlinear Optimization

Linear inequalities for bounded products of variables

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Mixed-integer nonlinear programming (MINLP) is a vast class of optimization problems with a broad range of applications. In its most general form, a MINLP problem can be formulated as

MINLP: min
$$g_0(x)$$

s.t. $g_i(x) \le 0$ $\forall i = 1, 2..., m$
 $x \in \mathbb{Z}^p \times \mathbb{R}^{n-p}$,

where $g_i: \mathbb{R}^n \to \mathbb{R}$ is, in general, a nonlinear function for all $i=0,1,\ldots,m$ and may be nonconvex. MINLP problems subsume two major difficulties of optimization problems, namely nonlinear g_i 's and integrality of a set of variables. Some well-known subclasses of MINLP are NP-hard: relaxing integrality on x yields a nonconvex (in general) nonlinear optimization problem, while assuming that both the objective function $g_0(x)$ and all constraints $g_i(x) \leq 0$ are convex yields the subclass of convex MINLP.

Global optima of MINLP problems can be computed by implicit enumeration schemes such as branch-and-bound [9], which relies on lower bounds obtained from a relaxation of the problem. Because a large lower bound can reduce the solution time, it is crucial to find a tight relaxation. Several MINLP solvers use Linear Programming (LP) relaxations computed by reformulating a MINLP into an equivalent problem with constraints of the form $x_k = f_k(x_1, x_2, \dots, x_{k-1})$, where f_k is a nonlinear function, and replacing each such constraint with a system of linear inequalities $A^k x \leq b^k$ [3, 18, 20].

Multilinear functions are an important class used in MINLP models. They are n-variate functions that are linear in each variable x_i , i.e., when the remaining n-1 variables are fixed. Among multilinear functions, the linear combination of products $\sum_{i=1}^k a_i \prod_{j \in S_i} x_j$, where $S_i \subseteq \{1, 2, ..., n\}$, is widely used in modeling practical MINLPs. Several practical applications arise in the bilinear case, where functions $\sum_{i=1}^n \sum_{j=1}^n a_{ij} x_i x_j$ are used: for instance, pooling and scheduling problems in Chemical Engineering [14, 17] and bidimensional bin packing [6].

This paper focuses on polyhedral relaxations of *monomials*, i.e., products of a set of variables: we aim to find valid linear inequalities for

$$M_n = \{x \in \mathbb{R}^{n+1} : x_{n+1} = \prod_{i=1}^n x_i, x \in [\ell, u]\},\$$

where $\ell, u \in \mathbb{R}^{n+1}$. We assume $0 \le \ell_i < u_i < +\infty$ for i = 1, 2, ..., n+1. M_n is bounded and nonconvex as the function $\xi(x) = \prod_{i=1}^n x_i$ is nonconvex.

Define $N = \{1, 2, ..., n\}$. The assumption $\ell \geq 0$ implies that trivial bounds on x_{n+1} are $\bar{\ell}_{n+1} = \prod_{i \in N} \ell_i$ and $\bar{u}_{n+1} = \prod_{i \in N} u_i$. In general, $\bar{\ell}_{n+1} \leq \ell_{n+1} < u_{n+1} \leq \bar{u}_{n+1}$; in the remainder, we denote as M_n^{\star} the special case of M_n where $\ell_{n+1} = \bar{\ell}_{n+1}$ and $u_{n+1} = \bar{u}_{n+1}$. We are interested in developing a convex set enclosing M_n , defined by a system of linear inequalities. This would also allow us to approximate rational terms:

$$Q_2 = \{x \in \mathbb{R}^3 : x_1 = \frac{x_3}{x_2}, x \in [\ell, u]\},\$$

and, in general, quotients with products as denominator: $Q_n = \{x \in \mathbb{R}^{n+1} : x_1 = \frac{x_{n+1}}{\prod_{k=2}^n x_k}, x \in [\ell, u]\}.$

1. Linear Inequalities for M_2

The following linear relaxation of M_2^{\star} was introduced by McCormick [12] and shown to be its tightest convex relaxation by Al-Khayyal and Falk [1]:

$$\begin{array}{rclrcrcr}
x_3 & \geq & \ell_2 x_1 & + & \ell_1 x_2 & - & \ell_1 \ell_2 \\
x_3 & \geq & u_2 x_1 & + & u_1 x_2 & - & u_1 u_2 \\
x_3 & \leq & \ell_2 x_1 & + & u_1 x_2 & - & \ell_1 u_2 \\
x_3 & \leq & u_2 x_1 & + & \ell_1 x_2 & - & u_1 \ell_2.
\end{array} \tag{1}$$

 M_2^{\star} and its convex hull are depicted in Figure 1.

As regards M_2 , Tawarmalani et al. [19] describe the convex hull of $\{x \in \mathbb{R}^3 : x_1x_2 + x_3 \geq c, \ell_i \leq x_i \leq u_i, i = 1, 2, 3\}$. This is a special case of M_2 , as $x_1x_2 + x_3 \geq c$ implies a lower bound ℓ_3 on x_1x_2 that is larger than $\bar{\ell}_3 = \ell_1\ell_2$ if $\ell_1\ell_2 + u_3 < c$. Tawarmalani and Sahinidis [20] describe the convex hull of

$$D_3 = \{x \in \mathbb{R}^3 : x_1 = \frac{x_3}{x_2}, \\ 0 < \ell_2 \le x_2 \le u_2, \ 0 \le \ell_3 \le x_3 \le u_3\},\$$

again a special case of M_2 where $\ell_1 = \frac{\ell_3}{u_2}$, $u_1 = \frac{u_3}{\ell_2}$. The set D_3 is also studied by Jach et al. [8], who generalize the approach of [20] to find the convex hull

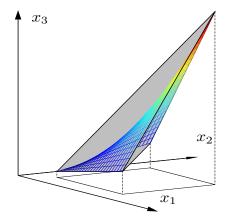


Figure 1: M_2^{\star} and its convex hull (1).

