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THE EIGENVALUES OF SECOND-ORDER SPECTRAL DIFFERENTIATION MATRICES*

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Abstract. The eigenvalues of the pseudospectral second derivative matrix with homogeneous Dirichlet boundary conditions are important in many applications of spectral methods. This paper investigates some of their properties. Numerical results show that a certain fraction of the eigenvalues approximate the eigenvalues of the continuous operator very accurately, but the errors in the remaining ones are large. It is demonstrated that the inaccurate eigenvalues correspond to those eigenfunctions of the continuous operator that cannot be resolved by polynomial interpolation in the spectral grid. In particular, it is proved that π points on average per wavelength are sufficient for successful interpolation of the eigenfunctions of the continuous operator in a Chebyshev distribution of nodes, and six points per wavelength for a uniform distribution. These results are in agreement with the observed fractions of accurate eigenvalues. By using the characteristic polynomial, a bound on the spectral radius of the differentiation matrix is derived that is accurate to 2% or better. The effect of filtering on the eigenvalues is studied numerically.

Key words. spectral methods, differentiation matrix, polynomial interpolation, filtering, stability

AMS(MOS) subject classifications. 65M10, 65D05, 65D25, 65F15

1. Introduction. The second-order (pseudo-) spectral differentiation process can be described as follows:

(1) Interpolate the data at prescribed grid points $x_1, \cdots, x_{N-1}$ by a global polynomial $p(x)$, which may be additionally constrained to satisfy certain boundary conditions at x_0 and x_N;

(2) Differentiate the interpolant twice to obtain estimates $p''(x_j)$ of the second derivative of the data at each grid point.

This simple idea is the basis of spectral collocation methods for the numerical solution of partial differential equations, which have become prominent in the past decade ([8], [10]). Since the differentiation process is linear it can be described by an $(N-1)\times(N-1)$ matrix D^2_{SP}. This matrix is typically neither sparse nor symmetric, in contrast to the situation with finite differences, where the differentiation matrix on a uniform grid with spacing h is given by

$$D^2_{FD}=\frac{1}{h^2}\begin{pmatrix} -2 & 1 & & 0 \\ 1 & -2 & 1 & \\ & & \ddots & \\ 0 & & 1 & -2 \end{pmatrix}. \tag{1}$$

For reasons discussed below it is of interest to know the eigenvalues of these differentiation matrices. The eigenvalues of D^2_{FD} can be obtained analytically, but not those of D^2_{SP}. The purpose of this paper is to investigate the eigenvalues of D^2_{SP} both experimentally and theoretically.

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The principal reason why the eigenvalues of D_{SP}^2 matter is that they affect numerical stability. To solve the equation $v_t = v_{xx}$, even if only a steady-state solution is the ultimate goal, the space derivative may be approximated by spectral differentiation and the time derivative by a linear multistep or Runge–Kutta formula. This combination can be stable for a fixed time step Δt only if the eigenvalues of D_{SP}^2 lie in the stability region in the complex plane for the given time-integration formula with the given timestep. The important quantity here is the spectral radius $\rho(D_{SP}^2)$, defined as the maximum of the moduli of the eigenvalues of D_{SP}^2. For finite differences or finite elements the spectral radius of the differentiation matrix is typically of size $O(N^2)$, but for spectral methods on nonperiodic domains this figure becomes $O(N^4)$. The result is that explicit time integration formulas are subject to painfully restrictive stability conditions of the form $\Delta t = O(N^{-4})$. It is desirable to be able to determine accurately what these restrictions are, and what can possibly be done to get around them.

Tight stability restrictions can be avoided by the use of implicit time-integration formulas, and this brings us to a second application of eigenvalue analysis. To implement an implicit formula, a direct inversion of a dense matrix is very expensive, and one alternative, proposed by Orszag [17], is a solution by an iteration based on a finite difference preconditioner. The efficiency of such an iteration depends on how the preconditioner affects the eigenvalues of D_{SP}^2. Haldenwang et al. have shown that in certain problems it reduces the range of magnitudes of the eigenvalues from $O(N^4)$ to $O(1)$, making a Richardson iteration extremely fast [13].

A third and more obvious reason to study the eigenvalues of D_{SP}^2 is that if some of them lie in the right half-plane (with increasing real parts as $N \to \infty$), then the spectral approximation to the partial differential equation will be ill-posed regardless of the formula for time integration. Although this does not occur with the spectral grids in general use, we show below that it does happen if one tries to use equidistant points in a nonperiodic problem.

Eigenvalues of first-order spectral differentiation matrices have been studied by various authors. Dubiner has obtained asymptotic eigenvalue estimates [4]; Solomonoff and Turkel have proved that under certain circumstances all eigenvalues lie in the left half-plane [18]; Dubiner and Tal-Ezer have studied the difference between Chebyshev and Legendre grid points [4]; and various further results and experiments have been provided by Trefethen and Trummer [20] and Funaro [6], [7]. Here, again, spectral methods face the problem that outlying eigenvalues of size $O(N^2)$ lead to stability restrictions $\Delta t = O(N^{-2})$ where we would get $O(N^{-1})$ for finite differences or finite elements. The first-order case is problematic, because the continuous problem has no eigenvalues at all and the matrices involved are nearly defective, with the result that time-stability bounds based on eigenvalues and stability regions may give highly unrealistic indications of true ("Lax"-) stability [20].

Eigenvalues of second-order differentiation matrices, the subject of this paper, have received less attention. The most important result, due to Gottlieb and Lustman [9], is that the eigenvalues are real and negative and distinct for second-order differentiation in Chebyshev extreme points, or in any other set of points for which the pseudospectral approximation to the corresponding first-order hyperbolic model problem is stable. The second-order case is better behaved than the first-order one: the corresponding continuous problem does have eigenvalues, which match those of the spectral approximation to some degree, and the eigenvalues appear to be much less sensitive to rounding error. As a result we expect that the time-stability bounds that follow from this paper also correspond closely to Lax-stability bounds, and hence are directly applicable to stability questions for practical spectral computations.

It is worth noting why eigenvalue analysis is appropriate for analyzing spectral methods, since it is usually unnecessary for finite differences or finite elements. The reason is that finite difference and finite element formulas, being translation invariant or nearly so, have eigenvectors that are Fourier modes or close to them, so that stability questions largely reduce to the study of amplification factors (von Neumann analysis) and wave reflection at boundaries (GKS analysis). But for spectral calculations the eigenvectors are by no means known a priori, and until a more general theory is devised, we have to study them explicitly.

Spectral methods are commonly applied on several kinds of grids. For periodic problems, the points are equally spaced and the interpolant is a trigonometric polynomial, but as this case offers no mysteries we will not consider it. For nonperiodic problems, we will take $[-1, 1]$ as our standard space interval, with $x_0 = -1$ and $x_N = 1$ and boundary conditions

$$p(x_0) = p(x_N) = 0. \tag{2}$$

This means that the polynomial $p(x)$ described in the first paragraph is constrained to satisfy the conditions (2). We will consider four sets of collocation points $x_1, \cdots, x_{N-1}$:

Chebyshev extreme points:	$x_j = -\cos(j\pi/N)$,
Chebyshev points:	$x_j = -\cos((2j-1)\pi/2(N-1))$,
Legendre points:	$x_j = j$th zero of P_{N-1},
Equispaced points:	$x_j = -1 + 2j/N$,

where P_{N-1} is the Legendre polynomial of degree $N-1$. The Chebyshev points can also be described as the zeros of the Chebyshev polynomial T_{N-1}, and the Chebyshev extreme points are the extrema of T_N. The first three of these sets of points are all used in various applications; they all have nonuniform distributions in $[-1, 1]$ with density proportional to $1/\sqrt{1-x^2}$ as $N \to \infty$. Equispaced points are not used in practice, for good reasons: interpolants based on these points diverge rapidly as $N \to \infty$—even for arbitrarily smooth data, if rounding errors are present. We include equispaced points in the investigation because they give valuable perspective on the other cases.

