

Asymptotic coefficients and errors for Chebyshev polynomial approximations with weak endpoint singularities: Effects of different bases

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Abstract When one solves differential equations by a spectral method, it is often convenient to shift from Chebyshev polynomials $T_n(x)$ with coefficients a_n to modified basis functions that incorporate the boundary conditions. For homogeneous Dirichlet boundary conditions, $u(\pm 1) = 0$, popular choices include the “Chebyshev difference basis” $\varsigma_n(x) \equiv T_{n+2}(x) - T_n(x)$ with coefficients here denoted by b_n and the “quadratic factor basis” $\varrho_n(x) \equiv (1 - x^2)T_n(x)$ with coefficients c_n . If $u(x)$ is weakly singular at the boundary, then the coefficients a_n decrease proportionally to $\mathcal{O}(A(n)/n^\kappa)$ for some positive constant κ , where $A(n)$ is a logarithm or a constant. We prove that the Chebyshev difference coefficients b_n decrease more slowly by a factor of $1/n$ while the quadratic factor coefficients c_n decrease more slowly still as $\mathcal{O}(A(n)/n^{\kappa-2})$. The error for the unconstrained Chebyshev series, truncated at degree $n = N$, is $\mathcal{O}(|A(N)|/N^\kappa)$ in the interior, but is worse by one power of N in narrow boundary layers near each of the endpoints. Despite having nearly identical error norms in interpolation, the error in the Chebyshev basis is concentrated in boundary layers near both endpoints, whereas the error in the quadratic factor and difference basis sets is nearly uniformly oscillating over the entire interval in x . Meanwhile, for Chebyshev polynomials, the values of their derivatives at the endpoints are $\mathcal{O}(n^2)$, but only $\mathcal{O}(n)$ for the difference basis. Furthermore, we give the asymptotic coefficients and rigorous error estimates of the approximations in these three bases, solved by the least squares method. We also find an interesting fact that on the face of it, the aliasing error is regarded as a bad thing; actually, the error norm associated with the downward curving spectral coefficients decreases even faster than the error norm of infinite truncation. But the premise is under the same basis, and when involving different bases, it may not be established yet.

Keywords Chebyshev polynomial, interpolation, endpoint singularities, least squares method

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1 Introduction

The success of Chebyshev polynomial spectral methods in solving differential and integral equations is comprehensively cataloged in a variety of standard texts such as [14, 16, 20, 25, 27], and a cornucopia of others including two by Boyd [6, 8]. There are, however, some areas of spectral methods where open questions remain and consensus has not been achieved. One is the best way to impose boundary conditions. Even if we narrow the focus to the “basis recombination”, which is to use basis functions that are linear combinations of Chebyshev polynomials such that each basis function individually and exactly satisfies homogeneous linear boundary conditions, it might also have multiple options. Weak endpoint singularities—“weak” in the sense that the spectral series converges—are still a topic of active exploration. In this paper, we analyze both issues and show that they are closely interrelated.

The standard Chebyshev coefficients of a function $u(x)$ are the coefficients a_n in the series

$$u(x) = \sum_{n=0}^{\infty} a_n T_n(x). \quad (1.1)$$

If $u(x)$ has weak endpoint singularities, then its Chebyshev coefficients a_n asymptotically (as $n \rightarrow \infty$) decrease proportional to $1/n^\kappa$ for some positive constant κ , which is the “algebraic convergence order”, perhaps modulo some slower-than-power functions of n such as $\ln^\vartheta(n)$, $\vartheta \in \mathbb{N}_+$. Here, “weak” (singularity) means that $u(x)$ is continuous everywhere on the interval $x \in [-1, 1]$, but its first derivative or higher derivatives are singular.

When a problem satisfies homogeneous Dirichlet boundary conditions $u(\pm 1) = 0$, it is often *desirable* to choose basis functions that satisfy the boundary conditions. Two possibilities are

$$u^{\text{diff}}(x) = \sum_{n=0}^{\infty} b_n \varsigma_n(x), \quad \varsigma_n(x) \equiv T_{n+2}(x) - T_n(x) \quad (\text{the difference basis}) \quad (1.2)$$

or

$$u^{\text{quad}}(x) = \sum_{n=0}^{\infty} c_n \varrho_n(x), \quad \varrho_n(x) \equiv (1 - x^2)T_n(x) \quad (\text{the quadratic factor basis}). \quad (1.3)$$

This was dubbed “basis recombination” in the book of Boyd, who discussed this strategy and its alternatives in [6, pp. 112–114]. The alternatives are “boundary-bordering”, which is to replace collocation or Galerkin projection conditions by rows of the discretization matrix that explicitly enforce the boundary conditions, and “penalty methods” [16]. Karageorghis [17] discussed the relationship between basis recombination and boundary-bordering for multidimensional problems in single and multiple domains.

Why “desirable”? Boyd gave an answer for eigenvalue problems in [3]. Boundary-bordering for an eigenvalue problem gives a discretization matrix in which the rows that impose the boundary conditions are independent of the eigenvalue. This was sufficient to wreck EISPACK, the premier eigensolver of its day. Forty years later, library matrix eigensolvers are made of sterner stuff, but the rows imposing boundary conditions are still bad for the condition number.

Heinrichs [15] pointed out that if one constructs the recombined basis functions to be, say, for symmetric functions for Dirichlet boundary conditions $T_{n+2}(x) - T_n(x)$ instead of $T_{2n+2}(x) - T_0(x)$, the oscillations of the two Chebyshev polynomials of similar degrees partially cancel, reducing the condition number of the discretization matrix. The improvement for a k -th order differential equation with a basis truncated to N Chebyshev polynomials is a factor of N^k reduction in the condition number, which is particularly significant for higher order differential equations¹⁾.

The widespread use of basis recombination is attested by texts like [16] as well as by other literature [13].

Convergence theory for Chebyshev polynomial series has coevolved with Chebyshev algorithms and applications [6, 16]. Boyd’s review [7] summarizes convergence theory up to 2009. More recent

¹⁾ Parenthetically, note that basis recombination is also very convenient when N is *small* and the discretized problem is solved by a computer algebra system; reducing the number of basis coefficients from N to $(N - 2)$ greatly reduces the complexity of the explicit, analytic answer [5].

contributions include [18, 19, 27, 29, 31, 35]. There is also active literature on closely related problems such as Gaussian quadrature and Clenshaw-Curtis quadrature for functions with various types of singularities [24, 26, 30, 34], which were not included in [7]. It is impossible to review this in detail, but the sheer mass of theory shows that this vein of mathematics is still being actively mined.

Gaps in the existing theory are: how do basis recombination and interpolation alter the convergence rate? In this paper, we fill in these gaps.

One unnoticed but significant aspect of spectral methods for problems with weak endpoint singularities is that all the three expansions have coefficients decreasing as inverse powers of n (or inverse powers of n multiplied by a factor of a logarithm function), but the exponents are *different* for each of the three as expressed by the first theorem below. Indeed, there are also other differences among these three basis sets when truncated.

Our comparisons employ three different ways to calculate the coefficients in these basis sets.

(1) The Chebyshev inner product projection is

$$a_0 = \frac{1}{\pi} \int_{-1}^1 \frac{T_0(x)}{\sqrt{1-x^2}} u(x) dx, \quad a_n = \frac{2}{\pi} \int_{-1}^1 \frac{T_n(x)}{\sqrt{1-x^2}} u(x) dx, \quad n > 0, \quad (1.4)$$

b_n and c_n are expressed by the difference equations given below. They are consistent with all the degrees with the infinite Chebyshev series as defined precisely in Lemma 2.1.

(2) The infinite sums are truncated and $(N+1)$ -point interpolation is applied.

(3) Least squares minimization of constraints is applied at M points, where $M > (N+1)$.

The least squares method yields a rectangular matrix problem. Interpolation is the limit in which the matrix is square ($M = N+1$), while the infinite series coefficients are the limit $M \rightarrow \infty$.

The effects on the *errors* when each of the expansions is truncated after N terms are subtle. These subtleties are explained in Section 3.

We compare the basis functions in Figure 1. The qualitative resemblance is strong, which makes the behavioral differences all the more remarkable.

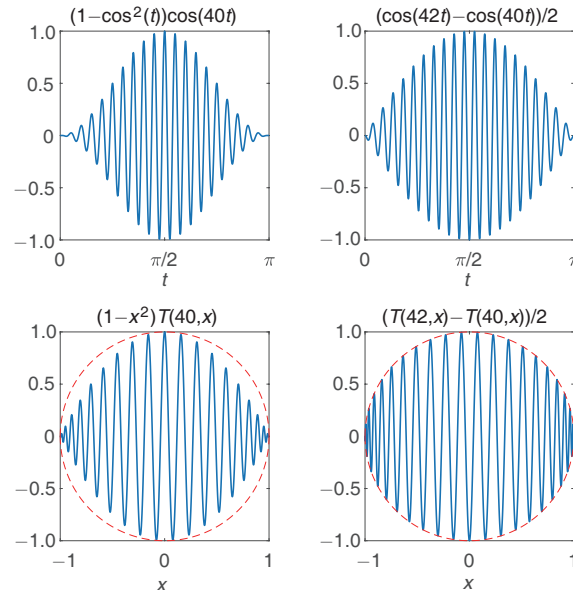


Figure 1 (Color online) The left two plots show a typical quadratic factor basis function, plotted versus t at the top and $x = \cos(t)$ at the bottom. Right: Same but for a basis function which is the difference of two Chebyshev polynomials, $\varsigma_{40}(x) = T_{42}(x) - T_{40}(x)$. The envelope of the bottom right curve is almost a circle of unit radius

2 Rates of decay of Chebyshev coefficients and basis functions

In this section, we compare the coefficients of the infinite series on each basis. Interpolation and least squares with a finite number of quadrature points are reserved for later sections.

Lemma 2.1 (Difference equations for infinite series coefficients). *Suppose that a function $u(x)$ is zero at both endpoints but analytic everywhere on $[-1, 1]$ except at the endpoints where $u(x)$ is allowed to be weakly singular. Here “weakly” is in the sense that $v(x) = u(x)/(1-x^2)$ is bounded at the endpoints. Let $u(x)$ have the three infinite series representations (1.1)–(1.3). Then the following statements hold:*

(i) $\varsigma_n(x)$ and $\varrho_n(x)$ are connected by the difference equation and initial conditions, i.e.,

$$\begin{aligned} \varsigma_0(x) &= T_2(x) - T_0(x) = -2\varrho_0(x), \quad \varsigma_1(x) = T_3(x) - T_1(x) = -4\varrho_1(x), \\ \varsigma_n(x) - \varsigma_{n-2}(x) &= -4\varrho_n(x), \quad n \geq 2. \end{aligned} \quad (2.1)$$

(ii) The condition $u^{\text{diff}}(x) = u(x)$ requires that the coefficients b_n be connected to a_n by the difference equation

$$b_0 = -a_0, \quad b_1 = -a_1, \quad b_{n-2} - b_n = a_n, \quad n \geq 2, \quad (2.2)$$

which implies that

$$b_{2n} = -\sum_{j=0}^n a_{2j}, \quad b_{2n+1} = -\sum_{j=0}^n a_{2j+1}. \quad (2.3)$$

(iii) Similarly, $u^{\text{quad}}(x) = u(x)$ only if

$$\begin{aligned} \frac{1}{2}c_0 - \frac{1}{4}c_2 &= a_0, \quad \frac{1}{4}c_1 - \frac{1}{4}c_3 = a_1, \quad -\frac{1}{2}c_0 - \frac{1}{4}c_4 + \frac{1}{2}c_2 = a_2, \\ -\frac{1}{4}(c_{n-2} + c_{n+2}) + \frac{1}{2}c_n &= a_n, \quad n > 2. \end{aligned} \quad (2.4)$$

(iv) The condition that $u^{\text{quad}}(x) = u^{\text{diff}}(x)$ demands that

$$c_0 - \frac{1}{2}c_2 = -2b_0, \quad c_{n-2} - c_n = -4b_{n-2}, \quad n \geq 3 \quad (2.5)$$

with the solution

$$c_0 = -2 \sum_{j=0}^{\infty} b_{2j}, \quad c_1 = -4 \sum_{j=0}^{\infty} b_{2j+1}, \quad c_{2n} = -4 \sum_{j=n}^{\infty} b_{2j}, \quad c_{2n+1} = -4 \sum_{j=n}^{\infty} b_{2j+1}, \quad n \geq 1. \quad (2.6)$$

Equivalently, using the infinite sums for c_0 and c_1 , we see that the higher coefficients can be written as finite sums as

$$c_{2n} = 2c_0 + 4 \sum_{j=0}^{n-1} b_{2j}, \quad c_{2n+1} = c_1 + 4 \sum_{j=0}^{n-1} b_{2j+1}, \quad n \geq 1. \quad (2.7)$$

(v) Given $u(x) = u^{\text{quad}}(x)$, the coefficients c_n can be defined without ambiguity as the Chebyshev coefficients of an auxiliary function $v(x)$:

$$v(x) \equiv \frac{u(x)}{1-x^2} = \sum_{n=0}^{\infty} c_n T_n(x), \quad (2.8)$$

where c_n can be calculated by the formula (1.4).

(vi) If $u^{\text{diff}}(x) = u^{\text{quad}}(x)$, the relation of b_n and c_n is

$$b_0 = \frac{c_2 - 2c_0}{4} = \frac{1}{2\pi} \int_{-1}^1 \sqrt{\frac{1}{1-x^2}} v(x) (T_2(x) - T_0(x)) dx, \quad (2.9)$$

$$b_n = \frac{c_{n+2} - c_n}{4} = \frac{1}{2\pi} \int_{-1}^1 \sqrt{\frac{1}{1-x^2}} v(x) \varsigma_n(x) dx, \quad n \in \mathbb{N}_+. \quad (2.10)$$

Proof. To show the first statement, recall the Chebyshev identity [6, 25]

$$T_m(x)T_n(x) = \frac{1}{2}(T_{m+n}(x) + T_{|m-n|}(x)).$$

We can easily verify that the quadratic factor basis can be written as

$$\varrho_0(x) = \frac{1}{2}(T_0(x) - T_2(x)), \quad \varrho_1(x) = \frac{1}{4}(T_1(x) - T_3(x)), \quad (2.11)$$

$$\varrho_n(x) = (1 - x^2)T_n(x) = -\frac{1}{4}(T_{n+2}(x) + T_{n-2}(x)) + \frac{1}{2}T_n(x), \quad n \geq 2. \quad (2.12)$$

The difference of two difference basis functions is

$$\varsigma_n(x) - \varsigma_{n-2}(x) = T_{n+2}(x) + T_{n-2}(x) - 2T_n(x), \quad n \geq 2,$$

which is just $-4\varrho_n(x)$.

