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The convergence of multi-shift QR algorithm for symmetric matrices

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ABSTRACT

In this paper, we discuss the convergence of the double-shift and multi-shift QR algorithms for symmetric tridiagonal matrices. We analyze how to choose multi-shifts by comparing the relationships between the number of iterations, CPU time and the number of multi-shifts. Numerical tests and figures are performed.

1. Introduction

To find the eigenvalues for a matrix, it is necessary to perform many iterations, then it will bring the matrix to the upper Hessenberg form first, for symmetric matrix this will be tridiagonal form by using a technique based on Householder reduction, with a finite sequence of orthogonal similarity transforms, somewhat like a two-sided QR decomposition. Symmetric matrices appear naturally in a variety of applications, and typical numerical linear algebra software makes special accommodations for them.

The QR algorithm, invented fifty years ago by Francis [8,9] and Kublanovskaya [10–12], is one of the most powerful eigenvalue methods. The usual QR algorithm for finding the eigenvalues of a Hessenberg matrix H is based on vector-vector operations, e.g., adding a multiple of one row to another, or one column to another[6,7]. There are several papers proposing parallel implementations of the QR algorithm, e.g. [1–3]. The QR algorithm with shift is a very good method for finding all eigenvalues of an irreducible symmetric matrix. There are two kinds of shifts in common use. One is called the Rayleigh quotient shift, and the other is called willkinson's shift [13–18].

Jiang discussed the convergence properties of double-shift and multishift QL algorithms [4]. In this paper, we try to get deeper understanding about the convergence behavior of the QR algorithm. We consider the QR algorithm with multi-shift applying to symmetric tridiagonal matrices. Furthermore, we give some numerical experiments to analyze the relationship between the number of iterations, CPU time and multi-shifts.

The rest of the paper is organized as follows. After addressing some known results of the QR iteration with double-shift in Section 2 we prove the convergence of multi-shift QR iteration in Section 3. Some comments on the convergence of QR iteration are contained in Section 4. Some numerical results are discussed in Section 5 and the conclusions are given in Section 6.

2. QR iteration with double-shift

In modern computational practice, the QR algorithm is performed in an implicit version which makes the use of multiple shifts easier to introduce. The matrix is first brought to an upper Hessenberg form $A_0 = Q^T AQ$ as in the explicit version; then, at each step, the first column of A_k is transformed via a small-size Householder similarity transformation to the first column

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of $(A_k - \mu_1 I)(A_k - \mu_2 I)$, where μ_1 and μ_2 are the two eigenvalues of the trailing 2×2 principal submatrix of A_k, this is the so-called implicit double-shift. The implicit double-shift QR algorithm is a very good method for finding complex eigenvalues of Hessenberg matrices. Unfortunately its convergence cannot be ensured. For example, the Hessenberg matrix

$$H = \begin{bmatrix} 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ & & \ddots & \ddots & \vdots \\ & & & 1 & 0 \end{bmatrix}$$

is invariant under the double-shift QR algorithm (actually, it is 0-shift), and therefore it does not converge. The convergence of the multi-shift QR algorithm is an even more complicated problem.

Given an $n \times n$ symmetric tridiagonal matrix

$$H = \begin{bmatrix} h_{11} & h_{12} & & & \\ h_{21} & h_{22} & h_{23} & & \\ & \ddots & \ddots & \ddots & \\ & & h_{n-1,n-2} & h_{n-1,n-1} & h_{n-1,n} \\ & & & h_{n,n-1} & h_{nn} \end{bmatrix},$$

where $h_{ij} = h_{ji}$ for $i,j = 1,2,\ldots,n$.

We use the double-shif QR algorithm to produce the sequence $\{H_k\}$ of symmectric tridiagonal matrices, where $H_1 = H$ and

$$H_k = \begin{bmatrix} h_{11}^{(k)} & h_{12}^{(k)} & & & \\ h_{21}^{(k)} & h_{22}^{(k)} & h_{23}^{(k)} & & \\ & \ddots & \ddots & \ddots & \\ & & h_{n-1,n-2}^{(k)} & h_{n-1,n-1}^{(k)} & h_{n-1,n}^{(k)} \\ & & & h_{n,n-1}^{(k)} & h_{nn}^{(k)} \end{bmatrix}.$$

The double-shift procedure is as follows (for $k = 1,2,\ldots$).

1. take the trail 2×2 matrix

$$T_k = \begin{bmatrix} h_{n-1,n-1}^{(k)} & h_{n-1,n}^{(k)} \\ h_{n,n-1}^{(k)} & h_{nn}^{(k)} \end{bmatrix}$$

and take the two eigenvalues of T_k as shifts $\mu_1^{(k)}$ and $\mu_2^{(k)}$.

2. do double-shift QR

(1) $H_k - \mu_1^{(k)} I = Q_k R_k$,
(2) $H_{k+1/2} = R_k Q_k + \mu_1^{(k)} I$,
(3) $H_{k+1/2} - \mu_2^{(k)} I = Q_{k+1/2} R_{k+1/2}$,
(4) $H_{k+1} = R_{k+1/2} Q_{k+1/2} + \mu_2^{(k)} I$,

where Q_k and $Q_{k+1/2}$ are orthogonal matrices, R_k and $R_{k+1/2}$ are upper triangular matrices that have nonnegative diagonal entries.

Let

$$\widetilde{Q}_k = Q_k Q_{k+1/2},$$

$$\widetilde{R}_k = R_{k+1/2} R_k,$$

then we have

$$H_{k+1} = \widetilde{Q}_k^T H_k \widetilde{Q}_k$$

and

$$M_k = [H_k - \mu_1^{(k)} I][H_k - \mu_2^{(k)} I] = \widetilde{Q}_k \widetilde{R}_k. \tag{1}$$