Once the boundary conditions (2) and collocation points x_j are fixed, the differentiation matrix D_{SP}^2 is implicitly determined, but there are various methods of applying D_{SP}^2 computationally. For Chebyshev points, a fast implementation can be based on the FFT (see § 5). For other point distributions it is necessary to form the matrix explicitly and then multiply. To derive the matrix entries, note that the polynomial $p(x)$ of degree N that interpolates the values $0, u_1, \cdots, u_{N-1}, 0$ at $x_0, \cdots, x_N$ can be written as

$$p(x) = \sum_{j=1}^{N-1} u_j l_j(x),$$

where

$$l_j(x) = \prod_{\substack{k=0 \\ k \neq j}}^{N} \frac{(x - x_k)}{(x_j - x_k)}.$$

Differentiating p twice at $x = x_i$ gives

$$(D_{SP}^2)_{ij} = l_j''(x_i), \qquad i, j = 1, \cdots, N-1. \tag{3}$$

More computationally practical methods for deriving these entries can be found in [8], [19], and [11], where explicit formulas are given.

An outline of the paper is as follows. First, § 2 presents numerical experiments to summarize the properties of the eigenvalues and eigenvectors of D^2_{SP}. We find that a proportion $2/\pi$ of the eigenvalues are accurate approximations to those of the continuous problem, or $1/3$ in the case of equispaced points. The figure $2/\pi$ results from the fact that only this proportion of the eigenfunctions of the continuous problem—sine and cosine functions of various wave numbers—can be resolved by polynomial interpolation, i.e., have at least two points per wavelength in the center of the Chebyshev or Legendre grid. The larger $O(N^4)$ outliers lie far off the scale in our eigenvalue plots, which emphasizes what tight stability restrictions they give rise to.

Section 3 is devoted to obtaining estimates for the largest outlying eigenvalues by means of the characteristic polynomial, which for cases of practical interest is known exactly. A simple root bound theorem of Newton provides surprisingly tight upper bounds that come within 2% of the exact (computed) values (Fig. 4 and Theorem 1). These bounds can readily be applied to derive timestep conditions for explicit time integrators that will guarantee time stability, a derivation that users of spectral methods have usually carried out empirically.

Section 4 shows that the ratios $2/\pi$ and $1/3$ that appeared in the numerical experiments have a theoretical basis. The question considered is, how many points per average wavelength must a grid possess in order to interpolate a sine or cosine successfully, in the limit $N\to\infty$? The answers turn out to be π and 6 for Chebyshev/Legendre and equispaced grids, respectively (Theorem 2). (A different proof of the latter result is implicit in a paper by Budd [1].) Since the eigenfunctions of the continuous second-order differentiation operator are sines and cosines, this result leads to an explanation of the numbers $2/\pi$ and $1/3$.

Finally, § 5 considers the possibility of modifying spectral methods by low-pass filters designed to alleviate stability problems. By plotting the eigenvalues of a filtered differentiation matrix, we can get a quick indication of whether the filtering is likely to be successful. Our experiments suggest that none of the filters proposed so far achieve the desired end without an unacceptable loss of accuracy.

2. Numerical observations. The eigenvalues of the continuous second derivative operator, with zero boundary conditions at $x=\pm 1$, are defined by

$$D^2u(x)=\lambda u(x), \qquad -1\leqq x\leqq 1, \tag{4}$$

$$u(\pm 1)=0.$$

This problem is easily solved; the eigenvalues are

$$\lambda_k=-\frac{k^2\pi^2}{4}, \qquad k=1,2,3,\cdots \tag{5}$$

with the corresponding normalized eigenfunctions

$$u(x)=\begin{cases}\cos\left(\frac{1}{2}k\pi x\right), & k \text{ odd},\\ \sin\left(\frac{1}{2}k\pi x\right), & k \text{ even}.\end{cases} \tag{6}$$

The finite-difference discretization of (4) on an N-grid is

$$D^2_{FD}u=\lambda u, \tag{7}$$

where D_{FD}^2 is the order $N-1$ matrix defined in (1). The eigenvalues of this problem are equally easy to obtain; see, e.g., [16, p. 50]. They are given by

$$\lambda_k = -N^2 \sin^2\left(\frac{k\pi}{2N}\right), \qquad k=1, \cdots, N-1, \tag{8}$$

with the corresponding eigenvectors

$$u_j = \begin{cases} \cos\left(\frac{1}{2}k\pi x_j\right), & k \text{ odd}, \\ \sin\left(\frac{1}{2}k\pi x_j\right), & k \text{ even}. \end{cases} \tag{9}$$

Notice that these eigenvectors are exact discretizations of the eigenfunctions (6) for the continuous problem, but that only the eigenvalues smallest in magnitude are approximated accurately. The error in λ_1 is $O(h^2)$, whereas λ_{N-1} is too small by the factor $4/\pi^2$ in the limit $N \to \infty$. Nevertheless, the spectral radius satisfies $\rho(D_{FD}^2) = O(N^2)$ as $N \to \infty$. Therefore the time-stability restriction for a typical explicit time integration scheme is $\Delta t \leqq O(N^{-2})$. In Fig. 1(a) the eigenvalues (8) of the finite-difference method are compared graphically with the eigenvalues (5) of the continuous problem.

Turning to spectral methods, we consider the matrix D_{SP}^2 defined in (3). The numerically computed eigenvalues of D_{SP}^2 for collocation at Chebyshev extrema are shown in Fig. 1(b). All of them are real, distinct, and negative, as has been proven by Gottlieb and Lustman [9]. Observe that the eigenvalues that are small in magnitude are spectrally accurate approximations to those of the continuous problem. (The spectral accuracy can be proved by the techniques of Calogero [2].) We refer to these eigenvalues as "inliers," in contrast with the remaining "outliers," the eigenvalues which do not approximate those of the continuous problem to any degree. The largest outliers grow explosively as $O(N^4)$, lying far off-scale in our plot (roughly 24 times the scale of the vertical axis!), and this restricts the timestep in typical explicit integration schemes to $\Delta t \leqq O(N^{-4})$.

The eigenvalues of Fig. 1(b) appear in approximate pairs. The reason for this is that the corresponding eigenfunctions occur in pairs of odd and even functions, as will be made clearer in equations (13), (15), and (17) of the next section.

Numerical calculations of this kind show that the proportion of eigenvalues that are inliers approaches $2/\pi$ as $N \to \infty$; the dashed line in Fig. 1(b) represents the value $k = (2/\pi)N$. (Haldenwang et al. have pointed out previously that the proportion of inliers appeared to be close to 2/3 [13].) The intuitive explanation of this critical value is simple. For $k > (2/\pi)N$, the sines and cosines that would be eigenfunctions for the continuous problem have fewer than two points per wavelength in the center of the Chebyshev mesh, i.e., they cannot be resolved by polynomial interpolation. The nonresolution of the higher eigenfunctions can be observed in Fig. 2, where selected eigenvectors of D_{SP}^2, based on Chebyshev extrema, are plotted. The eigenvectors corresponding to inliers are sines and cosines to a good approximation, but the eigenvectors corresponding to outliers are dominated by large oscillations near the boundary.

A more rigorous explanation of the critical value $k = (2/\pi)N$ is due to Gottlieb and Orszag [10, p. 35]. They consider the Chebyshev expansion of $\sin\left(\frac{1}{2}k\pi x\right)$, rather than interpolation, and show that the error decreases exponentially only if the degree of the expansion is larger than $\frac{1}{2}k\pi$. In § 4 we show that $k \leqq (2/\pi)N$ is indeed a sufficient condition to resolve $\sin\left(\frac{1}{2}k\pi x\right)$ or $\cos\left(\frac{1}{2}k\pi x\right)$ by polynomial interpolation of degree N on Chebyshev or Legendre grids. Numerical evidence of this result has been presented by Solomonoff and Turkel [18].

