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Prolate spheroidal wavefunctions as an alternative to Chebyshev and Legendre polynomials for spectral element and pseudospectral algorithms

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Abstract

Prolate spheroidal functions of order zero are generalizations of Legendre polynomials which, when the "bandwidth parameter" $c > 0$, oscillate more uniformly on $x \in [-1, 1]$ than either Chebyshev or Legendre polynomials. This suggests that, compared to these polynomials, prolate functions give more uniform spatial resolution. Further, when used as the spatial discretization for time-dependent partial differential equations in combination with explicit time-marching, prolate functions allow a longer stable timestep than Legendre polynomials. We show that these advantages are real and further, that it is almost trivial to modify existing pseudospectral and spectral element codes to use the prolate basis. However, improvements in spatial resolution are at most a factor of $\pi/2$, approached slowly as $N \to \infty$. The timestep can be lengthened by several times, but not by a factor that grows rapidly with N. The prolate basis is not likely to radically expand the range of problems that can be done on a workstation. However, for production runs on the "bleeding edge" edge of arithmurgy, such as numerical weather prediction, the rewards for switching to a prolate basis may be considerable.
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Keywords: Pseudospectral; Spectral element; Prolate spheroidal wavefunctions; Quasi-uniform spectral scheme

"Prolate Spheroidal Wave Functions are likely to be a better tool for the design of spectral and pseudo-spectral techniques than the orthogonal polynomials and related functions" – Xiao et al. [48, p. 837]

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1. Introduction

Pseudospectral methods using Chebyshev polynomials have been the method of choice for calculating high accuracy solutions to problems on a finite domain with non-periodic boundary conditions. The Chebyshev basis is the optimum *polynomial basis* for spectral and spectral methods when applied on a single domain [13,19,29,45]. When these algorithms are applied on multiple domains using variational principles and expansions of moderate degree on each element, Legendre polynomials are the best polynomial choice [35]. But what of *non-polynomial* basis sets for non-periodic problems on an interval?

Xiao et al. [48] proposed a non-polynomial alternative: expansion in prolate spheroidal functions of zeroth order. Their rationale is that the prolate functions are bandlimited and are known to be particularly useful in signal-processing applications. But is the Fourier transform property of bandlimitedness relevant to non-periodic problems on a finite interval? In any event, how can one compare non-polynomial basis functions with polynomials except through the crudest empirical tests?

This paper addresses these questions. First, we place prolate methods in context as one strategy for achieving a spectral method with a quasi-uniform grid, as opposed to the very non-uniform grids associated with Legendre and Chebyshev polynomials. Second, we codify an enlarged definition of convergence to include continuous adjustment of the bandwidth parameter c of the prolate functions with the truncation N. (As opposed to the usual definition of convergence, which is the limit $N \to \infty$ with all parameters of the basis set *fixed*.) Third, we make a beginning at convergence theory for prolate functions in the continuously adjusted limit. (Prolate functions degenerate to Legendre polynomials in the limit $N \to \infty$ for fixed bandwidth c, and thus we can profitably discuss their accuracy only when c varies linearly with N.) Finally, we summarize the usefulness of prolate series in the limits of small, one-off research projects and large, run-the-code-a-thousand-times operational computations.

2. The quest for quasi-uniform spectral schemes

Chebyshev and Legendre polynomial methods have been a splendid success as chronicled in books by Boyd [13], Deville et al. [24], Karniadakis and Sherwin [35], Fornberg [28], Mason and Handscomb [36] and Trefethen [45]. However, the many successful applications catalogued in these tomes cannot conceal unpleasant truths. The computational grids (Gaussian quadrature points) associated with Chebyshev and Legendre polynomials are highly non-uniform. For both sets of polynomials, the points are separated by only $O(1/N^2)$ near the endpoints at $x = \pm 1$. By using the identities $T_n(x) = \cos(n \arccos(x))$ and the asymptotic approximation for the Legendre polynomials, one can similarly show that points are separated by $(\pi/2)(2/N)$ near $x = 0$.

The non-uniform distribution of collocation points has two unfortunate consequences:

1. The resolution near $x = 0$ is *poorer* than of a uniformly spaced grid with the same number of points by a factor of $\pi/2$.
2. When a Chebyshev or Legendre spatial discretization is applied to a time-dependent problem, the Courant–Friedrichs–Lewy (CFL) time-stepping limit for an explicit scheme is roughly the *square* of that for a finite difference spatial discretization on a uniform grid.

These drawbacks have inspired considerable interest in modifying spectral methods so as to obtain what we will dub a "Quasi-Uniform Spectral Scheme" (QUSS), that is, a spectral method that employs a spatial grid which is more uniform than the Chebyshev or Legendre grids. Before describing the particular QUSS studied here, we must note that it is but one of a number of alternatives including the following:

1. *Tikhonov regularization*: a polynomial pseudospectral method with a *uniform* grid which is regularized by minimizing a functional that weights both smoothness of the approximation as well as the residual of the differential equation [10].

2. *Kosloff/Tal-Ezer basis*: Chebyshev basis with an arcsine change-of-coordinate [13,37].
3. *Theta-mapped cosine basis*: similar to Kosloff/Tal-Ezer but with a different, non-singular change-of-coordinate using Jacobian theta functions (to be published).
4. *Fourier Extension/Embedding*: solving a non-periodic problem using a Fourier basis and grid on a larger domain on which the solution is modified to be smoothly periodic [3,14,27,30].
5. *Fourier Embedding with Sum Acceleration*: similar to the previous scheme except that the solution is not required to be periodic on the extended domain, but instead is approximated by a Fourier series that is summed to exponential accuracy on the physical interval by a standard sequence acceleration algorithm such as the Euler summation or Levin's nonlinear sequence transformation (to be published).
6. *Extended KT or theta-mapped basis*: solving a non-periodic problem on an extended domain such that the non-uniform areas of the Kosloff/Tal-Ezer basis or the theta-mapped cosine basis are outside the physical domain, in the spirit of the Fourier Extension/Embedding family of methods (to be published).
7. Prolate spheroidal basis.

It would take us too far afield to attempt to discuss these alternatives in detail, but the existence of so many QUSSs makes it all the more imperative to carefully analyze the virtues and vices of the prolate basis. At the same time, it must be noted that two defects of the prolate basis are vices shared by the other six schemes as well: the annoyance of tuning a numerical parameter (here c) and the fact that the best theoretical performance is approached only slowly and asymptotically from below as the number of degrees of freedom N tends to infinity. The quest for QUSS is both important and difficult.

3. A visual and analytical rationale for prolate spheroidal functions

Why is the prolate spheroidal basis more uniform than Legendre polynomials? The answer is that Legendre polynomials are the axisymmetric eigenfunctions of the Laplace operator on the surface of a sphere while prolate functions of order zero are Laplace axisymmetric eigenfunctions on the surface of a prolate spheroid. This is a surface of revolution which is generated by rotating an ellipse around an axis connecting the north and south poles. The eccentricity of the ellipse is proportional to the so-called "bandwidth parameter" c whose role in prolate theory is explained in later sections. In the limit of infinite eccentricity – $c \to \infty$ – the prolate spheroid becomes an infinitely long cylinder as illustrated in Fig. 1. The

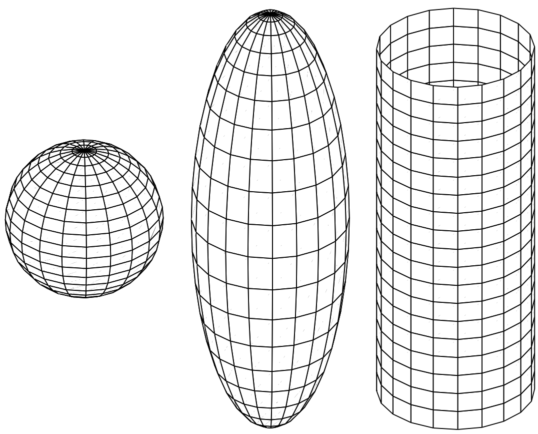

Fig. 1. The sphere (left) and the cylinder (right) are limits of a prolate spheroid for zero bandwidth c and infinite bandwidth c, where c is a measure of the "prolateness" of the prolate spheroid.

axisymmetric Laplace eigenfunctions are *trigonometric* functions in the axial coordinate z, which is equivalent to latitude. For large but finite eccentricity, the prolate spheroid resembles a cylinder over most of its length. It follows that the eigenfunctions of the Laplacian operator on the surface of an elongated prolate spheroid must resemble trigonometric functions except close to the poles.

Thus, by shifting to a prolate basis, we do indeed obtain basis functions that oscillate more uniformly in x than the Legendre or Chebyshev polynomials.

3.1. Large degree asymptotics for prolate spheroidal functions of order zero

The near-uniformity of the prolate basis can be demonstrated analytically through the asymptotic approximations of the prolate functions. Asymptotic approximations for prolate functions of order zero (or general order) have been derived by [1,25,26,38,41] and others cited by these authors. The quantity

$$c_*(n) \equiv (\pi/2)(n + 1/2) \qquad [\text{“Transition Bandwidth”}] \tag{1}$$

defined by Slepian and Miles, plays a crucial role in the asymptotic theory and indeed in all aspects of prolate spheroidal applications. When $c < c_*(n)$, the approximation

$$\psi_n(x; c) \sim \frac{\sqrt{\mathscr{E}(x; m)}}{(1 - x^2)^{1/4}(1 - mx^2)^{1/4}} J_0\left(\frac{c}{\sqrt{m}}\mathscr{E}(x; m)\right), \tag{2}$$

where J_0 is the usual Bessel function [2], is valid for all $x \in [-1, 1]$ where

$$\mathscr{E}(x; m) \equiv \int_x^1 \mathrm{d}t \, \frac{\sqrt{1 - mt^2}}{\sqrt{1 - t^2}} \equiv E(1; m) - E(x; m) \tag{3}$$

is the difference of the complete and incomplete elliptic integrals of the second kind [2] and the elliptic modulus m is

$$m \equiv c^2/\chi_n, \tag{4}$$

where $\chi_n(c)$ is the nth eigenvalue of the prolate differential equation (9). When the condition $c < c_*(n)$ is satisfied, as is necessary for the validity of the asymptotic approximation, then $m < 1$.

