A Note on the Double-Shift QL Algorithm

Jiang Erxiong
Department of Mathematics
Fudan University
Shanghai 200433, China

Submitted by Richard A. Brualdi

ABSTRACT

We discuss convergence properties of the double-shift and multishift QL algorithms.

INTRODUCTION

The implicit double-shift QL algorithm is a very sophisticated method for finding complex eigenvalues of Hessenberg matrices. Unfortunately its convergence cannot be ensured. For instance, the Hessenberg matrix

\[ H_1 = \begin{bmatrix}
0 & 1 \\
0 & 0 & 1 \\
& & \ddots & \ddots \\
0 & 0 & 0 & \cdots & 1 \\
1 & 0 & 0 & \cdots & 0
\end{bmatrix} \]

is invariant under the double-shift QL, and therefore does not converge. The convergence of the multi-shift QL algorithm is an even more complicated problem.

It is an interesting problem whether this method converges when it is applied to a symmetric tridiagonal matrix. A definite answer is given in this paper.

MAIN RESULTS

Given an $n \times n$ symmetric tridiagonal matrix

$$
T = \begin{bmatrix}
\alpha_1^{(1)} & \beta_1^{(1)} & 0 \\
\beta_1^{(1)} & \alpha_2^{(1)} & \beta_2^{(1)} \\
& \ddots & \ddots & \ddots \\
& & \beta_{n-2}^{(1)} & \alpha_{n-1}^{(1)} & \beta_{n-1}^{(1)} \\
0 & & \beta_{n-1}^{(1)} & \alpha_n^{(1)}
\end{bmatrix},
$$

consider the sequence $\{T_k\}$ of symmetric tridiagonal matrices produced by using the double-shift $QL$ algorithm, where $T_1 = T$ and

$$
T_k = \begin{bmatrix}
\alpha_1^{(k)} & \beta_1^{(k)} & 0 \\
\beta_1^{(k)} & \alpha_2^{(k)} & \beta_2^{(k)} \\
& \ddots & \ddots & \ddots \\
& & \beta_{n-2}^{(k)} & \alpha_{n-1}^{(k)} & \beta_{n-1}^{(k)} \\
0 & & \beta_{n-1}^{(k)} & \alpha_n^{(k)}
\end{bmatrix}.
$$

The procedure to obtain $T_{k+1}$ from $T_k$ is as follows (for $k = 1, 2, \ldots$):

1. Take the $2 \times 2$ matrix

$$
\begin{bmatrix}
\alpha_1^{(k)} & \beta_1^{(k)} \\
\beta_1^{(k)} & \alpha_2^{(k)}
\end{bmatrix}
$$

from the top of $T_k$, and use its two eigenvalues $\sigma_1^{(k)}, \sigma_2^{(k)}$ as shifts.

2. Do the double-shift $QL$

$$
(T_k - \sigma_1^{(k)}) = Q_k L_k, \quad (1)
$$

$$
T_{k+1/2} = L_k Q_k + \sigma_1^{(k)} I, \quad (2)
$$

$$
T_{k+1/2} - \sigma_2^{(k)} = Q_{k+1/2} L_{k+1/2}, \quad (3)
$$

$$
T_{k+1} = L_{k+1/2} Q_{k+1/2} + \sigma_2^{(k)} I, \quad (4)
$$
where $Q_k, Q_{k+1/2}$ are orthogonal matrices, and $L_k, L_{k+1/2}$ are lower triangular matrices that have nonnegative diagonal elements.

Let

$$\bar{Q}_k = Q_k Q_{k+1/2},$$  \hspace{1cm} (5)

$$\tilde{L}_k = L_{k+1/2} L_k.$$  \hspace{1cm} (6)

Obviously we have

$$T_{k+1} = \bar{Q}_k^T T_k \bar{Q}_k.$$  \hspace{1cm} (7)

It is also easy to show that

$$M_k = (T_k - \sigma_1^{(k)} I)(T_k - \sigma_2^{(k)} I) = \bar{Q}_k \tilde{L}_k.$$  \hspace{1cm} (8)

Denote the $n$ column vectors of the orthogonal matrix $\bar{Q}_k$ by $q_1^{(k)}, q_2^{(k)}, ..., q_n^{(k)}$, and the $i$th element of $q_j^{(k)}$ by $q_{ij}^{(k)}$. The elements of the lower triangular matrix $\tilde{L}_k$ are $l_{ij}^{(k)}$.

