

On a conjecture concerning interpolation by bivariate Bernstein polynomials

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Abstract

In this paper we discuss a conjecture of Schumaker that the principal submatrices of collocation matrices of bivariate Bernstein polynomials over triangular grids have positive determinant. It is easy to show that the conjecture holds for the 2×2 submatrices. In this paper we show that it also holds for the 3×3 submatrices, working with the equivalent ‘monomial form’ of the conjecture. This result generalizes to a class of 3×3 matrices which will be described.

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1 Introduction

In 2003, Schumaker made a conjecture, stated in [1], concerning the non-singularity of matrices arising from interpolation by bivariate Bernstein polynomials, which is as follows. To each integer $d \geq 1$ we associate the set of multi-indices

$$\mathcal{I}_d = \{\mathbf{i} = (i_1, i_2, i_3) : i_1, i_2, i_3 \geq 0, |\mathbf{i}| := i_1 + i_2 + i_3 = d\},$$

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whose cardinality is $\binom{d+2}{2}$. Given a triangle T with vertices v_1, v_2, v_3 in $\mathbb{R}^2$ we define the Bernstein basis polynomials of degree d as

$$B_{\mathbf{i}}^d(x) = \frac{d!}{i_1!i_2!i_3!} \lambda_1^{i_1} \lambda_2^{i_2} \lambda_3^{i_3}, \quad \mathbf{i} \in \mathcal{I}_d,$$

where $\lambda_1, \lambda_2, \lambda_3$ are the barycentric coordinates of x with respect to T ,

$$\lambda_1 + \lambda_2 + \lambda_3 = 1, \quad \lambda_1 v_1 + \lambda_2 v_2 + \lambda_3 v_3 = x.$$

To each multi-index $\mathbf{i} \in \mathcal{I}_d$ we can also associate the so-called domain point

$$\xi_{\mathbf{i}} = \frac{i_1}{d} v_1 + \frac{i_2}{d} v_2 + \frac{i_3}{d} v_3$$

in T . It is well known that interpolation from the linear space π_d of bivariate polynomials of degree $\leq d$ at these $\binom{d+2}{2}$ domain points is well-posed. Since the Bernstein basis polynomials of degree d are a basis for π_d it follows that the collocation matrix

$$M = [B_{\mathbf{j}}^d(\xi_{\mathbf{i}})]_{\mathbf{i}, \mathbf{j} \in \mathcal{I}_d}$$

is non-singular. Thus, given data $f_{\mathbf{i}} \in \mathbb{R}$, $\mathbf{i} \in \mathcal{I}_d$, at the domain points $\xi_{\mathbf{i}}$, there is a unique Bernstein polynomial

$$p(x) = \sum_{\mathbf{j} \in \mathcal{I}_d} c_{\mathbf{j}} B_{\mathbf{j}}^d(x),$$

that interpolates them, i.e., such that

$$p(\xi_{\mathbf{i}}) = f_{\mathbf{i}}, \quad \mathbf{i} \in \mathcal{I}_d.$$

However, one might consider the situation that some of the coefficients $c_{\mathbf{j}}$ are known and that we might try to find the remaining ones by just interpolating at the corresponding reduced set of domain points. This leads to the conjecture:

Conjecture 1 (Schumaker) *Let Γ be a subset of $\mathcal{I}_d$. Then the matrix*

$$M_{\Gamma} = [B_{\mathbf{j}}^d(\xi_{\mathbf{i}})]_{\mathbf{i}, \mathbf{j} \in \Gamma}$$

is non-singular, and moreover, $\det(M_{\Gamma}) > 0$.

We assume that the ordering of the multi-indices $\mathbf{i}$ in Γ is the same as for the $\mathbf{j}$, in which case $\det(M_\Gamma)$ is independent of the ordering. Another way of stating the conjecture is the claim that the whole matrix $M = M_{\mathcal{I}_d}$ is a P -matrix, meaning that all its principal minors are positive.

The conjecture was confirmed to be true in [10] for all $d \leq 7$ by simply computing the determinant of M_Γ for all possible $\Gamma \subset \mathcal{I}_d$. The conjecture has also been shown to hold in some special cases in [7].

