

Bounding the Range of a Sum of Multivariate Rational Functions

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Abstract Bounding the range of a sum of rational functions is an important task if, e.g., the global polynomial sum of ratios problem is solved by a branch and bound algorithm. In this paper, bounding methods are discussed which rely on the expansion of a multivariate polynomial into Bernstein polynomials.

Key words: Multivariate rational function, Range enclosure, Bernstein polynomial

1 Introduction

In this paper, we consider the expansion of a multivariate polynomial into Bernstein polynomials over a box, i.e., an axis-aligned region, in $\mathbb{R}^n$. This expansion has many applications, e.g., in computer aided geometric design, robust control, global optimization, differential and integral equations, and finite element analysis [8], [13]. A very useful property of this expansion is that the interval spanned by the minimum and maximum of the coefficients of this expansion, the so-called *Bernstein coefficients*, provides bounds for the range of the given polynomial over the considered

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box, see, e.g., [11]. A simple (but by no means economic) method for the computation of the Bernstein coefficients from the coefficients of the given polynomial is the use of formula (2) below. This formula (and also similar ones for the Bernstein coefficients over more general sets like simplices and polytopes) allows the symbolic computation of these quantities when the coefficients of the given polynomial depend on parameters. Some applications are making use of this symbolic computation: In [6, Sections 3.2 and 3.3] and the many references therein, the reachability computation and parameter synthesis with applications in biological modelling are considered. In [4, 5], parametric polynomial inequalities over parametric boxes and polytopes are treated. Applications in static program analysis and optimization include dependence testing between references with linearized subscripts, dead code elimination of conditional statements, and estimation of memory requirements in the development of embedded systems. Applications which involve polynomials of higher degree or many variables require a computation of the Bernstein coefficients which is more economic than by formula (2). In [21], the second and third authors have presented a matrix method for the computation of the Bernstein coefficients which is faster than the methods developed so far and which is included in version 12 of the MATLAB toolbox INTLAB [17].

In this paper, we aim at finding bounds for the range of a sum of rational functions over a box. This problem appears when the global polynomial sum of ratios problem is solved by a branch and bound method, see, e.g., [7], [10]. The sum of ratios problem is one of the most difficult fractional programming problems encountered so far¹.

After having introduced the Bernstein expansion in Section 2, we will extend in Section 3 the bounds for the range of a single rational function to a sum of rational functions. In the sequel we employ the following notation. Let $n \in \mathbb{N}$ (set of the non-negative integers) be the number of variables. A multi-index $(i_1, \dots, i_n) \in \mathbb{N}^n$ is abbreviated by i . In particular, we write 0 for $(0, \dots, 0)$. Arithmetic operations with multi-indices are defined entry-wise; the same applies to comparison between multi-indices. For $x = (x_1, \dots, x_n) \in \mathbb{R}^n$, its *monomials* are defined as $x^i := \prod_{s=1}^n x_s^{i_s}$. For $d = (d_1, \dots, d_n) \in \mathbb{N}^n$ such that $i \leq d$, we use the compact notations $\sum_{i=0}^d := \sum_{i_1=0}^{d_1} \cdots \sum_{i_n=0}^{d_n}$ and $\binom{d}{i} := \prod_{s=1}^n \binom{d_s}{i_s}$.

2 Bernstein Expansion

In this section, we present fundamental properties of the Bernstein expansion over a box, e.g., [8, Subsection 5.1], [11], [16], that are employed throughout the paper.

¹ The problem of optimizing one or several ratios of functions is called a *fractional program*. The ninth bibliography of fractional programming [18] covering mainly the period 2016-2018 lists 520 papers on fractional programming and its applications.

