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Convex Envelopes of Monomials of Odd Degree

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Abstract. Convex envelopes of nonconvex functions are widely used to calculate lower bounds to solutions of nonlinear programming problems (NLP), particularly within the context of spatial Branch-and-Bound methods for global optimization. This paper proposes a nonlinear continuous and differentiable convex envelope for monomial terms of odd degree, x^{2k+1}, where $k \in \mathbb{N}$ and the range of x includes zero. We prove that this envelope is the tightest possible. We also derive a linear relaxation from the proposed envelope, and compare both the nonlinear and linear formulations with relaxations obtained using other approaches.

Key words: Cubic, Odd degree, Monomial, Convex relaxation, Global optimization

1. Introduction

One of the most effective techniques for the solution of nonlinear programming problems (NLPs) to global optimality is the spatial Branch-and-Bound (sBB) method (Tuy, 1998). This requires the computation of a lower bound to the solution, usually obtained by solving a convex relaxation of the original NLP (Ryoo and Sahinidis, 1995; Maranas and Floudas, 1995; Adjiman and Floudas, 1996; Smith and Pantelides, 1997). The formation and tightness of such a convex relaxation are critical issues in any sBB implementation.

As shown in (Smith, 1996) and (Smith and Pantelides, 1997; Smith and Pantelides, 1999), it is, in principle, possible to form a convex relaxation of any NLP by isolating the nonconvex terms and replacing them with their convex relaxation. Tight convex underestimators are already available for many types of nonconvex term, including bilinear and trilinear products, linear fractional terms, and concave and convex univariate functions. However, terms which are piecewise concave and convex are not explicitly catered for. A frequently occurring example of such a term is x^{2k+1}, where $k \in \mathbb{N}$ and the range of x includes zero. A detailed analysis of the conditions required for concavity and convexity of polynomial functions has been given in (Maranas and Floudas, 1995); however, the results obtained therein only apply to the convex underestimation of multivariate polynomials with positive variable values. For monomials of odd degree, where the variable ranges over both negative and positive values, no special convex envelopes have been proposed in the literature, and one therefore has to rely either on generic convex relaxations such as those given by Floudas and co-workers (Androulakis et al., 1995; Adjiman

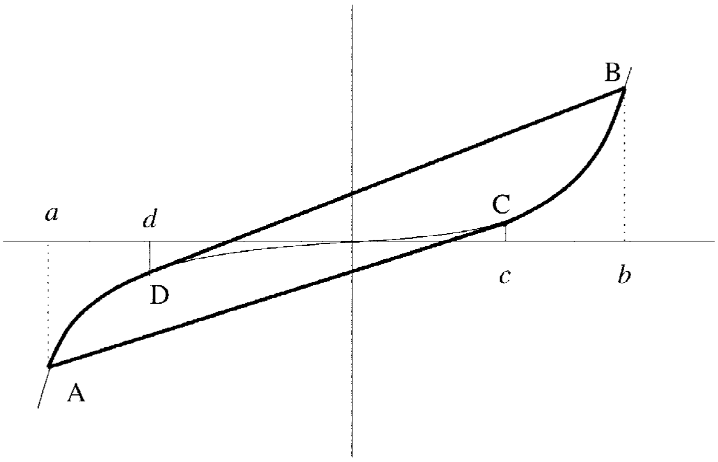

Figure 1. Tightest (nonlinear) convex envelope of x^{2k+1}.

and Floudas, 1996) or on reformulation in terms of other types of terms for which convex relaxations are available.

In this article, we propose a convex nonlinear envelope for odd power terms of the form x^{2k+1} ($k \in \mathbb{N}$), where $x \in [a, b]$ and $a < 0 < b$. The envelope derived is continuous and differentiable everywhere in $[a, b]$. We also derive a tight linear relaxation. We compare both of these relaxations with convex relaxations derived using other methods.

2. Statement of the problem

Maranas and Floudas (1995) discussed the generation of convex envelopes for general univariate functions. Here we consider the monomial x^{2k+1} in the range $x \in [a, b]$ where $a < 0 < b$. Let c, d be the x-coordinates of the points C, D where the tangents from points A and B respectively meet the curve (see Figure 1). The shape of the convex underestimator of x^{2k+1} depends on the relative magnitude of b and c. In particular, if $c < b$ (as is the case in Figure 1), a convex underestimator can be formed from the tangent from $x = a$ to $x = c$ followed by the curve x^{2k+1} from $x = c$ to $x = b$. On the other hand, if $c > b$ (cf. Figure 2), a convex underestimator is simply the straight line passing through A and B.