**Lemma 1.** For the above double-shift QL procedure, we have

$$M_k q_1^{(k)} = l_{11}^{(k)} e_1,$$  \hspace{1cm} (9)

where $e_1$ is the first column of unit matrix $I$.

**Proof.** Take the transpose of Equation (8):

$$M_k = M_k^T = \tilde{L}_k^T \bar{Q}_k^T.$$  

So

$$M_k \bar{Q}_k = \tilde{L}_k^T$$

Comparing the first columns of the two sides of the above equation, we have Equation (9).
The convergence theorems will be given in the following. In describing these theorems the superscript \( k \) is omitted for the sake of simplicity, i.e., the elements of \( T_k \) are \( \alpha_i, \beta_i \), and the elements of \( T_{k+1} \) are \( \hat{\alpha_i}, \hat{\beta_i} \).

**Theorem 1.** Let \( n \geq 5 \). Under the double-shift QL algorithm (1), (2), (3), (4), we have following conclusions:

1. \(|\beta_1 \beta_2|\) is a monotone nonincreasing sequence.
2. \(|\beta_1 \beta_2| \to 0\) or \(|\beta_3 \beta_4| \to 0\). In either case \( \beta_1 \beta_2 \beta_3 \beta_4 \to 0 \).
3. If \(|\beta_1 \beta_2| \to 0\) then \(|\beta_3 \beta_4| \to 0\), \(|q_{31}| \to 1\), \(|q_{13}| \to 1\), \(\alpha_3 - \alpha_1 \to 0\), and \(\beta_2^2 + \beta_3^2 - \beta_1^2 \to 0\).

**Proof.** Equation (9) has \( n \) equations, the first of which is

\[
\beta_1 \beta_2 q_{31} = l_{11}.
\] (10)

From (7)

\[
T_{k+1}^2 = \tilde{Q}_k^T T_k^2 \tilde{Q}_k\]

so

\[
\hat{\beta}_1 \hat{\beta}_2 = e_3^T T_{k+1}^2 e_1 = e_3^T \tilde{Q}_k^T T_k^2 \tilde{Q}_k e_1 = q_3^T T_k^2 q_1.
\]

From (9)

\[
\left[ T_k^2 - (\sigma_1 + \sigma_2) T_k + \sigma_1 \sigma_2 I \right] q_1 = l_{11} e_1.
\]

So

\[
T_k^2 q_1 = (\sigma_1 + \sigma_2) T_k q_1 - \sigma_1 \sigma_2 q_1 + l_{11} e_1,
\]

and

\[
\hat{\beta}_1 \hat{\beta}_2 = q_3^T \left[ (\sigma_1 + \sigma_2) T_k q_1 - \sigma_1 \sigma_2 q_1 + l_{11} e_1 \right].
\]

Because

\[
q_3^T T_k q_1 = e_3^T T_{k+1} e_1 = 0, \quad q_3^T q_1 = 0.
\]
So
\[ \hat{\beta}_1 \hat{\beta}_2 = l_{11} q_3^T v_1 = l_{11} q_{13} \]  
(11)

Substituting \( l_{11} \) of Equation (10) into (11), we have

\[ \hat{\beta}_1 \hat{\beta}_2 = \beta_1 \beta_2 q_{13} q_{31}. \]  
(12)

Because \( q_1, q_3 \) are unit vectors, \( |q_{13}| \leq 1, |q_{31}| \leq 1 \). Thus

\[ |\hat{\beta}_1 \hat{\beta}_2| \leq |\beta_1 \beta_2|, \]
i.e., \( |\beta_1 \beta_2| \) is a monotone nonincreasing sequence, which proves the first conclusion in the theorem.