Jaklič and Kanduč [6] showed by computation that the matrix $M + M^T$ is positive definite for $d \leq 16$ (but not for $d = 17$) which proves the conjecture for $d \leq 16$. Jaklič and Kanduč also observed that the conjecture can be simplified (somewhat) as follows: we can ignore any multi-index $\mathbf{i} = (i_1, i_2, i_3) \in \mathcal{I}_d$ for which any coordinate i_1, i_2 , or i_3 is zero. Such a multi-index has a corresponding domain point $\xi_{\mathbf{i}}$ that is either a vertex of T (two coordinates are zero), or an interior edge point of T (one coordinate is zero). More precisely, let

$$\mathcal{I}'_d = \{\mathbf{i} = (i_1, i_2, i_3) : i_1, i_2, i_3 \geq 1, |\mathbf{i}| = d\},$$

(the set of multi-indices $\mathbf{i} \in \mathcal{I}_d$ for which $\xi_{\mathbf{i}}$ is in the interior of T). Then it is sufficient to show

Conjecture 2 *For any subset Γ of the reduced set $\mathcal{I}'_d$, $\det(M_\Gamma) > 0$.*

The reason for this is that we can order the points $\mathbf{i}$ of $\mathcal{I}_d$ starting with $(d, 0, 0)$, $(0, d, 0)$, and $(0, 0, d)$, followed by the sequence $(i, d-i, 0)$, $i = 1, \dots, d-1$, and $(i, 0, d-i)$, $i = 1, \dots, d-1$, and $(0, i, d-i)$, $i = 1, \dots, d-1$, and the remaining points are those of $\mathcal{I}'_d$ (in any order). Then $M_{\mathcal{I}_d}$ has a block lower triangular structure, with seven square blocks on the diagonal, the first three of dimension 1, the next three of dimension $d-1$, and finally the block $M_{\mathcal{I}'_d}$ of dimension $\binom{d-1}{2}$. The three blocks of dimension $d-1$ are themselves P -matrices since they are totally positive, and so it is sufficient to show that $M_{\mathcal{I}'_d}$ is a P -matrix. An example of this block structure can be seen in Figures 3,4 of [6], in which the degree is $d = 4$.

Jaklič and Kanduč [6] showed that the matrix $M_{\mathcal{I}'_d} + M_{\mathcal{I}'_d}^T$ is positive definite for $d \leq 17$, which therefore proves the conjecture for $d \leq 17$. This result was also found by Foucart, who, moreover, has extended it to $d \leq 20$ using a refinement of this strategy [5].

Jaklič and Kanduč also observed that the problem can be restated in terms of a simpler matrix N_Γ , consisting only of multinomials. This

is because for $\mathbf{i}, \mathbf{j} \in \mathcal{I}_d$,

$$B_{\mathbf{j}}^d(\xi_{\mathbf{i}}) = \frac{d!}{j_1!j_2!j_3!} \left(\frac{i_1}{d}\right)^{j_1} \left(\frac{i_2}{d}\right)^{j_2} \left(\frac{i_3}{d}\right)^{j_3}.$$

Therefore, by the linearity of the determinant of M_{Γ} with respect to its columns, $\det(M_{\Gamma}) > 0$ if and only if $\det(N_{\Gamma}) > 0$, where

$$N_{\Gamma} = [i_1^{j_1} i_2^{j_2} i_3^{j_3}]_{\mathbf{i}, \mathbf{j} \in \Gamma}.$$

If we consider the number of points in Γ for $\Gamma \subset \mathcal{I}'_d$, then clearly $\det(N_{\Gamma}) > 0$ for $|\Gamma| = 1$. For $|\Gamma| = 2$, if $\Gamma = \{\mathbf{i}, \mathbf{j}\}$ for distinct $\mathbf{i}, \mathbf{j} \in \mathcal{I}'_d$ then

$$N_{\Gamma} = \begin{bmatrix} i_1^{i_1} i_2^{i_2} i_3^{i_3} & i_1^{j_1} i_2^{j_2} i_3^{j_3} \\ j_1^{i_1} j_2^{i_2} j_3^{i_3} & j_1^{j_1} j_2^{j_2} j_3^{j_3} \end{bmatrix},$$

and so

$$\det(N_{\Gamma}) = \prod_{k=1}^3 \left(i_k^{j_k} j_k^{i_k}\right) \left(\prod_{k=1}^3 \left(\frac{j_k}{i_k}\right)^{j_k - i_k} - 1\right) > 0$$

since $(j_k/i_k)^{j_k - i_k} \geq 1$ with equality only when $i_k = j_k$. However, it has not yet been shown that $\det(N_{\Gamma}) > 0$ for $|\Gamma| = 3$ in general.

2 A new conjecture and a theorem

Numerical tests suggest that the matrices N_{Γ} belong to a larger class of matrices with positive determinant, in which we allow the integer coordinates of $\mathbf{i} \in \Gamma$ to be real, and we no longer require that they should sum to some fixed d . For $x = (x_1, \dots, x_m)$ and $y = (y_1, \dots, y_m)$ in $\mathbb{R}^m$ let $x \cdot y = \sum_{i=1}^m x_i y_i$ be their scalar product and let $x^y = x_1^{y_1} \cdots x_m^{y_m}$. Let us also define $\ln(x) = (\ln(x_1), \dots, \ln(x_m)) \in \mathbb{R}^m$.

