SIAM J. MATRIX ANAL. APPL.
Vol. 12, No. 3, pp. 426-431, July 1991

$O(n^2)$ REDUCTION ALGORITHMS FOR THE CONSTRUCTION OF A BAND MATRIX FROM SPECTRAL DATA*

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Abstract. Efficient rotation patterns are presented that provide stable $O(n^2)$ algorithms for the construction of a real symmetric band matrix having specified eigenvalues and first p components of its normalized eigenvectors. These methods can also be used in the second phase of the construction of a band matrix from the interlacing eigenvalues as described in [*Linear Algebra Appl.*, 40 (1981), pp. 79–87]. Previously presented algorithms for these reductions that use elementary orthogonal similarity transformations require $O(n^3)$ arithmetic operations.

Key words. band matrix, inverse eigenvalue problem, Givens rotations

AMS(MOS) subject classification. 65F30

1. Introduction. Let A be a real symmetric $(2p+1)$-band matrix of order n, and let A_k denote the trailing principal submatrix of $A = A_n$ of order k. It is well known that the eigenvalues of A_k interlace those of A_{k+1} for each $k < n$, and moreover, given real numbers $\lambda_j^{(k)}$ $(1 \leqq j \leqq k,\ n-p \leqq k \leqq n)$ satisfying

$$\lambda_j^{(k+1)} \leqq \lambda_j^{(k)} \leqq \lambda_{j+1}^{(k+1)}, \tag{1}$$

there is a $(2p+1)$-band matrix $A = A_n$ such that the eigenvalues of A_k are $\{\lambda_j^{(k)}\}_{j=1}^{k}$ for each k. In general, this band matrix is not uniquely determined.

The problem of constructing a band matrix from the interlacing eigenvalues (1) is considered in [2] and [1]. A survey of this problem and some related inverse eigenvalue problems is given in [3]. In [2] the interlacing eigenvalues are used to determine the first p components of the normalized eigenvectors of A, and the remaining components of the eigenvectors (and hence A) are constructed using a block Lanczos process. In [1] a matrix of bordered structure (where the trailing principal submatrix of order p is diagonal) is constructed that satisfies the required spectral conditions. Householder transformations that preserve the eigenvalues of the trailing submatrices are then applied to reduce this bordered matrix to band form. This reduction procedure uses $O(n^3)$ arithmetic operations.

In this note we present efficient rotation patterns that provide stable $O(n^2)$ procedures that can be used in the second step (the reduction step) of either of the above methods. These algorithms provide solutions to the open problem posed in [3, p. 615]. The first rotation pattern we present can be considered as the generalization to band matrices of Rutishauser's procedure for the construction of Jacobi matrices from spectral data presented in [4].

2. Efficient reduction algorithms. The reduction step in [2] can be described as follows. Given $\{\lambda_j\}_{j=1}^{n}$ and an $n \times p$ matrix Q_1 with orthonormal columns, construct a

* Received by the editors October 24, 1988; accepted for publication (in revised form) January 31, 1990. This research was supported in part by National Science Foundation grant DMS-8704196.

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$(2p+1)$-band matrix A having eigenvalues λ_j such that Q_1^T forms the first p rows of the (orthogonal) eigenvector matrix for A. This reduction can be performed using a sequence of orthogonal similarity transformations whose composition results in an orthogonal transformation Q such that

$$(2)\qquad \begin{bmatrix} I_p & 0 \\ 0 & Q^T \end{bmatrix}\begin{bmatrix} X & Q_1^T \\ Q_1 & \Lambda \end{bmatrix}\begin{bmatrix} I_p & 0 \\ 0 & Q \end{bmatrix}=\begin{bmatrix} X & I_p & 0 \\ I_p & & A \\ 0 & & \end{bmatrix}$$

is a $(2p+1)$-band matrix of order $n+p$. The trailing principal submatrix $A = A_n$ then satisfies the required spectral conditions, and Q_1 comprises the first p columns of Q. (The matrix X is arbitrary and remains unchanged.)

