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AN INSTABILITY PHENOMENON IN SPECTRAL METHODS*

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Abstract. The eigenvalues of Chebyshev and Legendre spectral differentiation matrices, which determine the allowable time step in an explicit time integration, are extraordinarily sensitive to rounding errors and other perturbations. On a grid of N points per space dimension, machine rounding leads to errors in the eigenvalues of size $O(N^2)$. This phenomenon may lead to inconsistency between predicted and observed time step restrictions. One consequence of it is that spectral differentiation by interpolation in Legendre points, which has a favorable $O(N^{-1})$ time step restriction for the model problem $u_t = u_x$ in theory, is subject to an $O(N^{-2})$ restriction in practice. The same effect occurs with Chebyshev points for the model problem $u_t = -xu_x$. Another consequence is that a spectral calculation with a fixed time step may be stable in double precision but unstable in single precision. We know of no other examples in numerical computation of this kind of precision-dependent stability.

Key words. spectral method, instability, rounding error, differentiation matrix, boundary condition
AMS(MOS) subject classifications. 65M10, 65G05, 65D25, 65F15

1. Introduction. Spectral methods have become popular in the last decade for the numerical solution of partial differential equations [1], [8], [18]. The essential idea is to approximate spatial derivatives by constructing a global interpolant through discrete data points, and then differentiating the interpolant at each point. (Such a process is more properly known as a "pseudospectral" method.) On a periodic domain, as arises for example in global atmospheric circulation models, the data points are evenly spaced and the interpolant is a trigonometric function. On a domain with boundaries, as arises more often, the points are unevenly spaced, usually at the zeros or extrema of Chebyshev or Legendre polynomials, and the interpolant is a polynomial.

The advantage of spectral methods is that in favorable circumstances they are more accurate than finite differences or finite elements, so that fewer grid points are needed. A principal disadvantage is that in problems with boundaries, they are often subject to tight stability restrictions. On a grid of N points in one space dimension, an explicit finite difference formula will typically exhibit a time step restriction of $\Delta t = O(N^{-1})$ for hyperbolic and $\Delta t = O(N^{-2})$ for parabolic problems. For spectral methods the restrictions become $\Delta t = O(N^{-2})$ and $\Delta t = O(N^{-4})$, respectively. This presents one with the choice of taking wastefully short time steps to maintain stability, or of turning to implicit formulas. Since spectral differentiation matrices are dense, the latter course leads to difficult linear or nonlinear algebraic problems whose efficient solution—usually by preconditioned iterative or multigrid methods—is at present a topic of active research [13].

The stability of spectral methods for initial boundary value problems is not well understood. Certain model problems have been worked out in detail [4], [6], [15], but no general theory is available that is as readily applicable as the "Kreiss-Osher" theory for finite differences [9]. A recent contribution in this direction is by Gottlieb, Lustman and Tadmor [7].

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In most of this paper we consider the first-order hyperbolic initial boundary value problem

$$
\begin{aligned}
&u_t = u_x, && x\in(-1,1), \quad t>0,\\
&u(x,0)=f(x), && x\in(-1,1),\\
&u(1,t)=0, && t\geqq 0,
\end{aligned}
\tag{1}
$$

which can be viewed as a model of a more general hyperbolic system of equations with appropriately specified boundary conditions. Given $N\geqq 1$, let $x_1>x_2>\cdots>x_N$ be a set of points in $[-1,1)$. The **spectral differentiation matrix** $D_N:\mathbf{C}^N\to\mathbf{C}^N$ for these points is defined as the $N\times N$ matrix that effects the following mapping $v\mapsto w=D_Nv$:

(a) Let $v=\{v_j\}\in\mathbf{C}^N$ be a vector of data values at the points $\{x_j\}$;

(b) Let $p(x)$ be the unique polynomial of degree at most N with $p(x_j)=v_j$ and $p(1)=0$;

(c) Set $w_j=p'(x_j)$, $1\leqq j\leqq N$.

Notice the key point that the boundary condition of (1) is incorporated in (b). The explicit determination of the entries of D_N, given $\{x_j\}$, is straightforward and described in [15].

Two choices of $\{x_j\}$ are considered here: the **Chebyshev extreme points**

$$
x_j=\cos\frac{j\pi}{N}, \qquad 1\leqq j\leqq N,
\tag{2}
$$

which are the extrema of the Chebyshev polynomial $T_N(x)$, and the **Legendre points**, defined as the zeros of the Legendre polynomial $P_N(x)$. (The latter can be computed by the program GAUSSQ of Golub and Welsch [3].) Let D_N^C and D_N^L denote the corresponding differentiation matrices. Explicit formulas for the entries of D_N^C are given in § 4 of [5]. For comparison we will also mention D_N^F, the $N\times N$ Fourier spectral differentiation matrix on a periodic regular grid with no boundary conditions, which is subject to none of the instability phenomena to be discussed here. See [11] and § 1 of [5].

Our concern is with the eigenvalues of D_N. In a typical explicit spectral discretization of (1), the spatial derivative is approximated by D_N and the time derivative by an Adams–Bashforth or Runge–Kutta formula. For each time step Δt, such a formula has a **stability region** in the complex plane, defined as the set of all $\lambda\in\mathbf{C}$ for which it reduces to a stable recurrence relation when applied to the model problem $u_t=\lambda u$ [12]. The spectral model of (1) has bounded solutions as $t\to\infty$, for fixed Δt, if and only if all the eigenvalues of D_N lie in this stability region. (We ignore the borderline possibility of defective eigenvalues on the boundary of the stability region, which do not appear in the cases considered here.) The stability region expands in proportion to Δt^{-1}. Therefore if the eigenvalues of D_N are of size $O(N)$, the result is a stability restriction $\Delta t=O(N^{-1})$, while if they are of size $O(N^2)$, the restriction becomes $\Delta t=O(N^{-2})$.

To be more precise, the eigenvalues of D_N determine the "time-stability" of a spectral method ($t\to\infty$, Δt fixed), but not its "Lax-Richtmyer stability" ($\Delta t\to 0$, t fixed). Thus there is much more to the stability analysis of spectral methods than is mentioned in this paper; see [8]. But it appears that in a wide range of practical applications, time-stability is a good indicator of whether or not a spectral computation will be successful.

2. Exact vs. computed eigenvalues. Figure 1 shows the eigenvalues of D_N^F, D_N^C and D_N^L in the complex plane for $N=14$ and $N=28$. The computations were performed by EISPACK [14] routines in double precision on a Sun Workstation (≈ 16 digit accuracy), and $N=28$ was chosen because it is the largest value for which all three pictures are unaffected by rounding error.[1] It is important to note the following: the scale in plots (d)-(f) is half that of plots (a)-(c).

D_N^F is skew-symmetric, and its eigenvalues are pure imaginary and uniformly spaced along the complex interval $[-i\pi N/2, i\pi N/2]$. This is well known and easy to prove; the eigenvectors are complex exponentials [11]. When N is even, as in these figures, the eigenvalue at zero has multiplicity 2.