Conjecture 3 *Let $X = \{x^1, \dots, x^n\}$ be a set of distinct points x^i in $[1, \infty)^m$. Then the matrix*

$$A_X = [(x^i)^{(x^j)}]_{i,j=1,\dots,n} = [e^{x^j \cdot \ln(x^i)}]_{i,j=1,\dots,n} \quad (1)$$

has positive determinant.

This is already known to be true in the one-dimensional case $m = 1$ because the log function is increasing; see for example the discussion following equation (1.86) of [9].

In the remainder of the paper we are going to show

Theorem 1 *Conjecture 3 holds for $|X| \leq 3$ (and all $m \geq 1$).*

In particular, this proves Conjecture 2 (and therefore Conjecture 1) for $|\Gamma| \leq 3$.

The first non-trivial case of Theorem 1 is the case that $|X| = 2$. If $X = (x, y)$ for distinct $x, y \in [1, \infty)^m$, then

$$A_X = \begin{bmatrix} e^{x \cdot \ln(x)} & e^{y \cdot \ln(x)} \\ e^{x \cdot \ln(y)} & e^{y \cdot \ln(y)} \end{bmatrix}.$$

Then

$$\det(A_X) = e^{y \cdot \ln(x) + x \cdot \ln(y)} (e^{(y-x) \cdot (\ln y - \ln x)} - 1),$$

and since $(y_k - x_k)(\ln y_k - \ln x_k) \geq 0$, $k = 1, \dots, m$, with equality only when $x_k = y_k$, it follows that $\det(A_X) > 0$.

It remains to treat the case that $|X| = 3$.

3 Reduction to generic case

We can simplify the task of proving the $|X| = 3$ case of Theorem 1 by reducing it to the following ‘generic’ case. Let $X = \{x^1, \dots, x^n\}$ be a set of points $x^i = (x_1^i, x_2^i, \dots, x_m^i)$ in $\mathbb{R}^m$. We will say that these points are *coordinate-wise distinct* if the coordinates $x_k^1, x_k^2, \dots, x_k^n$ are distinct for all $k = 1, \dots, m$.

Theorem 2 *If $X = \{x^1, x^2, x^3\}$ is a set of three coordinate-wise distinct points in $[1, \infty)^m$ then $\det(A_X) > 0$.*

To explain why, we will denote by

$$A \circ B = [a_{ij}b_{ij}]_{i,j=1,\dots,n}$$

the Hadamard product of two real $n \times n$ matrices

$$A = [a_{ij}]_{i,j=1,\dots,n}, \quad B = [b_{ij}]_{i,j=1,\dots,n}$$

(see [12], [4], [11]).

Proof that Theorem 2 implies Theorem 1. Suppose $X = \{x^1, x^2, x^3\}$, with $x^1, x^2, x^3 \in \mathbb{R}^m$ distinct. The proof is by induction on m . Suppose first that $m = 1$. Then x_1^1, x_1^2, x_1^3 are distinct, and so Theorem 2 implies that $\det(A_X) > 0$.

Otherwise, $m \geq 2$. If x_k^1, x_k^2, x_k^3 are distinct for all $k = 1, \dots, m$ then $\det(A_X) > 0$ by Theorem 2. Otherwise, we may suppose without loss of generality that $x_m^2 = x_m^3$. We can write A_X as the Hadamard product

$$A_X = A \circ B,$$

where

$$A = [e^{y^j \cdot \ln(y^i)}]_{i,j=1,2,3},$$

and $y^i = (x_1^i, \dots, x_{m-1}^i)$, and

$$B = [e^{x_m^j \ln(x_m^i)}]_{i,j=1,2,3}.$$

Then, letting $a = x_m^1$ and $b = x_m^2 = x_m^3$,

$$B = \begin{bmatrix} e^{a \ln a} & e^{b \ln a} & e^{b \ln a} \\ e^{a \ln b} & e^{b \ln b} & e^{b \ln b} \\ e^{a \ln b} & e^{b \ln b} & e^{b \ln b} \end{bmatrix}.$$

Dividing column 1 of B by $e^{a \ln b}$ and columns 2 and 3 by $e^{b \ln b}$, and then dividing row 1 by $e^{b(\ln a - \ln b)}$, we see that

$$\det(A_X) = k \det(A \circ C),$$

where $k > 0$ and

$$C = \begin{bmatrix} e^{(a-b)(\ln a - \ln b)} & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}.$$