In the algorithm given in [1], an $n \times n$ matrix of the bordered form

$$(3)\qquad B=\begin{bmatrix} B_0 & B_1^T \\ B_1 & D \end{bmatrix},$$

where D is a diagonal matrix of order $n-p$, is constructed such that the trailing principal submatrices of orders $n-p$ through n of B have prescribed eigenvalues. Householder transformations that do not involve the first p coordinate axes are then used to transform B to a $(2p+1)$-band matrix A while preserving the eigenvalues of the trailing principal submatrices. In particular, the composition of these Householder transformations yields an orthogonal matrix U of order $n-p$ such that

$$(4)\qquad A=\begin{bmatrix} I_p & 0 \\ 0 & U^T \end{bmatrix}\begin{bmatrix} B_0 & B_1^T \\ B_1 & D \end{bmatrix}\begin{bmatrix} I_p & 0 \\ 0 & U \end{bmatrix}$$

is a $(2p+1)$-band matrix of order n. Thus, the reduction of the matrices in (2) and (4) is essentially the same problem. (Observe that the identity matrix in (2) arises because the columns of Q_1 are orthonormal.) We will describe our efficient rotation patterns in terms of the reduction of a matrix in the bordered form (3).

The efficient reduction to band form that generalizes the algorithm of [4] is obtained by performing plane rotations to introduce appropriate zeros in B row-by-row beginning at row $p+2$, in such a way that *the intermediate matrices remain sparse*. In contrast, a Householder transformation to introduce zeros in the first column of the matrix will result in a full matrix, and the subsequent Householder transformations must be performed on full matrices.

Let $R(A, j, k, l) = GAG^T$, where G is the elementary Givens rotation in the (j, k)-plane that annihilates a_{kl}. Thus, G is the identity matrix if $a_{kl} = 0$. If $a_{kl} \neq 0$, then G is the identity matrix apart from the 2×2 submatrix formed from rows and columns j and k, which is given by

$$G\begin{bmatrix} j, & k \\ j, & k \end{bmatrix}=\begin{bmatrix} c & s \\ -s & c \end{bmatrix},$$

where $c := a_{jl}/\sqrt{a_{jl}^2 + a_{kl}^2}$ and $s := a_{kl}/\sqrt{a_{jl}^2 + a_{kl}^2}$. Our algorithm for reducing the bordered matrix to band form is then given as follows.

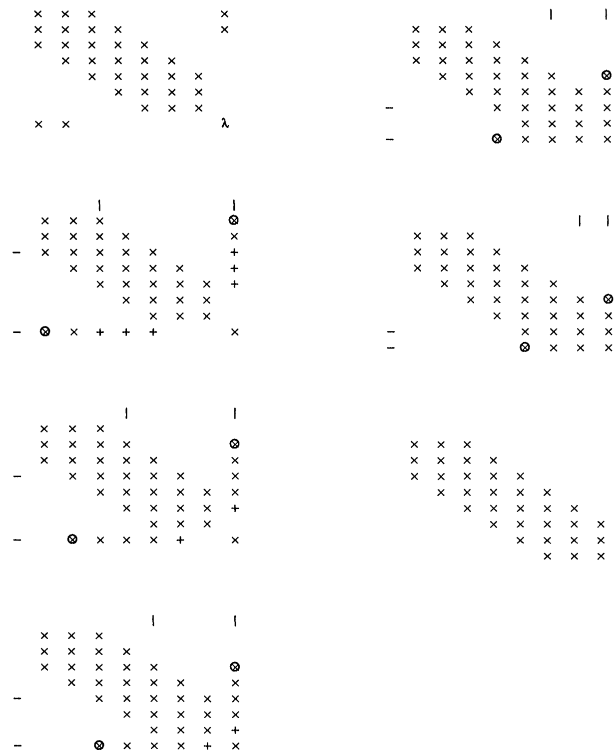

FIG. 1. *Rotations are performed in coordinate planes* (3, 8), (4, 8), (5, 8), (6, 8), *and* (7, 8) *to introduce the appropriate zeros in the eighth row.*

ALGORITHM 1.

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for k = p+2, ··· , n
  for j = p+1, ··· ,k−1
    A := R (A,j,k,j−p)
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To see how the sparsity is preserved, consider the example in Fig. 1. There $n = 8$, $p = 2$, and the necessary zeros have already been introduced in rows 4 through 7. Nonzero entries are represented by $\times$, a Givens rotation is performed in the indicated planes to annihilate the circled entry, and the symbol $+$ indicates the "fillin" (i.e., the additional nonzero entries) introduced by the rotation. The first rotation, in the (3, 8) plane, annihilates $a_{8,1}$ and creates $p + 1 = 3$ additional nonzero entries. (We count a_{ij} and a_{ji} as one element.) The successive rotations introduce at most one additional nonzero element each, so there are at most $2p + 1 = 5$ nonzero entries on the eighth row at any time. We can therefore perform each elementary similarity transformation on A in $O(p)$ arithmetic work. Thus the amount of computation required by the reduction is $O(pn^2)$.

