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Optimization-Aided Construction of Multivariate Chebyshev Polynomials

M. Dressler*, S. Foucart†, M. Joldes‡, E. de Klerk§, J. B. Lasserre¶, and Y. Xu||

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 monomials 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.

AMS classification: 41A10, 65D15, 90C22.

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 n th 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 $\text{coeff}_{x^n}(p) = 2^{n-1}$ —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 $\text{coeff}_{x^n}(p) = 2^{n-1}$ —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 $k = 1, 2, \dots, n$ —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 $k = 2, \dots, n$;
- T_n is the polynomial with the largest growth outside $[-1, 1]$, i.e., for every $t \notin [-1, 1]$ and every $k = 0, 1, \dots, n$, T_n maximizes $|p^{(k)}(t)|$ over all polynomials $p \in \mathcal{P}_n$ satisfying $\|p\|_{[-1,1]} \leq 1$;
- 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 [21] 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

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

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

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

The added constraints are polynomial nonnegativity constraints and, as such, can conceivably be dealt with using sum-of-squares (SOS) techniques. In fact, as clarified later, we will advantageously use the dual facet of the Moment-SOS hierarchy [14] 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

$$\deg \left(\sum_{k=(k_1, \dots, k_d)} c_{k_1, \dots, k_d} x_1^{k_1} \cdots x_d^{k_d} \right) = \max_{k: c_k \neq 0} |k|, \quad \text{where } |k| = k_1 + \cdots + k_d;$$

- 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

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

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

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

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

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

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

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 Knowledge

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 n th degree monomial and where \mathcal{V} is the space \mathcal{P}_{n-1}^d , 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

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

A folklore result in Approximation Theory shows that the latter can alternatively be expressed as a maximum, namely as

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

In optimization custom, this is viewed as a strong duality result, whose proof is informative to sketch here. To start, the inequality that the maximum in (5) does not exceed the minimum in (4) simply follows from the fact that, for any feasible $v \in \mathcal{V}$ and $\lambda \in C(\Omega)^*$, one has

$$\lambda(f) = \lambda(f - v) \leq \|\lambda\|_{C(\Omega)^*} \|f - v\|_{\Omega} = \|f - v\|_{\Omega}.$$

Next, for the reverse inequality, given a best approximant v^* , consider the linear functional $\tilde{\lambda}$ defined on $\mathcal{V}_f := \mathcal{V} \oplus \mathbb{R}f$ by

$$\tilde{\lambda}(v + tf) = t\|f - v^*\|_{\Omega}, \quad v \in \mathcal{V}, \quad t \in \mathbb{R}.$$

This linear functional has norm one: indeed, setting aside the trivial case $t = 0$, one has

$$|\tilde{\lambda}(v + tf)| = |t| \|f - v^*\|_{\Omega} \leq |t| \|f - (-v/t)\|_{\Omega} = \|v + tf\|_{\Omega},$$

with equality for $t = 1$ and $v = -v^*$. Therefore, by the Hahn–Banach extension theorem, there exists a linear functional λ defined on $C(\Omega)$ such that $\|\lambda\|_{C(\Omega)^*} = 1$ and $\lambda|_{\mathcal{V}_f} = \tilde{\lambda}|_{\mathcal{V}_f}$, implying in

particular $\lambda|_{\mathcal{V}} = 0$. The maximum in (5) is then larger than or equal to $\lambda(f) = \tilde{\lambda}(f) = \|f - v^*\|_{\Omega}$, i.e., than the minimum in (4). This concludes the sketch of strong duality.

