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ON POLYNOMIALS OF LEAST DEVIATION FROM ZERO IN SEVERAL VARIABLES

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ABSTRACT. A polynomial of the form $x^\alpha - p(x)$, where the degree of p is less than the total degree of x^α , is said to be least deviation from zero if it has the smallest uniform norm among all such polynomials. We study polynomials of least deviation from zero over the unit ball, the unit sphere and the standard simplex. For $d = 3$, extremal polynomial for $(x_1 x_2 x_3)^k$ on the ball and the sphere is found for $k = 2$ and 4. For $d \geq 3$, a family of polynomials of the form $(x_1 \cdots x_d)^2 - p(x)$ is explicit given and proved to be the least deviation from zero for $d = 3, 4, 5$, and it is conjectured to be the least deviation for all d .

1. INTRODUCTION

Let Π_n^d denote the space of polynomials of degree at most n in d variables and we write $\Pi_n = \Pi_n^1$. For $d = 1$, it is well-known that the 2^{1-n} multiple of the Chebyshev polynomial of the first kind

$$T_n(x) = \cos n(\arccos x) = 2^{n-1}x^n + q(x), \quad q \in \Pi_{n-1},$$

is the monic polynomial of least deviation from zero in Π_n in the space $C[-1, 1]$; that is,

$$\inf_{p \in \Pi_{n-1}} \|x^n - p(x)\|_{C[-1,1]} = 2^{1-n} \|T_n\|_{C[-1,1]} = 2^{1-n}.$$

Equivalently, we say that $x^n - 2^{1-n}T_n$ is the best approximation to x^n in $C[-1, 1]$.

Let Ω be a region in \mathbb{R}^d . For $f \in C(\Omega)$, the best approximation of f from Π_n^d in the uniform norm is the quantity

$$(1.1) \quad E_n(f; \Omega) = \inf_{p \in \Pi_{n-1}^d} \|f - p\|_{C(\Omega)},$$

where $\|f\|_{C(\Omega)} = \max_{x \in \Omega} |f(x)|$. We call p^* an extremal polynomial for f if $E_n(f; \Omega) = \|f - p^*\|_{C(\Omega)}$. For $x = (x_1, \dots, x_d) \in \mathbb{R}^d$ and $\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}_0^d$, we define the monomial $x^\alpha = x_1^{\alpha_1} \cdots x_d^{\alpha_d}$. The degree of the monomial x^α is $|\alpha| = \alpha_1 + \dots + \alpha_d$. If $p^*(x)$ is an extremal polynomial for the monomial x^α , we call $x^\alpha - p^*(x)$ the polynomial of least deviation from zero. For Ω being a region in \mathbb{R}^d , polynomials of least deviation are known only in the case that Ω is a cube. We are interested in the case of the unit ball $B^d = \{x : \|x\| \leq 1\}$, where $\|x\|$ is the usual Euclidean norm of x , the unit sphere $S^{d-1} = \{x : \|x\| = 1\}$ and the standard simplex $T^d = \{x : x_1 \geq 0, \dots, x_d \geq 0, 1 - x_1 - \dots - x_d \geq 0\}$.

For $d = 2$, the least deviation of $x^n y^m$ from Π_{n+m-1}^2 in the space $C(\Omega)$ has been studied for B^2 and T^2 (see, for example, [Gearhart, 73], [Reimer, 77], [Newman and Xu, 93],

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[Bojanov, Haussmann and Nikolov, 01]). For $d > 2$, the only case known is $x_1 \cdots x_d$ on B^d and S^{d-1} , which is a polynomial of least deviation by itself. This is shown recently in [Andreev and Yudin, 01],

$$(1.2) \quad \inf_{p \in \Pi_{d-1}^d} \|x_1 \cdots x_d - p(x)\|_{C(B^d)} = \inf_{p \in \Pi_{d-1}^d} \|x_1 \cdots x_d - p(x)\|_{C(S^{d-1})} \\ = \|x_1 \cdots x_d\|_{C(S^{d-1})} = d^{-d/2}.$$

In other word, the best approximation of $x_1 \cdots x_d$ from Π_{d-1}^d is the zero polynomial. Finding polynomials of least deviation on these regions appear to be a difficult problem. Only a handful of explicit non-trivial examples of extremal polynomials for $d \geq 3$ are known in the literature.

In the present paper, we study the least deviation from zero for monomials of lower degrees. We found extremal polynomials for $(x_1 x_2 x_3)^2$ and $(x_1 x_2 x_3)^4$ on B^3 and S^2 and a family of extremal polynomials for $x_1^2 \cdots x_d^2$ on B^d and S^{d-1} , which are derived from the extremal polynomials for $x_1 x_2 x_3$ and $(x_1 x_2 x_3)^2$ on T^3 and $x_1 \cdots x_d$ on T^d , respectively. We give an explicit construction of this family of polynomials and conjecture that they are the least deviation polynomials. The conjecture is proved for $d = 3, 4, 5$. The result provides, we believe, the first non-trivial example of polynomials of least deviation on these domains. For example, we have

$$\inf_{p \in \Pi_3^3} \|x_1^2 x_2^2 x_3^2 - p(x)\|_{C(B^3)} = \inf_{p \in \Pi_3^3} \|x_1^2 x_2^2 x_3^2 - p(x)\|_{C(S^3)} = 72^{-1}$$

and the minimum is attained by the extremal polynomial $R_3(x_1, x_2, x_3)$ defined by

$$R_3(x_1, x_2, x_3) = (72x_1^2 x_2^2 x_3^2 - 4(x_1^2 + x_2^2 + x_3^2) + 4(x_1^4 + x_2^4 + x_3^4)^2 + 1)/72.$$

The least deviation, 72^{-1} , is surprisingly small in view of the value $3^{-3/2}$ for $x_1 x_2 x_3$.

Our proof is based on a general result for the Chebyshev approximation in [Rivlin and Shapiro, 61], in which the best approximation element is characterized in terms of extremal signature. The most difficult part, however, is to identify a correct extremal polynomial. There is no general method for this purpose. We relied heavily on the computer algebra system *Mathematica* to test and verify conjectures. In retrospect, the explicit construction is natural and rather suggestive. For example, $R_3(x)$ agrees with the Chebyshev polynomial $T_2(x)$ on the three edges of the face of T^3 defined by $x_1 + x_2 + x_3 = 1$. The result allows first glimpse of what an extremal polynomial in more than two variables may look like.

