Optimization-Aided Construction of Multivariate Chebyshev Polynomials

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Abstract

This article is concerned with an extension of univariate Chebyshev polynomials of the first kind to the multivariate setting, where one chases best approximants to specific monomials by polynomials of lower degree relative to the uniform norm. Exploiting the Moment-SOS hierarchy, we devise a versatile semidefinite-programming-based procedure to compute such best approximants, as well as associated signatures. Applying this procedure in three variables leads to the values of best approximation errors for all mononials up to degree six on the euclidean ball, the simplex, and the cross-polytope. Furthermore, inspired by numerical experiments, we obtain explicit expressions for Chebyshev polynomials in two cases unresolved before, namely for the monomial $x_1^2 x_2^2 x_3$ on the euclidean ball and for the monomial $x_1^2 x_2 x_3$ on the simplex.

Key words and phrases: best approximation, Chebyshev polynomials, sum of squares, method of moments, semidefinite programming.

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1 Introduction

For $n \geq 1$, let $\mathcal{P}_n$ denote the space of univariate polynomials of degree less than or equal to n. The classical nth degree Chebyshev polynomial (of the first kind) is the polynomial T_n often implicitly defined via the relation $T_n(\cos\theta) = \cos(n\theta)$ for all $\theta \in [-\pi, \pi]$. It is characterized by a wealth of extremal properties, including:

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- $2^{-n+1}T_n$ is the monic polynomial that deviates least from zero in the uniform norm on $[-1,1]$, i.e., T_n minimizes $\|p\|_{[-1,1]} := \max\{|p(x)| : x \in [-1,1]\}$ over all polynomials $p \in \mathcal{P}_n$ satisfying $\mathrm{coeff}_{x^n}(p) = 2^{n-1}$—this is how Chebyshev polynomials were first introduced in [4];

- $2^{-n+1}T_n$ is the monic polynomial that deviates least from zero in the L_2-norm on $[-1,1]$ with respect to the inverse semicircle weight, i.e., T_n minimizes $\int_{-1}^{1} p(x)^2(1-x^2)^{-1/2}dx$ over all polynomials $p \in \mathcal{P}_n$ satisfying $\mathrm{coeff}_{x^n}(p) = 2^{n-1}$—this relates to the orthogonality of Chebyshev polynomials for this weight;

- T_n is the extremizer of every differentiation operator, i.e., T_n maximizes $\|p^{(k)}\|_{[-1,1]}$ over all polynomials $p \in \mathcal{P}_n$ satisfying $\|p\|_{[-1,1]} \leq 1$ for every $k = 1, 2, \ldots, n$—this is Markov's inequality due to A. A. Markov for $k = 1$ and Markov's inequality due to his younger brother V. A. Markov for $k = 2, \ldots, n$;

- T_n is the polynomial with the largest growth outside $[-1,1]$, i.e., T_n maximizes $|p^{(k)}(t)|$ over all polynomials $p \in \mathcal{P}_n$ satisfying $\|p\|_{[-1,1]} \leq 1$ for every $t \notin [-1,1]$ and every $k = 1, 2, \ldots, n$;

- T_n is the polynomial with largest arc-length on $[-1,1]$, i.e., T_n maximizes $\int_{-1}^{1} \sqrt{1 + p'(x)^2}dx$ over all polynomials $p \in \mathcal{P}_n$ satisfying $\|p\|_{[-1,1]} \leq 1$.

Each of these five properties, which are all found in the classic book [18] by Rivlin, could serve as a rationale for a generalization of Chebyshev polynomials to the multivariate setting. The generalization examined in this article is based on the first property. Thus, denoting by $\mathcal{P}_n^d$ the space of d-variate polynomials of degree $\leq n$ and considering a domain $\Omega \subseteq \mathbb{R}^d$, we intend to tackle the optimization program

$$\underset{p \in \mathcal{P}_n^d}{\text{minimize}} \ \|p\|_\Omega := \max_{x \in \Omega} |p(x)| \qquad \text{subject to } p \text{ being monic.}$$

Although this is a convex optimization program—the constraint is linear and the objective function is convex—solving it is far from trivial. By introducing a slack variable $c \in \mathbb{R}$, it is seen to be equivalent to

$$\text{(1)} \qquad \underset{c \in \mathbb{R},\, p \in \mathcal{P}_n^d}{\text{minimize}} \ c \qquad \text{subject to } p \text{ being monic and to } \begin{cases} c + p \geq 0 & \text{on } \Omega, \\ c - p \geq 0 & \text{on } \Omega. \end{cases}$$

The added constraints are polynomial nonnegativity constraints and, as such, can conceivably be dealt with using sum-of-squares (SOS) techniques. In fact, we will advantageously use the dual facet of the Moment-SOS hierarchy [12] to address our central optimization program.

But before delving into the technicalities, let us mention that the above formulation comes with some ambiguities about

- the notion of multivariate degree: we will concentrate exclusively on the total degree given by

$$\deg\left(\sum_{k=(k_1,\dots,k_d)} c_{k_1,\dots,k_d}\, x_1^{k_1}\cdots x_d^{k_d}\right) = \max_k |k|, \qquad \text{where } |k| = k_1+\cdots+k_d;$$

- the choice of domain Ω: we will consider only the simplex S, the cross-polytope C (ℓ_1-ball), the euclidean ball B (ℓ_2-ball), and the hypercube H (ℓ_∞-ball), which are given by

$$S = \left\{x\in\mathbb{R}^d : x_1,\dots,x_d \geq 0 \text{ and } \sum_{i=1}^d x_i \leq 1\right\}, \qquad C = \left\{x\in\mathbb{R}^d : \sum_{i=1}^d |x_i| \leq 1\right\},$$

$$B = \left\{x\in\mathbb{R}^d : \sum_{i=1}^d |x_i|^2 \leq 1\right\}, \qquad H = \left\{x\in\mathbb{R}^d : \max_{i=1,\dots,d} |x_i| \leq 1\right\};$$

- the meaning of 'monic' in the constraint: it can be interpreted as imposing that the coefficient on a fixed nth degree monomial equals one while the coefficients on all other nth degree monomials equal zero, leading to the best approximation problem

$$\text{(2)} \qquad \underset{p\in\mathcal{P}_{n-1}^d}{\text{minimize}}\ \|m_k - p\|_\Omega, \qquad \text{where} \quad m_k(x) = x_1^{k_1}\cdots x_d^{k_d} \quad \text{and} \quad |k| = n,$$

  or it could be interpreted as imposing that the coefficients on all the nth degree monomials sum up to one, leading to the program

$$\text{(3)} \qquad \underset{p\in\mathcal{P}_n^d}{\text{minimize}}\ \|p\|_\Omega \qquad \text{subject to} \sum_{|k|=n} \text{coeff}_{m_k}(p) = 1.$$

  The term Chebyshev polynomial will refer to the first interpretation. It is the subject of this article and necessitates a computational approach. The second interpretation comes, more classically, with explicit expressions for a large class of domains including S, C, B, and H. This is the subject of a companion article, see [5].

Here, our contribution includes the numerical—sometimes explicit—construction of all Chebyshev polynomials up to degree $n = 6$ for $d = 3$ variables. The whole list of errors of best approximation is assembled in Section 4, completing a partial catalog of known results recalled in Section 2. This section also provides a refresher on some important reductions and on the central concept of signature. The production of novel Chebyshev polynomials exploits a semidefinite programming procedure presented in Section 3. Arguably, this is the centerpiece of our work and we emphasize its versatility, which would allow one to make easy adjustments for related problems, e.g. multivariate Zolotarev's polynomials could be constructed with only small modifications of the procedure. It is also worth noting already at this point that the workflow is not only numerical: the experimental Chebyshev polynomials returned by our procedure can be verified explicitly or symbolically to be genuine Chebyshev polynomials. For instance, best approximants to the monomial $m_{(2,2,1)}$ relative to the euclidean ball and to the monomial $m_{(2,1,1)}$ relative to the simplex are derived analytically in Section 4. Finally, Section 5 gives an outlook on a possible augmentation of the procedure and its deployment into further computational endeavors.