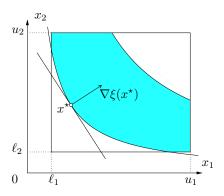


Figure 2: Projection of M_2 onto (x_1, x_2) .

of (n-1)-convex functions, i.e., nonconvex functions that are convex when any of their variables is fixed.

In order to find valid inequalities for the more general M_2 , consider its projection onto (x_1, x_2) : $P_2 = \{(x_1, x_2) \in \mathbb{R}^2 : \ell_i \leq x_i \leq u_i, i = 1, 2, \ell_3 \leq x_1x_2 \leq u_3\}$ (see Figure 2). It is safe to assume here that $\ell_3 \leq \ell_1u_2$ and $\ell_3 \leq u_1\ell_2$, as otherwise a tighter valid lower bound for x_1 (resp. x_2) would be $\ell_3/u_2 > \ell_1$ (resp. $\ell_3/u_1 > \ell_2$), or equivalently, the upper left (resp. lower right) corner of the bounding box would be cut out by $x_1x_2 \geq \ell_3$. Similarly, we assume that $u_3 \geq \ell_1u_2$ and $u_3 \geq u_1\ell_2$.

Before describing a valid linear inequality for M_2 , it is worth to briefly mention the particular case where $\ell_1 = \ell_2 = 0$ and $u_1 = u_2 = +\infty$. In that case, the convex hull is easily proved to be the intersection of $\{x \in \mathbb{R}^3 : \ell_3 \leq x_3 \leq u_3\}$ with the second order cone $\{x \in \mathbb{R}^3 : (x_3 + \sqrt{\ell_3 u_3})^2 \leq (\sqrt{\ell_3} + \sqrt{u_3})^2 x_1 x_2\}$.

Lifted Tangent Inequalities. We provide a more detailed derivation of the results below in [4]. Consider a point $x^* \in [\ell_1, u_1] \times [\ell_2, u_2]$ such that $x_1^* x_2^* = \ell_3$, therefore $\ell_1 \leq x_1^* \leq \min\{u_1, \ell_3/\ell_2\}$ and $\ell_2 \leq x_2^* = \ell_3/x_1^* \leq \min\{u_2, \ell_3/\ell_1\}$. The tangent to the curve $x_1x_2 = \ell_3$ at x^* gives a linear inequality $a_1(x_1-x_1^*)+a_2(x_2-x_2^*) \geq 0$ that is valid for P_2 (see Figure 2). The coefficients a_1 and a_2 are given by the gradient of the function $\xi(x) = x_1x_2$ at x^* , i.e., $a_1 = \frac{\partial \xi}{\partial x_1}(x^*) = x_2^*$ and $a_2 = \frac{\partial \xi}{\partial x_2}(x^*) = x_1^*$. Hence the inequality, which we call tangent inequality, is

$$x_2^{\star}(x_1 - x_1^{\star}) + x_1^{\star}(x_2 - x_2^{\star}) \ge 0.$$
 (2)

As this inequality is valid within P_2 and is independent from x_3 , it is also valid for M_2 .

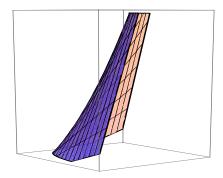


Figure 3: A representation of M_2 .

Consider now M_2 (depicted in Figure 3) rather than its projection. To give a hint as to why Mc-Cormick inequalities (1) are not sufficient in this case, consider the set Y obtained by intersecting M_2 with the set $\{x \in \mathbb{R}^3 : x_1 = x_2\}$, and suppose $\ell_1 = \ell_2 = 0$ and $u_1 = u_2 = 10$. Then Y can be represented as $\{(\lambda, y) \in \mathbb{R}^2 : y = \lambda^2\}$. The McCormick inequalities imply $y \leq 100\lambda$, which yields the convex relaxation given by the shaded area (both light and dark) in Figure 4, clearly not the tightest relaxation given that (2) tightens it. Furthermore, lifting (2) would restrict the relaxation to the darker area in Figure 4. We lift (2) as follows: the inequality

$$x_2^{\star}(x_1 - x_1^{\star}) + x_1^{\star}(x_2 - x_2^{\star}) + b(x_3 - \ell_3) \ge 0$$
 (3)

is clearly valid for $x_3 = \ell_3$. Validity for M_2 requires

$$g(b) = \min\{x_2^{\star}(x_1 - x_1^{\star}) + x_1^{\star}(x_2 - x_2^{\star}) + b(x_3 - \ell_3) : (x_1, x_2, x_3) \in M_2\} \ge 0.$$

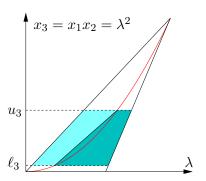


Figure 4: The relaxation of M_2 intersected with $\{x \in \mathbb{R}^3 : x_1 = x_2\}$ using McCormick inequalities only (the light shaded area) and with the lifted inequality (the dark shaded area).

Clearly, g(b) = 0 if $b \ge 0$ (a global optimum is given by (x_1^*, x_2^*)), hence we aim at finding the minimum b < 0 such that (3) is valid.

Observe that validity of (3) requires that it be satisfied by all points of $UC_2 = \{x \in [\ell, u] : x_3 = x_1x_2 = u_3\}$. If we relax the bounds u_1 and u_2 on x_1 and x_2 , the line $T = \{x \in \mathbb{R}^3 : x_3 = u_3, x_2^{\star}(x_1 - x_1^{\star}) + x_1^{\star}(x_2 - x_2^{\star}) + b(u_3 - \ell_3) = 0\}$ intersects UC_2 in either (i) none, (ii) one, or (iii) two points. The first two cases imply validity of the inequality, unlike the third one.

