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Note

Computing the Eigenvalues and Eigenvectors of Symmetric Arrowhead Matrices*

1. INTRODUCTION

In this paper we will be concerned with the eigenvalue problem for a symmetric matrix which is zero except for its main diagonal and one row and column. Such problems arise in the description of radiationless transitions in isolated molecules [1] and of oscillators vibrationally coupled with a Fermi liquid [6]. In these applications the order n of the matrix A can be in the thousands. The purpose of this paper is to present formulas and efficient algorithms for computing eigenvalues and eigenvectors of such matrices.

Since eigenvalues are invariant under similarity transformations, we can symmetrically rearrange the rows and columns of the matrix at our convenience, and we therefore assume without loss of generality that A has been ordered so that the nonzero row and column are last. Thus, we consider matrices of the form

$$A = \begin{pmatrix} d_1 & 0 & 0 & \cdots & 0 & e_1 \\ 0 & d_2 & 0 & \cdots & 0 & e_2 \\ 0 & 0 & d_3 & \cdots & 0 & e_3 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & d_{n-1} & e_{n-1} \\ e_1 & e_2 & e_3 & \cdots & e_{n-1} & p \end{pmatrix}. \tag{1.1}$$

which we will call (symmetric) *arrowhead* matrices. By further interchanges, we can arrange for the diagonal elements to be ordered so that $d_1 \leqslant d_2 \leqslant \cdots \leqslant d_{n-1}$. Hence, we will consider only *ordered* arrowhead matrices.

Since A is symmetric, its eigenvalues may in principle be computed by invoking any of a number of standard programs (e.g., the EISPACK programs [8]). However, these programs usually begin with an initial reduction of the matrix to tridiagonal form, which entails $O(n^3)$ operations and $O(n^2)$ storage. In this paper we propose an alternative which takes advantage of the structure of A: namely, we propose to solve the Eq. (2.1) below, which is closely related to the secular equation, for the eigenvalues of A. This results in an algorithm which requires only $O(n^2)$ computa-

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tions and $O(n)$ storage. Although the idea is conceptually simple and in fact has been used to solve other eigenvalue problems of special structure [2, 3, 5, 7], some care must be taken to show that the computation is stable.

In the next section we will give the basic properties of arrowhead matrices, and in the next we will describe how the equation $\varphi_A(\lambda)=0$ may be solved. In the last section we will discuss the computation of eigenvectors. We point out here that our algorithms are completely parallel; the computations for one simple eigenvalue are completely independent of those for another.

2. Properties of Eigenvalues of Arrowhead Matrices

We begin by disposing of a special case. If there is a zero in the last column, say $e_i=0$, then the diagonal element d_i is an eigenvalue whose eigenvector is the ith unit vector. To compute the remaining eigenvalues, we can reduce the size of the problem by deleting the ith row and column of the matrix, eventually obtaining a matrix for which all elements e_j are nonzero. We will call such an arrowhead matrix *irreducible*.

The basic results on the eigenvalues of arrowhead matrices are contained in the following theorem due to Wilkinson [10, pp. 94 ff]. Here we give a slightly different proof that contains results needed to derive our algorithm.

Theorem 2.1. *Let A be an ordered, irreducible arrowhead matrix of the form* (1.1). *Let*

$$d_0=\min\left\{d_1-|e_1|,\ \ldots,\ d_{n-1}-|e_{n-1}|,\ p-\sum_i |e_i|\right\}$$

and

$$d_n>\max\left\{d_1+|e_1|,\ \ldots,\ d_{n-1}+|e_{n-1}|,\ p+\sum_i |e_i|\right\}.$$

For $i=1,\ \ldots,\ n-2$ and $k>0$ if

$$d_{i-1}<d_i=\cdots=d_{i+k}<d_{i+k+1},$$

then d_i is an eigenvalue of A of multiplicity k. For each pair of distinct successive diagonals $d_{i-1}<d_i$, there is a single eigenvalue λ_i of A satisfying $d_{i-1}<\lambda_i<d_i$, and all such eigenvalues satisfy the equation $\varphi_A(\lambda_i)=0$, where

$$\varphi_A(\lambda)=p-\lambda-\sum_{i=1}^{n-1}\frac{e_i^2}{d_i-\lambda}. \tag{2.1}$$