We can express $\det(A)$ as

$$a_{11} \det(A[2, 3 : 2, 3]) - a_{21} \det(A[1, 3 : 2, 3]) + a_{31} \det(A[1, 2 : 2, 3]),$$

where $A[i_1, i_2 : j_1, j_2]$ denotes the 2×2 submatrix of A with rows i_1, i_2 , and columns j_1, j_2 , and we can express $\det(A \circ C)$ analogously. We then deduce that

$$\det(A \circ C) - \det(A) = (e^{(a-b)(\ln a - \ln b)} - 1) a_{11} \det(A[2, 3 : 2, 3]).$$

Since $x_m^2 = x_m^3$, the points y^2 and y^3 must be distinct, and therefore, $\det(A[2, 3 : 2, 3]) > 0$. We also have $a_{11} > 0$.

We now consider the two cases (i) $a \neq b$, (ii) $a = b$.

In case (i),

$$e^{(a-b)(\ln a - \ln b)} - 1 > 0,$$

and so

$$\det(A \circ C) > \det(A).$$

If y^1, y^2, y^3 are distinct then by the induction hypothesis, the case $m - 1$ implies that $\det(A) > 0$. If y^1, y^2, y^3 are not distinct then $\det(A) = 0$. In either case, $\det(A) \geq 0$ and therefore, $\det(A \circ C) > 0$.

In case (ii),

$$e^{(a-b)(\ln a - \ln b)} - 1 = 0,$$

and so

$$\det(A \circ C) = \det(A).$$

But $a = b$ implies that $x_m^1 = x_m^2 = x_m^3$. But then y^1, y^2, y^3 must be distinct. So by the induction hypothesis, the case $m - 1$ implies that $\det(A) > 0$. Therefore, $\det(A \circ C) > 0$. $\square$

4 Symmetrization

It remains to prove Theorem 2. The first step in establishing this is an observation about 3×3 non-negative matrices. Let $A = [a_{ij}]_{i,j=1,\dots,n}$ be an $n \times n$ non-negative real matrix. Then we can form an associated symmetric matrix A_{sym} by

$$A_{\text{sym}} = [\sqrt{a_{ij}a_{ji}}]_{i,j=1,\dots,n}. \quad (2)$$

The (i, j) -th element of A_{sym} is the geometric mean of a_{ij} and a_{ji} . The diagonal elements of A_{sym} are the same as those of A . For $n = 1, 2$ it is easy to check that $\det(A) = \det(A_{\text{sym}})$.

Lemma 1 *If $n = 3$ then $\det(A) \geq \det(A_{\text{sym}})$.*

Proof. By the Leibniz formula for $\det(A)$,

$$\det(A) = a + b + c - (d + e + f), \quad (3)$$

where

$$\begin{aligned} a &= a_{11}a_{22}a_{33}, & b &= a_{21}a_{32}a_{13}, & c &= a_{31}a_{12}a_{23}, \\ d &= a_{11}a_{32}a_{23}, & e &= a_{21}a_{12}a_{33}, & f &= a_{31}a_{22}a_{13}. \end{aligned}$$

Then,

$$\det(A_{\text{sym}}) = a + 2\sqrt{bc} - (d + e + f),$$

and therefore,

$$\det(A) - \det(A_{\text{sym}}) = b + c - 2\sqrt{bc} = (\sqrt{b} - \sqrt{c})^2 \geq 0.$$

$\square$

5 Positive definiteness

Due to Lemma 1 we can reduce the proof of Theorem 2 to a question of positive definiteness.

Lemma 2 *Let $A_1, \dots, A_m$ be a sequence of 3×3 non-negative matrices and let $A = A_1 \circ A_2 \circ \dots \circ A_m$. If $(A_k)_{\text{sym}}$ is positive-definite for all $k = 1, \dots, m$, then $\det(A) > 0$.*

Proof. Since A is a non-negative 3×3 matrix, Lemma 1 implies that $\det(A) \geq \det(A_{\text{sym}})$. Denote the elements of A by a_{ij} , $i, j = 1, 2, 3$, and the elements of A_k by $a_{ij}^{[k]}$, $i, j = 1, 2, 3$. Then the (i, j) -th element of A_{sym} is

$$\sqrt{a_{ij}a_{ji}} = \sqrt{\prod_{k=1}^m a_{ij}^{[k]} \prod_{k=1}^m a_{ji}^{[k]}} = \prod_{k=1}^m \sqrt{a_{ij}^{[k]} a_{ji}^{[k]}},$$

and therefore

$$A_{\text{sym}} = (A_1)_{\text{sym}} \circ (A_2)_{\text{sym}} \circ \dots \circ (A_m)_{\text{sym}}.$$

