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ORIGINAL PAPER

# Convex underestimation for posynomial functions of positive variables

**Han-Lin Li · Jung-Fa Tsai · Christodoulos A. Floudas**

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**Abstract** The approximation of the convex envelope of nonconvex functions is an essential part in deterministic global optimization techniques (Floudas in Deterministic Global Optimization: Theory, Methods and Application, 2000). Current convex underestimation algorithms for multilinear terms, based on arithmetic intervals or recursive arithmetic intervals (Hamed in Calculation of bounds on variables and underestimating convex functions for nonconvex functions, 1991; Maranas and Floudas in J Global Optim 7:143–182, (1995); Ryoo and Sahinidis in J Global Optim 19:403–424, (2001)), introduce a large number of linear cuts. Meyer and Floudas (Trilinear monomials with positive or negative domains: Facets of convex and concave envelopes, pp. 327–352, (2003); J Global Optim 29:125–155, (2004)), introduced the complete set of explicit facets for the convex and concave envelopes of trilinear monomials with general bounds. This study proposes a novel method to underestimate posynomial functions of strictly positive variables.

**Keywords** Convex envelopes · Convex underestimators · Posynomials

H.-L. Li (✉)
Institute of Information Management, National Chiao Tung University,
No. 1001, Ta Hsueh Road, Hsinchu 300, Taiwan
e-mail: hlli@cc.nctu.edu.tw

J.-F. Tsai
Department of Business Management, National Taipei University of Technology,
No. 1, Sec. 3, Chung-Hsiao E. Road, Taipei 10608, Taiwan
e-mail: jftsai@ntut.edu.tw

C. A. Floudas
Department of Chemical Engineering, Princeton University, Princeton, NJ 08544, USA
e-mail: floudas@titan.princeton.edu

## 1 Introduction

Convex underestimators of nonconvex functions are frequently applied in global optimization algorithms such as the $\alpha$ BB algorithm [1,2,10] to underestimate the nonconvex functions. A good convex underestimator should be as tight as possible and should contain minimal number of new variables and constraints thus to improve the computational effect of processing a node in a branch-bound tree [11].

Tawarmalani and Sahinidis [26] developed the convex envelope and concave envelope for *x/y* over a unit hypercube, proposed a semidefinite relaxation of *x/y*, and suggested convex envelopes for functions of the form $f(x)y^2$ and $f(x)/y$. Ryoo and Sahinidis [21] studied the use of arithmetic intervals, recursive arithmetic intervals, logarithmic transformation, and exponential transformation for multilinear functions. Tawarmalani et al. [24] studied the role of disaggregation in resulting tighter linear programming relaxations. Tawarmalani and Sahinidis [27] introduced the convex extensions for lower semi-continuous functions, proposed a technique for constructing convex envelopes for nonlinear functions, and studied the maximum separation distance for functions such as *x/y*. Tawarmalani et al. [25] studied 0–1 hyperbolic programs, and developed eight mixed-integer convex reformulations. Liberti and Pantelides [15] proposed a nonlinear continuous and differentiable convex envelope for monomials of odd degree, derived its linear relaxation, and compared to other relaxation. Pörn et al. [20] presented different convexification strategies for nonconvex optimization problems and illustrated how to convexified posynomials and negative binomials within the field of discrete optimization. Björk et al. [7] studied convexifications for signomial terms, introduced properties of power convex functions, compared the effect of the convexification schemes for heat exchanger network problems, and studied quasi-convex convexifications.

Meyer and Floudas [17] studied trilinear monomials with positive or negative domains, derived explicit expressions for the facets of the convex and concave envelopes and showed that these outperform the previously proposed relaxations based on arithmetic intervals or recursive arithmetic intervals. Meyer and Floudas [18] presented explicit expressions for the facets of convex and concave envelopes of trilinear monomials with mixed-sign domains. Tardella [23] studied the class of functions whose convex envelope on a polyhedron coincides with the convex envelope based on the polyhedron vertices, and proved important conditions for a vertex polyhedral convex envelope. Meyer and Floudas [19] described the structure of the polyhedral convex envelopes of edge–concave functions over polyhedral domains using geometric arguments and proposed an algorithm for computing the facets of the convex envelopes.