The paper is organized as follows. In the following section we recall the theoretic background needed to prove our result. The results for $d = 3$ are discussed in Section 3 and those for $d > 3$ are in Section 4.

2. EXTREMAL SIGNATURE AND BEST APPROXIMATION

We recall the characterization of the extremal polynomials in terms of the extremal signature. The study in [Rivlin and Shapiro, 61] is given in the general setting of approximation from a finite dimensional subspace of $C(\Omega)$ on a compact Hausdorff space Ω . We shall restrict the statement to our setting.

Let Ω be an infinite compact set in \mathbb{R}^d . A signature σ on the set Ω is a function with finite support, whose nonzero values are either $+1$ or -1 . A signature σ is

called extremal with respect to Π_n^d if there exists a subset \mathcal{S} in the support of σ and positive numbers λ_v , $v \in \mathcal{S}$, such that

$$\sum_{v \in \mathcal{S}} \lambda_v \sigma(v) p(v) = 0, \quad \text{for all } p \text{ in } \Pi_n^d.$$

Let $r > 0$ be a fixed number. For each $p \in \Pi_{n-1}^d$, we denote by $\mathcal{S}_r(p; f)$ the set

$$\mathcal{S}_r(p; f) = \{x \in \Omega : |f(x) - p(x)| = r\}.$$

If $r = \|f - p\|_{C(\Omega)}$, $\mathcal{S}_r(p; f)$ is the set of extremal points of $f - p$ and we denote it by $\mathcal{S}(p; f)$.

The characterization of the best approximation of f from Π_n^d is given by the following theorem in [Rivlin and Shapiro, 61]:

Theorem 2.1. *A polynomial p^* in Π_n^d satisfies $\|f - p^*\|_{C(\Omega)} = E_n(f; \Omega)$ if and only if there exists an extremal signature σ with support in $\mathcal{S}(p^*; f)$ such that $\sigma(v) = \text{sign}(f - p^*)(v)$ for all $v \in \mathcal{S}(p^*; f)$.*

The sufficient part of the theorem provides a method to verify if a polynomial p^* is extremal. One needs, however, to know the extremal polynomial in advance, as the extremal signature is supported on the set $\mathcal{S}(p^*; f)$ which depends on p^* . The sufficient part of the theorem can be extended to the signature support on $\mathcal{S}_r(p; f)$, in which r is not necessarily $\|f - p\|_{C(\Omega)}$. We will use this slightly extended version, which we state in the following. A simple proof is included for completeness; see [Rivlin and Shapiro, 61] for more details.

Theorem 2.2. *Suppose there exists a polynomial $p^* \in \Pi_n^d$ and an extremal signature σ supported on $\mathcal{S}_r(p^*; f)$. Then $E_n(f; \Omega) \geq r$.*

Proof. We can normalize the measure λ_μ for the extremal signature so that it is a probability measure; that is, $\sum_{v \in \mathcal{S}_r(p^*; f)} \lambda_v = 1$. Let $\mathcal{S}(r) = \mathcal{S}_r(p^*; f)$ in this proof. Since $\sum \lambda_v p(v) = 0$ for any polynomial $p \in \Pi_n^d$, we have

$$\begin{aligned} \|f(x) - p(x)\|_{C(\Omega)} &\geq \sum_{v \in \mathcal{S}(r)} \lambda_v |f(v) - p(v)| \\ &\geq \left| \sum_{v \in \mathcal{S}(r)} \lambda_v \sigma_v f(v) - \sum_{v \in \mathcal{S}(r)} \lambda_v \sigma_v p(v) \right| \\ &= \left| \sum_{v \in \mathcal{S}(r)} \lambda_v \sigma_v f(v) \right| = \left| \sum_{v \in \mathcal{S}(r)} \lambda_v \sigma_v (f(v) - p^*(v)) \right| \\ &= \sum_{v \in \mathcal{S}(r)} \lambda_v |f(v) - p^*(v)| = r \sum_{v \in \mathcal{S}(r)} \lambda_v = r. \end{aligned}$$

where we have used the fact that $f(v) - p^*(v) = \sigma_v r$ for $v \in \mathcal{S}(r)$. \square

The extension allows us to apply the result to the situation where a good candidate for p^* is identified but the norm of $f - p^*$ is hard to determine. This is precisely our case in Section 4.

Our construction is motivated by the recent study in [Andreev and Yudin, 01], in which it is shown that if f is invariant under a finite group G (that is, $f(xg) = f(x)$ for all $g \in G$), then the best approximation $E_n(f; S^{d-1})$ is attained at G invariant polynomials. (This result appeared early in [Ganzburg and Pichugov, 81] as

pointed out by a referee.) More precise, we state the result in [Andreev and Yudin, 01] as follows:

Proposition 2.3. *Let G be a subgroup of the rotation group $O(d)$ and let $G\Pi_n^d$ denote the polynomials in Π_n^d that are invariant under G . If f is invariant under G , then*

$$\inf_{p \in \Pi_{n-1}^d} \|f(x) - p(x)\|_{C(S^{d-1})} = \inf_{p \in G\Pi_{n-1}^d} \|f(x) - p(x)\|_{C(S^{d-1})}.$$

Using this fact, the best approximation of several invariant functions are given in [Andreev and Yudin, 01], including the case $x_1 \cdots x_d$ in (1.2) (invariant under the symmetric group). The proof in [Andreev and Yudin, 01] can be applied to any region Ω and f that are invariant under a finite group G . In particular, if f is invariant under a subgroup G of the symmetric group $S_d(T^d)$ of the simplex T^d , then an extremal polynomial of f can be taken as a G -invariant polynomial.