Proof. Let $\lambda_1\leqslant\cdots\leqslant\lambda_n$ be the eigenvalues of A. By Cauchy's interleaving

theorem [10, p. 98], the eigenvalues of A interlace the eigenvalues of the matrix formed by deleting the last row and column of A, so that

$$\lambda_1 \leqslant d_1 \leqslant \lambda_2 \leqslant \cdots \leqslant d_{n-1} \leqslant \lambda_n. \tag{2.2}$$

By Gerschgorin's theorem [9, p. 302], $d_0 < \lambda_1$ and $\lambda_n < d_n$. These inequalities immediately imply the statements about multiple eigenvalues.

We will next show that if λ is distinct from the numbers d_i, then λ is an eigenvalue of A if and only if $\varphi_A(\lambda) = 0$. If λ is an eigenvalue of A, then $\det(A - \lambda I) = 0$. If we multiply the first row of this determinant by $e_1/(d_1 - \lambda)$ and subtract it from the last row, multiply the second row by $e_2/(d_2 - \lambda)$ and subtract it from the last, and so on, we get the equation

$$\det \begin{pmatrix} d_1 - \lambda & 0 & 0 & \cdots & e_1 \\ 0 & d_2 - \lambda & 0 & \cdots & e_2 \\ 0 & 0 & d_3 - \lambda & \cdots & e_3 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \varphi_A(\lambda) \end{pmatrix} = 0.$$

Since this determinant is the product of the diagonals and $d_i - \lambda \neq 0$, we must have $\varphi_A(\lambda) = 0$. Conversely, if $\varphi_A(\lambda) = 0$, then $\det(A - \lambda I) = 0$.

Now assume that $d_{i-1} < d_i$, where $1 < i < n - 1$. Then for λ near to but greater than d_{i-1}, we have (remember $e_{i-1} \neq 0$)

$$\varphi_A(\lambda) \cong -\frac{e_{i-1}^2}{d_{i-1} - \lambda} > 0. \tag{2.3}$$

For λ near to but less than d_i, we have

$$\varphi_A(\lambda) \cong -\frac{e_i^2}{d_i - \lambda} < 0. \tag{2.4}$$

Therefore, $\varphi_A(\lambda)$ must change sign in the interval (d_{i-1}, d_i), and the point at which it does is an eigenvalue. The inequalities (2.2) ensure that the sign changes only once in the interval.

It remains only to show that there is an eigenvalue strictly less than d_1 and an eigenvalue strictly greater than d_{n-1}. If λ is near to but less than d_1, then

$$\varphi_A(\lambda) \cong -\frac{e_1^2}{d_1 - \lambda} < 0.$$

On the other hand, as $\lambda \to -\infty$ we have $\varphi_A(\lambda) \cong -\lambda > 0$. Hence $\varphi_A(\lambda)$ changes sign in $(-\infty, d_1)$. A similar argument shows that $\varphi_A(\lambda)$ has to change sign in (d_{n-1}, ∞). ∎

The theorem shows we can find eigenvalues corresponding to repeated values of the diagonal by inspection. The remaining eigenvalues are located strictly between

the d_i's and satisfy the equation $\varphi_A(\lambda)=0$. Since φ_A is very easy to compute, this suggests that we attempt to use a root-finding method to compute the eigenvalues of A. We will describe and analyze such a method in the next section.

