Block reduction of matrices to condensed forms for eigenvalue computations

Jack J. DONGARRA* and Danny C. SORENSEN**
Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL 60439, U.S.A.

Sven J. HAMMARLING
Numerical Algorithms Group Ltd., Wilkinson House, Jordan Hill Road, Oxford, United Kingdom OX2 8DR

Received 11 February 1988
Revised 7 October 1988

Abstract: In this paper we describe block algorithms for the reduction of a real symmetric matrix to tridiagonal form and for the reduction of a general real matrix to either bidiagonal or Hessenberg form using Householder transformations. The approach is to aggregate the transformations and to apply them in a blocked fashion, thus achieving algorithms that are rich in matrix–matrix operations. These reductions to condensed form typically comprise a preliminary step in the computation of eigenvalues or singular values. With this in mind, we also demonstrate how the initial reduction to tridiagonal or bidiagonal form may be pipelined with the divide and conquer technique for computing the eigensystem of a symmetric matrix or the singular value decomposition of a general matrix to achieve algorithms which are load balanced and rich in matrix–matrix operations.

Keywords: Eigenvalue computations, high-performance computing, block algorithms.

1. Introduction

The key to using a high-performance computer effectively is to avoid unnecessary memory references. In most computers, data flows from memory into and out of registers and from registers into and out of functional units, which perform the given instructions on the data. Algorithm performance can be dominated by the amount of memory traffic rather than by the number of floating-point operations involved. The movement of data between memory and registers can be as costly as arithmetic operations on the data. This provides considerable motivation to restructure existing algorithms and to devise new algorithms that minimize data movement.

Along these lines there has been much activity in the past few years involving redesign of some of the basic routines in linear algebra [7,9,10]. A number of researchers have demonstrated the effectiveness of block algorithms on a variety of modern computer architectures with vector-processing or parallel-processing capabilities, on which potentially high performance can easily

* Work supported in part by the National Science Foundation.

be degraded by excessive transfer of data between different levels of memory (vector registers, cache, local memory, main memory, or solid-state disks) [1–4,8,10,12]. The redesign has led to the development of algorithms that are based on matrix–vector and matrix–matrix techniques [2,10].

This approach to software construction is well suited to computers with a hierarchy of memory and true parallel-processing computers. A survey that provides a description of many advanced-computer architectures may be found in [6]. For those architectures it is often preferable to partition the matrix or matrices into blocks and to perform the computation by matrix–matrix operations on the blocks. By organizing the computation in this fashion we provide for full reuse of data while the block is held in cache or local memory. This approach avoids excessive movement of data to and from memory and gives a surface-to-volume effect for the ratio of arithmetic operations to data movement, i.e., \( O(n^3) \) arithmetic operations to \( O(n^2) \) data movement. In addition, on architectures that provide for parallel processing, parallelism can be exploited in two ways:

1. operations on distinct blocks may be performed in parallel; and
2. within the operations on each block, scalar or vector operations may be performed in parallel.

For a description of blocked implementation for Cholesky factorization, LU decomposition, and matrix multiply and the specifications for a set of building blocks to aid the development of block algorithms, see [5].

Many of the most successful algorithms for computing eigenvalues or singular values of matrices require an initial reduction to condensed form. Typically, this condensed form is well suited to the implementation of an underlying iterative process used to compute the eigenvalues or singular values. We present block algorithms suitable for computing three different condensed forms. These are the reduction of a symmetric matrix to tridiagonal form, and the reduction of a (real) general matrix to either upper Hessenberg form or bidiagonal form. The reduction of a symmetric matrix to tridiagonal form dominates the computation of eigenvalues if no eigenvectors are required and represents about half the work if both eigenvalues and eigenvectors are sought. A similar remark is appropriate for the reduction of a general matrix to bidiagonal form in preparation for the computation of singular values. When the full eigensystem or singular value decomposition is desired, divide and conquer techniques are appropriate for both of these computations, and we shall discuss how to pipeline the reduction to condensed form with a divide and conquer scheme.