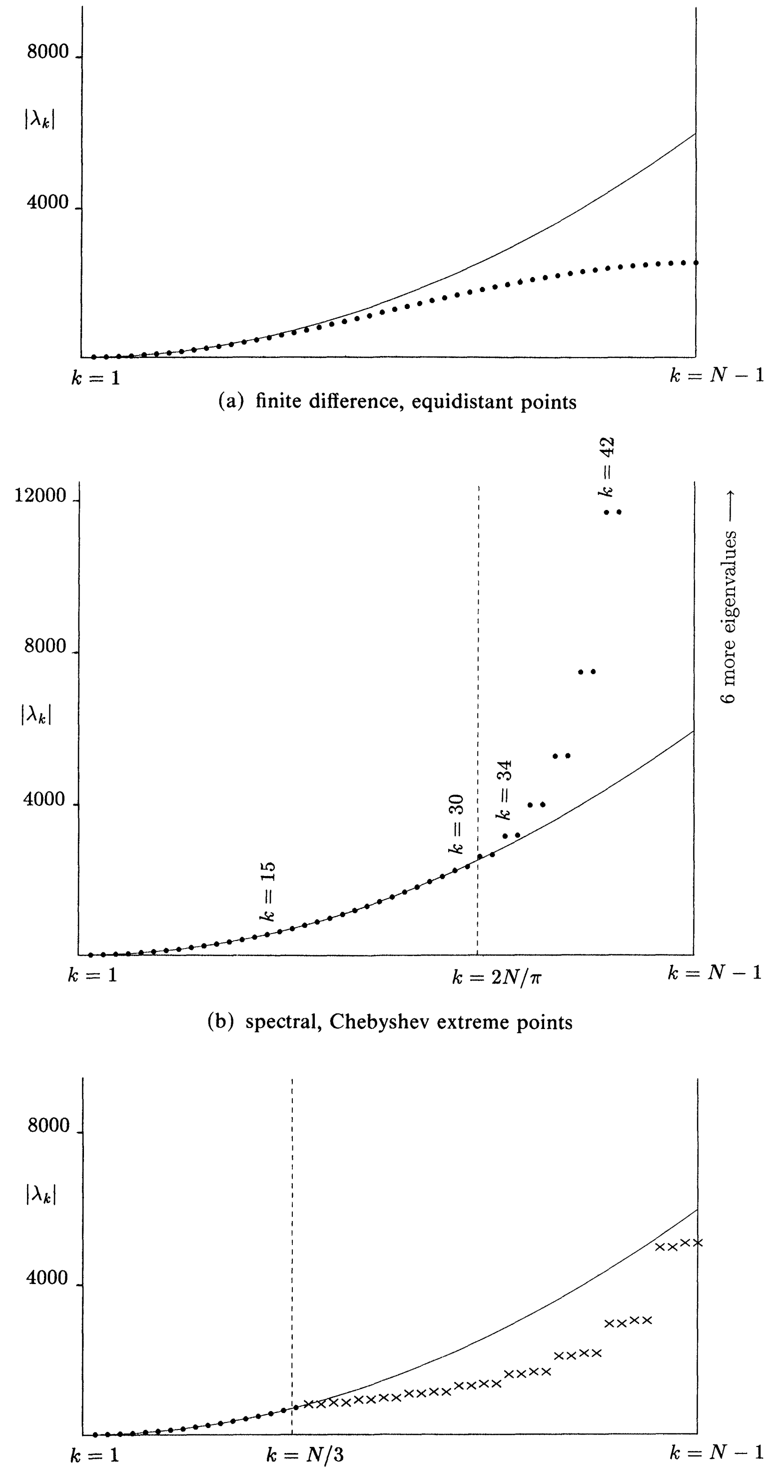


FIG. 1. *Eigenvalues of three second-order differentiation matrices with* $N = 50$ *compared with eigenvalues of the continuous problem* (4) (*located on the solid line*). *Crosses denote moduli of complex eigenvalues.*

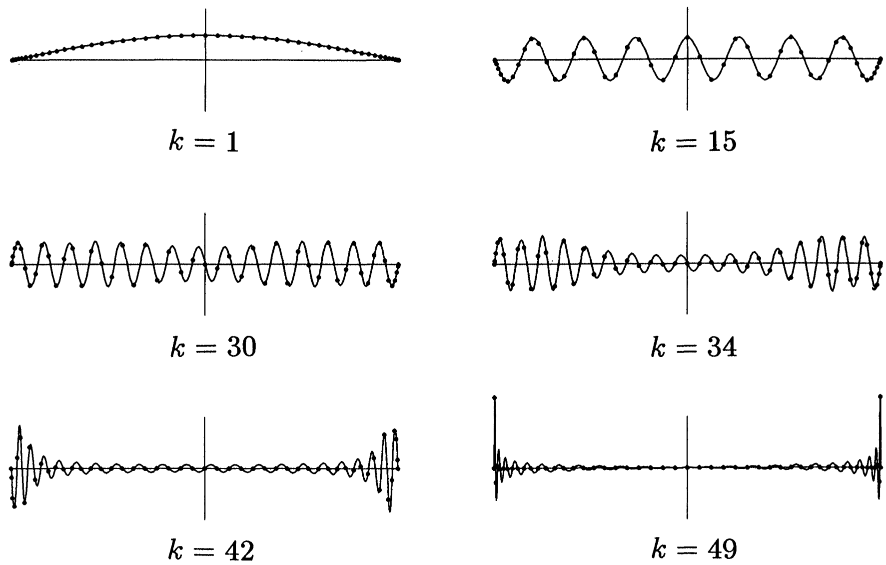


FIG. 2. *Selected eigenvectors of D^2_{SP}, based on Chebyshev extrema, for $N = 50$. The continuous line represents the polynomial interpolant. The corresponding eigenvalues are marked in Fig.* 1(b)

A naive way to get rid of the outliers is to replace the Chebyshev or Legendre meshes by a uniform mesh; there are then at least two points per wavelength for all the eigenfunctions to be approximated. Although this change indeed reduces the spectral radius to $O(N^2)$, the outliers turn out to be complex, as indicated in Fig. 1(c). Moreover, for N sufficiently large, some of the eigenvalues are located in the right half-plane, rendering the semidiscretization unstable. Figure 3 shows the eigenvalue locations in the case $N = 50$. Only one third of the eigenvalues are inliers (see Fig. 1(c)), suggesting that six points per wavelength are needed to resolve sines and cosines on equidistant points. We return to this observation in § 4.

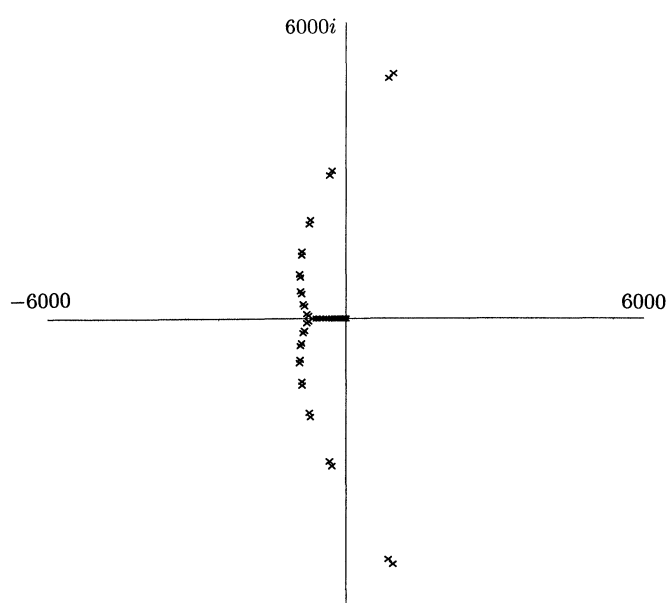


FIG. 3. *Eigenvalues in the complex plane of D^2_{SP} based on equidistant points.* $N = 50$.