Outside of a small neighborhood of the endpoints whose width is $O(1/\sqrt{c})$, the Bessel function can be approximated to yield

$$\psi_n(x; c) \sim \sqrt{\frac{2}{\pi}} \frac{m^{1/4}}{\sqrt{\chi_n}} \frac{1}{(1 - x^2)^{1/4}(1 - mx^2)^{1/4}} \cos\left(\frac{c}{\sqrt{m}}\mathscr{E} - \pi/4\right). \tag{5}$$

If the bandwidth c is chosen to equal the transition bandwidth $c_*(n)$, then using $\chi_n(c = c_*(n)) = c_*^2(1 + O(1/n^2))$ [16],

$$\psi_n(x; c = c_*(n)) \sim \sqrt{\frac{2}{\pi}} \frac{1}{c} \frac{1}{(1 - x^2)^{1/2}} \cos([\pi/2]n(1 - x)). \tag{6}$$

The important conclusion is that when the bandwidth parameter is close to the transition bandwidth, the prolate function is rather like $\cos([\pi/2]n(1 - x))$. This in turn suggests that the grid points associated with the prolate basis will be nearly uniform, as confirmed by numerical calculations, and the non-uniform resolution of Legendre expansions will be replaced by a more uniform approximation.

4. Definitions of rate of convergence: continuously adjusted spectral expansions

The classical definition of series convergence is to fix all internal parameters of the basis functions, and then ask how rapidly the error falls as $N \to \infty$, where N is the truncation of the expansion. For spectral series, the usual (and highly desired) situation is that the error falls as $\exp(-N\mu)$ for some positive constant μ. This is the same as the rate of decrease for the "geometric" series of introductory calculus, $1/(1-x) \sim 1 + x + x^2 + \cdots$, for which the error is proportional to $x^{N+1} = \exp(-[N+1]\log(x))$ for $|x| < 1$. This motivates the usual definition of "Asymptotic Rate of Geometric Convergence" which has been used in both the theory of linear algebra iterations and in spectral expansion theory [13]:

Definition 4.1 ((*Classical*) *Asymptotic rate of geometric convergence*). If the error in a series approximation, truncated after the Nth term, is decreasing proportional to $\exp(-N\mu)$, perhaps multiplied by algebraic functions of N or other factors that vary more slowly with N than an exponential, then μ is said to be the "asymptotic rate of geometric convergence". A more precise definition in terms of the *supremum* limit is:

$$\mu = \overline{\lim_{N\to\infty, c \text{ fixed}}}\{-\log|E_T(N)|/N\}, \tag{7}$$

where $E_T(N)$ is the L_∞ norm of the error in truncating the series after the Nth term.

However, when the basis functions contain an internal parameter, we must generalize the notion of convergence. The reason is that we can specify a value of this parameter c and a truncation N and then compute the error in approximating a given function $u(x)$. Choosing various c and N defines a two-dimensional array of errors. The classical definition is the "horizontal limit", that is, asking what happens as N varies while the basis function parameter c is *fixed*. However, it is almost never the case with spectral series that the contours of error are vertical in the c–N-plane so that the downgradient direction (the path of most rapid decrease of the error) is horizontal. Rather, error decreases most rapidly within the c–N plane when *c varies with the truncation N*.

This is hardly a novel observation. It has been made for Hermite series by [4,6], for rational Chebyshev series in [7–9], for the Cloot–Weideman basis by [22,23,46] and for Laguerre functions in [18]. However, even now, for some, the notion of basis functions which change with the truncation N is too wierd, too far from standard convergence theory.

Nevertheless, for each formula connecting c to N, we can compute a spectral series for a given function f, truncate after the Nth term, and plot the rate at which the errors fall. Note that in both the classical and continuously adjusted limits, the rate of convergence μ depends on the function $f(x)$ which is being expanded.

Definition 4.2 (*Continuously adjusted asymptotic rate of geometric convergence*). If the error in a series approximation, truncated after the Nth term, is decreasing proportional to $\exp(-N\nu)$ when the basis function parameter c varies according to some specified function $c(N)$, then ν is said to be the "continuously adjusted asymptotic rate of geometric convergence". A more precise definition in terms of the *supremum* limit is:

$$\nu = \overline{\lim_{N\to\infty}}\{-\log|E_T(N; c(N))|/N\}. \tag{8}$$

Fig. 2 shows the error contours in the truncation of the prolate series for a particular (but representative) function $u(x)$. The error decreases in the horizontal limit of fixed c, varying N, but this is not the most efficient approximation procedure. When the truncation N is 10, the best choice of bandwidth parameter c

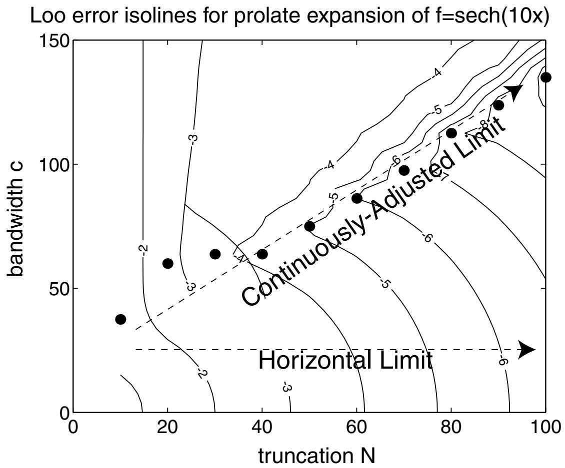

Fig. 2. Contours of the base-10 logarithm of the L_∞ error of the prolate spheroidal expansion in the N–c-plane, where c is the internal parameter (bandwidth parameter) of the prolate basis functions, computed for the particular function $u = \mathrm{sech}(10x)$. The black disks mark the minimum error for fixed truncation N.

is about 40. Keeping $c = 40$ as N increases reduces the error to about 3×10^{-7} when $N = 100$. However, increasing c linearly with N – following the line of the black dots in the figure – allows the error to be reduced by another factor of 300 at $N = 100$, for which the optimal c is not 40, but roughly 135.

The horizontal limit of fixed parameter is optimum only when the error contours are vertical, that is, the error is independent of c. This is obviously a very special case. It is typical, rather than unusual, for the best choice of an internal basis function parameter to vary with N.

Furthermore, when the prolate bandwidth c is fixed, the prolate functions turn into Legendre polynomials in the limit $N \to \infty$: $\lim_{n\to\infty} \psi_n(x; c) = P_n(x)$. All advantages of the prolate basis over Legendre series are lost unless c is allowed to vary with N.

5. Properties of prolate spheroidal wavefunctions of order zero

The prolate functions first appeared as the solutions to a differential equation which arose in separating variables to solve the Helmholtz equation in prolate spheroidal coordinates:

$$(1 - x^2)\psi_{n,xx} - 2x\psi_{n,x} + \{\chi_n - c^2x^2\}\psi_n = 0, \quad n = 0, 1, 2, \ldots, \tag{9}$$

where n is the mode number, χ_n is the eigenvalue and c is a constant that will be here called the "bandwidth" parameter. We must append the phrase "of order zero" because Eq. (9) is a special case of the general equation for the angular (latitude-like) factors in spheroidal coordinates.

The prolate functions will be orthonormalized so that

$$\int_{-1}^{1} \psi_m(x; c)\psi_n(x; c)\,\mathrm{d}x = \delta_{mn} = \begin{cases} 1, & m = n, \\ 0, & m \neq n. \end{cases} \tag{10}$$

The coefficients of an arbitrary function,

$$u(x) = \sum_{n=0}^{\infty} a_n \psi_n(x; c), \tag{11}$$

are

$$a_n = \int_{-1}^{1} f(x)\psi_n(x;c)\,\mathrm{d}x. \tag{12}$$

The prolate functions have properties typical of Sturm–Liouville eigenfunctions including the following:

Theorem 5.1 (Properties of prolate spheroidal functions).
1. *$\psi_n(x;c)$ is symmetric in x if n is even and $\psi_n(-x) = -\psi_n(x)$ is antisymmetric when n is odd.*
2. *ψ_n has exactly n zeros on the interval $x \in [-1, 1]$.*
3. *The ψ_n are orthogonal on $x \in [-1, 1]$ with unit weight function.*
4. *The ψ_n are complete in $L_2[-1, 1]$.*

All these properties are shared by the Legendre polynomials.

The proofs are given in [42,48].

One unique property among Sturm–Liouville eigenfunctions is that all prolate functions of order zero are bandlimited in the sense that their Fourier transforms are identically zero whenever the transform variable $|k| > c$.

One major complication is that prolate functions cannot be calculated by a three-term recurrence, as for Legendre polynomials. Instead, the most efficient method known is a Legendre–Galerkin eigenvalue algorithm. When the ψ_n are expanded in terms of normalized Legendre polynomials and the differential equation is discretized by a Galerkin method, the result is a symmetric tridiagonal matrix whose elements are given in the following section.

Prolate Gaussian quadrature points cannot be computed by the simple root-finding algorithms used for Legendre polynomials. Instead, one must employ more complicated procedures developed in [21,48] as described in the following section. Unfortunately, the calculation of eigenvalues, eigenfunctions, and Gaussian quadrature points must be done anew whenever c is changed.

Another unfortunate complication is the need to choose the bandwidth parameter c. There is no general theory, alas, but we can offer some guidelines.

Theorem 5.2 (Legendre and Hermite limits of prolate functions).
1. $\psi_n(x; c = 0) \equiv P_n(x)$. (13)
2. $\psi_n(x;c) \sim P_n(x) + \frac{c^2}{16n}\{P_{n-2}(x) - P_{n+2}(x)\}, \quad n \gg c^2, \quad x \in [-1, 1].$ (14)
3. $\lim_{n\to\infty} \psi_n(x;c) = P_n(x), \quad x \in [-1, 1].$ (15)
4. $\chi_n(c) \sim n(n+1)\left\{1 + \mathrm{O}\left(\frac{c^2}{2n^2}\right)\right\}.$ (16)
5. *As $c \to \infty$, fixed n*

$$\psi_n(x;c) \sim \exp(-cx^2/2)H_n(\sqrt{c}x), \tag{17}$$

$$\chi_n(c) \sim c(2n+1) - \frac{n^2 + n + (3/2)}{2} + \mathrm{O}(1/c). \tag{18}$$

The theorem implies that when c is zero, or even when c is small compared to N, then the omitted terms of the prolate series are all approximately Legendre polynomials and the error is as bad as the Legendre error. Who would work with a basis of transcendental functions when polynomials, computable by three-term recurrence, are as accurate?

On the other hand, the asymptotic, large-degree approximations to the prolate expansion give us the following guidance in choosing c:

Theorem 5.3 (Prolate "Dead Zone"). *When the bandwidth $c > c_*(N)$ where the "transition bandwidth" is defined by*

$$c_*(N) \equiv (\pi/2)(N + 1/2) \tag{19}$$

then all modes $\psi_n(x; c), n = 0, 1, 2, \ldots, N$ included in the truncated series are exponentially small in a neighborhood of $x = \pm 1$. It follows that it is stupid to choose $c > c_*(N)$ for a given N because then the truncated series cannot approximate a general function $u(x)$ over the entire interval, $x \in [-1, 1]$, but rather fails in this "dead zone" near the endpoints.

