Transport Eigenvalue Problems—Effect of Order of Approximation and Step Size on Solution Accuracy

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In the modeling of energy and mass transport processes, linear parabolic partial differential equations often result. By formulating series solutions these equations reduce to eigenvalue problems, which are more readily solved. Although evaluating eigenvalues and eigenfunctions is not trivial, we expect better accuracy than by numerically solving the original PDE. In addition, such analytical solutions are useful for checking numerical solutions of nonlinear problems that are extensions of their linear counterparts. Ybarra and Eckert (1980) use a finite-difference procedure to evaluate the eigenvalues and eigenfunctions in their solution of viscous heating problems in slit flow; Dinh and Armstrong (1982) then use these analytical results to check the accuracy of their approximate solutions.

Here we report how the accuracy of the eigenproblem calculations depends on the order of approximation of the differential equation and step size selected. Such knowledge provides a needed guideline to balance the order of approximation with the step size for an accurate solution with a reasonable expenditure of computer time. Although accuracy of the solution is the prime criterion, computer time can be important, particularly in process simulation packages where such a solution is required many times. We recommend use of higher-order approximations rather than smaller step size for accuracy and reduced computational costs.

For illustration we present the solution of the following differential equation:

$$(1-\eta^2)\frac{\partial\theta}{\partial\psi}=\frac{\partial^2\theta}{\partial\eta^2} \tag{1}$$

subject to the boundary conditions

$$\begin{aligned}&\frac{\partial\theta}{\partial\eta}=0 \text{ at } \eta=0\\ &\theta=0 \text{ at } \eta=1\\ &\theta=1 \text{ at } \psi=0\end{aligned} \tag{2}$$

This equation models either heat or mass transfer of a Newtonian fluid at large Peclet numbers in a plane Poiseuille flow. Brown (1960) published an accurate solution to this problem, and we shall use his results to assess the accuracy of our eigenvalues and eigenfunctions.

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A series solution can be constructed by the classical technique of separation of variables (Churchill, 1963)

$$\theta(\psi,\eta)=\sum_{n=1}^{\infty}C_nF_n(\eta)G_n(\psi) \tag{3}$$

The separation process yields a trivial solution for $G_n(\psi)$

$$G_n(\psi)=\exp(-\lambda_n\psi) \tag{4}$$

and results in the following Sturm-Liouville problem:

$$F''(\eta)+\lambda(1-\eta^2)F(\eta)=0 \tag{5}$$

subject to the boundary conditions

$$\begin{aligned}F'(0)&=0\\ F(1)&=0\end{aligned} \tag{6}$$

This boundary-value problem has an infinite set of solutions $F_n(\eta)$ corresponding to an infinite set of eigenvalues λ_n that can be evaluated, as now will be described.

SOLUTION PROCEDURE

Since Eq. 5 is a linear second-order differential equation of the form

$$y''(x)+f(x)y(x)=0 \tag{7}$$

the solution can be generated by approximating the differential equation and boundary conditions with a set of difference equations; the resulting set of algebraic equations must then be satisfied at equally spaced points in the relevant interval (Hildebrand, 1974). Ybarra and Eckert (1980) outlined the procedure of how the difference equations are constructed. The general form of the equation to solve is

$$\mathbf{Af}=\lambda\mathbf{Bf} \tag{8}$$

which is a generalized eigenvalue problem.

Since we are interested in the effect that the order of approximation has on the accuracy of the eigenproblem solution, we tested three orders of approximation: third, fifth, and seventh. Their difference equations follow:

Third-Order

For $n = 2,3,\ldots M$:

$$y_{n+1} - 2\left(1 - \frac{h^2}{2} f_n\right) y_n + y_{n-1} = 0 \tag{9}$$

Fifth-Order

For $n = 2,3,\ldots M$:

$$\left(1 + \frac{h^2}{12} f_{n+1}\right) y_{n+1} - 2\left(1 - \frac{5h^2}{12} f_n\right) y_n + \left(1 + \frac{h^2}{12} f_{n-1}\right) y_{n-1} = 0 \tag{10}$$

Seventh-Order

For $n = 3,4,\ldots M-1$:

$$-\frac{h^2}{240} f_{n+2} y_{n+2} + \left(1 + \frac{h^2}{10} f_{n+1}\right) y_{n+1} - 2\left(1 - \frac{97h^2}{240} f_n\right) y_n + \left(1 + \frac{h^2}{10} f_{n-1}\right) y_{n-1} - \frac{h^2}{240} f_{n-2} y_{n-2} = 0 \tag{11}$$