D_N^C is not skew-symmetric, and its eigenvalues have negative real part (see [5, § 6]). Most of them lie along a bow-shaped curve extending from $-iN$ to iN. But there are also a few outliers extending far beyond the bow, and these have size $O(N^2)$ as $N \to \infty$. (The corresponding eigenvectors are dominated by high wave number oscillations.) The number of these outlying eigenvalues is not fixed, but increases with N. Their presence is what makes time-stepping for Chebyshev spectral methods difficult. The exact eigenvalues of D_N^C are not known, but it is reported that asymptotic approximations have been derived by M. Dubiner [16].

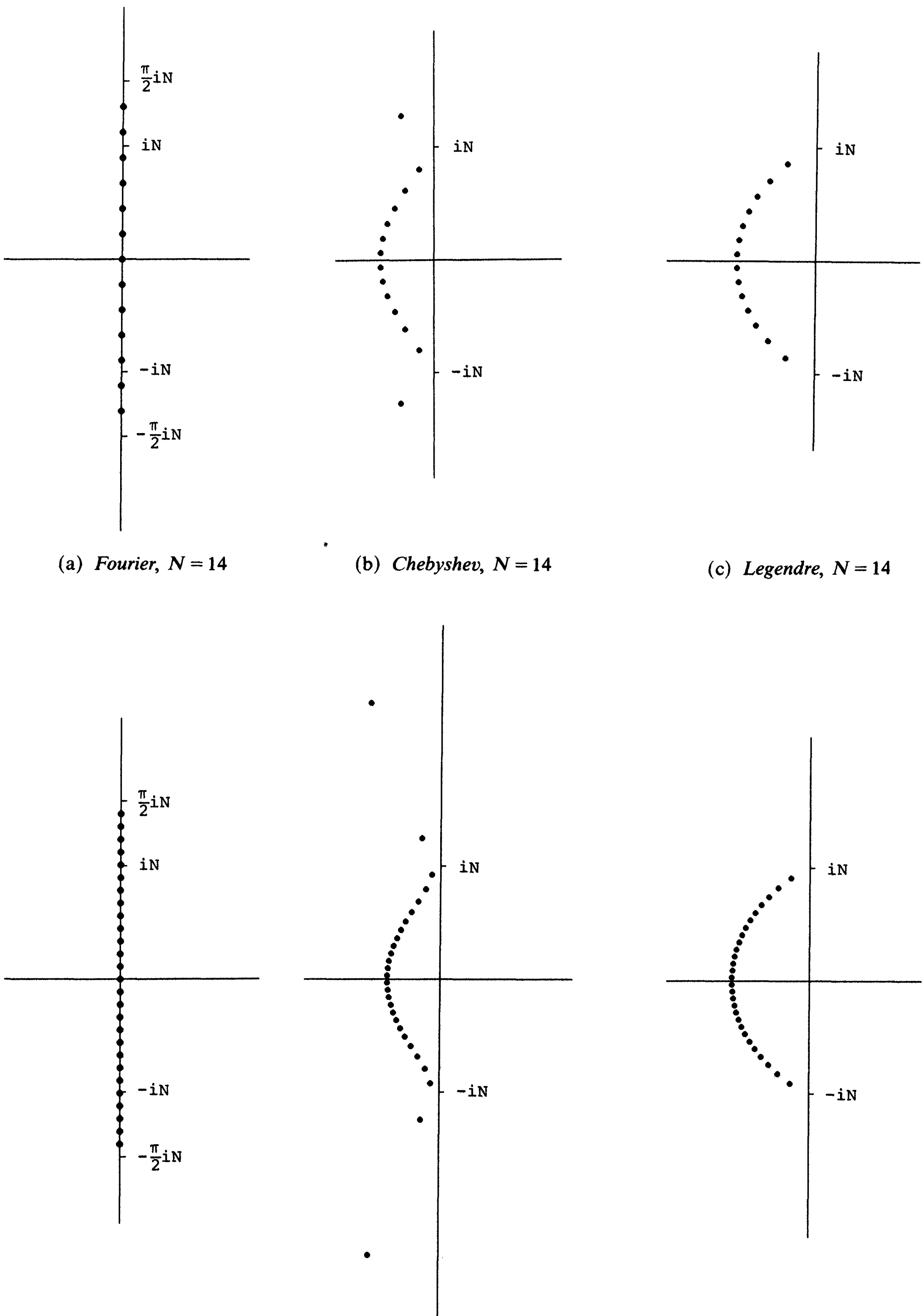
D_N^L is also not skew-symmetric, and again its eigenvalues have negative real part. In contrast to the Chebyshev case, all of them lie along an approximately circular curve extending from $-iN$ to iN, with no outliers. This discovery is due to Dubiner and Tal-Ezer [15], who have obtained exact formulas which show that in this case the eigenvalues are related to the zeros of a Hankel function [16]. Unfortunately, it appears to be difficult to generalize this well-behaved eigenvalue distribution to problems other than (1), and so Legendre points are not suitable at present as a general replacement for Chebyshev points in spectral calculations. They also have the disadvantage that interpolation in Legendre points cannot straightforwardly be carried out by a Fast Fourier Transform.

In summary, on the basis of Fig. 1 and what theory is available to support it, one would conclude that if a reasonable time-stepping formula is used, the Fourier, Legendre and Chebyshev spectral methods for the model problem (1) will have time step restrictions $\Delta t = O(N^{-1})$, $O(N^{-1})$ and $O(N^{-2})$, respectively.

But the pictures change when N is increased. In Fig. 2, N has been raised to 56 (with the scale of the plots reduced somewhat more than proportionately). The $O(N^2)$ outliers in the Chebyshev plot have become more dominant. But a more striking qualitative change is that in both the Chebyshev and Legendre cases, the smooth curve of smaller eigenvalues has split in two. *This bifurcation is entirely caused by rounding error.* In exact arithmetic, the eigenvalues would continue to line up along a single smooth curve.

To substantiate this claim, Figs. 3 (Chebyshev) and 4 (Legendre) hold N fixed and vary the precision. They show eigenvalues for $N=28$ computed with approximately 16-, 8- and 4-digit accuracy (simulated by introduction of random perturbations in the initial matrix). In both cases, the eigenvalues move dramatically as the precision is reduced, lining up along an arc far from the origin and a vertical straight line near the imaginary axis. Between Figs. 3(a) and (b), for example, perturbations of order 10^{-8} have moved the eigenvalues by distances greater than 10. The significance of the dashed lines in the figures is explained in the next section.

