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NOTE

Properties of Collocation Third-Derivative Operators

Spectral methods for solving partial differential equations have become increasingly popular because of their ability to achieve high accuracy using relatively few grid points [1–2]. Of these, collocation methods are particularly well suited for problems having nonlinearities or complicated boundary conditions. This is because the independent variable is represented in terms of its values at a set of collocation grid points rather than as the coefficients of a spectral expansion. Using $u(x_i)$, $i=0, ..., N$, to denote these values at the collocation points x_i, the spatial differentiation of u may be represented by the operation

$$u_x(x_i) = \sum_{j=0}^{N} D_{ij} u(x_j), \quad i=0, ..., N, \tag{1}$$

where D is the derivative matrix operator associated with a particular choice of the x_i. The implementation of collocation methods is therefore similar to that of finite difference methods, except that the derivative matrix operator is full rather than banded.

The primary purpose of this note is to point out a difficulty which is experienced by some commonly used collocation schemes when integrating equations containing third spatial derivatives, for example,

$$u_t + au_x + abu_{xxx} = 0, \tag{2}$$

where a and b are constants, which arises in the study of dispersive waves. (When considering u as a function of the continuous variable x, we shall take it to denote the solution to a spatially continuous equation; in contrast, $u(x_i, t)$ will denote the solution to a spatially discretized equation.) Dispersive waves occur when the temporal frequency ω of each Fourier wave component is not in direct proportion to its spatial wave number k, so that the phase velocity $c=\omega/k$ is dependent upon k. For ion-acoustic waves in a plasma [3] and shallow water waves [4], for example, the dispersion relation is of the form $\omega = ak(1-bk^2)$, and the evolution of a small-amplitude waveform u consequently is described by (2). If the nonlinearity of the wave is significant, then the Korteweg de Vries equation, which under an appropriate scaling of the variables can be written

$$u_t - 6uu_x + u_{xxx} = 0, \tag{3}$$

applies [5–6]. When solving equations such as these numerically, an adequate representation of the third spatial derivative clearly is needed.

As an example, consider the initial boundary value problem

$$u_t = u_{xxx}, \quad u(-1, t) = 0, \quad u(1, t) = 0, \quad u_x(-1, t) = 0. \tag{4}$$

with $-1 \leqslant x \leqslant 1$, $t \geqslant 0$. Upon choosing a set of collocation points x_i, $i=0, ..., N$, the spatial differentiation in (4) may be represented by applying the collocation third-derivative operator,

$$u_{xxx}(x_i, t) = \sum_{j=0}^{N} D_{ij}^{(3)} u(x_j, t). \tag{5}$$

It is evident that the first two boundary conditions require $u(x_0)=0$ and $u(x_N)=0$. The third boundary condition may be implemented by applying Eq. (1) at x_N and substituting the boundary values for $u(x_0, t)$ and $u(x_N, t)$, leading to

$$u(x_{N-1}, t) = -\sum_{j=1}^{N-2} \frac{D_{Nj}}{D_{N,N-1}} u(x_j, t). \tag{6}$$

Substituting these values into (5), we find that the third spatial derivative at the remaining points, $x_1 \cdots x_{N-2}$, is represented by

$$\tilde{D}_{ij}^{(3)} = D_{ij}^{(3)} - \frac{D_{Nj}}{D_{N,N-1}} D_{i,N-1}^{(3)}, \quad i, j = 1, ..., N-2, \tag{7}$$

and the spatial discretization of Eq. (4) may therefore be written

$$u_t(x_i, t) = \sum_{j=1}^{N-2} \tilde{D}_{ij}^{(3)} u(x_j, t), ..., \quad i=1, N-2. \tag{8}$$

A desirable property of the semi-discrete approximation (8) is that it be asymptotically stable, i.e., that for a given N the solution remains bounded on some norm as $t \to \infty$. That the analytical solution exhibits such a property can be

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demonstrated by multiplying both sides of Eq. (4) by u and integrating over the interval $[-1, 1]$. Integrating the right-hand side by parts and applying the boundary conditions then leads to

$$\frac{d}{dt}\int_{-1}^{1} u^2\,dx = -\frac{1}{2}u_x^2(1), \tag{9}$$

implying that the L_2 norm $\|u\|_2 = (\int_{-1}^{1} u^2\,dx)^{1/2}$ must remain bounded. However, the solution to (8), given formally by $u(x_i, t) = \exp(\tilde{D}^{(3)}t)\,u(x_i, 0)$, will satisfy this property only if all of the eigenvalues of $\tilde{D}^{(3)}$ have nonpositive real parts.