Proof. The asymptotic expansions given by [38,41]. Fig. 3 is a visual proof. □

The same point is made by the following theorem, which is a slight restatement of Theorem 5.3 of Chen et al. [20]:

Theorem 5.4 (Infinite order convergence of prolate functions). *Let $u(x)$ be a function in the Sobolev space $H^2[-1, 1]$ with the expansion*

$$u(x) = \sum_{n=0}^{\infty} a_n \psi_n(x; c). \tag{20}$$

Define a parameter

$$\rho \equiv c(N)/c_*(N) = c(N)/[(\pi/2)(N + 1/2)]. \tag{21}$$

Then for sufficiently large N,

$$|a_N| \leqslant D\left\{N^{-(2/3)s} \|u\|_{H^s[-1,1]} + (\rho[N])^{\delta N} \|u\|_{L^2[-1,1]}\right\}, \tag{22}$$

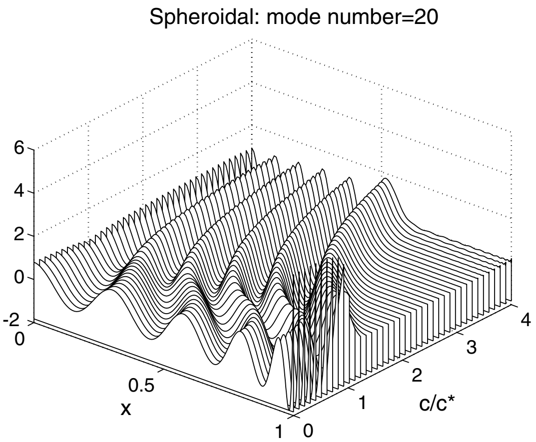

Fig. 3. A waterfall plot of $\psi_{20}(x; c)$ in the x–c-plane. The bandwidth has been scaled by dividing by $c_* = (\pi/2)(20.5)$ so that the transition point is at one in the scaled bandwidth. When $c/c_* > 1$, the prolate functions have WKB/Liouville–Green "turning points" for $|x_t| < 1$ where the eigenfunctions change from oscillation (inside the turning points) to exponential decay (for larger x), as confirmed by the asymptotic approximations. For $c = 0$ (foreground), $\psi_{20}(x; 0) = P_{20}(x)$. The eigenfunctions were scaled so that the maximum value at $x = 0$ is one.

where δ and D are positive constants. The constant s is a real-valued positive number, but is otherwise arbitrary; in practice, one would choose s as large as possible until the Sobolev norm H_s becomes unbounded. In particular, if u is analytic on $x \in [-1, 1]$, then one can take the limit $s \to \infty$ and the prolate coefficients of u converge faster than any finite inverse power of N ("infinite order convergence") provided that $\rho < 1$.

Proof. Chen et al. [20] state a similar theorem with ρ replaced by $q \equiv \sqrt{c^2/\chi_N}$, where χ_N is the Nth eigenvalue of the prolate differential equation. However, as shown in [16], $q = \rho/\sqrt{\omega(c;N)}$ where ω is a function that is: (i) always positive and (ii) asymptotes as $N \to \infty$ to a function $\Omega(\rho)$ which is *independent* of N. It follows that for sufficiently large N, q and ρ are proportional with a proportionality constant which is independent of N. □

The most important implication of the theorem arises when $c = c_*$; then $\Omega \approx 1$ so that $q \sim \rho \sim 1$. The theorem then does not require any decrease in the prolate coefficients as $N \to \infty$. This reinforces the conclusion that, when the prolate series is truncated at the Nth term, all useful choices of c satisfy the essential-for-accuracy inequality

$$\boxed{c < c_*(N)} \tag{23}$$

6. Numerical calculation of prolate functions

6.1. Solving the prolate differential equation

As shown by Bouwkamp [5], the prolate spheroidal wave equation can be converted into a symmetric, tridiagonal matrix by applying the Legendre–Galerkin method. Expand

$$\psi_j(x;c) = \sum_{j=0}^{M} B_{jk}\overline{P_k}(x). \tag{24}$$

The normalized Legendre polynomials (denoted by overbar) are defined in terms of the standard Legendre polynomials by

$$\overline{P_n}(x) \equiv P_n(x)\sqrt{n + 1/2}. \tag{25}$$

The standard Legendre polynomials can be computed by the recurrence

$$P_0 = 1, \quad P_1 = x, \quad P_{n+1}(x) = \frac{1}{n+1}\{(2n+1)P_n - nP_{n-1}\}. \tag{26}$$

The Legendre–Galerkin method [5,13] converts the differential equation into a matrix eigenvalue problem of the form

$$\vec{\vec{A}}\vec{b} = \chi\vec{b}, \tag{27}$$

where $\vec{b}$ is the column vector of Legendre coefficients, χ is the eigenvalue and the non-zero elements of the symmetric tridiagonal matrix $\vec{\vec{A}}$ are

$$A_{j,j-2} = c^2 \frac{j(j-1)}{(2j-1)\sqrt{(2j-3)(2j+1)}}, \tag{28}$$

$$A_{j,j} = j(j+1) + c^2 \frac{2j(j+1) - 1}{(2j+3)(2j-1)} - \chi, \tag{29}$$

$$A_{j,j+2} = c^2 \frac{(j+2)(j+1)}{(2j+3)\sqrt{(2j+5)(2j+1)}}, \quad j = 0, 1, 2, \ldots \tag{30}$$

The eigenvalues and eigenfunctions of a symmetric tridiagonal matrix can be computed very efficiently by the QR algorithm; the explicit code (in various languages) is given (TQLI) in [39,40].

Note that to accurately approximate N prolate functions, it is necessary to solve an $M \times M$ matrix problem where $M > N$. We recommend $M = 2N$ (at least); the acid test is to repeat the calculation with different M, and be satisfied only when the Legendre coefficients for the first N prolate functions are insensitive to M for sufficiently large M [11,13].

6.2. Grid points and quadrature weights

Pseudospectral and spectral element methods employ an associated grid. The choice of the optimum grid is controversial even in one dimension [12], but the conventional choice for orthogonal polynomials is the points of the associated Gauss–Lobatto quadrature. Xiao et al. [48] therefore advocated the same.

However, when the basis functions are no longer orthogonal polynomials, it is necessary to generalize the meaning of "Gaussian quadrature" [48]; note that these generalized definitions apply to an *arbitrary* basis set $\{\phi_j\}$ and not merely to prolate functions.

Definition 6.1 (*Generalized Gaussian quadrature*). An N-point quadrature formula is a Gaussian quadrature with respect to a set of $2N$ basis functions $\phi_0, \ldots, \phi_{2N-1}$ on an interval $x \in [a, b]$ with a weight function $\omega(x)$ if the formula is exact for each of the $2N$ integrals $I_n \equiv \int_a^b \phi_n(x)\omega(x)\,dx$, $n = 0, \ldots, 2N-1$.

In spectral elements, the endpoints are part of the grid. This requires a slight extension of Xiao et al.'s definition:

Definition 6.2 (*Generalized Gauss–Lobatto quadrature*). An N-point quadrature formula which includes the endpoints $x = a$ and $x = b$ as quadrature points is a Gauss–Lobatto quadrature with respect to a set of $2N-2$ basis functions $\phi_0, \ldots, \phi_{2N-3}$ on an interval $x \in [a, b]$ with a weight function $\omega(x)$ if the formula is exact for each of the $2N-2$ integrals $I_n \equiv \int_a^b \phi_n(x)\omega(x)\,dx$, $n = 0, \ldots, 2N-3$.

Because the Legendre polynomials have definite parity with respect to the origin, the quadrature points and weights for ordinary Legendre–Gauss and Legendre–Lobatto quadratures are symmetric with respect to $x = 0$. Boyd [17] shows that the prolate grid points and weights are also symmetric with respect to $x = 0$, which dramatically reduces the cost of computing the grid points and weights.

The task in Gauss–Lobatto quadrature is to choose the free grid points and the weights so that the integration residuals ρ_j are zero for $j = 0, \ldots, 2N-3$, where

$$\rho_j \equiv \int_{-1}^{1} \psi_j(x; c) - \sum_{k=1}^{N} w_k \psi_j(x_k; c). \tag{31}$$

If the grid points and weights are symmetric with respect to the origin, then the residuals of odd degree j are automatically zero because all the prolate functions of odd degree are antisymmetric with respect to the origin; the contributions from grid points $x_j > 0$ will exactly cancel those from $-x_j$, regardless of the numerical values of the grid points and weights.

The computational problem with symmetry is therefore reduced to the vanishing of the N residuals,

$$\rho_j = 0, \quad j = 0, 2, 4, \ldots, 2N-4. \tag{32}$$

If N is odd, $x=0$ is automatically a grid point; the unknowns are the location of the grid points on the interior of $x \in [0,1]$ plus the quadrature weights of these points and also the weights of $x=0$ and $x=1$. If N is even, then $x=0$ is not a grid point and the unknowns are the grid points on the interior of $x \in [0,1]$ plus their weights and the weight of the endpoint, $x=1$. For either N, there are always $N-1$ unknowns to be determined by solving (32).

If the prolate functions are expanded as Legendre series as in (24), then the exact integrals are

$$\int_{-1}^{1} \psi_j(x;c) = \sqrt{2} B_{j0}(c). \tag{33}$$

For fixed bandwidth c, the quadrature residuals are *nonlinear* in the grid points and quadrature weights w_j. It is therefore necessary to apply a Newton–Raphson iteration. For small c, the grid points and weights of the Legendre–Lobatto grid are a good initialization for the prolate iteration. The Legendre–Lobatto points and weights can be computed by using the short but complete software listings in [47, Matlab] and [19, Fortran].

For larger c, one can apply the continuation method as suggested in [21] or the improved initialization-by-extrapolation of [17].

The need to recompute the grid points and weights for *each* c is obviously an unpleasant complication compared to a basis of Legendre or Chebyshev polynomials. However, the grid-and-weight computation needs to be done only once even in a time-marching calculation of thousands of timesteps.

For pure "collocation" or "pseudospectral" methods, only the grid points x_j are needed. Chen et al. [20] experimented with what one may dub the "prolate-Lobatto" points, that is, choosing the x_j to be roots of $\mathrm{d}\psi_{N-2}/\mathrm{d}x$ plus $x = \pm 1$ – and reported little difference in performance from the Gaussian quadrature points.

6.3. Prolate cardinal functions

Spectral element methods, also known as p-type finite elements, commonly employ basis sets which are labeled by any of the following three interchangeable terms: "cardinal basis", "Lagrange basis" or "nodal basis". The cardinal functions are linear combinations of the orthogonal functions

$$C_j(x;c) = \sum_{m=0}^{N-1} C_{mj} \psi_m(x;c), \tag{34}$$

which are chosen so that the jth cardinal function is one at the jth grid point and is zero at all of the other grid points:

$$C_j(x_i;c) = \delta_{ij}, \tag{35}$$

where δ_{ij} is the usual Kronecker-delta function, equal to 1 if $i=j$ and zero otherwise. This property is very convenient for approximating the variational integrals of the spectral element method by an N-point numerical quadrature as explained in the standard texts [35]. It is easy to create a cardinal basis as we shall now describe.

