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 linearized version of the envelope, and compare both the nonlinear and linear forms with envelopes obtained using other approaches.

Keywords: monomial convexification 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 ([Tuy98]). This requires the computation of a lower bound to the solution, usually obtained by solving a convex relaxation of the original NLP (see [RS95, MF95, AF96, SP97]). The formation and tightness of such a convex relaxation are critical issues in any sBB implementation.

As shown in [Smi96] and [SP97, SP99], 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 [MF95]; 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 (see [AMF95, AF96]) 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 envelope. We compare both of these envelopes with convex envelopes derived using other methods.

2 Statement of the problem

[MF95] 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 fig. 1 below). The shape of the convex underestimator of x^{2k+1}

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depends on the relative magnitude of b and c. In particular, if $c < b$ (as is the case in fig. 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. fig. 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 fig. 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.

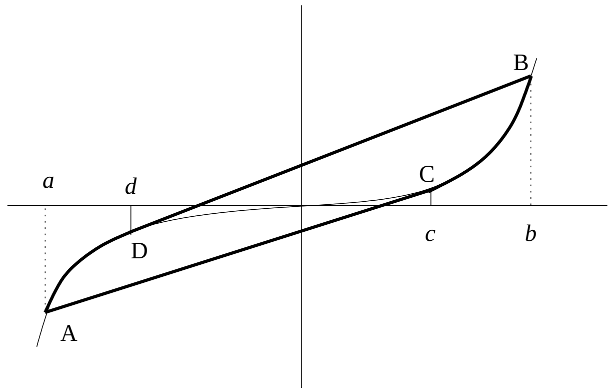


Figure 1: Tightest (nonlinear) convex envelope of x^{2k+1}.

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:

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

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[2] 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 [Ste89].

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 $k \geq 1$, and this lies in $[-1 + 1/2k, -0.5]$.

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

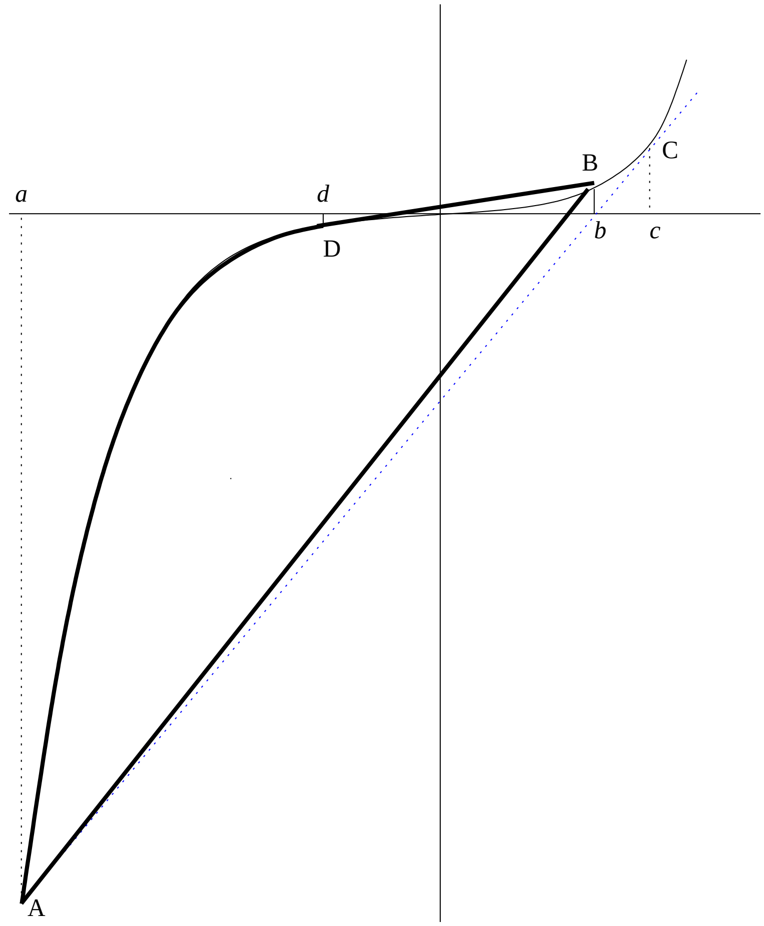


Figure 2: The case when $c > b$.