The situation is similar for the concave overestimator of x^{2k+1} in the range $x \in [a, b]$. If $d > a$, the overestimator is given by the upper tangent from B to D followed by the curve x^{2k+1} from D to A, as shown in Figure 1. On the other hand, if $d < a$, the overestimator is just the straight line from A and B. It should be noted that the conditions $c > b$ and $d < a$ cannot both hold simultaneously.

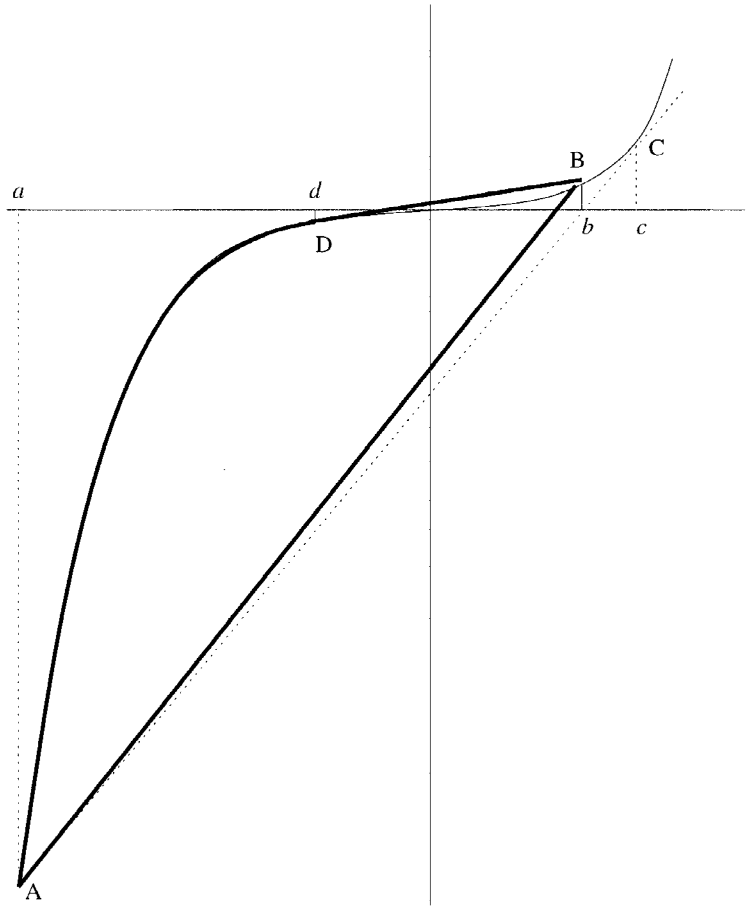

Figure 2. The case when $c > b$.

3. The tangent equations

The discussion in Section 2 indicates that forming the convex envelope of x^{2k+1} requires the determination of the tangents that pass through points A, C and B, D. Considering the first of these two tangents and equating the slope of the line $\overline{AC}$ to the gradient of x^{2k+1} at $x = c$, we derive the tangency condition:

$$\frac{c^{2k+1} - a^{2k+1}}{c - a} = (2k+1)c^{2k} \tag{1}$$

Hence c is a root of the polynomial:

$$P^k(x, a) \equiv (2k)x^{2k+1} - a(2k+1)x^{2k} + a^{2k+1} \tag{2}$$

It can be shown by induction on k that:

$$P^k(x, a) = a^{2k-1}(x - a)^2 Q^k(\frac{x}{a}) \tag{3}$$

Table 1. Numerical values of the roots of $Q^k(x)$ for $k = 1, .., 10$ (to 10 significant digits).

k	r_k	k	r_k
1	−0.5000000000	6	−0.7721416355
2	−0.6058295862	7	−0.7921778546
3	−0.6703320476	8	−0.8086048979
4	−0.7145377272	9	−0.8223534102
5	−0.7470540749	10	−0.8340533676

where the polynomial $Q^k(x)$ is defined as:

$$Q^k(x) \equiv 1 + \sum_{i=2}^{2k} i x^{i-1}. \tag{4}$$

Thus, the roots of $P^k(x, a)$ can be obtained from the roots* of $Q^k(x)$. Unfortunately, polynomials of degree greater than 4 cannot generally be solved by radicals (what is usually called an "analytic solution"). This is the case for $Q^k(x)$ for $k > 2$. For example, the Galois group of $Q^3(x) \equiv 6x^5 + 5x^4 + 4x^3 + 3x^2 + 2x + 1$ is isomorphic to S_5 (i.e., the symmetric group of order 5) which is not solvable since its biggest proper normal subgroup is A_5, the smallest non-solvable group. For details on Galois theory and the solvability of polynomials, see Stewart (1989).

