Lower bound functions for polynomials

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Abstract

Relaxation techniques for solving nonlinear systems and global optimisation problems require bounding from below the nonconvexities that occur in the constraints or in the objective function by affine or convex functions. In this paper we consider such lower bound functions in the case of problems involving multivariate polynomials. They are constructed by using Bernstein expansion. An error bound exhibiting quadratic convergence in the univariate case and some numerical examples are given.

1 Introduction

A frequently used approach for solving nonlinear systems, combinatorial optimisation problems, or constrained global optimisation problems is the generation of relaxations, and their use in a branch and bound framework. Generally speaking, a relaxation of a given problem has the properties that

(i) each feasible point of the given problem is feasible for the relaxation,

(ii) the relaxation is easier to solve than the given problem, and

(iii) the solutions of the relaxation converge to the solutions of the original problem, provided the maximal width of the set of feasible points converges to zero.

For many problems a relaxation can be constructed, if the functions which define the problem can be bounded from below by affine or convex functions. For example, if we want to check

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whether a given (complicated) function $f : X \to \mathbb{R}$ with $X \subseteq \mathbb{R}^n$ takes some negative values on a box X, we can formulate this problem in the form:

Is the set of feasible points $F := \{x \in X : f(x) \leq 0\}$ empty?

If f is an (arbitrarily) nonlinear function the set F may be very complicated. It is well-known that checking whether F is empty is an NP-hard problem, even for quadratic functions. If there exists an affine lower bound function $\underline{f}$ for f on X, then we define the relaxation as the problem

Is the set of (relaxed) feasible points $R := \{x \in X : \underline{f}(x) \leq 0\}$ empty?

Obviously, the inclusion $F \subseteq R$ holds valid such that property (i) is satisfied. The relaxation is a linear programming problem which, in contrast to the original problem, can be solved in polynomial time; that is, the check whether R is empty or not is much easier than the original test (see property (ii)). If the lower bound function $\underline{f}$ converges to the original function f for decreasing diameter of X then property (iii) is satisfied. Putting this relaxation into a branch and bound framework, under mild conditions we get either convergence to a point with negative value of f, or we find that F is empty. In a similar way, relaxations can be constructed to solve nonlinear systems and global optimisation problems.

Relaxation techniques were first discussed in the case of linear integer problems, and later also for special structured continuous global optimisation problems; see for example the monographs of Floudas [9], Horst and Pardalos [13], and Parker and Rardin [22]. Linear relaxations for bilinear problems were first considered by Al-Khayyal and Falk [2]. They use the convex envelope of bilinear terms in order to obtain a relaxation. For developments and improvements for special structured continuous global optimisation problems that include non-convexities introduced by concave univariate, bilinear and linear fractional terms the reader is referred to Zamora and Grossmann [29]. For constrained global optimisation problems and nonlinear systems which are defined by arbitrary arithmetical expressions, see Adjiman and Floudas [1] and Androulakis, Maranas, and Floudas [3]. There convex lower bound functions are constructed by augmenting the nonconvex expressions with the addition of separable quadratic functions, which aim to overpower the nonconvexities. In Adjiman and Floudas [1] special emphasis is placed on the construction of lower bound functions by computing eigenvalues of interval Hessian matrices. In Jansson [17], quasiconvex relaxations are defined by using interval arithmetic together with zero- and first-order information for constructing convex lower and concave upper bound functions of arbitrarily arithmetical expressions.

This paper addresses the construction of relaxations for problems involving multivariate polynomials. The major goal is to show how non-convex multivariate polynomial terms can be replaced by affine and convex lower bound functions which are computed by using Bernstein coefficients. These bound functions may be used in any relaxation method described in the above literature, whenever these approaches do not deliver satisfactory results for polynomial terms of higher degree. Moreover, several properties of these bound functions are discussed. For properties of Bernstein polynomials the reader is referred to Cargo and Shisha [5], Farin [7], Garloff [11], Garloff, Jansson and Smith [12], and Zettler and Garloff [30].

By using Bernstein coefficients, bounds for the range of a multivariate polynomial over a box can be computed. It was shown by Stahl [28] that in the univariate case these bounds are often tighter than bounds which are obtained by applying interval computation techniques (cf. Neumaier [21], Ratschek and Rokne [23]). In [19] a method is presented by which piecewise linear lower (and equally linear upper) bound functions for multivariate polynomials can be obtained. This leads to tight enclosures of the given polynomials which are important, e.g., in intersection testing. The construction is presented there in detail in the univariate and bivariate cases. However, these lower bound functions are in general not convex. So the convex envelope of the piecewise linear lower bound functions has to be taken, requiring additional effort.

The paper is organised as follows. In the next section some basic definitions and properties of Bernstein polynomials are given. Affine and convex lower bound functions based on the Bernstein expansion are presented in Section 3. An error bound for the affine lower bound functions is considered in Section 4. In the subsequent section some remarks are given, as to how algorithms for computing the bound functions have to be implemented such that these bounds are rigorous; that is, all roundings are taken into consideration. Section 6 contains a discussion of the question whether the lower bound function coincides with the lower convex envelope of the given polynomial. The results of the previous sections are illustrated by some numerical examples in Section 7. Finally, some conclusions are given.

2 Bernstein polynomials

We define multiindices $i = (i_1, \ldots, i_n)^T$ as vectors, where the n components are nonnegative integers. The vectors 0 and 1 denote the multiindices with all components equal to 0 or 1, respectively, which should not cause ambiguity. Comparisons and the absolute value $|.|$ are used entrywise. Also the division of multiindices i, l with $l > 0$ is defined componentwise in the form $i/l := (i_1/l_1, \ldots, i_n/l_n)^T$, and for $x \in \mathbb{R}^n$ its multipowers are

$$x^i := \prod_{\mu=1}^{n} x_\mu^{i_\mu}. \tag{1}$$

For the sum we use the notation

$$\sum_{i=0}^{l} := \sum_{i_1=0}^{l_1} \dots \sum_{i_n=0}^{l_n} . \tag{2}$$

A multivariate polynomial p of degree $l = (l_1, \dots, l_n)^T$ can be represented as

$$p(x) = \sum_{i=0}^{l} a_i x^i \quad \text{with} \quad a_i \in \mathrm{IR}, 0 \leq i \leq l, \text{ and } a_l \neq 0. \tag{3}$$