For $n = 2$:

$$\left(1 + \frac{3h^2}{40} f_1\right) y_1 - 2\left(1 - \frac{209h^2}{480} f_2\right) y_2 + \left(1 + \frac{h^2}{60} f_3\right) y_3 + \frac{7h^2}{120} f_4 y_4 - \frac{h^2}{40} f_5 y_5 + \frac{h^2}{240} f_6 y_6 = 0 \tag{12}$$

For $n = M$:

$$\frac{h^2}{240} f_{M-4} y_{M-4} - \frac{h^2}{40} f_{M-3} y_{M-3} + \frac{7h^2}{120} f_{M-2} y_{M-2} + \left(1 + \frac{h^2}{60} f_{M-1}\right) y_{M-1} - 2\left(1 - \frac{209h^2}{480} f_M\right) y_M + \left(1 + \frac{3h^2}{40} f_{M+1}\right) y_{M+1} = 0 \tag{13}$$

The difference equations determine the exact form of the six equal intervals ($M = 6$). For our example problem, we obtain the same $\boldsymbol{A}$ matrix for any approximation

$$\mathbf{A} = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 1 & -2 \end{bmatrix} \tag{14}$$

whereas the $\boldsymbol{B}$ matrix form we obtain is dependent on the order of approximation. In the following equation, the symbols X, +, and * represent the additional nonzero matrix elements entered as the order increases from third to fifth to seventh, respectively. Note the seventh row and column are excluded because at the external boundary $y_{M+1} = 0$.

$$\mathbf{B} = \begin{bmatrix} X & 0 & 0 & 0 & 0 & 0 \\ + & X & + & * & * & * \\ * & + & X & + & * & 0 \\ 0 & * & + & X & + & * \\ 0 & 0 & * & + & X & + \\ 0 & * & * & * & + & X \end{bmatrix} \tag{15}$$

Equations 9 through 13 can be used to determine all the elements of the matrix $\boldsymbol{B}$ except for the first row. The only nonzero element in that row is the first, which is $(h^2/2)f_1$.

The generalized eigenvalue problems were solved on Purdue University's CDC 6600 computer using the RGGEIG subroutine in the Argonne National Laboratory's EISPACK package. Since Sturm-Liouville problems possess only real eigenvalues, we modified the RGGEIG subroutine to obtain a accurate solution with reasonable computer time and storage allocation.

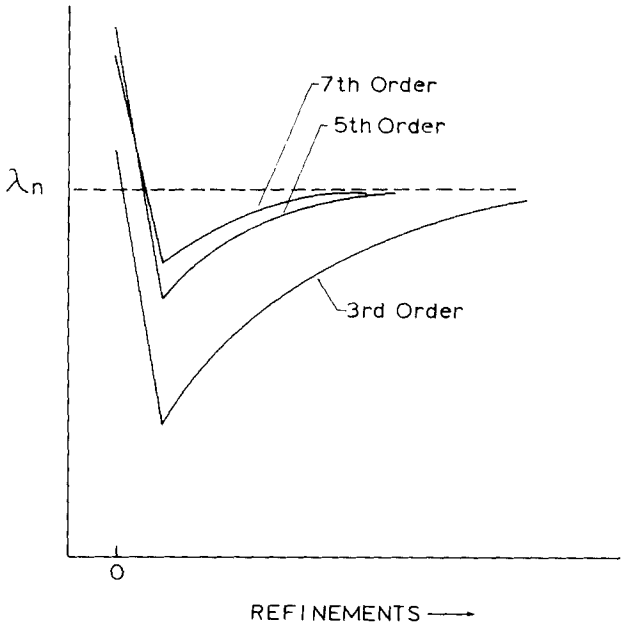

Figure 1. Comparison of an estimate of an eigenvalue with its true value depends on order of approximation and step size.

RESULTS AND DISCUSSION

Figure 1 is a generalization of how decreasing the step size (refining the difference scheme) improves the estimation of the nth eigenvalue. For all orders of approximation, the initial estimates of λ_n overshoot the true value, while successive refinements underestimate λ_n. The fifth and seventh orders converge to an accurate solution with fewer refinements than the third order. Each refinement introduces a higher eigenvalue and eigenfunction and improves the estimate.

Table 1 shows how the estimation of the tenth eigenvalue varies with the order of approximation and number of steps. Even after 100 steps the third-order approximation produces an eigenvalue that deviates from Brown's (1960) by nearly 1%. The fifth- and seventh-order approximations are closer to Brown's value in many fewer steps. The advantage of the seventh order over the fifth is that its initial eigenvalue estimates are always better. Table 1 also gives the CPU time consumed by subroutine RGGEIG to solve Eq. 8 for the eigenvalues and eigenvectors. The seventh order is preferred because it provides superior accuracy with less CPU time. For example, a 40-step, seventh-order scheme provides a better estimate to λ_{10} than a 100-step, third-order scheme, and does so in one-tenth the CPU time.