The discussion of this section was for the most part based on results for Chebyshev extrema, but the qualitative results concerning inlying and outlying eigenvalues remain the same for collocation in Chebyshev or Legendre zeros. The constant factors in the spectral radius do change, however, and we will now estimate them by considering the characteristic polynomial of D^2_{SP}.

3. Estimates based on the characteristic polynomial. A curious feature of spectral differentiation matrices is that although their eigenvalues are for the most part unknown, the coefficients of the associated characteristic polynomials can be determined exactly. In this section we make use of these coefficients to derive bounds on the largest and smallest eigenvalues of D^2_{SP} that are accurate to within a few percent. We simplify the notation by assuming that N is an even number.

To derive the characteristic polynomial for D^2_{SP}, we follow the ideas of Gottlieb and Lustman [9]. Let the components of each eigenvector be viewed as the nodal values of some polynomial $u_N(x)$ that satisfies the boundary conditions. The eigenvalues are then determined by

$$\begin{aligned} D^2u_N(x_j) &= \lambda u_N(x_j), \qquad j=1,\cdots,N-1,\\ u_N(\pm 1) &= 0, \end{aligned} \tag{10}$$

where D^2 is the continuous second derivative operator. This equation holds at the gridpoints, but we can interpret it as valid for all $x \in [-1, 1]$ if we add a suitably chosen polynomial of degree N that is zero at $x_1, \cdots, x_{N-1}$:

$$D^2u_N(x) = \lambda u_N(x) + (A+Bx)f_{N-1}(x), \qquad -1 \leqq x \leqq 1. \tag{11}$$

The appropriate choices are

$$f_{N-1}(x) = \begin{cases} T'_N(x) & \text{(collocation at Chebyshev extrema)},\\ T_{N-1}(x) & \text{(collocation at Chebyshev zeros)},\\ P_{N-1}(x) & \text{(collocation at Legendre zeros)},\\ \prod_{j=1}^{N-1}(x+1-2j/N) & \text{(collocation at equidistant points)}, \end{cases} \tag{12}$$

with A and B to be determined by the boundary conditions.

Since the solution to the homogeneous problem associated with (11) is not a polynomial in x, the general solution to (11) is given formally by

$$\begin{aligned} u_N(x) &= (D^2-\lambda)^{-1}(A+Bx)f_{N-1}(x)\\ &= -A\lambda^{-1}L(f_{N-1}) - B\lambda^{-1}L(xf_{N-1}), \end{aligned} \tag{13}$$

where L is the linear operator defined by

$$L = \sum_{k=0}^{N/2} \lambda^{-k}D^{2k}. \tag{14}$$

(We have assumed that all eigenvalues are nonzero, which follows from (11) since polynomials of exact degrees $\leqq N-2$ and $\geqq N-1$ cannot be equal.) Enforcing the boundary conditions $u_N(\pm 1) = 0$ in (13) yields

$$AL(f_{N-1}) + BL(xf_{N-1}) = 0 \quad \text{at} \quad x = \pm 1. \tag{15}$$

For A and B to be nontrivial we must have

$$L(f_{N-1})|_{x=1}L(xf_{N-1})|_{x=-1} - L(f_{N-1})|_{x=-1}L(xf_{N-1})|_{x=1} = 0. \tag{16}$$

Under the assumption that N is even, f_{N-1} is odd and xf_{N-1} is even, which implies that $L(f_{N-1})$ is odd and $L(xf_{N-1})$ is even. Therefore (16) reduces to

$$L(f_{N-1})|_{x=1}L(xf_{N-1})|_{x=1} = 0, \tag{17}$$

that is,

$$\sum_{k=0}^{N/2-1} a_{N-2k-2}\lambda^k = 0 \quad \text{or} \quad \sum_{k=0}^{N/2} b_{N-2k}\lambda^k = 0, \tag{18}$$

where

$$a_k := D^k(f_{N-1})|_{x=1}, \qquad b_k := D^k(xf_{N-1})|_{x=1} = a_k + ka_{k-1}. \tag{19}$$

The characteristic equations (18) provide the $N-1$ eigenvalues of D^2_{SP}.

Gottlieb and Lustman proceed to prove that for Chebyshev extreme points the eigenvalues are real, distinct, and negative, in accordance with the numerical observations reported in § 2. The proof is based on the theory of Hurwitz polynomials and relies on the fact that the eigenvalues of the corresponding first-order differentiation matrix lie in the left half-plane. Their theorem can be extended to cover the case of Legendre zeros, since the eigenvalues of the corresponding first-order differentiation matrix are all located in the left half-plane (see [8]). The theorem presumably applies to Chebyshev zeros too, as was confirmed numerically. However, it does not apply to equidistant points; numerical evidence of complex eigenvalues is presented in Fig. 3.

Having obtained the characteristic polynomials (18), we can derive bounds on the moduli of the eigenvalues by a number of methods. Two well-known possibilities are the Gershgorin circle theorem (applied to the companion matrices of (18)) and the Eneström–Kakeya theorem. (Funaro [7] and Trefethen and Trummer [20] have applied estimates of this kind to first-order differentiation matrices.) However, neither of these theorems provides particularly sharp bounds in the present problem. Instead, we utilize the a priori knowledge that all eigenvalues are real to employ the root bound theorem of Newton, which states that the roots of the polynomial $\lambda^m + c_1\lambda^{m-1} + \cdots + c_m = 0$ satisfy the following, provided that all of them are real:

$$|\lambda| \leqq \sqrt{c_1^2 - 2c_2}. \tag{20}$$

Proof. If $\lambda^m + c_1\lambda^{m-1} + \cdots + c_m = (\lambda - \lambda_1)\cdots(\lambda - \lambda_m)$, then $\lambda_1^2 + \cdots + \lambda_m^2 = (\lambda_1 + \cdots + \lambda_m)^2 - 2(\lambda_1\lambda_2 + \cdots + \lambda_{m-1}\lambda_m) = c_1^2 - 2c_2$. This lesser-known bound possesses a much better overestimation factor than the other methods quoted, as shown by van der Sluis [21].

To apply (20) to (18), explicit expressions for a_k and b_k are required. In the cases of Chebyshev or Legendre points, these can be obtained by differentiation of the Chebyshev or Legendre differential equations, as has been demonstrated by Funaro [7]. It is harder to derive expressions for a_k and b_k in the case of equidistant points, since no corresponding differential equation exists. However, even if the a_k and b_k could be computed explicitly, the fact that complex eigenvalues are present precludes the use of (20), and a less accurate root bound formula would have to be used. For these reasons equidistant points are excluded from the remainder of this section.

We can now derive upper bounds on the eigenvalues of D^2_{SP} by applying (20) to (18), and lower bounds by the same method after setting $\mu = \lambda^{-1}$. This yields

$$-\left(\frac{a_2^2}{a_0^2} - \frac{2a_4}{a_0}\right)^{1/2} \leqq \lambda_k \leqq -\left(\frac{a_{N-4}^2}{a_{N-2}^2} - \frac{2a_{N-6}}{a_{N-2}}\right)^{-1/2}, \tag{21}$$

$$-\left(\frac{b_2^2}{b_0^2} - \frac{2b_4}{b_0}\right)^{1/2} \leqq \lambda_k \leqq -\left(\frac{b_{N-2}^2}{b_N^2} - \frac{2b_{N-4}}{b_N}\right)^{-1/2}. \tag{22}$$

Equation (21) applies to roughly half of the eigenvalues (corresponding to the first equation in (18)), and (22) to the other half. The entire spectrum of D^2_{SP} is therefore located between the minimum of the left-hand sides of (21) and (22) and the maximum of the right-hand sides.