Consider case (ii) and denote $\bar{x} = (\bar{x}_1, \bar{x}_2)$ the only intersection; T is then tangent to UC_2 at \bar{x} . Thus, the gradient of ξ at \bar{x} must be parallel to $\nabla \xi(x^*)$, i.e., $\nabla \xi(\bar{x}) = \alpha \nabla \xi(x^*)$ for some $\alpha > 0$, hence $(\bar{x}_2, \bar{x}_1) = (\alpha x_2^*, \alpha x_1^*)$ and $\bar{x}_1 \bar{x}_2 = u_3 = \alpha^2 x_1^* x_2^* = \alpha^2 \ell_3$, therefore $\alpha = \sqrt{\frac{u_3}{\ell_3}}$. Since (\bar{x}_1, \bar{x}_2) satisfies (3) at equality,

$$\begin{array}{rcl} x_2^{\star}(\bar{x}_1 - x_1^{\star}) + x_1^{\star}(\bar{x}_2 - x_2^{\star}) + b(u_3 - \ell_3) & = \\ x_2^{\star}(\alpha x_1^{\star} - x_1^{\star}) + x_1^{\star}(\alpha x_2^{\star} - x_2^{\star}) + b(u_3 - \ell_3) & = 0, \end{array}$$

and as a result
$$b=\frac{2\left(1-\sqrt{\frac{u_3}{\ell_3}}\right)\ell_3}{u_3-\ell_3}$$
. The procedure outlined above does not work in

The procedure outlined above does not work in general as $\bar{x} = \alpha x^*$ may exceed one of the upper bounds on x_1 or x_2 . To this purpose, consider the parametric vector $\hat{x}(t)$ with $\hat{x}_i(t) = \min\{u_i, tx_i^*\}$. The set $\Gamma(x^*) = \{x \in \mathbb{R}^2 : x_i = \min\{u_i, tx_i^*\}, i = 1, 2, t \geq 1\}$, depicted in Figure 5 for two distinct vectors x^* , is a piecewise linear set. The function $\xi(t) = \hat{x}_1(t)\hat{x}_2(t)$ is monotonically non-decreasing and piecewise convex, and hence there exists a \hat{t}

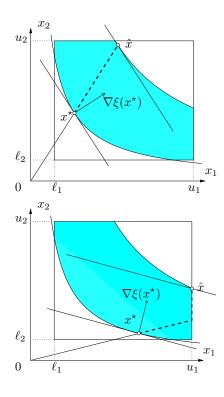


Figure 5: Construction of $\Gamma(x^*)$, \hat{t} , and \hat{x} . The set $\Gamma(x^*)$ is represented by the dashed line.

such that $\xi(\hat{t}) = u_3$. In order to compute \hat{t} , assume w.l.o.g. that $\frac{u_1}{x_1^*} \leq \frac{u_2}{x_2^*}$. Then

$$\xi(t) = \begin{cases} x_1^{\star} x_2^{\star} t^2 = \ell_3 t^2 & \text{if } 1 \le t \le \frac{u_1}{x_1^{\star}} \\ u_1 x_2^{\star} t & \text{if } \frac{u_1}{x_1^{\star}} \le t \le \frac{u_2}{x_2^{\star}} \\ u_1 u_2 & \text{if } t \ge \frac{u_2}{x_2^{\star}}, \end{cases}$$

and $\hat{t} = \xi^{-1}(u_3)$ is computed as follows: if $x_1^{\star}x_2^{\star}\left(\frac{u_1}{x_1^{\star}}\right)^2 = \frac{u_1^2x_2^{\star}}{x_1^{\star}} \geq u_3$, then $\hat{t} = \sqrt{\frac{u_3}{\ell_3}}$; otherwise, if $u_1x_2^{\star}\frac{u_2}{x_2^{\star}} = u_1u_2 \geq u_3$, $\hat{t} = \frac{u_3}{u_1x_1^{\star}}$. Note that these two cases exhaust all values of t as we assume $u_1u_2 \geq u_3$. Denote $\hat{x} = \hat{x}(\hat{t})$. Clearly $\hat{x} = (\hat{x}_1, \hat{x}_2, u_3) \in M_2$, and it satisfies (3) at equality if

$$b = \bar{b} := -\frac{x_2^{\star}(\hat{x}_1 - x_1^{\star}) + x_1^{\star}(\hat{x}_2 - x_2^{\star})}{u_3 - \ell_3},$$

which yields a valid inequality (3) for M_2 that we call lifted tangent inequality (LTI) – note that it only depends on x^* . The generalization to M_n is given in Section 3. LTIs are easily proven to be disjunctive cuts obtained from intersecting M_2 with the disjunction $x_3 = \ell_3 \vee x_3 = u_3$.

2. Linear Inequalities for M_n^*

The convex hull of sets defined by products of more than two terms has attracted interest for some decades. Meyer and Floudas [13] provide a set of linear inequalities describing the convex hull of a more general case of M_3^{\star} , where lower and upper bounds can also be negative.

Ryoo and Sahinidis [16] construct polyhedral relaxations of M_n^{\star} with n > 2 as follows: given an index set $I = \{i_1, i_2, \dots, i_K\}$ and the product of K > 2 variables $\prod_{i \in I} x_i$, add auxiliary variables y_2, y_3, \dots, y_K defined as

$$y_{2} = x_{i_{1}}x_{i_{2}}$$

$$y_{3} = y_{2}x_{i_{3}}$$

$$y_{4} = y_{3}x_{i_{4}}$$

$$\vdots$$

$$y_{K} = y_{K-1}x_{i_{K}}$$

where the bounds on y_k are determined by the bounds on the factors of the product. Then, add McCormick inequalities for $M_2^{(2)} = \{(x_{i_1}, x_{i_2}, y_2) \in [\ell_{i_1}, u_{i_1}] \times [\ell_{i_2}, u_{i_2}] \times [\ell(y_2), u(y_2)] : y_2 = x_{i_1}x_{i_2}\}$ and for each set $M_2^{(k)} = \{(y_{k-1}, x_{i_k}, y_k) \in [\ell(y_{k-1}), u(y_{k-1})] \times [\ell_{i_k}, u_{i_k}] \times [\ell(y_k), u(y_k)] : y_k = y_{k-1}x_{i_k}\}$, with $3 \leq k \leq K$. We define $\ell(y_k) := \ell(y_{k-1})\ell_{i_k}$, with $\ell(y_2) = \ell_{i_1}\ell_{i_2}$, and analogously define the upper bounds $u(y_k)$.