The eigenfunctions $F_n(\eta)$ have a convergence similar to the eigenvalues; Table 2 shows the sixth eigenfunction at selected values of η. The seventh-order approximation is superior to the lower-order ones throughout the interval $0 \leq \eta \leq 1$ except near zero, when few steps are used. With lower-order approximations the eigenfunctions are initially predicted better at η near zero because of the upper-row sparsity (boundary condition at $\eta = 0$) of matrix $\boldsymbol{B}$ in Eq. 15.

The errors in $F_n(\eta)$ are magnified at low η when the eigencoefficients are evaluated because the weighting function $(1 - \eta^2)$ is largest near $\eta = 0$, as can be seen in Eq. 16:

$$C_n = \frac{\int_0^1 (1 - \eta^2) F_n(\eta) d\eta}{\int_0^1 (1 - \eta^2) F_n^2(\eta) d\eta} \tag{16}$$

TABLE 1. ACCURACY OF THE TENTH EIGENVALUE DEPENDS ON THE ORDER OF APPROXIMATION AND NUMBER OF STEPS

	λ_{10}					
	Order					
Steps	Third		Fifth		Seventh	
20	1,118.97	(0.83)	1,335.58	(1.08)	1,370.58	(1.03)
40	1,341.17	(5.14)	1,412.22	(6.90)	1,414.74	(6.86).
80	1,399.19	(35.44)	1,418.19	(50.53)	1,418.36	(49.07)
100	1,406.24	(66.24)	1,418.51	(94.78)	1,418.58	(95.83)
		Brown (1960)	$\lambda_{10} = 1{,}418.80$			

CPU time(s) in parentheses is the time required to solve Eq. 8

Thus, the grid must be refined enough to insure $F_n(\eta)$ is reasonably predicted. The actual number of steps used in eigenproblems depends on the accuracy required by the user; however, we found that the nth eigencoefficient could be predicted within 1% of Brown's (1960) if we used $5n$ difference intervals. Since series solutions typically converge slowly as terms are added, more than 20 terms may be needed for a reasonable prediction of $\theta(\eta,\psi)$ at small ψ. If solutions only at $\psi > 0.01$ are of interest, fewer terms are needed because $G_n(\psi)$ exponentially reduces the nth term's contribution to $\theta(\eta,\psi)$. Therefore, a finely divided difference scheme is not be needed and computer time can be reduced by increasing the step size. Since the numerical errors are smoothed by averaging processes, low levels of refinement would also suffice for modeling of bulk transport effects.

Integration of Eq. 16 for the higher eigencoefficients can be subject to error because the higher eigenfunctions change rapidly between successive grid points. These eigenfunctions are of such a nature that they cross the η axis $n-1$ times between $0 < \eta < 1$. Estimates were improved at a fixed step size by spline fitting the eigenvector before integrating Eq. 16.

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NOTATION

A = matrix in the general eigenvalue problem
B = matrix in the general eigenvalue problem
C_n = eigencoefficients in Eq. 3
f = variable coefficient of x in Eq. 7
f = eigenvector representing the eigenfunction at the specified grid points
F = separation function in η only
G = separation function in ψ only
h = step size of finite difference
M = number of intervals in finite-difference scheme

TABLE 2. ACCURACY OF THE SIXTH EIGENFUNCTION DEPENDS ON THE ORDER OF APPROXIMATION AND NUMBER OF STEPS

		$F_6(\eta)$		
		Order		
η	Steps	Third	Fifth	Seventh
0.1	20	−0.58372	−0.60493	−0.60918
	40	−0.56606	−0.56570	−0.56564
	80	−0.56198	−0.56126	−0.56125
	100	−0.56149	−0.56096	−0.56095
		Brown (1960)	$F_6(0.1) = -0.56064$	
0.5	20	−0.53195	−0.59971	−0.60748
	40	−0.60504	−0.62435	−0.62480
	80	−0.62174	−0.62685	−0.62688
	100	−0.62370	−0.62701	−0.62702
		Brown (1960)	$F_6(0.5) = -0.62717$	
0.9	20	−0.98161	−1.06211	−1.07381
	40	−1.05020	−1.07116	−1.07167
	80	−1.06658	−1.07191	−1.07194
	100	−1.06853	−1.07195	−1.07196
		Brown (1960)	$F_6(0.9) = -1.07198$	

x = independent variable in Eq. 7
y = function of x in Eq. 7

Greek Letters

η = dimensional transverse distance
θ = dimensionless temperature
λ = eigenvalue
ψ = reduced axial distance

Subscripts

n = index corresponding to the nth eigenvector or eigenfunction as used in Eq. 3
n = grid point index used in Eqs. 9–13

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