By a theorem of Schur [12], if the matrices $(A_1)_{\text{sym}}, \dots, (A_m)_{\text{sym}}$ are positive definite then their Hadamard product is also positive definite. Therefore $\det(A_{\text{sym}}) > 0$, and consequently, $\det(A) > 0$ as well. $\square$

By applying this lemma we see that a sufficient condition for Theorem 2 to hold is that the symmetric matrix

$$[e^{(x_i \ln x_j + x_j \ln x_i)/2}]_{i,j=1,2,3}$$

is positive definite for any distinct $x_1, x_2, x_3 \geq 1$. By dividing the i -th row by $e^{x_i \ln x_i}$ and the j -th column by $e^{x_j \ln x_j}$, it follows that it is sufficient that

$$A = [e^{-(x_j - x_i)(\ln x_j - \ln x_i)/2}]_{i,j=1,2,3} \quad (4)$$

is positive definite. It is easy to see that the leading principal minors $\det(A[1 : 1])$ and $\det(A[1, 2 : 1, 2])$ are positive, and so it remains to show

Lemma 3 *The matrix A in (4) has positive determinant for distinct $x_1, x_2, x_3 \geq 1$.*

6 Determinant formula

As a first step to proving Lemma 3, consider next any matrix A of the form

$$A = \begin{bmatrix} 1 & a & b \\ a & 1 & c \\ b & c & 1 \end{bmatrix}, \quad (5)$$

where $0 < a, b, c < 1$. For such a matrix, there is a useful formula for its determinant, see [3] and [2]. Let

$$a = \cos \alpha, \quad b = \cos \beta, \quad c = \cos \gamma,$$

with $0 < \alpha, \beta, \gamma < \pi/2$.

Lemma 4 ([3],[2]) *The determinant of A in (5) is*

$$\det(A) = 4 \sin \left(\frac{\alpha + \beta + \gamma}{2} \right) \times \sin \left(\frac{\alpha + \beta - \gamma}{2} \right) \sin \left(\frac{\alpha + \gamma - \beta}{2} \right) \sin \left(\frac{\beta + \gamma - \alpha}{2} \right). \quad (6)$$

For the sake of completeness, the proof is as follows.

Proof. We can write the determinant of A as

$$\det(A) = 1 + 2abc - a^2 - b^2 - c^2 = (1 - a^2)(1 - b^2) - (c - ab)^2.$$

Therefore,

$$\begin{aligned} \det(A) &= \sin^2 \alpha \sin^2 \beta - (\cos \gamma - \cos \alpha \cos \beta)^2 \\ &= (\sin \alpha \sin \beta + \cos \gamma - \cos \alpha \cos \beta) \\ &\quad \times (\sin \alpha \sin \beta - \cos \gamma + \cos \alpha \cos \beta) \\ &= (\cos \gamma - \cos(\alpha + \beta))(\cos(\alpha - \beta) - \cos \gamma), \end{aligned}$$

which is the product of

$$\cos \gamma - \cos(\alpha + \beta) = 2 \sin \left(\frac{\alpha + \beta + \gamma}{2} \right) \sin \left(\frac{\alpha + \beta - \gamma}{2} \right),$$

and

$$\cos(\alpha - \beta) - \cos \gamma = 2 \sin \left(\frac{\alpha + \gamma - \beta}{2} \right) \sin \left(\frac{\beta + \gamma - \alpha}{2} \right).$$

□

If we then suppose that b is the smallest of a, b, c , we obtain the following condition for a positive determinant.

Theorem 3 *Suppose $a, b, c \in (0, 1)$ are distinct and $b < \min(a, c)$. Then the determinant of A in (5) is positive if $\alpha + \gamma > \beta$.*

Proof. Since $(\alpha + \beta + \gamma)/2 < 3\pi/4$, the first sine term in (6) is positive. Further, if $b < c$ then $\beta > \gamma$, and so $\beta + \alpha > \gamma$, and the second sine term is positive. Similarly, if $b < a$ then $\beta > \alpha$, and so $\beta + \gamma > \alpha$, and the fourth sine term is positive. Therefore, $\det(A) > 0$ if the remaining sine term is positive, i.e., if $\alpha + \gamma > \beta$. $\square$