Below is an explicit description of Algorithm 1 that involves only the lower-triangular part of the symmetric matrix A.

ALGORITHM 1.

Input: a symmetric matrix $A = [a_{j,k}]_{j,k=1}^{n}$ whose trailing principal submatrix of order $n - p$ is diagonal.

Output: a symmetric $(2p+1)$-band matrix A whose trailing principal submatrices of orders $n-p$ through n are orthogonally similar with those of the input matrix.

for $k=p+2, \cdots, n$
  for $j=p+1, \cdots, k-1$
    if $a_{k,j-p} \neq 0$ **then**
      $\rho := \sqrt{a_{j,j-p}^2 + a_{k,j-p}^2}$;
      $c := a_{j,j-p}/\rho$; $s := a_{k,j-p}/\rho$;
      $a_{j,j-p} := \rho$; $a_{k,j-p} := 0$;
      for $i=p-1, p-2, \cdots, 1$
        $\begin{bmatrix} a_{j,j-i} \\ a_{k,j-i} \end{bmatrix} := \begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} a_{j,j-i} \\ a_{k,j-i} \end{bmatrix}$
      for $i=j+1, j+2, \cdots, \min\{j+p, k-1\}$.
        $\begin{bmatrix} a_{i,j} \\ a_{k,i} \end{bmatrix} := \begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} a_{i,j} \\ a_{k,i} \end{bmatrix}$
      $u := a_{j,j}$; $v := a_{k,k}$; $w := a_{k,j}$;
      $a_{j,j} := c^2u + s^2v + 2csw$; $a_{k,k} := c^2v + s^2u - 2csw$;
      $a_{k,j} := cs(v-u) + (c^2 - s^2)w$.

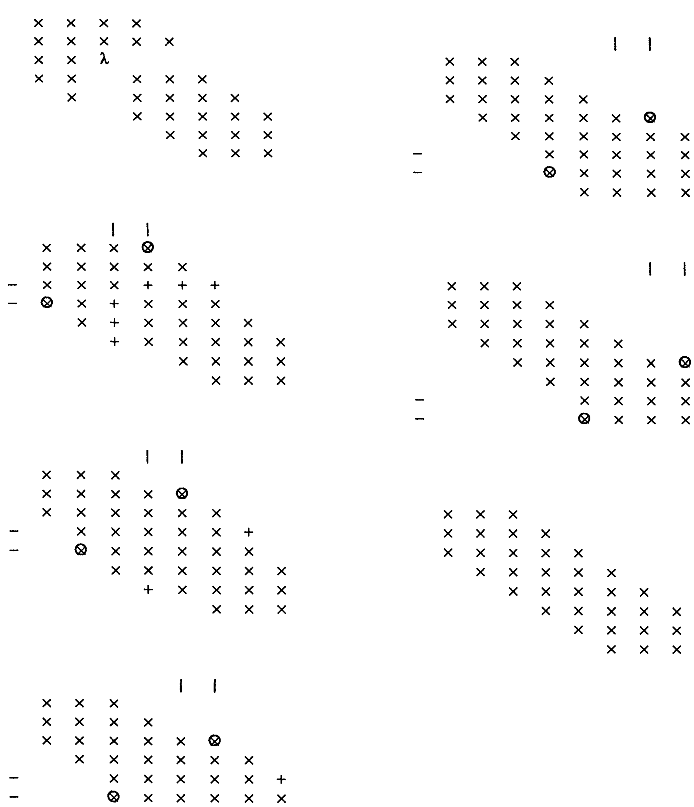

FIG. 2. *Rotations are performed in coordinate planes* (3, 4), (4, 5), (5, 6), (6, 7), *and* (7, 8) *to introduce the appropriate zeros.*

Another rotation pattern can be obtained by introducing the zeros in (3) from the bottom up along downwardly sloping diagonals.