3. Computing Eigenvalues

In this section we turn to the problem of computing the eigenvalue λ_i lying between d_{i-1} and d_i, assuming these diagonals are distinct. According to (2.3) and (2.4), if $\lambda \in (d_{i-1}, d_i)$ and $\varphi_A(\lambda)>0$, then $\lambda<\lambda_i$. If $\varphi_A(\lambda)<0$, then $\lambda>\lambda_i$. This suggests that we can compute λ_i by interval bisection. The following pseudo-code gives such an algorithm, computing an interval [b, c] of length at most eps which contains λ_i, and the midpoint of the interval as the estimate of the eigenvalue. The variable eps is a convergence tolerance, which must be greater than zero, and phi is a subprogram that returns the function φ_A.

```
a = d(i-1)
b = d(i)
while (b-a .gt. eps)
   c = (a+b)/2
   phic = phi(c)
   if (phic .eq. 0)
      a = b = c
      exit
   if (phic .lt. 0)
      b = c
   else
      a = c
   end if
end while
lambda = (a+b)/2
```

At each step of this algorithm, the size of the interval (a, b) containing the eigenvalue is reduced by a factor of two. In other words, the method adds about a bit of accuracy per iteration.

However, we recommend this procedure be used only to find brackets $a > d_{i-1}$ and $b < d_i$ for the eigenvalue. Once these brackets have been found, one should switch to a combination of the secant method and interval bisection. Although this method is complicated, it is available in library subroutine packages (e.g., zeroin in the IMSL library). The increased rate of convergence more than justifies the trouble.

There is one simplification which results when there are multiple eigenvalues. If $d_{i-1} < d_i = \cdots = d_{i+k} < d_{i+k+1}$, the terms

$$\sum_{j=i}^{i+k} \frac{e_j^2}{d_j - \lambda}.$$

in (2.1) collapse into

$$\frac{\sum_{j=i}^{i+k} e_j^2}{d_i - \lambda}.$$

Thus if we strike the rows and columns corresponding to $d_{i+1}, \ldots, d_{i+k}$ and replace e_i by $\sqrt{\sum_{j=i}^{i+k} e_j^2}$, the value of $\varphi_A(\lambda)$ is unchanged. When there are many repeated eigenvalues, this can result in large savings in the evaluation of ϕ_A.

At the end of the iteration, we have two numbers a and b within eps of each other such that phi(a) is nonnegative and phi(b) is nonpositive. However, phi and φ_A are not the same function, since phi is evaluated with rounding error. We now show that the effect of this rounding error is negligible.

We will assume that all computation is done in floating-point arithmetic with rounding unit ε_M. Specifically, we will assume that the result of any floating-point operation is to return a value that has relative error ε_M. For example, in computations to 10 decimal digits, ε_M is approximately 10^{-10}. Under these assumptions, we can show (see the Appendix to this paper) that if $n \geq 2$, $\varepsilon_M < 0.001$, and $n\varepsilon_M < 0.1$ then

$$\text{phi}(\lambda) = \varphi_{A+H}(\lambda),$$

where

$$|h_{in}| = |h_{ni}| \leq 1.06n\,|e_i|\,\varepsilon_M, \qquad i = 1, \ldots, n-1,$$

and

$$|h_{nn}| \leq 1.06n(|p| + |\lambda|)\varepsilon_M.$$

The other elements of H, which depends on λ, are zero.

This result shows that whatever we compute for $\varphi(\lambda)$, it is the same value we would have obtained by performing exact calculations with a slightly perturbed matrix $\tilde{A} = A + H$. Now it can be shown [9, p. 315] that such a perturbation can move the eigenvalues of A by no more than

$$\|H\|_\infty = \max_i \sum_j |h_{ij}|.$$

Since for our problem

$$\|H\|_\infty \leqslant 1.06n\left(|p| + |\lambda| + \sum_i |e_i|\right)\varepsilon_M \overset{\text{def}}{=} \eta(\lambda),$$