As an example, consider the case of collocation in Chebyshev extrema. From [10, p. 159], we have

$$D^k(T_N)_{x=1} = \prod_{l=0}^{k-1} \frac{N^2-l^2}{2l+1}, \tag{23}$$

and so by (12), (19) becomes

$$a_k = \prod_{l=0}^{k} \frac{N^2-l^2}{2l+1}, \tag{24}$$

$$b_k = \left(\frac{N^2-k^2}{2k+1}+k\right) \prod_{l=0}^{k-1} \frac{N^2-l^2}{2l+1}. \tag{25}$$

Inserting these expressions into (21) and (22) yields the bounds

$$\begin{aligned} -\left(\frac{11N^8+90N^6-2037N^4+7360N^2-5424}{4725}\right)^{1/2} \\ \leqq \lambda_k \leqq -\left(\frac{720N^3-2880N^2+3600N-1440}{8N^3-32N^2+40N-61}\right)^{1/2}, \end{aligned} \tag{26}$$

$$\begin{aligned} -\left(\frac{11N^8+150N^6+2583N^4-10700N^2+7956}{4725}\right)^{1/2} \\ \leqq \lambda_k \leqq -\left(\frac{48N^5-192N^4+240N^3-96N^2}{8N^5-32N^4+40N^3-19N^2+24N-24}\right)^{1/2}. \end{aligned} \tag{27}$$

Analogous estimates for collocation in Chebyshev and Legendre zeros are derived in the Appendix.

These expressions provide surprisingly tight bounds on the spectrum of D_{SP}^2. For example, a bound on the spectral radius is given by the largest of the absolute values of the left-hand sides of (26) and (27), which in this case is (27), and in Fig. 4 this bound is compared with the actual (computed) spectral radius for $4 \leqq N \leqq 40$. For most of the values shown the discrepancy is less than 2 percent. The sharpness of these bounds provides indirect evidence that in contrast to the situation for first-order problems discussed in [20], the spectral radius here is probably not highly sensitive to rounding errors, so that time stability may be a good approximation to Lax stability. The reason is that a computation with rounding errors will be equivalent to an exact computation involving a slightly perturbed matrix, and if the characteristic polynomial of that matrix has only slightly perturbed coefficients, then its eigenvalues must satisfy essentially the same bounds. For more direct evidence that time stability and Lax stability bounds are comparable, computations show that the 2-norm of D_{SP}^2 typically exceeds the spectral radius by only 1 or 2 percent.

If we consider the left-hand sides of (26) and (27) in the limit $N \to \infty$, as well as the corresponding bounds for Chebyshev and Lengendre zeros given in the Appendix, we obtain the following theorem.

THEOREM 1.

$$\limsup_{N\to\infty} \frac{\rho(D_{SP}^2)}{N^4} \leqq \begin{cases} \sqrt{\frac{11}{4725}} \approx 0.0482 & (\textit{Chebyshev extrema}), \\ \sqrt{\frac{29}{315}} \approx 0.3034 & (\textit{Chebyshev zeros}), \\ \sqrt{\frac{1}{96}} \approx 0.1021 & (\textit{Legendre zeros}). \end{cases} \tag{28}$$

We emphasize again that the result for Chebyshev zeros is based on the assumption that the eigenvalues are real and negative (see the remarks below (19)).

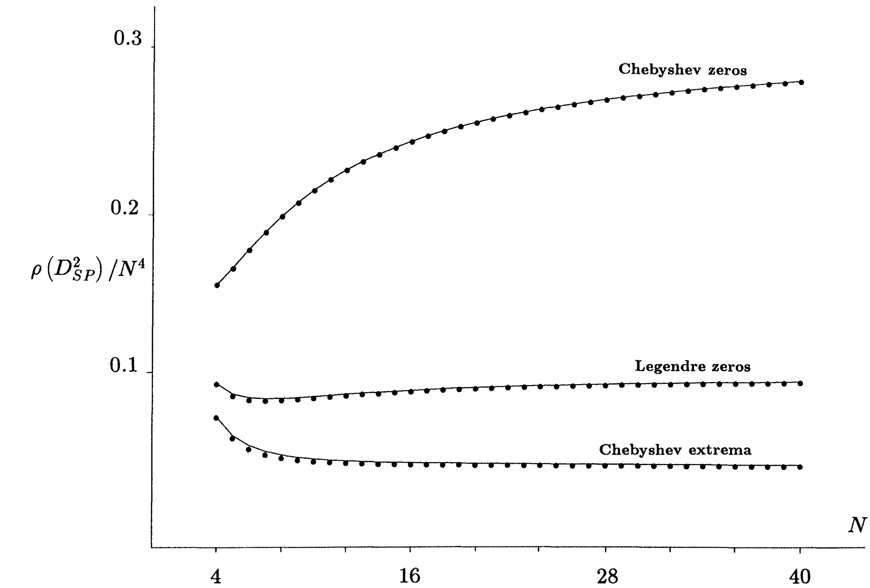


FIG. 4. *Spectral radius of D_{SP}^2 as a function of N, scaled by the factor N^4 (dots), compared with the theoretical bounds provided by the maximum absolute value of the left-hand sides of* (21) *and* (22) (*solid lines*).

The numerical results show that equality in (28) does not hold. However, they indicate that the bounds of Theorem 1 are accurate to within 2 percent, as indicated by the asymptotes in Fig. 4.

Equations such as (26), (27) provide accurate estimates not only of the moduli of the largest eigenvalues, but also of the smallest two eigenvalues. As $N \to \infty$ the actual eigenvalue λ_1 is a spectrally accurate approximation to the eigenvalue $-(\pi/2)^2 \approx -2.4674$ of the continuous problem, while the right-hand side of (27) yields $\lambda_1 \leqq -\sqrt{6} \approx -2.4495$. The discrepancy in these figures is less than 1 percent. Equation (26) yields an analogous bound $\lambda_2 \leqq -\sqrt{90} \approx -9.45$ for the second eigenvalue for sufficiently large N, and since λ_2 approaches $-\pi^2 \approx -9.87$ as $N \to \infty$, the discrepancy is about 4 percent. The inequalities listed in the Appendix show that Chebyshev and Legendre zeros lead to the same bounds $-\sqrt{6}$ and $-\sqrt{90}$ as in the case of Chebyshev extrema.

4. The resolution of the eigenfunctions by polynomial interpolation. In § 2 we observed that the appearance of outlying eigenvalues can be attributed to the nonresolution of the higher eigenfunctions of the continuous problem by polynomial interpolation (Figs. 1(b) and 1(c)). In this section we investigate this phenomenon further by considering the behavior of the error in interpolation of $\cos(\frac{1}{2}k\pi x)$ or $\sin(\frac{1}{2}k\pi x)$, $k = 1, \cdots, N-1$, as $N \to \infty$. Specifically, let α be a real parameter and define

$$f_N(x) = e^{i\alpha N x} \tag{29}$$

for $x \in [-1, 1]$. Let $p_N(x)$ denote the polynomial of degree N that interpolates $f_N(x)$ at the points

$$-1 = x_0 < x_1 < \cdots < x_{N-1} < x_N = 1. \tag{30}$$

We shall prove the following theorem.

THEOREM 2. *A sufficient condition for convergence in the sense of*

$$\max_{-1 \leqq x \leqq 1} |f_N(x) - p_N(x)| \to 0 \quad as \quad N \to \infty \tag{31}$$

is $|\alpha|<1$ *for Chebyshev extreme points, Chebyshev zeros, or Legendre zeros (i.e.,* $>\pi$ *points on average per wavelength), and* $|\alpha|<\pi/6$ *for equidistant points (i.e.,* >6 *points per wavelength).*

The result for equispaced points is valid for exact arithmetic only; as mentioned in the Introduction, rounding errors cause rapid divergence as $N\to\infty$.

Although we will not prove it here, the bounds in Theorem 2 appear to be sharp. They give a natural explanation of why the eigenvalues of D_{SP}^2 diverge from those of the continuous problem to the right of the dashed lines in Fig. 1.