A convex estimator can thus be obtained with 4(n-1) linear inequalities. This procedure, called Recursive Arithmetic Intervals (rAI), is shown by [16] to yield the convex hull of M_n^{\star} when $\ell=0$. Luedtke et al. [11] prove that this result also holds in the case where $\ell=-u$, and compare the tightness of the convex hull of bilinear functions to that of the McCormick relaxations.

A central result has been proved by Rikun [15] on the more general multilinear functions defined on polyhedra. For such functions, the validity of an inequality only needs to be checked at the vertices of the polyhedron on which they are defined, hence the convex hull of M_n^{\star} is polyhedral. However, said convex hull contains an exponential number of inequalities, which makes it impractical for use in global optimization solvers except for small n (see e.g. [2]). Inequalities for M_4^{\star} have been proposed by Cafieri et al. [5] by "composing" the convex hulls of bilinear and trilinear terms.

3. Linear Inequalities for M_n

The derivation of valid inequalities for M_n is a straightforward generalization of the method described in Section 1. Similar to M_2 , we assume $\ell_{n+1} \leq \min_{i \in N} \{\ell_i \prod_{j \in N \setminus \{i\}} u_j\}$ (resp. $u_{n+1} \geq \max_{i \in N} \{u_i \prod_{j \in N \setminus \{i\}} \ell_j\}$), as otherwise we can tighten one of the lower (resp. upper) bounds. Specifically, for i such that $\ell_{n+1} > \ell_i \prod_{j \in N \setminus \{i\}} u_j$, ℓ_i is increased to $\frac{\ell_{n+1}}{\prod_{j \in N \setminus \{i\}} u_j} > \ell_i$, and for all i such that $u_{n+1} < u_i \prod_{j \in N \setminus \{i\}} \ell_j$, u_i is reduced to $\frac{u_{n+1}}{\prod_{j \in N \setminus \{i\}} \ell_j} < u_i$.

Tangent Inequalities for M_n . Let us denote P_n the projection of M_n onto \mathbb{R}^n : $P_n = \{x \in \mathbb{R}^n : \ell_i \leq x_i \leq u_i, i \in N, \ell_{n+1} \leq \prod_{i \in N} x_i \leq u_{n+1} \}$. Define

$$LC_n := \{x \in P_n : \prod_{i \in N} x_i = \ell_{n+1}\};\ UC_n := \{x \in P_n : \prod_{i \in N} x_i = u_{n+1}\}.$$

The following simple result generalizes the validity of the tangent inequality (2).

Lemma 1 For any $x^* \in LC_n$, the inequality:

$$\sum_{i \in N} a_i(x_i - x_i^*) \ge 0, \tag{4}$$

where $a_i := \prod_{j \in N \setminus \{i\}} x_j^{\star}$, is valid for P_n .

For n=2, (4) reduces to (2). We lift (4) to obtain an inequality satisfied by a point on UC_n . To this purpose, consider the parametric point $\hat{x}(t)$ with components $\hat{x}_i(t) = \min\{u_i, tx_i^*\}$ and the set

$$\Gamma(x^*) = \{ x \in \mathbb{R}^n : x_i = \min\{u_i, tx_i^*\} \ \forall i \in \mathbb{N}, t \ge 1 \},$$

where x^* corresponds to t = 1. Also, consider the function $\xi(t) = \prod_{i \in N} \hat{x}_i(t)$, defined for all $t \geq 1$. Define $\hat{t} = \min\{\tau \geq 1 : \xi(\tau) = u_{n+1}\}$, i.e. the minimum t attaining a point in UC_n , and denote $\hat{x} = x(\hat{t})$. It can be shown that such a \hat{t} , in the general case, can be computed in O(n). Note that, for small values of t, the gradient of ξ at $\hat{x}(t)$ is proportional to $\nabla \xi(x^*)$.

Lifted Tangent Inequalities. A lifting of (4) that satisfies \hat{x} at equality yields a valid inequality for M_n . Then the inequality

$$\sum_{i \in N} a_i (x_i - x_i^*) + b(x_{n+1} - \ell_{n+1}) \ge 0$$
 (5)

holds at equality at x^* for any b, while it does at \hat{x} if $\sum_{i \in N} a_i(\hat{x}_i - x_i^*) + b(u_{n+1} - \ell_{n+1}) = 0$, or

$$b = \bar{b} := -\frac{\sum_{i \in N} a_i (\hat{x}_i - x_i^*)}{u_{n+1} - \ell_{n+1}}.$$

Note that, as for M_2 , \bar{b} is negative (a positive value yields a redundant inequality) and depends on x^* .

Theorem 1 Inequality (5) is valid for any $b \geq \bar{b}$.

A similar result can be proved when starting from any point x^* of UC_n , though the analogous inequality (4) is *not* valid unless lifted. The derivation is similar to the one above and is thus omitted.

Note that LTIs have to be amended to the LP relaxation; they do not dominate McCormick inequalities, and are thus not sufficient to describe the convex hull of M_n . For instance, the convex hull of M_2 is obtained by considering both McCormick inequalities and LTIs [4].

4. Computational Results

In order to assess the utility of the lifted tangent inequalities introduced above in the context of MINLP solvers, we have developed a procedure for generating LTIs and tested it on a set of MINLP problems.

