

MULTIVARIATE POLYNOMIAL APPROXIMATION IN THE HYPERCUBE

LLOYD N. TREFETHEN

(Communicated by)

ABSTRACT. A theorem is proved concerning approximation of analytic functions by multivariate polynomials in the s -dimensional hypercube. The geometric convergence rate is determined not by the usual notion of degree of a multivariate polynomial, but by the *Euclidean degree*, defined in terms of the 2-norm rather than the 1-norm of the exponent vector \mathbf{k} of a monomial $x_1^{k_1} \cdots x_s^{k_s}$.

1. INTRODUCTION

The aim of this paper is to prove a theorem concerning an effect identified in Section 6 of [12]. If an analytic function $f(\mathbf{x}) = f(x_1, \dots, x_s)$ is approximated by multivariate polynomials in the s -dimensional hypercube $[-1, 1]^s$, the usual notion of polynomial degree, namely the total degree, is not the right predictor of approximability. In the hypercube, the set of polynomials of a given total degree has \sqrt{s} times finer resolution along a direction aligned with an axis than along a diagonal. Conversely, the set of polynomials of a given maximal degree has \sqrt{s} times finer resolution along a diagonal than along an axis. To achieve balanced resolution in all directions one should work with polynomials of a given *Euclidean degree*.

Our definitions are as follows. With $s \geq 1$, we consider functions $f(\mathbf{x}) = f(x_1, \dots, x_s)$ in $[-1, 1]^s$, with $\|\cdot\|_{[-1,1]^s}$ representing the maximum norm over this set. For a monomial $x_1^{k_1} \cdots x_s^{k_s}$ we define

$$(1.1) \quad \text{Total degree :} \quad d_T = \|\mathbf{k}\|_1,$$

$$(1.2) \quad \text{Euclidean degree :} \quad d_E = \|\mathbf{k}\|_2,$$

$$(1.3) \quad \text{Maximal degree :} \quad d_{\max} = \|\mathbf{k}\|_{\infty},$$

where $\|\cdot\|_1$, $\|\cdot\|_2$, and $\|\cdot\|_{\infty}$ are the 1-, 2-, and ∞ - norms of the s -vector $\mathbf{k} = (k_1, \dots, k_s)$, and the degree of a multivariate polynomial is the maximum of the degrees of its nonzero monomial constituents. The total and maximal degree

2010 *Mathematics Subject Classification.* 41A63.

Supported by the European Research Council under the European Union's Seventh Framework Programme (FP7/2007–2013)/ERC grant agreement no. 291068. The views expressed in this article are not those of the ERC or the European Commission, and the European Union is not liable for any use that may be made of the information contained here.

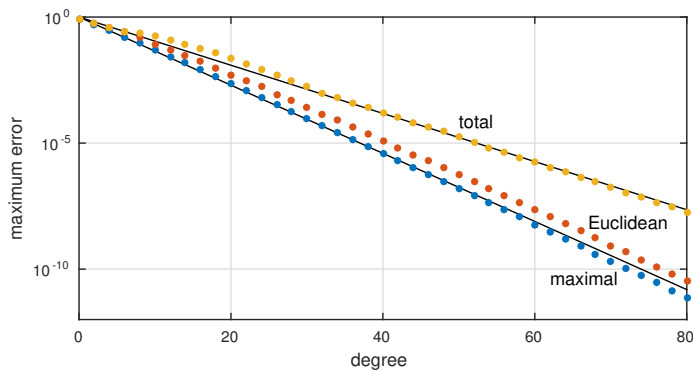


FIGURE 1. Maximum-norm errors in approximation of the Runge function (2.1) as a function of degree n in the unit square, for three different definitions of degree. The approximations come from least-squares minimization over a fine grid in $[-1, 1]^2$. Straight lines mark the convergence rates of Theorem 4.2.

definitions are standard and appear in publications like [8] and [10] where multivariate polynomial approximation in the hypercube is discussed, but the Euclidean degree seems to be new in [12]. Note that d_E is not in general an integer.

