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Valid Inequalities and Convex Hulls for Multilinear Functions

Pietro Belotti

Department of Industrial and Systems Engineering
Lehigh University

Andrew J. Miller [1]

Institut de Mathématiques de Bordeaux, Université Bordeaux 1, France
RealOpt, INRIA Bordeaux Sud-Ouest
andrew.miller@math.u-bordeaux1.fr

Mahdi Namazifar

Department of Industrial and Systems Engineering
University of Wisconsin-Madison

Abstract

We study the convex hull of the bounded, nonconvex set $M_n = \{(x_1, \ldots, x_n, x_{n+1}) \in \mathbb{R}^{n+1} : x_{n+1} = \prod_{i=1}^{n} x_i; \ell_i \leq x_i \leq u_i, i = 1, \ldots, n+1\}$ for any $n \geq 2$. We seek to derive strong valid linear inequalities for M_n; this is motivated by the fact that many exact solvers for nonconvex problems use polyhedral relaxations so as to compute a lower bound via linear programming solvers.

We present a class of linear inequalities that, together with the well-known McCormick inequalities, defines the convex hull of M_2. This class of inequalities, which we call *lifted tangent inequalities*, is uncountably infinite, which is not surprising given that the convex hull of M_2 is not a polyhedron. This class of inequalities

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generalizes directly to M_n for $n > 2$, allowing us to define strengthened relaxations for these higher dimensional sets as well.

Keywords: Mixed integer nonlinear programming, convex hulls, polyhedral analysis, strong formulation, multilinear functions

1 Motivation

Consider the following nonconvex, bounded set

$$M_n = \{x \in \mathbb{R}^{n+1} : x_{n+1} = \prod_{i=1}^{n} x_i, \ell_i \leq x_i \leq u_i, i = 1, 2 \ldots, n+1\},$$

where l and u are $(n+1)$-vectors. We assume $0 \leq \ell_i < u_i$ for $i = 1, \ldots, n+1$. The set M_n is nonconvex as the function $\xi_n(x) = \prod_{i=1}^{n} x_i$ is neither convex nor concave – its *epigraph* $\text{epi}(M) = \{x \in \mathbb{R}^{n+1} : x_{n+1} \geq \prod_{i=1}^{n} x_i, 0 < \ell_i \leq x_i \leq u_i, i = 1, \ldots, n\}$ and its *hypograph* $\text{hyp}(M) = \{x \in \mathbb{R}^{n+1} : x_{n+1} \leq \prod_{i=1}^{n} x_i, 0 < \ell_i \leq x_i \leq u_i, i = 1, 2 \ldots, n\}$ are both nonconvex sets.

Assuming M_n is contained in the first orthant, trivial bounds for x_{n+1} are given by $\prod_{i=1}^{n} \ell_i$ and $\prod_{i=1}^{n} u_i$, respectively. We denote these trivial bounds by $\bar{\ell}_{n+1}$ and $\bar{u}_{n+1}$ throughout. In general, $\bar{\ell}_{n+1} \leq \ell_{n+1} < u_{n+1} \leq \bar{u}_{n+1}$; in the remainder, we use the notation $M_n^{\star}$ for the set 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 superset C_n of M_n defined by a system of linear inequalities, therefore we seek a polyhedral set $C_n \supseteq M_n$. Our interest is motivated by the nonconvex optimization problem

$$\mathbf{P}: \qquad \min\{cx : x \in X\},$$

where X is, in general, a nonconvex set. In order to solve problems like $\mathbf{P}$ to optimality, one needs to implicitly enumerate all local optima, for instance by branch-and-bound algorithms (see, e.g., [1,10]). The bounding algorithms in such approaches often rely on linear relaxations of the nonconvex problem and can thus benefit from tighter linear relaxations.

Previous analysis has been focused primarily on M_n^*, that is, on the version in which *the product term in unbounded*. The well-known McCormick inequalities define the convex hull of M_2^* [5,2] in this case. It is known that the convex hull of M_n^* is a polyhedron, research on such polyhedra for $n > 2$ includes [8,6,7].

[1] Corresponding author

A set related to M_2 that is often used to approximate quotient terms in global optimization problems is

$$Q_2 = \{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_1 = \frac{x_3}{x_2}, \ell_i \leq x_i \leq u_i i = 1, 2, 3\}$$

The quotient set that is analogous to M_n is

$$Q_n = \{x \in \mathbb{R}^{n+1} : x_1 = \frac{x_{n+1}}{\prod_{k=2}^{n} x_k}, \ell_i \leq x_i \leq u_i i = 1, 2, \ldots, n+1\}$$

As with M_2 and M_n, previous research on such sets (e.g., [9,3]) has assumed that the quotient (here, x_1) is unbounded. As with M_2 and M_n, our model therefore generalizes these sets as well.