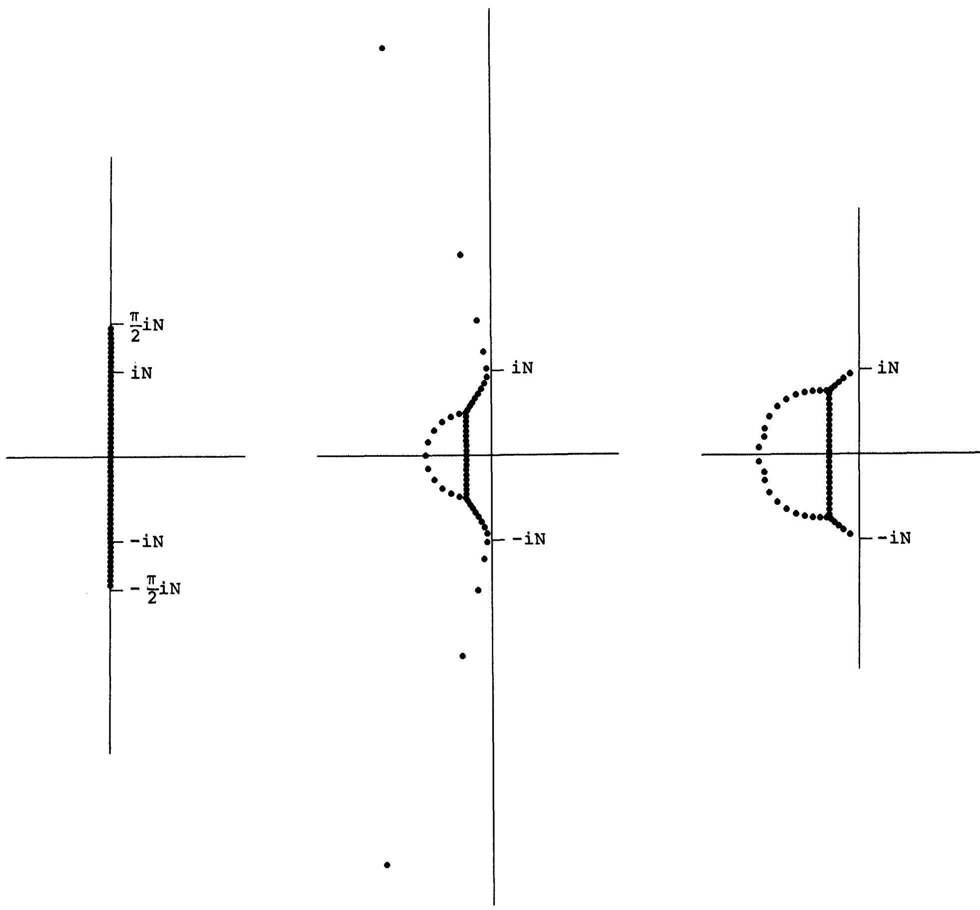
[1] Thus 28 is the most perfect number under the Sun.



(a) *Fourier,* $N = 14$ (b) *Chebyshev,* $N = 14$ (c) *Legendre,* $N = 14$

(d) *Fourier,* $N = 28$ (e) *Chebyshev,* $N = 28$ (f) *Legendre,* $N = 28$

FIG. 1. *Computed = exact eigenvalues of the Fourier, Chebyshev and Legendre spectral differentiation matrices with* $N = 14, 28$.



(a) *Fourier,* $N = 56$ (b) *Chebyshev,* $N = 56$ (c) *Legendre,* $N = 56$

FIG. 2. *Computed eigenvalues of the Fourier, Chebyshev and Legendre spectral differentiation matrices with* $N = 56$, *machine precision* $\varepsilon \approx 10^{-16}$.

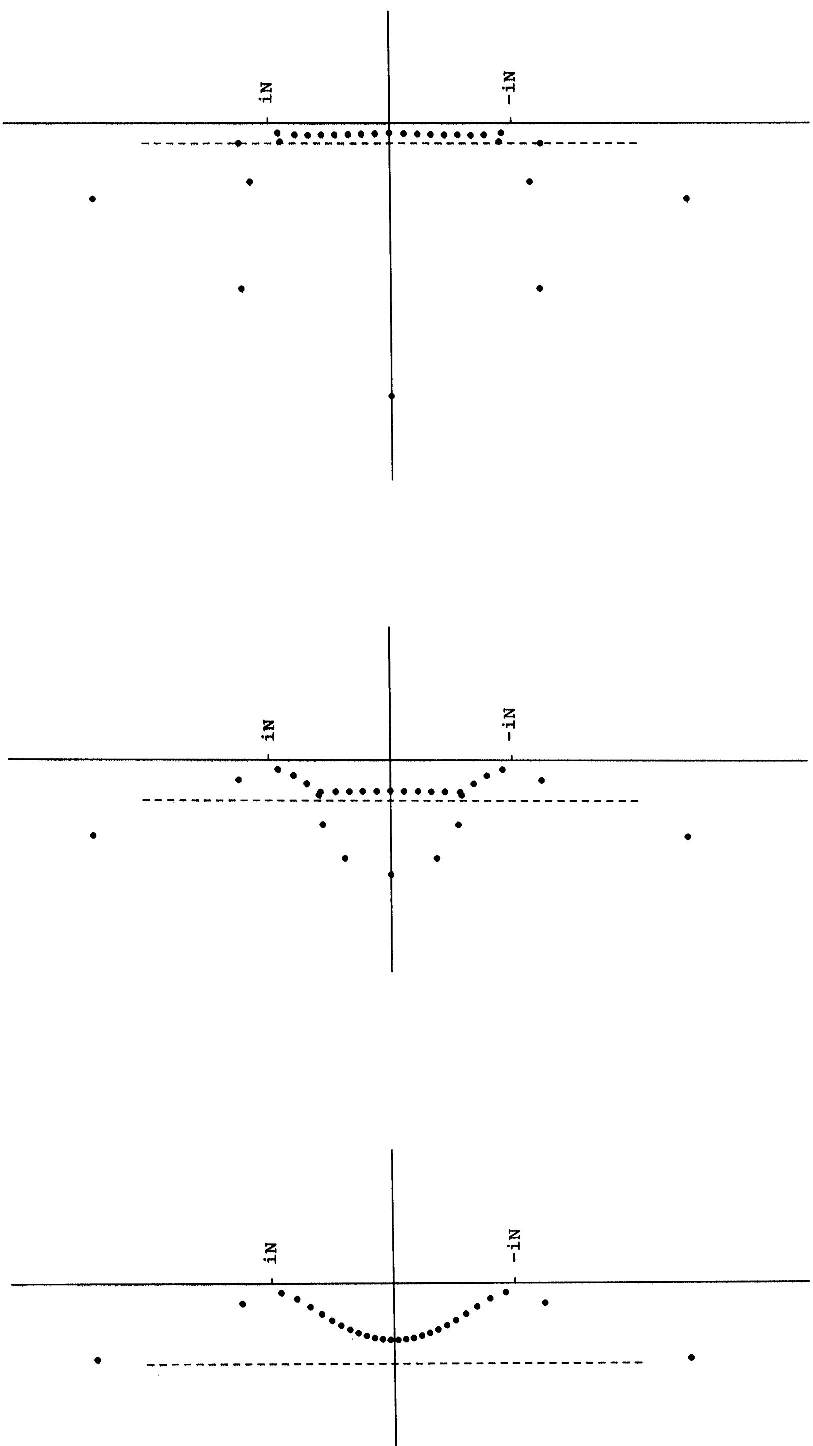
This phenomenon of great eigenvalue sensitivity is the central point of this paper. Similar figures will be obtained on any computer if N is large enough.