4. The roots of $Q^k(x)$ and their uniqueness

Unlike $P^k(x, a)$, the polynomial $Q^k(x)$ does not depend on the range of x being considered. Moreover, as shown formally in Section 4.1 below, $Q^k(x)$ has exactly one real root, r_k, for any $k \geqslant 1$, and this lies in $[-1 + 1/2k, -1/2]$. Hence, the roots of $Q^k(x)$ for different k can be computed *a priori* to arbitrary precision using simple numerical schemes (e.g., bisection). A table of these roots is presented in Table 1 for $k \leqslant 10$.

4.1. BOUNDING THE ROOTS OF $q^k(x)$

In this section, we show that $Q^k(x)$ has exactly one real root, which lies in the interval $[-1 + 1/2k, -1/2]$.

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* Although $P^k(x, a)$ has the additional root $x = a$, this is not of practical interest.

PROPOSITION 4.1. *For all $k \in \mathbb{N}$, the following properties hold:*

$$\left.\begin{array}{lcl} Q^k(0) & = & 1 \\ Q^k(-1) & = & -k \end{array}\right\} \tag{5}$$

$$\forall x > 0 \ \left(\frac{\mathrm{d}Q^k(x)}{\mathrm{d}x} > 0\right) \tag{6}$$

$$\forall x \leqslant -1 \ \left(Q^k(x) < 0\right) \tag{7}$$

Proof. (5): $Q^k(0) = 1$ by direct substitution in (4). Also $Q^k(-1) = 1 + \sum_{i=2}^{2k} i(-1)^{i-1} = \sum_{i=1}^{k}(2i-1) - \sum_{i=1}^{k} 2i = -k$.
(6): $\frac{\mathrm{d}Q^k(x)}{\mathrm{d}x} = \sum_{i=1}^{2k-1} i(i+1)x^{i-1}$, hence it is greater than zero whenever $x > 0$.
(7): For $x \neq 0$, we can rewrite $Q^k(x)$ as $\sum_{i=1}^{k} x^{2i-2}[2i(x+1)-1]$. For $x \leqslant -1$, we have $x^{2i-2} > 0$ and $[2i(x+1)-1] < 0$, thus each term of the sum is negative. □

From the above proposition and the continuity of x^{2k+1}, we can conclude that:

1. there is at least one root between -1 and 0 (property (5));
2. there are no roots for $x \geqslant 0$ (property (6) and the fact that $Q^k(0) > 0$);
3. there are no roots for $x \leqslant -1$ (property (7)).

LEMMA 4.2. *For all $k \in \mathbb{N}$, the real roots of $Q^k(x)$ lie in the interval* $[-1 + 1/2k, -1/2]$.

Proof. This is proved by induction on k. For $k = 1$, $Q^1(x) \equiv 1+2x$ has one real root at $x = -1/2$ which lies in the set $[-1+1/2, -1/2]$. In particular, $Q^1(x) < 0$ for all $x < -1+1/2$ and $Q^1(x) > 0$ for all $x > -1/2$.

We now make the inductive hypothesis that, for all $j < k$, $Q^j(x) > 0$ for all $x > -1/2$ and $Q^j(x) < 0$ for all $x < -1+1/(2j)$ and prove that the same holds for $j = k$. Using (4), we can write $Q^k(x) = Q^{k-1}(x) + x^{2k-2}(2kx + 2k - 1)$ for all $k > 1$. Since x^{2k-2} is always positive, we have that:

$$Q^k(x) > Q^{k-1}(x) \text{ if } x > -1 + \frac{1}{2k}$$
$$Q^k(x) < Q^{k-1}(x) \text{ if } x < -1 + \frac{1}{2k}$$

for all $k > 1$. Now, since $-1/2 > -1 + 1/(2k)$ for all $k > 1$, $Q^k(x) > Q^{k-1}(x) > 0$ for all $x > -1/2$ by inductive hypothesis.