Our interest is in leading order exponential effects, not algebraic fine points, and accordingly, we will make use of the notation O_ε defined as follows: $g(n) = O_\varepsilon(a^n)$ if for all $\varepsilon > 0$, $g(n) = O((a + \varepsilon)^n)$ as $n \rightarrow \infty$. By $O_\varepsilon(a^{-n})$ we mean $O_\varepsilon((1/a)^n)$, or equivalently, for all $\varepsilon > 0$, $O((a - \varepsilon)^{-n})$.

2. NUMERICAL ILLUSTRATION

The case $s = 2$ suffices for a numerical illustration. Let f be the 2D Runge function

$$(2.1) \quad f(x, y) = \frac{1}{1 + 10(x^2 + y^2)},$$

which is analytic for all real values of x and y and isotropic in the sense that it is invariant with respect to rotation in the x - y plane. Figure 1 gives an indication of the minimal error in approximation of f on $[-1, 1]^2$ by bivariate polynomials of various total, Euclidean, and maximal degrees. (Bivariate Chebyshev coefficients of f are plotted in Figure 6.4 of [12].) The figure is actually based on L^2 rather than L^∞ approximations, since these are much easier to compute, but this is enough to give an indication of the separation between the convergence rates when the degree is defined by d_T and when it is defined by d_E or d_{\max} .

The function (2.1) satisfies Assumption A of our theorem, Theorem 4.2, with $h^2 = 0.1$, and the data in the figure show convincing agreement with the predictions of the theorem. This function is analytic when x and y are real but not when they are complex. On the other hand the similar function

$$(2.2) \quad g(x, y) = \frac{1}{21 - 10(x^2 + y^2)}$$

has real singularities just outside the unit square. Theorem 4.2 applies with $h^2 = 0.1$ for this function too, and a plot of convergence rates (not shown) looks almost exactly like Figure 1.

3. CHEBYSHEV SERIES IN 1D

In the standard theory for a single variable x , for any $\rho > 1$, let E_ρ denote the open set bounded by the Bernstein ρ -ellipse in the complex x -plane, i.e., the image of the circle $|w| = \rho$ under the map $x = (w + w^{-1})/2$. A Lipschitz continuous function f defined on $[-1, 1]$ has an absolutely and uniformly convergent Chebyshev series

$$(3.1) \quad f(x) = \sum_{k=0}^{\infty} a_k T_k(x),$$

where T_k is the Chebyshev polynomial of degree k . Truncating the series at degree n gives the polynomial approximation

$$(3.2) \quad p_n(x) = \sum_{k=0}^n a_k T_k(x).$$

The following result goes back to Bernstein's prize-winning memoir of 1912 [2]. Here and elsewhere, when we say that f is analytic in a region, we mean that if necessary f can be analytically continued to that region.

Lemma 3.1. *If f is analytic in E_ρ , its Chebyshev coefficients and truncated Chebyshev expansions satisfy*

$$(3.3) \quad a_k = O_\varepsilon(\rho^{-k}), \quad \|f - p_n\|_{[-1,1]} = O_\varepsilon(\rho^{-n}).$$

Proof. The second estimate follows from the first, whose proof can be based on contour integrals over $\tilde{\rho}$ -ellipses with $\tilde{\rho} = \rho - \varepsilon$ for arbitrarily small $\varepsilon > 0$, or equivalently on contour integrals over circles in the z -plane after a change of variables from $x \in [-1, 1]$ to z on the unit circle. See Theorems 8.1 and 8.2 of [11]. \square

For our purposes it will be important to consider x^2 as well as x . When x ranges over E_ρ , with foci -1 and 1 and topmost point ih , x^2 ranges over another ellipse, with foci 0 and 1 and leftmost point $-h^2$, where h and ρ are related by

$$(3.4) \quad h = (\rho - \rho^{-1})/2, \quad \rho = h + \sqrt{1 + h^2}.$$

Arnol'd calls E_ρ a *Hooke ellipse* and E_ρ^2 a *Newton ellipse* [1]. We wish to parametrize the latter by h^2 rather than ρ , so we make the following definition.