Our analysis parallels the usual convergence proof of interpolation schemes (see, e.g., Krylov [14, p. 246], Davis [3, p. 80], or Warner [22]), except that the function to be interpolated depends on the degree of the interpolating polynomial. The starting point is the well-known Hermite formula for the error in polynomial interpolation on the grid (30):

$$f_N(x)-p_N(x)=\frac{\omega_{N+1}(x)}{2\pi i}\int_C \frac{f_N(z)}{\omega_{N+1}(z)(z-x)}\,dz, \tag{32}$$

where C is any closed contour in the complex plane that encloses $[-1,1]$, and

$$\omega_{N+1}(z):=\prod_{j=0}^{N}(z-x_j). \tag{33}$$

Taking absolute values yields

$$|f_N(x)-p_N(x)|\leqq\frac{1}{2\pi}\max_{-1\leqq x\leqq 1}|\omega_{N+1}(x)|\int_C\frac{|f_N(z)|}{|\omega_{N+1}(z)|\,|z-x|}\,|dz|. \tag{34}$$

Our aim is to determine for which values of α the right-hand side converges to zero as $N\to\infty$.

Consider the logarithmic potential of the point distribution (30) in the limit $N\to\infty$, namely

$$u(z)=\int_{-1}^{1}\ln\frac{1}{|z-t|}\,d\mu(t), \tag{35}$$

where $\mu(t)$ is the limiting distribution of the nodes as $N\to\infty$; in particular,

$$\mu(x)=\frac{1}{\pi}\int_{-1}^{x}(1-t^2)^{-1/2}\,dt \quad \text{(Chebyshev distribution)},$$

$$\mu(x)=\frac{1}{2}(x+1) \qquad \text{(uniform distribution)}$$

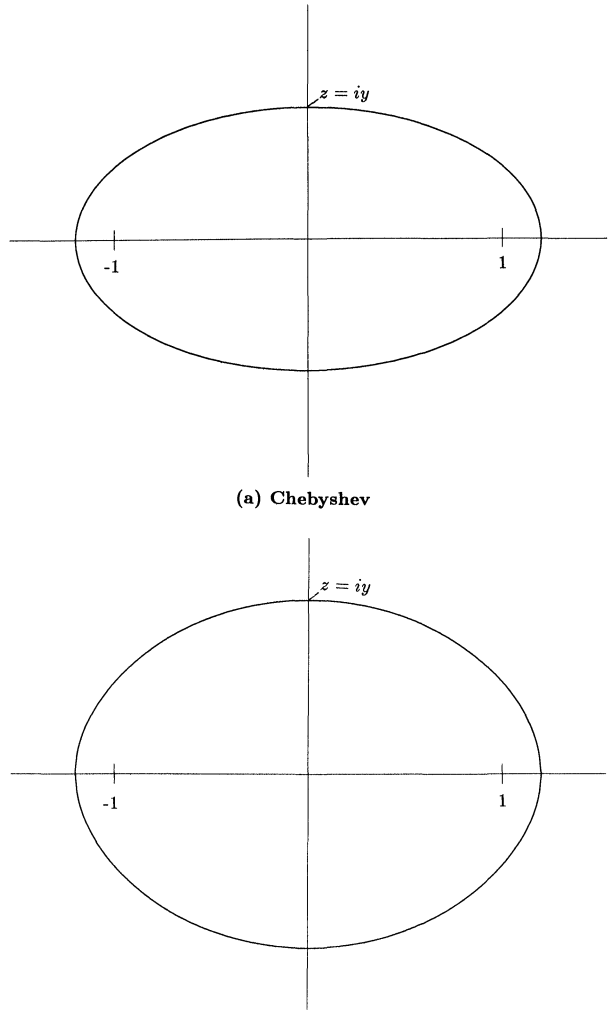
(see Krylov [14, pp. 252, 248]). Although we refer to the first of these as the Chebyshev distribution, it is appropriate for Chebyshev extrema, Chebyshev zeros, and Legendre zeros (and more generally for extrema or zeros of arbitrary Jacobi polynomials).

The curves $u(z)=c$, with c constant, are isopotential contours; smaller values of c correspond to bigger contours. The reason for introducing these contours is that if we integrate in (34) along one of them, the function $|\omega_{N+1}(z)|$ assumes a value independent of z in the limit $N\to\infty$, thereby simplifying the integration. Specifically, Krylov [14, p. 246] shows that

$$|\omega_{N+1}(z)|\to\exp(-(N+1)c) \quad \text{as} \quad N\to\infty \tag{36}$$

uniformly for all z on the curve

$$C=\{z\colon u(z)=c\}. \tag{37}$$



(b) Equidistant

FIG. 5. *Equipotential curves in the complex plane for two distributions of nodes of interpolation.*

Note that the constant c can be thought of as determined by the value y, where $z = iy$ is the intersection of C with the positive imaginary axis (see Fig. 5). From now on we will emphasize this by writing $c = c(y)$, since we will ultimately adjust y to get the sharpest estimate possible. With any such choice of C (34) yields

$$(38) \qquad |f_N(x) - p_N(x)| \leqq \frac{L}{2\pi S} \max_{-1 \leqq x \leqq 1} |\omega_{N+1}(x)| \max_{z \in C} |f_N(z)| \exp((N+1)c(y))$$

in the limit $N \to \infty$, where L is the length of C and S is the distance from C to $[-1, 1]$.

It remains to estimate the two terms (a) $\max_{-1 \leqq x \leqq 1} |\omega_{N+1}(x)|$ and (b) $\max_{z \in C} |f_N(z)|$. Both of these depend exponentially on N, and this dependence determines whether the right-hand side of (38) converges to zero as $N \to \infty$.

(a) Upper bounds for $\max_{-1 \leqq x \leqq 1} |\omega_{N+1}(x)|$ are readily obtained in the form

$$(39) \qquad \max_{-1 \leqq x \leqq 1} |\omega_{N+1}(x)| \leqq \phi(N) \exp(-Nd).$$

For example, in the case of Chebyshev extrema we have

$$\omega_{N+1}(x)=\frac{2^{1-N}}{N}(x^2-1)T'_N(x)$$

and therefore

$$|\omega_{N+1}(x)|=\frac{2^{1-N}}{N}|x^2-1||T'_N(x)|\leqq 2^{1-N},$$

since $|T'_N(x)|\leqq N/\sqrt{1-x^2}$ by Bernstein's inequality. This implies (39) with $\phi(N)=2$ and

$$d=\ln 2. \tag{40}$$

For interpolation in Chebyshev zeros and Legendre zeros the inequality (39) is again valid. The function $\phi(N)$ is different in each case, but its dependence on N is only algebraic and therefore unimportant. The crucial factor is the exponential $\exp(-Nd)$, which is the same for all three cases. That is, (39) holds with $d=\ln 2$ for Chebyshev extrema, Chebyshev zeros, and Legendre zeros.

For equidistant points, however, the exponential dependence on N is different, namely

$$d=1-\ln 2 \tag{41}$$

in the limit $N\to\infty$. To prove this, let $x_j=-1+2j/N$ and consider any $\chi\in[-1,1]$. If l is such that $x_l\leqq\chi\leqq x_{l+1}$, then

$$\begin{aligned}|\omega_{N+1}(\chi)|&=\prod_{j=0}^{l}(\chi-x_j)\prod_{j=l+1}^{N}(x_j-\chi)\\&\leqq\prod_{j=0}^{l}(x_{l+1}-x_j)\prod_{j=l+1}^{N}(x_j-x_l)\\&=\left(\frac{2}{N}\right)^{N+1}(l+1)!(N-l)!\\&\leqq\left(\frac{2}{N}\right)^{N+1}N!.\end{aligned}$$

An application of Stirling's formula shows that (39) is valid in the limit $N\to\infty$ with $\phi(N)=\sqrt{8\pi/N}$ and $d=1-\ln 2$.