The ith Bernstein polynomial of degree l is

$$B_i(x) := \binom{l}{i} x^i (1-x)^{l-i}, \tag{4}$$

where the generalised binomial coefficient is defined by $\binom{l}{i} := \prod_{\mu=1}^{n} \binom{l_\mu}{i_\mu}$, and x is contained in the unit box $I = [0,1]^n$. It is well-known that the Bernstein polynomials form a basis in the space of multivariate polynomials, and each polynomial in the form (3) can be represented in its Bernstein form over I

$$p(x) = \sum_{i=0}^{l} b_i B_i(x), \tag{5}$$

where the *Bernstein coefficients* b_i are given by

$$b_i = \sum_{j=0}^{i} \frac{\binom{i}{j}}{\binom{l}{j}} a_j \quad \text{for} \quad 0 \leq i \leq l. \tag{6}$$

A fundamental property for our approach is the *convex hull property*

$$\left\{ \begin{pmatrix} x \\ p(x) \end{pmatrix} : x \in I \right\} \subseteq conv \left\{ \begin{pmatrix} i/l \\ b_i \end{pmatrix} : 0 \leq i \leq l \right\}, \tag{7}$$

where the convex hull is denoted by *conv*. The points $\binom{i/l}{b_i}$ are called *control points* of p. This enclosure yields the inequalities

$$\min\{b_i : 0 \leq i \leq l\} \leq p(x) \leq \max\{b_i : 0 \leq i \leq l\} \tag{8}$$

for all $x \in I$.

3 Convex lower bound functions

In this section we show how special convex lower bound functions for multivariate polynomials can be constructed by using Bernstein expansion.

The simplest type of a convex lower bound function is a constant lower bound function. The left-hand side inequality (8) implies that the constant function

$$c(x) := \min\{b_i : 0 \le i \le l\} \tag{9}$$

is an affine lower bound function for the polynomial p over I with Bernstein coefficients $\{b_i\}_{i=0}^l$. The following theorem deals with nonconstant affine lower bound functions.

Theorem 3.1 *Let $\{b_i\}_{i=0}^l$ denote the Bernstein coefficients of an n-variate polynomial p of degree l. Let $\widehat{\imath}$ be a multiindex such that*

$$b_{\widehat{\imath}} := \min\{b_i : 0 \le i \le l\}, \tag{10}$$

and let $\widehat{J} \subseteq \{\widehat{\jmath} :\ 0 \le \widehat{\jmath} \le l,\ \widehat{\jmath} \ne \widehat{\imath}\}$ be a set of at least n multiindices such that

$$\frac{b_{\widehat{\jmath}} - b_{\widehat{\imath}}}{\|\widehat{\jmath}/l - \widehat{\imath}/l\|} \le \frac{b_i - b_{\widehat{\imath}}}{\|i/l - \widehat{\imath}/l\|} \quad \text{for each } \widehat{\jmath} \in \widehat{J},\ \ 0 \le i \le l,\ i \ne \widehat{\imath},\ i \notin \widehat{J}. \tag{11}$$

Here, $\|\cdot\|$ denotes some vector norm. Then the linear programming problem

$$\min\Big(\sum_{\widehat{\jmath} \in \widehat{J}} (\widehat{\jmath}/l - \widehat{\imath}/l)\Big)^T \cdot s \qquad \text{subject to} \tag{12}$$

$$(i/l - \widehat{\imath}/l)^T \cdot s \ge b_{\widehat{\imath}} - b_i \quad \text{for } \ 0 \le i \le l, i \ne \widehat{\imath} \tag{13}$$

has the following properties:

1. *It has an optimal solution $\widehat{s}$.*

2. *The affine function*

$$c(x) := -\widehat{s}^T \cdot x + (\widehat{s}^T \cdot (\widehat{\imath}/l) + b_{\widehat{\imath}}) \tag{14}$$

   is a lower bound function for p on I.

Proof.

1. Definition (10) implies $b_{\widehat{\imath}} - b_i \le 0$ for $0 \le i \le l$. Hence $s := 0$ satisfies the inequalities (13) and is feasible. Using (13) for $\widehat{\jmath} \in \widehat{J}$, i.e.

$$(\widehat{\jmath}/l - \widehat{\imath}/l)^T \cdot s \ge b_{\widehat{\imath}} - b_{\widehat{\jmath}},$$

it follows that the objective function (12) is bounded from below by $\sum_{\widehat{\jmath} \in \widehat{J}} b_{\widehat{\imath}} - b_{\widehat{\jmath}}$. A linear programming problem which has feasible solutions and a bounded objective function has at least one optimal solution $\widehat{s}$, so that the first statement is proved.

2. The convex hull property (7) yields

$$\begin{pmatrix} x \\ p(x) \end{pmatrix} = \sum_{i=0}^{l} \begin{pmatrix} i/l \\ b_i \end{pmatrix} \lambda_i, \quad \text{where } \ \lambda_i \ge 0,\ \sum_{i=0}^{l} \lambda_i = 1$$

for each $x \in I$. Therefore,

$$\begin{aligned}
\begin{pmatrix}\widehat{s}\\ 1\end{pmatrix}^T \cdot \begin{pmatrix}x\\ p(x)\end{pmatrix} &= \sum_{i=0}^{l} \lambda_i \widehat{s}^T \cdot (i/l) + \sum_{i=0}^{l} \lambda_i b_i \\
&= \sum_{i=0}^{l} \lambda_i \widehat{s}^T \cdot (i/l - \widehat{i}/l) + \sum_{i=0}^{l} \lambda_i \widehat{s}^T \cdot (\widehat{i}/l) \\
&\quad + \sum_{i=0}^{l} \lambda_i (b_i - b_{\widehat{i}}) + \sum_{i=0}^{l} \lambda_i b_{\widehat{i}} \\
&= \sum_{i=0}^{l} \lambda_i ((i/l - \widehat{i}/l)^T \cdot \widehat{s} + (b_i - b_{\widehat{i}})) + \sum_{i=0}^{l} (\widehat{s}^T \cdot (\widehat{i}/l) + b_{\widehat{i}}).
\end{aligned}$$

The inequalities (13) imply that the first sum is nonnegative. Hence,

$$p(x) + \widehat{s}^T \cdot x \geq \widehat{s}^T \cdot (\widehat{i}/l) + b_{\widehat{i}} \; ,$$

proving the last assertion. ■

Notice that due to the inequalities (13) each optimal solution $\widehat{s}$ must satisfy

$$(\widehat{j}/l - \widehat{i}/l)^T \cdot \widehat{s} \geq b_{\widehat{i}} - b_{\widehat{j}} \;\text{ for each }\; \widehat{j} \in \widehat{J}.$$

Hence, the objective function (12) tries to fulfil these inequalities as equations.