We have used COUENNE [7], an open-source software package included in the Coin-OR infrastructure [10], for all experiments. Couenne is a branch-and-bound solver that computes a lower bound with an LP relaxation obtained through reformulation techniques [12, 18, 20]. As for most MINLP solvers, COUENNE uses a procedure to gradually refine the LP relaxation by repeatedly solving the LP relaxation at each node of the branch-and-bound tree, obtaining a solution $x^{\rm LP}$, and seeking an inequality violated by $x^{\rm LP}$ which strengthens the relaxation.

Generating LTIs amounts to finding x^* associated with a violated LTI. We omit the details of the separation algorithm, but point out that the procedure finds a violated LTI in $\mathcal{O}(n)$. In these experiments, at each branch-and-bound node Couenne used up to four rounds of cuts to refine the LP relaxation.

Although LTIs can be separated for M_n , COUENNE does not generate inequalities for the convex hull of M_k^{\star} with $k \geq 3$, hence all of our experiments focus on bilinear terms. Products of more

than two variables are decomposed into a set of bilinear terms using the recursive Arithmetic Interval (rAI) technique [16] outlined in Section 2. Although each auxiliary y_k introduced by rAI has trivial bounds at the beginning, branching rules (which may also be imposed on y_k) and bound reduction techniques may reduce its bounds and thus require separation of LTIs for some, or all, of the bilinear terms generated.

Also, COUENNE can generate LTIs for bilinear sets M_2 not necessarily contained in \mathbb{R}^3_+ but in any other orthant, i.e., LTIs are generated when the bound interval of each variable does not have 0 as an interior point: if a variable x_i of a bilinear term has $\ell_i < u_i \le 0$, then a fictitious variable x_i' with inverted bound interval $[-u_i, -\ell_i]$ replaces x_i .

In order to show the utility of LTIs for M_2 , we have compared two variants of COUENNE, which we call COUENNE and COUENNELTI, on a set of MINLP instances. While the first variant only separates, for each bilinear term, inequalities (1), the second variant adds both these and LTIs—recall that there is no dominance relationship between these two families of inequalities.

We have performed tests on 474 instances from multiple online libraries: GLOBALLIB¹, MINLPLIB², and MACMINLP³. Both variants were allowed two hours of CPU time. All experiments have been carried out on the Palmetto cluster of Clemson University, which has machines with different CPUs and amounts of memory. Although a parallel version of COUENNE is currently being developed and the cluster allows running parallel jobs, we have used a serial version of the code for our tests. Also, in order to provide a fair comparison, each instance was solved by the two variants on the same machine.

Out of 474 instances, we only report on the 119 instances that took either or both algorithms more than one minute. Table 1 summarizes the comparison by showing, for each variant, the number of instances

- solved before the time limit (solved);
- solved in at most 90% of the other variant's time (best time);

Alg	Solved	Best time	Best nodes	Best lower
A1	26	15	7	24
A2	26	8	11	32

Table 1: Summary of the comparison between Couenne (A1) and CouenneLTI (A2).

- solved using at most 90% of the other variant's BB nodes (best nodes);
- for which the variant obtained the best lower bound (best lower).

The first three parameters refer to instances that at least one variant solved before the time limit, whereas the last one refers to the instances that neither algorithm could solve to optimality. It appears that separating LTIs on "easy" instances, i.e., those that can be solved within the time limit, is of limited impact (mainly on the number of BB nodes) and actually may lead to an increase in CPU time. However, when both algorithms take more than two hours, LTIs help obtain a better lower bound.

Table 2 shows in more detail the performance of both variants of Couenne for some of the instances where the difference in performance is significant, regardless of whether Couenne or CouenneLTI obtained a better result. A more complete report can be found in [4]. The better performance is in bold. The parameters reported in the columns are:

- Name, var, con: Name of the instance, number of variables and of constraints;
- T(lb): the CPU time taken to solve the problem to optimality, or, if no solution was found within the time limit, the lower bound in brackets;
- node: the number of BB nodes used before proving optimality or the time limit was passed;
- *ub*: the best known upper bound.

Although the results are only sketched here for reasons of space, it is apparent that some instances highly benefit from adding LTIs. Certain instances (nvs23, nvs24, st-e35) can be solved much more quickly, although it appears that for others (bayes2-10, bayes2-30, bayes2-50, tln5) LTIs have the opposite effect.

¹http://www.gamsworld.org/global/globallib.htm

²http://www.gamsworld.org/minlp/minlplib.htm

³http://www.mcs.anl.gov/~leyffer/MacMINLP

			Couenne		CouenneLTI		
Name	var	con	t(lb)	nodes	t(lb)	nodes	ub
bayes2-10	86	72	3553	124k	(0)	67k	2.55e-4
bayes2-30	86	75	3072	130k	(0)	$1.5 \mathrm{m}$	4.61e-4
bayes2-50	86	76	6140	1727	(0)	2057	0.9298
camcge	209	209	(-4036)	535	(-6092)	426	-191.74
ex5-2-5	32	19	(-4832)	$1.6 \mathrm{m}$	(-4775)	$2.1 \mathrm{m}$	-3500
ex5-4-4	27	19	(7257)	$3.1 \mathrm{m}$	(7801)	$2.1 \mathrm{m}$	10077.8
hhfair	27	25	252	30k	168	23k	-87.159
space-25	893	235	(89.4)	4388	(90.9)	5278	483.811
nvs23	9	9	(-1240)	$2.7 \mathrm{m}$	237	61k	-1125.2
nvs24	10	10	(-1200)	$2.5 \mathrm{m}$	6054	$1.7 \mathrm{m}$	-1033.2
st-e35	29	33	(42443)	$1.1 \mathrm{m}$	496	210k	64868
tln5	35	30	2506	$2.4 \mathrm{m}$	(9.86)	$4.5 \mathrm{m}$	10.3
tln7	63	42	(7.73)	123k	(9.31)	$1.5 \mathrm{m}$	15.6
water4	195	137	(716.7)	$1.3 \mathrm{m}$	(655.1)	957k	965.47
waterx	70	54	(636.7)	58k	(652.4)	106k	973.91

Table 2: Comparison between COUENNE and COUENNELTI on select instances. Under "t(lb)" columns are reported the CPU time or, if more than two hours, the lower bound in brackets; "ub" is the best known upper bound.