Furthermore, by the inductive hypothesis, $Q^{k-1}(x) < 0$ for all $x < -1 + 1/2(k-1)$; since $1/2k < 1/2(k-1)$, it is also true that $Q^{k-1}(x) < 0$ for all $x < -1+1/2k$. But since, as shown above, $Q^k(x) < Q^{k-1}(x)$ for all $x < -1+1/(2k)$, we can deduce that $Q^k(x) < 0$ for all $x < -1 + 1/(2k)$.

We have thus proved that, for all $k > 0$,

$$Q^k(x) > 0 \text{ if } x > -\frac{1}{2} \tag{8}$$

$$Q^k(x) < 0 \text{ if } x < -1 + \frac{1}{2k}. \tag{9}$$

The proof of the lemma follows from (8), (9) and the continuity of $Q^k(x)$. □

THEOREM 4.3. *For all $k \in \mathbb{N}$, $Q^k(x)$ has exactly one real root, which lies in the interval* $[-1 + 1/(2k), -1/2]$.

Proof. Consider the polynomial $P^k(x, 1) = 2kx^{2k+1} - (2k+1)x^{2k} + 1$ defined by (2). By virtue of (3), we have the relation $P^k(x, 1) = (x-1)^2 Q^k(x)$. Consequently, $P^k(x, 1)$ and $Q^k(x)$ have exactly the same roots for $x < 1$. Therefore (Lemma 4.2), all negative real roots of $P^k(x, 1)$ lie in the interval $[-1+1/(2k), -1/2]$, and there is at least one such root.

Now, $P^k(x, 1)$ can be written as $P^k(x, 1) = q_1^k(x) + q_2^k(x) + 1$, where $q_1^k(x) = 2kx^{2k+1}$ and $q_2^k(x) = -(2k + 1)x^{2k}$. Since q_1 is a monomial of odd degree, it is monotonically increasing in $[-1, 0]$. Since q_2 is a monomial of even degree with a negative coefficient, it is also monotonically increasing in $[-1, 0]$.

Overall, then, $P^k(x, 1)$ is monotonically increasing in $[-1, 0]$, and consequently in the interval $[-1 + 1/(2k), -1/2]$ where all its negative real roots lie. Therefore, there can be only one such root, which proves that $Q^k(x)$ also has a unique root in this interval. □

5. Nonlinear convex envelope

If the roots shown in the second column of Table 1 are denoted by r_k, then the tangent points c and d in Figure 1 are simply $c = r_k a$ and $d = r_k b$. The lower and upper tangent lines are given respectively by:

$$a^{2k+1} + \frac{c^{2k+1} - a^{2k+1}}{c - a}(x - a) \tag{10}$$

$$b^{2k+1} + \frac{d^{2k+1} - b^{2k+1}}{d - b}(x - b) \tag{11}$$

Hence, the convex/concave envelope for $z = x^{2k+1}$ when $x \in [a, b]$ and $a < 0 < b$:

$$l_k(x) \leqslant z \leqslant u_k(x) \tag{12}$$

is as follows:

– If $c < b$, then:

$$l_k(x) = \begin{cases} a^{2k+1}\left(1 + R_k\left(\frac{x}{a} - 1\right)\right) & \text{if } x < c \\ x^{2k+1} & \text{if } x \geqslant c \end{cases} \tag{13}$$

otherwise:

$$l_k(x) = a^{2k+1} + \frac{b^{2k+1} - a^{2k+1}}{b - a}(x - a) \tag{14}$$

– If $d > a$, then:

$$u_k(x) = \begin{cases} x^{2k+1} & \text{if } x \leqslant d \\ b^{2k+1}\left(1 + R_k\left(\frac{x}{b} - 1\right)\right) & \text{if } x > d \end{cases} \tag{15}$$

otherwise:

$$u_k(x) = a^{2k+1} + \frac{b^{2k+1} - a^{2k+1}}{b - a}(x - a) \tag{16}$$

where we have used the constant $R_k \equiv (r_k^{2k+1} - 1)/(r_k - 1)$.

By construction, the above convex underestimators and overestimators of x^{2k+1} are continuous and differentiable everywhere. Moreover, they form the convex envelope, as the following theorem shows.