Geometrically, the ratios in (11) describe slopes with respect to the Bernstein coefficients in direction $\widehat{j}/l - i/l$. There are many possibilities for the construction of an affine lower bound function c such that it passes through some of the control points. The intention of the previous theorem is to construct an affine lower bound function which comprises in a weighted form the n smallest slopes $\frac{b_{\widehat{j}} - b_{\widehat{i}}}{\|\widehat{j}/l - i/l\|}$; that is, c passes through a facet of the convex hull of the control points which has a minimal weighted slope.

In the univariate case, by definition (11), $\widehat{J}$ can be chosen such that it consists of exactly one element $\widehat{j}$ which may not be uniquely defined. The slope of the affine lower bound function c is equal to the smallest possible slope between the control points. Moreover, the optimal solution of the linear programming problem (12) and (13) can be given explicitly in the univariate case.

Theorem 3.2 *Suppose that all assumptions of Theorem 3.1 are satisfied, where $n = 1$ and where $\|\cdot\|$ denotes the absolute value. Choose $\widehat{J} = \{\widehat{j}\}$, where $\widehat{j}$ satisfies*

$$\frac{b_{\widehat{j}} - b_{\widehat{i}}}{|\widehat{j}/l - \widehat{i}/l|} = \min\left\{ \frac{b_i - b_{\widehat{i}}}{|i/l - \widehat{i}/l|} : \;\; 0 \leq i \leq l, \; i \neq \widehat{i} \right\}.$$

There then exists an optimal solution $\widehat{s}$ of the linear programming problem (12),(13) which satisfies

$$\widehat{s} = -\frac{b_{\widehat{j}} - b_{\widehat{i}}}{\widehat{j}/l - \widehat{i}/l}. \tag{15}$$

Proof. The condition (11) yields

$$-|i/l - \widehat{\imath}/l| \cdot \frac{b_{\widehat{\jmath}} - b_{\widehat{\imath}}}{|\widehat{\jmath}/l - \widehat{\imath}/l|} \geq b_{\widehat{\imath}} - b_i \tag{16}$$

for $0 \leq i \leq l$, $i \neq \widehat{\imath}$. We consider two cases, and prove in each case that $\widehat{s}$ is an optimal solution of the linear programming problem.

Case 1: We assume that $\widehat{\jmath} < \widehat{\imath}$. Then

$$\widehat{s} = \frac{b_{\widehat{\jmath}} - b_{\widehat{\imath}}}{|\widehat{\jmath}/l - \widehat{\imath}/l|} \geq 0. \tag{17}$$

Hence, for $i > \widehat{\imath}$, we have $i/l - \widehat{\imath}/l > 0$, and because of (10) we obtain

$$(i/l - \widehat{\imath}/l) \cdot \widehat{s} \geq 0 \geq b_{\widehat{\imath}} - b_i.$$

For $i < \widehat{\imath}$ the inequalities (16) and (17) yield

$$(i/l - \widehat{\imath}/l) \cdot \widehat{s} = -|i/l - \widehat{\imath}/l| \cdot \frac{b_{\widehat{\jmath}} - b_{\widehat{\imath}}}{|\widehat{\jmath}/l - \widehat{\imath}/l|} \geq b_{\widehat{\imath}} - b_i.$$

We have proved that $\widehat{s}$ satisfies the inequalities (13). For $i := \widehat{\jmath}$ the inequality (13) and (17) imply

$$b_{\widehat{\imath}} - b_{\widehat{\jmath}} \leq (\widehat{\jmath}/l - \widehat{\imath}/l) \cdot \widehat{s} = -(b_{\widehat{\jmath}} - b_{\widehat{\imath}}) = b_{\widehat{\imath}} - b_{\widehat{\jmath}},$$

which yields the optimality of $\widehat{s}$.

Case 2: We assume that $\widehat{\jmath} > \widehat{\imath}$. Then

$$\widehat{s} = -\frac{b_{\widehat{\jmath}} - b_{\widehat{\imath}}}{|\widehat{\jmath}/l - \widehat{\imath}/l|} \leq 0. \tag{18}$$

Hence, for $i < \widehat{\imath}$ we obtain

$$(i/l - \widehat{\imath}/l) \cdot \widehat{s} \geq 0 \geq b_{\widehat{\imath}} - b_i,$$

and for $i > \widehat{\imath}$ we obtain by using (16) and (18)

$$(i/l - \widehat{\imath}/l) \cdot \widehat{s} = -|i/l - \widehat{\imath}/l| \cdot \frac{b_{\widehat{\jmath}} - b_{\widehat{\imath}}}{|\widehat{\jmath}/l - \widehat{\imath}/l|} \geq b_{\widehat{\imath}} - b_i.$$

Therefore, $\widehat{s}$ is feasible and

$$b_{\widehat{\imath}} - b_{\widehat{\jmath}} \leq (\widehat{\jmath}/l - \widehat{\imath}/l) \cdot \widehat{s} = -(b_{\widehat{\jmath}} - b_{\widehat{\imath}}) = b_{\widehat{\imath}} - b_{\widehat{\jmath}}$$

yields the optimality of $\widehat{s}$. ∎

In the previous two theorems we have considered affine lower bound functions. The convex hull property (7) suggests that a convex lower bound function can be constructed which coincides with facets of the convex hull of the control points. This lower bound function is considered in the next theorem.