If f is even in each of its variables, then f is invariant under the sign changes of each variable (invariant under the group \mathbb{Z}_2^d); the extremal polynomial can be taken as a polynomial even in each of its variables. Furthermore, instead of B^d or S^{d-1} , we can work with T^d and T^{d-1} in this case. In fact, the following general proposition holds:

Proposition 2.4. *Let $\alpha \in \mathbb{N}_0^d$ and write $2\alpha = (2\alpha_1, \dots, 2\alpha_d)$ and $|\alpha| = n$. If $p^*(x)$ is an extremal polynomial for $E_n(x^\alpha; T^d)$ then $p^*(x_1^2, \dots, x_d^2)$ is an extremal polynomial for $E_n(x^{2\alpha}; B^d)$; conversely, if q^* is an extremal polynomial for $E_n(x^{2\alpha}; B^d)$ in the form $q^*(x) = p^*(x_1^2, \dots, x_d^2)$, then $p^*(x)$ is an extremal polynomial for $E_n(x^\alpha; T^d)$. Furthermore, let $f_\alpha(x_1, \dots, x_{d-1}) = x_1^{\alpha_1} \cdots x_{d-1}^{\alpha_{d-1}} (1 - x_1 - \cdots - x_{d-1})^{\alpha_d}$; then the above conclusion holds for $E_n(f_\alpha; T^{d-1})$ and $E_n(x^{2\alpha}; S^{d-1})$.*

We note that $f_\alpha(x_1^2, \dots, x_{d-1}^2) = x^{2\alpha}$ on S^{d-1} . The proposition follows easily from the fact that $x \mapsto (x_1^2, \dots, x_d^2)$ is one-to-one from T^d to $B_+^d = \{x \in B^d : x_i \geq 0\}$, and the map also induces a one-to-one mapping from Π_n^d to $G\Pi_{2n}^d$ with $G = \mathbb{Z}_2^d$, that is, the subspace of polynomials that are even in each of its variables. For $d = 2$ the proposition has been used in [Bojanov, Haussmann and Nikolov, 01]. The correspondence between polynomials on these domains also works for other problems involving polynomials, such as orthogonal polynomials and cubature formulae, see for example [Xu, 98].

3. LEAST DEVIATION FROM ZERO FOR $d = 3$

We consider best approximation to the monomials $x_1x_2x_3$ and $(x_1x_2x_3)^2$ in this section. The main task is to identify an extremal polynomial. The results in the previous section provide some guidance, but there is no general method for this purpose. Our first example, $R_3(x)$ given below, was found after many attempts. See the comments after the proof.

Theorem 3.1. *Define the polynomial $R_3(x)$ by*

$$R_3(x) = 72x_1x_2x_3 - 4(x_1 + x_2 + x_3) + 4(x_1 + x_2 + x_3)^2 - 8(x_1x_2 + x_2x_3 + x_1x_3) + 1.$$

Then $72^{-1}R_3(x)$ is a polynomial of least deviation from zero and

$$E_2(x_1x_2x_3; T^3) = E_2(x_1x_2(1 - x_1 - x_2); T^2) = 72^{-1}\|R_3\|_{C(T^3)} = 72^{-1}$$

Furthermore, $72^{-1}R_3(x_1^2, x_2^2, x_3^2)$ is a polynomial of least deviation from zero and

$$E_5(x_1^2 x_2^2 x_3^2; B^3) = E_5(x_1^2 x_2^2 x_3^2; S^2) = 72^{-1} \|R_3(x_1^2, x_2^2, x_3^2)\|_{C(B^3)} = 72^{-1}.$$

Proof. By Proposition 2.4 we only need to work with the simplex. It is easy to verify that $R_3(0, 0, 0) = 1$ and $R_3(1/2, 1/2, 0) = -1$. Solving the equations $\partial_i R_3(x) = 0$, $i = 1, 2, 3$, shows that R_3 has 4 critical points inside T_3 but none of them is maximum or minimum, since the values of $|R_3(x)|$ at these points are less than 1. Thus, $|R_3(x)|$ attains its maximum on the boundary of T^3 . It is easy to verify that the polynomial $R_3(x)$ satisfies

$$R_3(x, y, 0) = R_3(x, 0, y) = R_3(0, x, y) = (1 - 2x)^2 + (1 - 2y)^2 - 1$$

which is bounded by 1 in absolute value. Hence, we only need to show that $|R_3(x)|$ is bounded by one on the face of T^3 defined by $x_1 + x_2 + x_3 = 1$; that is, we need to show that $U_3(x_1, x_2) = R_3(x_1, x_2, 1 - x_1 - x_2)$ is bounded by 1 in absolute value on T^2 . Taking derivatives of $U_3(x_1, x_2)$ and solving for the critical points shows that it has 4 critical points inside T^2 , of which only the point $(1/3, 1/3)$ is a maximal, $U(1/3, 1/3) = 1$. Furthermore, it is easy to verify that

$$U_3(x, 0) = U_3(0, x) = U_3(x, 1 - x) = T_2(x);$$

that is, it agrees with Chebyshev polynomial of degree 2 on the boundary of the triangle. Hence, $|U_3(x)| \leq 1$. Furthermore, the above analysis also shows that

$$\begin{aligned} \mathcal{S}_+ &:= \{x : R_3(x) = 1\} = \{(0, 0, 0), (1, 0, 0), (0, 1, 0), (0, 0, 1), (1/3, 1/3, 1/3)\} \\ \mathcal{S}_- &:= \{x : R_3(x) = -1\} = \{(1/2, 1/2, 0), (1/2, 0, 1/2), (0, 1/2, 1/2)\}. \end{aligned}$$

Let $\sigma(v) = 1$ on $\mathcal{S}_+ \setminus \{(0, 0, 0)\}$ and $\sigma(v) = -1$ on \mathcal{S}_- . We show that σ is an extremal signature. Define $L_1 f$ and $L_2 f$ by

$$L_1 f = \frac{3}{4} f\left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right) + \frac{1}{12} (f(1, 0, 0) + f(0, 1, 0) + f(0, 0, 1))$$

and

$$L_2 f = \frac{1}{3} \left(f\left(\frac{1}{2}, \frac{1}{2}, 0\right) + f\left(\frac{1}{2}, 0, \frac{1}{2}\right) + f\left(0, \frac{1}{2}, \frac{1}{2}\right) \right).$$

Then $Lf := L_1 f - L_2 f$ satisfies $Lf = 0$, $f \in \Pi_2^3$. Thus, σ is an extremal signature for $x_1 x_2 x_3$ in $C(T^3)$. Furthermore, the support sets \mathcal{S}_+ and \mathcal{S}_- of σ are on the face of T^3 , which is identified with T^2 . This shows that σ is also an extremal signature for $x_1 x_2 (1 - x_1 - x_2)$ in $C(T^2)$. \square