2 Prior Scholarship

This section is exclusively concerned with (monomial-specific) multivariate Chebyshev polynomials, i.e., with solutions to the best approximation problem (2). We start by recalling a characterization of these solutions involving the notion of signature. Then we provide a catalog of previously derived multivariate Chebyshev polynomials—more precisely, of the known results that we are aware of. We point out from the outset that multivariate Chebyshev polynomials are generically not unique, explaining our tendency to manipulate signatures preferably to polynomials themselves.

2.1 Characterization via signatures

To be most general, let us assume that Ω is a compact set and that we are trying to approximate a continuous function $f \in C(\Omega)$ by elements of a finite-dimensional vector space $\mathcal{V} \subseteq C(\Omega)$, assuming of course that $f \notin \mathcal{V}$. We have in mind the case where f is a nth degree monomial and where $\mathcal{V}$ is the space $\mathcal{P}^d_{n-1}$, but the considerations of this subsection are valid beyond this specific case. The error of best approximation and (any one of) the best approximant(s) shall be denoted by $E_{\mathcal{V}}(f,\Omega)$ and by v^*, respectively, so that

$$E_{\mathcal{V}}(f,\Omega) = \min_{v \in \mathcal{V}} \|f - v\|_\Omega = \|f - v^*\|_\Omega. \tag{4}$$

It is well known that the error of best approximation can alternatively be expressed as a maximum (by duality, in optimization custom), namely as

$$E_{\mathcal{V}}(f,\Omega) = \max_{\lambda \in C(\Omega)^*} \lambda(f) \qquad \text{subject to } \lambda_{|\mathcal{V}} = 0 \text{ and } \|\lambda\|_{C(\Omega)^*} = 1. \tag{5}$$

The usual argument relies on the Hahn–Banach theorem to extend the norm-one linear functional $\widetilde{\lambda}$ defined on $\mathcal{V}_f := \mathcal{V} \oplus \mathbb{R}f$ by $\widetilde{\lambda}(v + tf) = t\|f - v^*\|_\Omega$. This linear functional can be expressed as a convex combination of $L \leq \dim(\mathcal{V}_f)$ extreme points[1] of the unit ball of the dual of $\mathcal{V}_f$. These extreme points are restrictions to $\mathcal{V}_f$ of some $\pm\delta_\omega$, $\omega \in \Omega$, where δ_ω represents the Dirac evaluation functional at a point ω. Thus, the Hahn–Banach extension takes the form $\lambda = \sum_{\ell=1}^L \tau_\ell \varepsilon_\ell \delta_{\omega_\ell}$ with

[1] Applying Krein–Milman and Carathéodory theorems gives $L \leq \dim(\mathcal{V}_f) + 1$. To obtain $L \leq \dim(\mathcal{V}_f)$, one should use the fact that a norm-one linear functional on a real finite-dimensional space $\mathcal{U}$ can be expressed as a convex combination of $L \leq \dim(\mathcal{U})$ extreme points of the unit ball of $\mathcal{U}^*$. This result can be found in [18, Theorem 2.13] when $\mathcal{U}$ is a space of continuous functions on a compact set $\mathcal{K}$, which always occurs with $\mathcal{K} = \mathrm{cl}[\mathrm{Ex}(B_{\mathcal{U}^*})]$. In the particular case $\mathcal{U} = \mathcal{P}^d_k$, it equates to Tchakaloff's theorem and its generalizations (notably by Richter [17]), stating that if a measure μ on $\mathbb{R}^d$ has moments up to degree k, then there exists an atomic measure with at most $\binom{k+d}{d}$ atoms in $\mathrm{supp}(\mu)$ and with same moments up to degree k.

$\omega_1, \ldots, \omega_L \in \Omega$, $\varepsilon_1, \ldots, \varepsilon_L = \pm 1$, and $\tau_1, \ldots, \tau_L > 0$ satisfying $\sum_{\ell=1}^{L} \tau_\ell = 1$. Notice that

$$
\begin{aligned}
E_{\mathcal{V}}(f, \Omega) = \lambda(f) = \lambda(f - v^*) &= \sum_{\ell=1}^{L} \tau_\ell \varepsilon_\ell (f - v^*)(\omega_\ell) \\
&\leq \sum_{\ell=1}^{L} \tau_\ell |(f - v^*)(\omega_\ell)| \leq \sum_{\ell=1}^{L} \tau_\ell \|f - v^*\|_\Omega = \|f - v^*\|_\Omega \\
&= E_{\mathcal{V}}(f, \Omega),
\end{aligned}
\tag{6}
$$

which implies that the equalities $\varepsilon_\ell (f - v^*)(\omega_\ell) = \|f - v^*\|_\Omega = E_{\mathcal{V}}(f, \Omega)$ hold for all $\ell = 1, \ldots, L$. This brings us to the notion of extremal signature associated with $f - v^*$, defined below along the lines of [18, Section 2.2].

Definition 1. A signature with support (aka base) $\mathcal{S} \subseteq \Omega$ is simply a function from $\mathcal{S}$ to $\{\pm 1\}$. A signature σ with support $\mathcal{S}$ is said to be extremal for $\mathcal{V}$ if there exist weights $\tau_\omega > 0$, $\omega \in \mathcal{S}$, such that $\sum_{\omega \in \mathcal{S}} \tau_\omega \sigma(\omega) v(\omega) = 0$ for all $v \in \mathcal{V}$. A signature σ with support $\mathcal{S}$ is said to be associated with a function $g \in C(\Omega)$ if $\mathcal{S}$ is included in the set $\{\omega \in \Omega : |g(\omega)| = \|g\|_\Omega\}$ of extremal points of g and if $\sigma(\omega) = \mathrm{sgn}(g(\omega))$ for all $\omega \in \mathcal{S}$.

The argument outlined before the definition leads to the following brief statement, found e.g. in [18, Theorem 2.6]. We emphasize that it does not provide a way to find extremal signatures and best approximants, but if one comes up with a guess for these (as we will do in Section 4), then it provides a way to verify that the guess is correct.

Theorem 2. An element $v^* \in \mathcal{V}$ is a best approximant to $f \in C(\Omega)$ from $\mathcal{V}$ if and only if there exists an extremal signature σ for $\mathcal{V}$ associated with $f - v^*$. Moreover, the support of such a signature can be chosen to have size $\leq \dim(\mathcal{V}) + 1$.

An important detail not made apparent in the above statement is the existence of a signature common to all best approximants—this is revealed by (6), because the involved arguments did not depend on the best approximant v^*. This fact explains our preference for solving (5) over (4), especially since (4) typically have nonunique solutions.

2.2 Simple reductions

Given a fixed number d of variables and a fixed degree n, completely solving the problem of d-variate nth degree Chebyshev polynomials requires finding best approximants to all d-variate nth degree monomials, so we would a priori need to tackle $\binom{n+d-1}{d-1}$ subproblems. For $d = 3$ and $n = 6$, it amounts to 28 subproblems and for $d = 3$ and $n = 10$, it amounts to 66 subproblems. Fortunately, this number can be decreased drastically by leveraging two simple reductions. The first reduction allows us to discard the indices $k_i = 0$ in the multiindex k of the monomial m_k, provided the full problem has been solved for all $d' < d$. The second reduction allows us to consider only indices $k_1, \dots, k_d$ that are ordered from largest to smallest, say. These facts are precisely stated in the two propositions below. In the first one, the domain Ω can be taken as any of our preferred choices—the simplex S, the cross-polytope C, the euclidean ball B, or the hypercube H—by selecting $\varphi = 0$. The argument, already found in [24, Proposition 4.1] for $\Omega = B$, is included here to also cover the case $\varphi \neq 0$.

