Computing Eigenvalues of Ordinary Differential Equations by Finite Differences

By John Gary

1. Introduction. We will be concerned with finite difference techniques for the solution of eigenvalue and eigenvector problems for ordinary differential equations. There are various methods by which the continuous eigenvalue problem may be transformed into a discrete problem. We will be concerned with methods which reduce to a matrix eigenvalue problem $| A + \lambda B | = 0$. This paper may be divided into two parts. The first deals with numerical methods for the solution of the matrix eigenvalue problem. The second deals with the convergence of the solution of the discrete problem.

The eigenvalues of the matrix are found by a "rootfinder" technique. The determinant $| A + \lambda B |$ is computed for a given λ, usually by Gaussian elimination using interchanges. This is coupled with a rootfinder such as Muller's or Newton's which locates the zeros of the determinant [5, 6]. This method is usually rather slow in comparison with other methods for computing eigenvalues such as the Q-R algorithm. However, the matrices arising from differential equations are frequently banded ($a_{ij} = b_{ij} = 0$ for $| i - j | > t$), with the "bandwidth" t small in comparison with the order of the matrices. In some cases, only a single eigenvalue of the matrix is required and a good approximation for this eigenvalue may be available for use by the rootfinder. This is the case in hydrodynamic stability problems where the "least stable mode" is computed as a function of a parameter such as the Reynolds number. A good approximation for the eigenvalue at a new value of the parameter can be obtained by extrapolation from values previously computed. For these problems, the use of Gaussian elimination with a rootfinder may be competitive with the Q-R algorithm.

In Section 2, a convergent difference scheme for a simple eigenvalue problem is described. This is to be compared with the non-convergent difference scheme for the same problem described in Section 5. In Section 3 a comparison of the Laguerre [4] and Muller [5] rootfinders is made on the basis of efficiency and accuracy. Since the rootfinder is the most critical element in this computational scheme, it is important to choose the best one.

A "block" Hyman's method may be used to compute the determinant in place of Gaussian elimination. This method was suggested by B. Parlett. It can be most efficiently applied to a "block" Hessenberg matrix of the form

$$\begin{vmatrix} E_1 & F_1 & 0 & & & \\ I & E_2 & F_2 & & & \\ 0 & & & & & \\ & & & & & \\ & & 0 & I & E_{N-1} & F_{N-1} \\ & & & 0 & I & E_N \end{vmatrix}.$$

The matrices E_i and F_i are matrices of low order, typically two-to-six. This type of matrix sometimes arises in eigenvalue problems. The "block" Hyman's method is described in Section 4.

The last three sections deal with the question of convergence. In Section 5 we give an example of a "natural" difference scheme for a simple eigenvalue problem which fails to converge. This scheme has truncation error of second order. A difference scheme for an initial-value problem must be stable as well as consistent in order to insure convergence. This example demonstrates that some sort of "stability" criterion is needed for difference schemes applied to boundary-value problems.

In Section 6 we note that a simple finite difference scheme, applied to a certain singular eigenvalue problem (that is, one with a continuous spectrum), converges. This simple example is included because finite difference methods are frequently applied to the singular equations which are generated by problems in inviscid hydrodynamic stability. It may be possible to prove some general results concerning convergence for singular equations.

In the last section we provide a convergence proof for a certain difference scheme for a self adjoint eigenvalue problem of arbitrary order. The fact that both the difference scheme and the differential equation allow a variational formulation is essential to the proof.

2. The Finite Difference Method. We wish to obtain the eigenvalues and eigenvectors of an ordinary differential equation or system of equations. The differential equation is replaced by a homogeneous system of difference equations [10]. The zeros of the determinant of this system, that is, the eigenvalues, are then found by using a rootfinder. We used a rootfinder due to Laguerre [4] and also one due to Muller [5].

For example, suppose we wish to solve the following eigenvalue problem,

$$u' - v = 0,$$

(2.1)

$$v' + \lambda u = 0, \qquad u(0) = u(\pi) = 0,$$

whose solution is $\lambda = m^2$, $u = \sin(mx)$, $v = m \cos(mx)$. The finite difference equations are

$$U_{i+1} - U_i - hV_i = 0, \quad \text{where} \quad U_i = u(ih), \qquad 0 \leq i \leq M, h = \pi/M,$$

$$V_{i+1} - V_i + h\lambda U_{i+1} = 0, \qquad V_i = v(ih + h/2), \qquad 0 \leq i \leq M - 1.$$

Note that the values of U and V are staggered. These equations can be written in the form of a matrix equation $A(\lambda)W = (B + \lambda C)W = 0$, where W is the vector $W = (U_0, V_0, \cdots, V_{M-1}, U_M)$. This is a generalized eigenvalue problem. The exact solution is easily seen to be $\lambda = 4(\sin mh/2)^2/h^2$, $U_i = \sin mih$, $V_i = \sqrt{\lambda} \cos m(ih + h/2)$ for $m = 1, \cdots, M - 1$. This is a good approximation, for small mh, to the solution of (2.1).

The numerical method consists in the use of Gaussian elimination to compute the determinant $A(\lambda) = B + \lambda C$. The zeros of the determinantal equation $A(\lambda) = 0$ are then found by using a rootfinder. In the above problem we gain a slight advantage in roundoff error by using a first-order system rather than a second-order equation. The term $2 + \lambda h^2$ appears in the difference equations for the second-order

equation. If our machine carries eight digits and $h = 0.001$, then we cannot expect to obtain much more than two digit accuracy for the root $\lambda = 1$. By using the first-order system we avoid this difficulty.

The eigenvectors are found as follows. Assume that λ_0 is a good approximation to an eigenvalue, that is, $A(\lambda_0)$ is nearly zero. To avoid working with a singular matrix, form $B = A(\lambda_0) + \epsilon I$ (we might have $\epsilon = 0.01$, for example). Now use the inverse power method to find the eigenvector of B corresponding to the smallest eigenvalue of B [11]. If ϵ is small enough this should be the eigenvector of A corresponding to the eigenvalue λ_0.