Caratzoulas and Floudas [8] proposed novel convex underestimators for trigonometric functions which are trigonometric functions themselves. Akrotirianakis and Floudas [4,5] introduced a new class of convex underestimators for twice continuously differentiable nonlinear programs, studied their theoretical properties, and proved that the resulting convex relaxation is improved compared to the $\alpha$ BB one. Meyer and Floudas [18] proposed two new classes of convex underestimators for general $C^2$ nonlinear programs which combine the $\alpha$ BB underestimators within a piecewise quadratic perturbation, derived properties for the smoothness of the convex underestimators, and showed the improvements over the classical $\alpha$ BB convex underestimators for box-constrained optimization problems.

Three popular convex underestimation methods, arithmetic intervals (AI) [12], recursive arithmetic intervals (rAI) [12,16,21], and explicit facets (EF) for convex envelopes of trilinear monomials [17,18], are effective to underestimate a trilinear term $x_1x_2x_3$ for $x_i$ to be bounded variables. However, these current methods have difficulty to treat a posynomial function. According to Ryoo and Sahinidis [21], the maximal number of required linear inequalities to lower bound a multilinear function $x_1x_2 \ldots x_n$ with $n$ variables, AI scheme needs to use $\prod_{k=2}^{n-1} \Theta_k^{\binom{n}{k}} \sum_{i=1}^{\left\lfloor \frac{n}{2} \right\rfloor} \binom{n}{2i}$ linear constraints maximally. $\Theta_k$ denotes the number of linear functions that the AI generates to lower bound $k$-cross-product terms, $k = 2, 3, \ldots, n-1$. Since the number of linear constraints of convex envelopes for a multilinear function with $n$ variables grows doubly exponentially in $n$, AI bounding scheme may only treat $n \leq 3$ cases. It is more difficult for AI to treat a posynomial function for $n > 3$ cases. More over, applying rAI scheme to underestimate a multilinear function $x_1x_2 \ldots x_n$ needs to use the maximum of exponentially many $2^{n-1}$ linear inequalities. Therefore, the rAI bounding scheme has difficulty to treat posynomial functions as well as AI scheme.

EF [17,18] provided the explicit facets of the convex and concave envelopes of trilinear monomials and demonstrated that these result in tighter bounds than the AI and rAI techniques. An important difference between EF and other bounding schemes is that these explicit facets are linear cuts which were proven to define the convex envelope. Explicit Facets, EF, of the convex envelope are effective in treating general trilinear monomials but the derivation of explicit facets for the convex envelope of general multilinear monomials and signomials is an open problem.

This study proposes a novel method for the convex relaxation of posynomial functions. This approach is different from the work of Maranas and Floudas [16] which provided an alternative way of generating convex underestimators for generalized geometric programming problems via the exponential transformation and linear underestimation of the concave terms. We first convexify a nonconvex posynomial function into a convex function and some bilinear functions, and subsequently we introduce linear underestimators for these bilinear functions. Comparing with current convex underestimation algorithms, the proposed method can deal with more general functions effectively. Applications of the proposed approach include the area of process synthesis and design of separations, phase equilibrium, nonisothermal complex reactor networks, and molecular conformation problems (e.g., [3,9,13]).

## 2 Proposed method

This section presents a new method to develop a convex underestimator for a posynomial function $f(X) = dx_1^{\alpha_1}x_2^{\alpha_2} \ldots x_n^{\alpha_n}$ where $X = (x_1, \ldots, x_n)$, $0 < \underline{x}_i \leq x_i \leq \bar{x}_i$, $\alpha_i \in \Re$ for $i = 1, 2, \ldots, n$, and $d > 0$.