The second statement follows from rewriting the series for $u^{\text{diff}}(x)$ as

$$u^{\text{diff}}(x) = \sum_{n=0}^{\infty} b_n \{T_{n+2}(x) - T_n(x)\} = -b_0T_0(x) - b_1T_1(x) + \sum_{n=2}^{\infty} (b_{n-2} - b_n)T_n(x), \quad (2.13)$$

and the term-by-term comparison with the standard Chebyshev series (1.1). The solution to the difference equation can be verified by direct substitution.

The reasoning for the third statement, which is the second-order difference equation for the c_n , is similar to that in the series for $u^{\text{quad}}(x)$, and here $\varrho_n(x)$ is replaced by its explicit expression in terms of Chebyshev polynomials, the sums are rearranged slightly so as to extract the multiplier of $T_n(x)$, and this multiplier is equated with a_n :

$$\begin{aligned} u^{\text{quad}}(x) &= \sum_{n=0}^{\infty} c_n \varrho_n(x) \\ &= \left(\frac{1}{2}c_0 - \frac{1}{4}c_2\right)T_0(x) + \left(\frac{1}{4}c_1 - \frac{1}{4}c_3\right)T_1(x) + \left(\frac{1}{2}c_2 - \frac{1}{2}c_0 - \frac{1}{4}c_4\right)T_2(x) \\ &\quad + \sum_{n=3}^{\infty} \left(-\frac{1}{4}c_{n-2} - \frac{1}{4}c_{n+2} + \frac{1}{2}c_n\right)T_n(x). \end{aligned}$$

Comparing this term by term with the Chebyshev series yields the difference equation. The solution to the difference equation can again be verified by direct substitution.

The fourth statement is demonstrated by similarly rewriting the series for $u^{\text{diff}}(x)$ and $u^{\text{quad}}(x)$, substituting the expression for $\varrho_n(x)$ in terms of differences of $\varsigma_n(x)$, and then comparing the two series [20, Subsection 2.5, Problem 19].

Solving the recurrence is complicated because the lowest degree involves two c_n 's. If we assume symbolic values for c_0 and c_1 , we obtain the formal solution

$$c_{2n} = 2c_0 + 4 \sum_{j=0}^{n-1} b_{2j}, \quad c_{2n+1} = c_1 + 4 \sum_{j=0}^{n-1} b_{2j+1}, \quad n \geq 1, \quad (2.14)$$

but this is not explicit without numerical values for c_0 and c_1 .

On the other hand, if we truncate the infinite series so that $c_{N+1} = c_{N+2} = 0$, then

$$c_N = -4b_N, \quad c_{N-1} = -4b_{N-1}. \quad (2.15)$$

The recurrence can now be solved backwards to yield

$$c_0 = -2 \sum_{j=0}^{N_e} b_{2j}, \quad c_{2n} = -4 \sum_{j=n}^{N_e} b_{2j}, \quad c_{2n+1} = -4 \sum_{j=n}^{N_o} b_{2j+1}, \quad n \geq 1, \quad (2.16)$$

where $N_e = N_o = (N - 1)/2$ if N is odd and $N_e = N/2$ and $N_o = N/2 - 1$ if N is even. The limit $N \rightarrow \infty$ yields the solution (2.6).

The fifth statement follows by dividing the series $u^{\text{quad}}(x)$ by $(1 - x^2)$ and then applying the usual integrals for Chebyshev coefficients.

Statement (vi) follows from combining the difference relations connecting b_n and c_n (the statement (iv) of this theorem) with the integrals for c_n proved as the statement (v). $\square$

Before analyzing the asymptotic decay rate of the Chebyshev coefficients of the infinite series for the functions with endpoint singularities, we shall give the exact representation of the Chebyshev coefficients for the function with an algebraic endpoint singularity.

Lemma 2.2 (See [28, (4.12)]). *For the function $u(x) = (x+1)^\varphi$ with $\varphi > -\frac{1}{2}$ and $\varphi \notin \mathbb{N}$, the Chebyshev expansion coefficients are*

$$a_n = \frac{(-1)^{n+1} \sin(\varphi\pi)}{\pi} \frac{1}{2^{\varphi-1}} B(2\varphi+1, n-\varphi), \quad n \geq \varphi+1, \quad (2.17)$$

where $B(x, y)$ denotes the Beta function.

Liu et al. [19] provided a detailed proof in the framework of fractional Sobolev-type spaces based on the generalized Gegenbauer functions of fractional degree (GGF-Fs). There is also other literature on the consequences for orthogonal polynomial series to the function $u(x)$ with an algebraic singularity [10, 28, 29, 31, 33, 35].

Theorem 2.3 (Orders of convergence for coefficients of infinite series). *Suppose that $u(x)$ owns weak singularities at the endpoints as*

$$u(x; \varphi, \vartheta) = g(x)(1-x^2)^\varphi \ln^\vartheta(1-x^2), \quad x \in [-1, 1], \quad (2.18)$$

where $\varphi > \frac{1}{2}$, $\vartheta \in \mathbb{N}_+$, $u(\pm 1; \varphi, \vartheta) = \lim_{x \rightarrow \pm 1} u(x; \varphi, \vartheta) = 0$ and the function $g(x)$ is analytic everywhere on $x \in [-1, 1]$. Then the coefficients of three expansions (1.1)–(1.3), respectively, satisfy

$$a_n \sim \frac{A(n)}{n^{2\varphi+1}}, \quad (2.19)$$

$$b_n \sim \frac{A(n)}{4\varphi} \frac{1}{n^{2\varphi}}, \quad (2.20)$$

$$c_n \sim -\frac{A(n)}{(2\varphi-1)(2\varphi)} \frac{1}{n^{2\varphi-1}} \quad (2.21)$$

for $n \gg 1$, where $A(n)$ varies more slowly than a power of n such as a logarithm or a constant. Specifically, $A(n) = \mathcal{O}(\ln^{\vartheta-1}(n))$, when $\varphi \in \mathbb{N}$; $A(n) = \mathcal{O}(\ln^\vartheta(n))$ when $\varphi \notin \mathbb{N}$. Moreover, we have the following expressions of $A(n)$:

(i) If $\vartheta = 1$, one has

$$A(n) = -\frac{2\Gamma(2\varphi+1)}{\pi} \{(-1)^n g(-1) + g(1)\} \{(\gamma_1 - \ln 2) \sin(\varphi\pi) + \pi \cos(\varphi\pi)\},$$

where $\gamma_1 = 2\psi_0(2\varphi+1) - \psi_0(n-\varphi) - \psi_0(n+\varphi+1)$ and $\psi_n(x)$ ($n \in \mathbb{N}$) is the polygamma function.

(ii) If $\vartheta = 2$, one has

$$A(n) = -\frac{2\Gamma(2\varphi+1)}{\pi} \{(-1)^n g(-1) + g(1)\} \{(\gamma_1^2 + \gamma_2 - 2\ln(2)\gamma_1 + \ln^2(2) - \pi^2) \sin(\varphi\pi) + 2\pi(\gamma_1 - \ln(2)) \cos(\varphi\pi)\},$$

where $\gamma_2 = 4\psi_1(2\varphi+1) + \psi_1(n-\varphi) - \psi_1(n+\varphi+1)$.

(iii) If $\vartheta \in \mathbb{N}_+$, one has the general formula

$$A(n) = -\frac{2}{\pi} \gamma_3 n^{2\varphi+1} \sum_{k=0}^{\vartheta} \binom{\vartheta}{k} \sum_{j=0}^k \binom{k}{j} \pi^j \sin\left(\frac{j}{2}\pi + \varphi\pi\right) \ln^{k-j}\left(\frac{1}{2}\right) \frac{d^{\vartheta-k}}{d\varphi^{\vartheta-k}} B(2\varphi+1, n-\varphi) \\ \sim -\frac{2\Gamma(2\varphi+1)}{\pi} \gamma_3 \{\ln^\vartheta(n) \sin(\varphi\pi) + \ln^{\vartheta-1}(n) \cos(\varphi\pi)\},$$

where

$$\gamma_3 = (-1)^n g(-1) + g(1).$$

Proof. The asymptotic behavior of the Chebyshev coefficients a_n follows from a theorem of Elliott [11] (see also [4, 12, 18, 19, 28, 30, 33, 35]). For simplicity, take $A(n)$ and $B(n)$ as constants below. Then for large n and assuming power-law behavior for b_n with the algebraic order of convergence k and the proportionality constant B , the difference equation (2.2) gives

$$\frac{B}{n^k} \left(\frac{1}{(1-2/n)^k} - 1 \right) = \frac{A}{n^{2\varphi+1}}.$$

For large n , $(1-2/n)^{-k} \approx 1 + 2k/n + \mathcal{O}(k^2/n^2)$ and then

$$\frac{2kB}{n^{k+1}} = \frac{A}{n^{2\varphi+1}},$$

from which it follows that $k = 2\varphi$ as claimed and $B = A/(2k) = A/(4\varphi)$.

To prove the third statement, define $v(x)$ as before by $u(x) = (1-x^2)v(x)$. c_n 's are the *standard* Chebyshev polynomial coefficients of the *modified* function $v = \sum_{n=0}^{\infty} c_n T_n(x)$, for which the asymptotic behavior of c_n follows from Elliott's theorem [11].

An alternative proof that gives the relative proportionality constant is as follows. Earlier, we proved in Lemma 2.1(iii) that

$$-\frac{1}{4}(c_{n-2} + c_{n+2}) + \frac{1}{2}c_n = a_n, \quad n \geq 2. \quad (2.22)$$

Assume that asymptotically for large n ,

$$c_n \sim \frac{C}{n^k}, \quad n \gg 1.$$

Substituting this into the second-order difference equation (2.4) gives

$$\frac{C}{2} \frac{1}{n^k} \left(-\frac{1}{2} \left(\frac{1}{(1-2/n)^k} + \frac{1}{(1+2/n)^k} \right) + 1 \right) = \frac{A}{n^{2\varphi+1}}.$$

Then it is not difficult to see that

$$\frac{Ck(k+1)}{n^{k+2}} = \frac{A}{n^{2\varphi+1}}.$$

Thus, it follows that $k = 2\varphi - 1$ and $C = -A/\{k(k+1)\} = -A/(4\varphi-2)\varphi$. The proof is not substantially changed if A is allowed to vary slowly, say logarithmically, with the degree.

Recently, Liu et al. [19, Subsection 6.2] gave the optimal decay rate of the Chebyshev expansion coefficients for this function $u(x; \varphi, \vartheta) = (1+x)^\varphi \ln^\vartheta(1+x)$ when $\vartheta = 1$. By the idea of this paper, we prove the optimal estimates of $A(n)$ given above, for the function (2.18) when $\vartheta = 1, 2$. By (1.4), for $n > 0$, the Chebyshev expansion coefficients are

$$\begin{aligned} a_n &= \frac{2}{\pi} \int_{-1}^1 g(x)(1-x^2)^\varphi \ln^\vartheta(1-x^2) \frac{T_n(x)}{\sqrt{1-x^2}} dx \\ &= \frac{2}{\pi} \int_{-1}^1 g(x)(1-x^2)^\varphi \left\{ \ln^\vartheta(1+x) + \ln^\vartheta(1-x) + \sum_{i=1}^{\vartheta-1} \binom{\vartheta}{i} \ln^i(1+x) \ln^{\vartheta-i}(1-x) \right\} \frac{T_n(x)}{\sqrt{1-x^2}} dx. \end{aligned}$$

As we know, the coefficients are dominated by terms who own the worst singularities, i.e., the terms whose lowest-order derivatives are unbounded and increase highest at the corresponding singularities. Thus, for $\vartheta > 1$,

$$a_n \simeq \frac{2}{\pi} \int_{-1}^1 g(x)(1-x^2)^\varphi \{\ln^\vartheta(1+x) + \ln^\vartheta(1-x)\} \frac{T_n(x)}{\sqrt{1-x^2}} dx$$

$$= \frac{2}{\pi} \int_{-1}^1 g(x)(1-x^2)^\varphi \ln^\vartheta(1+x) \frac{T_n(x)}{\sqrt{1-x^2}} dx + \frac{2}{\pi} \int_{-1}^1 g(x)(1-x^2)^\varphi \ln^\vartheta(1-x) \frac{T_n(x)}{\sqrt{1-x^2}} dx. \quad (2.23)$$

For convenience, we set

$$a_{n,1} := \frac{2}{\pi} \int_{-1}^1 g(x)(1-x^2)^\varphi \ln^\vartheta(1+x) \frac{T_n(x)}{\sqrt{1-x^2}} dx,$$

$$a_{n,2} := \frac{2}{\pi} \int_{-1}^1 g(x)(1-x^2)^\varphi \ln^\vartheta(1-x) \frac{T_n(x)}{\sqrt{1-x^2}} dx.$$

To obtain the asymptotic behavior of $a_{n,1}$, the dominant term of the integrand needs to be considered. Due to the fact that the function $g(x)$ is analytic on the interval $[-1, 1]$, it can be written as Taylor series at $x = -1$. Thus, the dominant contribution comes from the integral

$$a_{n,1} \simeq \frac{2^{\varphi+1}}{\pi} g(-1) \int_{-1}^1 (1+x)^\varphi \ln^\vartheta(1+x) \frac{T_n(x)}{\sqrt{1-x^2}} dx. \quad (2.24)$$

By Lemma 2.2, using L'Hospital's rule, we have

$$a_{n,1} \simeq \frac{2^{\varphi+1}}{\pi} g(-1) \int_{-1}^1 (1+x)^\varphi \left\{ \lim_{\varepsilon \rightarrow 0} \frac{((1+x)^\varepsilon - \sum_{j=0}^{\vartheta-1} \frac{\ln^j(1+x)}{j!} \varepsilon^j)}{\frac{\varepsilon^\vartheta}{\vartheta!}} \right\} \frac{T_n(x)}{\sqrt{1-x^2}} dx$$

$$= (-1)^{n+1} \frac{2}{\pi} g(-1) \sum_{k=0}^{\vartheta} \binom{\vartheta}{k} \sum_{j=0}^k \binom{k}{j} \pi^j \sin\left(\frac{j}{2}\pi + \varphi\pi\right) \ln^{k-j}\left(\frac{1}{2}\right) \frac{d^{\vartheta-k}}{d\varphi^{\vartheta-k}} B(2\varphi+1, n-\varphi).$$

Similarly, $a_{n,2}$ is equal to $a_{n,1}$ multiplied by a constant factor $\frac{(-1)^n g(1)}{g(-1)}$.