Figures 2–4 suggest a revised stability conclusion for spectral computations in floating-point arithmetic: Legendre as well as Chebyshev methods suffer a $\Delta t = O(N^{-2})$ time step restriction, and in both cases the constant involved may be affected by the machine precision.

3. A rough explanation. An explanation of these results can be found in the eigenvectors of D_N. We do not know these eigenvectors exactly, and so the explanation is not yet rigorous, but it correctly predicts at what value of N the instability phenomenon first appears, for any machine precision ε. In what follows we consider the Chebyshev case D_N^C, whose properties are clearer.

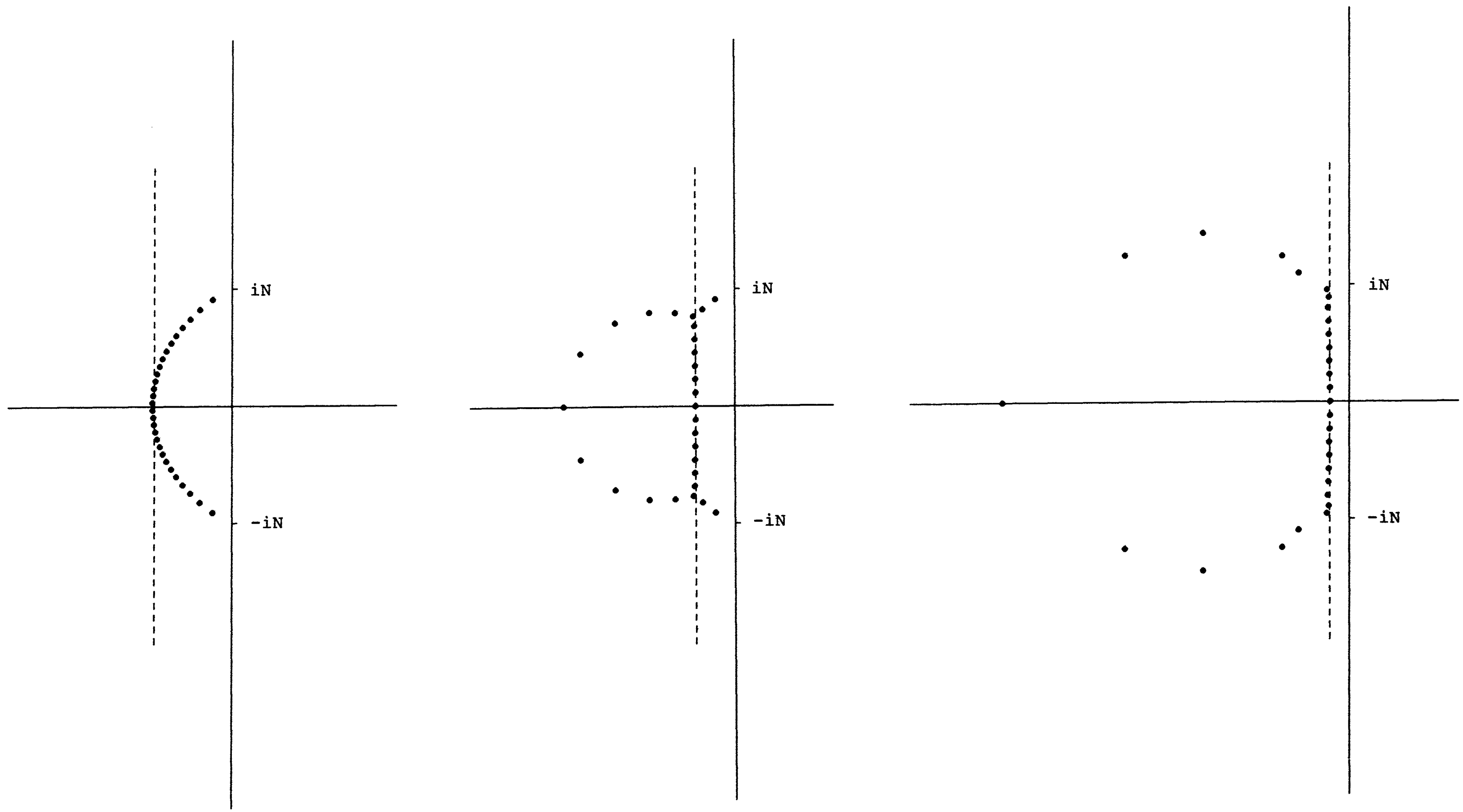
The key observation is that if λ is an exact eigenvalue of D_N^C, but not one of the outliers, then the corresponding eigenvector is closely approximated by

$$v_j \approx v_N\, e^{\lambda(x_j+1)}. \tag{3}$$



(a) 16 digits (b) 8 digits (c) 4 digits

FIG. 3. *Eigenvalues of the Chebyshev differentiation matrix* D_N^C *with* $N=28$, *computed in various precisions* ε. *The dashes indicate the line* $\operatorname{Re}\lambda=\frac{1}{2}\log_e\varepsilon$.



(a) 16 *digits* (b) 8 *digits* (c) 4 *digits*

FIG. 4. *Eigenvalues of the Legendre differentiation matrix D_N^L with $N = 28$, computed in various precisions ε. The dashes indicate the line* $\mathrm{Re}\,\lambda = \frac{1}{2}\log_e \varepsilon$.

(Recall from (2) that the Chebyshev points are numbered from right to left, so that v_N corresponds to $x=-1$.) It is not exactly of this form; an exact analysis would involve polynomials rather than exponentials. But it comes extremely close. The intuitive reason is that if the differentiation were exact and there were no boundary condition, (3) would be an exact eigenvector for any λ. Such a function is $e^{2\,\mathrm{Re}\,\lambda}$ times smaller in magnitude at $x=1$ than at $x=-1$. Therefore for $\mathrm{Re}\,\lambda \ll 0$, it is very small at $x=1$, which means that the boundary condition is nearly satisfied. In practice we observe that the exact eigenvectors of the discrete problem look like (3) plus a small oscillatory term with magnitude on the order of $e^{2\,\mathrm{Re}\,\lambda}$.

Some eigenvectors for the case $N=28$ are illustrated in Fig. 5. Figure 5(a) shows the eigenvalues of D_{28}^C in the upper half plane, and the real parts and moduli (plus and minus) of some corresponding eigenvectors. Each eigenvector is plotted as a function of x on $[-1, 1]$, i.e., $v_j = v(x_j)$, in a position just to the right of the imaginary axis. One sees that v_j decays rapidly in x for each λ except the outliers. Figure 5(b) clarifies the situation by showing the same eigenvectors after subtracting off the exponential term (3), and rescaling by $v_N e^{2\lambda}$:

$$(4) \qquad (v_j - v_N e^{\lambda(x_j+1)})/v_N e^{2\lambda}.$$

Since typically $\mathrm{Re}\,\lambda \approx -10$ in this figure, the denominator $e^{2\lambda}$ has magnitude around 10^{-9}. Yet the figure shows that even after division by this quantity, (4) has the form of an oscillatory signal of moderate amplitude. Thus the approximation (3) is accurate to around nine orders of magnitude.