For a twice-differentiable function $f(X)$, let $H(X)$ be the Hessian matrix of $f(X)$. The determinant of $H(X)$ can be expressed as $\det H(X) = (-1)^n(\prod_{i=1}^n d\alpha_i x_i^{n\alpha_i-2})(1-\sum_{i=1}^n \alpha_i)$. If $x_i \geq 0, \alpha_i < 0$ for all $i$ and $d > 0$ then $\det H(X) \geq 0$. Consider the following proposition:

**Proposition 1** *A twice-differentiable function $f(X)$ is convex for $x_i \geq 0, \alpha_i \leq 0, i = 1, 2, \ldots, n$, and $d > 0$* [6].

We then have two rules of underestimating $f(X)$ described below:

**Rule 1**. If $\alpha_i < 0, \forall i$, then $f(X)$ is already a convex function by Proposition 1. No convexification is required.
**Rule 2**. If $\alpha_i > 0$ for some $i$, then convert $f(X)$ into a new function $f(X,Y) = dx_1^{\alpha_1}\ldots y_i^{-\alpha_i}\ldots x_n^{\alpha_n}$ where $y_i = x_i^{-1}$. Since $f(X,Y)$ is already a convex function, we only need to underestimate functions $y_i = x_i^{-1}$ for all $i$.

**Theorem 1** *The lower bound of a nonconvex function $f(X) = dx_1^{\alpha_1}x_2^{\alpha_2}\ldots x_n^{\alpha_n}$, $0 < \underline{x}_i \leq x_i \leq \bar{x}_i$, where $d > 0, \alpha_i < 0, \quad i = 1, 2, \ldots, m, \alpha_i > 0, i = m+1, m+2, \ldots, n$, is obtained by solving the following convex program:*

$$Min f(X,Y) = dx_1^{\alpha_1}\ldots x_m^{\alpha_m} y_{m+1}^{-\alpha_{m+1}}\ldots y_n^{-\alpha_n}$$
$$subject\ to 1 \geq \frac{x_i}{\bar{x}_i} + \underline{x}_i y_i - \frac{\underline{x}_i}{\bar{x}_i}, \quad i = m+1, m+2, \ldots, n.$$

*Proof* By Rule 2, $f(X)$ is fully converted into a convex function $f(X,Y)$ where $y_i = x_i^{-1}$. The equality $x_i y_i = 1$ is nonconvex for $i = m+1, m+2, \ldots, n$. Denote $\underline{y}_i = \frac{1}{\bar{x}_i} \leq y_i \leq \frac{1}{\underline{x}_i} = \bar{y}_i$. The convex underestimators of the bilinear terms $x_i y_i$ for $i = m+1, m+2, \ldots, n$ are obtained based on the following inequalities:

$$(x_i - \underline{x}_i)(y_i - \underline{y}_i) \geq 0, \quad i = m+1, \quad m+2, \ldots, n,$$
$$(\bar{x}_i - x_i)(\bar{y}_i - y_i) \geq 0, \quad i = m+1, \quad m+2, \ldots, n,$$

which are expressed by the following inequalities:

$$x_i y_i \geq x_i \underline{y}_i + \underline{x}_i y_i - \underline{x}_i \underline{y}_i \Rightarrow 1 \geq \frac{x_i}{\bar{x}_i} + \underline{x}_i y_i - \frac{\underline{x}_i}{\bar{x}_i}, \quad i = m+1, \quad m+2, \ldots, n, \tag{1}$$

$$x_i y_i \geq x_i \bar{y}_i + \bar{x}_i y_i - \bar{x}_i \bar{y}_i \Rightarrow 1 \geq \frac{x_i}{\underline{x}_i} + \bar{x}_i y_i - \frac{\bar{x}_i}{\underline{x}_i}, \quad i = m+1, \quad m+2, \ldots, n. \tag{2}$$

Multiplying (1) by $\frac{\bar{x}_i}{\underline{x}_i}$, we have (2). Therefore, we only need constraint (1) to formulate the lower bound of $f(X)$.

*Remark 1* To form a convex underestimator for a posynomial function where $n$ variables having positive exponent, the proposed method at most requires $n$ additional variables and $n$ additional constraints.