2. The algorithm: reduction to tridiagonal form

We usually think of applying a sequence of Householder transformations to reduce the original symmetric matrix to symmetric tridiagonal form. We apply the transformations as similarity transformations to preserve the eigenvalues of the original matrix. The process can be described as follows:

\[
P_i = I - u_i u_i^T, \quad u_i^T u_i = 2, \quad T = P_{n-2} \cdots P_2 P_1 A P_1 P_2 \cdots P_{n-2}.
\]

Each transformation \( P_i \) is designed to introduce zeros in the \( i \)th column (and row) of the matrix below the subdiagonal (and above the superdiagonal) so as to leave the upper part of the matrix
in tridiagonal form and the lower part full and symmetric. At the $i$th step of the process, the matrix is of the form
\[
\begin{pmatrix}
    \times & \times & & & & & \\
    \times & \times & \times & & & & \\
    & \times & \times & \times & & & \\
    & & \times & \times & \times & & \\
    & & & \times & \times & \times & \\
    & & & & \times & \times & \\
    & & & & & \times & \\
\end{pmatrix}
\]

To describe the algorithmic details of this reduction, we use the notation $A^{(i:n,j:n)}$ to denote the $(n-i+1) \times (n-j+1)$ submatrix of $A$ beginning at the $(i, j)$ location of $A$; we denote the subvector of a vector $a$ beginning at the $i$th position by $a^{(i:n)}$; and the $i$th component of a vector $a$ by $a^{(i)}$. The vector $u_i$ is constructed from the $i$th column of the reduced matrix so that
\[
\alpha_i = -\text{sign}(a_i^{(i+1)})\|a_i^{(i+1:n)}\|_2, \quad u_i^{(i+1)} = \sqrt{1 - a_i^{(i+1)}/\alpha_i},
\]
\[
u_i^{(i+2:n)} = -a_i^{(i+2:n)}/(\alpha_i u_i^{(i+1)}), \quad u_i^{(1:i)} = 0.
\]

In practice $u_i$ is constructed and applied to the matrix as follows:
\[
y_i = A_i u_i, \quad v_i = y_i - \frac{1}{2} (v_i v_i^T) u_i, \quad A_{i+1} = A_i - u_i v_i^T - v_i u_i^T.
\]  \hfill (2.1)

In the process $A$ is repeatedly modified by a symmetric rank two update. This requires updates to half the $(n-i) \times (n-i)$ elements of the symmetric matrix at each stage of the process. (There are numerous ways to construct Householder vectors [14]; we have chosen this approach for simplicity and numerical properties.)

To achieve better memory utilization we can consider aggregating a sequence of transformations, say $p$ of them, so that the matrix will be updated by a rank $2p$ symmetric matrix. Such an implementation would be as follows: instead of explicitly updating the matrix with the rank two change, we form only the second column (row) of $A_2$, say $a_2$. We then update $a_2$ by applying (2.1) in the following way:
\[
a_2 = a_2 - v_2^{(2)} u_1 - u_2^{(2)} v_1.
\]
From this we can compute $u_2$; and $y_2$ would be formed as $y_2 = A_2 u_2$. However, we have not explicitly formed $A_2$. We can construct $y_2$ as follows:
\[
y_2 = A_2 u_2 = (A_1 - u_1 v_1^T - v_1 u_1^T) u_2 = A_1 u_2 - (v_1^T u_2) u_1 - (u_1^T u_2) v_1.
\]

We could then explicitly form $A_3$ as a symmetric rank four update as follows:
\[
A_3 = A_2 - u_2 v_2^T - v_2 u_2^T = A_1 - u_1 v_1^T - v_1 u_1^T - u_2 v_2^T - v_2 u_2^T.
\]

We could have continued the process and in general found for a rank $2p$ update
\[
A_{p+1} = A_1 - UV^T - VU^T,
\]
where

\[ U = (u_1, u_2, \ldots, u_p), \quad V = (v_1, v_2, \ldots, v_p), \quad v_p = y_p - \frac{1}{2}(y_p^T u_p) u_p, \]

\[ y_{p+1} = \left( A_{1} - UV^T - VU^T \right) u_{p+1}, \quad a_{p+1:p+1:n} = a_{p+1:p+1:n}^{(p+1:n)} - \sum_{i=1}^{p} (v_{i}^{(p+1:n)} u_{i} + u_{i}^{(p+1:n)} v_{i}). \]

Thus, \( A_{p+1} \) can be formed by a rank \( 2p \) symmetric update that is rich in matrix–matrix operations.