For simplicity we consider the unit box $\mathbf{u} := [0, 1]^n$, since any compact nonempty box $\mathbf{x}$ of $\mathbb{R}^n$ can be mapped affinely onto $\mathbf{u}$. Let $\ell \in \mathbb{N}^n$, $a_j \in \mathbb{R}$, with $j = 0, \dots, \ell$, such that for $s = 1, \dots, n$,

$$\ell_s := \max \{q \mid a_{j_1, \dots, j_{s-1}, q, j_{s+1}, \dots, j_n} \neq 0\}.$$

Let p be an ℓ -th degree n -variate polynomial with the power representation

$$p(x) = \sum_{j=0}^{\ell} a_j x^j. \quad (1)$$

We expand p into Bernstein polynomials of degree d , $d \geq \ell$, over $\mathbf{u}$ as

$$p(x) = \sum_{j=0}^d b_j^{(d)}(p) B_j^{(d)}(x),$$

where $B_j^{(d)}$ is the j -th Bernstein polynomial of degree d , defined as

$$B_j^{(d)}(x) := \binom{d}{j} x^j (1-x)^{d-j},$$

and $b_j^{(d)}(p)$ is the j -th Bernstein coefficient of p of degree d over $\mathbf{u}$ which is given by

$$b_j^{(d)}(p) = \sum_{i=0}^j \frac{\binom{j}{i}}{\binom{d}{i}} a_i, \quad 0 \leq j \leq d, \quad (2)$$

with the convention that $a_i := 0$ if $i \geq \ell$, $i \neq \ell$.

Note that by (2) the Bernstein coefficients are linear: Let p_1 and p_2 be polynomials with the power representations (1) with $\ell = \ell^{(1)}$ and $\ell = \ell^{(2)}$, respectively, and let $\ell := \max \{\ell^{(1)}, \ell^{(2)}\}$. If $p = \alpha p_1 + \beta p_2$, $\alpha, \beta \in \mathbb{R}$, then

$$b_j^{(d)}(p) = \alpha b_j^{(d)}(p_1) + \beta b_j^{(d)}(p_2), \quad i = 0, \dots, d. \quad (3)$$

3 Bounds for the Range of a Sum of Rational Functions

Let p and q be two n -variate real polynomials with the Bernstein coefficients over the unit box $\mathbf{u}$ given by $b_i^{(d)}(p)$ and $b_i^{(d)}(q)$, $0 \leq i \leq d$, respectively. We assume that the two polynomials have the same degree l since otherwise we can elevate the degree of the Bernstein expansion of either polynomial by component where necessary to ensure that their Bernstein coefficients are of the same order $d \geq l$. We consider the multivariate rational function $f := \frac{p}{q}$ over $\mathbf{u}$. In the sequel we assume

that all $b_i^{(d)}(q)$, $i = 0, \dots, d$, have the same strict sign (and without loss of generality we may assume that all of them are positive). We use the notation for the *rational* Bernstein coefficients of f

$$b_i^{(d)}(f) := \frac{b_i^{(d)}(p)}{b_i^{(d)}(q)}, \quad i = 0, \dots, d. \quad (4)$$

Then an enclosure for the range of f over $\mathbf{u}$ is given by the following theorem which includes also the polynomial case ($q = 1$).

Theorem 1 [15, Theorem 3.1], [12, Proposition 3] *The range of f over $\mathbf{u}$ can be bounded by*

$$\min_{i=0,\dots,d} b_i^{(d)}(f) \leq f(x) \leq \max_{i=0,\dots,d} b_i^{(d)}(f), \quad x \in \mathbf{u}. \quad (5)$$

(Vertex Condition) *Equality holds in the left or right inequality if and only if the minimum or the maximum of the Bernstein coefficients is attained at a vertex index i with $i_s \in \{0, d_s\}$, $s = 1, \dots, n$.*

Now we extend the bounds for the range over a box of a single rational function to a sum of such functions. Without loss of generality, we consider here only the case that we have solely two rational functions,

$$f = f_1 + f_2, \text{ where } f_1 = \frac{p_1}{q_1}, \quad f_2 = \frac{p_2}{q_2}. \quad (6)$$

We assume that both the numerator and denominator polynomials have the common degree ℓ and that all the Bernstein coefficients of each denominator polynomial have the same strict sign (but may be different for q_1 and q_2). By the additivity of the Bernstein coefficients (3) and the enclosure (5), one may conjecture that

$$\min_{i=0,\dots,d} (b_i^{(d)}(f_1) + b_i^{(d)}(f_2)) \leq f(x) \leq \max_{i=0,\dots,d} (b_i^{(d)}(f_1) + b_i^{(d)}(f_2)), \quad x \in \mathbf{u}. \quad (7)$$

However, this conjecture is not true even in the case of ratios of linear functions as the following example shows.