7 Triangle inequality

By applying Theorem 3 to the matrix A in (4) we have reduced the proof of Lemma 3, and consequently of Theorem 1, to showing that the function

$$\delta(x, y) := \arccos(e^{-(y-x)(\ln(y)-\ln(x))/2}),$$

satisfies the triangle inequality

$$\delta(x_1, x_2) + \delta(x_2, x_3) > \delta(x_1, x_3)$$

for

$$1 \leq x_1 < x_2 < x_3.$$

It turns out that this inequality does indeed hold and moreover generalizes to a class of functions f that replace the log function. Suppose that I is some real interval, and that $f : I \rightarrow \mathbb{R}$ is an increasing function, and that $f \in C^2(I)$. We will show

Theorem 4 (Triangle inequality) *Suppose*

$$\frac{|f''(x)|}{f'(x)^{3/2}} < c_*, \quad x \in I, \quad (7)$$

where $c_* \approx 2.2405365$. Then

$$\delta(x_1, x_2) + \delta(x_2, x_3) > \delta(x_1, x_3) \quad (8)$$

for any $x_1, x_2, x_3 \in I$ with $x_1 < x_2 < x_3$, where

$$\delta(x, y) := \arccos(e^{-(y-x)(f(y)-f(x))/2}). \quad (9)$$

Clearly, the condition (7) trivially holds for the case that $I = \mathbb{R}$ and $f(x) = x$. This then provides an alternative proof that the matrix

$$A = [e^{-(x_j - x_i)^2/2}]_{i,j=1,2,3} \quad (10)$$

is positive definite for distinct x_1, x_2, x_3 in $\mathbb{R}$, which is already known since the matrix elements are Gaussian radial basis functions; see, for example [8].

Next suppose that $f(x) = \ln x$ and suppose $x > 0$. Then

$$\frac{|f''(x)|}{(f'(x))^{3/2}} = \frac{1}{x^{1/2}}$$

and so (7) holds for $x \geq 1/c_*^2 \approx 0.1992$. Thus, the condition holds in particular for all $x \geq 1$, and thus Theorem 1 follows from Theorem 4.

8 Proof of Triangle Inequality

We will prove Theorem 4 in a series of steps, using partial derivatives of $\delta(x, y)$ in (9), which we will denote by

$$\delta_x = \frac{\partial \delta}{\partial x}, \quad \delta_y = \frac{\partial \delta}{\partial y}, \quad \delta_{xx} = \frac{\partial^2 \delta}{\partial x^2},$$

and so on.

Lemma 5 *A sufficient condition for the triangle inequality (8) to hold is that*

$$\delta_{xy}(x, y) > 0, \quad x, y \in I, \quad x < y.$$

Proof. Since $\delta(x_2, x_2) = 0$,

$$\begin{aligned} \delta(x_1, x_2) + \delta(x_2, x_3) - \delta(x_1, x_3) &= \int_{x_2}^{x_3} \delta_y(x_2, t) dt - \int_{x_2}^{x_3} \delta_y(x_1, t) dt \\ &= \int_{x_2}^{x_3} \int_{x_1}^{x_2} \delta_{xy}(s, t) ds dt > 0. \end{aligned}$$

□

We now compute the derivative δ_{xy} of δ in (9). Let

$$\phi(x, y) := (y - x)(f(y) - f(x)),$$

so that

$$\delta(x, y) = \arccos(e^{-\phi(x, y)/2}).$$

Lemma 6

$$\delta_{xy} = \frac{1}{4}e^\phi(e^\phi - 1)^{-3/2}\mu,$$

where

$$\begin{aligned}\mu(x, y) &= (f(y) - f(x))^2 + f'(x)f'(y)(y - x)^2 \\ &\quad - (2(1 - e^{-\phi}) - \phi)(f'(x) + f'(y)).\end{aligned}\tag{11}$$

Proof. By the chain rule,

$$\begin{aligned}\delta_x &= \frac{1}{2\sqrt{e^\phi - 1}}\phi_x, \\ \delta_y &= \frac{1}{2\sqrt{e^\phi - 1}}\phi_y, \\ \delta_{xy} &= \frac{e^\phi\mu}{4(e^\phi - 1)^{3/2}}, \quad \mu = 2(1 - e^{-\phi})\phi_{xy} - \phi_x\phi_y.\end{aligned}$$

The derivatives of ϕ are

$$\begin{aligned}\phi_x &= -f'(x)(y - x) - (f(y) - f(x)), \\ \phi_y &= f'(y)(y - x) + (f(y) - f(x)), \\ \phi_{xy} &= -f'(x) - f'(y),\end{aligned}$$

and substituting these into μ gives the result. $\square$

Thus a sufficient condition for the triangle inequality (8) to hold is that $\mu(x, y) > 0$ for $x < y$ in I . We next simplify this condition by replacing it by a stronger condition.