Definition 3.2. For any $s, a > 0$, $N_{s,a}$ is the open region in the complex plane bounded by the ellipse with foci 0 and s and leftmost point $-a$. Equivalently, it is the region consisting of points x satisfying $|x| + |x - s| < s + 2a$.

Thus $E_\rho^2 = N_{1,h^2}$, and Lemma 3.1 can be equivalently restated as follows.

Lemma 3.3. *Suppose that for some $h > 0$, $f(x)$ is analytic for all $x \in \mathbb{C}$ such that $x^2 \in N_{1,h^2}$. Then (3.3) holds with $\rho = h + \sqrt{1 + h^2}$.*

4. MAIN THEOREM

Now let f be a function of $\mathbf{x} \in [-1, 1]^s$ for some $s \geq 1$. If f is smooth, it has a uniformly and absolutely convergent multivariate Chebyshev series

$$(4.1) \quad p(\mathbf{x}) = \sum_{k_1=0}^{\infty} \cdots \sum_{k_s=0}^{\infty} a_{k_1, \dots, k_s} T_{k_1}(x_1) \cdots T_{k_s}(x_s)$$

(see e.g. Theorem 4.1 of [8]). Here is our analyticity assumption, generalizing that of Lemma 3.3.

Assumption A. *For some $h > 0$, $f(\mathbf{x})$ is analytic for all $\mathbf{x} \in \mathbb{C}^s$ in the s -dimensional region defined by the condition $x_1^2 + \cdots + x_s^2 \in N_{s, h^2}$.*

Note that a sufficient condition for Assumption A to hold is that $f(\mathbf{x})$ is analytic for all \mathbf{x} with $\Re(x_1^2 + \cdots + x_s^2) > -h^2$.

The following lemma will be proved in the next section.

Lemma 4.1. *If f satisfies Assumption A, its multivariate Chebyshev coefficients satisfy*

$$(4.2) \quad a_{\mathbf{k}} = O_{\varepsilon}(\rho^{-\|\mathbf{k}\|_2}),$$

where $\rho = h + \sqrt{1 + h^2}$.

Based on this result, our theorem bounds the convergence rates of polynomial approximations defined by total, Euclidean, and maximal degree.

Theorem 4.2. *If f satisfies Assumption A, then*

$$\inf_{d(p) \leq n} \|f - p\|_{[-1, 1]^s} = \begin{cases} O_{\varepsilon}(\rho^{-n/\sqrt{s}}) & \text{if } d = d_T, \\ O_{\varepsilon}(\rho^{-n}) & \text{if } d = d_E, \\ O_{\varepsilon}(\rho^{-n}) & \text{if } d = d_{\max}, \end{cases}$$

where $\rho = h + \sqrt{1 + h^2}$.

Proof of Theorem 4.2, assuming Lemma 4.1. The second (middle) assertion of the theorem follows from Lemma 4.1 by truncating the multivariate Chebyshev series (4.1), since $|T_{k_1}(x_1) \cdots T_{k_s}(x_s)| \leq 1$ for all \mathbf{k} for all $\mathbf{x} \in [-1, 1]^s$. The third assertion is a consequence of the second, since $d_{\max}(p) \leq d_E(p)$ for any multivariate polynomial p . The first assertion is also a consequence of the second since $d_T(p)/\sqrt{s} \leq d_E(p)$.

Theorem 4.2 is only an upper bound, so in principle, the difference it suggests between d_T and the other degrees d_E and d_{\max} might be illusory. However, numerical experiments such as that of Figure 1 and those reported in [12] make it clear that the difference is genuine. This could be made rigorous by the development of a converse theorem, as has been long established in the 1D case, again thanks to Bernstein (see Theorem 8.3 of [11]).