Example 1. Let $f_1(x) = \frac{2x+1}{x+1}$ and $f_2(x) = \frac{0.2x+1}{5x+1}$. Then $f = f_1 + f_2$ attains its global minimum ≈ 1.645445 on $[0, 1]$ at ≈ 0.4239 . The rational Bernstein coefficients of f_1 and f_2 are $b_0^{(1)}(f_1) = 1$, $b_1^{(1)}(f_1) = 1.5$, $b_0^{(1)}(f_2) = 1$, $b_1^{(1)}(f_2) = 0.2$, such that the lower bound in (7) is 1.7 which is greater than the global minimum of f .

We will return to (7) in Example 3.

3.1 The Naïve Bounds

To motivate the enclosure (11) below, we consider first the univariate case ($n = 1$). We start with recalling a formula for the Bernstein coefficients of the product pr of two polynomials p and r of degrees $\ell(p)$ and $\ell(r)$ in terms of their Bernstein coefficients, see [9, formula (44)]. In the sequel, we suppress in the presentation of the Bernstein coefficients the reference to their degrees. Since for the degree ℓ of the polynomial $p \cdot r$, $\ell = \ell(p) + \ell(r)$ holds, we obtain for $k = 0, 1, \dots, \ell$

$$\begin{aligned} b_k(pr) &= \sum_{\mu=\max\{0, k-\ell(r)\}}^{\min\{\ell(p), k\}} \frac{\binom{\ell(p)}{\mu} \binom{\ell(r)}{k-\mu}}{\binom{\ell}{k}} b_\mu(p) b_{k-\mu}(r) \\ &\leq \max_{\mu} b_\mu(p) b_{k-\mu}(r) \frac{1}{\binom{\ell}{k}} \sum_{\mu=\max\{0, k-\ell(r)\}}^{\min\{\ell(p), k\}} \binom{\ell(p)}{\mu} \binom{\ell(r)}{k-\mu}. \end{aligned} \quad (8)$$

By the Vandermonde convolution, the last sum in (8) equals $\binom{\ell}{k}$ such that we can conclude

$$b_k(pr) \leq \max_{\mu} b_\mu(p) b_{k-\mu}(r).$$

An analogous lower bound is provided by replacing the maximum by the minimum.

Returning to the two-term case in (6), we assume for simplicity that both the numerator and denominator polynomials have the common degree ℓ and that the Bernstein coefficients of q_1 and q_2 have the same strict sign. Put

$$M := \max_{i,j=0,\dots,\ell} (b_i(f_1) + b_j(f_2))$$

and

$$s := p_1 q_2 + q_1 p_2 - M q_1 q_2. \quad (9)$$

Then by (3), we obtain for $k = 0, 1, \dots, 2\ell$

$$b_k(s) := b_k(p_1 q_2) + b_k(q_1 p_2) - M b_k(q_1 q_2),$$

and by (8) with coefficients α_μ satisfying $\sum_{\mu} \alpha_\mu = 1$

$$\begin{aligned} b_k(s) &= \sum_{\mu=\max\{0, k-\ell\}}^{\min\{\ell, k\}} \alpha_\mu (b_\mu(p_1) b_{k-\mu}(q_2) + b_\mu(q_1) b_{k-\mu}(p_2) - M b_\mu(q_1) b_{k-\mu}(q_2)) \\ &= \sum_{\mu=\max\{0, k-\ell\}}^{\min\{\ell, k\}} \alpha_\mu b_\mu(q_1) b_{k-\mu}(q_2) \left(\frac{b_\mu(p_1)}{b_\mu(q_1)} + \frac{b_{k-\mu}(p_2)}{b_{k-\mu}(q_2)} - M \right) \\ &\leq 0, \end{aligned} \quad (10)$$