Theorem 3.3 *Let $\{b_i\}_{i=0}^l$ denote the Bernstein coefficients of an n-variate polynomial p of degree l. Let $\rho := \prod_{\mu=1}^{n} (l_\mu + 1)$. Then the function*

$$c(x) := \min \left\{ z \in \mathbb{R} : \; x \in \mathbb{R}^n, \begin{pmatrix} x \\ z \end{pmatrix} \in conv \left\{ \begin{pmatrix} i/l \\ b_i \end{pmatrix} : \; 0 \leq i \leq l \right\} \right\} \tag{19}$$

is a convex lower bound function for p on I. Moreover, this function can be characterised for each $x \in I$ as the optimal value of the linear programming problem

$$c(x) = \min \left\{ \sum_{i=0}^{l} b_i w_i : \; w \in W(x) \right\}, \tag{20}$$

with the set of feasible points

$$W(x) := \left\{ w \in \mathbb{R}^\rho : \; \sum_{i=0}^{l} (i/l) \cdot w_i = x, \; \sum_{i=0}^{l} w_i = 1, \; w_i \geq 0 \;\; for \; 0 \leq i \leq l \right\}. \tag{21}$$

Proof. Since the convex hull $C := conv\{\binom{i/l}{b_i} : \; 0 \leq i \leq l\}$ is compact and contains each point $\binom{x}{p(x)}$ with $x \in I$, it follows that the minimum in (19) exists for all $x \in I$ and $p(x) \geq c(x)$. Hence c is a lower bound function for p.

Let $x, y \in I$, then $\binom{x}{c(x)}, \binom{y}{c(y)} \in C$. Since C is a convex set, we have for $0 \leq \lambda \leq 1$:

$$\lambda \begin{pmatrix} x \\ c(x) \end{pmatrix} + (1 - \lambda) \begin{pmatrix} y \\ c(y) \end{pmatrix} = \begin{pmatrix} \lambda x + (1 - \lambda) y \\ \lambda c(x) + (1 - \lambda) c(y) \end{pmatrix} \in C.$$

Definition (19) yields $\lambda c(x) + (1 - \lambda) c(y) \geq c(\lambda x + (1 - \lambda) y)$, proving the convexity of c.

For $x \in I$ it follows by (19) that there exists a $w^x \in \mathbb{R}^\rho$ such that

$$\begin{pmatrix} x \\ c(x) \end{pmatrix} = \sum_{i=0}^{l} \begin{pmatrix} i/l \\ b_i \end{pmatrix} w_i^x, \; \sum_{i=0}^{l} w_i^x = 1, \; w_i^x \geq 0, \; 0 \leq i \leq l.$$

Hence $w^x \in W(x)$. From this observation the characterisations (20) and (21) follow immediately. ∎

The convex lower bound function c which is described in the previous theorem is the uniformly best underestimating convex function which can be obtained from the convex hull of the control points. But this function requires the solution of the linear programming problem (20) and (21) for each fixed $x \in I$. Therefore, this lower bound function should be applied in situations where only a few function evaluations are necessary. Notice that the lower bound function defined in Theorem 3.2 requires us to solve only *one* linear programming problem (cf.(12) and (13)); in this case a function evaluation requires only one scalar product (see (14)).

4 Error bound

In this section we shall deal with an error bound for the underestimating function (14) which was presented in Section 3. This bound coincides with an error bound given by Schaback [27].

Theorem 4.1 *Let $\{b_i\}_{i=0}^{l}$ denote the Bernstein coefficients of an n-variate polynomial p of degree l. Then the affine lower bound function (14) satisfies the a posteriori error bound*

$$0 \leq p(x) - c(x) \leq \max\{b_i - b_{\widehat{i}} + (i/l - \widehat{i}/l)^T \cdot \widehat{s} : \ 0 \leq i \leq l\}, \ x \in I. \tag{22}$$

Proof. For $x \in I$ *partition of unity* and *linear precision* (see for example [7]), i.e.,

$$1 = \sum_{i=0}^{l} B_i(x), \quad x = \sum_{i=0}^{l} (i/l) B_i(x), \tag{23}$$

imply

$$\begin{aligned} p(x) - c(x) &= (\sum_{i=0}^{l} b_i B_i(x)) + \widehat{s}^T \cdot x - \widehat{s}^T \cdot (\widehat{i}/l) - b_{\widehat{i}} \\ &= \sum_{i=0}^{l} (b_i + \widehat{s}^T \cdot (i/l) - \widehat{s}^T \cdot (\widehat{i}/l) - b_{\widehat{i}}) B_i(x) \\ &= \sum_{i=0}^{l} (b_i - b_{\widehat{i}} + (i/l - \widehat{i}/l)^T \cdot \widehat{s}) B_i(x). \end{aligned}$$

Using once more the partition of unity and the property that $B_i(x) \geq 0$ for $x \in I$ and $0 \leq i \leq l$, we obtain from this identity the error bound (22). ■

The quantities $b_i - b_{\widehat{i}} + (i/l - \widehat{i}/l)^T \cdot \widehat{s}$ are the defects of the inequalities in the linear programming problem (12) and (13), and can be obtained from the optimal simplex tableaux. Hence, the additional cost for computing this error bound is only the calculation of the maximal component, which is negligible.

In the univariate case, we can insert the representation (15) of the optimal solution $\widehat{s}$ into the error bound (22) to obtain the following result.

Corollary 4.1 *Suppose that the assumptions of Theorem 3.2 hold, then the affine lower bound function c satisfies the error bound*

$$0 \leq p(x) - c(x) \leq \max\left\{ \left(\frac{b_i - b_{\widehat{i}}}{i/l - \widehat{i}/l} - \frac{b_{\widehat{j}} - b_{\widehat{i}}}{\widehat{j}/l - \widehat{i}/l} \right) (i/l - \widehat{i}/l) : \ 0 \leq i \leq l, \ i \neq \widehat{i} \right\}, \ x \in I. \tag{24}$$

Remark: If we extend the construction of affine lower bound functions for polynomials in the univariate case from I to arbitrary intervals $[\underline{a}, \overline{a}]$ with $\underline{a} < \overline{a}$, then we can show similarly as in [27] that the error bound in Corollary 4.1 is quadratic with respect to the width of the interval , i.e., the right-hand side of (24) can be bounded from above by $C(p)(\overline{a}-\underline{a})^2$, where $C(p)$ is an constant depending only on p. The question whether quadratic convergence holds true in the multivariate case is open, but seems likely also to hold.