**Table 1** Comparison results of Example 1

| Scheme | AI | rAI | EF | BARON (root node) | ET [20] | Proposed method |
|---|---|---|---|---|---|---|
| Lower bound | 1 | 1 | 1 | 1 | 1 | 1 |
| No. of additional constraints | 16 | 18 | 6 | NA | NA | 3 |

## 3 Numerical examples

*Example 1* Underestimating a trilinear function $f(X) = x_1x_2x_3$, $1 \le x_1, x_2, x_3 \le 2$. The above function can be transformed into the following convex function:

$$f(Y) = y_1^{-1}y_2^{-1}y_3^{-1} \quad \text{where } x_1 = y_1^{-1}, \quad x_2 = y_2^{-1}, \quad x_3 = y_3^{-1},$$
$$\text{and} \quad 0.5 = \underline{y}_i \le y_i \le 1 = \bar{y}_i \quad \text{for } i = 1, 2, 3.$$

Then we have the convex underestimator for the trilinear function as below.

$$\begin{aligned} &\text{Min} f(Y) = y_1^{-1}y_2^{-1}y_3^{-1} \\ &\text{subject to } 1 \ge \frac{x_i}{\bar{x}_i} + \underline{x}_i y_i - \frac{\underline{x}_i}{\bar{x}_i}, \quad i = 1, 2, 3, \\ &\text{where } 1 = \underline{x}_i \le x_i \le 2 = \bar{x}_i, \quad 0.5 = \underline{y}_i \le y_i \le 1 = \bar{y}_i \quad \text{for} \quad i = 1, 2, 3. \end{aligned}$$

Solving the above convex relaxation program provides a lower bound of 1 and $(x_1, x_2, x_3, y_1, y_2, y_3) = (1, 1, 1, 1, 1, 1)$. The comparisons of the bounding schemes and the results obtained by BARON (2005) [22] at the root node and the exponential transformation (ET) approach of Pörn et al. [20] in the first iteration are listed in Table 1. The number of additional constraints of the proposed method is less than that of the other bounding schemes to find the same lower bound.

*Example 2* To construct the convex lower bound of a nonconvex function $f(X) = x_1x_2x_3x_4x_5 - x_2^{0.5}x_4^{0.5} - 3x_1 - x_5$, $1 \le x_1, x_2, x_3, x_4, x_5 \le 100$. According to the convexification rule (Proposition 5 of [14]), $-x_2^{0.5}x_4^{0.5}$ is a convex function without transformation and $f(X)$ can be transformed into a convex function as below:

$$f(X, Y) = y_1^{-1}y_2^{-1}y_3^{-1}y_4^{-1}y_5^{-1} - x_2^{0.5}x_4^{0.5} - 3x_1 - x_5$$
$$\text{where} \quad x_1 = y_1^{-1}, x_2 = y_2^{-1}, x_3 = y_3^{-1}, x_4 = y_4^{-1}, \quad \text{and } x_5 = y_5^{-1}.$$

Thus $x_i y_i = 1$, $0.01 = \underline{y}_i \le y_i \le 1 = \bar{y}_i$ for $i = 1, 2, \ldots, 5$.

The following is immediate:

$$(x_i - \underline{x}_i)(y_i - \underline{y}_i) \ge 0, \quad i = 1, 2, \ldots, 5,$$
$$(\bar{x}_i - x_i)(\bar{y}_i - y_i) \ge 0, \quad i = 1, 2, \ldots, 5.$$

**Table 2** Comparison results of Example 2

| Scheme | BARON (root node) | ET [20] | Proposed method | Optimal solution |
|---|---|---|---|---|
| Lower bound | −224.4 | −499 | −317.076 | −202 |

Then we have the convex underestimator for the multilinear function as below.