It is worth commenting on the form of the Hahn–Banch extension λ in the above argument. To do so, we notice that the linear functional $\tilde{\lambda} \in \mathcal{V}_f^*$ is expressed as a convex combination of L extreme points of the unit ball of \mathcal{V}_f^* , where one can take $L \leq \dim(\mathcal{V}_f) + 1$ by applying Krein–Milman and Carathéodory theorems. Since the extreme points of the unit ball of \mathcal{V}_f^* 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 , we can write $\tilde{\lambda} = \sum_{\ell=1}^L \tau_{\ell} \varepsilon_{\ell} \delta_{\omega_{\ell}}|_{\mathcal{V}_f}$ with $\omega_1, \dots, \omega_L \in \Omega$, $\varepsilon_1, \dots, \varepsilon_L = \pm 1$, and $\tau_1, \dots, \tau_L > 0$ satisfying $\sum_{\ell=1}^L \tau_{\ell} = 1$. It is then clear that the Hahn–Banach extension λ can be chosen as $\lambda = \sum_{\ell=1}^L \tau_{\ell} \varepsilon_{\ell} \delta_{\omega_{\ell}}$. Of note, the estimation of L can be refined to $L \leq \dim(\mathcal{V}_f)$ by calling upon Theorem 2.13 from Rivlin’s book [21], which states that a norm-one linear functional on a real finite-dimensional subspace \mathcal{U} of $C(\Omega)$ can be expressed as a convex combination of $L \leq \dim(\mathcal{U})$ extreme points of the unit ball of \mathcal{U}^* . In the particular case $\mathcal{U} = \mathcal{P}_k^d$, it equates to Tchakaloff’s theorem and its generalizations (notably by Richter [20]), 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 $\text{supp}(\mu)$ and with same moments up to degree k .

Closing the digression on the value of L and keeping the above notation, we point out that

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

which implies that the equalities $\varepsilon_{\ell} (f - v^*)(\omega_{\ell}) = \|f - v^*\|_{\Omega} = E_{\mathcal{V}}(f, \Omega)$ hold for all $\ell = 1, \dots, L$. This brings us to the notion of extremal signature associated with $f - v^*$, defined below along the lines of [21, 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 $\sigma(\omega) = \text{sgn}(g(\omega))$ for all $\omega \in \mathcal{S}$.

The argument outlined before the definition justifies the following brief statement, found e.g. in [21, 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 n th degree Chebyshev polynomials requires finding best approximants to all d -variate n th 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 [28, Proposition 4.1] for $\Omega = B$, is included here to also cover the case $\varphi \neq 0$. The statement uses the notation \mathbb{N}_0 for $\{0, 1, 2, \dots\}$, $\omega_I \in \mathbb{R}^I$ for the restriction of a vector $\omega \in \mathbb{R}^d$ to a subset I of $\{1, 2, \dots, d\}$, and I^c for the complement of I .

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

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

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

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

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

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

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

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

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

The second fact, stated hereafter, has been previously used to derive a number of examples in [1, 2, 27]. We include a standard argument (see e.g. [28, Theorem 3.2]) for the convenience of the reader. This fact is to be used with $\mathcal{V} = \mathcal{P}_{n-1}^d$ and G being the group of permutations 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 $h_g(\omega) = h(g\omega)$, $\omega \in \Omega$. If the domain Ω and the subspace $\mathcal{V} \subseteq C(\Omega)$ are invariant under the action of G , in the sense that

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

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 $g \in G$,

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

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 . \square

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 $k_1 + \dots + k_d = n$ and $k_1 \geq \dots \geq k_d \geq 1$. 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

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

since considering $k = (k_1, \dots, k_d)$ with $k_1 + \dots + k_d = n$ 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, \dots, p_d , as defined by $(p_1 \otimes \dots \otimes p_d)(x_1, \dots, x_d) = p_1(x_1) \dots p_d(x_d)$. It is not difficult to establish the following result by invoking signatures.

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

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

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

This result was proved by several authors, see e.g. [24, 6]. In [26], it has also been shown that $m_k - 2^{-n+d} T_{k_1} \otimes \dots \otimes T_{k_d}$ 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 $U_\ell = T'_{\ell+1}/(\ell+1)$ denoting the univariate ℓ th 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}_{n-1}^2 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, 19]. 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 $q \in \mathcal{P}_{n-3}^2$.

For $d > 2$, best approximants to monomials are known only for a few low-degree instances, such as $m_{(1,\dots,1)}(x) = x_1 x_2 \cdots x_d$ and $m_{(2,1,\dots,1)}(x) = x_1^2 x_2 \cdots x_d$, see [1, 2, 27]. Restricting our attention to the case $d = 3$, we now cite some articles and the result they contain:^{1,2}

- [1] : $E((1, 1, 1), B) = 3^{-3/2}$,
- [2] : $E((2, 1, 1), B) = (3 - \sqrt{8})/2$,
- [16] : $E((3, 1, 1), B) = (1 - a)(a^3/5)^{1/4}/5$, $a =$ smallest root of $9t^4 - 29t^3 + 24t^2 - 29t + 9$,
- [27] : $E((2, 2, 2), B) = 1/72$,
- [27] : $E((4, 4, 4), B) = b^{-1}/27^2$, $b \approx 21.8935834$.