Algorithm 1

\( U \) and \( V \) are temporary \( n \times p \) arrays, which are reused for each iteration of the \( k \) loop.

\( n \) is the order of the matrix

\( p \) is the blocking

\( N = (n - 2)/p \)

for \( k = 1, N \)

\( s = (k - 1)p + 1 \)

for \( j = s, s + p - 1 \)

\[ a_j = a_j - \sum_{i=s}^{j-1} (v_i^{(j+1)} u_i + u_i^{(j+1)} v_i) \]

\[ \alpha_j = -\text{sign}(a_j^{(j+1)}) \| a_j^{(j+1:n)} \|_2 \]

\[ u_j^{(j+1)} = \text{sqrt}(1 - a_j^{(j+1)}/\alpha_j) \]

\[ u_j^{(j+2:n)} = -a_j^{(j+2:n)}/(\alpha_j u_j^{(j+1)}) \]

\[ y_j = (A_j - U_{j-1} V_{j-1}^T - V_{j-1} U_{j-1}^T) u_j \]

\[ v_j = y_j - \frac{1}{2}(y_j^T u_j) u_j \]

\[ U_j = (U_{j-1}, u_j) \]

\[ V_j = (V_{j-1}, v_j) \]

end

\[ U = U_{s+p-1}, \quad V = V_{s+1-1} \]

perform symmetric rank \( 2p \) update on submatrix

\[ A^{(s:p:n,s+p:n)} = (A - UV^T - VU^T)^{(s:p:n,s+p:n)} \]

end

Note that for the following algorithms we assume that if in the construction of the Householder transformation, which takes \( x \) to \( (\alpha, 0, \ldots, 0)^T \), if the \( \max_{j=2,\ldots,n} |x_j| < \varepsilon |x_1| \), where \( \varepsilon \) is the machine precision, then the transformation is skipped.

\( U \) is a lower trapezoidal matrix with the first column having its first non-zero element in position \( s + 1 \) and the \( p \)th column having its first non-zero element in position \( s + p \). Notice that to aggregate the Householder transformations during the construction of the vector \( y_j \), we perform a matrix–vector multiplication with the submatrix \( A_{s} \) in the \( j \) loop.

Algorithm 1 constructs \( k \) block transformations and applies them to the matrix. We will call this a right-looking algorithm. Notice that at each of the \( k \) stages we are updating a submatrix of size \((n - s + 1) \times (n - s + 1)\). We can further reduce the amount of data referenced by the following algorithm.
Algorithm 2
for \( k = 1, N \)
\[ s = (k - 1)p + 1 \]
Apply the previous \( k - 1 \) block transformations to \( A^{(s-1,s:p-1)} \)
Compute \( U_k \) and \( V_k \)
end

At each stage of this algorithm we are only modifying an \((n - s + 1) \times p\) matrix. We will call this algorithm the \textit{left-looking algorithm}. This algorithm will require an access to the submatrix \( A_s \) in the loop; however, it avoids an update of the matrix at the end of the \( k \) loop.