It is also worth emphasizing that finding the convex envelope of M_2 allows us not only to describe the convex envelope of Q_2 (this description was derived in a much different way by [3]), but of a more general model as well. It is also important to emphasize that *all previous research* of which we are aware on both M_n and Q_n has focused on the case in which a function (either the product or the quotient) is unbounded. In other words, the model of M_n with nontrivial bounds has not been analyzed before. As a consequence, the convex hull of M_2 was, to our knowledge, unknown before this research. Another consequence is that the results discussed here generalize and dominate many of those presented previously.

2 Linear envelopes for $n = 2$

Here we develop convex envelopes for the set $M_2 = \{(x_1, x_2, x_3) \in [l, u] : x_3 = x_1 x_2\}$. Although this is the simplest case, many considerations generalize easily to the case when $n > 2$.

2.1 Unbounded x_3

The following linear relaxation of $M_2^\star$ was introduced by McCormick [5] and shown to be its tightest convex envelope by Al-Khayyal and Falk [2]:

$$\begin{aligned}
x_3 &\geq \ell_2 x_1 + \ell_1 x_2 - \ell_1 \ell_2 \\
x_3 &\geq u_2 x_1 + u_1 x_2 - u_1 u_2 \\
x_3 &\leq \ell_2 x_1 + u_1 x_2 - \ell_1 u_2 \\
x_3 &\leq u_2 x_1 + \ell_1 x_2 - u_1 \ell_2,
\end{aligned}$$

and is depicted in Figure 1 for convenience. The shaded tetrahedron is the linear envelope, while $M_2^\star$ is shown in colors.

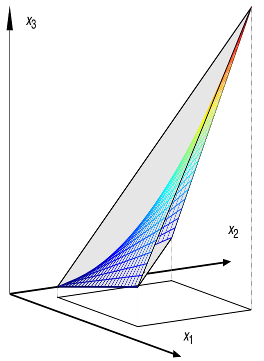

Fig. 1. Linear envelope of $M_2^\star$.

2.2 Nontrivial lower and upper bound for x_3

We consider first a finite lower bound, $\ell_3 > \bar{\ell}_3 = \ell_1\ell_2$. The darkest area in Figure 2 shows the projection of M_2 onto (x_1, x_2), that is, the set $P_2 = \{(x_1, x_2) \in \mathbb{R}^2 : \ell_i \leq x_i \leq u_i, i = 1, 2, x_1x_2 \geq \ell_3\}$. It is safe to assume here that $\ell_3 \leq \ell_1 u_2$ and $\ell_3 \leq u_1\ell_2$, as otherwise a 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. the lower right) corner of the bounding box in Figure 2 would be cut out by the convex set $x_1x_2 \geq \ell_3$. Similarly we assume that $u_3 \geq \ell_1 u_2$ and $u_3 \geq u_1\ell_2$.

Projecting M_2 onto (x_1, x_2) gives a convex set P_2. Consider a point $x^\star$ on the curve $x_1x_2 = \ell_3$ with $\ell_1 \leq x_1^\star \leq u_1$ and $\ell_2 \leq x_2^\star = \ell_3/x_1^\star \leq u_2$. The tangent to the curve $x_1x_2 = \ell_3$ at $x^\star$ gives a linear inequality $a_1(x_1-x_1^\star)+a_2(x_2-x_2^\star) \geq 0$, that is valid for P_2. The coefficients a_1 and a_2 are given by the gradient of the function $\xi_2(x) = x_1x_2$ at $x^\star$, i.e., $a_1 = \frac{\partial\pi}{\partial x_1}|_{x^\star} = x_2^\star$ and $a_2 = \frac{\partial\pi}{\partial x_2}|_{x^\star} = x_1^\star$. The lighter area within the bounding box above the tangent line is the set of points satisfying the above linear constraint, which we rewrite here:

$$x_2^\star(x_1 - x_1^\star) + x_1^\star(x_2 - x_2^\star) \geq 0. \tag{1}$$

As this inequality is valid within P_2 and is independent from x_3, it is also valid for M_2. We can lift it as follows: the inequality

$$x_2^\star(x_1 - x_1^\star) + x_1^\star(x_2 - x_2^\star) + a(x_3 - \ell_3) \geq 0 \tag{2}$$

is clearly valid for $x_3 = \ell_3$. For it to be valid for M_2,

$$g(a_3) = \min\{x_2^\star(x_1 - x_1^\star) + x_1^\star(x_2 - x_2^\star) + a(x_3 - \ell_3) : (x_1, x_2, x_3) \in M_2\} \geq 0$$

must hold. It is easy to show that $g(a_3) = 0$ if $a \geq 0$ (a global optimum is given by $(x_1^\star, x_2^\star)$), hence $a < 0$ in all lifted inequalities (2).