From the monotonicity of \( |\beta_1 \beta_2| \), there is a limit \( \tau \),

\[ |\beta_1 \beta_2| \rightarrow \tau, \]
where \( \tau \geq 0 \). If \( \tau \neq 0 \), then from Equation (12)

\[ \left| \frac{\hat{\beta}_1 \hat{\beta}_2}{\beta_1 \beta_2} \right| = |q_{13}| |q_{31}| \rightarrow 1. \]

This implies

\[ |q_{31}| \rightarrow 1, \quad |q_{13}| \rightarrow 1. \]

Because \( q_1 \) is a unit vector, the remaining elements of \( q_1 \) satisfy

\[ q_{i1} \rightarrow 0, \quad i = 1, 2, 4, 5, \ldots, n. \]

The fifth equation of (9) is

\[ \beta_3 \beta_4 q_{31} + \beta_4 (\alpha_4 \alpha_5 - \sigma_1 - \sigma_2) q_{41} l \left[ \beta_4^2 + \beta_5^2 + (\alpha_5 - \sigma_1)(\alpha_5 - \sigma_2) \right] q_{51} + \beta_5 (\alpha_5 + \alpha_6 - \sigma_1 - \sigma_2) q_{61} + \beta_5 \beta_6 q_{71} = 0. \]

Because the coefficients of \( q_{41}, q_{51}, q_{61}, \) and \( q_{71} \) are all bounded, we have \( \beta_3 \beta_4 \rightarrow 0. \)
For the second and third equations of (9) we have
\[
\beta_2^2 q_{21} + (\alpha_3 - \alpha_1) \beta_2 q_{31} + \beta_2 \beta_3 q_{41} = 0, \\
\beta_1 \beta_2 q_{11} + (\alpha_3 - \alpha_1) \beta_2 q_{21} + (\alpha_3(\alpha_3 - \alpha_1 - \alpha_2) + \alpha_1 \alpha_2 + \beta_2^2 + \beta_3^2 - \beta_2^2) q_{31} \\
+ (\alpha_4 + \alpha_3 - \alpha_2 - \alpha_1) \beta_3 q_{41} + \beta_3 \beta_4 q_{51} = 0,
\]
so we know \( \alpha_3 - \alpha_1 \to 0 \) and \( \beta_2^2 + \beta_3^2 - \beta_1^2 \to 0 \).

We can extend the above theorem to the \( s \)-shift case (i.e. shifting \( s \) times, \( s \geq 2 \)). Let

\[
T^{(k)}_{1:s} = \begin{bmatrix}
\alpha_1^{(k)} & \beta_1^{(k)} & 0 \\
\beta_1^{(k)} & \alpha_2^{(k)} & \beta_2^{(k)} \\
& \ddots & \ddots \\
& & \beta_{s-2}^{(k)} \alpha_{s-1}^{(k)} \beta_{s-1}^{(k)} \\
& & \beta_{s-1}^{(k)} \alpha_{s}^{(k)}
\end{bmatrix},
\]

and let its \( s \) eigenvalues be denoted \( \sigma_1^{(k)}, \sigma_2^{(k)}, \ldots, \sigma_s^{(k)} \). Do the following procedure:

\[
T_k - \sigma_1^{(k)} I = Q_k L_k, \\
T_{k+1/s} = L_k Q_k + \sigma_1^{(k)} I, \\
T_{k+1/s} - \sigma_2^{(k)} I = Q_{k+1/s} L_{k+1/s}, \\
T_{k+2/s} = L_{k+1/s} Q_{k+1/s} + \sigma_2^{(k)} I, \\
\vdots \\
T_{k+i/s} - \sigma_{i+1}^{(k)} I = Q_{k+i/s} L_{k+i/s}, \\
T_{k+(i+1)/s} = L_{k+i/s} Q_{k+i/s} + \sigma_{i+1}^{(k)} I, \\
\vdots \\
(T_{k+(s-1)/s} - \sigma_s^{(k)} I) = Q_{k+(s-1)/s} L_{k+(s-1)/s}, \\
T_{k+1} = L_{k+(s-1)/s} Q_{k+(s-1)/s} + \sigma_s^{(k)} I.
\]
The procedure that produces the above sequence \( \{T_k\} \) is called \( s \)-shift QL algorithm. Here \( Q_{k+i/s} \) \( (i = 0, 1, 2, \ldots, s - 1) \) is an orthogonal matrix; \( L_{k+i/s} \) \( (i = 1, 2, \ldots, s - 1) \) is a lower triangular matrix, and its diagonal elements are nonnegative.

**Theorem 2.** Let \( n \geq 2s + 1 \). For \( \{T_k\} \) produced by the \( s \)-shift QL procedure we have:

1. \( |\beta_1 \beta_2 \cdots \beta_s| \) is a monotone nonincreasing sequence.
2. \( |\beta_1 \beta_2 \cdots \beta_s| \to 0 \) or \( |\beta_{s+1} \beta_{s+2} \cdots \beta_{2s}| \to 0 \). If \( |\beta_1 \beta_2 \cdots \beta_s| \to 0 \), then \( |\beta_{s+1} \beta_{s+2} \cdots \beta_{2s}| \to 0 \), \( |q_{s+1,1}| \to 1 \), and \( |q_{1,s+1}| \to 1 \).

**Proof.** As in the case of \( s = 2 \), we have

\[
M_k = \prod_{i=1}^{s} (T_k - \sigma_i^{(k)}I) = \tilde{Q}_k \tilde{L}_k,
\]

where

\[
\tilde{Q}_k = Q_k Q_{k+1/s} \cdots Q_{k+(s-1)/s}
\]

is an orthogonal matrix, and

\[
\tilde{L}_k = L_{k+(s-1)/s} L_{k+(s-2)/s} \cdots L_k
\]

is a lower triangular matrix. So, as in the case \( s = 2 \) in Lemma 1, we get

\[
\prod_{i=1}^{s} (T_k - \sigma_i^{(k)}I)q_1 = l_{11} e_1, \tag{13}
\]

where \( q_1 \) is the first column of \( \tilde{Q}_k \), and \( l_{11} \) is the first diagonal element of \( \tilde{L}_k \).

We need to prove that the first equation of (13) is

\[
\beta_1 \beta_2 \cdots \beta_s q_{s+1,1} = l_{11}.
\]
Observe that

\[
e^T_1(T_k - \sigma_1^{(k)} I) = e^T_1 \begin{pmatrix} T_{1,s} - \sigma_1 I & \beta_s e_s e^T_1 \\ \beta_s e_1 e^T_s & T_{s+1,n} - \sigma_1 I \end{pmatrix}
\]

\[
= (e^T_1(T_{1,s} - \sigma_1 I), 0)
\]

\[
e^T_1(T_k - \sigma_1^{(k)} I)(T_k - \sigma_2^{(k)} I)
\]

\[
= (e^T_1(T_{1,s} - \sigma_1 I), 0) \begin{pmatrix} T_{1,s} - \sigma_2 I & \beta_s e_s e^T_1 \\ \beta_s e_1 e^T_s & T_{s+1,n} - \sigma_2 I \end{pmatrix}
\]

\[
= (e^T_1(T_{1,s} - \sigma_1 I)(T_{1,s} - \sigma_2 I), 0) \quad \text{(if } s \geq 3)\]

The first element of \((T_{1,s})^p e_s\) is zero when \(p \leq s - 2\), so we have

\[
e^T_1 \prod_{i=1}^{s-1} (T_k - \sigma_i I) = \left( e^T_1 \prod_{i=1}^{s-2} (T_{1,s} - \sigma_i I), 0 \right)
\]

\[
\times \begin{pmatrix} T_{1,s} - \sigma_{s-1} I & \beta_s e_s e^T_1 \\ \beta_s e_1 e^T_s & T_{s+1,n} - \sigma_{s-1} I \end{pmatrix}
\]

\[
= \left( e^T_1 \prod_{i=1}^{s-1} (T_{1,s} - \sigma_i I), 0 \right).
\]

