Handbook Series Linear Algebra

The Implicit QL Algorithm*

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1. Theoretical Background

In [1] an algorithm was described for carrying out the QL algorithm for a real symmetric matrix using shifts of origin. This algorithm is described by the relations

\[ Q_s(A_s - k_s I) = L_s, \quad A_{s+1} = L_s Q_s^T + k_s I, \]

\[ \text{giving} \quad A_{s+1} = Q_s A_s Q_s^T, \quad (1) \]

where \( Q_s \) is orthogonal, \( L_s \) is lower triangular and \( k_s \) is the shift of origin determined from the leading 2x2 matrix of \( A_s \).

When the elements of \( A_s \) vary widely in their orders of magnitude the subtraction of \( k_s \) from the diagonal elements may result in a severe loss of accuracy in the eigenvalues of smaller magnitude. This loss of accuracy can be avoided to some extent by an alternative algorithm due to FRANCIS [2] in which \( A_{s+1} \) defined by Eq. (1) is determined without subtracting \( k_s I \) from \( A_s \). With exact computation the \( A_{s+1} \) determined by the two algorithms would be identical, but the rounding errors are entirely different. The algorithm is based on the lemma that if \( A \) is symmetric and non-singular, and

\[ BQ = QA \]

(2)

with \( Q \) orthogonal and \( B \) tridiagonal with positive off-diagonal elements, then \( Q \) and \( B \) are fully determined when the last row of \( Q \) is specified. This can be verified by equating successively rows \( n, n-1, \ldots, 1 \) in Eq. (2). Hence if by any method we determine a tridiagonal matrix \( \tilde{A}_{s+1} \) such that

\[ \tilde{A}_{s+1} = \tilde{Q}_s A_s \tilde{Q}_s^T, \]

(3)

where \( \tilde{Q}_s \) is orthogonal, then provided \( \tilde{Q}_s \) has the same last row as the \( Q_s \) given by (1), \( \tilde{Q}_s = Q_s \) and \( \tilde{A}_{s+1} = A_{s+1} \). In the original algorithm \( Q_s \) is given as the product of \( n-1 \) plane rotations

\[ Q_s = P_1^{(i)} P_2^{(i)} \ldots P_{n-1}^{(i)}, \]

(4)

* Editor’s note. In this fascicle, prepublication of algorithms from the Linear Algebra Series of the Handbook for Automatic Computation is continued. Algorithms are published in ALGOL 60 reference language as approved by the IFIP. Contributions in this series should be styled after the most recently published ones.
where $P^{(i)}_i$ is a rotation in the plane $(i, i+1)$. It is clear that the last row of $Q$, is the last row of $P^{(i)}_{n-1}$. In the alternative algorithm a $Q$, is determined satisfying (3), again as the product of rotations $P^{(i)}_1 P^{(i)}_2 \ldots P^{(i)}_{n-2} P^{(i)}_{n-1}$, the rotation $P^{(i)}_{n-1}$ being that determined by the original algorithm. This ensures that $Q = Q_s$. Writing

$$\begin{bmatrix} 1 & \cdots & 1 \\ c_{n-1}^{(i)} & -s_{n-1}^{(i)} \\ s_{n-1}^{(i)} & c_{n-1}^{(i)} \end{bmatrix}, \quad A^{(i)} = \begin{bmatrix} d_1^{(i)} & e_1^{(i)} & \cdots & e_{n-1}^{(i)} \\ e_1^{(i)} & d_2^{(i)} & \cdots & e_{n-2}^{(i)} \\ \vdots & \vdots & \ddots & \vdots \\ e_{n-1}^{(i)} & e_{n-2}^{(i)} & \cdots & d_n^{(i)} \end{bmatrix},$$

where $P^{(i)}_{n-1}$ is defined as in the original algorithm, we have

$$c_{n-1}^{(i)} = \frac{d_n^{(i)} - k_s}{P_{n-1}^{(i)}}, \quad s_{n-1}^{(i)} = \frac{e_{n-1}^{(i)}}{P_{n-1}^{(i)}}, \quad P_{n-1}^{(i)} = [(d_n^{(i)} - k_s)^2 + (e_{n-1}^{(i)})^2]^{1/2}.$$  \hspace{1cm} \text{(6)}$$

The matrix $P_{n-1}^{(i)} A_s (P_{n-1}^{(i)})^T$ is of the form illustrated by

$$\begin{bmatrix} x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \end{bmatrix},$$

that is, it is equal to a tridiagonal matrix with additional elements in positions $(n, n-2)$ and $(n-2, n)$. This matrix can be reduced to tridiagonal form by $n-2$ orthogonal similarity transformations with matrices $P_{n-2}^{(i)}, \ldots, P_1^{(i)}$ respectively. (This is essentially Given's algorithm [3] for the reduction of a real symmetric matrix to tridiagonal form, performed starting with row $n$ rather than row 1 and taking advantage of the special form of the original matrix.) Immediately before the transformation with matrix $P_r^{(i)}$ the current matrix is of the form illustrated when $n = 6, r = 3$ by

$$\begin{bmatrix} x & x \\ x & x \\ x & x \\ x & x \\ x & x \end{bmatrix}. \hspace{1cm} \text{(8)}$$

Notice that the transformations are performed on matrix $A_s$ itself and not on $A_s - k_s I$.

As in the original algorithm economy of computation is achieved by examining the $e_i^{(i)}$ in order to determine whether the $A_s$ has effectively split into the direct sum of smaller tridiagonal matrices.

2. Applicability

The procedure intql5 is designed to find all the eigenvalues of a symmetric tridiagonal matrix.