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 [17]. 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}_{n-1}^2 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

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

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 [27] for the precise statement.

¹The value of $E((3, 1, 1), B)$ is implicit in [16, Theorem 2.1.(b)]—deriving the explicit value requires some work.

²There was a typographical error concerning the value of $E((4, 4, 4), B)$ in [27, Theorem 3.2].

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). Our implementation is available at https://github.com/foucart/Multivariate_Chebyshev_Polynomials. Although it limits itself to the best approximation from \mathcal{P}_{n-1}^d to monomials $m_k \in \mathcal{P}_n^d$ on the hypercube, the euclidean ball, the cross-polytope, and the simplex, the underpinning procedure is more general. Indeed, it could handle any polynomial $f \in \mathcal{P}_N^d$, $N \geq n$, instead of m_k , while the domain $\Omega \in \mathbb{R}^d$ could be any compact (with nonempty interior) basic semialgebraic set. This means that there exist polynomials g_1, \dots, g_H such that

$$(7) \quad \Omega = \{x \in \mathbb{R}^d : g_1(x) \geq 0, \dots, g_H(x) \geq 0\}.$$

We further assume that the polynomials describing Ω satisfy the Archimedean condition, meaning e.g. that there exist a constant $C > 0$ and sum-of-squares polynomials $\sigma_0, \sigma_1, \dots, \sigma_H$ such that

$$C - \|x\|_2^2 = \sigma_0(x) + \sum_{h=1}^H \sigma_h(x)g_h(x) \quad \text{for all } x \in \Omega.$$

This occurs for all four domains considered in this article—for instance, the argument for the simplex S can be found in [23, Example 12.49] and a similar argument applies to any compact convex polytope.

Our strategy to deal with the best approximation problem is to transform it into 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 [14]. This process leverages a combination of: (i) *semidefinite programming*³, an efficient machinery in Convex Optimization developed since the late seventies, and (ii) powerful positivity certificates and their dual analogs concerning the moment problem. These two ingredients were not available at the time of pioneering works such as the paper [22] 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 GloptiPoly 3, since many of the GMP components are built in this MATLAB/OCTAVE program, see [12].

Let us be more specific about the computation of the error of best approximation by polynomials from \mathcal{P}_{n-1}^d to a polynomial $f \in \mathcal{P}_N^d$, $N \geq n$, i.e., of $E^* := E_{\mathcal{P}_{n-1}^d}(f, \Omega)$, viewed as the optimal value of (4) or of (5)—which we call primal program and dual program, respectively. Looking at (4) first, it can be reformulated along the lines of (1) into

$$E^* = \min_{c \in \mathbb{R}, p \in \mathcal{P}_{n-1}^d} c \quad \text{subject to} \quad \begin{cases} c + f - p \in \mathcal{P}_+^d(\Omega), \\ c - f + p \in \mathcal{P}_+^d(\Omega), \end{cases}$$

³A 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. [15].

where $\mathcal{P}_+^d(\Omega)$ denotes the cone of d -variate polynomials that are nonnegative on Ω . As for (5), by identifying linear functionals $\lambda \in C(\Omega)^*$ with finite signed Borel measures μ on Ω through $\lambda(g) = \int_{\Omega} g d\mu$, $g \in C(\Omega)$, it can be rewritten as

$$(8) \quad E^* = \max_{\mu \in \mathcal{M}(\Omega)} \int_{\Omega} f d\mu \quad \text{s.to} \quad \int_{\Omega} p d\mu = 0 \text{ for all } p \in \mathcal{P}_{n-1}^d \quad \text{and} \quad \int_{\Omega} d|\mu| = 1.$$