Recall that if y is large and x is fixed, then

$$B(x, y) \sim \Gamma(x) y^{-x}. \quad (2.25)$$

By the induction method, using (2.25), we obtain

$$A(n) \sim -\frac{2\Gamma(2\varphi+1)}{\pi} \{(-1)^n g(-1) + g(1)\} \{\ln^\vartheta(n) \sin(\varphi\pi) + \ln^{\vartheta-1}(n) \cos(\varphi\pi)\}.$$

Note that using the above method, for $\vartheta = 1$, we see that the exact Chebyshev coefficients a_n can be obtained; for $\vartheta = 2$, we can obtain the optimal estimate of $A(n)$, i.e., the dominated terms can be exactly achieved. For a general $\vartheta \in \mathbb{N}$, the rough estimates of the Chebyshev coefficients can be found in [33, 36]. $\square$

Here, if $\vartheta = 0$, then $u(x; \varphi, \vartheta)$ is singular only if φ is not an integer, as is mentioned before this theorem. If not otherwise specified, $A(n)$ in the rest of this paper denotes the expression of $A(n)$ given in Theorem 2.3.

Remark 2.4. Here, the parameter $\varphi > \frac{1}{2}$ is required to make sure $2\varphi - 1 > 0$ in (2.21). In fact, when using the Chebyshev basis to approximate the function (2.18), it is only required $\varphi > -\frac{1}{2}$.

Remark 2.5. Because the natural logarithm function $\ln(n)$ increases very slowly as n increases, the differences in plots between $\ln(n)/n^\kappa$ and $1/n^\kappa$ are subtle in numerical experiments. It is very easy to believe that $A(n)$ is always a constant for all $\varphi > -\frac{1}{2}$. However, as demonstrated in this theorem, $A(n)$ is a constant only when $\vartheta = 1$ and $\varphi \in \mathbb{N}$.

Figure 2 confirms the coefficients' law in Theorem 2.3. Care must be exercised in interpreting this theorem. It applies when a_n 's obey an inverse power law, as is true for the exact Chebyshev coefficients of the infinite series. We later compute a variety of finite approximations to $u(x)$ and these, when represented in the Chebyshev basis, do not automatically have the inverse power-law behavior of the coefficients a_n .

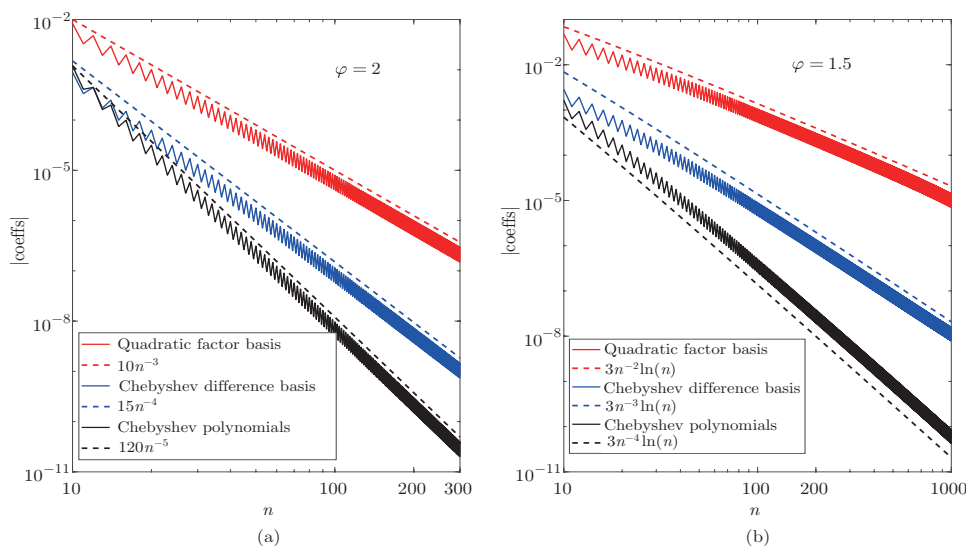


Figure 2 (Color online) Coefficients of the infinite series of the function $u(x) \equiv (1 + \frac{x}{2})(1 - x^2)^\varphi \ln(1 - x^2)$ in three different bases with (a) $\varphi = 2$ and (b) $\varphi = 1.5$

3 Errors in truncating infinite series

Suppose that we truncate each of the three series to a polynomial of degree N , i.e.,

$$u_N(x) = \sum_{n=0}^N a_n T_n(x), \quad (3.1)$$

$$u_N^{\text{diff}}(x) = \sum_{n=0}^{N-2} b_n \{T_{n+2}(x) - T_n(x)\} \quad (\text{the difference basis}), \quad (3.2)$$

$$u_N^{\text{quad}}(x) = \sum_{n=0}^{N-2} c_n (1 - x^2) T_n(x) \quad (\text{the quadratic factor basis}). \quad (3.3)$$

We have previously described the behavior of the *coefficients* a_n , b_n and c_n , but here a natural question arises: what are the *errors* in these truncations?

For the class of the function (2.18), Theorem 2.3 demonstrates that the Chebyshev coefficients fall as $\mathcal{O}(A(n)/n^{2\varphi+1})$ while the quadratic factor basis coefficients c_n decrease as $\mathcal{O}(A(n)/n^{2\varphi-1})$. A well-known theorem asserts that the truncation error in a Chebyshev series is bounded by the sum of the absolute values of all the neglected *terms*; because $|T_n(x)| \leq 1$ on $x \in [-1, 1]$, the bound is also the sum of the absolute values of all the neglected *coefficients*. One might suppose that the error in the L_∞ norm when the series is truncated at $n = N$ is the magnitude of the largest omitted coefficient, but in fact, the series error is worse by $\mathcal{O}(1/N)$ than the rate of convergence of the Chebyshev coefficients. Near the endpoints, the terms are all of the same sign or asymptotically strictly alternating. The order of convergence of the error then comes from the asymptotic sum approximation (3.4) below.

Lemma 3.1. For $\kappa \geq 2$ and $\vartheta \in \mathbb{N}$, then

$$\sum_{n=N+1}^{\infty} \frac{\ln^\vartheta(n)}{n^\kappa} \sim \frac{\ln^\vartheta(N)}{(\kappa - 1)N^{\kappa-1}}. \quad (3.4)$$

The lemma is proved in [1, Lemma 1] when $\vartheta = 0$ and in [36, Lemma 3.3] when $\vartheta \in \mathbb{N}$.

Figure 3(a) shows that this rises steeply in the error near the endpoints by the comparison of two different norms. The upper solid (black) curve, falling $1/N$ slower than the coefficients, is the usual maximum pointwise error

$$E_N^T = \max_{x \in [-1, 1]} |u(x) - u_N(x)|.$$

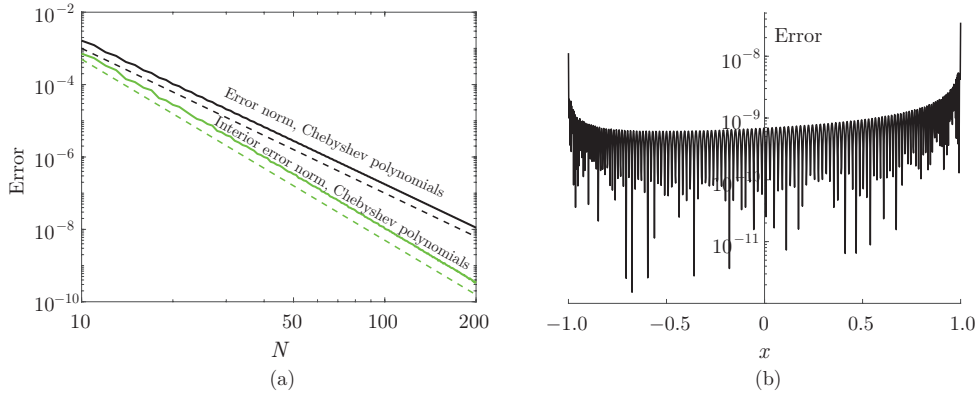


Figure 3 (Color online) (a) Green: the error norm of the Chebyshev polynomial series, truncated at $n = N$, when the norm is the maximum over the *middle* of the interval for $u(x) = (1 + x/2)(1 - x^2)^2 \ln(1 - x^2)$. The green dashes are the reference line, $30/N^5$. The Chebyshev coefficients (not shown) also exhibit the fifth-order convergence, matching the power-law exponent of the *interior* error, for this $u(x)$. Black: same except the error norm is computed over the *whole* of the interval, the usual norm. The black dashes are a graph of $1/N^4$. (b) The errors versus x of the Chebyshev polynomial series for $u(x)$, truncated after $N = 150$ terms, i.e., $E_N^T(x) \equiv |u(x) - u_N(x)|$

The lower curve, which decreases as rapidly as the coefficients a_n , represents the maximum error over the interval's *interior*, excluding the neighborhoods of both endpoints, i.e.,

$$E_N^{T, \text{interior}} = \max_{x \in [-0.8, 0.8]} |u(x) - u_N(x)|.$$

Instead of plotting norms versus truncation as in Figure 3(a), we can obtain a direct confirmation of the large errors in narrow boundary layers at the endpoints by plotting errors versus x as is shown in Figure 3(b).

Theorem 3.2 (Error in truncation of infinite series). *Suppose that we truncate each of the three series to a polynomial of degree N , as given in (3.1)–(3.3). Then the error estimates of the truncated series in L_∞ norm are presented in the following:*

(i) *For the Chebyshev series,*

$$E_N \equiv \max_{x \in [-1, 1]} |u(x) - u_N(x)| \sim \mathcal{O}(|A(N)|/N^{2\varphi}), \quad N \rightarrow \infty. \quad (3.5)$$

(ii) *For the difference basis,*

$$E_N^{\text{diff}} \equiv \max_{x \in [-1, 1]} |u(x) - u_N^{\text{diff}}(x)| \sim \mathcal{O}(|A(N)|/N^{2\varphi}), \quad N \rightarrow \infty. \quad (3.6)$$

(iii) *For the quadratic factor basis,*

$$E_N^{\text{quad}} \equiv \max_{x \in [-1, 1]} |u(x) - u_N^{\text{quad}}(x)| \sim \mathcal{O}(|A(N)|/N^{2\varphi-1}), \quad N \rightarrow \infty. \quad (3.7)$$

The $A(N)$ is given in Theorem 2.3.

Proof. The error in the Chebyshev series follows from the discussion preceding the theorem. To prove the remaining statements, note that the coefficients of the latter two expansions match up to degree $N - 2$ when expanded as Chebyshev series. However, the difference relations in Lemma 2.1 show that with $b_{N-1} = b_N = c_{N-1} = c_N = 0$,

$$\begin{aligned} u_N^{\text{diff}}(x) &= \sum_{n=0}^{N-2} a_n T_n(x) + b_{N-3} T_{N-1}(x) + b_{N-2} T_N(x), \\ &= u_N(x) + (b_{N-3} - a_{N-1}) T_{N-1}(x) + (b_{N-2} - a_N) T_N(x), \\ &= u_N(x) + b_{N-1} T_{N-1}(x) + b_N T_N(x). \end{aligned} \quad (3.8)$$

Now we know from Theorem 2.3 that

$$b_n \sim \mathcal{O}(A(n)/n^{2\varphi}).$$

This implies that b_{N-1} and b_N are proportional to the same power of N as the error in the truncated Chebyshev series. It follows that the error in the truncated series on the difference basis has the same rate of convergence as the truncation of the Chebyshev series.

To prove the final statement, observe that the truncated series on the quadratic factor basis can be written as

$$\begin{aligned} u_N^{\text{quad}}(x) &= \sum_{n=0}^{N-2} c_n(1-x^2)T_n(x) \\ &= \left(\frac{1}{2}c_0 - \frac{1}{4}c_2\right)T_0(x) + \left(\frac{1}{4}c_1 - \frac{1}{4}c_3\right)T_1(x) + \left(-\frac{1}{2}c_0 + \frac{1}{2}c_2 - \frac{1}{4}c_4\right)T_2(x) \\ &\quad + \sum_{n=3}^{N-2} \left(\frac{1}{2}c_n - \frac{1}{4}c_{n-2} - \frac{1}{4}c_{n+2}\right)T_n(x) - \frac{1}{4}c_{N-3}T_{N-1}(x) - \frac{1}{4}c_{N-2}T_N(x) \\ &\quad + \frac{1}{4}c_{N-1}T_{N-3}(x) + \frac{1}{4}c_NT_{N-2}(x) \\ &= u_N(x) + \frac{1}{4}c_{N-1}T_{N-3}(x) + \frac{1}{4}c_NT_{N-2}(x) + \left(\frac{1}{4}c_{N+1} - \frac{1}{2}c_{N-1}\right)T_{N-1}(x) \\ &\quad + \left(\frac{1}{4}c_{N+2} - \frac{1}{2}c_N\right)T_N(x). \end{aligned} \quad (3.9)$$

Lemma 2.1 shows that c_{N-1} and c_N are $\mathcal{O}(A(N)/N^{2\varphi-1})$. This is larger than the error in the truncated Chebyshev series by a factor of N . Thus this is the magnitude of the error in the truncated quadratic factor basis. $\square$

Figure 4 confirms the expected rates of decay for an arbitrary but representative example.