Define a matrix $\vec{\vec{\Psi}}$ to store the grid point values of the prolate functions as the matrix elements

$$\Psi_{ij} = \psi_j(x_i), \quad i,j = 0,1,2,\ldots,(N-1). \tag{36}$$

Arrange the Legendre coefficients of the prolate eigenfunctions into a matrix $\vec{\vec{B}}$, where

$$\psi_j(x;c) = \sum_{k=0}^{M-1} B_{jk}(c)\overline{P_k}(x). \tag{37}$$

Define the grid point values of the Legendre polynomials as the $N \times M$ rectangular matrix $\vec{\vec{\mathscr{P}}}$

$$\mathscr{P}_{ij} = P_j(x_i), \quad i = 0,1,2,\ldots(N-1), \quad j = 0,1,2,\ldots,(M-1) \tag{38}$$

then

$$\vec{\vec{\Psi}} = \vec{\vec{\mathscr{P}}}\vec{\vec{B}}^{\mathrm{T}}. \tag{39}$$

In matrix form, substituting the expansion of the cardinal functions into the definition of the grid point values of the cardinal functions gives

$$\vec{\vec{\Psi}}\vec{\vec{C}} = \vec{\vec{I}} \;\Rightarrow\; \vec{\vec{C}} = \vec{\vec{\Psi}}^{-1}, \tag{40}$$

where $\vec{\vec{I}}$ is the identity matrix.

7. Convergence theory, I: trigonometric functions

7.1. Introduction: model functions

There is, alas, little theory for the rate of convergence of prolate series. In this section and the next, we employ a strategy justified in [13], which is to examine the rates of convergence of representative prototype functions. When these graphs and asymptotics are extended to other functions, the result will be a cloud of conjectures rather than a flock of theorems. But conjecture-making has always been a valid part of mathematics, and we shall at least understand the reasoning that led Xiao et al. [48] to assert that the prolate basis is superior to either Chebyshev or Legendre polynomials.

7.2. Analytic coefficients of exp (ikx)

The spectral coefficients of the series for $\exp(-\mathrm{i}kx)$ are known for Chebyshev, Legendre and prolate bases:

$$b_n^{\mathrm{Cheb}}(k) \equiv \frac{2}{\pi}\int_{-1}^{1} \exp(-\mathrm{i}kx)T_n(1-x^2)^{-1/2}\,\mathrm{d}x = 2i^nJ_n(-k), \tag{41}$$

$$b_j^{\mathrm{Legendre}}(k) = i^j\Gamma(1/2)\left(\frac{2}{k}\right)^{1/2}(j+1/2)J_{j+1/2}(k), \tag{42}$$

$$b_n^{\mathrm{prolate}}(k) = \lambda_n(c)\psi_n(k/c;c), \tag{43}$$

where λ_n is the eigenvalue in the following integral equation which is satisfied by the prolate functions [42]: $\int_{-1}^{1}\exp(\mathrm{i}cxy)\psi_n(y;c)\,\mathrm{d}y = \lambda_n\psi_n(x;c)$.

From the asymptotics of the Bessel functions, one can show that both the Chebyshev and Legendre coefficients oscillate until $n \approx k$ and then fall steeply as n increases further.

In contrast, it is known that the prolate integral equation eigenvalue $\lambda_n \sim \sqrt{2\pi/c}$ for $n < (2/\pi)c$ but falls exponentially for larger n. If the bandwidth parameter c is chosen to equal the wave number k, as we shall show below is optimum in the limit $n \to \infty$, then $\lambda_n(c = k)$ falls exponentially for $n > (2/\pi)k$. These asymptotics prove the following.

Theorem 7.1 (Resolution of exp(ikx)). *In the limit $k \to \infty$,*

1. *Chebyshev and Legendre polynomials: the minimum useful truncation is*

$$N = k \quad [\textit{Chebyshev/Legendre threshold}]. \tag{44}$$

2. *For prolate spheroidal series of* $\exp(-\mathrm{i}kx)$ *with bandwidth parameter c chosen to equal k, the minimum useful truncation is*

$$N = (2/\pi)k \quad [\textit{prolate spheroidal threshold}]. \tag{45}$$

Together, these thresholds show that one can accurately approximate a sinusoidal function with $(2/\pi)$ fewer prolate functions than are needed for either basis of orthogonal polynomials. This claim is justified only in the limit $N, k \to \infty$; for finite (N, k), the prolate advantage is smaller than a factor of $\pi/2$.

Fig. 4 illustrates the convergence of the prolate coefficients for trigonometric functions. When the truncation N is scaled by dividing by $(\pi/2)k$, the graph confirms that the coefficients begin to fall steeply at $N/[(2/\pi)k] = 1$. In the limit $N \to \infty$, the graph is a step function as indicated by the heavy dashed curve. (Similar diagrams for Chebyshev and Legendre polynomials are Figs. 3.7 and 3.8 of [32].)

7.3. The cosine error function

The errors in the expansion of cos(kx) can be completely described by the trivariate function

$$E^{\cos}(N, k, c) \equiv \left\| \cos(kx) - \sum_{j=0}^{N-1} a_n(k; c)\psi_n(x; c) \right\|_{\infty}. \tag{46}$$

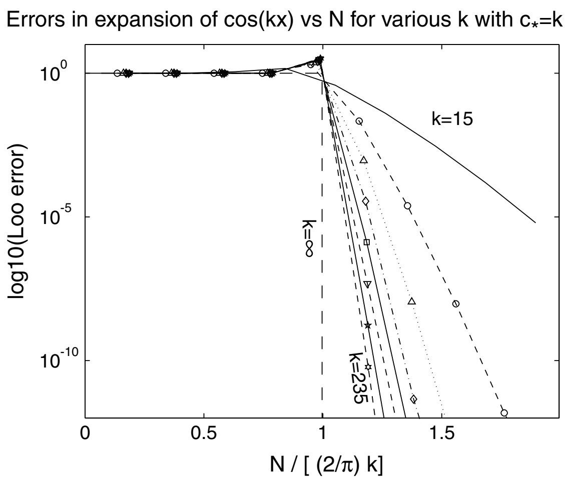

Fig. 4. Error in the expansion of cos(kx) versus N. The truncation N is scaled by dividing by $(2/\pi)k$. As N increases, the coefficients fall faster and faster when $N > (2/\pi)k$. The thick dashed curve shows the step function which is the asymptotic limit, $k, N \to \infty$.

A couple of scaling principles make it easier to visualize this three-dimensional function. First, the number of basis functions N must increase proportionately to k to obtain a reasonable approximation, i.e., "more wiggles $\rightarrow$ more basis functions" (Fig. 4). We therefore plot $E^{\cos}$ versus k/N (or equivalently, $k/c_*(N)$) because most of the dependence on N and k is through this ratio rather separately. Second, because of the special role of the transition bandwidth $c_*(N)$ in prolate theory, it is useful to plot the error function versus $c/c_*(N)$ rather than c.

Fig. 5 shows the contours of the logarithm of the error of the prolate expansion of $\exp(ikx)$ in the wave number-bandwidth plane for $N = 50$. The crucial point is that when $c = c_*(N)$, the error is O(1) for all wave numbers k. In other words, the obvious choice $c = c_*$ is *guaranteed to fail*. The best choice is to pick c to be perhaps one-half to two-thirds of $c_*(N)$ for moderate N; the ratio of c_{optimum}/c_* increases to one from below as $N \rightarrow \infty$.

Fig. 6 is similar to the preceding graph except that all the isolines are for the *same* error (10^{-6}) but for four different N, one of which is the limiting contour as $N \rightarrow \infty$. As N increases, the tops of all the error contours move closer and closer to the asymptotic limit, $c = c_*(N)$. Thus, the naive theory implied by the conjecture is true in the limit, but for *finite* N, some empirical correction to choose c smaller than $c_*(N)$ is desperately needed. A little crude curve-fitting yielded

$$\log(5E) \approx -1.2N\left\{1 - \frac{c}{c_*(N)}\right\} \;\leftrightarrow\; c(E;N) = c_*(N)\left\{1 + \frac{1}{1.2N}\log(5E)\right\}, \tag{47}$$

where E is the desired truncation error.

7.4. Anti-theorem: improvement in all wave numbers when $c > 0$

It would be highly desirable if one could make the broad statement: "in approximating $\exp(ikx)$, switching from Legendre polynomials to prolate spheroidal wavefunctions with some optimum $c(N)$ always improves the accuracy for all sufficiently small k for a given number of basis functions N". Unfortunately, this is not true as expressed by the following contradictory assertion:

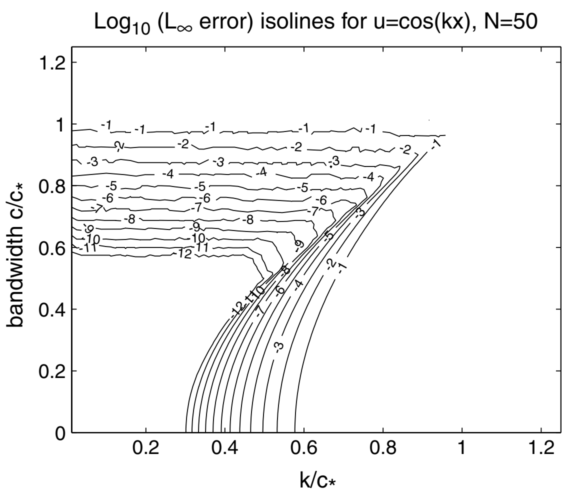

Fig. 5. Contours of the logarithm (base 10) of the maximum pointwise error (L_∞ error) for the expansion of $\cos(kx)$ as a 51 term prolate series, plotted in the k–c plane, where c is the prolate bandwidth. This is a fixed N plane through the three-dimensional parameter space spanned by (N, k, c).

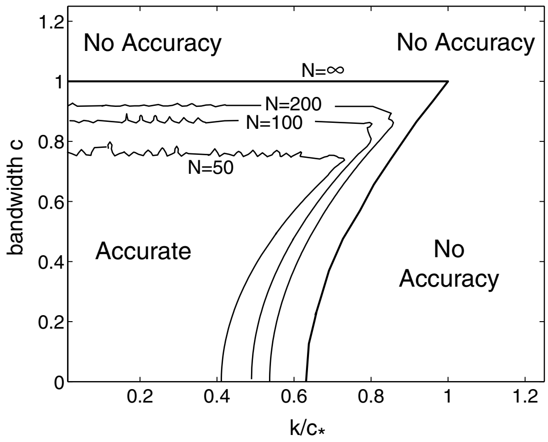

Fig. 6. The 10^{-6} isoline of the L_∞ error for the expansion of $\cos(kx)$ for four different N. Note that both the k and c axes have been scaled by $c_*(N)$.