The following theorem shows that affine polynomials coincide with their affine lower bounds; that is, the error bound is equal to zero for each $x \in I$.

Theorem 4.2 *Let $p(x) = a_0 + a_1x_1 + \ldots + a_nx_n$, with $a_i \in \mathrm{I\!R}$, for $i = 0, \ldots, n$, be an affine multivariate polynomial. Then the lower bound function (14) coincides with p on I.*

Proof. Let $l, i^\mu \in \mathrm{I\!R}^n$ for $\mu = 0, \ldots, n$ denote the n-multiindices with $l = 1, i^0 = 0, i^\mu = e_\mu$, where e_μ is the μth unit vector for $\mu = 1, ..., n$. By defining $a_{i^\mu} := a_\mu$ for $\mu = 0, \ldots, n$ and by using (1) and (3), it follows that the affine polynomial can be written in the form

$$p(x) = \sum_{\mu=0}^{n} a_{i^\mu} x^{i^\mu}.$$

A short calculation shows that the Bernstein coefficients (6) of this affine polynomial are

$$b_{i^0} = a_0, \quad b_{i^\mu} = a_0 + a_\mu \text{ for } \mu = 1, \ldots, n. \tag{25}$$

Using the notation $\widehat{i} := i^{\widehat{\mu}}$, the scalar products which occur in the linear programming problem (12) and (13) can be written in the form

$$(i^\mu/l - i^{\widehat{\mu}}/l)^T \cdot s = s_\mu - s_{\widehat{\mu}}, \tag{26}$$

and therefore problem (12), (13) is equivalent to

$$\min \sum_{\mu=0}^{n} s_\mu - s_{\widehat{\mu}} \qquad \text{subject to} \tag{27}$$

$$-s_{\widehat{\mu}} \geq a_{\widehat{\mu}} \tag{28}$$

$$s_\mu - s_{\widehat{\mu}} \geq a_{\widehat{\mu}} - a_\mu \text{ for } \mu = 1, \ldots, n, \ \mu \neq \widehat{\mu}. \tag{29}$$

The inequality (28) corresponds to (13) in the case where $i = 0$. Since the rank of the matrix corresponding to these inequalities is equal to n, it follows from the theory of linear programming, that an optimal vertex $\widehat{s}$ satisfies at least n inequalities as equations, and therefore

$$\begin{aligned} -\widehat{s}_{\widehat{\mu}} &= a_{\widehat{\mu}} \\ \widehat{s}_\mu - \widehat{s}_{\widehat{\mu}} &= a_{\widehat{\mu}} - a_\mu \text{ for } \mu = 1, \ldots, n, \ \mu \neq \widehat{\mu}. \end{aligned}$$

Hence $\widehat{s}_\mu = -a_\mu$ for $\mu = 1, \ldots, n$, and the affine lower bound function (14) can be written as

$$c(x) = -\sum_{\mu=1}^{n} (-a_\mu) x_\mu + (s_{\widehat{\mu}} + a_0 + a_{\widehat{\mu}}) = p(x)$$

for all $x \in I$. ■

Theorem 4.2 suggests that almost affine functions should be approximated rather well by the affine lower bound function (14). This coincides with our numerical experiences.

5 Verification

Due to rounding errors and cancellation, inaccuracies may be introduced into the calculation of the Bernstein coefficients and the lower bound functions. Especially, it may happen that the computed function value of a lower bound function is greater than the function value of the original function in some parts of the feasible domain. This may lead to erroneous conclusions in applications. In this section we give some suggestions for obtaining verified results.

Algorithms for calculating rigorous error bounds $\underline{b}_i \leq b_i \leq \overline{b}_i$ for the Bernstein coefficients are given by Fischer [8] and Rokne [24], [25]. These algorithms are based on interval arithmetic (see Neumaier [21]), and the case of polynomials with interval coefficients is also treated there. Using these algorithms, rigorous affine and convex lower bound functions can be computed in the univariate case.

In the multivariate case, the affine lower bound function (14) requires the solution of a linear programming problem, apart from the computation of the Bernstein coefficients. Due to rounding errors, the approximate solution $\widehat{s}$ may not be optimal or even not feasible. From the proof of Theorem 4.1 it follows immediately that c is a lower bound function for p iff for $x \in I$

$$0 \leq p(x) - c(x) = \sum_{i=0}^{l} (b_i - b_{\widehat{i}} + (i/l - \widehat{i}/l)^T \cdot \widehat{s}) B_i(x). \tag{30}$$

In other words, if $\widehat{s}$ satisfies

$$-(i/l - \widehat{i}/l)^T \cdot \widehat{s} \leq b_i - b_{\widehat{i}} \text{ for } 0 \leq i \leq l, i \neq \widehat{i}, \tag{31}$$

then $p(x) - c(x) \geq 0$, and therefore c is a lower bound function for p on I. Hence, if we compute a constant δ satisfying

$$\delta \leq \min\{(i/l - \widehat{i}/l)^T \cdot \widehat{s} + (b_i - b_{\widehat{i}}) : \ 0 \leq i \leq l, i \neq \widehat{i}\} \tag{32}$$

then

$$c(x) := -\widehat{s}^T \cdot x + (\widehat{s}^T \cdot (\widehat{i}/l) + b_{\widehat{i}} + \delta), x \in I,$$

is a verified affine lower bound function for p. The constant δ, which bounds the maximal violation of the inequalities (31) should be computed by using interval arithmetic. In order to obtain a rigorous lower bound for δ, the simplest possibility is to define the vectors $i-\widehat{i}, l, \widehat{s}$ and the real numbers $\underline{b}_i, \overline{b}_{\widehat{i}}$ as interval quantities, then to use the interval operations, and lastly to take the lower bound of the interval result. The same must be done for computing the constant term of $c(x)$. If interval arithmetic is not available the directed roundings *roundup* and *rounddown* can be used; but then the algorithm is more complicated since a distinction of cases is necessary. We emphasise that for this rigorous affine lower bound function it is not necessary to verify the feasibility or optimality of the approximate solution $\widehat{s}$ of the linear programming problem (12) and (13). We have only to add the constant δ, then c is a rigorous lower bound function.