The most commonly used orthogonal bases for functions on a bounded interval are the Legendre and Chebyshev polynomials. The usual choice for the collocation points is the Gauss–Lobatto points, corresponding to the extrema of an orthogonal polynomial of degree N, together with the end points $x_0 = -1$ and $x_N = 1$. The eigenvalues of the first and second derivative operators in these representations have eigenvalues that are negative definite when the corresponding analytical problem is bounded [7–8]. Such is not the case, however, for the eigenvalues of the third-derivative operator subject to the boundary conditions (4). In solving (6) analytically, it is found that the exact eigenvalues λ_n satisfy

$$\sqrt{3}\sin\sqrt{3}\,\lambda_n^{1/3} + \cos\sqrt{3}\,\lambda_n^{1/3} = e^{3\lambda_n^{1/3}} \tag{10}$$

and are real and negative definite. We computed the eigenvalues of the matrices $\tilde{D}^{(3)}$ in the Legendre and Chebyshev representations with 16-digit precision using an EISPACK-based routine. The eigenvalues, shown in Figs. 1–2, fall into two families: eigenvalues which are purely real and negative, and eigenvalues which are complex and lie along a bow-shaped curve. When $N = 42$, 20 of the 40 eigenvalues belong to each family. The eigenvalues of smallest modulus are in good agreement with the exact eigenvalues, the first 10 eigenvalues being accurate to one part in 10^6 when $N = 42$ (see Table I). The outlying complex eigenvalues have positive real parts. For sufficiently large N, we find that the real and imaginary parts of the eigenvalues having the largest positive real part for a given N grow in proportion to N^6. The approximate empirically determined constants of proportionality are given in Table II.

The Legendre and Chebyshev collocation techniques thus are unsuitable for solving Eq. (4) and are likely to be poor choices for solving any problem involving third derivatives.

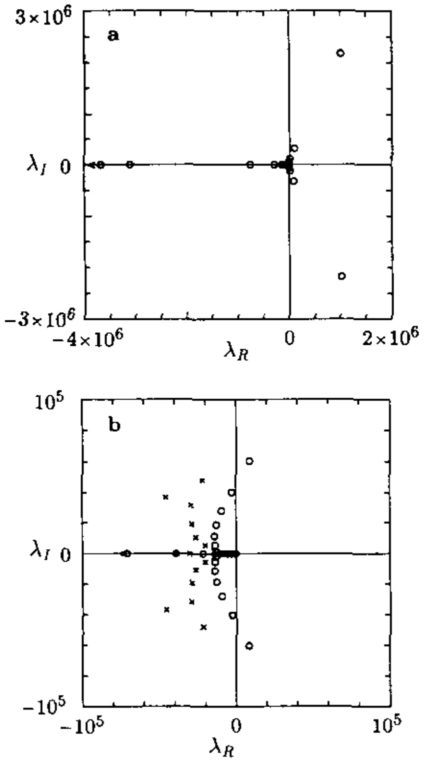

FIG. 1. Eigenvalues of $\tilde{D}^{(3)}$, the collocation third derivative operator for Eq. (4), in the Chebyshev representation with $N = 42$. In (a) all except an outlying eigenvalue at $(-4.77\times10^7, 0)$, indicated by the arrow, are plotted. In (b) the region near the origin is magnified (crosses indicate eigenvalues of $\hat{D}^{(3)}$).

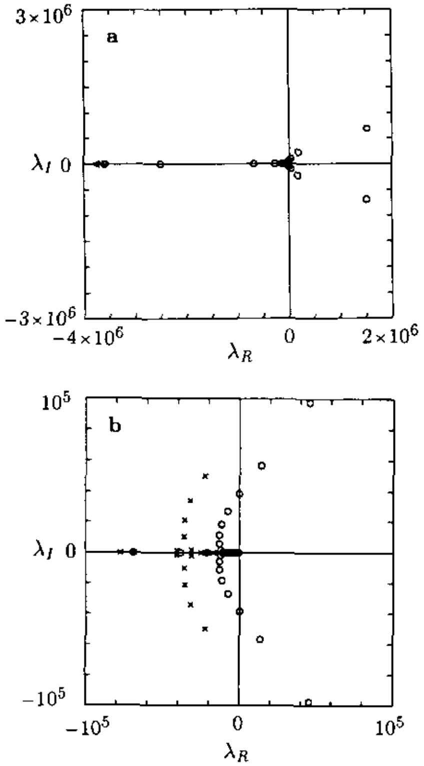

FIG. 2. Eigenvalues of $\tilde{D}^{(3)}$, the collocation third derivative operator for Eq. (4), in the Legendre representation with $N = 42$. In (a) all except an outlying eigenvalue at $(-2.68\times10^7, 0)$, indicated by the arrow, are plotted. In (b) the region near the origin is magnified (crosses indicate eigenvalues of $\hat{D}^{(3)}$.

TABLE I

Comparison of Exact and Approximate Eigenvalues[a]

n	Exact[b]	Cheb. collocation ($N=42$)	Cheb. τ ($N=42$)
1	9.4824069355200	9.4824069355629	9.4824131787527
2	60.693658411895	60.693658411071	60.693677806720
3	189.48497983854	189.48497984430	189.48485026156
4	431.65225182405	431.65225175753	431.65319541671
5	822.99854299525	822.99854351508	822.99355584868
6	1399.3268167680	1399.3268129680	1399.3471124458
7	2196.4400375254	2196.4400650976	2196.3783616258
8	3250.1411696432	3250.1409719368	3250.2066849998
9	4596.2331774974	4596.2346079268	4597.2232630109
10	6270.5190254638	6270.5163226666	6259.4004858211

[a] Of $\partial^3/\partial x^3$ for the boundary conditions of Eq. (4). All eigenvalues are negative.