Anti-Theorem 7.1. *In approximating* $\exp(ikx)$*, reduced error for moderate wave numbers k may be purchased at the price of* increased *error for* small *wave numbers.*

No analytical proof is known, but Fig. 7 clearly shows that the "anti-theorem" is true. The same message is carried by Fig. 6: the high accuracy contours, such as that for 10^{-12}, extend only to a bandwidth parameter (roughly $c/c_* \approx 0.6$) which is much smaller than the choice of bandwidth which is optimum for resolving a large number of wave numbers to an accuracy of 1/100 or better, which is $c/c_* \approx 0.9$.

It follows that if a function $u(x)$ has a Fourier transform that falls sufficiently fast, the prolate basis will be *worse* than Legendre. The prolate basis is most attractive for functions whose Fourier transform or series

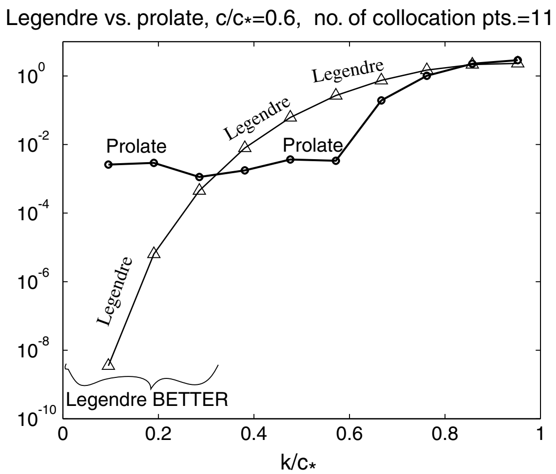

Fig. 7. Maximum pointwise errors for the approximation of $\cos(kx)$ for various k for 11-pt. Legendre collocation (thin curve with triangles) and prolate collocation with the same number of points and $c = 0.6c_*(N)$ (thick curve with black disks). For $k < c_*/3$, the Legendre basis is better.

is *broad* with a *slow* rate of decay; then, acceptable accuracy requires resolving as high a wave number k as possible, which the prolate basis does better than a Legendre series.

7.5. Connection with bandlimited functions

The superior properties of prolate spheroidal expansions of $\exp(\mathrm{i}kx)$ in at least some regions of the (k, N) plane is encouraging, but how can one extrapolate this to a broader class of functions? A partial answer is provided by bandlimited interpolation.

Definition 7.1 (*Bandlimited function*). A function $f^W(x)$ is said to be "bandlimited" of bandwidth W if it equals a Fourier integral with limits of integration that are not infinite but rather are $\pm W$

$$f^W(x) = \frac{1}{2\pi}\int_{-W}^{W} F(k)\exp(-\mathrm{i}kx)\,\mathrm{d}k, \quad x \in [-1, 1]. \tag{48}$$

Theorem 7.2 (Bandlimited approximation). *If $u(x)$ is analytic everywhere within the rectangle $\Re(x) \in [-1-\delta, 1+\delta] \otimes \Im(x) \in [-\delta, \delta]$ for some $\delta > 0$, then f can be approximated by a bandlimited function f^W of bandwidth W on $x \in [-1, 1]$ with error decreasing exponentially fast with bandwidth W [15].*

An explicit example is the "Lorentzian" or "Witch of Agnesi", discussed further in the next two sections, for which one can show that, with $a > 0$ a constant,

$$\left| \frac{1}{x^2 + a^2} - \frac{1}{2a}\int_{-W}^{W} \exp(-a|k|)\exp(-\mathrm{i}kx)\,\mathrm{d}k \right| \leqslant \exp(-aW)/a^2 \quad \forall \text{real } x. \tag{49}$$

A constructive proof that one can obtain similar bandlimited-approximation-with-exponential-accuracy is given in [15], but this notion of bandlimited approximation underlies a large part of signal-processing theory where windowed Fourier approximations are the very fabric of the field. Certainly Xiao et al. [48] were conceptualizing in terms of bandlimited approximation when they recommended prolate expansions for general $f(x)$ on a finite interval.

The good performance of prolate expansions for bandlimited functions is (partly) quantified by the following:

Theorem 7.3 (Fourier transform coefficient integral).

1. *Suppose $f(x)$ is a function, not necessarily bandlimited, with a Fourier transform $F(k) \equiv \int_{-\infty}^{\infty} f(x)\exp(\mathrm{i}kx)\,\mathrm{d}x$. Then the nth coefficient a_n of the prolate series for $f(x)$, $f(x) = \sum_{n=0}^{\infty} a_n \psi_n(x; c)$, where $a_n = \int_{-1}^{1} f(x)\psi_n(x; c)\,\mathrm{d}x$, can be written alternatively as*

$$a_n = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(-k) b_n(k)\,\mathrm{d}k, \tag{50}$$

where the b_n are the prolate or Legendre or Chebyshev coefficients of $\exp(\mathrm{i}kx)$ *as given by Eqs.* (41)–(43) *above.*

2. *If $f(x)$ is a bandlimited function of bandwidth W or less, which means that $|F(k)|$ is zero for $|k| > W$, then the coefficient integral is similarly bandlimited:*

$$a_n = \frac{1}{2\pi}\int_{-W}^{W} F(-k) b_n(k)\,\mathrm{d}k. \tag{51}$$

3. *The Chebyshev and Legendre coefficients $b_n(k)$ of a bandlimited function will fall supergeometrically $\forall |k| < W$ when*

$$\boxed{n > W} \quad [\textit{Chebyshev/Legendre threshold}]. \tag{52}$$

For prolate functions, if the bandwidth parameter c is chosen to equal W, the bandwidth of f(x), then the prolate coefficients fall exponentially for

$$\boxed{n > \frac{2}{\pi} W} \quad [\textit{Prolate threshold}]. \tag{53}$$

In other words, for bandlimited functions, prolate expansions are superior, by a factor of $\pi/2$, to Chebyshev and Legendre polynomials series at least in the limit $n \to \infty$.

Proof. Proposition 1: substitution of the Fourier representation of $f(x)$ into the integral for a_n, followed by substitution of the coefficients $b_n(k)$ for $\exp(ikx)$, Eq. (43), into the Fourier integral and simplification using the orthogonality of the prolate coefficients. (Note the replacement of k by $-k$.) Proposition 3 follows from the asymptotics of $b_n(k)$ as $n \to \infty$ for fixed k; when the thresholds are exceeded, the basis functions accurately approximate $\exp(-ikx)$ for all $k \in [-W, W]$. □

The reason for the qualifier "as $n \to \infty$" in the theorem is that when $n > n_{\text{threshold}}$, the coefficients fall off infinitely fast only when n is infinite.

7.6. Sinc function

The Whittaker cardinal function or "sinc" function is a good example for bandlimited functions because it has the most boring transform possible: a constant for all $k \in [-\pi, \pi]$ and zero for all larger $|k|$. The "sinc" is defined by

$$\text{sinc}(x) \equiv \frac{\sin(\pi x)}{\pi x}. \tag{54}$$

More generally, the function $\sin(bx)/(bx)$ is bandlimited with bandwidth b.

Fig. 8 shows that the error in a prolate expansion dives dramatically as soon as the bandwidth parameter c of the prolate basis is as large as the bandwidth of the sinc function. Unfortunately, the error rises steeply when the bandwidth parameter c becomes somewhat larger than the bandwidth of the sinc function. Once again, when $c = c_*(N)$, the prolate errors are much bigger than those of a Legendre series except for small N.

This graph illustrates the same phenomenon as shown in Fig. 7. When $c = 60$, for example, the prolate series is better than the Legendre series at resolving $\cos(60x)$ – but $\sin(30x)/(30x)$ has a bandwidth of only 30, and therefore has amplitude only in wave numbers between $k \in [-30, 30]$. For these low wave numbers, the Legendre expansion with 40 or more terms is more accurate.

The sinc function, with its one-or-nothing Fourier transform, is obviously special. However, it is typical of the Fourier transform of general functions in that the amplitude of the transform decays rapidly as $|k|$ increases, though the rate of decay is usually exponential rather than as a step function. For a function with rapid decay of its Fourier transform, the prolate expansion will be superior for the high wave numbers that have little amplitude, but inferior to Legendre for the small $|k|$ that contains most of the amplitude of the Fourier transform. This obviously is alarming.

7.7. Summary of bandlimited/prolate thinking

These examples and theory motivate the following "naive" prolate convergence theory. Choose k to be the largest wave number that can be accurately approximated by N functions, which is $c_*(N) = (\pi/2)$

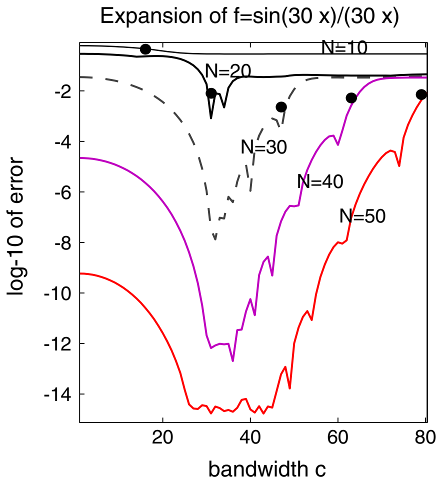

Fig. 8. L_∞ errors versus bandwidth c for prolate spheroidal expansions of $f = \sin(30x)/(30x)$ for various N. This sinc function is exactly bandlimited with a bandwidth of 30. The errors for the Legendre basis are the values of each curve at the left axis. The sharp minima in the error curves occur when the bandwidth parameter c of the prolate spheroidal basis functions matches the actual bandwidth of the sinc function; for a bandlimited function of bandwidth W, the best choice of c seems to be the bandwidth W. The heavy black dots denote the errors at $c = c_*(N)$. The fact that the dots are much higher (i. e., larger error) than the minima of the curves asserts that c must always be chosen *less than* $c_*(N)$.

$(N + 1/2)$. For large N, the prolate expansion with N basis functions will have negligible error for all $k \in [-c_*, c_*]$. Larger wave numbers will have $O(1)$ relative error, but because the error in approximating $f(x)$ by the bandlimited function $f^W(x; W = c_*(N))$ is exponentially small, so also will be the error caused by the inability of the prolate basis to approximate wave numbers $|k| > c_*$. For the Witch of Agnesi, for example, the approximation error for large N is proportional to $\exp(-a(\pi/2)N)$. For comparison, the error in a Chebyshev series (with small a) is $\exp(-aN)$ [13, Eq. (2.108), p. 57]. Thus, the asymptotic rate of convergence is $(\pi/2)$ greater than for the Chebyshev (or Legendre case), or to put it another way, we have gained 57% more digits of accuracy for the same truncation by switching to the prolate basis.