For the convex lower bound function (20), a rigorous lower bound for the function value requires the computation of a rigorous lower bound of the optimal value for the corresponding linear programming problem. Therefore, in contrast to the previous affine lower bound function, optimality has to be verified. Verification algorithms for linear programming problems are described in [16] and [18], for example.

6 Convex envelopes

Convex envelopes are of primary importance in many applications since they represent the uniformly best convex underestimating function, e.g., [2, 14]. Now the question arises under which conditions the lower bound functions introduced in Section 3 provide the lower convex envelope of a polynomial p. Of special interest is the case in which p is concave.

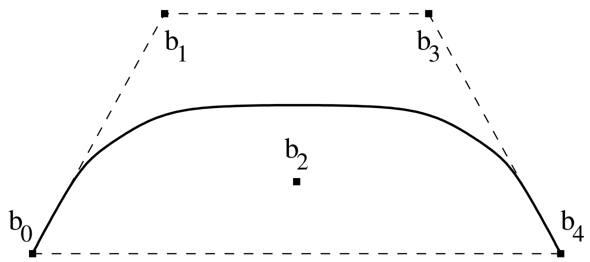

Figure 6.1 *The lower bound function coincides with the lower convex envelope.*

Question: *Let a univariate polynomial p be given which is concave over $[0, 1]$. Does the lower bound function c defined by (14) or (19) coincide with the lower convex envelope of p?*

Note that this is equivalent to stating that all control points of p occur on or above the lower convex envelope, cf. Figure 6.1. The constant and linear terms in the polynomial have no effect upon determining the placement of the control points relative to the lower convex envelope (since any adjustment of these terms affects the lower convex envelope and the control points identically), which permits us to consider the case

$$p(0) = p(1) = 0 \tag{33}$$

without loss of generality. In this case the question simplifies to the statement that all Bernstein coefficients are nonnegative.

The answer to this question is positive for $l \leq 4$. We give here the **proof for $\mathbf{l = 4}$:** Let p be represented as in (3) with Bernstein coefficients $b_i, i = 0, \ldots, 4$. Since by (6) we have $b_0 = a_0 = p(0)$ and $b_4 = \sum_{i=0}^4 a_i = p(1)$, it follows from (33) that $b_0 = b_4 = 0$. It is well-known, e.g. Chapter 4 of the monograph of Farin [7], that the Bernstein coefficients b'_i of the derivative of p are given by

$$b'_i = l(b_{i+1} - b_i), \ i = 0, 1, 2, 3. \tag{34}$$

Due to concavity it follows that $b_1 = \frac{1}{4}p'(0) \geq 0$ and $b_3 = -\frac{1}{4}p'(1) \geq 0$. We assume that $b_2 < 0$. Then by (34) we must have

$$\begin{array}{lll} b'_0 \geq 0, \ b'_1 < 0, & \text{with} & |b'_1| > |b'_0|, \\ b'_2 > 0, \ b'_3 \leq 0, & \text{with} & |b'_2| > |b'_3|. \end{array}$$

This implies $b'_2 - b'_1 > b'_0 - b'_3 = (b'_0 - b'_1) + (b'_1 - b'_2) + (b'_2 - b'_3)$, hence $2(b'_2 - b'_1) > -(b'_1 - b'_0) - (b'_3 - b'_2)$. If we denote the Bernstein coefficients of p'' by $b''_i, i = 0, 1, 2$, we can conclude that

$$2b''_1 > -b''_0 - b''_2$$

whence

$$\begin{aligned} & 4a_2 + 6a_3 > -4a_2 - 6a_3 - 12a_4, \quad \text{i.e.} \\ & 4(2a_2 + 3a_3 + 3a_4) = 4p''(\frac{1}{2}) > 0 \end{aligned}$$

which is impossible by the concavity of p. ∎

However, for general l the question has to be answered in the negative. The following counterexample was provided to us by Professor Dr. S. Rump. The polynomial of degree 7

$$p(x) = 11x - 72x^2 + 280x^3 - 602x^4 + 707x^5 - 424x^6 + 100x^7$$

is concave on I and satisfies conditions (33) but possesses a negative Bernstein coefficient.

7 Examples

In order to illustrate the previous theory, we consider the affine lower bound function (14) together with the error bound in Theorem 4.1 for some example polynomials. The following results were obtained from an implementation in `C++` , utilising the linear programming solver `LP_SOLVE` [4]. For the multivariate examples given, the computation time was less than 0.1s, on a PC equipped with a 450MHz processor.

Example 1: For degrees $l = 3, 8, 13, 17$ we have plotted in Figure 7.1 the univariate polynomials

$$p(x) = \sum_{i=0}^{l} \frac{(-1)^{i+1}}{i+1} x^i, \quad x \in [0,1],$$

together with their control points, and the corresponding affine lower bound functions. For each degree l we see that the affine lower bound function is rather close to the corresponding polynomial. In the two cases where p is a concave polynomial, the affine lower bound function is the convex envelope; that is the uniformly best convex underestimating function. Table 7.1 shows the error bound (22) for each degree l.