The finite difference matrix associated with a differential equation will be banded, that is, the elements a_{ij} of the matrix satisfy the condition $a_{ij} = 0$ if $|i - j| > s$, where s is the "bandwidth." Of course, the subroutines used to evaluate the determinant and the eigenvector take advantage of this fact.

3. Rootfinders. We will discuss two rootfinders, that of Laguerre [4] and that of Muller [5]. We assume that we wish to locate the roots of a polynomial $P_n(z)$ of degree n. The algorithm we use for the Laguerre rootfinder is that given by Parlett, although Parlett was not forced to use a finite difference representation for $P_n{}'(z)$ and $P_n{}''(z)$ [4]. If we have already located the roots $z_1, \cdots, z_s$, and if $z^{(k)}$ is an approximation to z_{s+1}, then a new approximation $z^{(k+1)}$ is computed by

$$(3.1) \qquad z^{(k+1)} = z^{(k)} - \frac{t}{S_1 \pm \sqrt{((t-1)[tS_2 - S_1{}^2])}}, \qquad t = n - s$$

where

$$S_1 = \frac{P_n{}'(z^{(k)})}{P_n(z^{(k)})} - \sum_{i=1}^{s} \frac{1}{(z^{(k)} - z_i)},$$

$$S_2 = \frac{(P_n{}')^2 - P_n P_n{}''}{P_n{}^2} - \sum_{i=1}^{s} \frac{1}{(z^{(k)} - z_i)^2}.$$

The sign in the denominator of equation (3.1) is chosen to minimize $|z^{(k+1)} - z^{(k)}|$. Derivatives are represented by finite differences, thus,

$$P_n{}'(z^{(k)}) = [P_n(z^{(k)} + \delta) - P_n(z^{(k)} - \delta)]/2\delta$$

and

$$P_n{}''(z^{(k)}) = [P_n(z^{(k)} + \delta) - 2P_n(z^{(k)}) + P_n(z^{(k)} - \delta)]/\delta^2.$$

The parameter δ was usually taken to be $\delta = 0.01$ for the problems described here. The selection of δ causes some difficulty. If two roots are separated by a distance less than δ they are not likely to be located accurately. If δ is too small, roundoff error can cause trouble. The algorithm used for Muller's method is that given by Frank [6]. That is,

$$z^{(k+3)} = z^{(k+2)} + (z^{(k+2)} - z^{(k+1)}) d_{k+3},$$

where

$$d_{k+3} = \frac{-2F_{k+2}(1 + d_{k+2})}{b_{k+2} \pm [b_{k+2}^2 - 4F_{k+2} d_{k+2}(1 + d_{k+2})[F_k d_{k+2} - F_{k+1}(1 + d_{k+2}) + F_{k+2}]]^{1/2}},$$

$$b_{k+2} = F_k d_{k+2}^2 - F_{k+1}(1 + d_{k+2})^2 + F_{k+2}(1 + 2d_{k+2}),$$

$$F_k = P_n(z^{(k)}) \Big/ \prod_{i=1}^{s} (z^{(k)} - z_i).$$

For both methods the test for convergence is

$$|z^{(k+1)} - z^{(k)}| < \epsilon_1(|z^{(k+1)}| + \epsilon_2).$$

We wish to apply these finite difference methods to problems of hydrodynamic instability. In these problems it is necessary to locate that root with the largest imaginary part. Usually it is necessary to find only this one root. Therefore, a desirable rootfinder would find that root z_i closest to the initial guess $z^{(0)}$. Then, if the initial guess is reasonably close, the rootfinder should converge to the desired root. Since we wish to tabulate this root as a function of a parameter, a reasonable initial guess can usually be obtained by extrapolation from values already known.

In order to test these two rootfinders we used the following polynomial: $P_{29}(z) = (z^6 - 1.3^6)D_{23}(z)$. Here, $D_{23}(z)$ is the determinant of the system of equations (5.1) (see Section 5) with $M = 24$. We know that 11 roots of $D_{23}(z) = 0$ are given by $(\sin (mh))^2/h^2$ for $m = 1, \cdots, 11$. There is also one root at the origin and, of course, six roots on the circle of radius 1.3. We are interested in the order in which the roots are located, their accuracy, and the average number of functional evaluations required to find a root.

A program was written to compute the roots of $P_{29}(z)$ using the two rootfinders. Figure 3.1 shows the order in which the first ten roots were found. Roots corresponding to missing numbers are outside the range of the graph. For each of the ten roots the initial approximation $z^{(0)}$ had the same value. The different figures show the effect of changing $z^{(0)}$ for each of the two rootfinders.

In the bottom four figures we used the polynomial

$$P_{27}(z) = (z - 1 - .5i)(z - 2 - i)(z - 3 - 1.5i)(z - 4 - 1.5i)D_{23}(z).$$

Clearly, neither rootfinder would consistently locate that root closest to the initial approximation. However, Laguerre's method is somewhat superior to Muller's method in this respect. When $z^{(0)} = -1$, neither rootfinder located the closest root ($z = -1.3$) first. This fact makes it difficult to track roots as a function of a parameter.

The behavior of a rootfinder doubtless depends on the relative location of the roots. Therefore, one needs to run more cases than we have to make a proper comparison of the rootfinders.

The average number of functional evaluations required to compute ten roots for some of the cases in Figure 3.1 are given in the table below. The parameter ϵ_1 used in the convergence test was $\epsilon_1 = 0.001$.