5. Concluding Remarks

We have described a family of linear inequalities of the convex hull of a class of nonconvex sets widely used in MINLP. Their efficiency has only been tested on products of two variables, but we expect to implement the more general procedure in the near future and apply it to MINLP problems with products of more than two variables.

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CyberInfrastructure for Mixed-Integer Nonlinear Programming

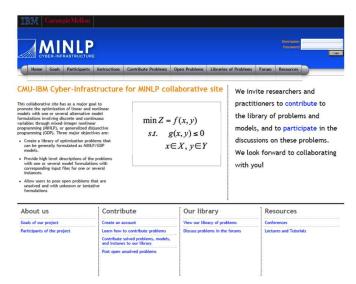
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Carnegie Mellon University and the IBM T. J. Watson Research Center researchers have developed a Collaborative CyberInfrastructure for Mixed-Integer Nonlinear Programming (MINLP): http://www.minlp.org, which is funded by the funded by the National Science Foundation under Grant OCI-0750826: "OpenCyberInfrastructure for Mixed-integer Nonlinear Programming: Collaboration and Deployment via Virtual Environments". The core team consists of: Larry Biegler, Ignacio E. Grossmann, François Margot and Nick Sahinidis of CMU, and Jon Lee and Andreas Wächter of IBM. Additional collaborators include: Pietro Belotti (Clemson University), Pedro Castro (INETI) and Juan Ruiz (CMU). The site was launched in October, 2009. The current homepage is shown below. Over the last 12 months the site has had between 500 and 1000 daily hits, and between 80 and 130 daily visits.



Optimization has been recognized as one of the strategic technologies for cyberinfrastructure computational tools. Many of the challenging optimization models require the use of discrete variables (often 0-1 variables) to represent logical choices, as well as the handling of nonlinearities in order to accurately predict the performance of physical, chemical, biological, financial or social systems. These optimization problems give rise to MINLP problems, which in 0-1 variables have the general form:

$$\begin{aligned} & \min \quad Z = f(x,y) \\ & \text{s.t.} \quad g(x,y) \leq 0 \\ & \quad x \in X, \ y \in Y \\ & X = \{x | x \in \mathbb{R}^n, \ x^L \leq x \leq x^U, \ Bx \leq b\} \\ & Y = \{y | y \in \{0,1\}, \ Ay \leq a\} \end{aligned}$$

In a form emphasizing the logical choices, such an MINLP can be represented as a Generalized Disjunctive Programming (GDP) problem in terms of Boolean and continuous variables and algebraic equations, disjunctions and logic propositions. Namely,

$$\min \quad Z = \sum_{k} c_k + f(x)$$
s.t.
$$r(x) \leq 0$$

$$\bigvee_{j \in J_k} \begin{bmatrix} Y_{jk} \\ g_{jk}(x) \leq 0 \\ c_k = \gamma_{jk} \end{bmatrix} \quad k \in K$$

$$\Omega(Y) = true$$

$$x \in \mathbb{R}^n, \ c_k \in \mathbb{R}^1$$

$$Y_{jk} \in \{true, \ false\}$$

While MINLP optimization methods can be successfully applied to a very wide class of MINLP problems, it represents one of the most challenging class of optimization problems. On the combinatorial side, MINLP are known to be "NP hard" (in fact, even undecidable as decision problems). On the side of continuous nonlinearities, many MINLP models are nonconvex, which implies that continuous relaxations typically give rise to many local solutions.

The number of computer codes for solving MINLP problems has increased in the last decade. The program DICOPT [9] is an MINLP solver that is available in the modeling system GAMS [4], and is based on the outer-approximation method [5] with heuristics for handling nonconvexities. A similar code to DICOPT, AAOA, is available in AIMMS. Codes that implement the branch-and-bound method include the code MINLP-BB that is based on an SQP

algorithm [8] and is available in AMPL, and the code SBB which is available in GAMS [9]. Both codes assume that the bounds are valid even though the original problem may be nonconvex. The code α -ECP that is available in GAMS implements the extended cutting plane method by Westerlund and Pettersson [12], including the extension by Westerlund and Pörn [13]. The open source code Bonmin [3] implements the branch-and-bound method, the outer-approximation and an extension of the LP/NLP-based branch-and-bound method in one single framework. FilMINT [1] also implements a variant of the LP/NLP-based branch-and-bound method. Codes for the global optimization that implement the spatial branch-and-bound method include BARON [9], LINDOGlobal [7], and Couenne [2]. As for codes for solving GDP problems the only ones that are currently available are LOGMIP [10] and EMP [6].

While there are a number of websites that have been aimed at comparing the computational performance of MINLP codes MacMINLP: AMPL collection of Mixed-Integer Nonlinear Programs http://wiki.mcs.anl.gov/ leyffer/index.php/MacMINLP, and MINLP World http://www.gamsworld.org/minlp/index.htm), the major goal of our website is to create a library of optimization problems, in different application areas, for which one or several alternative models are presented with the derivation of their mathematical formulations. The emphasis is on the formulation of models, because this is an area that is particularly critical in MINLP, where alternative formulations can often have vastly different computational performance [14]. One goal is to illustrate and discover good and bad practices of MINLP modeling. Each model has one or several instances that can serve to test various algorithms. While we are emphasizing MINLP models, MILP and NLP models can also be submitted, particularly if they are relevant to problems that also have MINLP formulations. Furthermore, we have recently added GDP problems, linear and nonlinear.

The MINLP cyberinfrastructure website is aimed at the optimization community that is increasingly interested in the solution and application of MINLP problems. This community involves academics and people from industry, and is highly multidisciplinary.