Here is the explanation of the instability phenomenon. An exact eigenvector of D_N^C is approximately $e^{2\,\mathrm{Re}\,\lambda}$ times smaller at $x=1$ than at $x=-1$: $|v_N| \approx e^{-2\,\mathrm{Re}\,\lambda}|v_1|$. On the other hand when v is multiplied by D_N, the entry v_N contributes to the entry $w_1 = (D_N v)_1$ in the product. If the multiplication is performed with rounding errors of relative size ε, then $(D_N v)_1$ will be degraded by a perturbation of order $\varepsilon |v_N| \approx \varepsilon\, e^{-2\,\mathrm{Re}\,\lambda}|v_1|$. All relative precision will be lost if

$$\varepsilon\, e^{-2\,\mathrm{Re}\,\lambda} \approx 1,$$

that is,

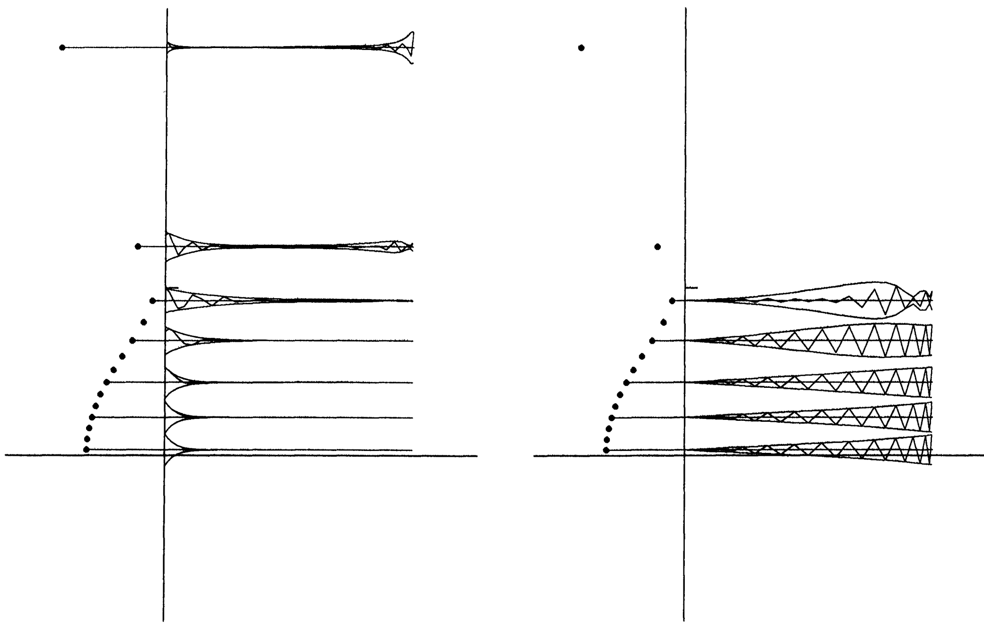
$$(5) \qquad \mathrm{Re}\,\lambda \approx \tfrac{1}{2}\log_e \varepsilon.$$

In other words, we cannot expect to obtain any eigenvectors numerically that are shaped like decaying exponentials in x, except when $\mathrm{Re}\,\lambda$ is greater than or equal to approximately $\frac{1}{2}\log_e \varepsilon$ (a negative number).

The dashed lines in Figs. 3 and 4 of the last section represented the condition (5). In confirmation of the argument above, the eigenvalues well to the right of the line in those figures appear to be unaffected by rounding errors, while those to the left are changed completely.

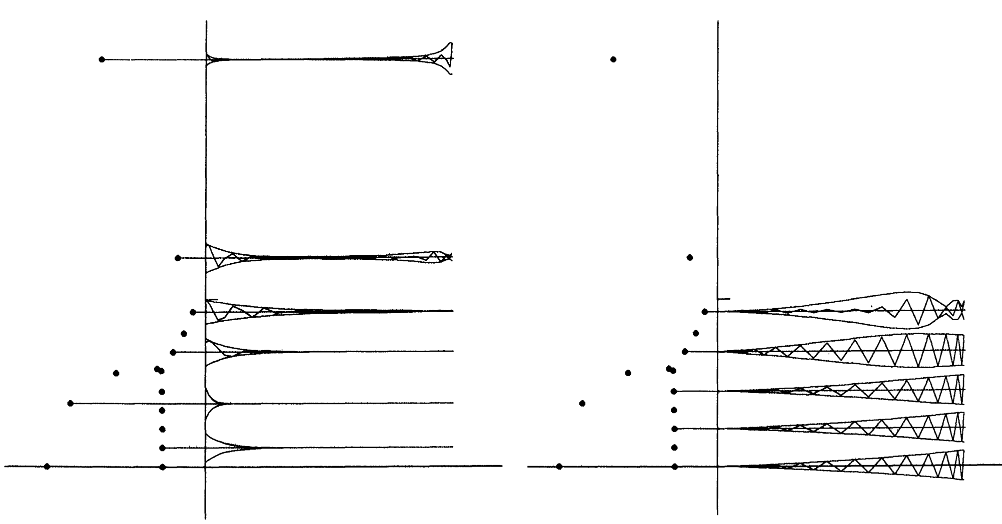
Figure 6 repeats Fig. 5, but with the matrix D_{28}^C modified by random perturbations of magnitude 10^{-8}, as in Fig. 3(b). Evidently the eigenvectors corresponding to eigenvalues on the vertical line still have the form (3), but with new values of λ that satisfy (5).

What about the spurious eigenvalues along the large curves in Figs. 2–4? Empirically, they have size $O(N^2)$ as $N \to \infty$. The following argument explains why at least some of the numerically computed eigenvalues must be very large. A sizable number of the eigenvalues lie along the line (5), with magnitudes much less than they would have had in exact arithmetic. On the other hand rounding errors have little effect on the product of all N eigenvalues—the determinant, which in these problems is a sum



(a) (b)

FIG. 5. *Exact ≈ computed eigenvectors of the Chebyshev differentiation matrix* D_N^C *with* $N = 28$. *Real parts and moduli are shown. Plot* (b) *shows what remains after the dominant exponential term is removed* (4).



(a) (b)

FIG. 6. *Same as Fig.* 5, *but computed in* 8*-digit precision.*

of products of matrix elements that is not subject to significant cancellation. Therefore some of the other eigenvalues must compensate by becoming much larger.