Functional Evaluations		
$z^{(0)}$	*Laguerre*	*Muller*
$10i$	24.0	30.5
$2i$	19.2	13.1
-1	16.8	10.6

$$Z^{(o)} = 10i$$

$$Z^{(o)} = 4i$$

$$Z^{(o)} = -1.5 + 0.2i$$

$$Z^{(o)} = -1$$

$$Z^{(o)} = 5i$$

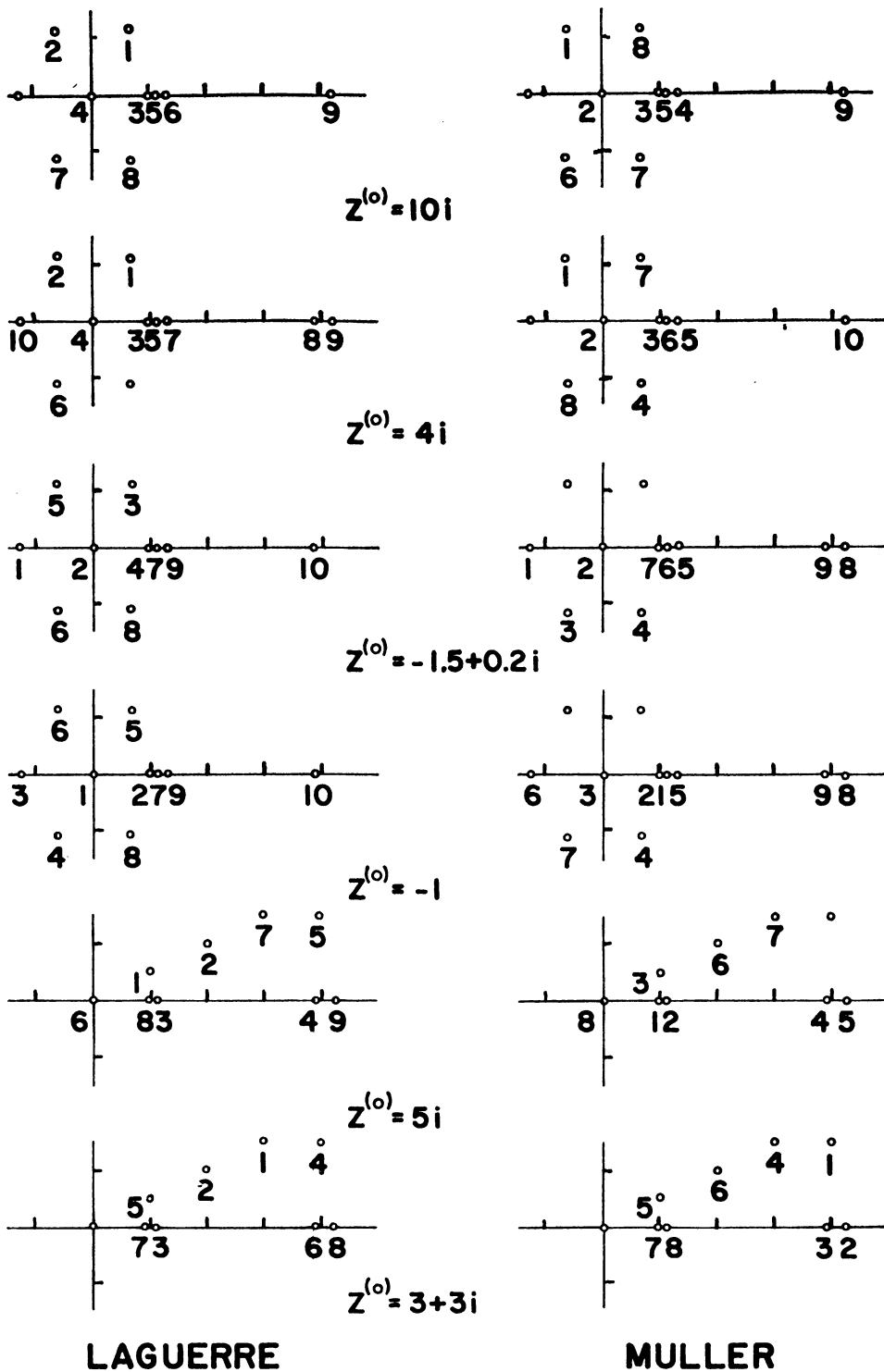$$Z^{(o)} = 3 + 3i$$

LAGUERRE   MULLER

FIGURE 3.1

An attempt was made to find all 29 roots using both rootfinders. The computed values for the last eleven roots are shown in the table below, along with the exact value of the root when known. The exact roots are given as real numbers, the computed roots are complex.

		Eigenvalues	
k	*Exact root*	*Laguerre's method*	*Muller's method*
19		$30.7692 + 10^{-14}i$	$14.5903 + 10^{-7}i$
20	36.7330	$36.7330 + 10^{-17}i$	$*36.7330 + 10^{-4}i$
21		$43.7708 + \text{'}10^{-10}i$	$8.54677 + 10^{-6}i$
22	43.7708	$38.3161 + 10^{-10}i$	$*50.7883 - 0.07i$
23		$45.1335 + 10^{-13}i$	$*54.9607 - 0.05i$
24	49.8142	$49.8142 + 10^{-10}i$	$*54.9607 + 0.06i$
25		$50.7843 + 10^{-14}i$	$*57.3763 + 0.04i$
26	54.4516	$54.4516 + 10^{-12}i$	$*45.1514 - 0.27i$
27		$54.9643 + 10^{-10}i$	$*37.4312 + 0.11i$
28	57.3667	$57.3667 + 10^{-10}i$	$*49.9389 - 0.14i$
29		$57.5094 + 10^{-15}i$	$57.5094 + 10^{-10}i$

* In these cases, the convergence criterion (with $\epsilon_1 = 1.E\text{-}6$) was not satisfied after 75 iterations.

In some cases, the iterates in Muller's method failed to satisfy the convergence criterion. Instead, the values of $z^{(k)}$ oscillated around the real axis.

As noted above, the values of $P_n'(z)$ and $P_n''(z)$ used in Laguerre's method are computed by finite differences using the increment δ. With $\delta = 0.01$ the method worked satisfactorily, but with $\delta = 0.001$ it sometimes failed to converge. This was apparently due to roundoff error in computing $P_n''(z)$. With $\delta = 0.01$ the computed values of $P_n'(z)$ did not change appreciably with small changes in δ; this was not true at $\delta = 0.001$. Therefore, the program should automatically vary δ if convergence is not obtained.