Proposition 3. Given $k \in \mathbb{N}_0^d$ with $|k| = k_1 + \cdots + k_d = n$, let $I := \{i = 1, \dots, d : k_i > 0\}$ and let $d' := |I|$. Let $\Omega' \subseteq \mathbb{R}^I$ be the d'-dimensional domain defined by $\Omega' = \{\omega_I, \omega \in \Omega\}$ and suppose that there is a $\varphi \in \mathbb{R}^{I^c}$ such that the element $\widetilde{\omega}$ defined by $\widetilde{\omega}_i = \omega_i$ for $i \in I$ and $\widetilde{\omega}_i = \varphi_i$ for $i \in I^c$ belongs to Ω whenever $\omega \in \Omega$. Then, with $k' := k_I \in \mathbb{N}_0^{d'}$, which satisfies $|k'| = k'_1 + \cdots + k'_{d'} = n$, one has

$$E_{\mathcal{P}^d_{n-1}}(m_k, \Omega) = E_{\mathcal{P}^{d'}_{n-1}}(m_{k'}, \Omega').$$

Proof. On the one hand, with $q' \in \mathcal{P}^{d'}_{n-1}$ such that $E_{\mathcal{P}^{d'}_{n-1}}(m_{k'}, \Omega') = \|m_{k'} - q'\|_{\Omega'}$ and with $q \in \mathcal{P}^d_{n-1}$ defined by $q(x) = q'(x_I)$, $x \in \mathbb{R}^d$, we have

$$\begin{aligned} E_{\mathcal{P}^{d'}_{n-1}}(m_{k'}, \Omega') &= \|m_{k'} - q'\|_{\Omega'} = \max_{\omega \in \Omega} |m_{k'}(\omega_I) - q'(\omega_I)| = \max_{\omega \in \Omega} |m_k(\omega) - q(\omega)| = \|m_k - q\|_\Omega \\ &\geq E_{\mathcal{P}^d_{n-1}}(m_k, \Omega). \end{aligned}$$

This inequality was obtained independently of the existence of φ. On the other hand, for the reverse inequality, given $p \in \mathcal{P}^d_{n-1}$, we have

$$\|m_k - p\|_\Omega = \max_{\omega \in \Omega} |m_k(\omega) - p(\omega)| \geq \max_{\omega \in \Omega} |m_k(\widetilde{\omega}) - p(\widetilde{\omega})| = \max_{\omega \in \Omega} |m_{k'}(\omega_I) - \widetilde{p}(\omega_I)|,$$

where $\widetilde{p}$ is implicitly defined as a polynomial in $\mathcal{P}^{d'}_{n-1}$. Therefore, we obtain

$$\|m_k - p\|_\Omega \geq \|m_{k'} - \widetilde{p}\|_{\Omega'} \geq E_{\mathcal{P}^{d'}_{n-1}}(m_{k'}, \Omega').$$

The inequality $E_{\mathcal{P}^d_{n-1}}(m_k, \Omega) \geq E_{\mathcal{P}^{d'}_{n-1}}(m_{k'}, \Omega')$ follows by taking the infimum over p. □

The second fact, stated hereafter, has been previously used to derive a number of examples in [1, 2, 23]. We include a standard argument (see e.g. [24, Theorem 3.2]) for the convenience of the reader. This fact is to be used with $\mathcal{V} = \mathcal{P}^d_{n-1}$ and G being the group of permutation of $\{1, 2, \dots, d\}$.

Proposition 4. Given a finite group G acting on a domain $\Omega \subseteq \mathbb{R}^d$, for $h \in C(\Omega)$ and $g \in G$, let $h_g \in C(\Omega)$ be defined by $h_g(\omega) = h(\omega g)$, $\omega \in \Omega$. If the domain Ω and the subspace $\mathcal{V} \subseteq C(\Omega)$ are invariant under the action of G, in the sense that

$$\begin{aligned} &\Omega_g := \{\omega g, \omega \in \Omega\} && \text{coincides with } \Omega \text{ for all } g \in G, \\ &\mathcal{V}_g := \{v_g, v \in \mathcal{V}\} && \text{coincides with } \mathcal{V} \text{ for all } g \in G, \end{aligned}$$

then, for any $f \in C(\Omega)$ and any $g \in G$,

$$E_{\mathcal{V}}(f, \Omega) = E_{\mathcal{V}}(f_g, \Omega).$$

Furthermore, if f is invariant under the action of G, i.e., if f_g coincides with f for all $g \in G$, then there is a best approximant v^* to f from $\mathcal{V}$ which is invariant under the action of G, i.e., $v^*_g = v^*$ for all $g \in G$.

Proof. For $f \in C(\Omega)$, let $v' \in \mathcal{V}$ be a best approximant to f from $\mathcal{V}$. The invariance of Ω implies that, for any $g \in G$,

$$\begin{aligned} E_{\mathcal{V}}(f, \Omega) &= \max_{\omega \in \Omega} |f(\omega) - v'(\omega)| = \max_{\omega \in \Omega} |f(\omega g) - v'(\omega g)| = \max_{\omega \in \Omega} |f_g(\omega) - v'_g(\omega)| \\ &\geq E_{\mathcal{V}}(f_g, \Omega), \end{aligned}$$

where the last step relied on the invariance of $\mathcal{V}$ to ensure that $v'_g \in \mathcal{V}$. A similar argument with f_g in place of f and g^{-1} in place of g would yield the reverse inequality $E_{\mathcal{V}}(f_g, \Omega) \geq E_{\mathcal{V}}(f, \Omega)$ and in turn the desired equality. Now, let us assume in addition that $f_g = f$ for all $g \in G$. Using the above, we have $\|f - v'\|_\Omega = \|f - v'_g\|_\Omega$, so that v'_g is also a best approximant to f from $\mathcal{V}$ for all $g \in G$. Consequently, the element $v^* := |G|^{-1} \sum_{g \in G} v'_g \in \mathcal{V}$, as a convex combination of best approximants, is itself a best approximant to f from $\mathcal{V}$. It is also readily seen that v^* thus defined is invariant under the action of G. □

As alluded to before, Propositions 3 and 4 imply that, for the simplex, the cross-polytope, the euclidean ball, and the hypercube, it is enough to consider the monomials m_k where $k \in \mathbb{N}_0^d$ satisfies $k_1 + \cdots + k_d = n$ and $k_1 \geq \cdots \geq k_d \geq 1$. The number of these monomials equals the number of partitions of the integer n into exactly d parts. This number $p_d(n)$ is known to obey the recurrence relation $p_d(n) = p_{d-1}(n-1) + p_d(n-d)$, which allows one to arrange them in a triangular table akin to Pascal's triangle. For instance, for $d = 3$ and $n = 10$, one has $p_3(10) = 8$. For $d = 3$ and $n = 6$, one has $p_3(6) = 3$, with the three partitions being $(4, 1, 1)$, $(3, 2, 1)$, and $(2, 2, 2)$. In case of the cross-polytope, the values of the three corresponding errors of best approximation are reported in the last column of Table 2, none of which were known before.

2.3 Known multivariate Chebyshev polynomials

In this section, we gather previously obtained results about multivariate Chebyshev polynomials for our domains of interest, with the exception of the cross-polytope, which seems to have been cast aside in the literature. We will use from now on the shorthand notation

$$E(k, \Omega) := E_{\mathcal{P}^d_{n-1}}(m_k, \Omega),$$

since considering $k = (k_1, \ldots, k_d)$ with $k_1 + \cdots + k_d = n$ implicitly tells us the value of d and n.

The hypercube. The case of the hypercube, i.e., $\Omega = H$, is completely resolved. Indeed, the geometry of the domain bodes well for calculations involving the tensor products of univariate polynomials $p_1, \ldots, p_d$, as defined by $(p_1 \otimes \cdots \otimes p_d)(x_1, \ldots, x_d) = p_1(x_1) \cdots p_d(x_d)$. It is not difficult to establish the following result by invoking signatures.

Theorem 5. Given $k \in \mathbb{N}^d$ with $k_1 + \cdots + k_d = n$, one has

$$E(k, H) = 2^{-n+d}$$

and a best approximant to m_k from $\mathcal{P}^d_{n-1}$ is given by $m_k - 2^{-n+d} T_{k_1} \otimes \cdots \otimes T_{k_d}$.