There has been some concern that spectral methods based on Legendre points may be unreliable for large N because of inaccuracy in computing these points. However, our experiments indicate that artificially introduced perturbations in the Legendre points generate a pattern of erroneous eigenvalues that is quite different from the ones shown in Figs. 2–4. This suggests that at least for $N < 100$ or so, errors in computing the Legendre points probably have less influence than errors in the subsequent matrix calculations. Legendre spectral methods are indeed more unreliable than Chebyshev, but only because they have no outlying eigenvalues to mask the effects of rounding error that are present in both cases.

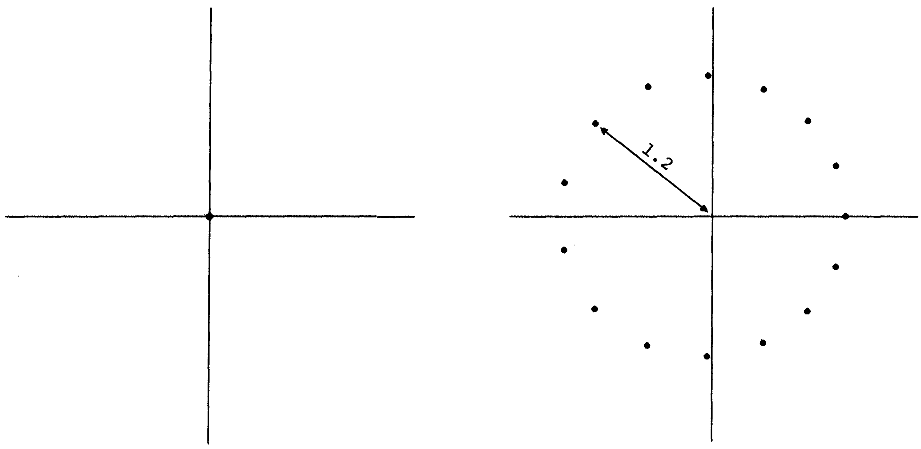
For *second*-order spectral differentiation, with zero boundary conditions at both endpoints, the eigenvalues of the differentiation matrix are real and negative [6] and have maximum magnitude $O(N^4)$ for both Chebyshev and Legendre points. Although these differentiation matrices are not normal, experiments show that their eigenvalues are less sensitive to perturbations than in the first-order case. Perhaps this is not too surprising, since the eigenvalues in the second-order problem are approximations to physically meaningful eigenvalues for the corresponding differential equation. The first-order differentiation operator of (1), by contrast, has no eigenvalues, so the eigenvalues of the corresponding differentiation matrix are wholly numerical in origin.

4. A related problem. It is well known that the eigenvalues of a skew-symmetric matrix are well conditioned as functions of the matrix elements, and therefore are affected negligibly by rounding errors [19]. This is the situation for the Fourier differentiation matrices of Figs. 1 and 2, and also for many finite difference differentiation matrices. On the other hand Figs. 3 and 4 show that the eigenvalues of D_N^C and D_N^L must be extremely ill conditioned. Neither of these matrices is skew-symmetric, and in fact, both are very close to being defective.

To see why this is so, consider what would have happened if the boundary condition $p(1)=0$ had not been imposed in step (b) of § 1. Specifically, let $\hat{D}_N^C$ be the differentiation matrix of dimension $N+1$ that results from degree-N polynomial interpolation of $N+1$ arbitrary data values v_j at $N+1$ Chebyshev points (2), including $x_0=1$, with no boundary condition. If v is interpolated by a polynomial $p(x)$ of degree N, $p'(x)$ will pass through the points $\hat{D}_N^C v$, p'' through $(\hat{D}_N^C)^2 v$, and so on. After $N+1$ differentiations the result is zero. Therefore $\hat{D}_N^C$ must be nilpotent, with $(\hat{D}_N^C)^{N+1}=0$. All of its eigenvalues are zero, but $(1, 1, \cdots, 1)^T$ is the only eigenvector: $\hat{D}_N^C$ is similar to a single Jordan block of dimension $N+1$. This means that $\hat{D}_N^C$ is completely defective, or "nonderogatory," with characteristic polynomial z^{N+1}. Therefore its eigenvalues will move distances of order $\varepsilon^{1/(N+1)}$ in response to a perturbation of the matrix entries, hence of the lower-order coefficients of the characteristic polynomial, of size ε.

Figure 7 confirms this prediction. The eigenvalues of $\hat{D}_N^C$ with $N=14$ have been computed in double precision with EISPACK. Instead of coinciding at the origin, they lie approximately on a circle of radius 1.2. It would be an exact circle centered at the origin if rounding errors affected only the degree-0 term in the characteristic polynomial.

This relatively familiar example illustrates how sensitive the eigenvalues of a defective matrix may be to small perturbations. The eigenvalue behavior of Figs. 2–4 is a more complicated manifestation of the same phenomenon. D_N^C is actually the same matrix as $\hat{D}_N^C$, but with the first row and column deleted. Thus it is a rank 2



(a) *Exact* (b) 16 *digits*

FIG. 7. *Exact and computed eigenvalues of the Chebyshev differentiation matrix* $\hat{D}_N^C$ (*no boundary conditions*) *with* $N=14$.

modification of $\hat{D}_N^C$, and in this sense very close to defective. The same argument holds for D_N^L.

An objection may be: What do EISPACK's errors in computing eigenvalues matter, since a spectral method needs only matrix multiplications? The answer is an elegant application of backward error analysis, as worked out by Wilkinson in the 1950s and 1960s [19]. The eigenvalues computed by EISPACK are the exact eigenvalues of some matrix $\tilde{D}$ that differs from D_N^C by order ε. Suppose that instead of an eigenvalue computation, we perform the various matrix-vector multiplications required by a spectral method. Again the result will be exact for some matrix $\tilde{\tilde{D}}$ that differs from D_N^C by order ε. $\tilde{\tilde{D}}-D_N^C$ may be five or ten times smaller than $\tilde{D}-D_N^C$, but the dashed barriers in Figs. 3 and 4 move relatively little if ε is changed by a constant factor. Therefore the eigenvalues of $\tilde{\tilde{D}}$ will still look approximately like those of $\tilde{D}$, as plotted in the figures, and these eigenvalues determine stability.

Indeed, the effects of Figs. 2-4 are felt even in exact arithmetic, if the initial differentiation matrix is rounded to machine precision just once.