by the definition of M . Since by Theorem 1 $s(x) \leq \max_{k=0,\dots,2\ell} b_k(s)$, $x \in \mathbf{u}$, we conclude that $s(x) \leq 0$ and therefore,

$$f_1(x) + f_2(x) \leq M, \quad x \in \mathbf{u}.$$

Similarly we obtain a lower bound for $f_1 + f_2$ on $\mathbf{u}$ if we replace the maximum by the minimum. The resulting enclosure for the range of $f = f_1 + f_2$ on $\mathbf{u}$

$$\min_{i,j=0,\dots,d} (b_i^{(d)}(f_1) + b_j^{(d)}(f_2)) \leq f(x) \leq \max_{i,j=0,\dots,d} (b_i^{(d)}(f_1) + b_j^{(d)}(f_2)), \quad x \in \mathbf{u}, \quad (11)$$

is simply the enclosure which we obtain if we form the (Minkowski) sum of the enclosure (5) for f_1 and f_2 . Therefore, this enclosure is obviously true also in the n -variate case which we will consider now again.

We put $\bar{f} := \max_{x \in \mathbf{u}} f(x)$ and for $d \geq \ell$,

$$\begin{aligned} \underline{m}^{(d)} &:= \min_{i,j=0,\dots,\ell} (b_i^{(d)}(f_1) + b_j^{(d)}(f_2)), \\ \overline{m}^{(d)} &:= \max_{i,j=0,\dots,\ell} (b_i^{(d)}(f_1) + b_j^{(d)}(f_2)). \end{aligned}$$

In the sequel, we present our results mainly only for the upper bounds. Analogous results hold for the lower bounds.

Theorem 2 *The following vertex condition holds*

$$\bar{f} = \overline{m}^{(d)} \quad \text{if and only if} \quad \overline{m}^{(d)} = b_{i^*}^{(d)}(f_1) + b_{i^*}^{(d)}(f_2) \quad \text{for a vertex index } i^*.$$

Proof Assume that $\overline{m}^{(d)}$ is attained at a vertex index i^* . Then the statement is clear because the sum of the related Bernstein coefficients is a function value of f , see [15, Remark 1]. Conversely, assume that $\bar{f} = \overline{m}^{(d)}$, and let $\hat{x} = f(\hat{x})$ for some $\hat{x} \in \mathbf{u}$. Define the polynomial s as in (9) with $M = \overline{m}^{(d)}$. Then we can conclude that

$$\frac{s(\hat{x})}{q_1(\hat{x})q_2(\hat{x})} = f(\hat{x}) - \overline{m}^{(d)} = 0,$$

hence $s(\hat{x}) = 0$. Since s is nonpositive on $\mathbf{u}$, it attains its maximum at $\hat{x}$.

On the other hand, in the multivariate case a straightforward extension of formula (8) for the product of two polynomials in the Bernstein representation exists, see [2, Section 3.3], by which we can conclude as in (10) that $b_i(s) \leq 0$, for $i = 0, \dots, 2d$. Since $s(x) \leq \max_{i=0,\dots,2d} b_i(s)$, it follows that there exists an index i^* with $b_{i^*}(s) = 0$, whence

$$\max_{x \in \mathbf{u}} s(x) = b_{i^*}(s).$$

By the polynomial vertex condition in Theorem 1, we can conclude that the index i^* is a vertex index. $\square$

In [12], some properties of the bounds in the case of a single rational function are presented. From Proposition 4 and Theorem 8 therein it immediately follows that also in the multi-term case the bounds are monotone, i.e., for $l \leq d \leq k$ it holds that $\underline{m}^{(d)} \leq \underline{m}^{(k)}$ and $\overline{m}^{(k)} \leq \overline{m}^{(d)}$, and that the so-called inclusion isotonicity of the interval function provided by the enclosure $[\underline{m}^{(d)}(f, \mathbf{x}), \overline{m}^{(d)}(f, \mathbf{x})]$ is valid. However, compared to the single-term case, we are losing one order of convergence of the bounds to the range. So, degree elevation may not result in linear convergence. This is shown by the following example.