It involves operations researchers, industrial, chemical and mechanical engineers, economists, chemists and biologists. This community, however, is largely disconnected, especially between algorithm developers and application domain researchers.

Our website provides a mechanism for the entire spectrum from researchers to users to contribute towards the creation of this library of optimization problems, and to provide a forum of discussion for algorithm developers and application users where alternative formulations, as well as performance and comparison of algorithms can be discussed. The website, which was launched in October 2009, contains information on tutorials, a bibliography and links to other resources on MINLP.

The information that is required for submitting a problem is structured as follows:

Problem Title.

- **Problem Statement:** pdf file that describes precisely the problem with all the required assumptions. The problem statement is independent of any model formulation.
- Overview of Session: pdf file that briefly expands on the problem (qualitatively) and describes major features of formulations submitted for that submission session.
- **Models:** pdf files describing the mathematical models and their derivation.
- **Instances:** GAMS/AMPL/AIMMS input and output files. The size of the model is specified by the user for each instance.
- Results, Analysis & Data: pdf file where the author reports results obtained with the supplied models and presents an analysis of them. The data for the various instances are included in an appendix of this file.

Admittedly, the effort involved in the submission of these problems is not small. However, in order to facilitate this task, we have provided a detailed guide as well as examples at the link http://www.minlp.org/goals/instructions.php. When authors submit a problem, it is examined by the administrator who either approves or suggests changes to the submission.

The functionality of the website is such that if an author submits problem with one or several models, instances and results, other authors or the same author can submit in subsequent sessions alternative models or instances for that problem. A possible scenario is as follows. Session 1: author X submits problem statement, models A & B, instances and results. Perhaps another researcher, author Y, finds a better model C, and submits Session 2 for that same problem, where author Y submits new model C, instances and results. Discussion between authors X and Y can then take place within a wiki forum that is available in the site. Next, perhaps author X finds that he/she can solve larger problems with his/her model and submits Session 3 in which author X submits new instances, and results for models A, B, C.

The library currently contains 27 MINLP problems that were submitted in areas such as engineering, operations management, physics and finance. The list is as follows:

- Crude-oil operations scheduling.
- Inventory-production-distribution problems with direct shipments.
- Optimal scheduling of multistage batch plants.
- Integrated process water networks design problem.
- Cutting stock optimization problem for the production of carton board boxes.
- Optimal simultaneous synthesis of heat exchangers network.
- Optimal scheduling of refined products pipelines and terminal operations.
- Disjunctive strategies for optimization of pipeline operations.
- Extended pooling problem with the summer time (EPA) complex emissions constraints.
- Optimization of metabolic networks in biotechnology.
- Close-enough vehicle routing problem.
- Simultaneous cyclic scheduling and control of a multiproduct continuous stirred tank reactor.

- Optimal separation sequences based on distillation: from conventional to fully thermally coupled systems.
- Close-enough traveling salesman problem.
- The delay constrained routing problem.
- A deterministic security constrained unit commitment model.
- Stochastic portfolio optimization with round lot trading constraints.
- Stabilizing controller design and the Belgian chocolate problem.
- Design of telecommunication networks with shared protection.
- Optimal design of multiproduct batch plant.
- Solving MINLPs with Dinkelbach's Algorithm and MINLP Methods.
- Polygeneration energy systems design.
- Periodic scheduling of continuous multiproduct plants.
- Optimization model for density modification based on single-crystal X-ray diffraction data.
- Supply chain design with stochastic inventory management.
- Optimization of a class of hybrid dynamic systems.
- Water treatment network design.

As an example, in the above list, the problem "Optimal design of multiproduct batch plant", describes a nonconvex MINLP and convexified MINLP formulation in which the performance of DICOPT is shown to be significantly faster than SBB and BARON. In the problem "Optimal periodic scheduling of continuous multiproduct plants", the MINLP has a linear fractional objective that is not solvable with many of the standard codes (DICOPT, SBB, α -ECP, BARON). The problem "Optimization model for density modification based on single-crystal X-ray diffraction data", describes alternative models, an MINLP and two MILPs, both extremely large

in size, which have not been solved to optimality. The "Water treatment process design problem" describes two alternative models, one in terms of flows and compositions, the other in terms of individual flows and split fractions. Both cannot solved be to global optimality without proper lower and upper bounds on the variables. Furthermore, the model with flows and composition leads to fewer nodes in the spatial branch and bound with BARON. The problem "Optimization of hybrid dynamic systems" compares a formulation with complementarity constraints, which leads to a continuous nonconvex NLP, that is shown to solve much faster than the corresponding MINLP model.

The GDP problems that have been submitted are the following:

- Process synthesis problem.
- 2-D constrained layout.
- Strip-packing problem.
- Job-shop scheduling.

In these problems, reformulation based on big-M transformation and convex-hull are compared. In the case of the "Process synthesis problem" the performance of the logic-based outer-approximation algorithm is also analyzed.

In summary, we believe that our cyberinfrastructure website for MINLP offers unique problems and capabilities. The site also provides information on various resources, meetings and an extensive bibliography. We welcome any new contributions to expand the library of problems. For feedback on this site, comments are welcome at: minlp@andrew.cmu.edu.

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Bulletin

Paul Tseng Lectureship Prize

The Mathematical Optimization Society invites nominations for the Paul Y. Tseng Memorial Lectureship in Continuous Optimization. This prize was established in 2011 and will be presented for the first time at the Twenty First International Symposium of Mathematical Programming (ISMP) in 2012, and triennially at each ISMP thereafter. The lectureship was established on the initiative of family and friends of Professor Tseng, with financial contributions to the endowment also from universities and companies in the Asia-Pacific region. The purposes of the lectureship are to commemorate the outstanding contributions of Professor Tseng in continuous optimization and to promote the research and applications of continuous optimization in the Asia-Pacific region.