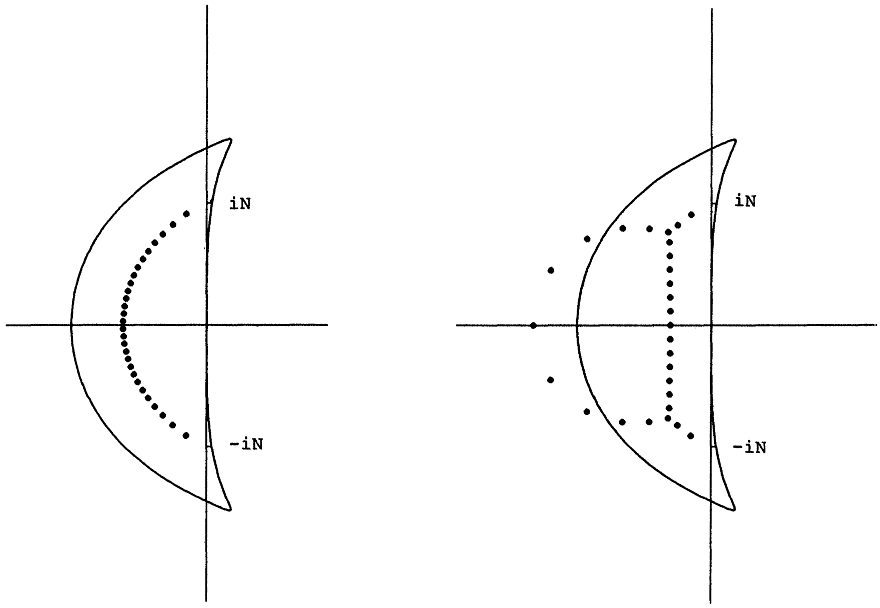
As a simpler example of the same kind of reasoning, is the matrix $\hat{D}_N^C$ of Fig. 7 power-bounded? Mathematically, yes, since it is nilpotent. Numerically, no—and this is confirmed by experiments.

5. Precision-dependent stability. For an indisputable demonstration that the erroneous eigenvalues of Figs. 2-4 should not be blamed on EISPACK, one can verify experimentally that they determine the stability or instability of a spectral method.

We took $N=28$ and solved (1) by Legendre spectral differentiation in space and the third-order Adams-Bashforth formula in time:

$$v^{n+1}=v^n+\tfrac{1}{12}D_N^L(23v^n-16v^{n-1}+5v^{n-2}). \tag{6}$$

The initial function was $f(x)=\cos^2(\pi x/2)$, with exact solution values taken at the three initial time steps. The time step was $\Delta t=\frac{1}{2}N^{-1}\approx .01786$. Figure 8 shows the computed eigenvalues of D_N^L in double and single precision, and superimposed on them, the stability region of the Adams-Bashforth formula for this value of Δt. Figure



(a) 16 *digits* (b) 8 *digits*

FIG. 8. *Computed eigenvalues of the Legendre differentiation matrix* D_N^L *with* $N=28$, *and the stability region for the third-order Adams-Bashforth formula with* $\Delta t = \frac{1}{2}N^{-1} \approx .01786$. *For stability the eigenvalues must lie within the stability region.*

8(a) indicates that in theory, the time integration ought to be stable. Figure 8(b) suggests that in 8-digit arithmetic, it will be unstable.

Here are the rather dramatic results at $t=1$, $x=x_N \approx -0.996442$:

$$\begin{aligned} \text{Exact:} \quad & u(x_N) \approx 0.999969, \\ \text{16-digit precision:} \quad & v_N \approx 0.995718, \\ \text{8-digit precision:} \quad & v_N \approx -6.93 \times 10^8. \end{aligned}$$

It is a familiar occurrence that problems of instability can be alleviated by switching to higher precision, but the usual reason is that the instability gets excited less strongly by rounding errors. The present example represents a very different situation, for in this case, higher precision makes the computation actually stable. We do not know of any other examples in which the machine precision determines the stability of a numerical calculation.

6. A variable-coefficient example involving Chebyshev points. After reading a preprint of this paper, Eli Turkel pointed out to us that he has encountered precision-dependent results in solving the following problem:

$$u_t = -xu_x, \qquad 1 \leqq x \leqq 1 \tag{7}$$

by a pseudospectral method based on Chebyshev points [17]. (The exact solution is $u(x,t) = u(x\,e^{-t}, 0)$.) The motivation for this problem is that both $x=1$ and $x=-1$ are outflow boundaries, so that no boundary conditions are mathematically required. Now the spectral differentiation process consists of interpolating $N+1$ data points at positions x_j for $0 \leqq j \leqq N$, differentiating the interpolant, and multiplying by $-x_j$. The exact eigenvectors are the monomials x^n, $0 \leqq n \leqq N$, sampled at the interpolation points, with corresponding eigenvalues $-n$. Thus this is a problem involving Chebyshev points that should nevertheless have a comfortable $\Delta t = O(N^{-1})$ stability restriction.

The eigenvalues may be real, but the matrix is by no means symmetric. If it were, rounding errors would have little effect. In fact, Fig. 9 shows that for $N = 64$ and 128, all but a few of the eigenvalues computed by EISPACK lie far from the real axis. (In both cases most of the eigenvalues lie in approximate pairs.) For larger N or lower machine precision, the situation becomes even worse, and Turkel reports that he has encountered instability even in double precision on a Cray computer (128 bits). Thus problem (7) provides another clear example of precision-dependent stability of spectral methods.

To confirm that the eigenvalues computed by EISPACK have relevance to the stability of time integrations, we again took initial data $f(x) = \cos^2(\pi x/2)$, and solved (7) by the third-order Adams–Bashforth formula (6) with $\Delta t = \frac{1}{2}N^{-1}$. Required additional starting values were taken from the exact solution. Table 1 shows some computed results at $x = x_{N/4} = 1/\sqrt{2}$, $t = 1$, where the exact value is ≈ 0.84212460. For the first column of results each spatial discretization was performed by explicit matrix multiplication, but the second is based on an FFT instead. At $N = 128$ the erroneous eigenvalues have once again had a catastrophic effect on stability. This happens eventually with $N = 64$, too, but only after a longer time integration.