Lemma 7 *A sufficient condition for $\mu(x, y) > 0$ for $x, y \in I$, $x < y$, is that*

$$2(f'(x)f'(y))^{1/2}\phi > (f'(x) + f'(y))(2(1 - e^{-\phi}) - \phi).$$

Proof. We can write μ in (11) as $\mu = a^2 + b^2 - c$, where

$$\begin{aligned}a &= f(y) - f(x), \quad b = (f'(x)f'(y))^{1/2}(y - x), \\ c &= (f'(x) + f'(y))(2(1 - e^{-\phi}) - \phi).\end{aligned}$$

Then $\mu \geq 2ab - c$, and so it is sufficient that $2ab > c$. $\square$

We can rearrange the condition of Lemma 7 in the form

$$\rho(x, y) > F(\phi(x, y)), \quad x, y \in I, \quad x < y, \quad (12)$$

where

$$\rho(x, y) = 2 \frac{(f'(x)f'(y))^{1/2}}{f'(x) + f'(y)}, \quad (13)$$

and

$$F(t) = 2t^{-1}(1 - e^{-t}) - 1, \quad t > 0.$$

We note that $\lim_{t \rightarrow 0+} F(t) = 1$ and $\lim_{t \rightarrow \infty} F(t) = -1$, and

$$F'(t) = \frac{-2e^{-t}}{t^2}(e^t - (1 + t)) < 0,$$

from which we see that F is decreasing. We also have

$$F''(t) = \frac{4e^{-t}}{t^3}(e^t - (1 + t + t^2/2)) > 0,$$

from which we see that F is convex. We next use an estimate of F to obtain a simpler condition.

Lemma 8 *Let $t_* > 0$ be the unique positive zero of F . We note that $t_* \approx 1.5936$. If*

$$\rho(x, y) > 1 - \frac{\phi(x, y)}{t_*}, \quad (14)$$

for all $x, y \in I$ with $x < y$ then $\mu(x, y) > 0$.

Proof. Since $F(0) = 1$ and F is convex, we have

$$F(t) \leq 1 - t/t_*, \quad 0 \leq t \leq t_*.$$

Now suppose that x and y satisfy (14). If $\phi(x, y) \leq t_*$ then (12) is satisfied. Otherwise, $\phi(x, y) > t_*$. But then (12) holds because $\rho(x, y) \geq 0$. $\square$

Thus the triangle inequality (8) holds if $\nu(x, y) > 0$ for $x < y$ in I , where

$$\nu(x, y) = \rho(x, y) - \left(1 - \frac{\phi(x, y)}{t_*}\right).$$

Lemma 9 *A sufficient condition for $\nu > 0$ to hold is that*

$$\nu_{xy}(x, y) < 0, \quad x, y \in I, \quad x < y.$$

Proof. Since $\nu(x, y) = \nu(y, x)$ and $\nu(x, x) = \nu(y, y) = 0$,

$$\begin{aligned}\nu(x, y) &= \frac{1}{2}(\nu(x, y) + \nu(y, x) - \nu(x, x) - \nu(y, y)) \\ &= \frac{1}{2} \left(\int_x^y \nu_y(x, t) dt - \int_x^y \nu_y(y, t) dt \right) \\ &= -\frac{1}{2} \int_x^y \int_x^y \nu_{xy}(s, t) ds dt > 0.\end{aligned}$$

□

This means that the triangle inequality (8) holds if

$$\nu_{xy} = \rho_{xy} + \frac{1}{t_*} \phi_{xy} < 0, \quad x, y \in I, \quad x < y.$$

Since $\phi_{xy} = -(f'(x) + f'(y))$, it is therefore sufficient that

$$|\rho_{xy}| < \frac{f'(x) + f'(y)}{t_*}. \quad (15)$$

We next compute ρ_{xy} . To simplify expressions we define

$$a = f'(x), \quad b = f'(y), \quad (16)$$

so that

$$\rho = \frac{2a^{1/2}b^{1/2}}{a+b}. \quad (17)$$

When differentiating ρ we will also use the notation

$$a' = f''(x), \quad b' = f''(y). \quad (18)$$

Lemma 10

$$\rho_{xy} = \frac{a'b'}{2a^{1/2}b^{1/2}} \frac{(6ab - a^2 - b^2)}{(a+b)^3}.$$

Proof. Differentiating ρ in (17) with respect to x gives

$$\rho_x = \frac{a^{-1/2}a'b^{1/2}}{a+b} - \frac{2a^{1/2}b^{1/2}a'}{(a+b)^2} = \frac{a'}{a^{1/2}}\sigma,$$