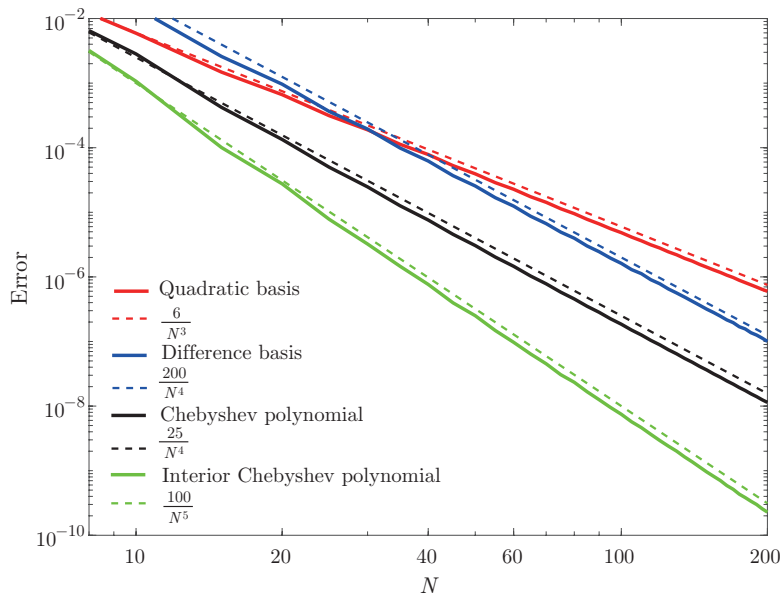


Figure 4 (Color online) Maximum pointwise errors (the L_∞ norm) in the truncated infinite series in three different basis sets for various truncations N for the typical example $u(x) = (1 + x/2)(1 - x^2)^2 \ln(1 - x^2)$. The upper solid line (red) is the error norm for the quadratic factor basis; the dashed red line is $6/N^3$. The solid blue curve is the error norm for the difference basis; the dashed blue line is $200/N^4$. The solid black curve is the error norm for the truncation of the standard Chebyshev series; the black dashed curve is $25/N^4$. The green solid curve is the maximum pointwise error for $x \in [-1/2, 1/2]$, the interior of the interval $x \in [-1, 1]$; the dashed green curve is $100/N^5$.

4 Equivalence theorem

Theorem 4.1 (Dirichlet-enforcing basis equivalence). *If two polynomial approximations, constrained to satisfy homogeneous Dirichlet boundary conditions, are determined by the same set of interpolation constraints or least squares conditions, then the approximations are identical and must have identical errors, i.e.,*

$$u_N^{\text{diff}}(x) = u_N^{\text{quad}}(x). \quad (4.1)$$

Proof. By definition, $u_N^{\text{diff}}(x)$ is a polynomial of degree N which is zero at both endpoints. The fundamental theorem of algebra asserts that any polynomial can be written in the factored form. Therefore,

$$u_N^{\text{diff}}(x) = (1 - x^2)p_{N-2}(x), \quad N \geq 2, \quad (4.2)$$

where $p_{N-2}(x)$ is a polynomial of degree $(N - 2)$. This is identical in the form to $u_N^{\text{quad}}(x)$. If, for example, we determine the approximations by $N - 1$ interpolation conditions, these constraints uniquely determine $p_{N-2}(x)$ as the interpolant of $v(x)$, the same as for $u_N^{\text{quad}}(x)$. Therefore $u_N^{\text{diff}}(x) = u_N^{\text{quad}}(x)$ for interpolation. The argument extends to any other reasonable mechanism to determine the approximations provided that the same conditions are applied to both $u_N^{\text{diff}}(x)$ and $u_N^{\text{quad}}(x)$. $\square$

This equivalence theorem greatly simplifies error analysis. However, we have already shown that the coefficients b_n and c_n are *different*. Furthermore, the error of an unconstrained series of Chebyshev polynomials is different from that of the constrained approximations.

5 Interpolation and aliasing errors in Chebyshev polynomial coefficients

5.1 Grids and uniqueness

There are two canonical interpolation grids associated with Chebyshev polynomials. The “roots” grid is

$$x_k = -\cos\left(\frac{2k+1}{2N+2}\pi\right), \quad k = 0, 1, \dots, N \quad (\text{“Chebyshev-Gauss” grid}). \quad (5.1)$$

The “endpoints-and-extrema” or “Lobatto” grid is

$$x_k = -\cos\left(\frac{k}{N}\pi\right), \quad k = 0, 1, \dots, N \quad (\text{“Chebyshev-Lobatto” grid}). \quad (5.2)$$

If the Lobatto grid is chosen, then the interpolating polynomial must be 0 at $x = \pm 1$ in order to satisfy the interpolation condition at the endpoints. It follows that whether we represent the interpolated polynomial using Chebyshev polynomials, the difference basis or the quadratic factor basis, we always obtain the same polynomial.

In contrast, if the interpolation points are those of the roots grid, which does not include the endpoints, then the standard Chebyshev polynomial interpolation gives an interpolating polynomial which is not exactly equal to 0 at the endpoints. If we use either the quadratic factor basis or the difference basis, the result, by the polynomial factorization theorem, can be written in the form

$$u_N^{I,\text{con}}(x) = (1 - x^2)v_{N-2}^{I,\text{con}}(x), \quad (5.3)$$

where $u_N^{I,\text{con}}(x)$ and $v_{N-2}^{I,\text{con}}(x)$ are Chebyshev interpolants on Chebyshev-Lobatto grids for the functions $u(x)$ and $v(x) = u(x)/(1 - x^2)$, respectively, and they satisfy the homogeneous Dirichlet boundary conditions. Thus, there are *two* distinct interpolants on the *roots* grid, being the Chebyshev interpolant (lacking zeros at the endpoints) and the difference-and-quadratic-factor interpolant (which vanishes at both endpoints by construction). In contrast, the interpolant on the *Lobatto* (endpoint-including) grid is always *unique*.

5.2 Aliasing errors in the Chebyshev coefficients of the interpolant

The Chebyshev coefficients of both the interpolant, $a_n^I(N)$, and the infinite series a_n can be computed by Gauss-Chebyshev quadrature as given in [6, p. 99]. When the number of quadrature points M is equal to $N + 1$, then the coefficients are the result from interpolation; the coefficients of the infinite series are $a_n = \lim_{M \rightarrow \infty, \text{fixed } N} a_n^I(N)$. But what is the relationship between series and interpolant coefficients for finite N ? The following provides an answer.

Theorem 5.1 (Aliasing formula for Chebyshev coefficients). *Let $u(x)$ be Lipschitz continuous on $[-1, 1]$ and let $u_N^I(x)$ be its Chebyshev interpolant, i.e.,*

$$u_N^I(x) = \frac{1}{2}a_0^I + \sum_{n=1}^N a_n^I T_n(x), \quad (5.4)$$

which is obtained by choosing the Chebyshev-Gauss grids as interpolation points. Let a_n (without the superscript) denote the coefficients of the infinite series

$$u(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n T_n(x). \quad (5.5)$$

Then one has

(i)

$$a_n^I = a_n + \mathcal{E}_n, \quad \mathcal{E}_n = \sum_{j=1}^{\infty} (a_{-n+2j(N+1)} + a_{n+2j(N+1)}) (-1)^j, \quad n = 0, 1, \dots, N; \quad (5.6)$$

(ii)

$$\begin{aligned} a_n^I &\approx a_n - a_{2N+2-n} - a_{2N+2+n} + \mathcal{O}(a_{3N}), \quad n = 0, \dots, N, \\ a_{\frac{1}{2}(N+1)}^I &\approx a_{\frac{1}{2}(N+1)} - a_{\frac{3}{2}(N+1)} + \mathcal{O}(a_{\frac{5}{2}(N+1)}), \\ a_{N+1-m}^I &\approx a_{N+1-m} - a_{N+1+m} + \mathcal{O}(a_{3N}), \quad m \in \mathbb{N}_+, \quad m \ll N. \end{aligned} \quad (5.7)$$

Proof. The first statement was proved by Fox and Parker [14, Subsection 4.3]. The second comes from specializing n to particular ranges in degree and then making obvious approximations. $\square$

Theorem 5.2. *Suppose that the Chebyshev coefficients in (5.5) for large n are*

$$a_n \sim A \frac{\ln^{\vartheta}(n)}{n^{\kappa}}, \quad \text{where } n \gg 1, \quad \kappa > 0, \quad A \text{ is a constant and } \vartheta \in \mathbb{N}.$$

Then one has the following estimates:

(i) *For small degree n , the aliasing error in Chebyshev coefficients is*

$$\mathcal{E}_n \sim -\frac{A \ln^{\vartheta}(2N)}{2^{\kappa-1} N^{\kappa}}, \quad (5.8)$$

and the relative error is

$$\frac{|\mathcal{E}_n|}{|a_n|} \sim \frac{1}{2^{\kappa-1}} \frac{n^{\kappa} \ln^{\vartheta}(2N)}{N^{\kappa} \ln^{\vartheta}(n)}. \quad (5.9)$$

Specially, if the coefficients a_n are well approximated by the power law A/n^{κ} , for small degree n such that $n \ll \frac{2}{\kappa}(N+1)$, then

$$\mathcal{E}_n \sim \frac{A}{2^{\kappa-1}} \frac{1}{N^{\kappa}} \sum_{j=1}^{\infty} \frac{(-1)^j}{j^{\kappa}}, \quad \frac{|\mathcal{E}_n|}{|a_n|} \leq \frac{1}{2^{\kappa-1}} \frac{n^{\kappa}}{N^{\kappa}}. \quad (5.10)$$

(ii) *For $n = N + 1 - m$, when m is a small positive integer, the relative error is*

$$\frac{|\mathcal{E}_{N+1-m}|}{|a_{N+1-m}|} \sim 1 + \mathcal{O}\left(\frac{\kappa m}{N+1}\right). \quad (5.11)$$

Proof. Substituting the coefficients into the terms in the error sum gives

$$\begin{aligned} a_{2j(N+1)\pm n} &\sim \frac{A \ln^\vartheta(2jN)}{(2j(N+1)\pm n)^\kappa} \sim \frac{A \ln^\vartheta(2jN)}{2^\kappa(N+1)^\kappa} \frac{1}{j^\kappa \{1 \pm n/(2j(N+1))\}^\kappa}, \\ a_{2j(N+1)-n} + a_{2j(N+1)+n} &\approx \frac{A \ln^\vartheta(2jN)}{2^{k-1}(N+1)^\kappa} \frac{1}{j^\kappa} \left\{ 1 + \mathcal{O}\left(\frac{\kappa^2 n^2}{4j^2(N+1)^2}\right) \right\}. \end{aligned}$$

The asymptotic expression (5.8) then follows.

If we assume that n is sufficiently large such that $a_n \sim A/n^\kappa$, then the relative coefficient error follows immediately upon invoking

$$\sum_{j=1}^{\infty} \frac{(-1)^{j+1}}{j^\kappa} < 1, \quad \forall \kappa > 0. \quad (5.12)$$

To prove the second statement, substitute the coefficients decay law into the equation (5.7) from the general aliasing theorem, Theorem 5.1. Using asymptotic tools, we see that (5.11) will be obtained. $\square$

The second statement implies that coefficients whose degree is near the aliasing limit, $n = N$, are badly in error. When the Chebyshev coefficients decay slowly, as $\mathcal{O}(\ln^\vartheta(n)/n^\kappa)$, $a_{N+1-m} \approx a_{N+1+m}$; the relationship $a_{N+1-m}^I \approx a_{N+1-m} - a_{N+1+m}$ implies strong cancellation so that

$$|a_{N+1-m}^I| \ll |a_{N+1-m}| \quad (5.13)$$

and the relative error is near 100%. When $\vartheta = 0$, a log-log plot of the interpolation points $|a_n^I|$ is a straight line for the intermediate n , but dives to small values as $n \rightarrow N$, curving downward below the line. For general $\vartheta \in \mathbb{N}_+$, the plot of interpolation coefficients $|a_n^I|$ still curls downward much more than the curve of Chebyshev coefficients $|a_n|$ as $n \rightarrow N$.

The first statement shows that in contrast, low-degree coefficients can be computed with a small relative error, but for fixed degree n , the relative error falls with N as $\ln^\vartheta(N)/N^k$, the same decay rate as that of the coefficients. In a word, if a_n diminishes with $\ln^\vartheta(n)/n^k$ the coefficient can be computed as the corresponding coefficient of the $(N+1)$ -point interpolant with a relative error that is order k in N by a factor of $\ln^\vartheta(N)$.

6 Interpolants and interpolation errors with Dirichlet boundary conditions

6.1 Interpolants and their similarities and differences

Because the Lobatto grid includes the endpoints, the standard, unconstrained Chebyshev interpolant is zero at both endpoints for any function satisfying $u(\pm 1) = 0$. As noted in Subsection 5.1, the interpolant on the Lobatto grid is unique and therefore,

$$u_N^{\text{Cheb,Lob},I}(x) = u_N^{\text{diff,Lob},I}(x) = u_N^{\text{quad,Lob},I}(x). \quad (6.1)$$

So let us turn to the roots grid. Define $v(x) \equiv u(x)/(1-x^2)$ as before. There exists a polynomial of degree $(N-2)$, which we will denote by $v_{N-2}^{\text{Cheb},I}(x)$, that interpolates $v(x)$ at all of the points on the $(N-1)$ -point roots grid.

Theorem 6.1 (Interpolants on the roots grid). *Suppose that $u(x)$ satisfies Dirichlet boundary conditions $u(\pm 1) = 0$ and the $(N-1)$ -point Chebyshev interpolant of $v(x)$ is*

$$v_{N-2}^{\text{Cheb},I}(x) = \sum_{n=0}^{N-2} \tilde{c}_n^I T_n(x). \quad (6.2)$$

Compute $u_N^{\text{quad},I}(x)$ by $(N-1)$ -point interpolation of $u(x)$, where

$$u_N^{\text{quad},I}(x) = \sum_{n=0}^{N-2} c_n^I (1-x^2) T_n(x). \quad (6.3)$$

Similarly, compute $u_N^{\text{diff},I}(x)$ by $(N-1)$ -point interpolation, where

$$u_N^{\text{diff},I}(x) = \sum_{n=0}^{N-2} b_n^I \{T_{n+2}(x) - T_n(x)\}. \quad (6.4)$$

Then it leads to

$$u_N^{\text{quad},I}(x) = (1-x^2)v_{N-2}^{\text{Cheb},I}(x), \quad (6.5)$$

$$u_N^{\text{diff},I}(x) = (1-x^2)v_{N-2}^{\text{Cheb},I}(x), \quad (6.6)$$

$$u_N^{\text{diff},I}(x) = u_N^{\text{quad},I}(x), \quad (6.7)$$

$$c_n^I = \tilde{c}_n^I, \quad i = 0, 1, \dots, N-2 \quad (6.8)$$

and

$$b_0^I = \frac{c_2^I - 2c_0^I}{4}, \quad b_n^I = \frac{c_{n+2}^I - c_n^I}{4}, \quad n = 1, 2, \dots, (N-4), \quad b_{N-3}^I = -\frac{c_{N-3}^I}{4}, \quad b_{N-2}^I = -\frac{c_{N-2}^I}{4}. \quad (6.9)$$

Proof. The interpolation conditions for $u(x)$ in the quadratic factor basis are

$$u(x_j) = u_N^{\text{quad},I}(x_j) = \sum_{n=0}^{N-2} c_n^I (1-x_j^2) T_n(x_j). \quad (6.10)$$

The same for $v(x)$ multiplied by $(1-x^2)$ are

$$(1-x_j^2)v(x_j) = (1-x_j^2)v_{N-2}^{\text{Cheb},I}(x_j) = \sum_{n=0}^{N-2} \tilde{c}_n^I (1-x_j^2) T_n(x_j). \quad (6.11)$$

The left-hand side of (6.11) is $u(x_j)$. The right-hand side is identical in the form to the interpolant of $u(x)$ by $u_N^{\text{quad},I}(x)$. Therefore, $\tilde{c}_n^I = c_n^I$ from which $u_N^{\text{quad},I}(x) = (1-x^2)v_{N-2}^{\text{Cheb},I}(x)$ follows. The second and third lines, (6.6) and (6.7), follow from the equivalence Theorem 4.1. The formulas for b_n^I follow from the difference equations in Lemma 2.1(vi). $\square$

6.2 Interpolation errors and error norms

Suppose that the Chebyshev polynomial coefficients a_n of a function $u(x)$ are decreasing as

$$a_n \sim A \ln^\vartheta(n)/n^\kappa, \quad (6.12)$$

where $\kappa = 2\varphi + 1 > 0$ and $\vartheta \in \mathbb{N}$. The error in the Chebyshev interpolant of $u(x)$ is expected to be $\mathcal{O}(\ln^\vartheta(N)/N^\kappa)$ on the interior of the interval, by slowing to $\mathcal{O}(\ln^\vartheta(N)/N^{\kappa-1})$ in the endpoint boundary layers.