5. PROOF OF LEMMA 4.1

To complete the proof of Theorem 4.2 we must prove Lemma 4.1. For this we will make use of a result in the book by Bochner and Martin [3]. Let $\boldsymbol{\rho} = (\rho_1, \dots, \rho_s)$ be an s -vector with $\rho_j > 1$ for each j , and let $E(\boldsymbol{\rho}) \subset \mathbb{C}^s$ be the *elliptic polycylinder* defined as the set of all points $\mathbf{x} \in \mathbb{C}^s$ such that $x_j \in E_{\rho_j}$ for each j . The result in question is an s -dimensional generalization of Lemma 3.1.

Lemma 5.1. *Let f be analytic in $E(\boldsymbol{\rho})$. Then its multivariate Chebyshev coefficients satisfy*

$$(5.1) \quad a_{\mathbf{k}} = O_{\varepsilon}(\rho_1^{-k_1} \cdots \rho_s^{-k_s})$$

as $k_1 + \cdots + k_s \rightarrow \infty$.

Proof. Equation (5.1) means that for any $\varepsilon > 0$, $a_{\mathbf{k}} = O((\rho_1 - \varepsilon)^{-k_1} \cdots (\rho_s - \varepsilon)^{-k_s})$. This is essentially Theorem 11 on p. 95 of [3], which is derived by contour integrals. For further discussion see [4]. \square

Proof of Lemma 4.1. For any s -vector \mathbf{k} of nonnegative indices, define

$$c_j = \frac{k_j}{\|\mathbf{k}\|_2} \leq 1$$

and

$$h_j = c_j h.$$

Then $h_1^2 + \cdots + h_s^2 = h^2$, so by Assumption A, $f(\mathbf{x})$ is analytic in the subset of \mathbb{C}^s defined by the condition $x_1^2 + \cdots + x_s^2 \in N_{s, h^2}$. From Lemma 5.2 below, we have

$$(5.2) \quad N_{1, h_1^2} \oplus \cdots \oplus N_{1, h_s^2} \subseteq N_{s, h_1^2 + \cdots + h_s^2},$$

where \oplus denotes the standard Minkowski sum of sets. It follows that $f(\mathbf{x})$ is analytic whenever $x_j \in N_{1, h_j^2}$ for each j . In other words, $f(\mathbf{x})$ is analytic in the elliptic polycylinder $E(\hat{\boldsymbol{\rho}})$ with $\hat{\rho}_j$ defined by

$$\hat{\rho}_j = h_j + \sqrt{1 + h_j^2} = c_j h + \sqrt{1 + (c_j h)^2}.$$

It can be shown (Lemma 5.3, below) that this final quantity is greater than or equal to the number ρ_j which we define by

$$\rho_j = (h + \sqrt{1 + h^2})^{c_j} = \rho^{k_j / \|\mathbf{k}\|_2}.$$

Therefore if $\boldsymbol{\rho}$ is the s -vector with components given by this formula, then the associated polycylinder satisfies $E(\boldsymbol{\rho}) \subseteq E(\hat{\boldsymbol{\rho}})$, and $f(\mathbf{x})$ is analytic in $E(\boldsymbol{\rho})$. We now calculate

$$(5.3) \quad \rho_1^{-k_1} \cdots \rho_s^{-k_s} = \rho^{-(k_1^2 + \cdots + k_s^2) / \|\mathbf{k}\|_2} = \rho^{-\|\mathbf{k}\|_2},$$

and inserting this identity in (5.1) gives (4.2), as required. \square

Here are the two lemmas just used.