3. Reduction to Hessenberg form

Not surprisingly, the same approach can be used in the reduction to Hessenberg form. Here we have
\[ H = P_{n-2} \cdots P_2 P_1 A P_1 P_2 \cdots P_{n-2}, \]
where \( H \) is upper Hessenberg. The idea of using a rank two or higher update in this context was discussed in [9]. Here it is convenient to use slightly modified formulas to those in [9] given by
\[
\begin{align*}
y_i &= A_i^T v_i, \quad z_i = A_i v_i, \quad v_i = y_i - \frac{1}{2} (z_i^T u_i) u_i, \quad w_i = z_i - \frac{1}{2} (y_i^T u_i) u_i, \quad A_{i+1} = A_i - u_i v_i^T - w_i u_i^T.
\end{align*}
\]
When \( A \) is symmetric, \( y_i = z_i \), and \( v_i = w_i \) and these equations are as in the tridiagonal case. The vector \( u_i \) is computed from the same equations as for the tridiagonal case. Here \( A \) is updated as
\[ A_{p+1} = A_1 - UV^T - WU^T, \]
where
\[
\begin{align*}
U &= (u_1, u_2, \ldots, u_p), \quad V = (v_1, v_2, \ldots, v_p), \quad W = (w_1, w_2, \ldots, w_p), \\
y_{p+1} &= (A_1^T - UV^T - UW^T) u_{p+1}, \quad z_{p+1} = (A_1 - UV^T - WU^T) u_{p+1}.
\end{align*}
\]
\( U, V, \) and \( Y \) are trapezoidal, but \( Z \) and \( W \) are not.

4. Reduction to bidiagonal form

A problem that is closely associated with the eigenvalue problem is to compute the Singular Value Decomposition (SVD) of a real \( m \times n \) matrix \( A \). This decomposition is directly related to the symmetric eigenvalue problem in that the singular values of \( A \) are the square roots of the eigenvalues of the symmetric positive semidefinite matrix \( A^T A \). It is numerically preferable to avoid formation of \( A^T A \), and the algorithm of choice involves an initial reduction of \( A \) to upper bidiagonal form \( B \) through a sequence of Householder transformations to obtain
\[ A = U B V^T \]
with \( U \) and \( V \) orthogonal and \( B \) upper bidiagonal.
This initial reduction may be treated with an algorithm similar to those already presented. In this case
\[ B = P_{n-1}^T \cdots P_2^T P_1^T A Q_1 Q_2 \cdots Q_{n-2}, \]
where each \( P_j \) is an \( m \times m \) Householder transformation and each \( Q_j \) is an \( n \times n \) Householder transformation. Again we may achieve efficient memory utilization by aggregating a sequence of transformations, say \( p \) of them, so that the matrix will be updated by a matrix of rank \( 2p \). However, there are data dependencies within this reduction that require additional attention.

Let us suppose for the moment that the sequences \( \{u_j\} \) and \( \{v_j\} \) can be computed at will. In general,
\[ (I-uu^T)(I-vv^T) = A - uw^T - yv^T, \]
where
\[ y = Av, \quad z = A^Tu \quad \text{and} \quad w = z - (u^Ty)v; \]
see [9] for more details. Thus, a straightforward extension of the tridiagonalization scheme presented in Section 2 gives the following algorithm:

**Algorithm 3**

\( U \) and \( V \) are temporary \( m \times p \) arrays, which are reused for each iteration of the \( k \) loop
\( V \) and \( W \) are temporary \( n \times p \) arrays, which are reused for each iteration of the \( k \) loop
\( n \) is the number of columns in the matrix
\( m \) is the number of rows in the matrix
\( p \) is the blocking
\( N = (n-2)/p \)
for \( k = 1, N \)
\( s = (k-1)p + 1 \)
for \( j = s, s+p-1 \)
    compute \( u_j \)
    compute \( v_j \)
    \[ y_j = (A - U_{j-1}W_{j-1}^T - Y_{j-1}V_{j-1}^T)v_j \]
    \[ h_j = (A - U_{j-1}W_{j-1}^T - Y_{j-1}V_{j-1}^T)^Tu_j \]
    \[ w_j = h_j - (u_j^Tv_j)v_j \]
    \[ U_j = (U_{j-1}, u_j) \]
    \[ V_j = (V_{j-1}, v_j) \]
    \[ W_j = (W_{j-1}, w_j) \]
    \[ Y_j = (Y_{j-1}, y_j) \]
end