where

$$\sigma = \frac{b^{1/2}(b-a)}{(a+b)^2}.$$

Then differentiating σ with respect to y gives

$$\begin{aligned}\sigma_y &= \frac{(1/2)b^{-1/2}b'(b-a) + b^{1/2}b'}{(a+b)^2} - \frac{2b^{1/2}(b-a)b'}{(a+b)^3} \\ &= \frac{b'}{2b^{1/2}} \frac{(6ab - a^2 - b^2)}{(a+b)^3},\end{aligned}$$

and hence the result follows. $\square$

Using Lemma 10, the inequality (15) expands to

$$\frac{|a'||b'|}{2a^{1/2}b^{1/2}} \frac{|6ab - a^2 - b^2|}{(a+b)^4} < \frac{1}{t_*},$$

where, as before, $a = f'(x)$ and $b = f'(y)$. Since

$$|6ab - a^2 - b^2| = |4ab - (a-b)^2| \leq 4ab + (a-b)^2 = (a+b)^2,$$

and

$$\frac{1}{(a+b)^2} \leq \frac{1}{4ab},$$

it follows that another sufficient condition for the triangle inequality (8) is that

$$\frac{|a'||b'|}{a^{3/2}b^{3/2}} < \frac{8}{t_*},$$

or in terms of f , that

$$\frac{|f''(x)||f''(y)|}{(f'(x))^{3/2}(f'(y))^{3/2}} < \frac{8}{t_*}.$$

Therefore it is sufficient that

$$\frac{|f''(x)|}{f'(x)^{3/2}} < c_*, \quad x \in I,$$

where

$$c_* = \left(\frac{8}{t_*}\right)^{1/2} \approx 2.2405365.$$

Thus we have proved Theorem 4.

9 Final remarks

We note that condition (7) has the property that it is the same if we replace f by its functional inverse g , i.e., $g = f^{-1}$. With $g(y) = x$ and $y = f(x)$, we find that

$$g'(y) = \frac{1}{f'(x)}, \quad g''(y) = -\frac{f''(x)}{(f'(x))^3},$$

and so

$$\frac{g''(y)}{g'(y)^{3/2}} = -\frac{f''(x)}{f'(x)^{3/2}}.$$

Therefore, the condition (7) for g is the same as for f .

Another example of a function which satisfies condition (7) is $f(x) = \arctan(x)$, for $x \in I$, where $I = \mathbb{R}$. This is because

$$\frac{|f''(x)|}{(f'(x))^{3/2}} = \frac{2|x|}{\sqrt{1+x^2}} < 2 < c_*, \quad x \in \mathbb{R}.$$

Due to Theorem 4, we have a generalization of Theorem 1. Define $f : \mathbb{R}^m \rightarrow \mathbb{R}$ by $f(x) = (f_1(x_1), \dots, f_m(x_m))$ for $x = (x_1, \dots, x_m) \in \mathbb{R}^m$, where each function f_i is a function $f_i : I_i \rightarrow \mathbb{R}$, with I_i a real interval, such that f_i is increasing and belongs to $C^2(I_i)$ and satisfies condition (7). Let $I = I_1 \times \dots \times I_m$. Then, using the same proof as that of Theorem 1, we deduce

Corollary 1 *Let $X = \{x^1, x^2, x^3\}$ be distinct points in I . Then the matrix*

$$[e^{x^j \cdot f(x^i)}]_{i,j=1,2,3} \tag{19}$$

has positive determinant.

There is a natural generalization of Conjecture 1 to m -variate Bernstein polynomials on a simplex in $\mathbb{R}^m$ for any $m \geq 1$. Since Theorem 1 holds for points in $\mathbb{R}^k$ for all $k \leq m+1$, it follows that this generalized conjecture holds for $n = |\Gamma| \leq 3$. Similar to the bivariate case, it is sufficient to consider triples of multi-indices that correspond to domain points on a common (interior) face of any dimension of the simplex (edges, 2-faces and so on).

As regards Conjecture 3 for $n \geq 4$, numerical tests suggest two things: (i) that the inequality $\det(A_X) \geq \det((A_X)_{\text{sym}})$ may hold for

all n for the specific class of matrices A_X in (1), and (ii) that the matrix $(A_X)_{\text{sym}}$, or equivalently the matrix

$$[e^{-(x^j - x^i) \cdot (\ln(x^j) - \ln(x^i))/2}]_{i,j=1,\dots,n},$$

may be positive definite for all distinct $x^1, \dots, x^n \in [1, \infty)^m$. However, for $n \geq 4$ there does not seem to be any simple reason why the determinant inequality $\det(A_X) \geq \det((A_X)_{\text{sym}})$ should hold.

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