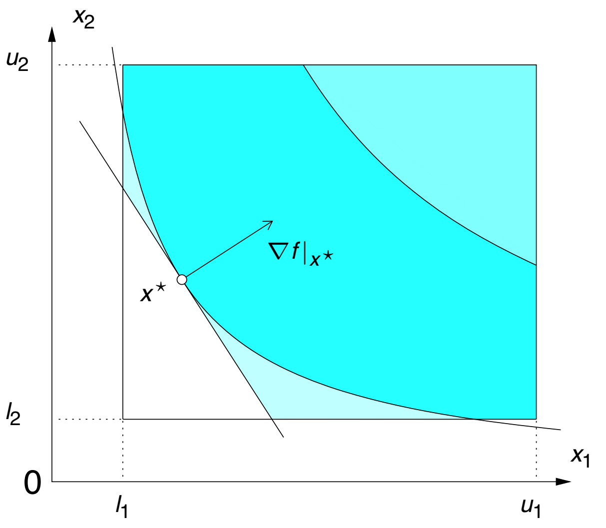

Fig. 2. A projection of M_2 with non-trivial lower and upper bounds ℓ_3, u_3.

We next show how to calculate a. First we will show how to get this coefficient and then we will prove that the inequalities we get are not dominated by any other valid inequality. To find the coefficient a in the inequality (2), intuitively we know that the plane

(3) $$x_2^\star(x_1 - x_1^\star) + x_1^\star(x_2 - x_2^\star) + a(x_3 - \ell_3) = 0$$

should touch the curve $x_1x_2 = u_3$ at exactly one point; let's call this point $(\bar{x}_1, \bar{x}_2)$. If for a moment we disregard the bounds on x_1 and x_2, the fact that the plane (3) touches the curve $x_1x_2 = u_3$ at $(\bar{x}_1, \bar{x}_2)$ means that the plane would be tangent to the curve $x_1x_2 = u_3$ at this point. This means that the gradient of the curve at $(\bar{x}_1, \bar{x}_2)$ is parallel to the projection of the normal to the plane onto the (x_1, x_2) space. The gradient of the curve $x_1x_2 = u_3$ at $(\bar{x}_1, \bar{x}_2)$ is $(\bar{x}_2, \bar{x}_1)$ and the projection of the normal to the plane onto the (x_1, x_2) space is $(x_2^\star, x_1^\star)$. As a result we will have:

(4) $$\exists \alpha \in \mathbb{R} : \bar{x}_2 = \alpha x_2^\star, \bar{x}_1 = \alpha x_1^\star.$$

But we know that $\bar{x}_1\bar{x}_2 = u_3$; so we will have:

(5) $$\bar{x}_1\bar{x}_2 = u_3 = \alpha^2 x_1^\star x_2^\star = \alpha^2 \ell_3,$$

and as a result

(6) $$\alpha = \sqrt{\frac{u_3}{\ell_3}}.$$

On the other hand we know that $(\bar{x}_1, \bar{x}_2)$ is on the plane (3), which implies

(7) $$x_2^\star(\bar{x}_1 - x_1^\star) + x_1^\star(\bar{x}_2 - x_2^\star) + a(u_3 - \ell_3) = 0,$$

As a result,

(8) $$x_2^\star(\alpha x_1^\star - x_1^\star) + x_1^\star(\alpha x_2^\star - x_2^\star) + a(u_3 - \ell_3) = 0.$$

By (6) and (8), the value for a is:

(9) $$a = \frac{2(1 - \sqrt{\frac{u_3}{\ell_3}})\ell_3}{u_3 - \ell_3}.$$

Notice that the value of a does not depend on the value of $x_1^\star$ and $x_2^\star$, and that it is less than zero. Intuitively this value for a will give a tight valid inequality for M_2 if $\ell_1 \le \bar{x}_1 \le u_1$ and $\ell_2 \le \bar{x}_2 \le u_2$ (the proof will come later). But if $(\bar{x}_1, \bar{x}_2)$ is not in the domain of (x_1, x_2) we need to find a point on the curve $x_1x_2 = u_3$ at which the plane (3) touches the curve. Intuitively this point would be one of the end points of the curve $x_1x_2 = u_3; \ell_1 \le x_1 \le u_1, \ell_2 \le x_2 \le u_2$. That is, the tangent point on the curve $x_1x_2 = u_3$ will need to be chosen to be either $(u_1, \frac{u_3}{u_1}, u_3)$ or $(\frac{u_3}{u_2}, u_2, u_3)$.