4. A Block Hyman's Method. In this section we will describe a second method for evaluating the determinant of the finite difference equations. This method was suggested to the author by B. Parlett. It is a modification of Hyman's method [4]. We will illustrate the method by applying it to the following system of differential equations. These equations are similar to the linearized Navier-Stokes equations for parallel flow.

$$\frac{Du}{Dx} = w, \qquad \frac{Dv}{Dx} = -i\alpha u,$$

$$\frac{Dw}{Dx} = (f(x) - \lambda)u + g(x)v + i\alpha z,$$

$$\frac{Dz}{Dx} = -(f(x) - \lambda)v - i\alpha w.$$

In the above, u, v, w, z are complex functions of the real variable x, $f(x)$ and $g(x)$ are known functions, and α is a constant. The boundary conditions are $u(a) = v(a) = u(b) = v(b) = 0$. We let $h = (b - a)/M$, $x_j = a + jh$, $U_j = u(x_j)$, $V_j = v(x_j)$, $W_j = w(x_j + h/2)$, $Z_j = z(x_j + h/2)$.

The difference equations are the following:

$$U_0 = V_0 = U_M = V_M = 0,$$

$$U_{j+1} - U_j - hW_j = 0,$$

$$V_{j+1} - V_j + \frac{i\alpha h}{2}(U_{j+1} + U_j) = 0,$$

$$W_j - W_{j-1} - h(f_j - \lambda)U_j - hg_j\, V_j - \frac{i\alpha h}{2}(Z_j + Z_{j-1}) = 0,$$

$$Z_j - Z_{j-1} + h(f_j - \lambda)V_j + \frac{i\alpha h}{2}(W_j + W_{j-1}) = 0.$$

Define the vector W to be $W = (U_0, V_0, W_0, Z_0, \cdots, U_M, V_M)$. Then the difference equations can be written in matrix form as $AW = 0$, where $A(\lambda) = B + \lambda C$. The matrices A, B, C, can be written in block tridiagonal form where the blocks are two-by-two matrices. That is,

$$A = \begin{vmatrix} A_{1,2} & A_{1,3} & & \\ A_{2,1} & A_{2,2} & A_{2,3} & \\ & \vdots & & \\ & & A_{J,1} & A_{J,2} \end{vmatrix},$$

where $J = 2M + 1$, and similarly for B and C. For example,

$$B_{1,2} = \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix},$$

$$B_{j,1} = \begin{vmatrix} -1 & 0 \\ +\dfrac{i\alpha h}{2} & -1 \end{vmatrix} \qquad \text{if} \quad j = 2, 4, \cdots, 2M.$$

For these equations, we have $A_{j,1} = -I + O(h)$, $j \leq 2M$, and $C_{j,1} = C_{j,3} = 0$. We can alter the matrix A by multiplying the jth row by $-A_{j,1}^{-1}$ and adding the last column to the next-to-last column to obtain a matrix $A' = B' + \lambda C'$, where

$$A' = \begin{vmatrix} A'_{1,2} & A'_{1,3} & & & \\ I & A'_{2,2} & A'_{2,3} & & \\ & I & A'_{3,2} & A'_{3,3} & \\ & & \vdots & & \\ & & I & A'_{J-1,2} & A'_{J-1,3} \\ & & & I & A'_{J,2} \end{vmatrix}.$$

Note that the zeros of $|A'(\lambda)|$ coincide with those of $|A(\lambda)|$. We will now define a "block Hyman's method" to compute the determinant of A'. Define the matrix X such that

$$
X = \begin{vmatrix} I & 0 \cdots \cdots \cdots X_1 \\ 0 & I & 0 \cdots \cdots X_2 \\ & & \vdots \\ & & I & X_{J-1} \\ & & & X_J \end{vmatrix}, \qquad A'X = \begin{vmatrix} A'_{1,2} & A'_{1,3} & 0 \cdots \cdots \cdots \cdots Y \\ I & A'_{2,2} & A'_{2,3} & & 0 \\ & & \vdots \\ & & I & A'_{J-1,2} & 0 \\ & & & I & 0 \end{vmatrix}.
$$

Thus we may take X_J to be an arbitrary non-singular two-by-two matrix, and the remainder of the X_j are given by the recursive formula below,

$$
X_{J-1} + A'_{J,2}X_J = 0,
$$

$$
X_{j-1} + A'_{j,2}X_j + A'_{j,3}X_{j+1} = 0,
$$

$$
Y = A'_{1,2}X_1 + A'_{1,3}X_2 .
$$

Since $\det(X) = \det(X_J)$, we have $\det(A') = \det(Y)/\det(X_J)$. Therefore, the eigenvalues are those values of λ which make the determinant of Y zero. These values are found with a rootfinder. Of course, we must go through the transformation from A' to Y each time the determinant is evaluated.

An algorithm to compute the eigenvectors of A' is easily found, although we have no guarantee the algorithm will produce accurate results. Suppose λ has been chosen such that $\det(Y)$ is nearly zero. Then we can obtain an approximate solution for $Yq = 0$ by various methods. Note that the order of Y is low. Then we form the vector

$$
w' = \begin{vmatrix} X_1 q \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ X_J q \end{vmatrix} = X \begin{vmatrix} 0 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ q \end{vmatrix}.
$$

If $Yq = 0$, then it is easy to see from the form of the matrix $A'X$ that $A'W' = 0$.

An operational count indicates that the block Hyman's method should be slightly faster than Gaussian elimination when applied to matrices in the form of A'. If S is the order of the matrices $A'_{k,j}$, then the number of multiplications required to evaluate the determinant is approximately $2S^3 J$ for Hyman's method and $\frac{1}{2}(5S^3 + S^2)J$ for Gaussian elimination. The number of additions is approximately the same in each case. Of course, $3S^3 J$ multiplications are required to put the matrix into the form of A', but this need be done only once, whereas the determinant must be evaluated many times per eigenvalue. If the matrix is in the form of A, then Gaussian elimination requires $\frac{1}{6}(23S^3 - 3S^2 - 2S)J$ multiplications. Hyman's method has the advantage of requiring slightly less storage. If the calculation of Y in Hyman's method causes an overflow on the machine it is only necessary to multiply the matrix X_J by a small constant to scale the computation. Thus Hyman's method might have some slight advantage over Gaussian elimination. However, if the differential equation is singular, then it is difficult to produce the identity matrices on the sub-diagonal of A'. In this case, Gaussian elimination is probably superior.