THEOREM 5.1. *The convex relaxation of x^{2k+1} for $x \in [a, b]$ where $a < 0 < b$ and $k \in \mathbb{N}$ given in equations (12)-(16) is the tightest possible.*

Proof. First, consider the case where $a < d < 0 < c < b$. As the convex underestimator between c and b is the curve itself, no tighter one can be found in that range. Furthermore, the convex underestimator between a and c is a straight line connecting two points on the original curve, so again it is the tightest possible.

It only remains to show that $l_k(x)$ is convex for any small neighbourhood of c. Consider the open interval $(c - \varepsilon, c + \varepsilon)$, and the straight line segment $\Gamma(c, c + \varepsilon)$ with endpoints $(c, l_k(c))$, $(c + \varepsilon, l_k(c + \varepsilon))$. Because for all $x \geqslant c$, $l_k(x) \equiv x^{2k+1}$ is convex, all points in $\Gamma(c, c + \varepsilon)$ lie above the underestimator. If we now consider $\Gamma(c - \varepsilon, c + \varepsilon)$, its slope is smaller than the slope of $\Gamma(c, c + \varepsilon)$ (because the point with coordinate $c - \varepsilon$ moves on the tangent of the curve at c), yet the right endpoint $c + \varepsilon$ of the segments is common. Thus all points in $\Gamma(c - \varepsilon, c + \varepsilon)$ also lie above the underestimator $l_k(x)$. Since ε is arbitrary, the claim holds. A similar argument holds for the overestimator between a and d.

The cases where $a < d < 0 < b \leqslant c$ and $d \leqslant a < 0 < c < b$ are simpler as the underestimator is a straight line in the whole range of x. □

6. Linear relaxation

The convex envelope presented in Section 5 is nonlinear. As convex relaxations are used to solve a local optimization problem at each node of the search tree examined

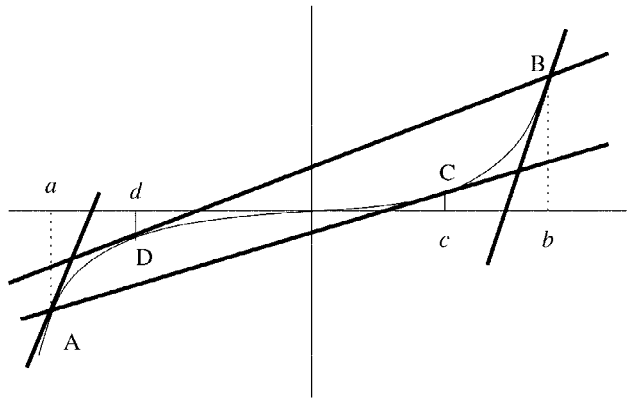

Figure 3. Linear relaxation of x^{2k+1}.

by the sBB algorithm, using a linear envelope instead may have a significant impact on computational cost. We can relax the nonlinear convex envelope to a linear relaxation by dropping the "follow the curve" requirements on either side of the tangency points, and using the lower and upper tangent as convex underestimator and concave overestimator respectively, as follows:

$$a^{2k+1}\left(1+R_k\left(\frac{x}{a}-1\right)\right) \leqslant z \leqslant b^{2k+1}\left(1+R_k\left(\frac{x}{b}-1\right)\right) \tag{17}$$

We can tighten the relaxation further by drawing the tangents to the curve at the endpoints A, B, as shown in Figure 3. This is equivalent to employing the following constraints:

$$(2k+1)b^{2k}x - 2kb^{2k+1} \leqslant z \leqslant (2k+1)a^{2k}x - 2ka^{2k+1} \tag{18}$$

in addition to those in (17).

As has been noted in Section 2, when $c > b$, the underestimators on the left hand sides of (17) and (18) should be replaced by the line $a^{2k+1}+(b^{2k+1}-a^{2k+1})/(b-a)(x-a)$ through points A and B (see Figure 2). On the other hand, if $d < a$, this line should be used to replace the concave overestimators on the right hand sides of (17) and (18). The linear relaxation constraints are summarized in Table 2.

7. Comparison to other convex relaxations

This section considers two alternative convex relaxations of the monomial x^{2k+1} where the range of x includes 0, and compares them with both the nonlinear envelope and the linear relaxation proposed in this paper.