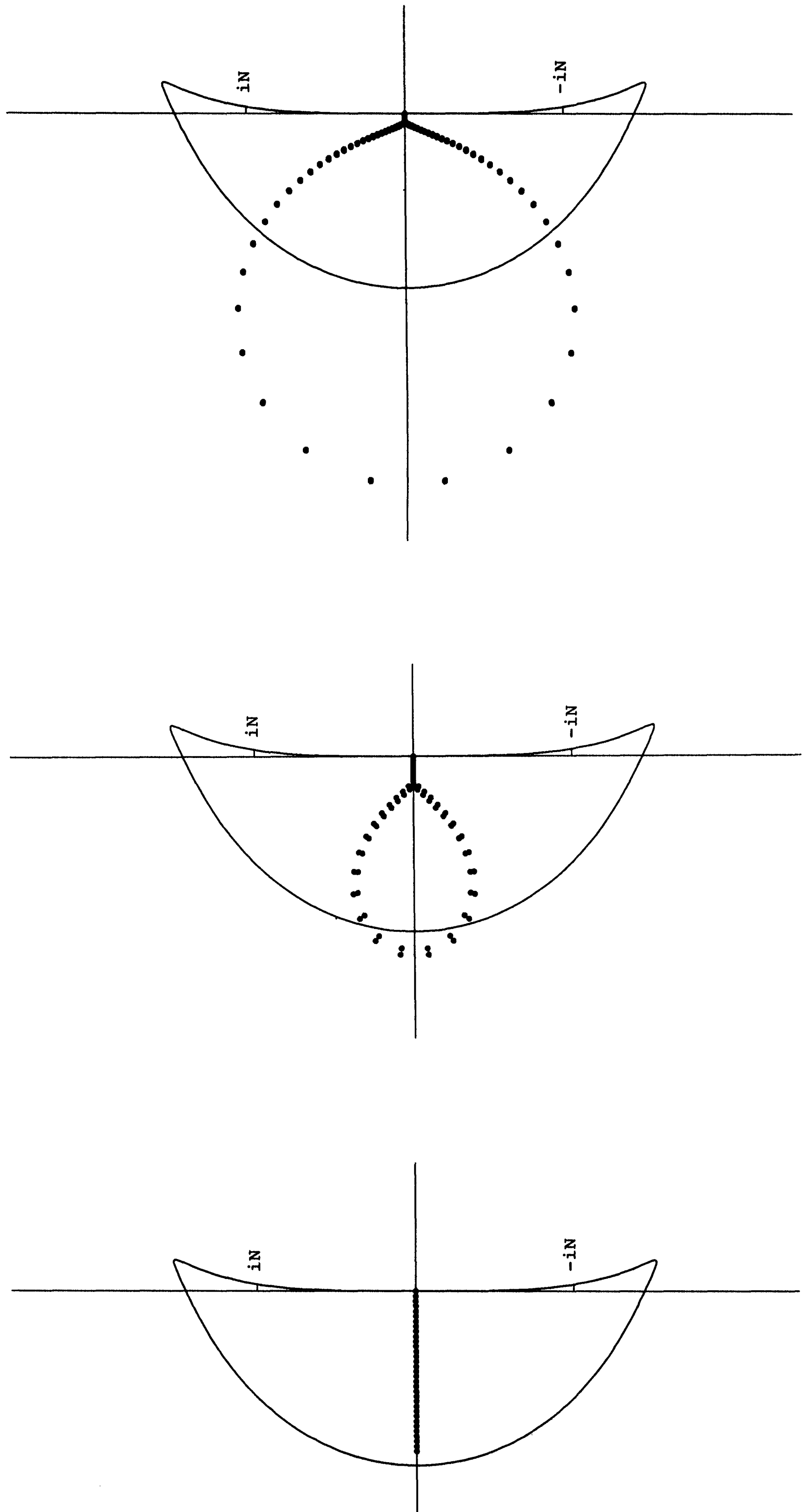
The second column above shows that the use of the FFT does not eliminate the stability problem in spectral differentiation. Now no matrix appears explicitly in the numerical algorithm, and certainly no matrix eigenvalues, but the eigenvalues still have their effect.

TABLE 1

	Matrix	FFT
$N = 32$	0.84212530	0.84212530
$N = 64$	0.84212470	0.84212470
$N = 128$	1.6×10^{60}	-7.2×10^{45}

7. Eigenvalue estimates based on the characteristic polynomial. We have considered three model problems: $u_t = u_x$ with Chebyshev points, $u_t = u_x$ with Legendre points, and $u_t = -xu_x$ with Chebyshev points. In all three cases the coefficients of the characteristic polynomial of the differentiation matrix are known exactly. (See [5, § 6] for the first problem. The coefficients for the second can be determined by the same method, and for the third they are easily obtained since the eigenvalues are $0, -1, \cdots, -N$.) Funaro [2] has pointed out that lower and upper bounds for the moduli of the matrix eigenvalues can be derived from these coefficients. But in several cases these bounds miss the correct order of dependence by a factor of N. Analogously disappointing results are obtained if one tries to estimate eigenvalues by means of matrix norms. The instability phenomenon described in this paper can explain these discrepancies.

Let the characteristic polynomial be $c_0 + \cdots + c_N z^N$, or $c_0 + \cdots + c_{N+1} z^{N+1}$ for the problem $u_t = -xu_x$, since the matrix there has dimension $N+1$. In each case the



(a) $N=32$ (b) $N=64$ (c) $N=128$

FIG. 9. *Computed eigenvalues (16-digit precision) of the Chebyshev differentiation matrix for* $u_t = -xu_x$, $N = 32, 64, 128$. *In each case the exact eigenvalues are* $-k$, $0 \leqq k \leqq N$. *The stability regions for the third-order Adams–Bashforth formula with* $\Delta t = \frac{1}{2}N^{-1}$ *are also shown.*

coefficients are all nonnegative; otherwise there would be eigenvalues in the right half plane. Therefore by the Eneström–Kakeya Theorem [10], we have

$$r \leqq |\lambda_k| \leqq R \tag{8}$$

for all eigenvalues λ_k, where

$$r = \min_k \left|\frac{c_k}{c_{k+1}}\right|, \qquad R = \max_k \left|\frac{c_k}{c_{k+1}}\right|. \tag{9}$$

Table 2 compares these bounds, as functions of N, with estimates of the actual eigenvalues in both exact and floating-point arithmetic.

In four of the six cases listed in Table 2, the rigorous bound (8) is too conservative by a factor $O(N)$ for the exact eigenvalues, yet in every case it is on target for the eigenvalues computed with rounding errors. This can be explained as follows. Rounding errors are equivalent to the introduction of small perturbations in the entries of the differentiation matrix, and these induce small relative perturbations in the coefficients of the characteristic polynomial.[2] Therefore, a bound such as (8) that is based solely on the relative magnitude of these coefficients must also approximately hold for eigenvalues computed with rounding errors. But we know that in the presence of rounding errors, all three of these problems have minimum and maximum eigenvalue moduli $O(1)$ and $O(N^2)$, respectively, not $O(N)$.

Thus eigenvalue estimates based on the characteristic polynomial, although far from sharp for the exact problem, have the virtue that they remain valid even in inexact arithmetic.

TABLE 2
Minimum and maximum moduli of eigenvalues of spectral differentiation matrices.

	$\min\|\lambda_k\|$			$\max\|\lambda_k\|$		
	Exact	Flt.-pt.	r	Exact	Flt.-pt.	R
Chebyshev, $u_t = u_x$	$\approx .46N$	$O(1)$	$1-\frac{1}{N+1}$	$\approx .089N^2$	$O(N^2)$	$\frac{1}{3}N^2+\frac{1}{6}$
Legendre, $u_t = u_x$	$\approx .66N$	$O(1)$	1	$\approx N$	$O(N^2)$	$\frac{1}{2}N^2+\frac{1}{2}N$
Chebyshev, $u_t = -xu_x$	0	0	0	N	$O(N^2)$	$\frac{1}{2}N^2+\frac{1}{2}N$

Note added in proof. A paper surveying what is known about the eigenvalues of spectral differentiation matrices is in preparation [20].

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[2] A characteristic polynomial is not always well conditioned as a function of the matrix elements, since cancellation may occur, but numerical experiments confirm that for these matrices the characteristic polynomial is well conditioned. For example, the dominant diagonal elements of D_N^C and D_N^L are large and negative, so no significant cancellation occurs in computing the trace, which is the coefficient of the term of second highest degree.

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