In order to compare the accuracy of Hyman's method with that of Gaussian elimination, we used the non-convergent difference scheme described in Section 5. Since we know some exact solutions for this problem, we can determine the error in the computed eigenvalues. Of course, this does not directly measure the roundoff error in the determinantal evaluation, but it is the eigenvalues we wish to compute. In both cases the Laguerre rootfinder was used. The exact solutions were computed double precision, the two methods used single precision on an eight digit machine (IBM 7090). The eigenvectors in the case of Gaussian elimination were computed by the method described in Section 2. The results are given in the table below.

For this problem there was considerable difficulty in computing the eigenvectors by the inverse power method. The inverse power method is defined by $DX^{(k)} = X^{(k-1)}$, where $X^{(0)} = (1, 1, \cdots, 1)$, $D = A(\lambda_0) + \epsilon I$, and λ_0 is a computed eigenvalue, that is, the determinant of $A(\lambda_0)$ is nearly zero. The eigenvector is taken to be the limit of the sequence $X^{(k)}$. This method works well if the eigenvalues of D are well separated. In our case they are not well separated. With $M = 24$ and $\lambda_0 = 0.99430150$, the matrix A had eigenvalues $\pm 0.0001i$. After 200 iterations with $\epsilon = 10^{-5}$, the vector $X^{(200)}$ differed from the exact eigenvector by the error shown in the last column of the table below. For larger values of ϵ the method converged too slowly. The fact that the method worked this well is somewhat surprising. Note that the roots of $|A(\lambda)| = 0$ may be well separated even though the eigenvalues of D are not. For this problem, Hyman's method is clearly superior for the eigenvector calculation.

	Hyman's Method		Gaussian Elimination	
h	*Error in computed e-value*	*Max. error in e-vector*	*Error in computed e-value*	*Max. error in e-vector*
0.132	$5. \times 10^{-8}$	6.0×10^{-8}	$5. \times 10^{-8}$	4.4×10^{-3}
0.065	$5. \times 10^{-8}$	7.3×10^{-8}	$4. \times 10^{-8}$	1.7×10^{-4}
0.031	$6. \times 10^{-8}$	3.0×10^{-7}	$7. \times 10^{-8}$	3.3×10^{-4}
0.016	$7. \times 10^{-8}$	3.0×10^{-8}	$4. \times 10^{-8}$	5.1×10^{-4}
0.008	$3. \times 10^{-8}$	1.2×10^{-6}	not computed	

5. A Non-Convergent Difference Scheme. We will define a second difference scheme for solving the trivial eigenvalue problem given in Section 2. Instead of using a staggered mesh, we put both variables at the same mesh point. We assume the equation $v' + \lambda u = 0$ is satisfied at the boundary and use a three-point, one-sided difference quotient to approximate v' at the boundary. The difference equations are

$$U_0 = 0,$$
$$-3V_0 + 4V_1 - V_2 = 0,$$
$$U_{i+1} - U_{i-1} - 2hV_i = 0,$$
(5.1)
$$V_{i+1} - V_{i-1} + 2h\lambda U_i = 0, \qquad i = 1, \cdots, M - 1.$$
$$V_{M-2} - 4V_{M-1} + 3V_M = 0,$$
$$U_M = 0,$$

If the number of mesh points is odd, we can obtain a partial analytic solution to these equations. By combining the equations we obtain the following system for the variables $\{U_0, U_2, \cdots, U_M\}$: $U_{i-2} - 2U_i + U_{i+2} + 4h^2\lambda U_i = 0$, where $i = 2, 4, \cdots, M - 2$. To obtain a non-trivial solution for the latter system, we must have $\lambda \equiv \lambda_m = (\sin (mh))^2/h^2$, with $m = 1, 2, \cdots, M/2 - 1$. Remember that we have assumed M to be even. With a little algebra these solutions can be obtained explicitly. They are

$$U_i = \sin (imh), \qquad V_i = B\sqrt{\lambda_m} \cos (imh), \qquad\qquad i = 0, 2, \cdots, M,$$

$$U_i = B \sin (imh), \qquad V_i = \sqrt{\lambda_m} \cos (imh), \qquad i = 1, 3, \cdots, M - 1,$$

where

$$B = 4 \cos (mh)/(3 + \cos (2mh)), \qquad m = 1, 2, \cdots, M/2 - 1.$$

Note that $B = 1 + O(h^2)$, $\lambda_m = m^2 + O(h^2)$. Therefore, these solutions agree with those of the differential equation (2.1) to within $O(h^2)$ for fixed m.

However, we can obtain additional solutions of (4.1) by setting certain variables to zero, namely,

$$U_0 = V_1 = U_2 = \cdots = V_{M-1} = U_M = 0.$$

Then a non-trivial solution is obtained by solving the following eigenvalue problem for the variables $\{V_0, U_1, \cdots, U_{M-1}, V_M\}$:

$$3V_0 + V_2 = 0,$$

$$V_{i+1} - V_{i-1} + 2h\lambda U_i = 0, \qquad i = 1, 3, \cdots, M - 1,$$

$$U_{i+1} - U_{i-1} - 2hV_i = 0, \qquad i = 2, 4, \cdots, M - 2,$$

$$3V_M + V_{M-2} = 0.$$

One solution of this system is clearly $\lambda = 0$, $V_i = 0$, $U_i = $ constant. Of course, the eigenvectors are highly "discontinuous" and, therefore, not an approximation to the solution of the differential equation (2.1). However, the table below indicates that the eigenvalues, with the exception of the first, approximate those of equation (2.1) to within $O(h)$. The zero eigenvalue can be eliminated by modifying the difference scheme at the boundary so that the matrix is no longer reducible when $\lambda = 0$. However, the "double" eigenvalues remain. This eigenvalue problem was solved numerically by the method described in Section 4. The results are given in the table below (K is simply the number of the eigenvalue numbered in order of magnitude).