The Chebyshev polynomial coefficients of $v(x) \equiv u(x)/(1-x^2)$ converge more slowly than those of $u(x)$ by a factor of about n^2 (see [28]). Define

$$E_N^v(x) \equiv |v(x) - v_{N-1}^{I,\text{con}}(x)|. \quad (6.13)$$

It follows that $E_N^v(x)$ will be $\mathcal{O}(\ln^\vartheta(N)/N^{\kappa-1})$ on the interior of the interval. To obtain the corresponding error in $u(x)$, we must multiply by the factor of $(1-x^2)$ which is the ratio of $u(x)$ to $v(x)$, i.e.,

$$E_N^u(x) = (1-x^2)E_N^v(x). \quad (6.14)$$

It follows that

$$\max_{x \in [-1,1]} (E_N^u(x)) \sim \frac{A \ln^\vartheta(N)}{N^{\kappa-1}}. \quad (6.15)$$

As explained in [6, Chapter 2], the error in truncating the infinite Chebyshev series by discarding all the terms of degree $(N + 1)$ and higher can be bounded rigorously by the sum of the absolute values of the neglected coefficients, i.e.,

$$E_N(x) \equiv |u(x) - u_N(x)| \leq \sum_{n=N+1}^{\infty} |a_n|. \quad (6.16)$$

Chebyshev interpolation on either the roots grid or the Lobatto grid is bounded by *twice* the sum of the absolute values of the neglected coefficients, i.e.,

$$E_N^I(x) \equiv |u(x) - u_N^I(x)| \leq 2 \sum_{n=N+1}^{\infty} |a_n|. \quad (6.17)$$

It is difficult to make more precise statements; for $u(x) = T_{\frac{3}{2}(N+1)}(x)$, for example,

$$\begin{aligned} u_{N+1}(x) &= 0, & E_{N+1}(x) &= T_{\frac{3}{2}(N+1)}(x), \\ u_N^I &= -T_{\frac{1}{2}(N+1)}(x), & E_{N+1}^I(x) &= T_{\frac{3}{2}(N+1)}(x) + T_{\frac{1}{2}(N+1)}(x). \end{aligned}$$

Nevertheless, it follows that $E_N^I(x)$ is roughly double the error in truncating the infinite Chebyshev series and therefore its L_∞ norm is $\mathcal{O}(\ln^\vartheta(N)/N^{\kappa-1})$.

Because of the endpoint singularities, the usual nearly-uniform error for truncated Chebyshev series (or Chebyshev interpolants) of *smooth* functions, analytic on the entire interval, is replaced by an error which is huge in boundary layers near each endpoint and smaller outside of these boundary layers by a factor of $\mathcal{O}(1/N)$ (the bottom curve in Figure 5).

Applying this same reasoning to $v(x) \equiv u(x)/(1 - x^2)$ gives an error for $v(x)$ which is $\mathcal{O}(N)$ times as large as the error for $u(x)$ (note that the order κ of singularities for $v(x)$ is one less than that for $u(x)$ and each decrease in κ by *one* reduces the order of the Chebyshev coefficients by *two*). To obtain the approximation in the quadratic factor basis for $u(x)$, we must multiply the Chebyshev series for $v(x)$ by $(1 - x^2)$. Similarly, the highly nonuniform error in $v(x)$ (the blue dotted curve in Figure 5) must be replaced, to obtain the error for interpolation of $u(x)$ by either of the constrained basis sets, by $(1 - x^2)$ times the error for $v(x)$. The zeros at the endpoints wipe out the boundary layers of large errors in $v(x)$ to yield an error which is nearly uniform over $x \in [-1, 1]$ as shown by the gold dashed curve in Figure 5.

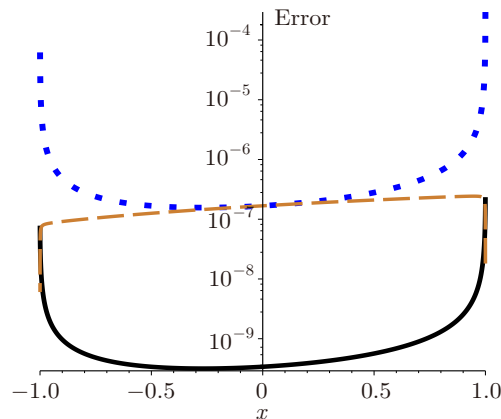


Figure 5 (Color online) Errors versus x for interpolation of $u(x) = (1 + x/2)(1 - x^2)^2 \ln(1 - x^2)$, the same function as employed in the previous figure, by means of 100 interpolation points on the roots grid. Top (blue dots): $|v(x) - v_N^{\text{Cheb},I}(x)|$, the interpolant of $v(x) = u(x)/(1 - x^2)$. Bottom (the solid black curve): $|u(x) - u_N^{\text{Cheb},I}(x)|$, the error in the classic Chebyshev interpolation on the roots grid. The dashed gold line is the error for the quadratic factor basis, the error in $u_N^{\text{quad},I}(x) = (1 - x^2)v_{N-2}^{\text{Cheb},I}(x)$; this is identical to the error in the difference basis since (for interpolation) $u_N^{\text{quad},I}(x) = u_N^{\text{diff},I}(x)$

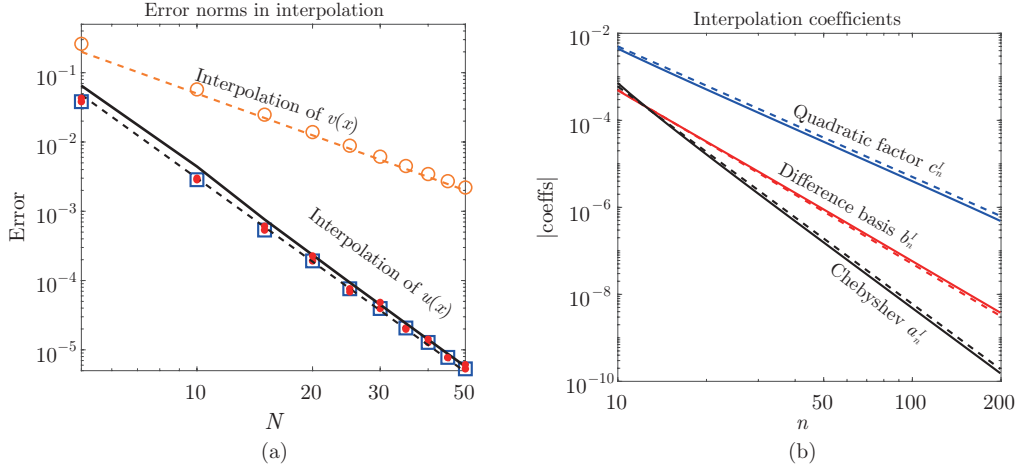


Figure 6 (Color online) (a) Log-log plot of the error norms versus the number of interpolation points N for interpolation of $u(x) = (1 + x/2)(1 - x^2)^2 \ln(1 - x^2)$, the same function as employed in the previous figure. The top circle gold curve: the error norm $\max_{x \in [-1, 1]} |v(x) - v_N^{\text{Cheb}, I}(x)|$, the interpolant of $v(x) = u(x)/(1 - x^2)$. The gold dashed curve is $5/N^2$, proportional to $1/N^{\kappa-3}$. The bottom three curves, almost superimposed and hard to distinguish, are the error norms for the approximation of $u_N^{\text{Cheb}, I}(x)$ by the Chebyshev interpolant (the black curve), $u_N^{\text{quad}, I}(x)$ (blue boxes) and $u_N^{\text{diff}, I}(x)$ (red solid disks). The red disks are at the centers of the blue boxes because $u_N^{\text{quad}, I}(x)$ is identically equal to $u_N^{\text{diff}, I}(x)$, as asserted by Theorem 4.1. The black dashed curve is $30/N^4$, proportional to $1/N^{\kappa-1} = 1/N^{2\varphi}$. (b) Odd degree coefficients versus degrees for interpolation, the same function as employed in the previous figure, by means of 400 interpolation points on the roots grid. To minimize aliasing contamination, only the coefficients up to degree 199 are plotted. Top (the blue solid line): c_n^I , which are simultaneously the Chebyshev coefficients of $v(x)$ and also the coefficients of $u(x)$ in the quadratic factor basis where $v(x) = u(x)/(1 - x^2)$. Middle (the red solid curve): coefficients b_n^I of the difference basis for $u(x)$. Bottom (the solid black curve): the Chebyshev coefficients a_n^I of the interpolant on the roots grid. The dashed lines are proportional to $1/n^3$ (top/blue), $1/n^4$ (middle/red) and $1/n^5$ (bottom/black). The parameter $\varphi = 2$ while $\kappa = 2\varphi + 1 = 5$

Plain classical Chebyshev interpolation, although not better than the other two basis sets in the L_∞ norm, is superior because the pointwise Chebyshev interpolation is as bad as the norm only in boundary layers whereas the quadratic factor and difference errors are as bad as the norm over the entire interval.

Figure 6(a) displays error norms instead of pointwise errors. The close agreement between the dashed curves and the matching solid curves confirms the theoretical predictions given above.

6.3 Coefficients of interpolants

Figure 6(b) shows how the coefficients vary. Even though the *errors* of the difference basis and quadratic factor basis interpolants are *identical*, their *coefficients* obey *different power laws*. The quadratic factor coefficients c_n decay more slowly by one order than the difference basis coefficients b_n . The power laws for all the three basis sets are the same as those for truncation of the infinite series, so no further discussion will be given.

7 Least squares

Least squares is a third strategy that provides an alternative to the interpolation and truncation of infinite series. Is it better? Is it worse? One complication is that least squares is actually a family of methods because the approximation varies with the choice of the inner product.

The next two subsections describe the basic methods with and without Lagrange multipliers. In the rest of this section, we shall analyze the least squares for three bases in turn. When the inner product is integration over the interval, we shall show that least squares yields approximations *different* from the interpolation and truncation for the constrained-to-vanish-at-the-endpoints basis sets.

7.1 Least squares without Lagrange multipliers: The general basis

The goal of least squares is to minimize the “cost function”

$$\mathfrak{J} = \frac{1}{2} \langle u(x) - u_N(x), u(x) - u_N(x) \rangle, \quad (7.1)$$

where

$$u_N(x) = \sum_{n=0}^N d_n \phi_n(x). \quad (7.2)$$

For the moment, the choices of the inner product $\langle f(x), g(x) \rangle$ and the basis functions $\phi_n(x)$ are unspecified.

Proposition 7.1. *Suppose that the cost function and $u_N(x)$ are as above. Define an $(N+1) \times (N+1)$ matrix $\mathbf{G}$ as the matrix with the elements*

$$G_{mn} = \langle \phi_m(x), \phi_n(x) \rangle, \quad m, n = 0, 1, \dots, N. \quad (7.3)$$

Define $\mathbf{f}$ as the vector with elements

$$f_n \equiv \langle \phi_n(x), u(x) \rangle, \quad n = 0, 1, \dots, N. \quad (7.4)$$

Then $u_N(x)$ is the unique minimizer if and only if the spectral coefficients d_n are the elements of the $(N+1)$ -dimensional vector $\mathbf{d}$ which solves

$$\mathbf{G}\mathbf{d} = \mathbf{f}. \quad (7.5)$$

Proof. Substitute the series into the cost function and apply the condition for a minimum that the derivatives of the cost function with respect to the coefficients d_j are all zero. This gives

$$\frac{\partial \mathfrak{J}}{\partial d_m} = 0 = -\langle u(x), \phi_m(x) \rangle + \sum_{n=0}^N d_n \langle \phi_m(x), \phi_n(x) \rangle, \quad (7.6)$$

which is the linear algebra problem (7.5). □

Let us suppose that the inner product is approximated by Gaussian quadrature with N_{col} points. For the Chebyshev weight,

$$\begin{aligned} \langle f(x), g(x) \rangle &\equiv \int_{-1}^1 \frac{1}{\sqrt{1-x^2}} f(x)g(x)dx \approx \langle f, g \rangle_{Gq} \equiv \frac{\pi}{N_{\text{col}}} \sum_{j=1}^{N_{\text{col}}} f(x_j)g(x_j), \\ x_j &= \cos\left(\frac{2j-1}{2N_{\text{col}}}\pi\right), \quad j = 1, 2, \dots, N_{\text{col}}. \end{aligned}$$

The quadrature approximation has all the properties to be an inner product, so we use $\langle \cdot, \cdot \rangle_{Gq}$ as the inner product in the rest of this subsection. This inner product varies from interpolation (when $N_{\text{col}} = N+1$ as explained below) to integration over the interval in the limit $N_{\text{col}} \rightarrow \infty$.