Table 2. Summary of linear relaxations for $z = x^{2k+1}$, $x \in [a, b]$, $a < 0 < b$

$c < b$ and $d > a$	$c > b$ and $d > a$	$c < b$ and $d < a$
$z \geqslant a^{2k+1}(1 + R_k(\frac{x}{a} - 1))$	$z \geqslant a^{2k+1} + \frac{b^{2k+1}-a^{2k+1}}{b-a}(x-a)$	$z \geqslant a^{2k+1}(1 + R_k(\frac{x}{a} - 1))$
$z \leqslant b^{2k+1}(1 + R_k(\frac{x}{b} - 1))$	$z \leqslant b^{2k+1}(1 + R_k(\frac{x}{b} - 1))$	$z \leqslant a^{2k+1} + \frac{b^{2k+1}-a^{2k+1}}{b-a}(x-a)$
$z \geqslant (2k+1)b^{2k}x - 2kb^{2k+1}$	$z \leqslant (2k+1)a^{2k}x - 2ka^{2k+1}$	–
$z \leqslant (2k+1)a^{2k}x - 2ka^{2k+1}$	–	$z \geqslant (2k+1)b^{2k}x - 2kb^{2k+1}$

7.1. REFORMULATION IN TERMS OF BILINEAR PRODUCTS

One possible way of determining a convex relaxation for $z = x^{2k+1}$, where $a \leqslant x \leqslant b$ and $a < 0 < b$, is via its reformulation in terms of a bilinear product of x and the convex monomial x^{2k}:

$$
\begin{aligned}
& z = wx \\
& w = x^{2k} \\
& a \leqslant x \leqslant b \\
& 0 \leqslant w \leqslant w^U = \max\{a^{2k}, b^{2k}\}
\end{aligned}
$$

By replacing the bilinear term wx with the standard linear convex envelope proposed by (McCormick, 1976), and the convex univariate term x^{2k} with the convex envelope given by the function itself as the underestimator and the secant as the overestimator, we obtain the following constraints:

$$
\begin{aligned}
& aw \leqslant z \leqslant bw \\
& w^U x + bw - w^U b \leqslant z \leqslant w^U x + aw - w^U a \\
& x^{2k} \leqslant w \leqslant a^{2k} + \frac{b^{2k} - a^{2k}}{b - a}(x - a) \\
& a \leqslant x \leqslant b \\
& 0 \leqslant w \leqslant w^U
\end{aligned}
$$

After some algebraic manipulation, we can eliminate w to obtain the following nonlinear convex relaxation for z:

$$\frac{w^U a}{a - b}(x - b) \leqslant z \leqslant \frac{w^U b}{b - a}(x - a) \tag{19}$$

$$bx^{2k} + w^U(x - b) \leqslant z \leqslant ax^{2k} + w^U(x - a) \tag{20}$$

$$a\left(a^{2k} + \frac{b^{2k} - a^{2k}}{b - a}(x - a)\right) \leqslant z \leqslant b\left(a^{2k} + \frac{b^{2k} - a^{2k}}{b - a}(x - a)\right) \tag{21}$$

Figure 4 shows the convex/concave relaxations for x^3 for $x \in [-1, 1]$ obtained using (19)–(21). It also compares them with the nonlinear envelope of section 5 (dashed lines in Figure 4a) and the linear relaxations of section 6 (dashed lines in Figure 4b).

As can be seen from Figure 4a, the convex relaxation (19)–(21) is generally similar to that of Section 5 (in that both the underestimator and the overestimator consist of a straight line joined to a curve), but not as tight. This is to be expected in view of Theorem 5.1.

On the other hand, the convex relaxation (19)–(21) is slightly tighter than the linear relaxation of Section 6 in the sub-interval $[a, e]$ where e is the point at which the curve on the right hand side of (20) intersects the tangent line on the right hand side of (18); and also in the sub-interval $[f, b]$ where f is the point at which the curve on the left hand side of (20) intersects the tangent line on the left hand side of (18). However, the linear relaxation of section 6 is tighter everywhere else.