Let us mention a connection between cubature formulae and the extremal signature for $R_3(x)$. A cubature formula is a linear combination of function evaluations that gives an approximation to an integral ([Stroud, 71]). Let $d\mu$ be a positive measure on $\Omega \subset \mathbb{R}^d$. If

$$\int_{\Omega} f(x) d\mu = \sum_{k=1}^N \lambda_k f(x_k), \quad f \in \Pi_n^d,$$

and there is at least one $f \in \Pi_{n+1}^d$ such that the equality fails, then the cubature formula is said to be of degree n . It is called positive, if all λ_k are positive numbers. For the extremal signature for $R_3(x)$, it is easy to verify that both $L_1 f$ and $L_2 f$ are

cubature formulae of degree 2 for dx on the set $\Sigma^2 = \{x \in T^3 : x_1 + x_2 + x_3 = 1\}$; that is,

$$\int_{\Sigma^2} f(x) dx = L_1 f = L_2 f, \quad \text{for all } f \text{ in } \Pi_2^2.$$

Since we identify Σ^2 with T^2 , one can write L_1 and L_2 as linear combinations of function evaluations for functions of two variables. Thus, the extremal signature is given by the difference of two positive cubature formulae.

During our search for $R_3(x)$, we found $U_3(x)$ first. In retrospect, the formula of $U_3(x)$, which can be written as

$$U_3(x_1, x_2) = 72x_1x_2(1 - x_1 - x_2) - 3 + 4(x_1^2 + x_2^2 + (1 - x_1 - x_2)^2),$$

is quite natural since it agrees with the Chebyshev polynomials of degree 2 on the boundary of T^2 . This also suggests the possibility that other monomials may also have extremal polynomials that agree with Chebyshev polynomials on the boundary of T^3 . For example, for $(x_1x_2x_3)^n$, one may look for a polynomial that agrees with Chebyshev polynomials of n -th degree on the boundary of the simplex. One example of such a polynomial is $T_n(R_3(x))$, where $T_n(t)$ denotes the Chebyshev polynomial of degree n . Although this function is not a polynomial of least deviation, it helps us to find a solution for the monomial $(x_1x_2x_3)^2$.

Theorem 3.2. *Define polynomial $R_5(x)$ by*

$$\begin{aligned} R_5(x) = & 27^2b(x_1x_2x_3)^2 - 1 + 2(x_1 + x_2 + x_3) - 2(x_1 + x_2 + x_3)^2 \\ & + 2[1 - 4(x_1 + x_2 + x_3) + 4(x_1^2 + x_2^2 + x_3^2)]^2 \\ & - 27x_1x_2x_3[(32/9 - 2a + b)(x_1 + x_2 + x_3)^2 + 6a(x_1x_2 + x_1x_3 + x_2x_3)]. \end{aligned}$$

Then $27^{-2}b^{-1}R_5(x)$ is a polynomial of least deviation from zero,

$$E_5(x_1^2x_2^2x_3^2; T^3) = E_5(x_1^2x_2^2(1 - x_1 - x_2)^2; T^2) = 27^{-2}b^{-1}\|R_5\|_{C(T^3)} = 27^{-2}b^{-1},$$

where the constant a, b and the reciprocal of the least deviation is given by

$$a = 28.5926243, \quad b = 21.8935834, \quad 27^2b = 15960.4223.$$

Furthermore, $72^{-2}b^{-1}R_3(x_1^2, x_2^2, x_3^2)$ is a polynomial of least deviation from zero,

$$E_5(x_1^2x_2^2x_3^2; B^3) = E_5(x_1^2x_2^2x_3^2; S^2) = 72^{-2}b^{-1}\|R_5(x_1^2, x_2^2, x_3^2)\|_{C(B^3)} = 27^{-2}b^{-1}.$$

Just like the case of $R_3(x)$, the proof amounts to showing that $|R_5(x)| \leq 1$ on T^3 and there exists an extremal signature. It is not difficult once the formula of R_5 is identified. We first give an account on how R_5 is discovered.

Following the construction of $R_3(x)$, we look for a polynomial in the form of

$$\begin{aligned} U_5(x, y) = & 27xy(1 - x - y)[27bxy(1 - x - y) + 3a(x^2 + y^2 + (1 - x - y)^2) - c] \\ & + 2[-3 + 4(x^2 + y^2 + (1 - x - y)^2)]^2 - 1 \end{aligned}$$

that will be a polynomial of least deviation on T^2 with leading monomial $x^2y^2(1 - x - y)^2$. Note that the Chebyshev polynomial of degree 2 is $T_2(t) = 2t^2 - 1$ and $T_2(2t - 1) = -3 + 4(t^2 + (1 - t)^2)$. The form of U_5 is chosen so that on the boundary of T^2 it satisfies

$$U_5(x, 0) = U_5(0, x) = U_5(x, 1 - x) = T_2(T_2(2x - 1)) = T_4(2x - 1).$$

We then choose $c = 32/9 + a + b$ so that $U_5(1/3, 1/3) = 1$. It follows that $1 - U_5(x, x)$ can be factored as

$$1 - U_5(x, x) = x(1 - 2x)(1 - 3x)^2(64 - 54ax + 27bx + 162bx^2).$$

We need to choose a and b so that the last factor is positive for $0 \leq x \leq 1/2$. One choice is to make this factor $2b(9x + d)^2$. This leads to $a = 16(3 - 4d)/(3d^2)$ and $b = 32/d^2$. At this point, it becomes apparent that there need to be more points on which $U_5(x, y) = -1$ inside T^2 . We therefore solve the equations $U_5(x, x) = -1$ and $U_5'(x, x) = 0$. This leads to $d = -1.208972894$, which gives the values for a and b in the theorem. It turns out that this choice does work out and $|U_5(x, y)| \leq 1$ on T^2 . The final step is to identify the formula of $R_5(x_1, x_2, x_3)$ from that of $U_5(x_1, x_2)$ with the requirement that $R_5(x_1, x_2, 1 - x_1 - x_2) = U_5(x_1, x_2)$ and $|R_5(x, y)| \leq 1$ on T^3 . This step is not trivial since an additional multiple of $(x_1 + x_2 + x_3)^k$ to any term in $R_5(x)$ does not change the value of the polynomial on the face of T^3 defined by $x_3 = 1 - x_1 - x_2$. The polynomial $U_5(x_1, x_2)$ is an extremal polynomial on the triangle T^2 that agrees with the Chebyshev polynomials of degree 4 on the three boundary lines of T^2 , its graph is depicted below.