Lemma 5.2. *For any $s, t > 0$ and $a, b > 0$,*

$$(5.4) \quad N_{s, a} \oplus N_{t, b} \subseteq N_{s+t, a+b}.$$

Proof. If $x \in N_{s, a}$ and $y \in N_{t, b}$, then we have

$$|x| + |x - s| < s + 2a, \quad |y| + |y - t| < t + 2b.$$

Therefore by the triangle inequality,

$$|x + y| + |(x + y) - (s + t)| < (s + 2a) + (t + 2b),$$

that is,

$$|x + y| + |(x + y) - (s + t)| < (s + t) + 2(a + b),$$

which implies $x + y \in N_{s+t, a+b}$. \square

Lemma 5.3. *For any $h \geq 0$ and $c \in [0, 1]$, $ch + (1 + c^2h^2)^{1/2} \geq (h + (1 + h^2)^{1/2})^c$.*

Proof. Given h , define $\varphi(c) = ch + (1 + c^2h^2)^{1/2}$. We must show $\varphi(c) \geq \varphi(1)^c$, or equivalently

$$(5.5) \quad \psi(c) \geq c\psi(1), \quad 0 \leq c \leq 1,$$

where

$$\psi(c) = \log(\varphi(c)) = \log(ch + (1 + c^2h^2)^{1/2}).$$

Since $\psi(0) = 0$, a sufficient condition for (5.5) to hold is that ψ is convex in the sense that $\psi''(c) \leq 0$ for $c \in [0, 1]$. This follows from the identity $\psi''(c) = -ch^3(1 + c^2h^2)^{-3/2}$. \square

6. DISCUSSION

This work is motivated by computational applications, since for computation in higher dimensions, a hypercube is usually the domain of choice. Theorem 4.2 suggests that any method for computation in a hypercube that is based on one of the familiar definitions of the degree of a multivariate polynomial, namely total degree or maximal degree, is likely to be suboptimal. For example, a standard idea of multidimensional quadrature (cubature) is the exact integration of multivariate polynomial approximations of a given total degree, an idea going back to Maxwell [7, 9]. The theorem casts doubt upon the appropriateness of that approach.

Quantifying this assertion reveals that when s is moderate or large, the differences in efficiency of different approximation strategies may be considerable. The portions of the unit balls in the 1-, 2-, and ∞ -norms restricted to the positive orthant have volumes

$$(6.1) \quad V_1 = \frac{1}{s!} \sim \frac{1}{\sqrt{2\pi s}} \left(\frac{e}{s}\right)^s, \quad V_2 = \frac{(\pi/4)^{s/2}}{(s/2)!} \sim \frac{1}{\sqrt{\pi s}} \left(\frac{\pi e}{2s}\right)^{s/2}, \quad V_\infty = 1,$$

and with $s = 10$, for example, we have

$$(6.2) \quad V_1 \approx 0.000000276, \quad V_2 \approx 0.00249, \quad V_\infty = 1.$$

For fixed s and $n \rightarrow \infty$, the dimensions of the spaces of polynomials of degree n defined by d_T , d_E , and d_{\max} scale as n^s times these numbers. By putting such estimates together with Theorem 4.2, we can work out consequences for approximation.

First of all let us compare Euclidean and maximal degree. According to the theorem, we expect to need similar values of n for both d_E and d_{\max} to achieve a given approximation accuracy. This suggests that in the 10-hypercube, a fit based on d_{\max} will require $V_\infty/V_2 \approx 402$ times as many parameters as one based on d_E , where V_∞ and V_2 are the numbers given in (6.2). The general formula for the s -hypercube based on (6.1) is

$$(6.3) \quad \frac{\text{no. of parameters for approx. based on } d_{\max}}{\text{no. of parameters for approx. based on } d_E} \approx \frac{V_\infty}{V_2} \sim \sqrt{\pi s} \left(\frac{2s}{\pi e}\right)^{s/2}.$$