7.2. UNDERESTIMATION THROUGH α PARAMETER

An alternative approach to deriving convex relaxations of general non-convex functions is the αBB algorithm (Androulakis et al., 1995; Adjiman and Floudas, 1996). In this case, the convex underestimator $\mathcal{L}_k(x)$ is given by $x^{2k+1} + \alpha_k(x-a)(x-b)$, where α_k is a positive constant that is sufficiently large to render the second derivative $d^2\mathcal{L}_k(x)/dx^2$ positive for all $x \in [a, b]$. Similarly, the concave overestimator $\mathcal{U}_k(x)$ is given by $x^{2k+1} - \beta_k(x-a)(x-b)$ where β_k is sufficiently large to render $d^2\mathcal{U}_k(x)/dx^2$ negative for all $x \in [a, b]$. It can easily be shown that the above conditions are satisfied by the values:

$$\alpha_k = k(2k+1)|a|^{2k-1} \tag{22}$$

$$\beta_k = k(2k+1)b^{2k-1}. \tag{23}$$

The convex relaxation for the case of $k = 1$ (i.e., the function x^3) obtained using the above approach in the domain $x \in [-1, +1]$ is shown in Figure 5. It is evident that it is looser than those shown in Figures 1 and 3.

8. Conclusion

We have derived a convex nonlinear envelope for monomials of the form x^{2k+1} where 0 is included in the range of x. The constraints defining it are continuous and differentiable everywhere in the domain of interest. It can also form the basis for the derivation of a linear (convex) relaxation that may be more efficient for use within sBB-type algorithms. Both the envelope and the linear relaxation are generally tighter than relaxations obtained using reformulation to bilinear products or using the α-parameter method.