With $\mathcal{M}_+(\Omega)$ denoting the cone of finite nonnegative Borel measures on Ω , the latter can further be rewritten as⁴

$$(9) \quad E^* = \max_{\mu^{\pm} \in \mathcal{M}_+(\Omega)} \int_{\Omega} f d(\mu^+ - \mu^-) \quad \text{s.to} \quad \int_{\Omega} p d(\mu^+ - \mu^-) = 0 \text{ for all } p \in \mathcal{P}_{n-1}^d$$

$$\text{and} \quad \int_{\Omega} d(\mu^+ + \mu^-) = 1.$$

This is an instance of the Generalized Moment Problem (GMP), mentioned above. Note that $\mathcal{P}_+^d(\Omega)$ is the dual cone of $\mathcal{M}_+(\Omega)$ (and vice versa) with respect to the pairing $\langle p, \mu \rangle := \int_{\Omega} p d\mu$. In other words, one has $\mathcal{M}_+(\Omega)^* = \mathcal{P}_+^d(\Omega)$, where the dual cone is defined in the usual way, i.e.,

$$\mathcal{M}_+(\Omega)^* := \left\{ p \in \mathcal{P}^d(\Omega) : \langle p, \nu \rangle \geq 0 \text{ for all } \nu \in \mathcal{M}_+(\Omega) \right\}.$$

The *quadratic module* of g_1, \dots, g_H , denoted by $\mathcal{Q}(g_1, \dots, g_H)$, is an important subcone of $\mathcal{P}_+^d(\Omega)$. It consists of all polynomials of the form

$$(10) \quad p = \sigma_0 + \sigma_1 g_1 + \dots + \sigma_H g_H$$

for some sum-of-squares polynomials $\sigma_0, \sigma_1, \dots, \sigma_H$. The associated *truncated* quadratic module of degree $2t$, denoted by $\mathcal{Q}(g_1, \dots, g_H)_t$, is the subset of $\mathcal{Q}(g_1, \dots, g_H)$ obtained by restricting all the terms in (10) to have degree at most $2t$, i.e., $\deg(\sigma_0) \leq 2t$ and $\deg(\sigma_h g_h) \leq 2t$ for $h = 1, \dots, H$.

By definition, the dual cone of $\mathcal{Q}(g_1, \dots, g_H)$ consists of linear functionals λ on \mathcal{P}^d such that $\lambda(p) \geq 0$ for all $p \in \mathcal{Q}(g_1, \dots, g_H)$. This dual cone can be described in terms of sequences of positive semidefinite matrices. To this end, we denote by $\text{Hank}_t(y)$ the Hankel matrices of size $\binom{t+d}{d} \times \binom{t+d}{d}$ built from a sequence y indexed by \mathbb{N}_0^d as having entries y_{i+j} for $i, j \in \{0, \dots, t\}^d$. Similarly, we construct matrices $\text{Hank}_t(G_h y)$ from sequence $G_h y$ associated with each g_h , namely $(G_h y)_{\ell} = \sum_{|\ell'| \leq \deg(g_h)} \text{coeff}_{m_{\ell'}}(g_h) y_{\ell+\ell'}$ for any $\ell \in \mathbb{N}_0^d$.

The following theorem by Putinar [18] describes the relation between $\mathcal{P}_+^d(\Omega)$ and $\mathcal{Q}(g_1, \dots, g_H)$, and, on the dual side, between $\mathcal{M}_+(\Omega)$ and $\mathcal{Q}(g_1, \dots, g_H)^*$.

⁴(8) \leq (9) holds by considering the Jordan decomposition $\mu =: \mu^+ - \mu^-$ of a $\mu \in \mathcal{M}(\Omega)$ which is optimal for (8) and (9) \leq (8) holds by considering $\mu := (\mu^+ - \mu^-) / \int_{\Omega} d|\mu^+ - \mu^-|$ where $\mu^+, \mu^- \in \mathcal{M}_+(\Omega)$ are optimal for (9).