Example 2. We choose $n = 1$, $f_1(x) = \frac{x}{2-x}$, $f_2(x) = \frac{2-2x}{2-x}$. Then $f(x) = 1$, $x \in \mathbf{u}$. The two Bernstein coefficients for $d = 1$ of f_1 as well as of f_2 are 0 and 1. So $\overline{m}^{(1)} = 2$ which cannot be improved by degree elevation because both coefficients are function values.

To enforce convergence of the bounds to the range we apply subdivision. The convergence result (Theorem 4) will immediately follow from the linear convergence of the bounds with respect to the width of the box.

Theorem 3 *Let $\mathbf{x} = [\underline{x}, \overline{x}]$ be any subbox of $\mathbf{u}$. Then*

$$\max_{i,j=0,\dots,d} (b_i^{(d)}(f_1, \mathbf{x}) + b_j^{(d)}(f_2, \mathbf{x})) - \max_{x \in \mathbf{x}} f(x) \leq \delta \|\overline{x} - \underline{x}\|_\infty,$$

where δ is a constant not depending on $\mathbf{x}$.

Proof Let $\max_{x \in \mathbf{x}} f(x) = f(x')$, with $x' \in \mathbf{x}$, and define $\overline{f}_m := \max_{x \in \mathbf{x}} f_m(x)$, $m = 1, 2$. Then $f(x')$ can be written as

$$f(x') = \overline{f}_1 + \overline{f}_2 + f_1(x') - \overline{f}_1 + f_2(x') - \overline{f}_2.$$

We apply the results on quadratic convergence in the single-term case [12, Theorem 6] and a standard argument involving the Mean Value Theorem, e.g., [14, Theorem 4.1.18] to f_1 and f_2 to obtain

$$\max_{i=0,\dots,d} b_i^{(d)}(f_1, \mathbf{x}) + \max_{j=0,\dots,d} b_j^{(d)}(f_2, \mathbf{x}) - f(x') \leq \delta_1 \|\overline{x} - \underline{x}\|_\infty^2 + \delta_2 \|\overline{x} - \underline{x}\|_\infty,$$

where δ_1 and δ_2 are constants not depending on $\mathbf{x}$. Since $\|\overline{x} - \underline{x}\|_\infty \leq 1$ the proof is complete. $\square$

To simplify the presentation, we will reserve in the sequel the upper index of the Bernstein coefficients for the subdivision level. Repeated bisection of $\mathbf{u}^{(0,1)} := \mathbf{u}$ in all n coordinate directions results at subdivision level $1 \leq h$ in subboxes $\mathbf{u}^{(h,\nu)}$ of edge length 2^{-h} , $\nu = 1, \dots, 2^{nh}$. Denote the Bernstein coefficients of f over $\mathbf{u}^{(h,\nu)}$ by $b_i^{(h,\nu)}(f)$. For their computation see [21].

Theorem 4 *(Linear convergence with respect to subdivision) For $1 \leq h$ it holds*

$$\max_{i,j=0,\dots,l; \nu=1,\dots,2^{nh}} (b_i^{(h,\nu)}(f_1) + b_j^{(h,\nu)}(f_2)) - \overline{f} \leq \delta 2^{-h},$$

where δ is a constant not depending on h .

With increasing subdivision level, the chances are becoming better and better that the vertex condition holds on subboxes.

In the subdivision process, it may be advantageous to check the vertex condition of Theorem 1 term-wise because then we will be able to detect terms for which we have already found the true minimum or maximum of the respective rational functions such that a further division of the boxes under consideration is not necessary for these terms. If the vertex condition is satisfied for the lower or the upper bounds for all terms and the individual vertex indices coincide for at least one index, then the vertex condition in Theorem 2 is fulfilled, and we already have found the true minimum or maximum of the sum of ratios.