Unfortunately, this naive prolate convergence theory has a couple of defects. First, unlike the Witch of Agnesi, most functions on $x \in [-1, 1]$ do not have nice Fourier transforms; an unbounded function like $x^4/(x^2 + a^2)$ is an example. However, one can always find a so-called "windowed" function $\tilde{f}$ that approximates f accurately on $x \in [-1, 1]$, but has a well-behaved transform; a constructive proof is given in [15].

The second difficulty is that a bandlimited function is always an *entire* function whereas most solutions to differential equations have poles or branch points somewhere in the finite complex x-plane. In the next two sections, the complications of singularities are explained.

8. Darboux's principle: singularities control asymptotic rate of convergence

Singularities come in a bewildering profusion of simple poles, double poles, logarithms, fractional powers, etc. How can numerical experiments sort out all this complexity? A couple of general principles help.

Theorem 8.1 (Darboux's principle: singularities and convergence). *For all types of spectral expansions* (*and for ordinary power series*), *both the* domain *of* convergence *in the complex plane and also the* rate *of* convergence *are controlled by the* location *and* strength *of the* gravest singularity *in the complex plane. "Singularity" in this context denotes poles, fractional powers, logarithms and other branch points, and discontinuities of $f(z)$ or any of its derivatives.*

Each such singularity gives its own additive contribution to the coefficients a_n in the asymptotic limit $n \to \infty$. The "gravest" singularity is the one whose contribution is larger than the others in this limit; there may be two or more of equal strength.

For the special case of power series, this is "Darboux's theorem" [13], *Theorem 1, p. 32.*

In words, Darboux's principle means that it is unnecessary to experiment with functions that have lots and lots of singularities; it is always sufficient (for large N) to consider functions that have only a single pole or branch point. (In order to obtain real-valued models, it is often convenient to examine $f(x)$ which have a pair of singularities at locations that are complex conjugates.)

Theorem 8.2 (Location and type dependence). *The asymptotic spectral coefficients a_n for sufficiently large n decrease at a rate which is an* algebraic *function of the* type *of the singularity but an* exponential *function of the* location *of the singularity. For example, the coefficients of two functions that have (gravest) singularities at the same point in the complex plane, but one is a simple pole whereas the other is a logarithm, will differ by a factor proportional to n. In contrast, the coefficients of two functions with simple poles at different locations will usually differ asymptotically as $n \to \infty$ by a factor proportional to* $\exp(-qn)$ *for some constant q* [13, Chapter 2].

Both theorems are provably true for all known spectral expansions (Legendre, Hermite, Laguerre, Chebyshev, etc.) as well as for ordinary power series. However, there are two technical complications:

1. Neither theorem has been proved for prolate functions.
2. A *useful* proof for prolate functions must consider the simultaneous, "continuously adjusted" limit that N and c increase *together*.

The adjective "useful" is required because in the limit $N \to \infty$ for *fixed* bandwidth c, $\psi_N(x; c) \to P_N(x)$, and therefore the extension from the known Legendre theorems to the prolate basis is trivial in this "horizontal limit", as the fixed c limit was dubbed in Section 2. However, we reiterate that prolate functions are interesting only when they are *different* from Legendre polynomials, and this requires the "continuously adjusted" limit.

Darboux-ish thinking has other limitations illustrated in Fig. 9. This compares the spectral coefficients for three related functions:

$$f^{\mathrm{Witch}}(x; a) \equiv \frac{1}{x^2 + a^2} = \frac{1}{2a} \int_{-\infty}^{\infty} \exp(-a|k|) \exp(-\mathrm{i}kx)\, \mathrm{d}k \quad \text{[Witch of Agnesi]}, \tag{55}$$

the bandlimited-Witch

$$\begin{aligned} f^{\mathrm{bW}}(x; a, W) &\equiv \frac{1}{2a} \int_{-W}^{W} \exp(-a|k|) \exp(-\mathrm{i}kx)\, \mathrm{d}k \\ &= \frac{1}{x^2 + a^2} \left\{ 1 - \exp(-aW)[\cos(Wx) - \frac{x}{a} \sin(Wx)] \right\} \quad \text{[Bandlimited-Witch]} \end{aligned} \tag{56}$$

and their difference

$$\delta^{W}(x; a, W) \equiv f^{\mathrm{Witch}}(x) - f^{\mathrm{bW}}(x; W) = \frac{1}{a} \frac{\exp(-aW)}{x^2 + a^2} \{a \cos(Wx) - x \sin(Wx)\}. \tag{57}$$

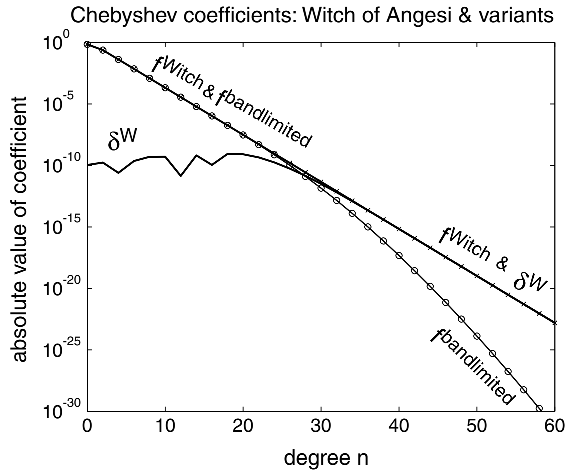

Fig. 9. Even degree coefficients for three related functions which are symmetric with respect to the origin: the Witch of Agnesi, $f^{\mathrm{Witch}} \equiv 1/(x^2 + a^2)$, the bandlimited-Witch function, f^{bW}, which is obtained by truncating the Fourier integral representation of the "Witch" to a bandwidth of $\pm W$, and the function δ^{W}, which is the difference between the other two. The coefficients are those of Chebyshev polynomial series, though the Legendre coefficients would differ only slightly. The parameters are $a = 1$ and $W = 20$ where a is the location of the poles of the Witch on the imaginary axis and W is the bandwidth of the bandlimited-Witch. The qualitative behavior is insensitive to a and W, but the numerical values of the transitions from one asymptotic regime to another do depend on these parameters.

In the limit $W \to \infty$, $f^{\mathrm{bW}}(x; a, W) \to f^{\mathrm{Witch}}(x; a)$:

$$\left\|\delta^{W}(x, a, W)\right\|_{\infty} = \frac{\exp(-aW)}{a^2}. \tag{58}$$

Thus, the difference between the Witch of Agnesi and its bandlimited approximation can be made arbitrarily small by taking W sufficiently large, and the maximum pointwise value of δ^W can equivalently be made as small as we please. However, a bandlimited function is always an entire function, as long as the Fourier integrand is in the class L_2, whereas f^{Witch} and δ^W have poles at $x = \pm ia$.

Nevertheless, the spectral coefficients of the large function f^{Witch} and the tiny function δ^W *asymptote* to one another as $n \to \infty$ because by construction, both functions have *identical* singularities in the complex x-plane. In another blow to over-reliance on asymptotics, the first 15 even coefficients of $\delta^W(x; a = 1, W = 12)$ are unaffected by the poles at $x = \pm\mathrm{i}$, but are instead less than 10^{-9} because the maximum value of δ^W for the given (a, W) is only 0.2×10^{-8}: asymptotic thinking must be applied only asymptotically. Similarly, the leading coefficients of the entire function, the bandlimited-Witch, are almost identical to those of the singular function, the Witch of Agnesi. For large degree, however, the coefficients of the bandlimited-Witch fall off supergeometrically, far faster than those of the two singular functions.

When the Witch of Agnesi is translated by a real constant s, the accuracy of its approximation by $f^{\mathrm{bW}}(x - s; a, W)$ is independent of the translation s:

$$f^{\mathrm{Witch}}(x - s; a) \equiv \frac{1}{[x - s]^2 + a^2} = \frac{1}{2a}\int_{-\infty}^{\infty} \exp(\mathrm{i}ks)\exp(-a|k|)\exp(-\mathrm{i}kx)\,\mathrm{d}k \tag{59}$$

since the translational factor in the Fourier integral representation, $\exp(\mathrm{i}ks)$, always has unit modulus. Nevertheless, the value of s has a profound effect on the rate of convergence of Legendre and prolate spheroidal series.

Thus, we have two reasons to be careful in using bandlimited approximations to estimate the relative performance of prolate versus Legendre expansions:

1. Except when $f(x)$ is an entire function, the *error* in bandlimited approximation ultimately controls the spectral coefficients a_n as $n \to \infty$, even though the error function (such as δ^W) may be made arbitrarily small for real x.
2. Bandlimited approximation is indifferent to translation whereas the spectral coefficients of a function $f(x-s)$ are in general very sensitive to s.

It follows that we are well-advised to examine the performance of prolate series for a singular functions, too.

9. Pole error function

Darboux's Principle and the Location and Type Dependence Theorems imply that it is unnecessary to explore all possible types of singular functions. Instead, the Witch of Agnesi (with translation) is a satisfactory model for all functions with singularities at finite x, but off the real interval $x \in [-1, 1]$. The singularities of the Witch of Agnesi are simple poles, but if we examined the prolate and Legendre series for a function with logarithmic singularities or double poles, the results would change only a little as made more precise in the theorem. If we compared the Witch of Agnesi to another function that had additional singularities farther from the expansion interval, again the differences would fall, in this case exponentially with degree, as $n \to \infty$.

It is convenient to define a real-valued function which has poles of unit magnitude at the conjugate points $x = s \pm \mathrm{i}a$:

$$u_{pole}(x; a, s) = -\mathrm{i}\left\{\frac{1}{x-(s-\mathrm{i}a)} - \frac{1}{x-(s+\mathrm{i}a)}\right\} = \frac{2a}{(x-s)^2+a^2}. \tag{60}$$

We then define the four-parameter error function

$$E^{\mathrm{pole}}(N, c; a, s) \equiv \left\| u_{pole}(x, a, s) - \sum_{j=0}^{N-1} a_n(k; c)\psi_n(x; c) \right\|_{\infty}. \tag{61}$$

It is impossible to depict a four-dimensional function in our three-dimensional world, but there are some powerful simplifications.

First, the isosurfaces of error for different truncations N are all similar in shape: as N increases, a given error isosurface migrates to smaller a, meaning that a larger number of prolate functions can achieve the same accuracy when the poles are closer to the real axis. Thus, showing a fixed-N slice through the four-dimensional parameter space will provide most of the information we want.