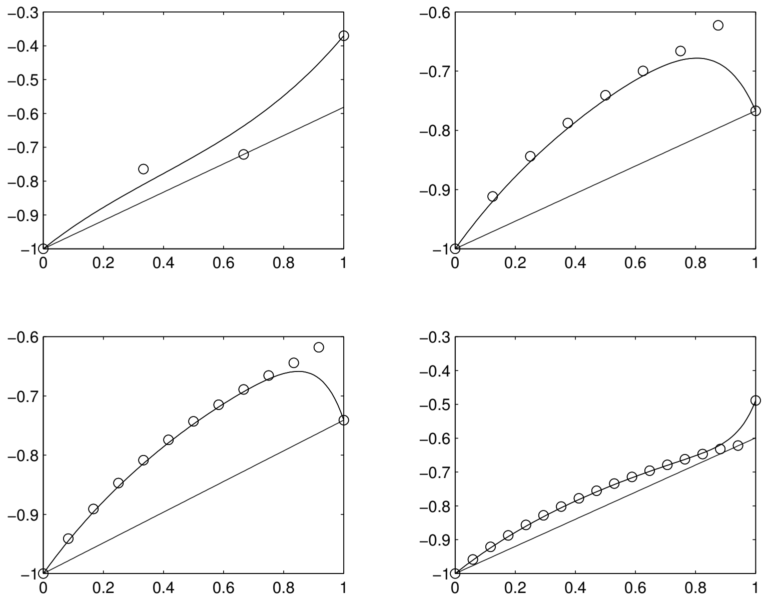

Figure 7.1 *Control points and lower bound functions for Example 1.*

l	3	8	12	17
error (22)	0.2113	0.1735	0.1446	0.1103

Table 7.1 *Error bounds for the polynomials of Example 1.*

Figure 7.1 and the error bounds in Table 7.1 demonstrate that for these examples the functions (14) are very close approximations of the lower convex envelopes.

Example 2: We consider three univariate polynomials from the literature. The first two polynomials

$$p_1(x) = \frac{1}{6}x^6 - \frac{52}{25}x^5 + \frac{39}{80}x^4 + \frac{71}{10}x^3 - \frac{79}{20}x^2 - x + \frac{1}{10}, \quad x \in [-1.5, 11]$$

and

$$p_2(x) = (x-1)^{10}, \quad x \in [0, 2]$$

can be found in [6]. They are also considered in [24]. In Figures 7.2 and 7.3 a plot of these polynomials together with their control points and their affine lower bound functions is shown. In each case the domain is transformed to the unit interval I. The third univariate polynomial is considered in [26]

$$p_3(x) = (x - 10^{-3})(x + 0.5 \times 10^{-3})(x - 0.25 \times 10^{-3}), \quad x \in [-1, 1]$$

and has three zeros clustered at $10^{-3}, -0.5 \times 10^{-3}, 0.25 \times 10^{-3}$. It is displayed in Figure 7.4.

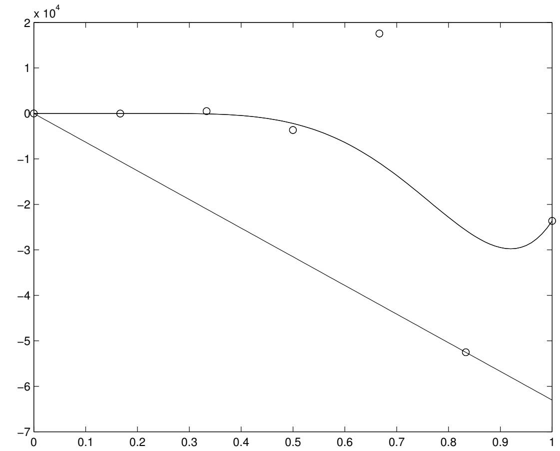

Figure 7.2 *Control points and lower bound function for p_1.*

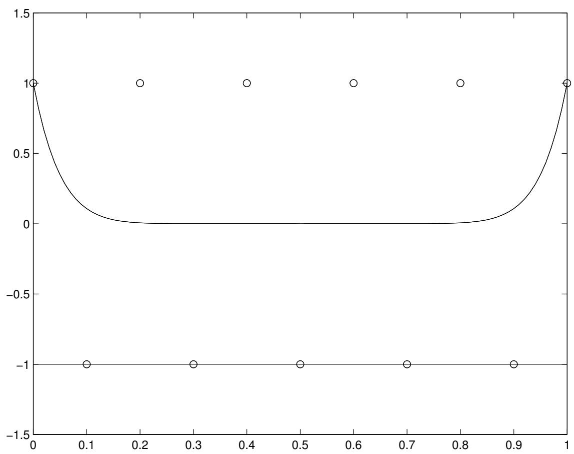

Figure 7.3 *Control points and lower bound function for p_2.*

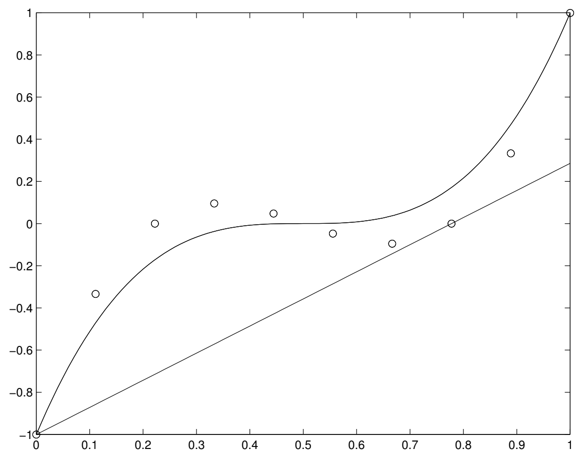

Figure 7.4 *Control points and lower bound function for* p_3*.*

The error bounds (22) for the polynomials p_1, p_2, and p_3 are 5.9582×10^4, 2.0, and 0.7147, respectively.

Example 3: We display in Figure 7.5 for the famous Wilkinson polynomial

$$p(x) = \prod_{i=1}^{20}(x - i), \quad x \in [1, 3]$$

the control points and the affine lower bound function.

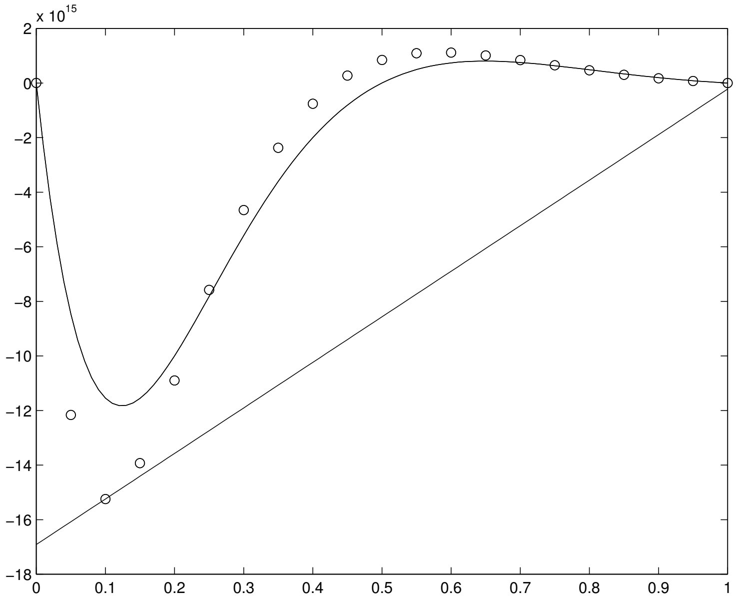

Figure 7.5 *Control points and lower bound functions for the Wilkinson polynomial.*

The error bound (22) is 1.6912×10^{16}.