Theorem 8. Let $\Omega = \{x \in \mathbb{R}^d : g_1(x) \geq 0, \dots, g_H(x) \geq 0\}$ be a compact semialgebraic set such that g_1, \dots, g_H satisfy an Archimedean condition. Then:

(Real analysis facet): A real sequence $y = (y_\ell)_{\ell \in \mathbb{N}_0^d}$ has a representing measure on Ω if and only if

$$\text{Hank}_t(y) \succeq 0, \text{Hank}_t(G_1 y) \succeq 0, \dots, \text{Hank}_t(G_H y) \succeq 0 \quad \text{for all } t \in \mathbb{N}.$$

Thus, a linear functional λ on \mathcal{P}^d is (identified with an element) in $\mathcal{M}_+(\Omega)$ if and only if the sequence $y = (\lambda(m_\ell))_{\ell \in \mathbb{N}_0^d}$ satisfies the above semidefinite conditions.

(Real algebraic geometry facet): If $p \in \mathcal{P}^d$ is strictly positive on Ω , then $p \in \mathcal{Q}(g_1, \dots, g_H)$. Conversely, any $p \in \mathcal{Q}(g_1, \dots, g_H)$ is nonnegative on Ω .

Putinar's Positivstellensatz may also be formulated as follows: if a polynomial $p \in \mathcal{P}^d$ is strictly positive on Ω , then there exists $t \in \mathbb{N}$ such that $p \in \mathcal{Q}(g_1, \dots, g_H)_t$. As a result, one has

$$\begin{aligned} (11) \quad E^* &= \inf_{c \in \mathbb{R}, p \in \mathcal{P}_{n-1}^d} \{c : c \pm (f - p)(x) > 0 \text{ for all } x \in \Omega\} \\ &= \inf_{c \in \mathbb{R}, p \in \mathcal{P}_{n-1}^d} \{c : c \pm (f - p) \in \mathcal{Q}(g_1, \dots, g_H)_t \text{ for some } t \in \mathbb{N}\}. \end{aligned}$$

Since sums-of-squares can be modeled using semidefinite matrices, semidefinite programming can be used to compute, for any fixed $t \in \mathbb{N}$ large enough⁵, an upper bound for E^* as

$$(12) \quad \text{ub}_t := \inf_{c \in \mathbb{R}, p \in \mathcal{P}_{n-1}^d} c \quad \text{subject to} \quad \begin{cases} c + f - p \in \mathcal{Q}(g_1, \dots, g_H)_t, \\ c - f + p \in \mathcal{Q}(g_1, \dots, g_H)_t. \end{cases}$$

Notice that (ub_t) forms a nonincreasing sequence and, according to (11), that $\lim_{t \rightarrow \infty} \text{ub}_t = E^*$. The idea to construct such a sequence of semidefinite programs is originally due to Lasserre [13].

The sequence of dual semidefinite programs leads us to consider, for each $t \in \mathbb{N}$,

$$(13) \quad \text{ub}'_t := \sup_{y^\pm \in \mathbb{R}^{\{0, \dots, 2t\}^d}} \sum_{|\ell| \leq N} \text{coeff}_{m_\ell}(f)(y_\ell^+ - y_\ell^-) \quad \text{s.to } y_\ell^+ - y_\ell^- = 0, |\ell| \leq n-1, y_0^+ + y_0^- = 1, \\ \text{and} \quad \text{Hank}_t(y^\pm) \succeq 0, \text{Hank}_{t-n'_1}(G_1 y^\pm) \succeq 0, \dots, \text{Hank}_{t-n'_H}(G_H y^\pm) \succeq 0,$$

where $n'_1 := \lceil \deg(g_1)/2 \rceil, \dots, n'_H := \lceil \deg(g_H)/2 \rceil$. This program can be thought of as a truncation at level t of the program (9) in which $\mu^\pm \in \mathcal{M}_+(\Omega)$ would be replaced by their infinite sequences of moments $y_\ell^\pm = \int_\Omega m_\ell d\mu^\pm$, $\ell \in \mathbb{N}_0^d$. Here, the finite sequence y^\pm represents pseudo-moments. Since the feasibility set of (9) is contained in the feasibility set of (13), one has $E^* \leq \text{ub}'_t$, i.e., the ub'_t are also upper bounds for E^* . Furthermore, by weak duality for semidefinite programs, one always has $\text{ub}'_t \leq \text{ub}_t$. In view of $\lim_{t \rightarrow \infty} \text{ub}_t = E^*$, it is therefore immediate that $\lim_{t \rightarrow \infty} \text{ub}'_t = E^*$, too. The strong duality result $\text{ub}'_t = \text{ub}_t$ is actually valid, since a constraint qualification always holds,