Second, the dependence on the translational parameter s turns out to be rather simple: $s = 0$, where the poles are the imaginary axis, is always the hardest case. When $s = \pm 1$ [i.e., poles near endpoints ± 1], the errors are much smaller, but there is a qualitative change, too: the prolate basis has no advantage over the Legendre polynomial expansion, or in other words $c = 0$ is optimum when $|s| = 1$. (The reason is intuitively obvious: the Legendre–Lobatto grid has a high density of points near $x = \pm 1$, precisely the points on the real axis which are nearest the poles of $u_{\mathrm{pole}}(x; a, \pm 1)$; when $c > 0$, the grid points migrate towards the center of the interval, away from the singularities, and the error of a truncated series increases.)

Consequently, it is sufficient to show two-dimensional slices in the *c*–*a* plane for fixed truncation N and for the two extreme cases of the translational parameter s: $s = 0$ and $s = 1$, as done in Fig. 10. For $c = 0$, the Legendre polynomial case which is the lower edge of each contour plot, the isolines are nearly vertical,

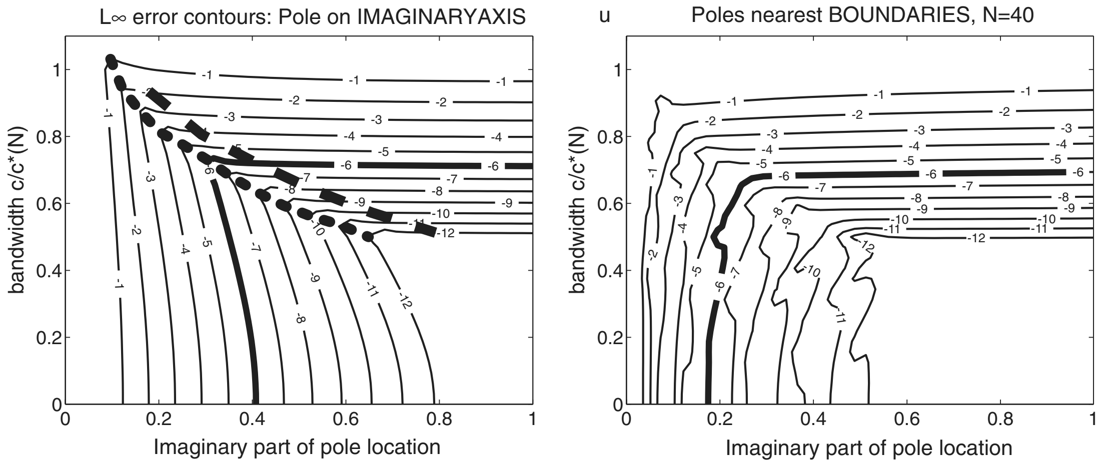

Fig. 10. Contours of the base-10 logarithm of the maximum pointwise error in the approximation of the function u_{pole} by the prolate functions $\{\psi_0(x;c),\ldots,\psi_{40}(x;c)\}$, plotted versus a (horizontal axis; denotes the imaginary part of the location of the poles) and the prolate bandwidth parameter $c/c_*(N=40)$ (vertical axis). The bottom axis of the plot gives the errors for Legendre polynomial series (i.e., $c=0$). Left panel: $u_{\text{pole}}(x,N,0,a)=2a/(x^2+a^2)$ [poles on the imaginary axis]. The thick dotted contour contains points that have the smallest error for a given a, which is the distance of the poles from the real axis. The thick dashed contour connects points where the error is equal to the Legendre error. The graph shows that there is only a small margin of error in choosing c. Right panel: same but for the function $u_{\text{pole}}(x,N,1,a)+u_{\text{pole}}(x,N,-1,a)=2a/([x-1]^2+a^2)+2a/([x+1]^2+a^2)$, which has simple poles at $x=\pm 1\pm ia$. In both panels, the thick solid contour distinguishes the isoline where the L_∞ error is 10^{-6}. This contour is much farther to the right in the left panel, meaning that this accuracy can be achieved when the poles are closer to the real axis so as long as the poles are near the endpoints and not the center of the interval.

and the errors decrease as a, which gives the distance of the poles from the real axis, increases. This is in accord with common sense: the farther the singularities are from the real axis, the smaller the numerical challenge (and also, the smoother $u_{\text{pole}}(x)$ appears for real x). In the left panel, where the poles are on the imaginary axis, the error isolines bend leftward to smaller a – poles near the real axis – as c increases. This implies that the prolate series are able to resolve near-axis singularities *better* than Legendre polynomials. Hurrah! Prolate is better than Legendre, and not just for bandlimited functions!

9.1. Boundary-layer anti-theorem

Now for the bad news. First, the lack of any leftward movement in the contours in the right panel implies the following:

Anti-Theorem 9.1 (Universality/boundary layer). *The prolate spheroidal basis is* not *optimum for expanding all classes of analytic functions $u(x)$; in particular, it is inferior to Legendre or Chebyshev polynomials for approximating functions whose main numerical challenge is thin boundary layers or off-interval singularities close to* ± 1.

The reason that the prolate basis is counter-productive for a function with singularities near $x=\pm 1$ or more generally, for functions with boundary layers, is that when the major numerical challenge is near the endpoints, it is obviously desirable to have a high density of grid points near the endpoints – exactly as true of a Legendre or Chebyshev method. Because prolate expansions (for $c>0$) reduce the density of grid points near the boundaries compared to the Legendre grid, it is hardly surprising that prolate methods are *inferior* to Legendre for solutions with *boundary layers* or near-endpoint singularities.

9.2. Difficulty of choosing bandwidth parameter c

The second unpleasant development in Fig. 10 is that all the error isolines in turn sharply to become approximately horizontal, that is, parallel to the a-axis, for sufficiently large c. In all cases, the turn occurs for $c/c_*(N)$ less than one.

When the poles are on the imaginary x-axis (left panel), there is an optimum c that is nonzero as marked by the dotted line. The thick dashed line connects points where the error is equal to the Legendre polynomial error for the same value of a. Unfortunately,

1. The optimum c varies rather strongly with a, the distance of the poles from the real axis, so it is impossible to predict $c_{\text{optimum}}(a)$ accurately unless the distance of singularities in the complex x-plane is known in advance.
2. The thick dashed line is very close to the dotted line, implying that even a slight overshoot in the choice of c [relative to $c_{\text{optimum}}(a)$] will yield errors no better or perhaps worse than a Legendre expansion.

Since the location of complex-valued singularities of the solution to a nonlinear differential equation are almost never known a priori, the sensible strategy is to choose c *conservatively*, such as $c = c_*(N)/2$. However, the error will then be only *moderately* better than for Legendre polynomials.

9.3. The unimportance of translation

The errors are sensitive to the real part of s, the location of the singularities. However, as noted earlier, the worst case is always when the singularities are on the imaginary axis. If we apply prolate basis functions in a multidomain formulation to solve a differential equation or systems of equations, the various singularities are likely to be at rather random and unpredictable locations relative to each subdomain. If the prolate basis is employed for the spatial discretization of a time-dependent fluid flow, then the singularities will in fact move around over time. What happens then?

The answer is that the prolate basis is no better than Legendre for boundary layers or near-subdomain-wall singularities, but since near-endpoint poles are the easiest to resolve, the prolate basis will still give an accurate approximation. The maximum pointwise error over the global domain will be controlled by those singularities which are both close to the center of a subdomain, and also near the real axis. For this most difficult case of center-of-the-subdomain singularities, the prolate basis will be *superior* to the Legendre. Thus, the global accuracy of a multidomain spectral element method should be better with a prolate basis than with a Legendre basis.

The improvement will not be the $\pi/2$ factor per dimension predicted by the naive arguments given in the early sections because the practical difficulties of choosing c will reduce the rewards of a prolate basis. Further, although the prolate basis will be at least moderately superior to Legendre for flows with travelling fronts or other high-gradient interior features, the prolate basis is no better than Legendre for a flow with no structure except boundary layers.

But these exceptions are rare and numerically easy. Prolate functions are advantageous for complicated, challenging problems where it is important to wring every bit of performance from a given number of grid points.

10. Prolate element method: theory

When the order of the polynomials in a finite element method is sufficiently high (sixth or higher order, though "higher" is always defined somewhat arbitrarily), the algorithms are most efficiently implemented using the technology of spectral methods. The resulting schemes are then called "spectral elements" [24,35] or "*p*-type finite elements". The critical feature is that spectral elements employ the Legendre–Lobatto grid in combination with Legendre–Lobatto cardinal functions.

Therefore, to change basis to prolate spheroidal functions, it is merely necessary to

1. Replace the vectors that store the Gauss–Lobatto quadrature points and weights.
2. Replace the matrices that store the derivatives of the cardinal functions at the Gauss–Lobatto points.

Otherwise, the prolate spectral element method is *identical* to the Legendre spectral element.

11. Prolate element method: numerical example

To illustrate this, we took an existing spectral element code in Matlab, and converted it to a prolate spheroidal method by changing the numbers in the two arrays and one (first derivative) matrix described above. The techniques for computing the grid points and prolate cardinal functions were described in Section 4.

The problem is only a humble second order linear boundary value problem, solved on a single domain. There is not a lot of point in multiplying examples because the *mechanics* of the prolate spectral element algorithm are identical to the Legendre spectral element algorithm except for the change of basis. The success or failure of the switch therefore hinges entirely on the faster convergence of the prolate spheroidal basis as explained with many illustrations above.

12. Time-marching and eigenvalues of derivative matrices

Chen et al. [20] have performed an independent analysis of prolate spectral methods, focusing on time-dependent partial differential equations. Because of the thoroughness with which they analyze first order hyperbolic PDEs, our discussion of timestep limits will be brief.

When the spatial discretization is a Legendre or Chebyshev spectral method, the resulting system of ODEs in time is very "stiff", that is, has a maximum stable timestep which is extremely small. For a second order (in space) PDE such as the diffusion equation, the maximum stable timestep is $O(N^{-4})$. In contrast, a second order finite difference discretization would have a timestep limit proportional to $1/N^2$. Xiao, Rokhlin and Yarvin claim [48] that a prolate basis can split the difference with a maximum stable timestep which is $O(1/N^3)$. The timestep limit is the inverse of the largest eigenvalue of the spatial differentiation matrix, so an equivalent statement is that the largest eigenvalues of the second derivative discretization matrix are $O(N^2)$ for finite differences, $O(N^3)$ for prolate and $O(N^4)$ for Legendre.

Unfortunately, the prolate basis does less well than claimed by Xiao, Rokhlin and Yarvin. Chen et al. [20] have noted that for hyperbolic equations at least, the stability limit is improved by imposing boundary conditions using a penalty method instead of the usual strategy of a strong constraint. Although penalty boundary conditions have a variety of attractive features, it is unfortunate that one must change the boundary condition algorithm just to maximize the effects of changing the basis in an existing Legendre or Chebyshev code (see Fig. 11).