Thus

\[
e^T_1 \prod_{i=1}^{s} (T_k - \sigma_i I) = \left( e^T_1 \prod_{i=1}^{s-1} (T_{1,s} - \sigma_i I), 0 \right) \begin{pmatrix} T_{1,s} - \sigma_s I & \beta_s e_s e^T_1 \\ \beta_s e_1 e^T_s & T_{s+1,n} - \sigma_s I \end{pmatrix}
\]

\[
= \left( e^T_1 \prod_{i=1}^{s} (T_{1,s} - \sigma_i I), \beta_s e^T_1 \prod_{i=1}^{s-1} (T_{1,s} - \sigma_i I) e_s e^T_1 \right).
\]
Observe that the first element of \((T_{1,s})^{s-1}e_s\) is \(\beta_1 \beta_2 \cdots \beta_{s-1}\), so
\[
 e_1^T \prod_{i=1}^{s} (T_k - \sigma_i I) = \left( e_1^T \prod_{i=1}^{s} (T_{1,s} - \sigma_i I) \cdot \beta_1 \beta_2 \cdots \beta_s, 0, \ldots, 0 \right)
 - \left( 0, \ldots, 0, \beta_1 \beta_2 \cdots \beta_s, 0, \ldots, 0 \right).
\]
Therefore the first equation of (13) is
\[
\beta_1 \beta_2 \cdots \beta_s q_{s+1,1} = l_{11}.
\] (14)

Because the element in row \(s + 1\) of the first column of \(\hat{T}^*\) is \(\hat{\beta}_1 \hat{\beta}_2 \cdots \hat{\beta}_s\), we obtain
\[
\hat{\beta}_1 \hat{\beta}_2 \cdots \hat{\beta}_s = e_{s+1}^T \hat{T}^* e_1 = e_{s+1}^T \tilde{Q}^T \hat{T}^* \tilde{Q} e_1 = q_{s+1}^T T^* q_1.
\]
But using Equation (13), we have
\[
T^* q_1 = \sum_{j=0}^{s-1} d_j T^j q_1 + l_{11} e_1,
\]
where
\[
d_0 = \sigma_1 \sigma_2 \cdots \sigma_s, \quad d_{s-1} = \sum_{i=1}^{s} \sigma_i, \quad \text{etc.}
\]
On the other hand
\[
q_{s+1}^T T^j q_1 = e_{s+1}^T \hat{T}^j e_1 = 0 \quad \text{when} \quad j < s - 1,
\]
so
\[
\hat{\beta}_1 \hat{\beta}_2 \cdots \hat{\beta}_s = l_{11} q_{s+1}^T e_1 = l_{11} q_{1,s+1}.
\] (15)
Substituting Equation (14) into the above equation, we have

\[ \hat{\beta}_1 \hat{\beta}_2 \cdots \hat{\beta}_s = \beta_1 \beta_2 \cdots \beta_s q_{s+1,1} q_{1,s+1}. \]  

(16)

Because \( |q_{s+1,1}| \leq 1 \) and \( |q_{1,s+1}| \leq 1 \), \( \{\beta_1 \beta_2 \cdots \beta_s\} \) is a monotone nonincreasing sequence. The first conclusion of this theorem has been proved.

\(|\beta_1 \beta_2 \cdots \beta_s|\) must have a limit \( \tau \geq 0 \). If \( \tau = 0 \) then \( |\beta_1 \beta_2 \cdots \beta_s| \rightarrow 0 \).