\( U = U_{s+p-1}, V = V_{s+1}^{s+1-1} \)
\( Y = Y_{s+p-1}, W = W_{s+1}^{s+1-1} \)
perform rank \( 2p \) update on submatrix
\[ A_{s+p:s+p:n+s+p:n} = (A - UW^T - YV^T)_{s+p:s+p:n} \]
end
Unfortunately, it is not so straightforward to compute \( u_j \) and \( v_j \) at will. At step \( j \) of the usual bidiagonalization process, the vector \( u_j \) is non-zero in the \( j \)th entry. Hence application on the left by the corresponding Householder transformation alters the \( j \)th row of the reduced matrix \( A_j \) and knowledge of this row is required to compute the vector \( v_j \) which is non-zero in the \( j+1 \)st entry. The dependencies now become even more complicated because it would appear that the transformation corresponding to \( v_j \) must be applied from the right before \( u_{j+1} \) can be computed and so on. However, we note that the above algorithm will be valid if there is an independent formula for computing the \( v_j \) since the \( u_j \) may be computed as in the previous algorithms by knowing the \( j \)th column of the reduced matrix. Indeed, there is an independent formula for computing the \( v_j \) which may be found by noting that

\[ V^T A^T A V = B^T B = T \]

where \( V = Q_1 Q_2 \cdots Q_{n-2} \) is precisely the sequence of transformations that would be computed in Algorithm 1 to reduce the matrix \( A^T A \) to tridiagonal form \( T = B^T B \). This leads to the following procedure for computing the \( v_j \):

**Procedure compute \( v_j \)**

\[
\begin{align*}
  z_j &= A_j^T a_j^{(s:j)} - \sum_{i=s}^{j-1} (v_i x_i^{(j+1)} + x_i v_i^{(j+1)}) \\
  \xi_j &= -\text{sign}(z_j^{(j+1)}) \frac{\|z_j^{(j+1:n)}\|_2}{\xi_j} \\
  v_j^{(j+1)} &= \text{sqrt}(1 - z_j^{(j+1)}/\xi_j) \\
  v_j^{(j+2:n)} &= -z_j^{(j+2:n)}/(\xi_j v_j^{(j+1)}) \\
  t_j &= (A_s^T A_s - V_{j-1} X_{j-1}^T - X_{j-1} V_{j-1}^T) v_j, \quad A_s = A^{(s:m,j:n)} \\
  x_j &= t_j - \frac{1}{2}(t_j v_j) v_j \\
  X_j &= (X_{j-1}, x_j)
\end{align*}
\]

Computation of the \( u_j \) only depends upon the \( j \)th column of the reduced matrix being in place before the \( j \)th step. Therefore, the column-oriented formula given in Algorithm 1 may be adapted to give

**Procedure compute \( u_j \)**

\[
\begin{align*}
  a_j &= a_j - \sum_{i=s}^{j-1} (u_i w_i^{(j+1)} + y_i v_i^{(j+1)}) \\
  \alpha_j &= -\text{sign}(a_j^{(j)}) \frac{\|a_j^{(j:m)}\|_2}{\alpha_j} \\
  u_j^{(j)} &= \text{sqrt}(1 - a_j^{(j)}/\alpha_j) \\
  u_j^{(j+1:m)} &= -a_j^{(j+1:m)}/(\alpha_j u_j^{(j)})
\end{align*}
\]

If these two procedures are substituted for "compute \( u \)" and "compute \( v \)" in Algorithm 3, then it be well defined. In all of these we do not explicitly form the indicated matrix products. Instead, the matrix–vector products are accumulated.
5. Relationship to the WY-factorization

The algorithm presented here for aggregating Householder transformations is closely related to the WY-representation for the product of Householder matrices presented by Bischof and Van Loan [2]. The relationship is most clearly seen in the contexts of the QR-factorization of a general rectangular matrix. The WY-representation has the following form:

**QR-Factorization (Bischof and Van Loan)**

- $n$ is the number of columns in the matrix
- $p$ is the blocking
- $N = n/p$
- for $k = 1, N$
  - $s = (k-1)p + 1$
  - for $j = s, s+p-1$
    - $a_j = a_j - \sum_{i=s}^{j-1} z_i^{(j)} u_i$ where $z_i = A_i u_i$
    - compute Householder vector $u_j$
      - $Y_k^{(s:j)} = (Y_k^{(s:j-1)} - u_j u_j^T Y_k^{(s:j-1)}, -2u_j)$
  - end
  - perform rank $2p$ update on submatrix
    - $A^{(s+p:n,s+p:n)} = A^{(s+p:n,s+p:n)} - U Y_k^{T} A^{(s+p:n,s+p:n)}$
  - end

If one implements the reduction along the lines of the algorithm described in Section 2, the factorization can be described as follows:

**QR-Factorization (Alternative Algorithm)**

- $n$ is the order of the matrix
- $p$ is the blocking
- $N = n/p$
- for $k = 1, N$
  - $s = (k-1)p + 1$
  - for $j = s, s+p-1$
    - $a_j = a_j - \sum_{i=s}^{j-1} v_i^{(j+1)} u_i$
    - compute Householder vector $u_j$
      - $v_j = (A_s^T - V_k^{(s:j-1)} U_k^{(s:j-1)^T}) u_j$
  - end
  - perform rank $2p$ update on submatrix
    - $A^{(s+p:n,s+p:n)} = (A - U V_k^T)^{(s+p:n,s+p:n)}$
  - end

The two differences between the block algorithms are in the formation of $v_j$ and $Y_j$ and also in the update of the matrix $A$. For the Alternative Algorithm the vector $v_j$ is updated using the
submatrix $A$, and the Bischof and Van Loan algorithm uses information from $u_i$ and $Y^{(s:j-1)}$. Thus the Bischof and Van Loan algorithm will have fewer accesses to the data. In the update of the matrix $A$ for the Bischof and Van Loan factorization, the update is of the form

$$A^{(s+p:n,s+p:n)} = A^{(s+p:n,s+p:n)} - UY^\top A^{(s+p:n,s+p:n)},$$

and for the alternative factorization, the update is of the form

$$A^{(s+p:n,s+p:n)} = A^{(s+p:n,s+p:n)} - UV^\top.$$

The Alternative Algorithm incorporates the information about the matrix $A$ in the matrix $V$.

We can describe the reduction to tridiagonal form for the symmetric eigenvalue problem using the Bischof and Van Loan approach as

$$A_{p+1} = (I - USU^\top)A_1(I - USU^\top).$$

If we multiply out and combine terms, we can reduce the expression to

$$A_{p+1} = A_1 - ZU^\top - UZ^\top$$

where

$$W = A_1US^\top$$

and

$$Z = W - \frac{1}{2}USU^\top W$$

which is of the form described in Section 2.

With the WY-representation it is simple to apply the set of transformations to another matrix, as is required in back substitution for the eigenvector computation; one simply applies $(I - WY^\top)$ to the matrix. To apply the transformation using the formulation in Section 2, one can use the Householder vectors to construct the matrix $S$ such that $I - USU^\top$ can be used to apply the transformations to the eigenvectors of the symmetric tridiagonal matrix, back transforming them to the eigenvectors of the original problem. The matrix $S$ is a $p \times p$ upper triangular matrix whose $k$th column is formed as follows:

$$(I - USU^\top)(I - uu^\top) = I - uu^\top - USU^\top + USU^\top uu^\top$$

$$= I - [U, u]
\begin{pmatrix}
S & -SU^\top u \\
0 & u^\top
\end{pmatrix}
= I - [U, u]
\begin{pmatrix}
S & -SU^\top u \\
0 & 1
\end{pmatrix}
\begin{pmatrix}
U^\top \\
u^\top
\end{pmatrix}.$$ 