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 $k \leq 10$.

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

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

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 $[-1 + \frac{1}{2k}, -\frac{1}{2}]$.

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

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

$$\forall x > 0 \ \left(\frac{dQ^k(x)}{dx} > 0\right) \tag{6}$$

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

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): $\frac{dQ^k(x)}{dx} = \sum_{i=1}^{2k-1} i(i+1)x^{i-1}$, 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 $x \leq -1$, 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 $x \geq 0$ (property (6) and the fact that $Q^k(0) > 0$);
3. there are no roots for $x \leq -1$ (property (7)).

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

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

We now make the inductive hypothesis that, for all $j < k$, $Q^j(x) > 0$ for all $x > -\frac{1}{2}$ and $Q^j(x) < 0$ for all $x < -1 + \frac{1}{2j}$ 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:

$$\begin{aligned} Q^k(x) > Q^{k-1}(x) \quad &\text{if} \quad x > -1 + \frac{1}{2k} \\ Q^k(x) < Q^{k-1}(x) \quad &\text{if} \quad x < -1 + \frac{1}{2k} \end{aligned}$$

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

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

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

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

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

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

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

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 $P^k(x,1) = (x-1)^2Q^k(x)$. 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 The 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 fig. 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 envelope for $z = x^{2k+1}$ when $x \in [a, b]$ and $a < 0 < b$:

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

is as follows:

- If $c < b$, then:

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

  otherwise:

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

- If $d > a$, then:

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

  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 $R_k \equiv \frac{r_k^{2k+1} - 1}{r_k - 1}$.

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

5.1 Theorem
The convex envelope 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 $x \geq c$, $l_k(x) \equiv x^{2k+1}$ 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 $a < d < 0 < b \leq c$ and $d \leq a < 0 < c < b$ are simpler as the underestimator is a straight line in the whole range of x. $\square$

6 Linear convex envelope

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

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

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

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

in addition to those in (17).

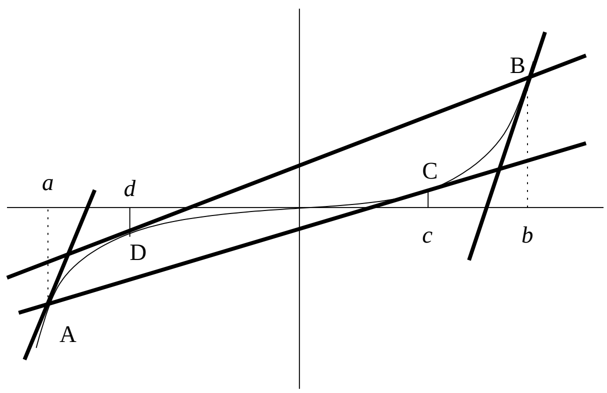


Figure 3: Linear envelope of x^{2k+1}.

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 $a^{2k+1} + \frac{b^{2k+1}-a^{2k+1}}{b-a}(x-a)$ through points A and B (see fig. 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 convex envelope constraints are summarized in table 2.

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

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

7 Comparison to other convex envelopes

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

7.1 Reformulation in terms of bilinear products

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

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

By replacing the bilinear term wx with the standard linear convex envelope proposed by [McC76], 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:

$$\begin{array}{rcl} aw \leq & z & \leq bw \\ w^U x + bw - w^U b \leq & z & \leq w^U x + aw - w^U a \\ x^{2k} \leq & w & \leq a^{2k} + \dfrac{b^{2k} - a^{2k}}{b - a}(x - a) \\ a \leq & x & \leq b \\ 0 \leq & w & \leq w^U \end{array}$$