The polynomial U_3

Let us point out that there does not seem to be a closed form for the values of a and b . In fact, the value of d in the above paragraph is one of the real roots of the following polynomial:

$$\begin{aligned} & -612220032 - 1365527808t - 835528041t^2 - 101556504t^3 \\ & + 23270976t^4 + 26037504t^5 + 7670016t^6 + 929280t^7 + 41984t^8. \end{aligned}$$

This polynomial has 4 real roots and 4 complex roots, and it cannot be factored over the integers.

We now give a formal proof of Theorem 3.2.

Proof of Theorem 3.2. First of all, we need to show that $|R_5(x)| \leq 1$ for $x \in T^3$. Solving $\partial_i R_5(x) = 0$, $i = 1, 2, 3$, numerically for critical points shows that $|R_5(x)|$ attains its maximum on the boundary of T^3 . Furthermore,

$$\begin{aligned} R_5(x, y, 0) &= R_5(x, 0, y) = R_5(0, x, y) \\ &= -1 + 2(x + y) - 2(x + y)^2 + 2(1 - 4(x + y) + 4(x^2 + y^2))^2, \end{aligned}$$

and the polynomial has no critical point inside T^2 . Consequently, the maximum of $|R_5(x)|$ is attained on the face of T^3 defined by $x_1 + x_2 + x_3 = 1$. In other words, we only need to show that $|U_5(x_1, x_2)| \leq 1$ on T^2 . Again this can be proved by solving $\partial_i U_5(x_1, x_2) = 0$, $i = 1, 2$, and the maximum is attained on the boundary. This proves that $|R_5(x)| \leq 1$ on T^3 and it also gives the set $\mathcal{S}_+ = \{x : |R_5(x)| = 1\}$ and the set $\mathcal{S}_- = \{x : |R_5(x)| = -1\}$. Let S_3 be the symmetric group of three elements. For $a = (a_1, a_2, a_3) \in \mathbb{R}^3$ we define $a\tau := (a_{\tau_1}, a_{\tau_2}, a_{\tau_3})$, $\tau \in S_3$ and $(a)_G := \{a\tau : \tau \in S_3\}$. Then

$$\begin{aligned} \mathcal{S}_+ &= \{(1/3, 1/3, 1/3), (0, 0, 0), (1, 0, 0)_G, (1/2, 1/2, 0)_G, (t_1, t_1, 1 - 2t_1)_G\} \\ \mathcal{S}_- &= \{((2 - \sqrt{2})/4, (2 + \sqrt{2})/4, 0)_G, (t_2, t_2, 1 - 2t_2)_G\}, \end{aligned}$$

where $t_1 = 0.4588164122$ and $t_2 = 0.1343303216$. We consider the signature σ defined by $\sigma(v) = 1$, $v \in \mathcal{S}_+ \setminus \{(0, 0, 0)\}$ and $\sigma(v) = -1$, $v \in \mathcal{S}_-$. To show that σ is an extremal signature, we define Lf by

$$\begin{aligned} Lf &= c_0 f(1/3, 1/3, 1/3) + c_1 \sum_{\tau} f((1, 0, 0)\tau) \\ &\quad + c_2 \sum_{\tau} f((1/2, 1/2, 0)\tau) + c_3 \sum_{\tau} f((t_1, t_1, 1 - 2t_1)\tau) \\ &\quad - c_4 \sum_{\tau} f(((2 - \sqrt{2})/4, (2 + \sqrt{2})/4, 0)\tau) - c_5 \sum_{\tau} f((t_2, t_2, 1 - 2t_2)\tau), \end{aligned}$$

where the sum is taken over all distinct permutations of the base point and the coefficients are given by

$$\begin{aligned} c_0 &= 0.0997251873, & c_1 &= 0.0097228135, & c_2 &= 0.0621246411, \\ c_3 &= 0.0243979796, & c_4 &= 0.0615774830, & c_5 &= 0.1178707075. \end{aligned}$$

Then $Lf = 0$ for all $f \in \Pi_4^3$, which shows that σ is an extremal signature. This completes the proof of Theorem 3.1. \square

The linear functional Lf given above is evidently a sum of two linear functionals with positive coefficients. Unlike the case of R_3 , however, the two linear functionals are not cubature formulas of degree 5 with respect to the Lebesgue measure.

The two cases solved in this section appear to indicate a surprisingly complicated picture for the best approximation of monomials in three variables, and the picture is remarkably different from that of one and two variables. We make two remarks in this regard.

Remark 3.1. One surprising fact of Theorem 3.2 is that the least deviation is not given by a reciprocal of an integer. This indicates a major difference between the case of three variables and that of one and two variables. In the case of one variable, the polynomial of least deviation from zero is the classical Chebyshev polynomial,

for which the least deviation of x^n to Π_{n-1} in $C[-1, 1]$ is 2^{1-n} . In the case of two variables, we know for example

$$E_n(x^k y^{n-k}; B^2) = \inf_{p \in \Pi_{n-1}^2} \|x^k y^{n-k} - p(x)\|_{C(B^2)} = 2^{1-n}.$$

For three variables, however, we do not know if the least deviation of x^α to $\Pi_{|\alpha|-1}^d$ could be represented by a simple formula that depends only on the total degree of the monomial. The result in this section seems to indicate that such a formula does not exist.

