On the Coding of Jacobi's Method for Computing Eigenvalues and Eigenvectors of Real Symmetric Matrices*

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Abstract. A technique is given which allows the coding of Jacobi's Method such that the computing time is proportional to the cube of the order of the matrix for large order matrices. The method used is one where successive rotations are chosen such that the largest magnitude off-diagonal element is the pivot; these tactics lead to a small number of rotations and a corresponding high accuracy and reduction in computing time. An algorithm for coding is offered.

Jacobi's method [1, 2, 3, 6, 7] consists of performing consecutive 2-by-2 rotations of a real symmetric matrix H with elements $H(km)$, $k \leqq m$, where the largest magnitude off-diagonal element $H(ij)$ is used as a "pivot." A rotation is defined as the following unitary transformation where the primes indicate the new elements.

$$
\begin{aligned}
H'(km) &= H(km) && \text{for } k \text{ and } m \neq i \text{ or } j \\
H'(ki) &= cH(ki) + sH(kj) && \text{for } k \neq i \text{ or } j \\
H'(kj) &= -sH(ki) + cH(kj) && \text{for } k \neq i \text{ or } j \\
H'(ii) &= c^2[H(ii) + 2tH(ij) + t^2H(jj)] && \\
H'(jj) &= c^2[H(jj) - 2tH(ij) + t^2H(ii)] && \\
H'(ij) &= 0 &&
\end{aligned}
$$

with the last equation leading to:

$$
t = \frac{\text{sign of } \{[H(ii) - H(jj)]\} \cdot 2H(ij)}{|H(ii) - H(jj)| + \sqrt{(H(ii) - H(jj))^2 + 4(H(ij))^2}}
$$

$$
c = \frac{1}{\sqrt{1 + t^2}}
$$

$$
s = tc
$$

A square matrix U, which is initially set to be a unit matrix, is also successively rotated into a unitary matrix of the eigenvectors by the transformations:

$$
\begin{aligned}
U'(km) &= U(km) && \text{for } m \neq i \text{ or } j \\
U'(ki) &= cU(ki) + sU(kj) && \\
U'(kj) &= -sU(ki) + cU(kj) &&
\end{aligned}
$$

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It is important to note that the form of t is always numerically accurate and approaches zero as $H(ij)$ becomes small. In addition, the form of $H'(ii)$ and $H'(jj)$, which do not utilize the invariance of the trace, are chosen so as to maintain accuracy with ill-conditioned matrices. These choices also eliminate improper overflows as the $H(ij)$ become small. This prescription does *not* order the eigenvalues. Because ordered eigenvalues are a convenience, an interchange procedure should be introduced whenever $H'(ii) < H'(jj)$ occurs so that the roles (i.e. labels) of i and j are reversed in the above equations. It is to be emphasized that the above process is only a *pseudo-ordering* one since different submatrices of the matrix may not have any connecting off-diagonal elements and hence cannot be ordered (e.g. in an extreme case, an already diagonal matrix).

In a computer with B significant figures, the diagonalization is concluded either when the trivial case $|H(ij)| = 0$ occurs or when

$$|H(ij)| < 2^{-p} |H(kk)|_{\min}, \ (p = B),$$

is satisfied. The latter condition guarantees the accuracy of the eigenvalues of even an ill-conditioned degenerate matrix. It should be noted that though $p = B/2$ would be good enough for the accuracy of the eigenvalues of a non-degenerate matrix the accuracy of the eigenvectors requires $p = B$; moreover, the diagonalization process accelerates as the rotations proceed so that looking for more careful stopping procedures is probably not very fruitful.

The advantages of picking the largest magnitude off-diagonal element as a rotation "pivot" are twofold. Firstly, the number of rotations is minimized (roughly half the number required as when picking the $H(ij)$ at random), so that computation time is reduced. Secondly, the truncation and round-off error propagation appears empirically to be proportional to the number of rotations [4].

A special programming technique [5] has been developed to search for the largest magnitude off-diagonal element required for each rotation in a time having only a linear dependence on n, the matrix order. This is the same form of time-dependence as the rotation itself and is in contrast to the time of the obvious searching procedure which would depend on $n(n-1)/2$, the number of off-diagonal elements. This new search procedure basically utilizes the fact that only two columns and two rows of the matrix H are affected by the rotation. Consequently, by keeping two vectors giving the magnitude and location of the largest magnitude element in each column, it is possible to preserve a history according to the effect of the current rotation. This would be a straightforward procedure if it were not for the fact that the rotation also affects two rows. A brief outline of the procedure is now given for the case of a matrix $H(km)$ stored in triangular form, where $k = 1, 2, \cdots, m$ is the row number and $m = 1, 2, \cdots, n$ is the column number.

0. Initially for $m = 2, \cdots, n$, find $X(m) = |H(pm)|$ and $Y(m) = p$ where p is such that $|H(pm)|$ is the largest value over the range $1 \leqq p < m$.
1. Find $X(q)$, $Y(q)$ where q is such that $X(q)$ is the largest value over the range $1 < q \leqq n$, thus determining the largest magnitude off-diagonal element; check $X(q)$ to determine if diagonalization is finished.

2. Set $i = Y(q)$, $j = q$ thus locating the indices of the largest magnitude off-diagonal element.
3. Compute $H'(ii)$, $H'(jj)$, c, s and set $H'(ij) = 0$.
4. Examine $Y(m)$ over the range $i < m < j$; if $Y(m) = i$, temporarily replace $H(im)$ by zero, compute a new $X(m)$ and $Y(m)$, and restore the $H(im)$ element. Similarly examine $Y(m)$ over the range $j < m \leqq n$; if $Y(m) = i$ or j, temporarily replace $H(im)$ and $H(jm)$ by zero, compute a new $X(m)$ and $Y(m)$, and restore the $H(im)$ and $H(jm)$ elements.
5. Compute $H'(ki)$ and $H'(kj)$ over the range $1 \leqq k < i$. Compute $H'(im)$ and $H'(mj)$ over the range $i < m < j$; replace $X(m)$ by $|H'(im)|$ if the latter is larger and if replacement is made, set $Y(m) = i$. Compute $H'(im)$ and $H'(jm)$ over the range $j < m \leqq n$; replace $X(m)$ by the larger of $X(m)$, $|H'(im)|$ or $|H'(jm)|$ and set $Y(m)$ to the value $Y(m)$, i, or j, respectively.
6. Compute new values of $X(i)$, $Y(i)$ and $X(j)$, $Y(j)$.
7. Compute $U'(ki)$ and $U'(kj)$ for $1 \leqq k \leqq n$.
8. Repeat procedure starting from Step 1.

In general, the accuracy appears to be near that allowed by the conditioning of the matrix and the truncation error of the original matrix elements of H. Thus, if the condition number (the ratio of the largest magnitude eigenvalue to the smallest) is of d significant figures, the smallest eigenvalue may (but not always) lose up to approximately d significant figures. The eigenvectors will be accurate to roughly an absolute error of 2^{-B} plus cumulative round-off error.

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5. Subprograms using these techniques have been written in the SAP and Fortran languages for use with the IBM 704 and 7090 computers. They are available from the SHARE Distribution Agency in Distributions 705 and 731.
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