So the new column of $S$ is

$$\begin{pmatrix}
-SU^\top u \\
1
\end{pmatrix}.$$ 

6. Pipelining reduction to condensed form with determination of eigenvalues

Recently, algorithms have been developed based upon divide and conquer strategies for the determination of eigenvalues and singular values for a matrix in condensed form [11,13]. These methods are also rich in matrix—matrix operations and mesh very well with the block reductions presented here. This is accomplished through pipelining the initial phase with the computation of eigenvalues and back transformation of eigenvectors. These considerations are of little consequence on serial computers but have significant performance advantages on parallel-vector processors.
We use the block reduction algorithm as described above to introduce zeros in a block of the matrix; say we are at the kth stage and have just introduced zeros into the kth block. As we start the next block reduction, on the k + 1st block, we can start in parallel the eigenvalue computation on that part of the tridiagonal matrix generated from the kth block reduction of the matrix. When we have completed eigenvalue computations from two tridiagonal segments, we can use the technique applied in the divide and conquer algorithm as described by Dongarra and Sorensen [11] to determine the eigenvalues and eigenvectors of a pair of tridiagonal matrices. Then the eigenvalues of successive pairs of blocks can be found, then pairs of pairs, etc., until the full set is determined. When the reduction to condensed form and the divide and conquer strategy are used in this pipelined fashion, a highly efficient parallel algorithm can be constructed.

This discussion is made more explicit in the following example. We consider a symmetric matrix that is to be partitioned into four block columns as shown in Fig. 1.

Let us associate $H_k$ with the process of reducing the kth block $A_k$ of the partitioned matrix to tridiagonal form using Householder transformations. Thus $H_k$ executes a block step of Algorithm 1 (see the k loop) on the block $A_k$. In this algorithm we have the possibility of spawning parallel processes. Processes may cooperate in applying the resulting transformation shown in

$$A^{(s+p:n,s+p:n)} = A^{(s+p:n,s+p:n)} - U_k V_k^T - V_k U_k^T$$

in parallel. Let us denote these parallel processes by $M_{kj}$ so that process $M_{kj}$ is responsible for a portion of the work in the matrix multiply in the performance of Algorithm 1 by process $H_k$.

On completion of process $H_k$ the tridiagonal matrix $T_k$ is exposed and the algorithm TQL2 may be applied to compute the eigensystem of $T_k$ after the rank one tearing has been computed. Let us denote this process by $E_k$.

Once processes $E_1$ and $E_2$ have completed, then the eigensystem of

$$\begin{pmatrix} T_1 & 0 \\ 0 & T_2 \end{pmatrix} = \begin{pmatrix} Q_1 & 0 \\ 0 & Q_2 \end{pmatrix} \begin{pmatrix} D_1 & 0 \\ 0 & D_2 \end{pmatrix} + \beta \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} \begin{pmatrix} q_1^T \\ q_2^T \end{pmatrix} \begin{pmatrix} Q_1^T & 0 \\ 0 & Q_2^T \end{pmatrix}$$

(6.1)

may be computed using the rank one updating scheme. Similarly, once processes $E_3$ and $E_4$ have completed, the eigensystem of $\text{diag}(T_3, T_4)$ may be computed. Finally the entire eigensystem may be obtained through rank one updating of these two eigensystems. Let us denote these processes as $U_1$, $U_2$ and $U_0$, respectively. With the proper storage arrangements these processes obey the large-grain control flow graph of Fig. 2. In this control flow graph a node denotes a process, for example, a subroutine name together with the pointers to the data which the subroutine is to operate upon. A process $P$ becomes schedulable or ready to execute when there are no incoming arcs to the node representing process $P$. This signifies that all of the data dependencies for process $P$ have been satisfied through the completion of the processes that it was dependent
upon. This graph indicates that processes $M_{ij}$ can execute immediately. Once they have completed, $H_1$ may report to $H_2$, and this process may execute and spawn processes $M_{2j}$. At the same time $H_1$ reports to process $E_1$, and it may begin execution. When $E_1$ and $E_2$ have both completed, process $U_1$ may start and so on.

To accumulate a matrix of eigenvectors, the successive Householder transformations must be multiplied from left to right in the order they are applied:

$$Q = \prod_{i=1}^{n-2} \left( I - 2u_iu_i^T \right)$$  \hspace{1cm} (6.2)

and we observe that when accumulated this way, successive applications of $I - u_iu_i^T$ affect only the last $n - i + 1$ columns of $Q$. Thus, application of the Givens transformations associated with $E_1$ may be applied as soon as the products of the Householder transformations associated with $H_1$ have been multiplied out. These transformations may be applied independently of the computation of $H_k$ for $k > 1$ because these matrices affect columns that are independent of the columns affected by $E_i$.