ALGORITHM 2.

for $k = n-1, n-2, \cdots, p+1$
  for $j = k+1, \cdots, n$
    $A := R(A, k-1, k, j-k)$

One step of this procedure is illustrated in Fig. 2. Observe that Algorithm 2 creates the same amount of fillin as Algorithm 1.

In fact, several patterns of rotations exist that preserve the sparsity of the intermediate matrices. For example, Algorithms 1 and 2 can be combined to build the band matrix according to any ordering for which the intermediate band (sub)matrices occupy contiguous rows and columns of the work array.

3. Numerical results. Numerical experiments verify that our efficient rotation pattern produces accurate results in lower-order work than the Householder reduction technique. These experiments were performed on the VAX 11/750 at Northern Illinois University. We will not attempt to analyze the numerical sensitivity of the inverse eigenproblem. Our only aim is to show that an efficient rotation pattern produces errors comparable with the Householder reduction technique in lower-order work.

The following experiment was performed. The method of [1] was used to create a bordered matrix whose trailing principal matrices of order $n-p$ through n have specified eigenvalues. This matrix was then reduced to $(2p+1)$-band form using

I. The Householder reduction procedure of [1];

II. The efficient rotation pattern of Algorithm 1.

We calculated the average and maximum error among the assigned eigenvalues of the trailing principal submatrices of orders $n-p$ through n relative to the Frobenius norm of the band matrix. The results displayed in Table 1 were obtained by assigning the eigenvalues of A_k, $n-p \leqq k \leqq n$, to be the integers $2j+(n-k-1)$, $1 \leqq j \leqq k$. Experiments were carried out on a variety of other problems with similar results.

Tables 2(a) and 2(b) show average CPU times used by each reduction scheme for various values of n and p. Table 2(c) shows the corresponding ratios of the time used by the Householder reduction to that of our rotation pattern. These ratios represent the speedup factors of Procedure II relative to Procedure I. Note that for fixed n, the amount

TABLE 1
Relative errors in eigenvalues.

		Average error		Maximum error	
n	p	I	II	I	II
10	2	3.39e−08	1.58e−08	2.61e−07	5.23e−08
20	2	3.58e−08	2.16e−08	2.21e−07	9.42e−08
50	2	2.40e−08	2.96e−08	1.31e−07	1.12e−07
10	4	3.52e−08	1.50e−08	1.57e−07	5.23e−08
20	4	2.00e−08	2.86e−08	1.10e−07	1.11e−07
50	4	2.71e−08	2.94e−08	1.12e−07	1.68e−07
10	6	2.08e−08	1.29e−08	7.84e−08	5.23e−08
20	6	2.73e−08	3.18e−08	7.39e−08	1.11e−07
50	6	2.91e−08	5.04e−08	1.68e−07	1.50e−07

TABLE 2(a)
Average timings for Procedure I (CPU *seconds*).

n / p	10	20	30	40	50	100	200
1	0.029	0.182	0.550	1.231	2.342	17.858	140.070
2	0.023	0.163	0.534	1.199	2.286	17.632	139.693
5	0.013	0.131	0.456	1.081	2.119	17.127	137.837
10		0.072	0.327	0.868	1.796	15.852	133.120
20			0.117	0.476	1.178	13.503	123.227

TABLE 2(b)
Average timings for Procedure II (CPU *seconds*).

n / p	10	20	30	40	50	100	200
1	0.022	0.087	0.207	0.381	0.596	2.493	10.273
2	0.018	0.099	0.244	0.453	0.734	3.112	13.037
5	0.009	0.103	0.302	0.618	1.044	4.807	20.757
10		0.063	0.287	0.692	1.275	6.937	32.130
20			0.104	0.451	1.110	9.250	50.007

TABLE 2(c)
Ratios of CPU *times*.

n / p	10	20	30	40	50	100	200
1	1.346	2.096	2.661	3.232	3.931	7.162	13.634
2	1.333	1.639	2.188	2.645	3.114	5.666	10.715
5	1.364	1.266	1.511	1.748	2.030	3.563	6.641
10		1.147	1.136	1.253	1.408	2.285	4.143
20			1.128	1.055	1.062	1.460	2.464

of computation required by Procedure I decreases as p increases, while that of Procedure II is often increasing as a function of p when p is small. These results show that our rotation pattern is consistently more efficient than the Householder reduction technique. The relative efficiency of the rotation pattern generally increases as n increases and decreases as p increases.

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