On the other hand let us compare Euclidean and total degree. According to the theorem, if a fit based on d_E needs degree n , we can expect a fit based on d_T to need degree $n\sqrt{s}$. Thus in the 10-hypercube, we must compare total degree $(\sqrt{10})^{10}n$ against Euclidean degree n , suggesting that a fit based on d_T will

require $(\sqrt{10})^{10} V_1/V_2 \approx 11.1$ times as many parameters as one based on d_E , where V_1 and V_2 are as given in (6.2). The general formula based on (6.1) is

$$(6.4) \quad \frac{\text{no. of parameters for approx. based on } d_T}{\text{no. of parameters for approx. based on } d_E} \approx \frac{s^{s/2} V_1}{V_2} \sim 2^{-1/2} \left(\frac{2e}{\pi} \right)^{s/2}.$$

Equations (6.3) and (6.4) show that both total and maximal degree may be exponentially less efficient for polynomial approximation than Euclidean degree. All these estimates apply to functions f whose complexity is approximately isotropic in the sense that the implications of Assumption A are reasonably sharp. A more extensive discussion of such differences can be found in Section 6 of [12].

In closing I would like to highlight a conceptual link between this note and my earlier paper [6] with Nick Hale. The central observation of [6] is that the resolving power of (univariate) polynomials on an interval $[-1, 1]$ is nonuniform, making polynomials fall short of optimality by a factor of $\pi/2$ in representing functions whose complexity on $[-1, 1]$ is uniform. In the present work, the issue is again nonuniformity of polynomials, but now they are multivariate and the uniformity issue pertains to rotation rather than translation. As pointed out in Section 7 of [12], the translational issue is present in multiple dimensions too.

ACKNOWLEDGMENTS

I have benefitted from extensive discussions of approximation and cubature in the hypercube with Hadrien Montanelli and Klaus Wang. I thank also Jared Aurentz, Stefan Güttel, Nick Hale, Allan Pinkus, and Alex Townsend for helpful suggestions. It was Aurentz who proposed the term “Euclidean degree.”

REFERENCES

1. V. I. ARNOL'D, *Huygens & Barrow, Newton & Hooke: Pioneers in Mathematical Analysis and Catastrophe Theory from Evolvants to Quasicrystals*, Birkhäuser, 1990.
2. S. N. BERNSTEIN, Sur l'ordre de la meilleure approximation des fonctions continues par des polynômes de degré donné, *Mém. Acad. Roy. Belg.*, 1912, pp. 1–104.
3. S. BOCHNER AND W. T. MARTIN, *Several Complex Variables*, Princeton U. Press, 1948.
4. J. BOYD, Large-degree asymptotics and exponential asymptotics for Fourier, Chebyshev and Hermite coefficients and Fourier transforms, *J. Eng. Math.* 63 (2009), 355–399.
5. T. A. DRISCOLL, N. HALE, AND L. N. TREFETHEN, *Chebfun User's Guide*, Pafnuty Publications, Oxford, 2014. See also www.chebfun.org.
6. N. HALE AND L. N. TREFETHEN, New quadrature formulas from conformal maps, *SIAM J. Numer. Anal.* 46 (2008), 930–948.
7. A. R. KROMMER AND C. W. UEBERHUBER, *Computational Integration*, SIAM, 1998.
8. J. C. MASON, Near-best multivariate approximation by Fourier series, Chebyshev series and Chebyshev interpolation, *J. Approx. Th.* 28 (1980), 349–358.
9. J. C. MAXWELL, On approximate multiple integration between limits of summation, *Proc. Camb. Phil. Soc.* 3 (1877), 39–47.
10. A. F. TIMAN, *Theory of Approximation of Functions of a Real Variable*, Dover, 1994.
11. L. N. TREFETHEN, *Approximation Theory and Approximation Practice*, SIAM, 2013.
12. L. N. TREFETHEN, Cubature, approximation, and isotropy in the hypercube, *SIAM Rev.*, to appear.

MATHEMATICAL INSTITUTE, UNIVERSITY OF OXFORD, OXFORD, OX2 6GG, UK
 E-mail address: trefethen@maths.ox.ac.uk