Define an $N_{\text{col}} \times (N+1)$ matrix $\mathbf{H}$ whose elements are

$$H_{jn} \equiv \phi_n(x_j), \quad j = 1, 2, \dots, N_{\text{col}}, \quad n = 0, 1, \dots, N, \quad (7.7)$$

and let $\mathbf{u}$ denote the vector whose elements are the samples of $u(x)$, i.e.,

$$u_j \equiv u(x_j), \quad j = 1, 2, \dots, N_{\text{col}}. \quad (7.8)$$

The interpolation problem is

$$\mathbf{H}\mathbf{d}^I = \mathbf{u}. \quad (7.9)$$

Here, we have added a superscript to the vector of spectral coefficients because the solution to the interpolation problem is not necessarily the same as the solution that minimizes $\mathfrak{J}$. Note that the matrix problem is an overdetermined system, but still well-posed if $N_{\text{col}} > N+1$.

Proposition 7.2. *The solution $\mathbf{d}$ of the least squares with an inner product using $N_{\text{col}} = N + 1$ quadrature points is identical to the solution $\mathbf{d}^I$ to the $(N + 1)$ -point interpolation problem. The matrices for least squares and interpolation are connected by*

$$\mathbf{G} = \frac{\pi}{N_{\text{col}}} \mathbf{H}^T \mathbf{H}, \quad \mathbf{f} = \frac{\pi}{N_{\text{col}}} \mathbf{H}^T \mathbf{u}. \quad (7.10)$$

To prove this proposition, one can refer to the proof of [8, Theorem 16].

When the basis functions are orthogonal, the n -th element of the solution is independent of N so long as $N \geq n$. The quadratic factor and difference basis are not orthogonal, and the solution elements depend on N .

7.2 Lagrange multiplier theorem: The equality of minimizers

When a “cost” function $\mathcal{J}$ is to be minimized subject to the constraints $\Psi = 0$ and $\Omega = 0$, it is very convenient to convert the problem to the unconstrained minimization of the modified “cost” function

$$J = \mathcal{J} + \lambda \Psi + \mu \Omega, \quad (7.11)$$

where λ and μ are additional unknowns called “Lagrange multipliers”, and Ψ and Ω denote the boundary constraints $u(1) = 0$ and $u(-1) = 0$, respectively. Take the original unknowns to be d_j , and the conditions for a minimum are

$$\frac{\partial J}{\partial d_j} = 0, \quad j = 0, 1, \dots, N, \quad (7.12)$$

$$\frac{\partial J}{\partial \lambda} = \Psi = 0, \quad (7.13)$$

$$\frac{\partial J}{\partial \mu} = \Omega = 0. \quad (7.14)$$

Here, the constraints are $u(\pm 1) = 0$; expressed in terms of Chebyshev coefficients, these are

$$\sum_{j=0}^N d_j = 0 \quad (\Leftrightarrow u(1) = 0), \quad \sum_{j=0}^N (-1)^j d_j = 0 \quad (\Leftrightarrow u(-1) = 0). \quad (7.15)$$

Theorem 7.3. *Consider two minimization problems.*

(i) *Suppose that $u_N^{\text{con}}(x)$ is a solution to the cost function*

$$\mathcal{J} \equiv \langle u(x) - u_N^{\text{con}}(x), u(x) - u_N^{\text{con}}(x) \rangle, \quad (7.16)$$

where $u_N^{\text{con}}(x)$ is a polynomial of degree N constructed so that $\Psi = 0$ and $\Omega = 0$, independent of the remaining unknowns, are satisfied. For example,

$$u_N^{\text{con}}(x) = \sum_{n=0}^{N-2} b_n \{T_{n+2}(x) - T_n(x)\}. \quad (7.17)$$

(ii) *Suppose that $u_N(x)$ is a solution to the cost function*

$$J \equiv \langle u(x) - u_N(x), u(x) - u_N(x) \rangle + \lambda \Psi + \mu \Omega, \quad (7.18)$$

where $u_N(x)$ is a polynomial of degree N , to be an unconstrained-at-the-endpoints minimizer of the cost function. Then the two solutions $u_N^{\text{con}}(x)$ and $u_N(x)$ to the minimization problems $\mathcal{J}$ and J , respectively, are identical.

Proof. Now the solution to the second minimization problem is forced to satisfy the constraint as well. At the minimum, $\Psi = \Omega = 0$, so the cost function reduces to

$$J \equiv \langle u(x) - u_N(x), u(x) - u_N(x) \rangle. \quad (7.19)$$

It follows that $u_N(x)$ and $u_N^{\text{con}}(x)$ both minimize $\langle u(x) - u_N^{\text{approx}}(x), u(x) - u_N^{\text{approx}}(x) \rangle$, where $u_N^{\text{approx}}(x)$ is either $u_N(x)$ or $u_N^{\text{con}}(x)$. Therefore, $u_N(x) \neq u_N^{\text{con}}(x)$ if and only if $u_N^{\text{approx}}(x)$ is not unique. However, the cost function is quadratic in the unknowns. The gradient of the cost function is therefore a linear function of the unknowns. The vanishing of its gradient implies it must have a unique solution. Therefore, the solutions to both the minimization problems are identical. $\square$

The theorem shows that the imposition of the zeros at the endpoints by the Lagrange multiplier gives nothing new when one represents $u_N(x)$ as a finite sum in either the difference basis or the quadratic factor basis.

7.3 Splitting the least squares problem into two via parity

An arbitrary function can always be split into its parts which are symmetric with respect to reflection about the origin, $S(x)$, and antisymmetric with respect to reflection, $A(x)$ (see [6, Chapter 8]). Symmetry means $S(-x) = S(x)$, $\forall x \in \Omega$, while $A(-x) = -A(x)$, $\forall x \in \Omega$, where the Ω is the domain of a function. The parts are $S(x) = (u(x) + u(-x))/2$ and $A(x) = (u(x) - u(-x))/2$.

If we apply this splitting to $u_N(x)$, the cost function becomes

$$\mathcal{J} = \mathcal{J}_S + \mathcal{J}_A + \lambda\Psi + \mu\Upsilon, \quad (7.20)$$

where

$$\mathcal{J}_S = \langle S - S_N, S - S_N \rangle, \quad \mathcal{J}_A = \langle A - A_N, A - A_N \rangle.$$

Here, $\mathcal{J}_S$ is a function of the even degree spectral coefficients only while $\mathcal{J}_A$ is a function only of $\{d_1, d_3, d_5, \dots\}$. After expanding the integrand of the original cost function to

$$\langle (S - S_n), (S - S_n) \rangle + \langle (A - A_n), (A - A_n) \rangle + \langle (S - S_n), (A - A_n) \rangle + \langle (A - A_n), (S - S_n) \rangle,$$

we invoke the fact that the product of a symmetric function and an antisymmetric function is antisymmetric; the integral of an antisymmetric function over a symmetric interval is always zero.

The cost function is not completely decoupled because the constraints depend on both even and odd coefficients. However, both constraints are always zero at the solution. It follows that any linear combination of the constraints is also a legitimate constraint. Define

$$\Theta = (\Psi + \Upsilon)/2 = \sum_{n=0} d_{2n}, \quad \chi = (\Psi - \Upsilon)/2 = \sum_{n=0} d_{2n+1}. \quad (7.21)$$

Least squares is now split into two completely independent problems. One is to minimize, using only symmetric basis functions,

$$\mathcal{J}_S + \lambda'\Theta \quad (7.22)$$

and the other, using only basis functions antisymmetric with respect to the origin, is to minimize

$$\mathcal{J}_A + \mu'\chi. \quad (7.23)$$

Since the methods of attack are similar for each, we shall only discuss the even parity problem in detail.

7.4 Unconstrained least squares with the quadratic factor basis

Define

$$v_{N-2}^{\text{quad}, LS}(x) = \sum_{n=0}^{N-2} c_n^{LS} T_n(x), \quad (7.24)$$

$$u_N^{\text{quad}, LS}(x) = \sum_{n=0}^{N-2} c_n^{LS} (1 - x^2) T_n(x) \quad (7.25)$$

and the cost function

$$\mathfrak{J} = \frac{1}{2} \langle u(x) - u_N^{\text{quad}, LS}(x), u(x) - u_N^{\text{quad}, LS}(x) \rangle, \quad (7.26)$$

and the definition of function $v(x)$ is given in (2.8). Then

$$\begin{aligned} \mathfrak{J} &= \frac{1}{2} \langle v(x) - v^{\text{quad}, LS}(x), (1-x^2)^2 v(x) - v^{\text{quad}, LS}(x) \rangle \\ &= \frac{1}{2} \int_{-1}^1 (v(x) - v^{\text{quad}, LS}(x))^2 (1-x^2)^{3/2} dx. \end{aligned} \quad (7.27)$$

It follows that $v^{\text{quad}, LS}(x)$ is a standard polynomial approximation to $v(x)$, but the weight function is not the usual Chebyshev weight of $1/\sqrt{1-x^2}$ but rather $(1-x^2)^{3/2}$. The orthogonal basis with this weight is the set of Gegenbauer polynomials of order 2. The Gegenbauer polynomials are defined as those polynomials satisfying the orthogonality condition

$$\int_{-1}^1 (1-x^2)^{m-1/2} \hat{C}_n^m(x) \hat{C}_k^m(x) dx = 0, \quad k \neq n, \quad (7.28)$$

where the subscript is the degree of the polynomial and the polynomials are normalized so that $\hat{C}_n^m(1) = 1$. (Warning: this is not the standard textbook normalization, but is convenient for comparing rates of convergence near the endpoints; we have added a caret to the symbol for the Gegenbauer polynomials to emphasize this.)

The Gegenbauer coefficients are *not* equal to the Chebyshev coefficients. However, Theorem 6 of [10] is a specialization of a theorem in proving $a_n^2 \sim \mathcal{O}(1/n^{2\varphi-1})$. Note that a_n^2 's are not the coefficients of $u(x)$ but rather are the coefficients of $v(x) = u(x)/(1-x^2)$ which has branch points proportional to $(1-x^2)^{\varphi-1} \ln(1-x^2)$ instead of $(1-x^2)^\varphi \ln(1-x^2)$ when $\varphi \in \mathbb{N}$; Theorem 2.3 must be applied with $\varphi \rightarrow \varphi - 1$ so that the coefficients of $v(x)$ decrease more slowly than those of $u(x)$ by a factor of $1/n^2$. The error near the endpoints is one order worse than the rate of convergence of the coefficients. For $\varphi \notin \mathbb{N}$ and $\vartheta \in \mathbb{N}_+$, by [33, Corollary 3.4], the coefficients decay rate of the standard Gegenbauer polynomials ($C_n^m(x)$ without the caret) expansion for the function $(1-x^2)^{\varphi-1} \ln^\vartheta(1-x^2)$ is proportional to $\mathcal{O}(\ln^\vartheta(n)/n^{2\varphi+2m-2})$. By the equality $C_n^m(x) = \frac{\Gamma(n+2m)}{\Gamma(2m)\Gamma(n+1)} \hat{C}_n^m(x)$, it is easy to see that the normalized Gegenbauer coefficients decay as

$$a_n^2 \sim \ln^\vartheta(n)/n^{2\varphi-1}, \quad n \gg 1. \quad (7.29)$$

The N -term truncation of the Gegenbauer series has an L_∞ error norm for $v(x)$ of $\mathcal{O}(\ln^\vartheta(N)/N^{2\varphi-2})$. Lemma 3.1 allows us to convert the asymptotic behavior of the Gegenbauer coefficients into a bound on the slowness of the rate of convergence of the error norm.

Theorem 7.4. Suppose that the coefficients a_n^m of a spectral series in Gegenbauer polynomials $\hat{C}_n^m(x)$ or Chebyshev polynomials $T_n(x)$ ($m = 0$) satisfy the bound

$$|a_n^m| \leq W \frac{\ln^\vartheta(n)}{n^\kappa}, \quad \forall n \geq 1, \quad \text{fixed } m, \quad \vartheta \in \mathbb{N}, \quad \text{and } \kappa > 1, \quad (7.30)$$

where W is a positive constant. Then the error in truncating the spectral series after the N -th term satisfies the inequality

$$\left| v(x) - \sum_{n=0}^N a_n^m \hat{C}_n^m(x) \right| \leq W \frac{\ln^\vartheta(N)}{(\kappa-1)N^{\kappa-1}}. \quad (7.31)$$

Proof. By the Baszenski-Delvos Lemma 3.1, the theorem is easy to be proved. $\square$

The theorem (combined with Tuan and Elliott's theorem [28] for Gegenbauer coefficients) yields the maximum pointwise error for $v(x)$. The error for $u(x) \equiv (1 - x^2)v(x)$ is

$$E_N^u(x) = \sum_{n=N+1}^{\infty} a_n^2(1 - x^2)\hat{C}_n^2(x). \quad (7.32)$$

To proceed further, we need two additional lemmas.

Lemma 7.5 (Gegenbauer as Chebyshev derivative). *Normalize the Gegenbauer polynomials so that each is one at the right endpoint. Then*

$$\hat{C}_{n-k}^k(x) = \frac{1}{\prod_{j=0}^{k-1} \frac{n^2-j^2}{2j+1}} \frac{d^k T_n(x)}{dx^k}. \quad (7.33)$$

Proof. It has long been known (see [22, Subsection 18.9.19, p.446]) that the k -th derivative of a Gegenbauer polynomial $\hat{C}_n^m(x)$ is proportional to $\hat{C}_{n-k}^{m+k}(x)$. It only remains to deduce the proportionality constant. Since the Gegenbauer polynomials are normalized to be one at the right endpoint, this constant must be the reciprocal of the value of the derivative at the origin which is known analytically to be (see [6, Appendix A])

$$\left. \frac{d^k T_n(x)}{dx^k} \right|_{x=1} = \prod_{j=0}^{k-1} \frac{n^2 - j^2}{2j+1}. \quad (7.34)$$

This completes the proof. $\square$

Applying Lemma 7.5, we see that the error (7.32) in the variational approximation of $u(x)$ is transformed to

$$E_N^u(x) = \sum_{n=N+1}^{\infty} a_n^2(1 - x^2) \frac{3}{(n+2)^2((n+2)^2 - 1)} \frac{d^2 T_{n+2}(x)}{dx^2}. \quad (7.35)$$

Bernstein [2] proved the following elegant theorem in a paper written in French. Here, P_n denotes the space of all the polynomials whose degrees are not more than n .