the eigenvalues $\tilde{\lambda}_i$ of $A + H$ satisfy

$$|\tilde{\lambda}_i - \lambda_i| \leqslant \eta(\lambda). \tag{3.1}$$

Let us now apply these results to the output a and b of our algorithm. From our rounding-error analysis, we have $\varphi_{A+H}(\mathsf{a}) \geqslant 0$. Since $A + H$ is an ordered, irreducible arrowhead matrix with diagonals d_i, its ith eigenvalue must be greater than or equal to a. It follows from (3.1) that $\lambda_i \geqslant \mathsf{a} - \eta(\mathsf{a})$. A similar argument shows that $\lambda_i \leqslant \mathsf{b} + \eta(\mathsf{b})$. In other words, our algorithm—either simple bisection or the composite method—always returns numbers a and b such that

$$\lambda_i \in [\mathsf{a} - \eta(\mathsf{a}), \mathsf{b} + \eta(\mathsf{b})] \cap (d_{i-1}, d_i).$$

4. Computing Eigenvectors

Next we consider the computation of eigenvectors of ordered, irreducible arrowhead matrices (we have already mentioned in Section 2 that if $e_i = 0$, then d_i is an eigenvalue whose eigenvector is the ith unit vector). We will first consider eigenvectors corresponding to nonmultiple eigenvalues. Let z_i be the eigenvector corresponding to λ_i, and assume that it has been normalized so that its nth component $z_n^{(i)}$ is one. Then it is easily verified from the equation $Az_i = \lambda_i z_i$ that the remaining components of z_i are given by the formulas

$$z_j^{(i)} = \frac{e_j}{\lambda_i - d_j}.$$

Since $d_{i-1} < \lambda_i < d_i$, the denominators in these formulas are nonzero.

The chief difficulty with these formulas is that we must use an approximate eigenvalue $\tilde{\lambda}_i$ in place of the true value, which gives an approximate eigenvector $\tilde{z}_i$. If we set

$$\delta_i = \min_{k \neq i} |\lambda_k - \tilde{\lambda}_i|,$$

then it follows [4] that the sine of the angle between z_i and $\tilde{z}_i$ satisfies

$$\sin \angle(z_i, \tilde{z}_i) \leqslant \frac{\|(A-\tilde{\lambda}_i I)\tilde{z}_i\|}{\delta_i \|\tilde{z}_i\|},$$

where $\|\cdot\|$ is the usual Euclidean norm. It is easily verified that $(A-\tilde{\lambda}_i I)\tilde{z}_i = (0, ..., 0, \varphi(\tilde{\lambda}_i))^T$. Hence

$$\sin \angle(z_i, \tilde{z}_i) \leqslant \frac{|\varphi(\tilde{\lambda}_i)|}{\delta_i \sqrt{1+\sum_{j=1}^{n-1} \tilde{z}_{j2}^{(i)}}}.$$

Since our algorithm returns intervals containing the eigenvalues, we may obtain a lower bound on δ_i from their endpoints.

The eigenvectors $z_{i+1}, ..., z_{i+k}$ of an eigenvalue $\lambda = d_i = d_{i+1} = \cdots = d_{i+k}$ of multiplicity k are zero except for the elements in positions i through $i+k$. From the last row of the equation $Az = \lambda z$, we see that these components must satisfy

$$e_i z_i^{(j)} + e_{i+1} z_{i+1}^{(j)} + \cdots + e_{i+k} z_{i+k}^{(j)} = 0, \qquad j = i+1, ..., i+k.$$

One way to define these vectors is to set

$$z_{i+m}^{(j)} = \begin{cases} \dfrac{e_{i+m} e_{i+j}}{e_i^2 + \cdots + e_{i+j-1}^2}, & m = 0, ..., j-1 \\ -1, & m = j \\ 0, & m = j+1, ..., k. \end{cases}$$

With this definition, the vectors z_j are mutually orthogonal.

APPENDIX: Rounding Error Analysis

The assumptions about our computer arithmetic amount to saying that the computed value of a floating point operation, say $a+b$, is $(a+b)(1+\varepsilon)$, where $|\varepsilon| \leqslant \varepsilon_M$. In deriving our bounds we will be faced with expressions of the form

$$\frac{(1+\varepsilon_1)(1+\varepsilon_2)\cdots(1+\varepsilon_j)}{(1+\varepsilon_{j+1})(1+\varepsilon_{j+2})\cdots(1+\varepsilon_k)}.$$

Eventually, we will replace such expressions by a bound independent of j, and in anticipation of this we let $\langle k \rangle$ be a generic symbol for such an expression. Clearly $\langle k \rangle \langle l \rangle = \langle k+l \rangle$.