Remark 3.2. The values of the least deviation in Theorems 3.1 and 3.2 are surprisingly small. Let us examine the case of the unit ball. We know

$$(3.1) \quad E_n(x_1^k x_2^{n-k}; B^3) = E_n(x_1^k x_3^{n-k}; B^3) = E_n(x_2^k x_3^{n-k}; B^3) = 2^{1-n}.$$

This follows from the fact that an extremal polynomial p^* for $x_1^m x_2^n$ must be even in x_3 since $x_1^m x_2^n$ is invariant under the group \mathbb{Z}_2 applied on the third variable. Let p^* be so chosen; then

$$\begin{aligned} \|x_1^{n-m} x_2^m - p^*(x_1, x_2, x_3)\|_{C(B^3)} &\geq \|x_1^{n-m} x_2^m - p^*(x_1, x_2, \sqrt{1-x_1^2-x_2^2})\|_{C(B^2)} \\ &\geq \inf_{p \in \Pi_n^2} \|x_1^{n-m} x_2^m - p(x_1, x_2)\|_{C(B^2)} = 2^{1-n}. \end{aligned}$$

Furthermore, the equality holds since an extremal polynomial for $x_1^{n-m} x_2^m$ on B^2 can also serve as an extremal polynomial on B^3 . Below is a list of other cases that we know on the unit ball:

$$\begin{aligned} E_n(x_1 x_2 x_3; B^3) &= 3^{-3/2}, \quad E_n(x_1^2 x_2^2 x_3^2; B^3) = 2^{-3} \cdot 3^{-1}, \\ E_n(x_1^4 x_2^4 x_3^4; B^3) &= 0.456755 \cdot 2^{-6} \cdot 3^{-6}, \end{aligned}$$

where we rewrite the value of the third one, which is given in Theorem 3.2, for easier comparison. The value of $E_n(x_1^2 x_2^2 x_3^2; B^3)$ appears to be strikingly small. For other degree 6 monomials given in (3.1), the value of the best approximation is only 2^{-5} . Also note the fast decrease shown in these three values.

4. LEAST DEVIATION FROM ZERO FOR $d > 3$

We consider the best approximation to $(x_1 \cdots x_d)^2$ on B^d or S^{d-1} , and the best approximation to $x_1 \cdots x_d$ on T^d or T^{d-1} in this section. The extremal polynomial can be taken as symmetric polynomials by Proposition 2.3. It is well known that every symmetric polynomial can be written in terms of elementary symmetric polynomials ([Macdonald, 95]).

The elementary symmetric polynomials of degree k in variables x_1, x_2, \dots, x_N are defined by

$$e_k(x) = \sum_{1 \leq i_1 < \dots < i_k \leq N} x_{i_1} x_{i_2} \cdots x_{i_k}, \quad 1 \leq k \leq N.$$

In particular, $e_1(x_1, \dots, x_N) = x_1 + \dots + x_N$ and $e_N(x_1, \dots, x_N) = x_1 \cdots x_N$. As it is often the case with the symmetric functions, we assume that N is sufficiently large and do not write the dependence of e_k on the number of variables. We will use the notation $\mathbf{1}^k = (1, 1, \dots, 1) \in \mathbb{R}^k$.

Definition 4.1. Using elementary symmetric functions, define $T_3(x)$ by

$$T_3(x) = 72e_3(x) - 4e_1(x) + 4e_1^2(x) - 8e_2(x) + 1$$

and $T_k(x)$ for $k > 3$ by the recursive formula

$$T_k(x) = r_k e_k(x) - T_{k-1}(x),$$

where the constant r_k is determined by $r_k = k^k [T_{k-1}(k^{-1}\mathbf{1}^k) + 1]$.

Note that $k^{-1}\mathbf{1}^k = (k^{-1}, \dots, k^{-1}) \in \mathbb{R}^k$; we use the evaluation of T_{k-1} , as a function of \mathbb{R}^k , at this point in the definition of r_k . Clearly r_k is uniquely determined. For $x \in \mathbb{R}^d$, the function $T_d(x)$ will serve as extremal polynomials. In particular, the polynomial $T_3(x)$ for $x \in \mathbb{R}^3$ is the same as $R_3(x)$ in the previous section. For $x \in \mathbb{R}^4$, the explicit formula of T_4 is given by

$$\begin{aligned} T_4(x) &= 896x_1x_2x_3x_4 - 72(x_1x_2x_3 + x_1x_2x_4 + x_1x_3x_4 + x_2x_3x_4) \\ &\quad + 4(x_1 + x_2 + x_3 + x_4) - 4(x_1 + x_2 + x_3 + x_4)^2 \\ &\quad + 8(x_1x_2 + x_1x_3 + x_1x_4 + x_2x_3 + x_2x_4 + x_3x_4) - 1. \end{aligned}$$

The value of r_d is of particular importance. It can be computed using the following formula.

Lemma 4.2. For $d \geq 3$,

$$r_d = d \sum_{k=4}^d k^{d-3} \binom{d}{k} [(-1)^k (9k^2 - 32k + 24) + k^2].$$

In particular, $r_3 = 72$, $r_4 = 896$, $r_5 = 14400$, and $r_6 = 283392$.

We defer the proof to the end of the section and continue to state our main result of this section.

Theorem 4.3. For $d \geq 3$, on the d -dimensional simplex

$$E_{d-1}(x_1 \cdots x_d; T^d) = E_{d-1}(x_1 \cdots x_{d-1}(1 - x_1 - \cdots - x_{d-1}); T^{d-1}) \geq r_d^{-1},$$

and the equality holds for $d = 3, 4, 5$ with $r_d^{-1}T_d(x)$ as a polynomial of least deviation from zero. Furthermore, on B^d and S^{d-1} ,

$$E_{2d-1}(x_1^2 \cdots x_d^2; B^d) = E_{2d-1}(x_1^2 \cdots x_d^2; S^{d-1}) \geq r_d^{-1}$$

and the equality holds for $d = 3, 4, 5$ with $r_d^{-1}T_d(x_1^2, \dots, x_d^2)$ as a polynomial of least deviation from zero.

We believe that the equality still holds for $d \geq 6$. In fact, all that is missing is to prove that $|T_d(x)| \leq 1$ for $x \in T^d$. We state it as a conjecture.

Conjecture 4.4. For $d \geq 6$, the inequality $\|T_d(x)\|_{C(T^d)} \leq 1$ holds. In particular, the equality in the above two theorems holds for $d \geq 6$.