This result was proved by several authors, see e.g. [20, 6]. In [22], it has also been shown that $m_k - 2^{-n+d} T_{k_1} \otimes \cdots \otimes T_{k_d}$ is a unique best approximant when and only when $d = 2$ and $k_1 = k_2$.

The euclidean ball. The case of the euclidean ball, i.e., $\Omega = B$, is partially resolved: it is solved for $d = 2$ variables but not completely in $d \geq 3$ variables. With U_ℓ denoting the univariate ℓth degree Chebyshev polynomial of the second kind, the result for $d = 2$ reads as follows.

Theorem 6. Given $k \in \mathbb{N}^2$ with $k_1 + k_2 = n$, one has

$$E(k, B) = 2^{-n+1}$$

and a best approximant to m_k from $\mathcal{P}^2_{n-1}$ is given by $m_k - 2^{-n}(U_{k_1} \otimes U_{k_2} - U_{k_2-2} \otimes U_{k_1-2})$, with the understanding that $U_{-1} = 0$.

This was obtained for the first time in [10]. Other explicit best approximants can be found in [3, 16]. It is also known that the difference between two best approximants has the form $(1 - x_1^2 - x_2^2) q(x_1, x_2)$ for some $q \in \mathcal{P}^2_{n-3}$.

For $d > 2$, best approximants to monomials are known only for a few low-degree instances, such as $m_{(1,\ldots,1)}(x) = x_1 x_2 \cdots x_d$ and $m_{(2,1,\ldots,1)}(x) = x_1^2 x_2 \cdots x_d$, see [1, 2, 23]. Restricting our attention to the case $d = 3$, we now cite some articles and the result they contain:[2,3]

$$\begin{aligned}
[1]: &\quad E((1,1,1), B) = 3^{-3/2}, \\
[2]: &\quad E((2,1,1), B) = (3 - \sqrt{8})/2, \\
[14]: &\quad E((3,1,1), B) = (1-a)(a^3/5)^{1/4}/5, \quad a = \text{smallest root of } 9t^4 - 29t^3 + 24t^2 - 29t + 9, \\
[23]: &\quad E((2,2,2), B) = 1/72, \\
[23]: &\quad E((4,4,4), B) = b^{-1}/27^2, \qquad\qquad b \approx 21.8935834.
\end{aligned}$$

[2]The value of $E((3,1,1), B)$ is implicit in [14, Theorem 2.1.(b)]—deriving the explicit value requires some work.
[3]There was a typographical error concerning the value of $E((4,4,4), B)$ in [23, Theorem 3.2].

The simplex. The case of the simplex, i.e., $\Omega = S$, is also partially resolved. Indeed, for $d = 2$, best approximants to monomials are presented in [15]. The result is recalled below.

Theorem 7. Given $k \in \mathbb{N}^2$ with $k_1 + k_2 = n$, one has

$$E(k, S) = 2^{-2n+1}$$

and a best approximant to m_k from $\mathcal{P}^2_{n-1}$ is given by $m_k - T_{k_1,k_2}$, where

$$T_{k_1,k_2}(x, y) = T_{k_1-k_2}(2x-1)T_{k_2}(8xy-1) + 8xy(2x-1)U_{k_1-k_2-1}(2x-1)U_{k_2-1}(8xy-1)$$

for $k_1 \geq k_2$, with the understanding that $U_{-1} = 0$.

In the case $d = 3$, we mention the results

$$[23]: \qquad E((1, 1, 1), S) = 1/72,$$
$$[23]: \qquad E((2, 2, 2), S) = b^{-1}/27^2, \qquad b \approx 21.8935834.$$

Note that there is a close connection between the best approximants on the simplex S to the monomial $m_k(x) = x_1^{k_1} \cdots x_k^{k_d}$ and the best approximants on the euclidean ball B to the monomial $m_{2k}(x) = x_1^{2k_1} \cdots x_k^{2k_d}$, see [23] for the precise statement.

3 Description of the Computational Procedure

In this section, we explain the procedure that we derived and exploited in order to produce a number of new multivariate Chebyshev polynomials (uncovered in Section 4). Although our implementation, available at `https://github.com/foucart/Multivariate_Chebyshev_Polynomials`, limits itself to the best approximation from $\mathcal{P}^d_{n-1}$ to monomials $m_k \in \mathcal{P}^d_n$ on the hypercube, the euclidean ball, the cross-polytope, and the simplex, the underpinning procedure is more general, as it could handle any polynomial $f \in \mathcal{P}^d_N$, $N \geq n$, instead of m_k, while the domain $\Omega \in \mathbb{R}^d$ could be any (compact with nonempty interior) basic semialgebraic set, meaning that there exist polynomials $g_1, \ldots, g_H$ such that

$$\Omega = \{x \in \mathbb{R}^d : g_1(x) \geq 0, \ldots, g_H(x) \geq 0\}.$$

The strategy is to view the best approximation problem as an instance of the Generalized Moment Problem (GMP), so that we can invoke the Moment-SOS hierarchy designed to solve a GMP whose data are algebraic (polynomials and semialgebraic sets), see [12]. This process leverages a combination of: (i) *semidefinite programming*[4], an efficient machinery in Convex Optimization developed since the late seventies, and (ii) powerful positivity certificates and their dual analogs

[4]A semidefinite program (SDP) is a conic convex optimization problem which can be solved in time polynomial in its input size, up to arbitrary (fixed) precision (e.g. with interior point methods); for more details see e.g. [13].

concerning the moment problem. These two ingredients were not available at the time of pioneering works such as the paper [19] by Rivlin and Shapiro, in which dual formulations were mostly used to prove the existence of optimal solutions and to characterize them. For the numerical computations, we will rely on GlobtiPoly 3, since many of the GMP components are built in this MATLAB/OCTAVE program, see [11].

Let us be more specific about the computation of the error of best approximation by polynomials from $\mathcal{P}^d_{n-1}$ to a polynomial $f \in \mathcal{P}^d_N$, $N \geq n$, i.e., of $E^* := E_{\mathcal{P}^d_{n-1}}(f, \Omega)$, viewed as the optimal value of (4) or of (5). We have already indicated that the program (4)—which we call primal—can be reformulated along the lines of (1). There, the polynomial nonnegativity constraints can be expressed as sum-of-squares constraints, unfortunately not guaranteed to be finite-dimensional. To make the constraints manageable, we force them to be finite-dimensional by way of some integer parameter s. Thus, having strengthen the constraints, we obtain an upper bound ub_s for E^*. The sequence of $(\mathrm{ub}_s)_{s\in\mathbb{N}}$ of upper bounds can be shown to be monotone nonincreasing and convergent to E^*. As for the program (5)—which we call dual—it produces alongside a nondecreasing sequence $(\mathrm{lb}_t)_{t\in\mathbb{N}}$ of lower bounds converging to E^*, which is to be justified in greater details in Theorem 8 below. These ideas have been implemented in the commands ChebPoly_primal and ChebPoly_dual and we emphasize that a precise estimation of the error of best approximation through $\mathrm{lb}_t \leq E^* \leq \mathrm{ub}_s$ is already available at this point. But the situation is more favorable than that: it often happens that the convergence of ub_s and lb_t occurs in a finite number of steps, which seems to be the case for the problem at hand. Lacking an *a priori* knowledge of the necessary number of steps, we compute ub_s and lb_t until these quantities stabilize, i.e., until $\mathrm{ub}_{s+1} = \mathrm{ub}_s$ and $\mathrm{lb}_{t+1} = \mathrm{lb}_t$. Actually, we do not need theoretical guarantees that this stabilization occurs either. Indeed, the process only serves as a *prediction* phase in our workflow, providing candidates for a best approximant v^* and a signature σ, as output by ChebPoly_primal and ChebPoly_dual, respectively. Then comes a *verification* phase, where the candidates v^* and σ (maybe cleaned up of numerical inaccuracies and imported into a symbolic system) can be verified to be genuine best approximant and associated signature by invoking Theorem 2.