⁵The semidefinite program of (12) may be infeasible for small t 's, in which case one has $\text{ub}_t = \infty$, but Putinar's Positivstellensatz guarantees that it is feasible for sufficiently large t .

by a similar argument to [13, Theorem 4.2(a)]. For instance, one may construct a strictly feasible solution to the dual semidefinite program by setting $\mu^+ = \mu^-$ equal to the uniform measure on Ω . Having assumed that Ω has a nonempty interior, this implies that μ^+ and μ^- lie in the interior of $(\mathcal{Q}(g_1, \dots, g_H)_t)^*$. The interested reader can find more details in the proof of [13, Theorem 4.2(a)]. In particular, the dual semidefinite program is unbounded if the primal program (12) is infeasible.

In summary, the following result constituting the basis for our computational procedure has been established.

Theorem 9. Let $\Omega = \{x \in \mathbb{R}^d : g_1(x) \geq 0, \dots, g_H(x) \geq 0\}$ be a compact semialgebraic set such that g_1, \dots, g_H satisfy an Archimedean condition and let $f \in \mathcal{P}_N^d$ a polynomial f of degree $N \geq n$. The values ub_t and ub'_t computed in (12) and (13) with $t \geq N + \max\{n'_1, \dots, n'_H\}$, $n'_h := \lceil \deg(g_h)/2 \rceil$, form nonincreasing sequences of upper bounds for the error $E_{\mathcal{P}_{n-1}^d}(f, \Omega)$ of best approximation to f from \mathcal{P}_{n-1}^d relative to Ω . Moreover, these sequences converge to the error of best approximation, i.e.,

$$\lim_{t \rightarrow \infty} \text{ub}_t = \lim_{t \rightarrow \infty} \text{ub}'_t = E_{\mathcal{P}_{n-1}^d}(f, \Omega).$$

The above ideas have been implemented in the commands `ChebPoly_primal` and `ChebPoly_dual`, which require `GloptiPoly 3`. Although any semidefinite solver could have been used to solve (12) and (13), we chose `GloptiPoly 3` because it offers a more user-friendly way to formulate the problems. Another advantage is that, when solving (13), `GloptiPoly 3` not only outputs moments but it can also extract the atomic measure generating them—the procedure used to do so is described in [11]. This corresponds to situations where the convergence of the sequence of upper bounds occurs in a finite number of steps, which is often the case in practice. While we do not know this number of steps in advance, in such cases, the precise value of $E_{\mathcal{P}_{n-1}^d}(f, \Omega)$ can be obtained by computing ub'_t (for t large enough) and certifying its genuine optimality “numerically” within `GloptiPoly 3`. Indeed, based on a deep result of Curto and Fialkow, `GloptiPoly 3` verifies a condition ensuring that $\text{ub}'_t = E_{\mathcal{P}_{n-1}^d}(f, \Omega)$ through a numerical estimation a rank drop in the Hankel matrices, see [11]. Such certificates substantiate the numerical values presented in the next section.

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}_{n-1}^3 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. Their content can be reproduced by running the codes made available on https://github.com/foucart/Multivariate_Chebyshev_Polynomials. Note that an asterisk

(*) appended to a value means that it could not be numerically certified⁶ by GloptiPoly 3. In a few instances, we could distill explicit expressions for previously unknown Chebyshev polynomials, see Theorems 10 and 11.

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. Here and in other tables, the value of $E(k, \Omega)$ needs to be multiplied by the factor presented at the top of its column, so e.g. $E((4, 1, 1), B) \approx 1.923 \times 10^{-2}$.

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

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

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

while a Chebyshev polynomial is given by

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

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—

⁶To be sure, it is the value of the error of best approximation that is certified, not the extracted atomic measure. In the case of $m_{(2,2,1)}$ on the simplex, for instance, even though the value $E((2, 2, 1), S) \approx 4.695 \times 10^{-4}$ is certified, the extracted atomic measure suffers from numerical inaccuracies. This case is challenging—we have tried to derive an explicit solutions from our computations, without any success.