Theorem 7.6 (Bernstein polynomial derivative bound). *If $P(x)$ is a polynomial of degree less than or equal to n in P_n , then for $k \leq n$ and $x \in [-1, 1]$,*

$$\left| \frac{d^k P(x)}{dx^k} \right| \leq B_n^{(k)} \|P(x)\|_{\infty}, \quad (7.36)$$

where

$$B_n^{(k)} = \sup_P \{|P^{(k)}(x)| : \|P\|_{\infty} \leq 1 \text{ and } P \in P_n\}.$$

Moreover, when n is large, for $x \in (-1, 1)$,

$$B_n^{(k)} \simeq \left(\frac{n}{\sqrt{1-x^2}} \right)^k, \quad n \rightarrow \infty. \quad (7.37)$$

In this theorem, the inequality holds with increasing precision in the asymptotic limit of increasing degrees. A complete proof in English was given by Whitley [32].

Multiplying the equation (7.36) by $(1 - x^2)$ and taking $k = 2$ and $P(x) = T_n(x)$ give

$$\left| (1 - x^2) \frac{d^2 T_n(x)}{dx^2} \right| \leq (1 + c)n^2, \quad n \rightarrow \infty, \quad (7.38)$$

where the small parameter satisfies $0 < c < 1$. It is easy to prove that

$$(1 - x^2) \frac{d^2 T_n(x)}{dx^2} = n(nT_n(x) - xU_{n-1}(x)). \quad (7.39)$$

Thus, when $n \in \mathbb{N}$ and $n \geq 2$, it holds that

$$\left| (1 - x^2) \frac{d^2 T_n(x)}{dx^2} \right| \leq 2n^2, \quad x \in [-1, 1]. \quad (7.40)$$

Theorem 7.7 (Error bound for $u(x)$ in the least squares/quadratic factor basis). *The error $E_N^u(x)$ in the degree N approximation in the quadratic factor basis using least squares with the inner product $\langle f(x), g(x) \rangle = \int_{-1}^1 f(x)g(x)dx$ satisfies the inequality*

$$|E_N^u(x)| \leq 6 \frac{W \ln^\vartheta(N)}{2\varphi N^{2\varphi}}. \quad (7.41)$$

Proof. To prove this theorem, we use (7.35) again:

$$E_N^u(x) = \sum_{n=N+1}^{\infty} a_n^2 \frac{3}{(n+2)^2((n+2)^2-1)} (1-x^2) \frac{d^2 T_{n+2}(x)}{dx^2}.$$

Recall that we previously demonstrated that a_n^2 's are proportional to $\ln^\vartheta(n)/n^{2\varphi-1}$ in (7.29). Applying the bound on the second derivative of the Chebyshev polynomials (7.38), we see that the error bound is transformed to

$$|E_N^u(x)| \leq W \sum_{n=N+1}^{\infty} \frac{\ln^\vartheta(n)}{n^{2\varphi-1}} \frac{6}{(n+2)^2((n+2)^2-1)} (n+2)^2 \leq 6W \sum_{n=N+1}^{\infty} \frac{\ln^\vartheta(n)}{n^{2\varphi-1+2}}.$$

Applying Lemma 3.1 with $k = 2\varphi + 1$ proves the theorem. $\square$

By (7.37), it is not hard to see that when N is large, one can obtain a sharper estimate

$$|E_N^u(x)| \leq (3+c) \frac{W \ln^\vartheta(N)}{2\varphi N^{2\varphi}}, \quad N \rightarrow \infty, \quad (7.42)$$

where c is a small parameter in $(0, 1)$.

7.5 Least squares with the difference basis

In this basis, the square matrix $\mathbf{G}$ has elements

$$\begin{aligned} G_{mn} &= \langle T_{2m}(x) - T_{2m-2}(x), T_{2n}(x) - T_{2n-2}(x) \rangle \\ &= \begin{cases} \pi, & m = n > 3, \\ 3\pi/2, & m = n = 1, \\ -\pi/2, & m = n + 1, \\ -\pi/2, & n = m + 1, \end{cases} \quad m = 1, 2, \dots, \quad n = 1, 2, \dots \end{aligned} \quad (7.43)$$

Thus, the 6×6 case is

$$\frac{2}{\pi} \mathbf{G} = \begin{vmatrix} 3 & -1 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 \end{vmatrix} \quad (7.44)$$

and with a_n denoting Chebyshev coefficients of the usual infinite series, unconstrained to vanish at the endpoints,

$$\frac{2}{\pi} \mathbf{f} = \begin{vmatrix} a_2 - 2a_0 \\ a_4 - a_2 \\ a_6 - a_4 \\ a_8 - a_6 \\ a_{10} - a_8 \\ a_{12} - a_{10} \end{vmatrix}. \quad (7.45)$$

Because of its sparsity, the matrix equation $\mathbf{G}\mathbf{d} = \mathbf{f}$, with the b_{2n}^{LS} now denoting the elements of $\mathbf{d}$, can be written as the difference system

$$3b_0^{LS} - b_2^{LS} = a_2 - 2a_0, \quad (7.46)$$

$$-b_{2n-2}^{LS} + 2b_{2n}^{LS} - b_{2n+2}^{LS} = a_{2n+2} - a_{2n}, \quad n = 1, 2, \dots, (N-2), \quad (7.47)$$

$$-b_{2N-4}^{LS} + 2b_{2N-2}^{LS} = a_{2N} - a_{2N-2}. \quad (7.48)$$

The solution is

$$b_{2n}^{LS} = -\frac{1-n/N}{1+1/(2N)} \sum_{m=0}^n a_{2m} + \frac{n+1/2}{N+1/2} \sum_{m=n+1}^N a_{2m}, \quad n = 0, \dots, (N-1).$$

The infinite series limit, already analyzed in Section 2, is

$$\lim_{N \rightarrow \infty, \text{fixed } n} b_{2n} = -\sum_{m=0}^n a_{2m}, \quad n = 0, \dots, \infty.$$

If both n and N are large but finite, the solution is simplified to

$$b_{2n}^{LS} = -\left(1 - \frac{n}{N}\right) \sum_{m=0}^n a_{2m} + \frac{n}{N} \sum_{m=n+1}^N a_{2m}, \quad n = 0, \dots, (N-1).$$

Now the Chebyshev coefficients of $u(x)$ must satisfy the condition $u(1) = 0$ which demands

$$\sum_{m=0}^n a_{2m} = -\sum_{m=n+1}^{\infty} a_{2m}. \quad (7.49)$$

Similarly, the second sum in b_{2n}^{LS} can be rewritten in terms of infinite summations as

$$\sum_{m=n+1}^N a_{2m} = \sum_{m=n+1}^{\infty} a_{2m} - \sum_{m=N+1}^{\infty} a_{2m}. \quad (7.50)$$

Then

$$\begin{aligned} b_{2n}^{LS} &= \left(1 - \frac{n}{N}\right) \sum_{m=n+1}^{\infty} a_{2m} + \frac{n}{N} \sum_{m=n+1}^{\infty} a_{2m} - \frac{n}{N} \sum_{m=N+1}^{\infty} a_{2m}, \\ b_{2n}^{LS} &= \sum_{m=n+1}^{\infty} a_{2m} - \frac{n}{N} \sum_{m=N+1}^{\infty} a_{2m}. \end{aligned}$$

Recall from Lemma 3.1 that (3.4) is equivalent to

$$\sum_{n=N+1}^{\infty} \frac{\ln^{\vartheta}(n)}{(2n)^{\kappa}} \sim \frac{1}{(\kappa-1)N^{\kappa-1}} \frac{\ln^{\vartheta}(N)}{2^{\kappa}} \left\{1 + \mathcal{O}\left(\frac{1}{N}\right)\right\}, \quad \vartheta \in \mathbb{N}. \quad (7.51)$$

If $a_n \sim \mathcal{O}(\ln^{\vartheta}(n)/n^{\kappa})$, then

$$b_{2n}^{LS} \sim \frac{A}{(\kappa-1)} \frac{1}{2^{\kappa}} \left\{ \frac{\ln^{\vartheta}(n)}{n^{\kappa-1}} - \frac{n}{N} \frac{\ln^{\vartheta}(N)}{N^{\kappa-1}} \right\} \sim \frac{A \ln^{\vartheta}(n)}{(\kappa-1)n^{\kappa-1}} \frac{1}{2^{\kappa}} \left\{ 1 - \frac{n^{\kappa} \ln^{\vartheta}(N)}{N^{\kappa} \ln^{\vartheta}(n)} \right\}. \quad (7.52)$$

The coefficients in the infinite series are $b_{2n}^{LS} \sim \mathcal{O}(\ln^{\vartheta}(n)/n^{\kappa-1})$, which is the same power law of the rate of decay as that for its least squares counterparts. However, the least squares coefficients—but not the infinite series coefficients—are $\ln^{\vartheta}(n)/n^{\kappa}$ multiplied by $(1 - (\frac{n}{N})^{\kappa} \frac{\ln^{\vartheta}(N)}{\ln^{\vartheta}(n)})$. On a log-log plot, b_{2n}^{LS} curves sharply downward as $n \rightarrow N$.

7.6 Least squares for Chebyshev series with Lagrange multipliers

If a constraint is not built-in to the approximation $u_N(x)$, it can alternatively be added by means of a Lagrange multiplier. The goal is to enforce two boundary conditions, but a function can always be split by parity and then only one constraint for each symmetry is needed.

The goal of least squares is to minimize the “cost function”

$$J = \frac{1}{2} \langle u(x) - S_N(x), u(x) - S_N(x) \rangle + \lambda \Psi, \quad (7.53)$$

where, for the even parity case,

$$S_N(x) = \sum_{n=0}^N a_{2n}^{LS} T_{2n}(x), \quad \Psi = \sum_{n=0}^N a_{2n}^{LS}. \quad (7.54)$$

Setting the gradients of the cost function with respect to all the unknowns gives

$$\frac{\partial J}{\partial \lambda} = \Psi = 0, \quad (7.55)$$

which merely insists that the constraint be satisfied, and also

$$\frac{\partial J}{\partial a_{2m}^{LS}} = 0 = \lambda - \langle u(x), T_{2m}(x) \rangle + \sum_{n=0}^N a_{2n}^{LS} \langle T_{2m}(x), T_{2n}(x) \rangle. \quad (7.56)$$

Because of orthogonality of the Chebyshev polynomials and using the identities $\langle T_0(x), T_0(x) \rangle = \pi$ and $\langle T_{2n}(x), T_{2n}(x) \rangle = \pi/2$ for $n \geq 1$, we have that the equations are simplified to

$$\lambda = \langle u(x), T_0(x) \rangle - a_0^{LS} \pi, \quad \lambda = \langle u(x), T_{2n}(x) \rangle - a_{2n}^{LS} \pi/2, \quad n \geq 1. \quad (7.57)$$

Let a_n denote the Chebyshev coefficients of the infinite series for $u(x)$. Recall that $a_0 = \frac{1}{\pi} \langle u(x), T_0(x) \rangle$ and $a_{2n} = \frac{2}{\pi} \langle u(x), T_{2n}(x) \rangle$. Then

$$\frac{1}{\pi} \lambda = a_0 - a_0^{LS}, \quad \frac{2}{\pi} \lambda = a_{2n} - a_{2n}^{LS}, \quad n \geq 1. \quad (7.58)$$

Adding these equations and then invoking $\Psi = 0$ gives

$$\lambda = \frac{\pi}{(2N+1)} \sum_{n=0}^N a_{2n}. \quad (7.59)$$

The Chebyshev coefficients of the solution to the variational problem are then

$$a_0^{LS} = -\frac{1}{\pi} \lambda + a_0, \quad a_{2n}^{LS} = -\frac{2}{\pi} \lambda + a_{2n}, \quad n \geq 1. \quad (7.60)$$

If the $a_{2n} \sim A \ln^\vartheta(2n)/(2n)^\kappa$ ($\kappa > 0, \vartheta \in \mathbb{N}$) as demanded by Theorem 2.3, then the error at the endpoints is

$$\Upsilon \equiv \sum_{n=0}^N a_{2n} = - \sum_{n=N+1}^{\infty} a_{2n} \approx \mathcal{O}\left(\frac{\ln^\vartheta(N)}{N^{\kappa-1}}\right), \quad (7.61)$$

the same as the L_∞ error norm of the Chebyshev series. (The error norm in fact is Υ for some of our exemplary $u(x)$.) It follows that

$$\lambda \sim \mathcal{O}(\ln^\vartheta(N)/N^\kappa), \quad \vartheta \in \mathbb{N}. \quad (7.62)$$

It is deserving to point out that the least squares approximation varies with the choice of the weight function. The Chebyshev weight function above is selected as $(1-x^2)^{-1/2}$ for any of the three bases. However, only the Chebyshev basis is orthogonal with the weight function, and the other two are not. Next, the weight functions to make the difference basis and the quadratic basis orthogonal are, respectively, given in this subsection.