To finish the description of our computational procedure, we deem it appropriate to present an explanation of the arguments underpinning the hierarchy of semidefinite programs which is at the heart of our optimization-aided strategy for tackling the best approximation problem. In view of our preference for the dual formulation (5), we outline the moment-based methodology at stake here—the complete justification in the most general setting can be found in [21], as well as the sum-of-squares-based methodology. The forthcoming details can be useful for solving the hierarchy with an arbitrary semidefinite solver. They are not fully necessary in GlobtiPoly 3, as the latter offers a more user-friendly way to formulate the problem. Another advantage of GlobtiPoly 3 is that, in addition to outputting moments, it can also extract the atomic measure they came from, i.e., the signature we are looking for. In the formal statement below, the matrices $\mathrm{Hank}_t(y)$ and $\mathrm{Hank}_\infty(y)$ built from an infinite sequence y indexed by $\mathbb{N}_0^d$ are the $\binom{t+d}{d} \times \binom{t+d}{d}$ and infinite Hankel matrices with entries y_{i+j}, $i, j \in \mathbb{N}_0^d$ with $|i|, |j| \leq t$ and $i, j \in \mathbb{N}_0^d$, respectively. As for the operators G_h defined on $\mathbb{R}^{\mathbb{N}_0^d}$, they represent the linear maps transforming the sequence of moments of a Borel measure ν into the sequence of moments of the Borel measure $g_h \times \nu$, so that $(G_h y)_\ell = \sum_{|\ell'| \le \deg(g_h)} \mathrm{coeff}_{m_{\ell'}}(g_h) y_{\ell+\ell'}$ for any $\ell \in \mathbb{N}_0^d$.

Theorem 8. Given a semialgebraic set $\Omega = \{x \in \mathbb{R}^d : g_1(x) \ge 0, \ldots, g_H(x) \ge 0\}$ and a polynomial $f \in \mathcal{P}_N^d$, $N \ge n$, the error of best approximation to f from $\mathcal{P}_{n-1}^d$ relative to Ω is equal to

$$E_{\mathcal{P}_{n-1}^d}(f, \Omega) = \lim_{t \to \infty} \mathrm{lb}_t,$$

where the nondecreasing sequence (lb_t) contains the optimal values of the following finite-dimensional semidefinite programs, parametrized by $t \ge N + \max\{n_1', \ldots, n_H'\}$, $n_h' := \lceil \deg(g_h)/2 \rceil$:

$$\underset{y^\pm}{\text{maximize}} \sum_{|\ell| \le N} \mathrm{coeff}_{m_\ell}(f)(y_\ell^+ - y_\ell^-) \qquad \text{s.to } \; y_\ell^+ - y_\ell^- = 0 \text{ for } |\ell| \le n-1, \;\; y_0^+ + y_0^- = 1,$$
$$\text{and} \quad \mathrm{Hank}_t(y^\pm) \succeq 0, \mathrm{Hank}_{t-n_1'}(G_1 y^\pm) \succeq 0, \ldots, \mathrm{Hank}_{t-n_H'}(G_H y^\pm) \succeq 0.$$

Proof (Sketch). From the dual representation (5) for the error of best approximation and from the identification of linear functionals $\lambda \in C(\Omega)^*$ with Borel measures μ on Ω via $\lambda(g) = \int_\Omega g d\mu$, $g \in C(\Omega)$, we arrive at

$$E_{\mathcal{P}_{n-1}^d}(f, \Omega) = \sup_\mu \int_\Omega f d\mu \qquad \text{s.to} \int_\Omega m_\ell d\mu = 0 \quad \text{for } |\ell| \le n-1 \quad \text{and} \quad \int_\Omega d|\mu| = 1.$$

Next, we consider the Jordan decomposition of μ as $\mu^+ - \mu^-$ where μ^+, μ^- are nonnegative Borel measures on Ω, so that $|\mu| = \mu^+ + \mu^-$. We think of these nonnegative Borel measures through their infinite sequences of moments given by

$$y_\ell^\pm = \int m_\ell d\mu^\pm, \qquad \ell \in \mathbb{N}_0^d.$$

The multivariate Hamburger moment problem establishes a one-to-one correspondence between sequences of moments of a nonnegative Borel measures ν on $\mathbb{R}^d$ and sequences $y \in \mathbb{R}^{\mathbb{N}_0^d}$ satisfying $\mathrm{Hank}_\infty(y) \succeq 0$. The same holds for nonnegative Borel measures ν supported on Ω provided one adds localization conditions entailing to the fact that $g_1 \times \nu, \ldots, g_H \times \nu$, too, must be nonnegative Borel measures. Altogether, this yields

$$E_{\mathcal{P}_{n-1}^d}(f, \Omega) = \sup_{y^\pm \in \mathbb{R}^{\mathbb{N}_0^d}} \sum_{|\ell| \le N} \mathrm{coeff}_{m_\ell}(f)(y_\ell^+ - y_\ell^-) \quad \text{s.to } y_\ell^+ - y_\ell^- = 0 \text{ for } |\ell| \le n-1, \;\; y_0^+ + y_0^- = 1,$$
$$\text{and} \quad \mathrm{Hank}_\infty(y^\pm) \succeq 0, \mathrm{Hank}_\infty(G_1 y^\pm) \succeq 0, \ldots, \mathrm{Hank}_\infty(G_H y^\pm) \succeq 0.$$

The semidefinite program announced in the statement of the theorem is a truncation of the above infinite-dimensional program to a finite-dimensional one at a level $t \in \mathbb{N}$ large enough to involve all the moments $\mu_\ell^\pm$, $|\ell| \le N$, into each Hankel matrix. The nondecreasingness of (lb_t) owes to the fact that finite sequences $y^\pm$ optimal for lb_t generate, when padded with zeroes, feasible sequences for lb_{t+1}, hence $\mathrm{lb}_{t+1} \ge \mathrm{lb}_t$. The justification that lb_t converges to $E_{\mathcal{P}_{n-1}^d}(f, \Omega)$ as $t \to \infty$ involves lengthy technicalities and is not sketched here. □

4 New Explicit Results

In this section, we present the discoveries that were made by exploiting the computational procedure just described. In particular, we consider the situation of $d = 3$ variables and give the values of the errors of best approximation from $\mathcal{P}^3_{n-1}$ to (essentially) all monomials m_k of degree n up to 6. Excluding the already settled case where Ω is the hypercube, we report, from largest to smallest Ω, on the cases of the euclidean ball, the cross-polytope, and the simplex in Tables 1, 2, and 3, respectively. The corresponding numerical values can be reproduced by running the codes made available on `https://github.com/foucart/Multivariate_Chebyshev_Polynomials`. In a few instances, we could even distill explicit expressions for previously unknown Chebyshev polynomials.

4.1 The euclidean ball

When $\Omega = B$, the values of $E(k, \Omega)$ had earlier been found when $|k| = 3$ and $|k| = 4$, but not for $|k| = 5$ (except $k = (3, 1, 1)$) nor $|k| = 6$ (except $k = (2, 2, 2)$). All these values are shown in Table 1.

degree $n = 3$ ($\times 10^{-1}$)	degree $n = 4$ ($\times 10^{-2}$)	degree $n = 5$ ($\times 10^{-2}$)	degree $n = 6$ ($\times 10^{-2}$)
$E(1,1,1),B) \approx 1.924$	$E((2,1,1),B) \approx 8.578$	$E((3,1,1),B) \approx 4.016$	$\mathbf{E((4,1,1),B) \approx 1.923}$
		$\mathbf{E((2,2,1),B) \approx 3.630}$	$\mathbf{E((3,2,1),B) \approx 1.652}$
			$E((2,2,2),B) \approx 1.388$

Table 1: Euclidean ball in dimension $d = 3$: the previously unknown values are shown in boldface.

In the case $k = (2, 2, 1)$, it was possible to recognize (part of) the signature points, which led us to deriving a Chebyshev polynomial explicitly. The result reads as follows.