Suppose \( \tau \neq 0 \). Then from Equation (16) it is known that

\[ |q_{s+1,1}| \rightarrow 1, \quad |q_{1,s+1}| \rightarrow 1. \]

When \( |q_{s+1,1}| \rightarrow 1 \) the other elements of \( q_1 \) tend to zero, i.e.,

\[ q_{j,1} \rightarrow 0, \quad j = 1, 2, \ldots, s, s+2, \ldots, n. \]

Consider the \( 2s+1 \)st equation of (13), which is

\[ \beta_{s+1} \beta_{s+2} \cdots \beta_{2s} q_{s+1,1} + h_{s+2} q_{s+2,1} + \cdots = 0. \]

Except for \( q_{s+1,1} \), every \( q_{j,1} \) has limit zero, and in the above equation the coefficients of \( q_{j,1} \) are bounded. When we take the limit, \( |q_{j,1}| \rightarrow 0 \), \( |q_{s+1,1}| \rightarrow 1 \), so it must be that

\[ \beta_{s+1} \beta_{s+2} \cdots \beta_{2s} \rightarrow 0. \]

Now the whole theorem has been proved.

Corollary [1]. For \( s = 1 \) (Rayleigh quotient shift) the following statements hold:

1. \( |\beta_1| \) is a monotone nonincreasing sequence.
2. Either \( \beta_1 \rightarrow 0 \), or \( \beta_2 \rightarrow 0 \), \( |q_{2,1}| \rightarrow 1 \), and \( |q_{1,2}| \rightarrow 1 \).

Proof. When \( s = 1 \), it is easy to see that the equalities (14), (15), (16) also hold, so conclusions 1 and 2 are also true.

In [2] there is a result concerning the convergence rate for the \( s \)-shift QL algorithm: if \( \beta_s \rightarrow 0 \) then \( \hat{\beta}_s = O(\beta^2) \).

Applying the above double-shift procedure to the matrix \( W_2^+ \), taking \( \varepsilon = 10^{-3} \) (\( \varepsilon = 10^{-10} \)), after 25 (29) iterations all eigenvalues are obtained. For \( W_2^+ \), with \( \varepsilon = 10^{-3} \) (\( \varepsilon = 10^{-10} \)), 24 (29) iterations were required.
In the process, the first step is to check whether $\beta_4 < \varepsilon$. If so, four eigenvalues can be obtained, and then the order of the matrix can be decreased by 4. If not, we check $\beta_3$; we can get three eigenvalues if $\beta_3 < \varepsilon$. If not, we check $\beta_2$, and when $\beta_2 < \varepsilon$, we have two eigenvalues. When the above three conditions are all false, we consider whether $\beta_1 < \varepsilon$. If so, one eigenvalue is obtained. Otherwise continue the iteration.

A lot of numerical examples show that $\beta_1, \beta_2$ usually will be very small. But we give an example in which $\beta_1, \beta_2$ do not converge to 0. Let

$$T = \begin{pmatrix} \alpha_1 & 1 & 0 & 0 & 0 \\ 1 & \alpha_2 & 1 & 0 & 0 \\ 0 & 1 & \alpha_3 & 0 & 0 \\ 0 & 0 & \alpha_3 & 0 & 0 \\ 0 & 0 & 0 & \alpha_4 & 0 \end{pmatrix},$$

where $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ are real numbers, and let

$$M = (T - \sigma_1 I)(T - \sigma_2 I) = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & h_1 & 0 & 0 \\ 0 & 0 & 0 & h_2 & 0 \end{pmatrix},$$

where $h_1 = \alpha_3^2 - (\alpha_1 + \alpha_2)\alpha_3 + (\alpha_1\alpha_2 - 1)$, $h_2 = \alpha_4^2 - (\alpha_1 + \alpha_2)\alpha_4 + (\alpha_1\alpha_2 - 1)$. It is easy to show that

$$\tilde{Q} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix};$$

here $M = \tilde{Q}L$ is the QL decomposition of $M$. Thus $\hat{T} = \tilde{Q}^T T \tilde{Q}$ and $\hat{T} = T$. This tells us that $T$ is invariant under the above double-shift QL process, so $\beta_1$ and $\beta_2$ do not converge to 0.

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