(b) To determine the contribution to (38) of the term $\max_{z\in C}|f_N(z)|$, we require explicit expressions for the equipotential curves in the limit $N\to\infty$. These are given by

$$u(z)=\ln(2/|z+\sqrt{z^2-1}|), \tag{42}$$

$$u(z)=\tfrac{1}{2}\operatorname{Re}\{2+(z-1)\ln(z-1)-(z+1)\ln(z+1)\} \tag{43}$$

for Chebyshev and equidistant distributions, respectively (see Krylov [14, pp. 253, 248]). In the Chebyshev case the curves $u(z)=c$ are confocal ellipses with foci at $z=\pm 1$. For equidistant points they are ovals of a thicker shape. (These curves are depicted in Fig. 5. See also Krylov [14, p. 249] and Warner [22] for illustrations.) In either of these cases we have

$$\max_{z\in C}|f_N(z)|=e^{|\alpha|Ny}, \tag{44}$$

where $z=iy$ is again the point of intersection of C with the positive imaginary axis.

We are now in a position to estimate the right-hand side of (38). Substitution of (39) and (44) into (38) shows that the convergence of the interpolation process is determined by the behavior of $\exp(N(|\alpha|y+c(y)-d))$ as $N\to\infty$, and convergence is guaranteed if the argument of this exponential is negative. That is, a sufficient condition for convergence is

$$|a|<\frac{d-c(y)}{y}. \tag{45}$$

To determine the maximum range of values of α over which (45) is valid, we define

$$g(y)=\frac{d-c(y)}{y} \tag{46}$$

and look for the maximum value of this function. In other words, the idea is to vary the contour of integration (determined by y) so as to get the best estimate.

For Chebyshev points we have from (40) and (42) that

$$g(y)=\frac{\ln(y+\sqrt{y^2+1})}{y}, \tag{47}$$

with maximum value $g(y)=1$ if $y\to 0$. Hence (45) becomes

$$|\alpha|<1. \tag{48}$$

Similarly, for equidistant points (41) and (43) show that

$$g(y)=\frac{\ln\sqrt{1+y^2}+\frac{1}{2}y(\pi-2\tan^{-1}y)-\ln 2}{y}. \tag{49}$$

The maximum value of this function is $g(\sqrt{3})=\pi/6$, and accordingly (45) yields

$$|\alpha|<\frac{\pi}{6}. \tag{50}$$

This completes the proof of Theorem 2. □

5. The effect of filtering on the eigenvalues. In the previous sections we have explored the fact that the spectral radius of the Chebyshev second derivative operator is of magnitude $O(N^4)$, with the result that explicit time integration methods typically must satisfy an extremely restrictive timestep restriction $\Delta t\leqq O(N^{-4})$. It has been suggested by Gottlieb and Turkel [12], and others, that judicious filtering of the high modes might alleviate this problem.

In order to explain the filtering process, it is necessary to describe an algorithm based on the FFT by which spectral differentiation is commonly performed on the Chebyshev extreme points (see [8] or [11]). The polynomial $u_N(x)$ is expanded as

$$u_N(x)=\sum_{l=0}^{N} a_l T_l(x), \tag{51}$$

where

$$a_l=\frac{2}{\bar{c}_l N}\sum_{j=0}^{N}\frac{1}{\bar{c}_j}u_N(x_j)T_l(x_j) \tag{52}$$

and

$$\bar{c}_l = \begin{cases} 2 & l = 0, N, \\ 1 & \text{otherwise.} \end{cases}$$

Differentiation of (51) yields

$$D^2 u_N(x) = \sum_{l=0}^{N-2} b_l T_l(x), \tag{53}$$

with

$$b_l = \frac{1}{c_l} \sum_{\substack{n=l+2 \\ n+l \text{ even}}}^{N} n(n^2 - l^2) a_n \tag{54}$$

and

$$c_l = \begin{cases} 2 & l = 0, \\ 1 & \text{otherwise} \end{cases}$$

(see [10, p. 160]).

The second derivative is computed by the following three steps. (a) Given the data $u_N(x_j)$, compute the coefficients a_l by an FFT from (52). (b) Compute the coefficients b_l using (54). (c) Compute the derivative $D^2 u_N(x_j)$ at the gridpoints via another FFT from (53).

Although the use of the FFT obviates the need to calculate the entries of D_{SP}^2 explicitly in a computer program, for studying the effects of filtering it is convenient to use (51)-(53) to obtain them. To do this, we substitute (52) into (54), and substitute the result into (53). If the resulting expression is evaluated at the gridpoints x_i, we find that the entries of the differentiation matrix are given by

$$(D_{SP}^2)_{ij} = \frac{2}{\bar{c}_j N} \sum_{l=0}^{N-2} \sum_{\substack{n=l+2 \\ n+l \text{ even}}}^{N} \frac{1}{c_l \bar{c}_n} n(n^2 - l^2) T_l(x_i) T_n(x_j). \tag{55}$$

The filtering idea is to smooth the interpolant before differentiation, i.e., to replace (51) by

$$u_N(x) = \sum_{l=0}^{N} \beta_l a_l T_l(x), \tag{56}$$

where the filter function β_l satisfies $0 \leqq \beta_l \leqq 1$ for all $l = 0, \cdots, N$, $\beta_l \approx 1$ for $l \ll N$, and $|\beta_l| \ll 1$ for $l \approx N$. The effect of this function is to leave the low modes approximately intact, but to reduce the energy content of the higher modes.

To explain why this type of filtering reduces the spectral radius, we rewrite (54) in matrix form as

$$b = Aa, \tag{57}$$

where $b = \{b_0, \cdots, b_{N-2}\}^T$ and $a = \{a_2, \cdots, a_N\}^T$. The differentiation operator in transform space is then represented by the matrix A. It is easy to check that the maximum column sum of A is attained in the final column, and this gives $\|A\|_1 = O(N^4)$. Filtering of the high modes amounts to replacing A by $\tilde{A}$, where the lth column of $\tilde{A}$ is β_l times the lth column of A. Since $\beta_l \ll 1$ for $l \approx N$, a reduced maximum column sum can be expected and therefore also a reduced spectral radius.

Some possible filter functions were suggested by Gottlieb and Turkel [12] and Majda et al. [15]. (In the latter paper the purpose of filtering was to reduce the oscillations associated with discontinuous initial data, rather than to improve the time stability of the method. However, the filter introduced there may also be used for our purpose, since it satisfies the properties described below (56).) As an example we will consider the following filter function, suggested in [15]:

$$\beta_l = \begin{cases} 1, & 0 \leqq l \leqq l_0, \\ \exp\left[-\gamma\left(\dfrac{l-l_0}{N-l_0}\right)^4\right], & l_0 < l \leqq N, \end{cases} \tag{58}$$

where l_0 and γ are positive parameters. Note that it is easy to set up the filtered matrix D_{SP}^2—a factor of β_n is simply included in (55).

Figure 6 shows β_l and the corresponding eigenvalues of D_{SP}^2 for $N=16$, $l_0=10$, and $\gamma=0, 2, 5$. Notice that the spectral radius is indeed decreased by the filtering, but