$$\begin{aligned}&\text{Min}\, f(X,Y) = y_1^{-1}y_2^{-1}y_3^{-1}y_4^{-1}y_5^{-1} - x_2^{0.5}x_4^{0.5} - 3x_1 - x_5\\&\text{subject to } 1 \geq \frac{x_i}{\bar{x}_i} + \underline{x}_i y_i - \frac{\underline{x}_i}{\bar{x}_i}, \quad i = 1, 2, \ldots, 5,\\&\text{where } 1 = \underline{x}_i \leq x_i \leq 100 = \bar{x}_i, \quad 0.01 = \underline{y}_i \leq y_i \leq 1 = \bar{y}_i \quad \text{for} \quad i = 1, 2, \ldots, 5.\end{aligned}$$

Solving the above convex relaxation results in a lower bound of $f(X)$ is −317.076 and $(x_1, x_2, x_3, x_4, x_5, y_1, y_2, y_3, y_4, y_5) = (88.4717, 25.8304, 1, 25.8304, 63.4152, 0.1253, 0.7517, 1, 0.7517, 0.3758)$. The maximal number of required additional linear constraints is 5. Since the bounding schemes AI, rAI and EF have difficulties of generating too many extra constraints and without explicit facets for the convex envelope of general multilinear monomials and signomials to treat this nonconvex function, Table 2 only lists the results of BARON, ET, and the proposed method. The optimal solution of the original problem is −202. Table 2 shows that BARON's lower bound obtained at the root node is tighter than those obtained by the other two approaches in the first iteration and the proposed convex relaxation results in a tighter lower bound than ET.

*Example 3* Underestimating a nonconvex function

$$f(X) = x_1^{-2}x_2^{-1.5}x_3^{1.2}x_4^{3} - 3x_3^{0.5} + x_2 - 4x_4,$$

$1 \leq x_1, x_2, x_3, x_4 \leq 10$. The function can not be underestimated by the bounding schemes AI, rAI and EF. Transforming the function into the following convex function:

$$\begin{aligned}&f(X,Y) = x_1^{-2}x_2^{-1.5}y_3^{-1.2}y_4^{-3} - 3x_3^{0.5} + x_2 - 4x_4\\&\qquad\text{where} \quad x_3 = y_3^{-1}, x_4 = y_4^{-1}, \text{ and } 0.1 = \underline{y}_i \leq y_i \leq 1 = \bar{y}_i \quad \text{for } i = 3, 4.\end{aligned}$$

Then we have the convex underestimator for the nonconvex function as below.

$$\begin{aligned}&\text{Min}\, f(X,Y) = x_1^{-2}x_2^{-1.5}y_3^{-1.2}y_4^{-3} - 3x_3^{0.5} + x_2 - 4x_4\\&\text{subject to } 1 \geq \frac{x_i}{\bar{x}_i} + \underline{x}_i y_i - \frac{\underline{x}_i}{\bar{x}_i}, \quad i = 3, 4,\\&\text{where} \quad 1 = \underline{x}_i \leq x_i \leq 10 = \bar{x}_i, 0.1 = \underline{y}_i \leq y_i \leq 1 = \bar{y}_i \quad \text{for } i = 3, 4.\end{aligned}$$

Solving the above convex relaxation results in a lower bound of −41.2442 and $(x_1, x_2, x_3, x_4, y_3, y_4) = (10, 2.9045, 6.9239, 9.5478, 0.4076, 0.1452)$. Only 2 additional linear constraints and 2 variables are added to the convex program. The optimal

**Table 3** Comparison results of Example 3

| Scheme | BARON (root node) | ET [20] | Proposed method | Optimal solution |
|---|---|---|---|---|
| Lower bound | −40 | −48.4868 | −41.2442 | −38.08 |

solution of the original problem is −38.08 and the comparison results are shown in Table 3. By Table 3, we know that BARON gives a tighter lower bound than the others two approaches and the proposed convex relaxation results in a tighter lower bound than ET.

## 4 Conclusion

This study integrates the convexification techniques and the bounding schemes to construct a convex lower bound for a posynomial function of strictly positive variables which is difficult to be treated by the current methods. Less number of variables and constraints are used in the proposed method than being used by current methods. Computational results of the examples illustrate that the proposed convex relaxation can effectively derive a tight lower bound for a posynomial function.

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