Let us point out that there does not appear to exist a closed formula for r_d . Below is a list of the first few values of r_d and their prime factorization:

$$\begin{aligned} r_3 &= 72 = 2^3 \cdot 3^2, & r_4 &= 896 = 2^7 \cdot 7, & r_5 &= 14400 = 2^6 \cdot 3^2 \cdot 5^2, \\ r_6 &= 283392 = 2^8 \cdot 3^3 \cdot 41, & r_7 &= 6598144 = 2^9 \cdot 7^2 \cdot 263, \\ r_8 &= 177373184 = 2^{15} \cdot 5413, & r_9 &= 5406289920 = 2^{12} \cdot 5 \cdot 3^4 \cdot 3259, \\ r_{10} &= 184223744000 = 2^{14} \cdot 5^3 \cdot 23 \cdot 3911, \\ r_{11} &= 6939874934784 = 2^{14} \cdot 3^3 \cdot 11^2 \cdot 137 \cdot 409. \end{aligned}$$

A closed formula will have to catch the pattern of the prime numbers presented in these formulae, which seems unlikely. We also note that the values of r_d appear to indicate that the best approximation to monomials becomes increasingly more complicated as d increases. See also the Remark 3.1.

The proof of Theorem 4.3 is split into several propositions. As before, we only need to prove the case of polynomials on the simplex. We start with the point set at which $T_d(x) = \pm 1$.

We will work with sets of points that are invariant under the symmetric group S_d . For $a \in \mathbb{R}^d$ we use the notation $(a)_G$ to denote the set of points that consist of all distinct permutations of x ; that is

$$(a_1, \dots, a_d)_G = \{(a_{\tau_1}, \dots, a_{\tau_d}) : \tau = (\tau_1, \dots, \tau_d) \in S_d\}$$

and we sometimes write $a\tau = (a_{\tau_1}, \dots, a_{\tau_d})$ for $\tau \in S_d$.

Proposition 4.5. *Let $\mathcal{S}_+(T^d)$ and $\mathcal{S}_-(T^d)$ be the subsets of T^d on which $T_d(x) = 1$ and $T_d(x) = -1$, respectively. For odd d ,*

$$\mathcal{S}_+ = \left\{ \left(\frac{1}{d}, \dots, \frac{1}{d}\right)_G, \left(\frac{1}{d-2}, \dots, \frac{1}{d-2}, 0, 0\right)_G, \dots, \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 0, \dots, 0\right)_G, (1, 0, \dots, 0)_G \right\}$$

is a subset of $\mathcal{S}_+(T^d)$ and

$$\mathcal{S}_- = \left\{ \left(\frac{1}{d-1}, \dots, \frac{1}{d-1}, 0\right)_G, \left(\frac{1}{d-3}, \dots, \frac{1}{d-3}, 0, 0, 0\right)_G, \dots, \left(\frac{1}{2}, \frac{1}{2}, 0, \dots, 0\right)_G \right\}$$

is a subset of $\mathcal{S}_-(T^d)$. For even d ,

$$\mathcal{S}_+ = \left\{ \left(\frac{1}{d}, \dots, \frac{1}{d}\right)_G, \left(\frac{1}{d-2}, \dots, \frac{1}{d-2}, 0, 0\right)_G, \dots, \left(\frac{1}{2}, \frac{1}{2}, 0, \dots, 0\right)_G \right\}$$

is a subset of $\mathcal{S}_+(T^d)$ and

$$\mathcal{S}_- = \left\{ \left(\frac{1}{d-1}, \dots, \frac{1}{d-1}, 0\right)_G, \left(\frac{1}{d-3}, \dots, \frac{1}{d-3}, 0, 0, 0\right)_G, \dots, (1, 0, \dots, 0)_G \right\}$$

is a subset of $\mathcal{S}_-(T^d)$. Furthermore, all these points are on the face of T^d defined by the equation $x_1 + \dots + x_d = 1$.

Proof. In the definition of T_d , the value of r_d is chosen so that $T_d(\frac{1}{d+1}, \dots, \frac{1}{d+1}) = 1$. All other points in the given set contain at least one zero component. This allows us to use induction. For $T_3(x)$, it is easy to verify that $T_3(x) = 1$ if $x = (1, 0, 0)_G$ and $x = (1/3, 1/3, 1/3)$, and $T_3(x) = -1$ if $x = (1/2, 1/2, 0)_G$. The induction is based on the formula

$$T_d(x_1, \dots, x_{d-1}, 0) = -T_{d-1}(x_1, \dots, x_{d-1})$$

and similar formulae obtained by a permutation of (x_1, \dots, x_{d-1}) , which follow from the definition of T_d and the fact that $e_d(x_1, \dots, x_{d-1}, 0) = 0$. \square

Proposition 4.6. *The signature σ , defined by $\sigma(v) = 1$ if $v \in \mathcal{S}_+$ and $\sigma(v) = -1$ if $v \in \mathcal{S}_-$, is an extremal signature of T_d . More precisely, define*

$$\begin{aligned} Lg &= d^{d-1}g\left(\frac{1}{d}, \dots, \frac{1}{d}\right) - (d-1)^{d-1} \sum_{\tau} g\left(\left(\frac{1}{d-1}, \dots, \frac{1}{d-1}, 0\right)\tau\right) \\ &\quad + \dots + (-1)^{d-2}2^{d-1} \sum_{\tau} g\left(\left(\frac{1}{2}, \frac{1}{2}, 0, \dots, 0\right)\tau\right) + (-1)^{d-1} \sum_{\tau} g((1, 0, \dots, 0)\tau); \end{aligned}$$

then $Lp = 0$ for all $p \in \Pi_{d-1}^d$.