Example 4: In [20] a problem from combustion chemistry, the hydrogen combustion with excess fuel, is presented. The model is described by cubic equations with the polynomials

$$\begin{aligned} p_1(x_1,x_2) &= \alpha_1 x_1^2 x_2 + \alpha_2 x_1^2 + \alpha_3 x_1 x_2 + \alpha_4 x_1 + \alpha_5 x_2, \\ p_2(x_1,x_2) &= \alpha_6 x_1^2 x_2 + \alpha_7 x_1 x_2^2 + \alpha_8 x_1 x_2 + \alpha_9 x_2^3 + \alpha_{10} x_2^2 + \alpha_{11} x_2 + \alpha_{12}, \end{aligned}$$

where

$$\begin{array}{ll} \alpha_1 = -1.697 \times 10^7 & \alpha_7 = 4.126 \times 10^7 \\ \alpha_2 = 2.177 \times 10^7 & \alpha_8 = -8.285 \times 10^6 \\ \alpha_3 = 0.5500 & \alpha_9 = 2.284 \times 10^7 \\ \alpha_4 = 0.4500 \times 10^7 & \alpha_{10} = 1.918 \times 10^7 \\ \alpha_5 = -1.0000 \times 10^7 & \alpha_{11} = 48.40 \\ \alpha_6 = 1.585 \times 10^{14} & \alpha_{12} = -27.73 \end{array}$$

Both polynomials are displayed in Figure 7.6.

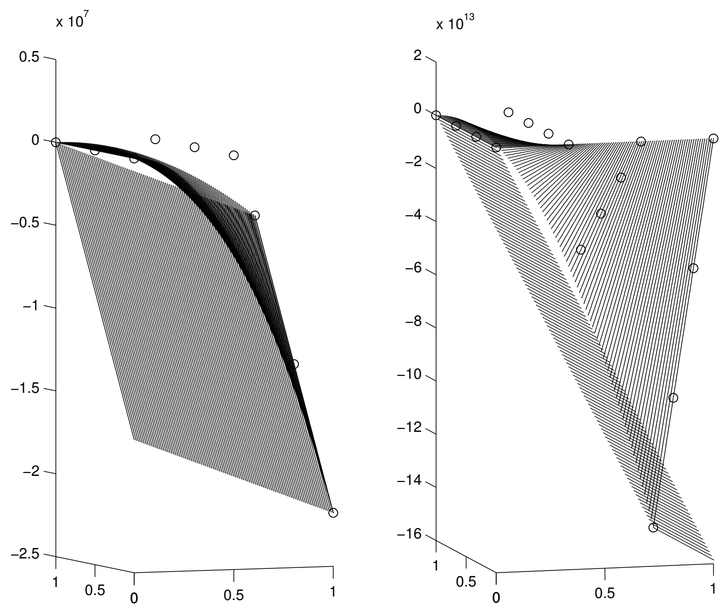

Figure 7.6 *Control points and lower bound functions for p_1 and p_2.*

The error bounds (22) for p_1 and p_2 are 1.937×10^7 and 1.585×10^4, respectively.

Example 5: The following two three-variate polynomials are taken from [15]:

$$\begin{aligned} p_1(x_1,x_2,x_3) &= 5x_1^9 - 6x_1^5 x_2^2 + x_1 x_2^4 + 2x_1 x_3, \quad x_i \in [0,1] \\ p_2(x_1,x_2,x_3) &= -2x_1^6 x_2 + 2x_1^2 x_2^3 + 2x_2 x_3, \quad x_i \in [0,1] \end{aligned}$$

The corresponding lower bound functions are

$$\begin{aligned} c_1(x_1,x_2,x_3) &= -0.125x_1 - 1.625x_2 - 0.04167 \\ c_2(x_1,x_2,x_3) &= -0.125x_1 - 1.75x_2 - 0.04167 \end{aligned}$$

with error bounds (22) 7.573 and 5.229, respectively.

Example 6: The following five-variate polynomial is taken from [10]:

$$p(x_1, x_2, x_3, x_4, x_5) = -0.0022053x_3x_5 + 0.0056858x_2x_5 + 0.0006262x_1x_4 - 6.665593,$$
$$x_1 \in [78, 102],\ x_2 \in [33, 45],\ x_3 \in [27, 45],\ x_4 \in [27, 45],\ x_5 \in [27, 45]$$

The corresponding lower bound function is

$$c(x_1, x_2, x_3, x_4, x_5) = 0.0169074x_1 + 0.153517x_2 - 0.0595431x_3 + 0.0488436x_4 + 0.0883929x_5 - 10.371$$

with error bound (22) 2.21317.

Conclusions

In this paper we have presented affine and convex lower bound functions which are based on Bernstein expansion. Moreover, an error bound is given, and its specialisation to the univariate case is treated. Some numerical examples illustrate the properties of the affine lower bound functions. For these examples the error bound describes rather accurately the real maximal error between the original function and the lower bound function. Moreover, this error is of the same order of magnitude as the maximal error between the original function and its convex envelope. In our future work we intend to incorporate these bound functions into algorithms for solving nonlinear polynomial systems and global optimisation problems with polynomial constraints.

Acknowledgement

The authors gratefully acknowledge support from the Ministry of Education and Research of the Federal Republic of Germany under contract no. 1707001. They also thank Professor Dr. Siegfried Rump for his counterexample presented in Section 6.

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