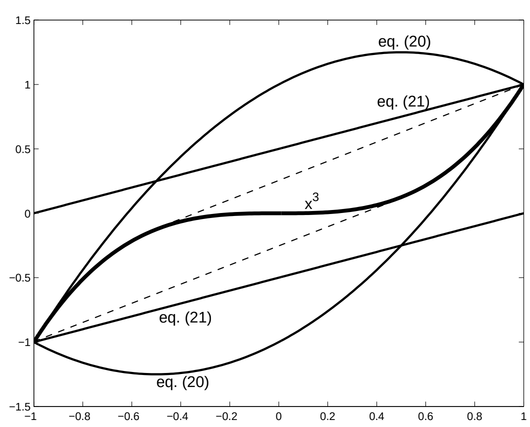
After some algebraic manipulation, we can eliminate w to obtain the following nonlinear convex envelope for z:

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

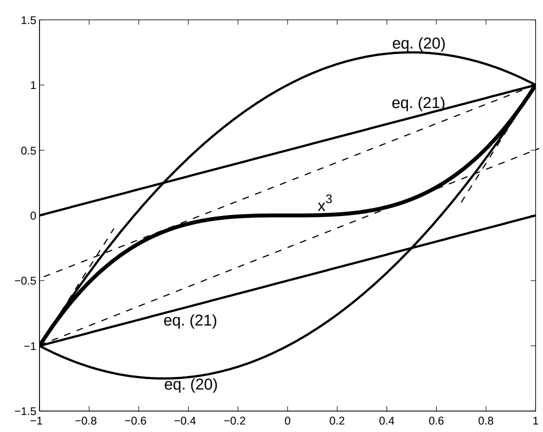
$$bx^{2k} + w^U(x - b) \quad \leq z \leq \quad ax^{2k} + w^U(x - a) \tag{20}$$

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

Fig. 4 shows the convex envelope for x^3 for $x \in [-1, 1]$ obtained using (19)-(21). It also compares it with the nonlinear convex envelope of section 5 (dashed lines in fig. 4a) and the linear one of section 6 (dashed lines in fig. 4b).



a. Comparison with nonlinear convex envelope



b. Comparison with linear convex envelope

Figure 4: Convex envelope of x^3 by reformulation to bilinear product.

As can be seen from fig. 4a, the convex envelope (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 envelope (19)-(21) is slightly tighter than the linear envelope 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 envelope of section 6 is tighter everywhere else.

7.2 Underestimation through α parameter

An alternative approach to deriving convex envelopes of general non-convex functions is the αBB algorithm (see [AMF95], [AF96]). 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 envelope 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 fig. 5. It is evident that it is looser than those shown in figs. 1 and 3.

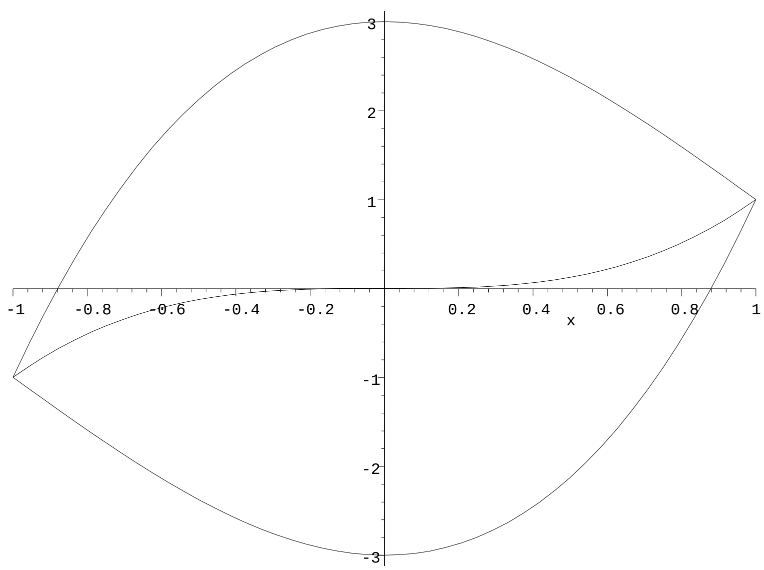


Figure 5: Convex envelope of x^3 by α relaxation.

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. This is the tightest possible envelope and 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 envelope that may be more efficient for use within sBB-type algorithms. Both of these envelopes are generally tighter than those obtained using reformulation to bilinear products or relaxation using the α-parameter method.

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