Theorem 9. With $a := \max\left\{(1 + t)^2(1 - t)t/(4(1 + 4t + 4t^2)), t \in [0, 1]\right\} \approx 3.63000825 \times 10^{-2}$, the error of best approximation on the euclidean ball to $m_{(2,2,1)}(x_1, x_2, x_2) = x_1^2 x_2^2 x_3$ by trivariate polynomials of degree at most 4 is

$$E_{\mathcal{P}^3_4}(m_{(2,2,1)}, B) = a,$$

while a Chebyshev polynomial is given by

$$P(x) = m_{(2,2,1)}(x_1, x_2, x_2) + a\, T_3(x_3),$$

where $T_3(t) = 4t^3 - 3t$ is the univariate Chebyshev polynomial of degree 3.

Proof. Guided by our computational procedure, we make the guess—which we are about to verify—

that a signature has support $\mathcal{S} = \mathcal{S}^+ \cup \mathcal{S}^-$, where $\mathcal{S}^- = -\mathcal{S}^+$ and

$$\mathcal{S}^+ = \left\{ \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} \sqrt{3}/2 \\ 0 \\ -1/2 \end{pmatrix}, \begin{pmatrix} -\sqrt{3}/2 \\ 0 \\ -1/2 \end{pmatrix}, \begin{pmatrix} 0 \\ \sqrt{3}/2 \\ -1/2 \end{pmatrix}, \begin{pmatrix} 0 \\ -\sqrt{3}/2 \\ -1/2 \end{pmatrix}, \right.$$
$$\left. \begin{pmatrix} \sqrt{(1-\tau^2)/2} \\ \sqrt{(1-\tau^2)/2} \\ \tau \end{pmatrix}, \begin{pmatrix} \sqrt{(1-\tau^2)/2} \\ -\sqrt{(1-\tau^2)/2} \\ \tau \end{pmatrix}, \begin{pmatrix} -\sqrt{(1-\tau^2)/2} \\ -\sqrt{(1-\tau^2)/2} \\ \tau \end{pmatrix}, \begin{pmatrix} \sqrt{(1-\tau^2)/2} \\ -\sqrt{(1-\tau^2)/2} \\ \tau \end{pmatrix} \right\}.$$

For reasons soon to become apparent, the parameter $\tau \approx 0.4052$ is chosen as the maximizer of $(1+t)^2(1-t)t/(4(1+4t+4t^2))$ over $t \in [0,1]$, so that $(1+\tau)^2(1-\tau)\tau/4 = a(1+4\tau+4\tau^2)$. Multiplying throughout by $(1-\tau)$ yields $((1-\tau^2)/2)^2\tau = a(1-T_3(\tau))$. As for best approximants to $m_{(2,2,1)}$ from $\mathcal{P}_4^3$, we shall show, in two steps, that $p^*(x_1,x_2,x_3) := -aT_3(x_3)$ is one of them.

The first step consists in proving that $|(m_{(2,2,1)} - p^*)(x)| = \|m_{(2,2,1)} - p^*\|_B$ for all $x \in \mathcal{S}$. To see this, we start by noticing that $(m_{(2,2,1)} - p^*)(x) = a$ for all $x \in \mathcal{S}^+$—this is a simple verification by plugging in the values $x \in \mathcal{S}^+$ into $(m_{(2,2,1)} - p^*)(x)$, but we emphasize that $(m_{(2,2,1)} - p^*)(\pm\sqrt{1-\tau^2}, \pm\sqrt{1-\tau^2}, \tau) = ((1-\tau^2)/2)^2\tau + aT_3(\tau) = a$ owes to our choice of τ. Then, from $\mathcal{S}^- = -\mathcal{S}^+$ and the oddity of $m_{(2,2,1)}$, it follows that $(m_{(2,2,1)} - p^*)(x) = -a$ for all $x \in \mathcal{S}^-$. All in all, we arrived at $|(m_{(2,2,1)} - p^*)(x)| = a$ for all $x \in \mathcal{S}$. Next, we claim that $|(m_{(2,2,1)} - p^*)(x)| \le a$ for all $x \in B$. By the oddity of $m_{(2,2,1)}$ again, it is enough to establish, for all $x \in B$, that $(m_{(2,2,1)} - p^*)(x) \le a$, i.e., that $x_1^2x_2^2x_3 \le a(1-T_3(x_3))$. If $x_3 \in [-1,0]$, this is clear. If $x_3 \in [0,1]$, it relies on the definition of a in the last inequality of the chain

$$\begin{aligned} x_1^2x_2^2x_3 &\le \frac{(x_1^2+x_2^2)^2}{4}x_3 \le \frac{(1-x_3^2)^2}{4}x_3 = (1-x_3)\left[\frac{(1+x_3)^2(1-x_3)x_3}{4}\right] \\ &\le (1-x_3)\Big[a(1+4x_3+4x_3^2)\Big] = a(1-T_3(x_3)). \end{aligned}$$

Altogether, we have obtained $|(m_{(2,2,1)} - p^*)(x)| = \|m_{(2,2,1)} - p^*\|_B = a$ for all $x \in \mathcal{S}$, as announced.

The second step comprises showing that $\|m_{(2,2,1)} - p\|_B \ge a$ for any $p \in \mathcal{P}_4^3$, or in fact for some best approximant p to $m_{(2,2,1)}$ from $\mathcal{P}_4^3$. Let us momentarily take for granted that $v = p^* - p$ satisfies $v(x) \ge 0$ for some $x \in \mathcal{S}^+$. With the help of this $x \in \mathcal{S}^+$, we derive

$$\|m_{(2,2,1)} - p\|_B \ge (m_{(2,2,1)} - p)(x) = (m_{(2,2,1)} - p^*)(x) + (p^* - p)(x) = a + v(x) \ge a,$$

as desired. Thus, it remains to justify that existence of $x \in \mathcal{S}^+$ such that $v(x) \ge 0$. According to Proposition 4, the best approximant p can be chosen to inherit properties of $m_{(2,2,1)}$, in particular being odd in x_3, even in x_1 and x_2, and symmetric when swapping x_1 and x_2. Therefore, one can choose p to contain only the terms x_3, x_3^3, and $(x_1^2+x_2^2)x_3$, and when restricted to the boundary of B, it contains only the terms x_3 and x_3^3, just like p^*. As a consequence, we write, for some $c, d \in \mathbb{R}$, $v(x) = cx_3 + dx_3^3$ for all $x \in \mathcal{S}^+$. Now assume by contradiction that $v(x) < 0$ for all $x \in \mathcal{S}^+$. This translates, after simplification, into $c + d < 0$, $-4c - d < 0$, and $\tau^{-2}c + d < 0$. Adding the second to the first yields $-3c < 0$, while adding the second to the third yields $(\tau^{-2} - 4)c < 0$, which is impossible since $\tau^{-2} \approx 6.088 > 4$. Thanks to this contradiction, the proof is complete. □

We have seen that the signature in the above proof was supported on the boundary of the ball. As a matter of fact, this is a phenomenon we noticed in all cases (where we could extract signatures). We thus conjecture that, for the approximation of monomials on the euclidean ball, signatures actually live on the sphere.

4.2 The cross-polytope

To the best of our knowledge, Chebyshev polynomials relative to the cross-polytope have not been investigated in the literature, hence the values of $E(k, C)$ reported in Table 2 seem to all be new. As expected, they are smaller than the values of $E(k, B)$ presented in Table 1 and larger than the values of $E(k, S)$ shown in Table 3.

degree $n = 3$ ($\times 10^{-2}$)	degree $n = 4$ ($\times 10^{-2}$)	degree $n = 5$ ($\times 10^{-3}$)	degree $n = 6$ ($\times 10^{-3}$)
$\mathbf{E((1,1,1),C) \approx 3.703}$	$\mathbf{E((2,1,1),C) \approx 1.273}$	$\mathbf{E((3,1,1),C) \approx 4.764}$	$\mathbf{E((4,1,1),C) \approx 1.853}$
		$\mathbf{E((2,2,1),C) \approx 3.398}$	$\mathbf{E((3,2,1),C) \approx 1.087}$
			$\mathbf{E((2,2,2),C) \approx 0.661}$

Table 2: Cross-polytope in dimension $d = 3$: all values were previously unknown.