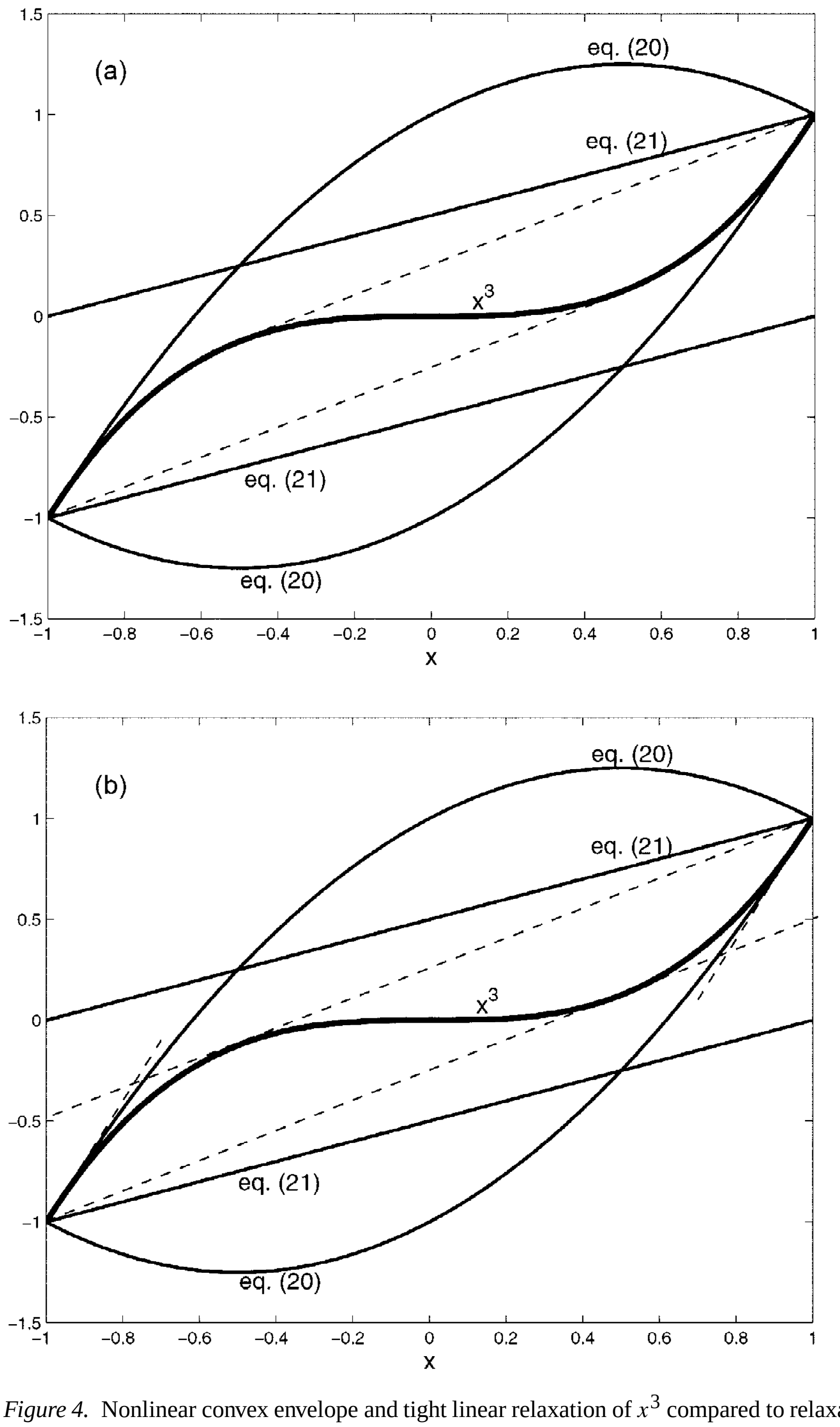

Figure 4. Nonlinear convex envelope and tight linear relaxation of x^3 compared to relaxations obtained by reformulation to bilinear product.

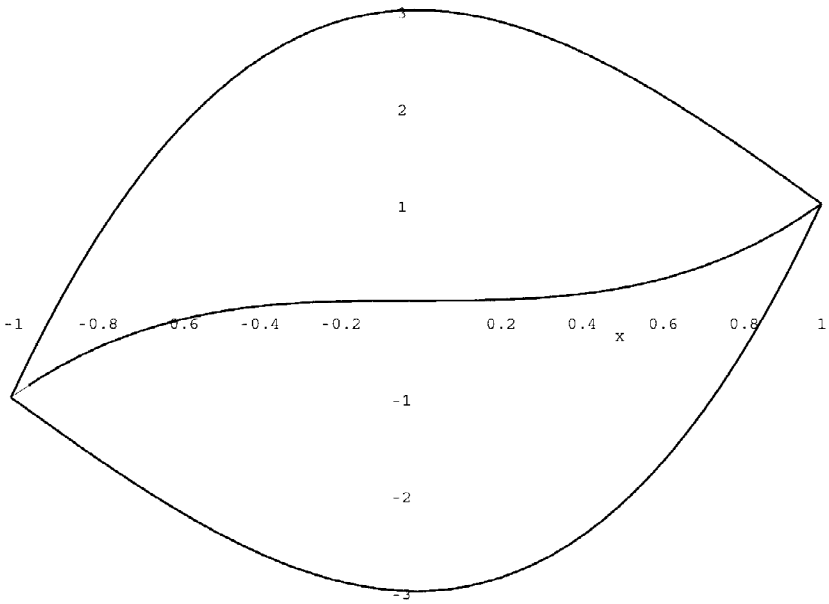

Figure 5. Convex/concave relaxations of x^3 by α parameter.

References

Adjiman, C. S. and Floudas, C. A. (1996), Rigorous convex underestimators for general twice-differentiable problems, *Journal of Global Optimization* 9(1), 23–40.

Androulakis, I. P., Maranas, C. D. and Floudas, C. A. (1995), α BB: A global optimization method for general constrained nonconvex problems, *Journal of Global Optimization* 7(4), 337–363.

Maranas, C. D. and Floudas, C. A. (1995), Finding all solutions to nonlinearly constrained systems of equations, *Journal of Global Optimization* 7(2), 143–182.

McCormick, G. P. (1976), Computability of global solutions to factorable nonconvex programs: Part I – Convex underestimating problems, *Mathematical Programming* 10, 146–175.

Ryoo, H. S. and Sahinidis, N. V. (1995), Global optimization of nonconvex NLPs and MINLPs with applications in process design, *Computers & Chemical Engineering* 19(5), 551–566.

Smith, E. M. (1996), On the optimal design of continuous processes, Ph.D. thesis, Imperial College of Science, Technology and Medicine, University of London.

Smith, E. M. and Pantelides, C. C. (1997), Global Optimisation of Nonconvex MINLPs, *Computers and Chemical Engineering* 21, S791–S796.

Smith, E. M. and Pantelides, C. C. (1999), A symbolic reformulation/spatial branch-and-bound algorithm for the global optimisation of nonconvex MINLPs, *Computers and Chemical Engineering* 23, 457–478.

Stewart, I. (1989), *Galois Theory*. 2nd edition Chapman & Hall, London.

Tuy, H. (1998), *Convex Analysis and Global Optimization*. Kluwer Academic Publishers, Dodrecht.