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

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

For reasons soon to become apparent, the parameter $\tau \approx 0.4052$ is chosen as the maximizer of $(1+t)^2(1-t)/(4(1+4t+4t^2))$ 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 $|(m_{(2,2,1)} - p^*)(x)| \leq a$ 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 $(m_{(2,2,1)} - p^*)(x) \leq a$, i.e., that $x_1^2x_2^2x_3 \leq a(1-T_3(x_3))$. 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

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

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 $\|m_{(2,2,1)} - p\|_B \geq a$ 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 $v(x) \geq 0$ for some $x \in \mathcal{S}^+$. With the help of this $x \in \mathcal{S}^+$, we derive

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

as desired. Thus, it remains to justify that existence of $x \in \mathcal{S}^+$ such that $v(x) \geq 0$. 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. \square

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

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

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 11. With $\tau \in [0, 1/4]$ being the solution to $\max \{y(1-2y)(y-\tau)^2, y \in [0, 1/2]\} = \tau^2/18$ 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

$$P(x) = x_1^2 x_2 x_3 + \frac{1}{2c^2} [-16x_1^2(x_2 + x_3) + 16x_1(x_2 + x_3)^2 - 2(64 + 12c + c^2)x_1 x_2 x_3 + 8x_2 x_3 - 2(x_2 + x_3) + 1].$$

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

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

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

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

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

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

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 $P(x^{(t)}) \leq P(x)$ reads $P(x_1, y, y) - (z+t)^2q(x_1) \leq P(x_1, y, y) - z^2q(x_1)$ 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 $x_1, y \geq 0$ and $x_1 + 2y \leq 1$, we recall from (14) that

$$(15) \quad P(x_1, y, y) = \frac{1}{2c^2} [2c^2x_1^2y^2 - 32x_1^2y - 2(32 + 12c + c^2)x_1y^2 + 8y^2 - 4y + 1],$$

so that

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

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

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

It follows that $|P(x_1, y, y)| \leq 1/(2c^2)$ at any critical point, since $[-16x_1^2y - 2y + 1] \leq 1$ is clear, while $[-16x_1^2y - 2y + 1] \geq -1$ holds because $16x_1^2y + 2y = 2y(8x_1^2 + 1) \leq (1 - x_1)(8x_1^2 + 1)$, the latter having maximal value $(68 + 5\sqrt{10})/54 \approx 1.5520 \leq 2$ over $x_1 \in [0, 1]$. At this point, it remains to verify that $|P(x_1, y, y)| \leq 1/(2c^2)$ on the boundary of the domain $\{x_1 \geq 0, y \geq 0, x_1 + 2y \leq 1\}$. 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 (15) and recalling that $\tau = -3/c$, we arrive at

$$(16) \quad P(1 - 2y, y, y) = \frac{1}{2c^2} - 2y(1 - 2y)(y - \tau)^2, \quad y \in [0, 1/2].$$

The inequality $P(1 - 2y, y, y) \leq 1/(2c^2)$ is obvious from here. The parameter τ is chosen to secure the other inequality $P(1 - 2y, y, y) \geq -1/(2c^2)$, which is equivalent to $y(1 - 2y)(y - \tau)^2 \leq 1/(2c^2)$ for all $y \in [0, 1/2]$ and thus follows from the equation $\max \{y(1 - 2y)(y - \tau)^2, y \in [0, 1/2]\} = \tau^2/18$. 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 $\max \{y(1 - 2y)(y - \tau)^2, y \in [0, 1/2]\}$ decreases from a positive quantity to $1/512$ there. In consequence, we have now established that $|P(x)| \leq 1/(2c^2)$ 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 (16), 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

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

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 $|P(x)| = \|P\|_{\mathcal{S}} = 1/(2c^2)$ for all $x \in \mathcal{S}$, as announced.

The second step consists in proving that $\|m_{(2,1,1)} - p\|_{\mathcal{S}} \geq 1/(2c^2)$ 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

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

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 $E_{\mathcal{P}_3^3}(m_{(2,1,1)}, \mathcal{S}) \approx 2.68850 \times 10^{-3}$. 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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