Eigenvalues

h	K						
	1	2	3	4	5	6	7
.12	0	.99443	1.0788	3.9115	4.242	8.557	9.273
.06	0	.99868	1.0397	3.9789	4.141	8.893	9.252
.03	0	.99967	1.0199	3.9947	4.075	8.973	9.154
.015	0	.99992	1.0099	3.9986	4.038	8.993	9.083

Apparently the difference scheme (5.1) effectively doubles the mesh spacing and thus introduces solutions which are poor approximations to those of the differential equation. In fact, the two sets of variables $(U_0, V_1, \cdots, V_{M-1}, U_M)$ and $(V_0, U_1, \cdots, U_{M-1}, V_M)$ are coupled only through the two equations

$$-3V_0 + 4V_1 - V_2 = 0,$$

$$V_{M-2} - 4V_{M-1} + 3V_M = 0.$$

The system (5.1) approximates the differential equation with truncation error $O(h^2)$ and is, therefore, consistent. In order to insure the convergence of a difference scheme for an initial value problem, we must have stability as well as consistency. This example makes it clear that some sort of "stability" is also required for boundary value problems. It would be very worthwhile to know just how this "stability" should be defined.

6. A Singular Differential Equation. We are interested in applying finite difference techniques to problems in hydrodynamic stability. These problems are frequently singular eigenvalue problems in ordinary differential equations. Therefore, the following example, although quite simple, may be of some interest.

We consider an eigenvalue problem with a continuous spectrum, namely, $(x - \lambda)(Y''(x) - \alpha^2 Y(x)) = 0$, $Y(0) = Y(1) = 0$. The solution is the Green's function

$$Y(x) = \begin{cases} \dfrac{\sinh \alpha x}{\sinh \alpha \lambda}, & x \leq \lambda, \\[2mm] \dfrac{\sinh \alpha(x - 1)}{\sinh \alpha(\lambda - 1)}, & x \geq \lambda, \end{cases} \qquad 0 < \lambda < 1.$$

The obvious finite difference scheme will produce a good approximation to this solution. The difference scheme is

$$(x_i - \lambda)(Y_{i+1} - (2 + \alpha^2 h^2)Y_i + Y_{i-1}) = 0, \qquad i = 1, \cdots, M - 1,$$

$$Y_0 = Y_M = 0, \qquad x_i = ih, \qquad h = 1/M.$$

If a non-trivial solution exists, we must have $\lambda = x_k$ for some k $(1 \leq k \leq M - 1)$. Then we can normalize the solution by requiring that $Y_k = 1$, in which case the problem reduces to two boundary value problems

$$Y_{i+1} - (2 + \alpha^2 h^2)Y_i + Y_{i-1} = 0, \qquad 1 \leq i \leq k - 1,$$

$$Y_0 = 0, \qquad Y_k = 1,$$

$$Y_{i+1} - (2 + \alpha^2 h^2)Y_i + Y_{i-1} = 0, \qquad k + 1 \leq i \leq M - 1,$$

$$Y_k = 1, \qquad Y_M = 0.$$

For fixed $x_k = \lambda$, the solution of these difference equations will converge to a solution of the differential equation (assume the subdivision is such that λ is always a mesh point) [15]. It is clear that the difference equations will yield the continuous spectrum in the limit.

It is probable that the finite difference method will also yield convergent ap-

proximate solutions for the more complicated equations arising in the theory of hydrodynamic stability. Green has applied the finite difference method to the problem of atmospheric instability with apparent success [14].

7. A Convergence Proof. In this section we will obtain a convergence proof for the difference formulation, but only for a special case. We will assume the differential eigenvalue problem is self adjoint with special boundary conditions. We define our difference equations using the variational formulation of the differential eigenvalue problem. The proof follows the methods of Courant-Friedrichs-Levy [1]. Weinberger has outlined a method for obtaining lower bounds for the eigenvalues of higher-order elliptic operators [2]. His method could probably be used to obtain convergence in this special case, but it would probably produce a more complicated proof. Forsythe has obtained asymptotic error estimates for a finite difference scheme applied to a second-order elliptic operator, but his method is not obviously applicable to higher-order operators [3].

We let

$$L(y) = a_0(x) \frac{d^n y}{dx^n} + \cdots + a_n(x)y = -\lambda y$$

be an eigenvalue problem with certain homogenous boundary conditions, presently unspecified. We assume the eigenvalues $\{\lambda_k\}$ of L are real and simple with $\lambda_1 < \lambda_2 < \cdots$. We also assume the eigenfunctions $\{y_k\}$ of L and the coefficients $a_k(x)$ to be as smooth as desired. Assume that A_h is a symmetric matrix such that the system of equations $A_h Y = 0$ is a consistent finite difference approximation for $L(y) = 0$ (here, h is the mesh spacing). That is, if y is any sufficiently smooth function and $Y_{hi} = y(x_i)$, then $L(y) = A_h Y_h + O(h^s)$, where $s > 0$. In fact, we will require that $s \geq 1$. We let $\mu_h^{(k)}$, $U_h^{(k)}$ be the eigenvalues and eigenvectors of A_h (we assume $\mu_h^{(1)} \leq \mu_h^{(2)} \leq \cdots$). In essence, we are assuming that the problem is self adjoint and that it is differenced in such a way that the symmetry is preserved.