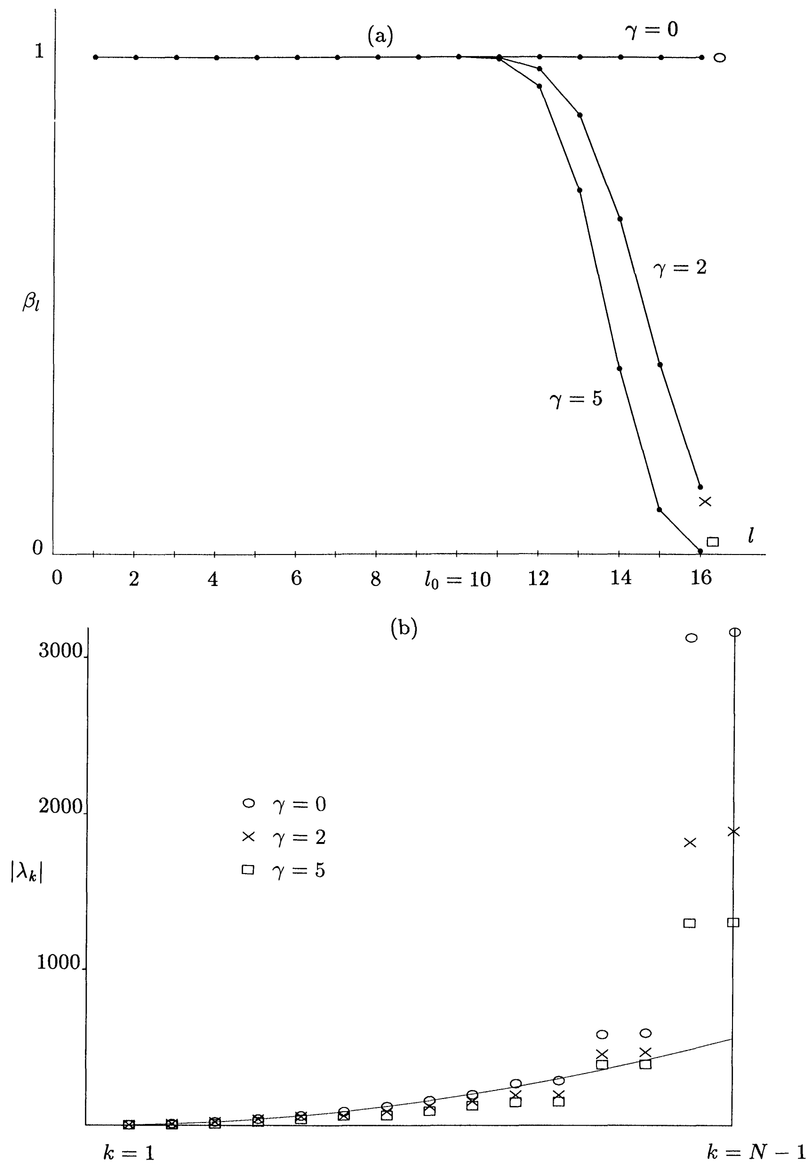


FIG. 6: (a) *The filter function* (58) *with* $N=16$, $l_0=10$, *and* $\gamma=0, 2, 5$. (b) *Eigenvalues of the corresponding differentiation matrices.*

at the cost of the loss of spectral accuracy in the lower eigenvalues. Different values of l_0 do not improve the situation significantly. These discouraging results are not peculiar to the filter function (58), since the filters suggested in [12] also lead to the same conclusion: small amounts of filtering do not improve the spectral radius significantly; moderate amounts destroy the spectral accuracy in the low eigenvalues.

Similar observations were reported by Fulton and Taylor [5] in a study of filtering for the first-order Chebyshev differencing operator. Their assessment of filters was based on the computation of the spectral radius of the growth matrix of a Runge-Kutta time integrator applied to the semidiscrete system, and on computations of the solutions to the first-order wave equation. We believe that the examination of the eigenvalues of the differentiation matrix is a more straightforward method for analyzing such questions.

Another possible strategy for the removal of the outliers has been suggested to us. First, compute the eigenvalue decomposition of D_{SP}^2 in the form $D_{SP}^2 = S\Lambda S^{-1}$. Then replace the outlying eigenvalues (λ_k, $k > 2N/\pi$) by some innocuous values (we tried the corresponding eigenvalues of the continuous problem) to form a new diagonal matrix $\tilde{\Lambda}$, and assemble a modified "differentiation" matrix $\tilde{D}_{SP}^2 = S\tilde{\Lambda}S^{-1}$. Although $\tilde{D}_{SP}^2$ now has eigenvalues almost identical to that of the continuous problem, applying it to various test functions shows that it does not differentiate properly. That is, the error $|(\tilde{D}_{SP}^2 y)_j - y''(x_j)|$ does not in general converge to zero as $N \to \infty$, even for smooth functions $y(x)$.

We are unaware of any filtering strategy that eliminates the outliers without sacrificing a great deal of accuracy.

Appendix. In this Appendix we derive bounds on the eigenvalues of the spectral differentiation matrices D_{SP}^2 based on Chebyshev and Legendre zeros, analogous to the bounds (26) and (27) for Chebyshev extreme points.

Chebyshev zeros. Let $f_{N-1} = T_{N-1}$. By (19) and (23) we obtain

$$a_k = \prod_{l=0}^{k-1} \frac{(N-1)^2 - l^2}{2l+1}, \tag{59}$$

$$b_k = \left(\frac{(N-1)^2 - (k-1)^2}{2k-1} + k \right) \prod_{l=0}^{k-2} \frac{(N-1)^2 - l^2}{2l+1}. \tag{60}$$

Inserting these expressions into (21) and (22) yields the bounds

$$-\left(\frac{29N^8 - 232N^7 + 826N^6 - 1708N^5 + 1981N^4 - 868N^3 - 316N^2 + 288N}{315} \right)^{1/2}$$
$$\leqq \lambda_k \leqq -\left(\frac{720N^3 - 5040N^2 + 11520N - 8640}{8N^3 - 56N^2 + 128N - 141} \right)^{1/2},$$
$$-\left(\frac{29N^8 - 232N^7 + 1078N^6 - 3220N^5 + 7441N^4 - 12628N^3 + 12872N^2 - 6600N + 1260}{315} \right)^{1/2}$$
$$\leqq \lambda_k \leqq -\left(\frac{48N^4 - 240N^3 + 288N^2}{8N^4 - 40N^3 + 48N^2 - 3N + 18} \right)^{1/2}.$$

Legendre zeros. The Legendre polynomial of degree N satisfies the differential equation

$$(1 - x^2)P_N''(x) - 2xP_N'(x) + N(N+1)P_N(x) = 0, \tag{61}$$

and differentiating k times yields

$$(62)\quad (1-x^2)P_N^{(k+2)}(x)-2(k+1)xP_N^{(k+1)}(x)+(N(N+1)-k(k+1))P_N^{(k)}(x)=0.$$

If this equation is evaluated at $x=1$, we obtain the recurrence relation

$$(63)\qquad P_N^{(k+1)}(1)=\frac{N(N+1)-k(k+1)}{2(k+1)}P_N^{(k)}(1), \qquad P_N(1)=1,$$

and therefore

$$(64)\qquad D^k(P_N)_{x=1}=\prod_{l=0}^{k-1}\frac{N(N+1)-l(l+1)}{2(l+1)}.$$

If we now let $f_{N-1}=P_{N-1}$, (19) becomes

$$(65)\qquad a_k=\prod_{l=0}^{k-1}\frac{N(N-1)-l(l+1)}{2(l+1)},$$

$$(66)\qquad b_k=\left(\frac{N(N-1)-k(k-1)}{2k}+k\right)\prod_{l=0}^{k-2}\frac{N(N-1)-l(l+1)}{2(l+1)}.$$

The corresponding bounds on the eigenvalues are

$$-\left(\frac{N^8-4N^7+10N^6-16N^5-35N^4+92N^3+24N^2-72N}{96}\right)^{1/2}$$

$$\leqq \lambda_k \leqq -\left(\frac{360N^3-1980N^2+3510N-2025}{4N^3-22N^2+39N-45}\right)^{1/2} \quad \text{and}$$

$$-\left(\frac{N^8-4N^7+18N^6-40N^5+165N^4-268N^3+8N^2+120N}{96}\right)^{1/2}$$

$$\leqq \lambda_k \leqq -\left(\frac{24N^5-132N^4+234N^3-135N^2}{4N^5-22N^4+39N^3-24N^2+12N-15}\right)^{1/2}.$$

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Notes added in proof. 1. The eigenvalue bounds of Theorem 1 closely match the empirical results reported on p. 100 of the new book by Canuto et al. [23]. We have also been informed that theoretical results along these lines have been obtained by Hervé Vandeven of the University of Paris, VI, and will be published shortly.

2. Details related to the "6 points per wavelength" statement of Theorem 2 and other aspects of equispaced interpolation have been worked out in [24].

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