Furthermore, when c varies with the number of degrees of freedom N so that the ratio $\rho \equiv c(N)/c_*(N)$ is fixed, it is indeed possible to use a much larger timestep with the prolate basis than with the Legendre polynomial basis; equivalently, the prolate differentiation matrix eigenvalues grow more slowly with N than for Legendre. However, the ratio of the largest Legendre eigenvalue divided by the largest prolate eigenvalue exhibits two asymptotic regimes. For *small* N, the ratio is large, i.e., hurrah for prolate wavefunctions! For large N, however, the eigenvalue ratio *flattens* to a *constant*, as seen in Fig. 8 of Chen et al. [20]. The "breakpoint" between these two regimes is at very large N with ρ close to one, but as we have shown above,

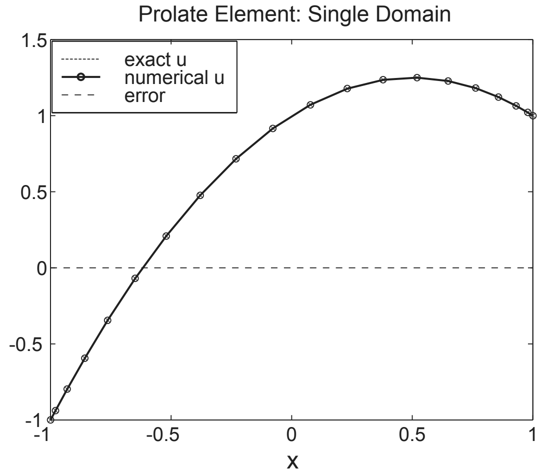

Fig. 11. $N = 20$ solution to $((1+x/2)u_x)_x - (4+x+x^2)u = x^4 + 2x^2 - 7x - (11/2)$ subject to the boundary conditions that $\sqrt{2}u_x(-1) + 2u(-1) = 3\sqrt{2} - 2$ and $\sqrt{2}u_x(1) + 2u(1) = 2 - \sqrt{2}$ with the exact solution $u = 1 + x - x^2$. The maximum pointwise error is 1.4E − 6.

accuracy is terrible when $c \approx c_*$. For smaller ρ, the approximation of $u(x)$ by an N-term prolate series is better, but unfortunately, the breakpoint then occurs for rather small N.

Fig. 12 illustrates that this same phenomenon arises for the second derivative matrix, as would arise in discretizing the diffusion equation, as opposed to the first order derivatives examined by Chen et al. [20]. The larger c/c_*, the longer before the ratio of Legendre to prolate eigenvalues asymptotes to a horizontal line. Indeed, for the highest ratio shown, $c/c_* = 0.95$, the flattening is literally off the plot.

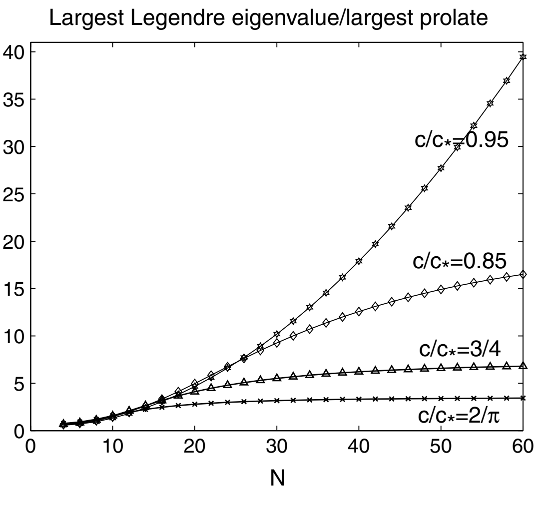

Fig. 12. Ratio of the largest eigenvalue of the second derivative collocation matrix (with homogeneous Dirichlet boundary conditions) for Legendre polynomials, divided by the largest eigenvalue for the corresponding matrix in the prolate basis. The bandwidth c was increased with N so as to keep the fixed ratio of $c(N)/c_*(N)$ which labels each of the four curves. The collocation points were the roots of $\mathrm{d}\psi_{N-2}/\mathrm{d}x$ plus the endpoints ± 1 or the Legendre–Lobatto grid. The maximum ratios of the eigenvalues for the second derivative matrix as shown in the graph are 3.5, 7, 17 and 41.

Once again, the most efficient use of the prolate basis requires a delicate dance – some careful tuning – to find an N-dependent and problem-dependent choice of c/c_* which simultaneously yields high accuracy but also a long timestep limit. The claim of an improvement of a factor of N for a second order PDE is not supported by the numerical results.

13. Summary: a new enhancement for the bleeding edge of arithmurgy

13.1. Desiderata or a theoretical and practical wish-list

This paper has only made a start on prolate spheroidal theory, building on the work of Xiao et al. [48]. Desired theoretical improvements include the following:

1. Explicit prolate coefficients for a function with poles or logarithmic singularities, such as $u_{\text{pole}}(x; s, a)$ whose properties were studied here only numerically.
2. Proof that Darboux's Principle applies to prolate series in the continuously adjusted limit ($(N, c) \to \infty$ simultaneously).
3. More detailed theory for asymptotic approximations for prolate coefficients in the continuously adjusted limit.
4. Publicly available libraries to compute the prolate functions, their derivatives, and the Gaussian quadrature points.
5. Prolate versus Legendre for a suite of difficult test examples.

The reason for the first wish is that for other basis sets, the theory of convergence is based on the asymptotic spectral coefficients of model functions with singularities. For prolate functions, we have only been able to evaluate the "pole error function" numerically. It would be more satisfying, at least mathematically, to have a formula for the prolate coefficients of the Witch of Agnesi similar to that for its Chebyshev coefficients.

The second wish is that Darboux' Principle, which we have implicitly relied upon in our analysis, is rigorously demonstrated for prolate functions. "Probably true" and "likely valid" are alarming words to a mathematician, and many an engineer and physicist have uttered them only to fall into the pit of genuine mistake.

The third wish is that for Chebyshev, Hermite, and Fourier series, it has been possible to build up a fairly complete theory of asymptotic approximations to the coefficients for various classes of functions using residues, steepest descent for integrals and so on. None of these powerful weapons has so far penetrated the mighty armor of prolate functions.

The fourth is fulfilled by the Matlab library in [17].

The fifth wish reflects the reality that the structure of the singularities for complex fluid flows and other interesting engineering and scientific solutions is not well-known. It is a truism among baseball players that even with the sophistication of modern pitching machines, practice in the batting cage is never the same as hitting in a big league game. The same is true in numerical analysis; the literature is littered with the tombs of algorithms that were heroic on simple problems but expired on all interesting applications. But such comparisons are beyond the scope of this already-rather-long paper.

13.2. Practicalities: research, one-offs, and operational supercomputing

Gottlieb et al. [20] obtained similar unimpressive improvements when the Legendre polynomial basis is replaced by prolate spheroidal wavefunctions of order zero. Nevertheless, there *is* some modest improvement.

There are three kinds of costs for employing the prolate basis:

1. Learning cost: the person-hours invested in learning the folklore of prolate functions and acquiring the necessary software.

2. Initialization/preprocessing costs: computing the prolate grid points, quadrature weights, and values of the basis functions and derivatives at the grid points.
3. Run-time costs: the each-and-every-time-step expenses.

To minimize "learning cost", we have developed a Matlab library, easily translated into other languages, which computes all these quantities for the prolate basis [17]. It is still necessary to learn a little bit about prolate functions, as reviewed here and in [17], but it is a one-article, once-in-a-lifetime expense.

It does take longer to calculate the prolate grid points, weights and derivatives than for the Legendre basis, but the preprocessing costs are so small – a fraction of a second on a workstation – that this preprocessing cost difference is negligible.

The run-time costs are the most significant. It is important to note, though, that because the substitution of prolate functions for Legendre polynomials is merely a change of basis, the operation count and programming complexity are *unchanged* by the switch in basis functions for a given number of grid points N. In other words, the run-time costs for the prolate and Legendre basis are *identical* for the same number of degrees of freedom N.

Thus, the prolate/Legendre battle is all about achieving a given accuracy with the smallest N, and here the prolate basis seems to have a modest advantage. To assess this, it is helpful distinguish between two limiting cases.

One extreme is the one-off, modest-scale research code. By this we mean that sort of a code that a scientist will write himself to solve a novel differential equation for a few cases on a workstation. For such computations, the switch from a Legendre to prolate basis would be a significant extra commitment of human resources even if the prolate basis functions and grid were computed using code from a publicly available library. An increase in resolution of perhaps 20% to 30% in each dimension, and perhaps an increase of a factor of two or three in timestep, would be insufficient to radically change the range of feasible problems. An all-night workstation calculation might be reduced, by switching to a prolate basis, to perhaps a two-hour calculation. But this is not terribly significant; "a good workstation never sleeps". Additional programming effort is a poor tradeoff for increasing the idleness of a workstation in the wee small hours of a morning; it is better to "program quick, let workstation compute all night".

The other extreme is represented by a numerical weather prediction code. At present, the global model of the National Center for Environmental Prediction is spectral, but at least three major spectral element models for either atmosphere or ocean have been developed [31,33,43,44].

Weather prediction models are normally run at least once a day on a state-of-the-art, multimillion dollar supercomputer. Typically, the resolution is changed only at intervals of a thousand days or so. Doubling resolution or timestep is equivalent to buying another ten million dollars of hardware. It follows that it is exceedingly worthwhile to make a dozen test runs to optimize a numerical parameter such as the bandwidth parameter c for a given model and a given resolution even if the reward is only a factor-of-two improvement. The programmer cost will be amortized over a thousand production runs; the payoff is the equivalent of millions of dollars of chips.

The European Centre for Medium-Range Forecasting (ECMWF) spectral model, for example, incorporates several improvements whose rewards are more modest than the switch to a prolate basis. For example, a uniform latitude-longitude grid leads to a high density of grid points near the poles. The latest ECMWF model therefore implements a "reduced grid" which selectively deletes points near the poles [34]. Although the cost reduction is only about 30% and the programming effort was non-trivial because the reduced grid voids the simple structure of a tensor product grid, the results were considered well worth the cost. Because a prolate basis would require only changing the grid points, and not the logical structure of the method, it would require less effort and yield a bigger payoff than the switch to a reduced grid.

Consequently, once a supercomputer spectral element code has been developed, it seems almost inevitable that it will be improved, modestly, by experimenting with a prolate basis. The enhancement will not succeed in all cases, and the payoff will be limited even when prolate basis is superior to Legendre. But it is very much the sort of tweak that is worthwhile at the "beta" stage just before the code goes into thousand-run production.

It follows that the prolate basis is unlikely to be useful for computing projects that are modest in programmer and execution time. However, the prolate basis could be literally worth millions in the opposite limit of very large, expensive-to-develop codes at the bleeding edge of supercomputing.

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