LEMMA 7.1. *If $\lambda_p \leq \mu_h^{(p)} + O(h)$ for $p = 1, 2, \cdots, t + 1$, then $|\mu_h^{(t)} - \lambda_t| = O(h^s)$ and $\|Y_h^{(t)} - U_h^{(t)}\| = O(h^s)$. Here, $Y_{hi}^{(t)} = y_t(x_i)$, where y_t is the tth eigenfunction of L and x_i is the ith mesh point.*

Proof. The proof is by induction on t. We have $Y_h^{(t)} = \beta_1 U_h^{(1)} + \cdots + \beta_M U_h^{(M)}$, where $U_h^{(k)}$ are the eigenvectors of A_h normalized such that $\|U_h^{(k)}\| = 1$. We define the norm by $\|U\|^2 = h \sum_{i=1}^M U_i^2$. Also, normalize y_t such that $\|Y_h^{(t)}\| = 1$. By assumption, $L(y_t) - A_h Y_h^{(t)} = \tau_h$, where $\|\tau_h\| = O(h^s)$. Hereafter, we drop the subscript h. Since $L(y_t) = \lambda_t y_t$, $(A - \lambda_t)Y^{(t)} = -\tau$. Therefore,

$$\sum_{i=1}^M \beta_i(\mu^{(i)} - \lambda_t)U^{(i)} = -\tau.$$

By the induction assumption, $\mu^{(i)} - \lambda_i = O(h^s)$ for $1 \leq i \leq t - 1$. Since $\lambda_1 < \lambda_2 < \cdots < \lambda_t$ for small enough h and $1 \leq i \leq t - 1$, we have $a \leq \frac{1}{2}|\lambda_t - \lambda_{t-1}| < |\mu^{(i)} - \lambda_t|$, where $a = \frac{1}{2} \min\{(\lambda_t - \lambda_{t-1}), (\lambda_{t+1} - \lambda_t)\}$. By the hypothesis of the lemma, and the fact that $\mu^{(t+1)} \leq \mu^{(i)}$ for $i \geq t + 1$, we have $a < |\mu^{(i)} - \lambda_t|$ if $t < i$.

The eigenvectors $U^{(k)}$ are orthogonal and $\|U^{tk}\| = 1$, therefore,

(7.1)
$$\sum_{i=1}^{M} \beta_i^2 (\mu^{(i)} - \lambda_t)^2 = \| \tau \|^2$$

and

$$\sum_{i \neq t} \beta_i^2 \leq \frac{1}{a^2} \| \tau \|^2 = O(h^{2s}).$$

Since $\| Y^{(t)} \| = 1$, $\beta_t^2 + \sum_{i \neq t} \beta_i^2 = 1$. Therefore, for h small, $\beta_t^2 > \frac{1}{2}$. From equation (7.1), $(\mu^{(t)} - \lambda_t)^2 \leq 2 \| \tau \|^2 = O(h^{2s})$. Therefore, $\mu^{(t)} - \lambda_t = O(h^s)$.

Next we will prove convergence for the eigenvector. We must normalize $Y^{(t)}$ such that $\beta_t \geq 0$. Since $1 - \beta_t^2 = O(h^{2s})$, we then have $1 - \beta_t = O(h^{2s})$. We have already proved $\sum_{i \neq t} \beta_i^2 = O(h^{2s})$, therefore,

$$\| Y^{(t)} - U^{(t)} \|^2 = \sum_{i \neq t} \beta_i^2 + (\beta_t - 1)^2 = O(h^{2s}).$$

The case $t = 1$ can be proved in the same manner. Therefore, our induction proof is complete.

In order to prove the next lemma we will assume the eigenvalue problem is given in the following variational form [8], [9]. Let $\mathfrak{D}(u) = \int_0^1 \sum_{s=0}^{k} a_s(x)[d^s u/dx^s]^2 \, dx$ and consider the set of functions $v^{(1)}(x), \cdots, v^{(p)}(x)$. We assume that the boundary conditions are $u(0) = u(1) = \cdots = (d^k u/dx^k)(0) = (d^k u/dx^k)(1) = 0$. The admissible functions u satisfy the boundary conditions and have piecewise continuous kth derivatives. The admissible function u which yields the maximum of the minimum of $\mathfrak{D}(u)/\| u \|$ subject to the conditions $u \cdot v^{(i)} = 0$, $1 \leq i \leq p$ is the $(p + 1)$st eigenfunction and the eigenvalue is this maximum. That is,

(7.2)
$$\lambda_{p+1} = \underset{v^{(1)}, \cdots, v^{(p)}}{\text{Max}} \quad \underset{u; u \cdot v^{(i)} = 0}{\text{Min}} \frac{\mathfrak{D}(u)}{\| u \|}.$$

We also assume that $a_k(x) > \epsilon > 0$ and $a_s(x) \geq 0$ for $s = 0, \cdots, k - 1$. Note that $k = n/2$.

We let $x_i = ih$, where $h = 1/M$ is the mesh spacing. The finite difference representation of equation (7.2) is given by

$$\mu_h^{(p+1)} = \underset{V^{(1)}, \cdots, V^{(p)}}{\text{Max}} \quad \underset{U; U \cdot V^{(i)} = 0}{\text{Min}} \frac{D_h(U)}{\| U \|},$$

where $D_h(U) = h \sum_{i=0}^{M} \sum_{s=0}^{k} a_s(x_i)[\Delta^s U_i]^2$ and $\Delta U_i = (U_{i+1} - U_i)/h$. The test vectors U satisfy the conditions $U_0 = \cdots = U_{k-1} = U_{M-k+1} = U_M = 0$. This is a first-order approximation to the boundary conditions in the differential problem. This formulation in terms of minimizing a quadratic form is equivalent to a matrix eigenvalue problem. Hereafter, we will usually supress the subscript h. We will now prove the following lemma.

LEMMA 7.2. *If $\mu^{(p)}$ and λ_p are the eigenvalues of the difference and differential problem, respectively, then $\lambda_p \leq \mu^{(p)} + O(h)$.*

Clearly, Lemma 7.1 and Lemma 7.2 together imply convergence of the difference scheme. In the proof of this lemma, we need only consider those h for which $\mu_h^{(p)} \leq \lambda_p$ and, thus, we can assume the set $\{\mu_h^{(p)}\}$ is bounded. We first note the following inequalities which are basic in the proof.

$$\| \Delta^k U \| \leq \frac{1}{\epsilon} D(U), \qquad \text{where } 0 < \epsilon \leq a_k(x),$$

(7.3)

$$| \Delta^s U_i | \leq \| \Delta^k U \|, \qquad 0 \leq i \leq M, 0 \leq s < k.$$

These inequalities follow easily from the fact that $U_0 = \cdots = U_{k-1} = 0$.