Theorem 7.8. If the weight function is chosen as $(1 - x^2)^{-3/2}$, then the difference basis $\{\varsigma_n(x)\}$ is orthogonal, i.e.,

$$\int_{-1}^1 \varsigma_m(x) \varsigma_n(x) (1 - x^2)^{-\frac{3}{2}} dx = 2\pi \delta_{mn}, \quad m, n = 0, 1, \dots \quad (7.63)$$

Proof. It holds that

$$\begin{aligned} \int_{-1}^1 \varsigma_n(x) \varsigma_m(x) (1 - x^2)^{-\frac{3}{2}} dx &= \int_0^\pi [\cos((n+2)t) - \cos(nt)] \cdot [\cos((m+2)t) - \cos(mt)] \frac{1}{\sin^2(t)} dt \\ &= 4 \int_0^\pi \sin[(m+1)t] \sin(t) \cdot \sin[(n+1)t] \sin(t) \cdot \frac{1}{\sin^2(t)} dt \\ &= 4 \int_0^\pi \sin[(m+1)t] \cdot \sin[(n+1)t] dt \\ &= 2\pi \delta_{mn}. \end{aligned}$$

This completes the proof. $\square$

Following the steps of least squares in Subsection 7.1, like (7.5), for the difference basis with the weight function $(1 - x^2)^{-3/2}$, one obtains

$$\tilde{\mathbf{G}} \tilde{\mathbf{d}} = \tilde{\mathbf{f}}, \quad (7.64)$$

where

$$\begin{aligned} \tilde{\mathbf{G}}_{mn} &= \langle \varsigma_m(x), \varsigma_n(x) \rangle = \int_{-1}^1 \varsigma_n(x) \varsigma_m(x) (1 - x^2)^{-\frac{3}{2}} dx \\ &= 4 \int_0^\pi \sin[(m+1)t] \cdot \sin[(n+1)t] dt \\ &\approx 4 \cdot \frac{\pi}{N_{\text{col}}} \sum_{k=0}^{N_{\text{col}}} \sin\left((m+1) \frac{(2k-1)\pi}{2N_{\text{col}}}\right) \sin\left((n+1) \frac{(2k-1)\pi}{2N_{\text{col}}}\right) \\ &= 4 \cdot \frac{\pi}{N_{\text{col}}} \cdot \frac{N_{\text{col}}}{2} \delta_{mn} = 2\pi \delta_{mn}, \quad m, n = 0, 1, \dots, N, \quad N_{\text{col}} > N + 1, \end{aligned}$$

which is a consequence of the orthogonality of the sine function with respect to the points $t_k = \frac{\pi(2k-1)}{N_{\text{col}}}$, $k = 1, 2, \dots, N_{\text{col}}$,

$$\sum_{k=1}^{N_{\text{col}}} \sin\left((m+1) \frac{(2k-1)\pi}{2N_{\text{col}}}\right) \sin\left((n+1) \frac{(2k-1)\pi}{2N_{\text{col}}}\right) = \frac{N_{\text{col}}}{2} \delta_{mn}$$

and

$$\begin{aligned} \tilde{\mathbf{f}}_n &= \langle u(x), \varsigma_n(x) \rangle = \int_{-1}^1 \varsigma_n(x) u(x) (1 - x^2)^{-\frac{3}{2}} dx \\ &= \int_0^\pi \varsigma_n(\cos(t)) u(\cos(t)) \cdot \frac{1}{\sin^2(t)} dt \\ &\approx \frac{\pi}{N_{\text{col}}} \sum_{k=1}^{N_{\text{col}}} \varsigma_n\left(\cos\left(\frac{(2k-1)\pi}{2N_{\text{col}}}\right)\right) u\left(\cos\left(\frac{(2k-1)\pi}{2N_{\text{col}}}\right)\right) \cdot \sin^{-2}\left(\frac{(2k-1)\pi}{2N_{\text{col}}}\right). \end{aligned}$$

When the number of the interpolation N_{col} is bigger than the number of the basis $N + 1$, the coefficients of the difference basis decrease as $\mathcal{O}(\ln^\vartheta(n)/n^{2\varphi})$ as $n \rightarrow \infty$, which obeys the same law of the counterpart coefficients in infinite series truncation as is shown in Figure 2. There is no curl up or curl down as $n \rightarrow N$. Thus the error norm is also the same as the error norm of the infinite series truncation.

In fact, to approximate the function $u(x)$, using the difference basis $\varsigma_n(x)$ with the weight function $(1 - x^2)^{-3/2}$ is equivalent to using the second Chebyshev function $U_n(x)$ with the weight function $\sqrt{1 - x^2}$.

Theorem 7.9. *If the weight function is chosen as $(1 - x^2)^{-5/2}$, then the quadratic basis $\{\varrho_n(x)\}$ is orthogonal, i.e.,*

$$\int_{-1}^1 \varrho_m(x) \varrho_n(x) (1 - x^2)^{-5/2} dx = \begin{cases} \pi, & m = n = 0, \\ \frac{1}{2} \pi \delta_{mn}, & m, n \in \mathbb{N}_+. \end{cases} \quad (7.65)$$

The theorem is easy to be proved. In a way similar to the procedure of least squares for the difference basis with the weight function $(1 - x^2)^{-3/2}$, one can also conclude that the least squares coefficients for the quadratic basis with the weight function $(1 - x^2)^{-5/2}$ decrease as $\mathcal{O}(A(n)/n^{2\varphi-1})$ as $n \rightarrow \infty$. The error decreases as $\mathcal{O}(|A(N)|/N^{2\varphi-1})$, which is also the same as the error of the infinite series truncation for the same basis. In the rest of this paper, we still use the inner product $\langle \cdot, \cdot \rangle$ mentioned in Subsection 7.1.

8 Comparing different approximations using the difference basis

The spectral coefficients and error norms are so similar that the most illuminating way to compare them is to tabulate ratios. Table 1 shows that when $n \ll N$, $b_n \approx b_n^I \approx b_n^{LS}$. When n nears N , the interpolation coefficients swell to nearly double those of the infinite series while $b_{LS} \ll b_n$.

We compare the ratio of error norms in Table 2. Least squares with integration as the inner product is only slightly worse than the truncation of the infinite series (less than 10%). The maximum pointwise error for interpolation is roughly double that of truncation of the infinite series, independent of N .

9 Comparing different quadratic factor basis approximations

Figure 7(a) shows that the coefficients of all the three approximation schemes in the basis $\varrho_n(x) = (1 - x^2)T_n(x)$ have the same slope, $1/n^{2\varphi-1}$, over most of the range in degree. The interpolant's coefficients and those obtained by least squares with the inner product

$$\langle f(x), g(x) \rangle = \int_{-1}^1 f(x)g(x)/\sqrt{1 - x^2} dx$$

both bend sharply downward as $n \rightarrow N$.

How do these fast-tail decreases affect the error norms? Figure 7(b) provides an answer.

The aliasing error, which produces the downward curve in the spectral coefficients for interpolation in Figure 7, is generally regarded as a bad thing. Therefore, the even sharper deviation from a power law for the least squares coefficients should be an even worse thing. Actually, the error norms associated with the downward curving spectral coefficients decrease faster by $O(N)$ than the error norm of the truncated infinite series with its pure power law (the black straight line in Figure 7(a)).

We have no explanation. However, note that some acceleration methods such as Euler acceleration [9, 21, 23] taper the high degree coefficients to improve accuracy. Something similar seems to be happening with aliased spectral series.

Table 1 Coefficient ratios for the difference basis, $\varsigma_n = T_{n+2}(x) - T_n(x)$, for $(1 + x/2)(1 - x^2)^\varphi \ln(1 - x^2)^\vartheta$ with $\vartheta = 1$ and $\varphi = 2$. b_n 's are the coefficients in the infinite series, b_n^I 's are the coefficients of the interpolant using 100 collocation points and b_n^{LS} 's are the result of least squares with integration as the inner product

n	10	20	30	40	50	60	70	80	90	92	94	96	98	99
b_n^I/b_n	1.00	1.00	1.00	1.00	1.01	1.03	1.08	1.19	1.43	1.51	1.60	1.71	1.83	1.900
b_n^{LS}/b_n	1.00	1.00	1.00	0.99	0.97	0.93	0.85	0.71	0.47	0.40	0.34	0.26	0.18	0.095

Table 2 The function and basis are the same as in the previous table except that the ratios are now of errors in the L_∞ norm, and these are listed versus the truncation N rather than degree n

N	10	20	30	40	50	60	70	80	90	100
E_N^{interp}/E_N	1.98	1.96	1.96	1.97	1.94	1.93	1.98	1.98	1.96	1.85
E_N^{LS}/E_N	0.96	1.03	1.06	1.07	1.08	1.09	1.07	1.09	1.04	1.07

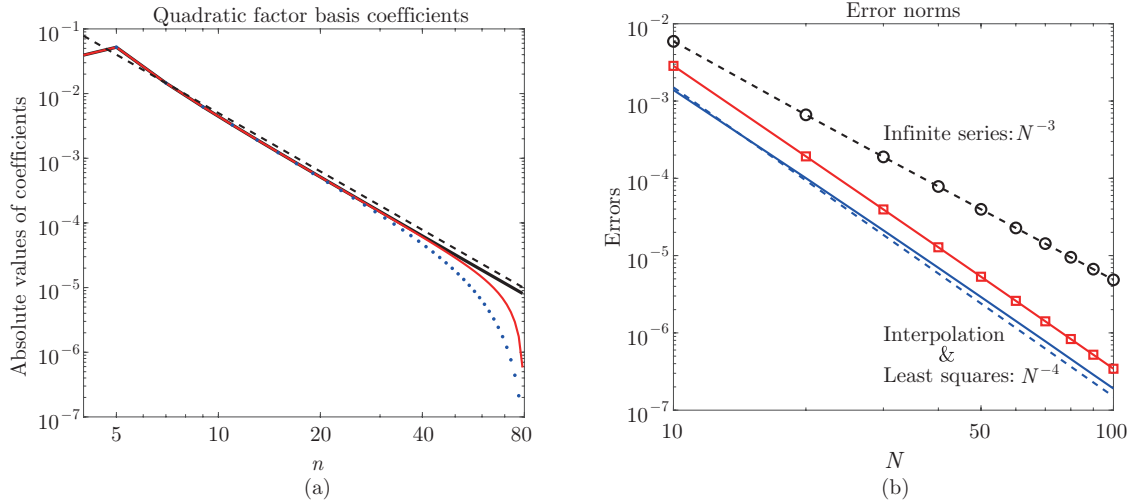


Figure 7 (Color online) (a) Odd degree coefficients versus degrees for approximations using the quadratic factor basis for $u(x) = (1 + x/2)(1 - x^2)^2 \ln(1 - x^2)$, the same function as employed in the previous figure, and $N = 80$. The thick black curve is the coefficients c_n of the infinite series. The thin red curve connects the absolute values of the coefficients of the 79-point interpolant in the quadratic factor basis. The blue dotted curve is the coefficients of least squares with the integral inner product. The black dashed line is proportional to $n^{\kappa-2}$. (b) Quadratic factor basis, the same as in the previous figure but showing error norms versus N instead of coefficients versus n . Black dashed circles: errors in truncation of the infinite series in the basis $\varrho_n(x)$. The red curve: errors in interpolation. The blue solid curve: errors of least squares approximations. The blue dash reference line is proportional to N^{-4}

10 Conclusion

The concern of this paper is to address the Chebyshev expansion of the weak singularity functions on three bases, both theoretically and computationally. The main results are concluded in the following.

1. The coefficients and errors of several kinds of approximations are summarized in Table 3.
2. There are *two* distinct interpolants on the *roots* grid, but the interpolant on the *Lobatto* (endpoint-including) grid is always *unique*.
3. The error norms in N -point interpolation on the roots grid are *identical* for all the three basis sets, i.e.,

$$\text{Error}_N^{\text{Cheb,Lob,I}} = \text{Error}_N^{\text{diff,Lob,I}} = \text{Error}_N^{\text{quad,Lob,I}} \sim \mathcal{O}(|A(N)|/N^{2\varphi}). \quad (10.1)$$

4. The pointwise errors for interpolation using the quadratic factor basis and the difference basis are identical for all x because $u_N^{\text{diff}}(x) = u_N^{\text{quad}}(x)$ for all x .

5. The pointwise error in standard Chebyshev interpolation, unconstrained by $u_N(\pm 1) = 0$, is *different* from the errors (not error norms) of the constrained basis sets, the quadratic factor basis and the difference basis; the errors of the constrained basis sets are *nearly-uniform* in x whereas the Chebyshev error is one order smaller than that of the constrained bases except in narrow *boundary layers* where the Chebyshev error rises to equal that of the constrained bases.

6. If the Chebyshev coefficients decay as $a_n \sim A \ln^\vartheta(n)/n^\kappa$ where A is a constant, ϑ is a nonnegative integer and $\kappa > 0$, then

Table 3 Results for $(1 - x^2)^\varphi \ln^\vartheta(1 - x^2)$ with $\varphi > \frac{1}{2}$ and $\vartheta \in \mathbb{N}$. The labels “u” and “d”, respectively, denote that the coefficients a_n curl up or curl down as $n \rightarrow N$, deviating from the correct asymptotic line because of aliasing errors as described in Theorem 5.2. The expression of $A(n)$ is given in Theorem 2.3. TS, IT, LS, and B.C.s represent Truncated Series, Interpolation, Least Squares and Boundary Conditions, respectively

Bases	Chebyshev	Difference	Quadratic	Chebyshev Lagrange
TS: Coeffs	$a_n \sim A(n)/n^{2\varphi+1}$	$b_n \sim A(n)/n^{2\varphi}$	$c_n \sim -A(n)/n^{2\varphi-1}$	-
TS: Errors	$ A(N) /N^{2\varphi}$	$ A(N) /N^{2\varphi}$	$ A(N) /N^{2\varphi-1}$	-
IT: Coeffs	$a_n^I \sim A(n)/n^{2\varphi+1}$ (d)	$b_n^I \sim A(n)/n^{2\varphi}$ (u)	$c_n^I \sim -A(n)/n^{2\varphi-1}$ (d)	-
IT: Errors	$ A(N) /N^{2\varphi}$	$ A(N) /N^{2\varphi}$	$ A(N) /N^{2\varphi}$	-
LS: Coeffs	$a_n^{LS} \sim A(n)/n^{2\varphi+1}$	$b_n^{LS} \sim A(n)/n^{2\varphi}$ (d)	$c_n^{LS} \sim -A(n)/n^{2\varphi-1}$ (d)	$a_n^{CL} \sim A(n)/n^{2\varphi+1}$
LS: Errors	$ A(N) /N^{2\varphi}$	$ A(N) /N^{2\varphi}$	$ A(N) /N^{2\varphi}$	$ A(N) /N^{2\varphi}$
B.C.s	Not imposed	Satisfied	Satisfied	Imposed by Lagrange a multiplier

(a) For small degree n ($1 < n \ll N$), the relative error in the Chebyshev coefficient is

$$\frac{|\mathcal{E}_n|}{|a_n|} \leq \frac{1}{2^{\kappa-1}} \frac{n^\kappa}{N^\kappa} \frac{\ln^\vartheta(N)}{\ln^\vartheta(n)}. \quad (10.2)$$

(b) For $n = N - m$ with m being small, the relative error is

$$\frac{|\mathcal{E}_{N-m}|}{|a_{N-m}|} \sim 1 + \mathcal{O}\left(\frac{\kappa m}{N}\right). \quad (10.3)$$

When $\vartheta = 0$, a_n^I is plotted versus n with logarithmic axes, and as a result the curve on the log-log plot should, for power-law decay, approach a straight line. The aliasing errors create a sharp downward turn in a_n^I as $n \rightarrow N$. (The coefficients for the difference basis exhibit a sharp upturn for similar reasons.)

7. The values of the derivatives at the endpoints are $\mathcal{O}(n^2)$ for Chebyshev polynomials, but only $\mathcal{O}(n)$ for the difference basis.

The most important conclusion is that those different choices of approximation schemes and bases can alter the rate of convergence by a factor of N or N^2 . For series that converge proportionally to small inverse powers of N due to weak endpoint singularities, this is significant. Knowing how to solve the singular problems using spectral methods is important, but giving the optimal basis seems more practically significant, especially in high-dimensional spaces.

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