[b] Exact eigenvalues are given by Eq. (10).

Indeed, we have found computational instability to be inevitable when solving the Korteweg–de Vries equation (3) by these means. One is thus motivated to seek modifications to the collocation technique which restore stability to such computations. One such modification was suggested by Bresson and Pavoni [9], who consider Chebyshev collocation solutions to

$$u_t + (\delta + \sigma u)\, u_x + \alpha u_{xxx} = 0, \qquad u(-1, t) = u(1, t) = u_x(1, t) = 0, \tag{11}$$

where $-1 \leqslant x \leqslant 1$, $t \geqslant 0$, and δ, σ, and α are constants. They attempt to impose the derivative boundary condition by constructing the third-derivative operator according to $D^{(3)} = D^2 \hat{I} D$, where D is the first-derivative operator, $\hat{I}_{ij} = \delta_{ij} - \delta_{i0}\delta_{j0}$, $i, j = 0 \cdots N$, and δ_{ij} is the Kroneker delta. The homogeneous Dirichlet conditions are subsequently imposed. The resulting third-derivative operator has eigenvalues that are negative definite, and the integration of Eq. (1) consequently is stable. However, we find that the numerical solution does not exactly satisfy the derivative boundary condition when this method is employed.

TABLE II

Proportionality to N^6 of Eigenvalue of $\tilde{D}^{(3)}$ with Maximum Positive Real Part[a]

Type	λ_R	λ_I
Chebychev	2.8×10^6	6.1×10^6
Legendre	4.0×10^6	4.0×10^6

[a] This eigenvalue, denoted λ_{max}, is given by $\lambda_{max} = (\lambda_R + i\lambda_I)(N/50)^6$.

An alternative approach is to consider problem (4) initially in the tau formulation [2], representing $u(x, t)$ as a truncated expansion $\sum_{k=0}^{N} \hat{u}_k R_k(x)$ in the orthogonal functions $R_k(x)$ and choosing the final three coefficients to satisfy the boundary conditions. In the Chebyshev tau representation, the third-derivative operator is $A^{(3)} = A^3$, where $A_{ij} = 2j/(1 + \delta_{i0})$, $i + j$ odd, $A_{ij} = 0$, $i + j$ even. The boundary conditions (4) are imposed by eliminating $\hat{u}_{N-2}$, $\hat{u}_{N-1}$, and $\hat{u}_N$ through the relations

$$\hat{u}_{N-2} + \hat{u}_{N-1} + \hat{u}_N = -\sum_{k=0}^{N-3} u_k, \tag{12}$$

$$\hat{u}_{N-2} - \hat{u}_{N-1} + \hat{u}_N = -\sum_{k=0}^{N-3} (-1)^k u_k, \tag{13}$$

$$(N-2)^2 \hat{u}_{N-2} + (N-1)^2 \hat{u}_{N-1} + N^2 \hat{u}_N = -\sum_{k=0}^{N-3} k^2 u_k, \tag{14}$$

yielding a reduced operator $\tilde{A}^{(3)}$ whose eigenvalues have negative real parts. The differentiation algorithm can then be imposed on the collocation variables u_i, $i = 2, ..., N-1$, through the operator $\hat{D}^{(3)} = \tilde{T} \tilde{A}^{(3)} \tilde{T}^{-1}$, where

$$\tilde{T}_{ij} = T_j(x_i), \quad i = 2, ..., N-1, j = 0, ..., N-3, \tag{15}$$

and $T_j(x)$ is the Chebyshev polynomial of degree j. The similarity transform preserves the negative-definite eigenvalues of $\tilde{A}^{(3)}$, and $\hat{D}^{(3)}$ is therefore suitable for integrating Eq. (4). We found that employing $\hat{D}^{(3)}$ to treat the third derivative led to satisfactory solutions of Eq. (11), whereas employing $\tilde{D}^{(3)}$ always led to numerical instability. Similar results were obtained in the Legendre polynomial representation.

To summarize, we have found that the collocation third-derivative operators in the Legendre and Chebyshev representations possess eigenvalues having sizable positive real parts, and are, therefore, unsuitable for computing solutions to problems such as (4). While these results do not directly bear on the usefulness of these methods for solving more complicated equations such as (2), (3), or (11), they do suggest that the Legendre and Chebyshev collocation methods are best avoided when solving equations containing third spatial derivatives. Such caution is borne out by our observation that numerical instability is inevitable when solving Eqs. (3) or (11) by such means. The Legendre and Chebyshev tau approximations are not so hindered, and the spectral solution of equations involving third derivatives on a bounded interval should, therefore, be approached either by these methods or by transforming the tau third-derivative operator to a collocation basis as described above.

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