Proof. The general idea of the proof is to let $v_1, \cdots, v_p$ be the first p eigenfunctions of the differential equation and define the vectors $V^{(s)}$ by $V_i^{(s)} = v_s(x_i)$. Then let U be the minimizing function defined by

$$\operatorname*{Min}_{U; U \cdot V^{(s)} = 0, 1 \leq s \leq p} \frac{D(U)}{\| U \|}$$

subject to the boundary conditions. Then $\dot{D}(U)/\| U \| \leq \mu^{(p+1)}$. Using U we define a function $u(x)$ which is an admissible function for the differential variational problem (7.2) and which satisfies the conditions

(a) $\int_0^1 v^{(s)} \cdot u \, dx = 0, \; 0 \leq s \leq p,$ (b) $\int_0^1 u^2 = 1,$

(7.4)

(c) $\mathfrak{D}(u) = D(U) + O(h),$ (d) $\dfrac{d^s u}{dX^s} = 0 \text{ at } X = 0, 1 \text{ for } 0 \leq s \leq k - 1.$

This will complete the proof, since $\lambda_{p+1} \leq \mathfrak{D}(u)$ and $\mathfrak{D}(u) = D(U) + O(h) \leq \mu^{(p+1)} + O(h)$. Note that λ_{p+1} is obtained by minimizing $\mathfrak{D}(u)/\| u \|$ subject to $u \cdot v^{(s)} = 0, 1 \leq s \leq p$.

We extend the vector U by setting $U_{M+1} = \cdots = U_{M+k} = 0$. Then define $\psi_k(x)$ by $\psi_k(x) = \Delta^k U_i$ for $x_i < x \leq x_{i+1}$. Define $u(x)$ by

$$u(x) = \int_0^x \int_0^{\tau_{k-1}} \cdots \int_0^{\tau_1} \psi_k(\tau_0) \, d\tau_0 \cdots d\tau_{k-1} .$$

Define $\varphi(x)$ by $\varphi(x) = x - x_i, x_i \leq x < x_{i+1}$. Thus $\varphi(x)$ is a "sawtooth" function. By first differentiating the expression for u k times, then integrating back again, we obtain:

$$\frac{d^k u}{dx^k} = \Delta^k U_i , \qquad\qquad\qquad x_i < x < x_{i+1},$$

$$\frac{d^{k-1} u}{dx^{k-1}} = \Delta^{k-1} U_i + \varphi(x) \Delta^k U_i , \qquad\qquad x_i \leq x < x_{i+1},$$

(7.5)

$$u(x) = U_i + \varphi(x) \Delta U_i + \int_0^x \varphi(\tau_0) \Delta^2 U_i \, d\tau_0$$

$$+ \cdots + \int_0^x \int_0^{\tau_{k-2}} \cdots \int_0^{\tau_1} \varphi(\tau_0) \Delta^k U_i \, d\tau_0 \cdots d\tau_{k-2} .$$

To verify the above equations note that

$$\int_0^x \psi_k(x) = h \sum_{j=0}^{i-1} \Delta^k U_j + (x - x_i) \Delta^k U_i$$

$$= \Delta^{k-1} U_i + \varphi(x) \Delta^k U_i, \qquad\qquad x_i \leq x < x_{i+1} .$$

To prove this lemma we need consider only those values of h such that $\mu_h^{(p+1)} \leq \lambda^{(p+1)}$. Since $D(U) \leq \mu_h^{(p+1)}$ for all h, $D(U)$ is also bounded. Therefore, from the

basic inequality (7.3), we have the sum $h\sum_{i=1}^{M}|\Delta^s U_i|^2$ bounded for $0 \leq s \leq k$. Consequently, $h\sum_{i=1}^{M}|\Delta^s U_i|$ is also bounded independently of h. Define the functions $\xi_s(x)$ by the equations below (see equations (7.5)).

$$(7.6)\qquad \frac{d^s u}{dx^s} = \Delta^s U + h\xi_s(x),\qquad\qquad 0 \leq s \leq k.$$

From equations (7.5), we see that $\xi_s(1)$ and $\int_0^1 \xi_s^2(x)\,dx$ are bounded independently of h for $0 \leq s < k$. It is obvious that

$$(7.7)\quad \int_0^1 a^s(x)\left[\frac{d^s u}{dx^s}\right]^2 dx = \int_0^1 a^s(x)[\psi_s]^2\,dx + O(h) = h\sum_{i=1}^{M} a^s(x_i)[\Delta^s U_i]^2 + O(h).$$

Therefore, $\mathfrak{D}(u) = D_h(U) + O(h)$. From the definition of $u(x)$ and the fact that $U_0 = \cdots = U_{k-1} = 0$ we have $(d^s u/dx^s)(0) = 0$ for $0 \leq s \leq k - 1$. Also, since $\xi_s(1)$ is bounded, $(d^s u_j/dx^s)(1) = O(h)$.

Define functions $g_j(x), 0 \leq j \leq k - 1$, such that (a) $g_j \in C^k$, (b) $(d^s g_j/dx^s)(0) = 0$, $s = 0, \cdots, k - 1$, and (c) $(d^s g_j/dx^s)(1) = \delta_{sj}$, where δ_{sj} is the Kronecker delta. Then replace u by $u - \sum_{j=0}^{k-1} hg_j\xi_j(1)$, where $\xi_j(x)$ is defined in equation (7.6). By this modification, u satisfies condition (7.4d). Equation (7.7) is still true. By the definition of U we have $\sum_{i=1}^{M} U_i v_j(x_i) = 0, 1 \leq j \leq p$. Therefore, $\int_0^1 u(x)v_j(x) = \gamma_j = O(h)$. Note that $u(x) = U_i + O(h)$ for $x_i < x < x_{i+1}$. We replace $u(x)$ by $u(x) - \sum_{j=1}^{p} \gamma_j v_j(x)$. Since the functions $v_j(x)$ satisfy equation (7.4d), and since $\{v_j\}$ is an orthonormal set, the new function u satisfies equations (7.4a, c, d). Since $h\sum_{i=1}^{M} U_i^2 = 1$, we can replace $u(x)$ by $u(x)/\int_0^1 u^2\,dx$ and conditions (7.4) are all satisfied by u.

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