The convergence can possibly be speeded up by employing term-wise the monotonicity and dominance tests presented in [19, Section 6.1].

Example 3. In [1, Example 3], see also [10, (5.14)], the function f

$$\begin{aligned} f := & \frac{-x_1^2 + 16x_1 - x_2^2 + 16x_2 - x_3^2 + 16x_3 - x_4^2 + 16x_4 - 214}{2x_1 - x_2 - x_3 + x_4 + 2} \\ & + \frac{-x_1^2 + 16x_1 - 2x_2^2 + 20x_2 - 3x_3^2 + 60x_3 - 4x_4^2 + 56x_4 - 586}{-x_1 + x_2 + x_3 - x_4 + 10} \\ & + \frac{-x_1^2 + 20x_1 - x_2^2 + 20x_2 - x_3^2 + 20x_3 - x_4^2 + 20x_4 - 324}{x_1^2 - 4x_4}, \end{aligned}$$

where

$$x_1 \in [6, 10], \quad x_2 \in [4, 6], \quad x_3 \in [8, 12], \quad x_4 \in [6, 8],$$

is to maximize. We have chosen the precision $\epsilon = 10^{-5}$ and have used an HP OMEN laptop with Intel®Core™ i7-10750H with CPU 2.20-5.0 GHz and 16 GB RAM. The method presented in Section 3 results in 0.043 ms at subdivision level $h = 7$ in the upper bound 16.16667 for f attained at $(6, 6, 10.05502, 8)$. The upper bound is very close to the bounds presented in [1] (computed with precision 10^{-2}) and [10] (computed with precision 10^{-4} , according to a private communication). Interestingly, the conjectured bound (7) provides nearly the same bound attained at the same place but for $h = 94$. The much higher subdivision level is not surprising because we cannot employ a vertex condition which is very useful to speed up the subdivision process.

We noticed a similar situation for the minimum. Our algorithm finds in 0.015 ms in only one subdivision step ($h = 1$) the lower bound 0.976190 attained at $(6, 4, 12, 6)$ for the minimum of f . Since this bound is attained at a vertex index, the vertex condition in Theorem 2 holds, and we know that we already have found the minimum of f . The same lower bound is provided by (7) at the same place but for $h = 72$ which confirms our experience that (7) is true in many cases.

3.2 Improved Bounds

In the single-term case, the bounds converge quadratically if subdivision is applied [12, Theorem 7]. Therefore, it appears advantageous to reduce the multi-term case to the single-term case by extending all ratios to the same denominator to obtain a single rational function which is to optimize. In Example 2, this gives the exact range $\{1\}$ of f . But such a procedure is not appropriate for a larger number of terms because the degrees of the resulting numerator and denominator polynomials become potentially large. However, we may partition the totality of the terms into groups of two or three terms and apply the procedure to each group. Finally, we form the (Minkowski) sum of all resulting enclosures. This procedure requires to compute the Bernstein coefficients of a product of two polynomials given the Bernstein coefficients of both polynomials. For this task it is beneficial to use one of the methods which are presented in [22, Section 4].

In passing, we note that most of the results presented in this paper easily extend to the Bernstein expansion over simplices [15, Remark 6], [19], [20], [23] which allow more general regions over which a sum of ratios is to optimize.

4 Future Work

To fight the increase of the degrees inherent in the method described in Section 3.2, one can use the least common multiple of the denominators. To compute this, one employs the greatest common divisor of the polynomials. A method which appears suitable for this task is the method for the division of two polynomials in Bernstein form presented in [3]. However, the focus herein is on the univariate case. Division algorithms for the multivariate case and analogues in the multivariate Bernstein setting of Gröbner bases are also discussed but have to be adapted to our problem. An important point here is that the methods allow all the computations to be performed using only Bernstein coefficients such that no conversion to the monomial coefficients is required.

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