When we do not wish to find eigenvectors, there is no reason to store the product $Q$ of these Householder transformations. Nor is it necessary to accumulate the product of the successive eigenvector transformations resulting from the updating problem. That is, we do not need to overwrite $Q$ with

$$Q \leftarrow Q \begin{pmatrix} Q_1 & 0 \\ 0 & Q_2 \end{pmatrix} \hat{Q}$$

where $Q_1$ and $Q_2$ are the matrices appearing in equation (6.1), $\hat{Q}$ is the matrix of eigenvectors for the interior matrix in (6.1), and $Q$ is the matrix appearing in (6.2) above. Instead, we may simply discard $Q$. Then the vector $q_1$ may be formed as $\hat{T}_1$ is transformed to $D_1$ in (2.2) by
accumulating the products of the transformations constructed in TQL2 that make up \( Q_1 \) against the vector \( e_k \). If there is more than one division, then \( Q_1 \) will have been calculated with the updating scheme. In this case we do not calculate all of \( Q_1 \) but instead use the component-wise formula for the eigenvectors to pick off the appropriate components needed to form \( q_1 \) (for details see [11,13]).

7. Operations counts and storage

An analysis of the number of floating-point operations (counting additions and multiplications) for the reduction to tridiagonal form of the standard algorithm reveals an operation count of

\[
 \frac{4}{3}n^3 + \frac{7}{2}n^2 + \frac{1}{6}n - 25 \text{ flops.}
\]

In aggregating the transformations to perform the block reduction, additional work is required in the formulation of \( y_j \) in Algorithm 1. The additional work for a block size \( p \) amounts to

\[
(2p - \frac{3}{2})n^2 + (-\frac{1}{3}p^2 - 2p + \frac{11}{2})n + (-\frac{4}{3}p^2 - 4p)
\]

floating-point additions and multiplications being performed.

The algorithm can be organized so that the vectors \( u_i \) overwrite the lower part of the matrix (as we do in the standard version of the software), but additional workspace of size \( n \times p \) is required to store the current block of \( V \).

8. Experimental results

The results in Table 1 were generated on an Alliant FX/8 computer using eight processors. The Alliant FX/8 is a parallel processor where each of the processors has vector registers and can perform vector operations. The results in Table 2 were generated on the CRAY X-MP using one processor.

<table>
<thead>
<tr>
<th>Order</th>
<th>( \frac{\text{TRED1}}{\text{TREDB}} )</th>
<th>( \frac{\text{ORTHES}}{\text{ORTHSB}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>1.94</td>
<td>2.59</td>
</tr>
<tr>
<td>200</td>
<td>2.39</td>
<td>3.01</td>
</tr>
<tr>
<td>300</td>
<td>2.40</td>
<td>3.23</td>
</tr>
<tr>
<td>400</td>
<td>2.39</td>
<td>3.35</td>
</tr>
<tr>
<td>500</td>
<td>2.36</td>
<td>3.46</td>
</tr>
</tbody>
</table>
Table 2
Ratio of execution times (speedups) between the EISPACK routine and the blocked version on the CRAY X-MP (Blocksize = 10)

<table>
<thead>
<tr>
<th>Order</th>
<th>Ratio</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>TRED1/TREDB</td>
<td>ORTHES/ORTHSB</td>
</tr>
<tr>
<td>100</td>
<td>1.03</td>
<td>1.29</td>
</tr>
<tr>
<td>200</td>
<td>1.10</td>
<td>1.52</td>
</tr>
<tr>
<td>300</td>
<td>1.21</td>
<td>1.65</td>
</tr>
<tr>
<td>400</td>
<td>1.23</td>
<td>1.79</td>
</tr>
<tr>
<td>500</td>
<td>1.28</td>
<td>1.92</td>
</tr>
</tbody>
</table>

References