4.3 The simplex

When $\Omega = S$, the values of $E(k, \Omega)$ had earlier been found when $|k| = 3$, but not for $|k| = 4$, $|k| = 5$, and $|k| = 6$ (except $k = (2, 2, 2)$). All these values are shown in Table 3. It appears empirically that signatures (when they could be extracted) live on the boundary of the domain, and more precisely here on the face of equation $x_1 + x_2 + x_3 = 1$. Note that this would imply, due to the close connection between the approximation of m_k on S and the approximation of m_{2k} on B, some particular cases of the conjecture relative to B.

degree $n = 3$ ($\times 10^{-2}$)	degree $n = 4$ ($\times 10^{-3}$)	degree $n = 5$ ($\times 10^{-4}$)	degree $n = 6$ ($\times 10^{-4}$)
$E((1,1,1),S) \approx 1.388$	$\mathbf{E((2,1,1),S) \approx 2.688}$	$\mathbf{E((3,1,1),S) \approx 5.984}$	$\mathbf{E((4,1,1),S) \approx 1.405}$
		$\mathbf{E((2,2,1),S) \approx 4.695}$	$\mathbf{E((3,2,1),S) \approx 1.000}$
			$E((2,2,2),S) \approx 0.6265$

Table 3: Simplex in dimension $d = 3$: the previously unknown values are shown in boldface.

In the case $k = (2,1,1)$, we could use the insight brought forward by our computations to derive a Chebyshev polynomial explicitly. The result reads as follows.

Theorem 10. With $\tau \in [0,1/4]$ being the solution to $\max\big\{y(1-2y)(y-\tau)^2, y \in [0,1/2]\big\} = \tau^2/18$ and with $c := -3/\tau$, the error of best approximation on the simplex to $m_{(2,1,1)}(x_1,x_2,x_3) = x_1^2 x_2 x_3$ by trivariate polynomials of degree at most 3 is

$$E_{\mathcal{P}_3^3}(m_{(2,1,1)}, S) = \frac{1}{2c^2},$$

while a Chebyshev polynomial is given by

$$\begin{aligned} P(x) &= x_1^2 x_2 x_3 \\ &\quad + \frac{1}{2c^2}\left[-16x_1^2(x_2+x_3) + 16x_1(x_2+x_3)^2 - 2(64+12c+c^2)x_1x_2x_3 + 8x_2x_3 - 2(x_2+x_3) + 1\right]. \end{aligned}$$

Proof. Guided by our computational procedure, we make the guess—which we are about to verify—that there is a signature with support $\mathcal{S} = \mathcal{S}^+ \cup \mathcal{S}^-$, where

$$\mathcal{S}^+ = \left\{ \begin{pmatrix}1/4\\3/4\\0\end{pmatrix}, \begin{pmatrix}1/4\\0\\3/4\end{pmatrix}, \begin{pmatrix}0\\1/2\\1/2\end{pmatrix}, \begin{pmatrix}1\\0\\0\end{pmatrix}, \begin{pmatrix}1-2\tau\\\tau\\\tau\end{pmatrix} \right\},$$

$$\mathcal{S}^- = \left\{ \begin{pmatrix}3/4\\1/4\\0\end{pmatrix}, \begin{pmatrix}3/4\\0\\1/4\end{pmatrix}, \begin{pmatrix}0\\0\\1\end{pmatrix}, \begin{pmatrix}0\\1\\0\end{pmatrix}, \begin{pmatrix}1-2\sigma\\\sigma\\\sigma\end{pmatrix} \right\}.$$

The parameters $\tau, \sigma \in [0,1/2]$ are considered free for now—their specific choice will be revealed later.

The first step consists in proving that $|P(x)| = \|P\|_S$ for all $x \in \mathcal{S}$. To this end, we start by proving that $\|P\|_S \le 1/(2c^2)$, i.e., that $|P(x_1,x_2,x_3)| \le 1/(2c^2)$ whenever $x_1,x_2,x_3 \ge 0$ and $x_1+x_2+x_3 \le 1$. This is easy to see if $x_1 = 0$, since then $2c^2\,P(0,x_2,x_3) = 8x_2x_3 - 2(x_2+x_3)+1$ is bounded as

$$\begin{cases} \ge -2(x_2+x_3)+1 \ge -2+1 & = -1, \\ \le 2(x_2+x_3)^2 - 2(x_2+x_3) + 1 & \le 1. \end{cases}$$

Using the fact that $8t(1-2t) \le 1$ for all $t \in \mathbb{R}$, it is also easy to see that $|P(x_1,x_2,x_3)| \le 1/(2c^2)$ if $x_2 = 0$ or $x_3 = 0$, since, e.g., $2c^2\,P(x_1,x_2,0) = -16x_1^2x_2 + 16x_1x_2^2 - 2x_2 + 1$ is

$$= \begin{cases} -2x_1[8x_2(x_1-x_2)] - 2x_2 + 1 & \ge & -2x_1[8x_2(1-2x_2)] - 2x_2 + 1 \ge -2x_1 - 2x_2 + 1 \ge -1, \\ 2x_2[8x_1(x_2-x_1)] - 2x_2 + 1 & \le & 2x_2[8x_1(1-2x_1)] - 2x_2 + 1 \le 2x_2 - 2x_2 + 1 = 1. \end{cases}$$

We therefore consider the case where x_1,x_2,x_3 are all nonzero and we notice that we can assume $x_2 = x_3$. Indeed, if we reparametrize by setting $y = (x_2+x_3)/2$ and $z = (x_2-x_3)/2$, so that

$x_2x_3 = y^2 - z^2$, then the expression for $P(x)$ becomes

$$(7)\qquad \begin{aligned} P(x) &= x_1^2y^2 + \frac{1}{2c^2}\left[-32x_1^2y + 64x_1y^2 - 2(64+12c+c^2)x_1y^2 + 8y^2 - 4y + 1\right] \\ &\quad - x_1^2z^2 + \frac{1}{2c^2}\left[\qquad\qquad 2(64+12c+c^2)x_1z^2 - 8z^2 \qquad\qquad \right] \\ &= \frac{1}{2c^2}\left[2c^2x_1^2y^2 - 32x_1^2y - 2(32+12c+c^2)x_1y^2 + 8y^2 - 4y + 1\right] - z^2q(x_1) \end{aligned}$$

for some univariate quadratic polynomial q. Thus, given $x \in S$ such that $|P(x)| = \|P\|_S$ and $t \in \mathbb{R}$ small enough, we define $x^{(t)} \in S$ by $x_1^{(t)} = x_1$, $x_2^{(t)} = x_2 + t$, and $x_3^{(t)} = x_3 - t$. In view of $(x_2^{(t)} + x_3^{(t)}) = (x_2 + x_3)/2 =: y$ and of $(x_2^{(t)} - x_3^{(t)}) = (x_2 - x_3)/2 + t =: z + t$, while supposing e.g. that $P(x) > 0$, the inequality $P(x^{(t)}) \le P(x)$ reads $P(x_1, y, y) - (z+t)^2q(x_1) \le P(x_1, y, y) - z^2q(x_1)$ whenever $|t|$ is small enough. This implies that $zq(x_1) = 0$, hence that $P(x) = P(x_1, y, y)$, meaning that the last two coordinates of an extremal point can be assumed to be equal, as claimed. Now, to determine the maximum of $|P(x_1, y, y)|$ when $x_1, y \ge 0$ and $x_1 + 2y \le 1$, we recall from (7) that

$$(8)\qquad P(x_1, y, y) = \frac{1}{2c^2}\left[2c^2x_1^2y^2 - 32x_1^2y - 2(32+12c+c^2)x_1y^2 + 8y^2 - 4y + 1\right],$$

so that

$$\frac{\partial P(x_1, y, y)}{\partial y} = \frac{1}{2c^2}\left[4c^2x_1^2y - 32x_1^2 - 4(32+12c+c^2)x_1y + 16y - 4\right].$$