The lectureship is awarded to an individual for outstanding contributions in the area of continuous optimization, consisting of original theoretical results, innovative applications, or successful software development. The primary consideration in the selection process is the quality and impact of the candidate's work in continuous optimization. A secondary consideration is to select candidates with strong interests to promote continuous optimization research in the Asia-Pacific region. However, there is no geographic restriction on the candidates.

The prize will be presented at the 2012 International Symposium on Mathematical Programming (ISMP), to be held August 19-24, 2012, in Berlin, Germany. The Tseng lecture will be arranged in a time slot devoted to the presentation of named lectures at ISMP-2012.

Nomination Material. The nomination must include a nomination letter of no more than two pages and a short CV of the candidate (no more than two pages, including selected publications). In addition, the nominator should also arrange for 1-2 letters of recommendation. All nomination materials should be sent (preferably in electronic form, as pdf documents) to the chair of the selection committee,

Sven Leyffer, Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL 60439, USA, leyffer@mcs.anl.gov.

Deadline. All nomination materials must be received by November 15, 2011.

Paul Y. Tseng Memorial Lectureship Committee.

- Sven Leyffer (chair), Argonne National Laboratory, USA.
- Duan Li, Chinese University of Hong Kong, Hong Kong.
- Stefan Ulbrich, Technical University of Darmstadt, Germany.
- Naihua Xiu, Beijing Jiaotong University, China.

Chairman's Column

I feel honored to have been selected as the chair of the SIAM Activity Group on Optimization for the next three years. I and the other new officers, Mihai Anitescu, Miguel Anjos, and Marina Epelman, will try to maintain its exemplary status and activities. Please feel free to contact us with any suggestions: our email addresses are available at the group's home page, http://www.siam.org/activity/optimization.

Let me start by thanking our predecessors, Michael Ferris and his team of Tom McCormick, Steve Vavasis, and Yinyu Ye, for leaving us in such a great state. We are the second largest activity group (trailing Computational Science and Engineering), with a large international representation, a high proportion of student members, and diverse representation in different academic disciplines and employment types. We have a distinguished journal, an outstanding series of conferences starting with the first in Boulder in 1984 and leading up to Darmstadt this year, and an excellent newsletter edited with flair and efficiency by Sven Leyffer; I am very glad to report that Sven has agreed to continue in this role.

I like to think of the optimization people in SIAM not so much as a group and more as a community. Our colleagues tend to exhibit less of the competition and infighting typical in other areas (a recent quote from Larry Summers of Harvard: "I'm one of the few people who went to Washington to get out of politics"), with a healthy willingness to get involved and help the profession. And so I'd like to devote this first column to the theme of collaboration.

While our job evaluation criteria may at times seem to encourage us to be proprietorial about our research, those of us who have been around a few years know the great benefits of research collaboration, both in advancing science and in personal satisfaction. Of course, junior scientists need to move out of the shadow of their advisors, but working with a variety of collaborators, possibly in a range of disciplines, can be very rewarding. My own research went through a "phase transition" about ten years after my Ph.D., from almost wholly singly-authored papers to almost wholly co-authored — and the change should have happened earlier!

One venue in which to meet new colleagues, share new ideas, and explore new collaborations is that of professional meetings. We all enjoy the intense atmosphere of focused workshops in our own specialty, where young researchers rub shoulders with established leaders and advance the state of the art. Perhaps even more stimulating are such workshops on topics closely related but distinct from our own specialties, where we learn about cutting-edge research to which our perspective and experience might contribute. There is also great value in more general meetings, like the triennial SIAM conferences on optimization, where we are exposed to a wide range of topics and get to appreciate the broad applicability of all areas of optimization.

So I hope you will take full advantage of the upcoming conference in Darmstadt. The organizing committee has put together an outstanding program with a wide range of invited presentations covering theory, computation, and applications. I invite you to step a little outside your comfort zone in attending sessions where you will be exposed to new techniques and areas of application. Optimization is involved in so many disciplines beyond its initial applications in logistics, planning, and engineering design: for example in service industries, with problems in call center staffing and emergency vehicle location and scheduling; in image reconstruction, sensor location, compressed sensing, and high-dimensional structured statistics; and in medicine and biology.

The last issue of Views-and-News contained a fascinating article by Fengqi You and Sven Leyffer on applying optimization to remediation efforts after the Gulf oil spill, and a 2009 issue was devoted to the public side of optimization. These examples show that our field addresses pressing social problems as well as those of economic efficiency. One hopes that optimization can also play a role in dealing with natural disasters such as the recent ones in Haiti, Pakistan, New Zealand, and Japan. I am sure Sven would be pleased to hear of such stories.

I look forward to seeing you in Darmstadt!

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Comments from the Editor

Over the past years, mixed-integer nonlinear programming (MINLP) has steadily grown in importance. An IMA hot-topics workshop on MINLP in 2008 was followed by a second workshop in Marseille on the same topic in 2010, and a third workshop is in the planning stages. The 2009 ISMP meeting included for the first time a cluster explicitly devoted to MINLP. The two papers in the issue describe different aspects of this burgeoning field.

The first paper by Belotti, Miller, and Namazifar shows how to obtain strong linear inequalities for simple mixed-integer nonlinear sets that involve nonconvex multilinear functions. This paper exemplifies some current research activities in MINLP, where authors study simple sets of nonlinear functions to obtain tight polyhedral or conic relaxations.

The second paper by Grossmann and Lee describes a new cyber-infrastructure for MINLP. Their

goal is to collect and annotate applications of MINLP, providing a focus for multi-disciplinary users of MINLP. The web-site, http://www.minlp.org, allows users to compare formulations, and promotes good modeling practices in optimization.

We are already planning the next issue of Viewsand-News, which will feature a number of short papers from the SIAM Conference on Optimization. Our long-term goal is to increase the number of issues from two to three per year. Please contact Mike Todd, or myself if you have suggestions for topical issues that you'd like to edit, or papers that you'd like to contribute.

Send your comments, suggestions, papers, or complaints to:

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