An analogous problem occurs if there exists a point $(\bar{x}_1, \bar{x}_2, \bar{x}_3)$ such that $\bar{x}_1\bar{x}_2 = u_3$, $\ell_1 \le \bar{x}_1 \le u_1$, and $\ell_2 \le \bar{x}_2 \le u_2$, *but* for which either $x_1^\star < \ell_1$ or $x_2^\star < \ell_2$, where $x_1^* = \frac{\bar{x}_1}{\alpha}$ and $x_2^* = \frac{\bar{x}_2}{\alpha}$. (As before $\alpha = \sqrt{\frac{u_3}{\ell_3}}$.) In this case, we have to computer the lifting coefficient that allows us to lift a linear inequality tangent to $(\bar{x}_1, \bar{x}_2, \bar{x}_3)$ so that it supports the curve $x_1x_2 = \ell_3$ at either the point $(\ell_1, \frac{\ell_3}{\ell_1}, \ell_3)$ or $(\frac{\ell_3}{\ell_2}, \ell_2, \ell_3)$. In this case, the lifting is necessary to ensure validity rather than to strengthen the inequality. It nevertheless results in an inequality that supports the convex hull of M_2 in as many points as possible.

We call all of the inequalities defined in the above way *lifted tangent inequalities*, whether they are lifted "inward" to strengthen them from a point on $x_1x_2 = \ell_3$ or "outward" to ensure their validity from a point on $x_1x_2 = u_3$. Space considerations prevent us from presenting any more of the development here. However, we have been able to develop these results sufficiently to prove the following theorem.

Theorem 2.1 *For M_2, the McCormick inequalities, the bounds $\ell_3 \le x_3 \le u_3$, and the lifted tangent inequalities define the convex hull.*

3 Results for M_n^*

Things become more complicated when $n > 2$. One obvious issue is that there is no compact description of the convex hull known. It is easy enough to define the set of extreme points of M_n^*: there is exactly one extreme point for each assignment of each of the first n variables to either its lower bound or its upper bound ([8]). This set, however, is exponential in number, and therefore an extended formulation based on enumerating the extreme points would be exponential as well.

An interesting related question is whether optimizing over M_n^* can be done in polynomial time. In other words, consider the model

$$\min\ x_{n+1} + \sum_{i \in N} a_i x_i$$
$$\text{s.t. } x_{n+1} = \prod_{i \in N} x_i; \quad \ell_i \le x_i \le u_i,\ i = 1, ..., n.$$

Here $a_i \in \mathbb{R}$ is a rational number for $i = 1, ..., n$. We continue to assume also that $0 \le \ell_i < u_i,\ i = 1, ..., n$. We call this model MLOpt. We have a number of results for MLOpt, including optimization algorithms and extended formulations for special cases. While the special cases are restricted, they are still much more general than previously known cases (very few) for which polynomial time algorithms were known.

Our results suggest that the complexity of the problem depends directly on the possible number of values that x_{n+1} can take in an extreme point solution of M_2^*. Interestingly, the fact that this number is in general exponential leads to the following negative conclusion:

Conjecture 3.1 *The general case of MLOpt is $\mathcal{NP}$-complete.*

We have not yet been able to prove this conjecture, but all the evidence points to this conclusion. Moreover, if this conjecture is true, this would strongly suggest that no compact description of the convex hull of M_n^* can be determined for the general case [4]. This would imply that the best one can hope to in general to get a strong formulation for M_n^* is to define an extended formulation by enumerating the extreme points.

4 Results for M_n

Most of the results for M_2 generalize to the model with $n > 2$ and nontrivial bounds ℓ_{n+1} and u_{n+1}. Defining valid inequalities and separating them can be done in the same way, with minor modifications to generalize the procedure to higher dimensions.

The general case seems to be too complicated to allow us to hope to prove that we have a complete description (even assuming that we can add lifted tangent inequalities to a projection of an exponential extended formulation such as that described in the previous section). However, we can prove that they suffice to define the convex hull for some special cases:

Proposition 4.1 *If $\ell_{n+1} = \bar{\ell}_{n+1}$, then conv($M_n$) is defined by intersecting conv(M_n^*) with the set of lifted tangent inequalities.*

Proposition 4.2 *If $u_{n+1} = \bar{u}_{n+1}$, then conv(M_n) is defined by intersecting conv(M_n^*) with the set of lifted tangent inequalities.*

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