As a consequence, at a critical point, we have $(32+12c+c^2)x_1y = c^2x_1^2y - 8x_1^2 + 4y - 1$ and in turn

$$P(x_1, y, y) = \frac{1}{2c^2}\left[-16x_1^2y - 2y + 1\right].$$

It follows that $|P(x_1, y, y)| \le 1/(2c^2)$ at any critical point, since $[-16x_1^2y - 2y + 1] \le 1$ is clear, while $[-16x_1^2y - 2y + 1] \ge -1$ holds because $16x_1^2y + 2y = 2y(8x_1^2 + 1) \le (1 - x_1)(8x_1^2 + 1)$, the latter having maximal value $(68 + 5\sqrt{10})/54 \approx 1.5520 \le 2$ over $x_1 \in [0, 1]$. At this point, it remains to verify that $|P(x_1, y, y)| \le 1/(2c^2)$ on the boundary of the domain $\{x_1 \ge 0, y \ge 0, x_1 + 2y \le 1\}$. Since the cases $x_1 = 0$ and $y = 0$ have already been dealt with, we need to consider the case $x_1 = 1 - 2y$, $y \in [0, 1/2]$. After some technical calculations left to the reader, starting from (8) and recalling that $\tau = -3/c$, we arrive at

$$(9)\qquad P(1-2y, y, y) = \frac{1}{2c^2} - 2y(1-2y)(y-\tau)^2, \qquad y \in [0, 1/2].$$

The inequality $P(1 - 2y, y, y) \le 1/(2c^2)$ is obvious from here. The parameter τ is chosen to secure the other inequality $P(1 - 2y, y, y) \ge -1/(2c^2)$, which is equivalent to $y(1 - 2y)(y - \tau)^2 \le 1/(2c^2)$ for all $y \in [0, 1/2]$ and thus follows from the equation $\max\left\{y(1-2y)(y-\tau)^2, y \in [0, 1/2]\right\} = \tau^2/18$. Note that this equation has a (unique) solution in $[0, 1/4]$, because $\tau^2/18$ increases from 0 to 1/288 on this interval and $\max\left\{y(1-2y)(y-\tau)^2, y \in [0, 1/2]\right\}$ decreases from a positive quantity to 1/512 there. In consequence, we have now established that $|P(x)| \le 1/(2c^2)$ for all $x \in S$, as announced. Let us turn to the justification that $|P(x)| = 1/(2c^2)$ for all signature points $x \in \mathcal{S} = \mathcal{S}^+ \cup \mathcal{S}^-$. From (9), we immediately see that $P(x) = 1/(2c^2)$ for the last three points of $\mathcal{S}^+$. The fact that

$P(x) = -1/(2c^2)$ for the last point of $\mathcal{S}^-$ is due to the choice of σ, as we take it to be the maximizer of $y(1-2y)(y-\tau)^2$ over $y \in [0, 1/2]$, ensuring that $\sigma(1-2\sigma)(\sigma-\tau)^2 = 1/(2c^2)$ and hence that $P(1-2\sigma, \sigma, \sigma) = -1/(2c^2)$. As for the other signature points, notice that they are of the form $(1-y, y, 0)$ or $(1-y, 0, y)$, for which technical calculations left to the reader yield

$$P(1-y, y, 0) = P(1-y, 0, y) = -\frac{1}{2c^2} T_3(2y-1), \qquad y \in [0, 1],$$

where, as usual, $T_3(t) = 4t^3 - 3t$ is the univariate Chebyshev polynomial of degree 3. It then easily follows that $P(x) = 1/(2c^2)$ for the first two points of $\mathcal{S}^+$ and that $P(x) = -1/(2c^2)$ for the first four points of $\mathcal{S}^-$. Altogether, we have now obtained $|P(x)| = \|P\|_S = 1/(2c^2)$ for all $x \in \mathcal{S}$, as announced.

The second step consists in proving that $\|m_{(2,1,1)} - p\|_S \geq 1/(2c^2)$ for any $p \in \mathcal{P}_3^3$. To this end, we notice that all signature points $x \in \mathcal{S}$ lie on the face $\mathcal{F} := \{x_1 \geq 0, x_2 \geq 0, x_3 \geq 0, x_1 + x_2 + x_3 = 1\}$ and we remark that $\{(x_1, x_2) : x \in \mathcal{S}\}$ is the support of an extremal signature for $\mathcal{P}_3^2$ associated with $P_{|\mathcal{F}}$, in the sense that there exist $c_x > 0$, $x \in \mathcal{S}$, such that $\sum_{x \in \mathcal{S}} c_x \operatorname{sgn}(P(x))\, r(x_1, x_2) = 0$ for all $r \in \mathcal{P}_3^2$. This can be verified (numerically) by looking at the null space of the 10×10 matrix with entry $\operatorname{sgn}(P(x)) m_{(k_1,k_2)}(x_1, x_2)$ on the row indexed by (k_1, k_2) with $k_1 + k_2 \leq 3$ and on the column indexed by $x \in \mathcal{S}$. Theorem 2 could now be invoked. Alternatively, given $p \in \mathcal{P}_3^3$, we can write $m_{(2,1,1)} - p = P - q$ for some $q \in \mathcal{P}_3^3$ and consider an $x \in \mathcal{S}$ such that $\operatorname{sgn}(P(x))\, q(x) \leq 0$, which is possible for otherwise $\sum_{x \in \mathcal{S}} c_x \operatorname{sgn}(P(x))\, q(x_1, x_2, 1 - x_2 - x_3) = 0$ would be violated. In this way, the desired inequality follows from

$$\|m_{(2,1,1)} - p\|_S \geq |P(x) - q(x)| \geq |P(x)| = \frac{1}{2c^2}.$$

The proof is now complete. □

Remark. The numerical values of the parameters τ and σ are $\tau \approx 0.21998$ and $\sigma \approx 0.41942$, leading to the error of best approximation the numerical value $E_{\mathcal{P}_3^3}(m_{(2,1,1)}, S) \approx 2.68850 \times 10^{-3}$. In fact, it can be shown (a computer algebra system will facilitate the task) that τ is the smallest real root of the quartic polynomial $2880t^4 - 5472t^3 + 4880t^2 - 1944t + 243$.

5 Conclusion

In this article, we proposed a semidefinite-programming method to compute best approximants to monomials by multivariate polynomials of lower degree. More than providing numerical values, the method allows us to make guesses for the multivariate analogs of Chebyshev polynomials that can—sometimes—be *a posteriori* certified explicitly or symbolically. Of note, the generic nonuniqueness of such analogs prompted us to preferentially solve the dual optimization program, putting the classical notion of signature at center stage. We emphasize that the underlying methodology is quite versatile and should enable to attack other problems in multivariate Approximation Theory by relying on modern tools from Optimization Theory, so long as one is ready to give up on purely analytical solutions. This is a point of view already brought forward by a subset of the authors to determine minimal projections (exploiting moments, see [7]) and Chebyshev polynomials associated to union of intervals (exploiting sums-of-squares, see [8]). In the multivariate setting, we should also be able to deal with unions of domains, as well as tackling norms other than L_∞ (notably L_1 and L_{2m}, $m \in \mathbb{N}$), adding convex constraints (e.g. interpolatory, shape-enforcing, etc), in the spirit of the proof-of-concept software Basc, short for 'Best Approximations by Splines under Constraints', see [9]. We note, though, that the semidefinite programs encountered in Basc could only be handled thanks to the benefits of representing univariate polynomials in the Chebyshev basis rather than in the monomial basis, so a similar approach should be taken in the multivariate setting. This is indeed realizable, at least in theory, and we give pointers on how to do this in some supplementary material. Still, bringing Basc to the multivariate realm will be a mighty task, but certainly one worth taking by a fresh generation of approximators/optimizers.

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