Proof. Since the points in \mathcal{S}_+ and \mathcal{S}_- are symmetric with respect to S_d , a moments reflection shows that we only need to verify $Lg = 0$ for symmetric polynomials. One basis of symmetric polynomials in Π_{d-1}^d consists of $m_k(x) = x_1^k + \dots + x_d^k$ for $k = 0, 1, \dots, d-1$. We show $Lm_k = 0$. Let $a_j = (1/j, \dots, 1/j, 0, \dots, 0) \in T^d$, which contains exactly j nonzero entries. Then the sum $\sum_{\tau \in S_d} g(a_j\tau)$ contains $\binom{d}{j}$ terms and $m_k(a_j) = j(1/j)^k$. Consequently, for $k \geq 1$,

$$Lm_k = d^{d-k} - \binom{d}{1}(d-1)^{d-k} + \binom{d}{2}(d-2)^{d-k} + \dots + (-1)^{d-1} \binom{d}{d-1}.$$

Furthermore, it is easy to see that $L1$ gives the same formula as Lm_1 (recall that points in \mathcal{S}_+ and \mathcal{S}_- satisfy $x_1 + \dots + x_d = 1$). Hence, we need to show, changing $n - k$ to k ,

$$(4.1) \quad \sum_{j=0}^d (-1)^j \binom{d}{j} j^k = 0, \quad k = 1, 2, \dots, d-1.$$

This is well known and can be proved by induction on d . □

By Theorem 3.2, the above proposition has proved that

$$\inf_{p \in \Pi_{d-1}^d} \|x_1 \dots x_d - p(x)\|_{C(T^d)} \geq r_d^{-1}.$$

In order to show that the equality holds, we only need to prove that $|T_d(x)| \leq 1$ for $x \in T^d$. However, we are able to establish this inequality only for $d = 3, 4, 5$.

Proposition 4.7. *For $d = 3, 4, 5$,*

$$|T_d(x)| \leq \|T_d\|_{C(T^{d-1})} = 1, \quad x \in T^d.$$

Proof. There does not seem to be an easy way of proving this. We use the standard method of finding critical points upon solving $(\partial_i T_d(x)/\partial x_i) = 0$, $1 \leq i \leq d$. The case $d = 3$ is in the previous section and the equations can be solved algebraically. The cases $d = 4$ and $d = 5$ are solved numerically. The details are omitted. Once the critical points are found, we can then verify that the inequality $|T_d(x)| < 1$ holds on these points, which shows that the maximum of $|T_d(x)|$ is attained on the boundary of T^d . Since $T_d(x_1, \dots, x_{d-1}, 0) = -T_{d-1}(x_1, \dots, x_{d-1})$, by induction, we only need to prove that $|T_d(x_1, \dots, x_{d-1}, 1 - x_1 - \dots - x_{d-1})| \leq 1$ for $x \in T^{d-1}$. Again, this is done by computing the critical points and evaluating. □

Putting the above propositions together, we have completed the proof of Theorem 4.3.

We still need to prove Lemma 4.2. First we note that the definition of T_d implies

$$T_d(x) = \sum_{k=4}^d (-1)^{d-k} r_k e_k(x) + (-1)^{d-3} T_3(x).$$

Proof of Lemma 4.2. Setting $x = a_{d+1} = (d+1)^{-1} \mathbf{1}^{d+1}$ and using the fact that $e_k(a_{d+1}) = \binom{d+1}{k} (d+1)^{-k}$ leads to the relation

$$(d+1)^{-(d+1)} r_{d+1} = \sum_{k=4}^d (-1)^{d-k} \binom{d+1}{k} (d+1)^{-k} r_k + (-1)^{d-3} T_3(a_{d+1}) + 1.$$

Replacing $d+1$ by d we can write the above equation as

$$\sum_{k=4}^d (-1)^{d-k} \binom{d}{k} d^{-k} r_k = (-1)^d T_3(d^{-1} \mathbf{1}^d) + 1 := A_d.$$

We want to reverse this relation so that $r_d = \sum_{j=4}^d b_j A_j$. A standard argument shows that, with b_j given below, this will follow from the combinatoric relation

$$J_{k,d} := \sum_{j=k}^d b_j (-1)^{j-k} \binom{j}{k} j^{-k} = \delta_{k,d}, \quad b_j = d \binom{d}{j} j^{d-1},$$

where $\delta_{k,d} = 1$ if $k = d$ and 0 otherwise. For $k = d$, $J_{d,d} = 1$ holds trivially. For $k < d$, a change of summation index gives

$$J_{k,d} = \binom{d}{k} \sum_{j=k}^d (-1)^{j-k} \binom{d-k}{j-k} j^{d-1-k} = \binom{d}{k} \sum_{j=0}^{d-k} (-1)^j \binom{d-k}{j} (k+j)^{d-1-k}.$$

By (4.1), the last formula shows that $J_{k,d} = 0$. Finally, the definition of T_3 shows that

$$T_3(d^{-1} \mathbf{1}^d) = 72 \binom{d}{3} d^{-3} - 8 \binom{d}{2} d^{-2} + 1 = d^{-2} (9d^2 - 32d + 24),$$

which gives the explicit value of A_d . Putting these relations together completes the proof. \square

We conjecture that $|T_d(x)| \leq 1$ for all d and the points in \mathcal{S}_+ and \mathcal{S}_- are the only ones on the face of T^d defined by $x_1 + \dots + x_d = 1$ on which $|T_d(x)| = 1$. The following fact is helpful for the case $d = 5$ and could be useful for $d > 5$. Let

$$D_d(x) = \det \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_d \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{d-3} & x_2^{d-3} & \dots & x_d^{d-3} \\ \partial_1 T_d(x) & \partial_2 T_d(x) & \dots & \partial_d T_d(x) \end{bmatrix},$$

where $\partial_i = \partial/\partial x_i$. Then $D_d(x)$ can be factored completely. We have, for example,

$$D_5(x) = -64 \prod_{1 \leq i < j \leq 4} (x_i - x_j) (-14 + 225x_5).$$

At the critical points of T_5 , $D_5(x) = 0$ and $D_5(x\tau) = 0$ for $\tau \in S_5$. One could use it to confirm the conjecture for $d > 5$. We did not try hard to push for larger d , since the method does not seem to lead to a proof for all d .

Our conjecture implies that $T_d(x)$ attains its maximum on the boundary of T^d . Part of this can be proved as follows: Let Δ denote the Laplacian operator $\Delta = \partial_1^2 + \dots + \partial_d^2$. Then it is easy to verify that $\Delta T_d(x) = (-1)^{d-1}8d$. In particular, this shows that $(-1)^{d-1}T_d(x)$ is a subharmonic function. Hence, by the maximum principle ([John, 82]) for the subharmonic functions, we can conclude that $(-1)^{d-1}T_d(x) \leq \max_{x \in \partial T^d} (-1)^{d-1}T_d(x)$.

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