In evaluating $\varphi_A(\lambda)$ we must first compute $p-\lambda$ which gives a value $(p-\lambda)\langle 1 \rangle$. Next we must compute $e_1^2/(d_1-\lambda)$, which gives $e_1^2\langle 3 \rangle/(d_1-\lambda)$. When the latter is subtracted from the former, we get

$$(p-\lambda)\langle 2 \rangle - \frac{e_1^2\langle 4 \rangle}{d_1-\lambda}.$$

Computing and subtracting the next term gives

$$(p-\lambda)\langle 3\rangle - \frac{e_1^2\langle 5\rangle}{d_1-\lambda} - \frac{e_2^2\langle 4\rangle}{d_2-\lambda}.$$

When φ is finally evaluated, we have

$$(p-\lambda)\langle n\rangle - \frac{e_1^2\langle n+2\rangle}{d_1-\lambda} - \frac{e_2^2\langle n+1\rangle}{d_2-\lambda} - \cdots - \frac{e_{n-1}^2\langle 4\rangle}{d_{n-1}-\lambda}.$$

If we now define

$$\tilde{p} = p\langle n\rangle - \lambda(\langle n\rangle - 1)$$

and

$$\tilde{e}_i = e_i\langle n-i+3\rangle^{1/2},$$

then the entire computation is equivalent to performing exact computations on the arrowhead matrix $\tilde{A}$ formed from $\tilde{p}$, the $\tilde{e}_i$ and the d_i. It remains to get bounds on the elements of $H = \tilde{A} - A$.

We begin with $h_{nn} = (p-\lambda)(1-\langle n\rangle)$. If $\varepsilon_M < 0.001$ and $n\varepsilon_M < 0.1$ then[1]

$$|1-\langle n\rangle| \leqslant 1.06n\varepsilon_M.$$

Hence

$$|h_{nn}| \leqslant 1.06n(|p|+|\lambda|)\varepsilon_M.$$

Similarly, we may show that

$$\begin{aligned}
|h_{in}| &\leqslant |1-\langle n-i+3\rangle^{1/2}|\ |e_i| \\
&\leqslant |1-(1+1.06(n-i+3)\varepsilon_M)^{1/2}|\ |e_i| \\
&\leqslant \left|1-\left(1+\frac{1.06(n-i+3)\varepsilon_M}{2}\right)\right|\ |e_i| \\
&\leqslant 1.06n\varepsilon_M\ |e_i|,
\end{aligned}$$

the last inequality holding when $n \geqslant 2$.

[1] This Wilkinson-style inequality can be established as follows. First observe that if $\varepsilon < 0.001$, then $(1-\varepsilon)^{-1} < 1+\varepsilon/0.999$. Hence $|\langle n\rangle - 1| < (1+\varepsilon_M/0.999)^n - 1$. Now $n\ln(1+\varepsilon_M/0.999) < n\varepsilon_M/0.999$, and hence $(1+\varepsilon_M/0.999)^n < \exp(n\varepsilon_M/0.999) < 1+(n\varepsilon_M/0.999)[1+n\varepsilon_M \exp(n\varepsilon_M/0.999)/1.998]$, the last inequality following from Taylor's theorem with remainder. The desired inequality now follows from evaluating $[1+n\varepsilon_M \exp(n\varepsilon_M/0.99)]/0.999$ for $n\varepsilon_M = 0.1$.

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D. P. O'LEARY
G. W. STEWART

Department of Computer Science
Institute for Advanced Computer Studies
University of Maryland
College Park, Maryland 20742
Center for Computational and Applied Mathematics
National Institute of Standards and Technology
Gaithersburg, Maryland 20879