Convergence of the tridiagonal QR algorithm

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Abstract

By use of the three-term recurrence relation, an elementary and constructive proof is given for the global convergence of the symmetric tridiagonal QR algorithm with Wilkinson’s shift. It is further illustrated why the asymptotic rate of convergence is essentially cubic, as has long been observed in numerical experiments. A general mixed shift strategy with global convergence and cubic rate is also presented. © 2001 Published by Elsevier Science Inc. All rights reserved.

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1. Introduction

Given a real symmetric tridiagonal matrix

\[ T := \begin{bmatrix}
\alpha_1 & \beta_1 \\
\beta_1 & \alpha_2 & \beta_2 \\
& \ddots & \ddots & \ddots \\
& & \beta_{n-1} & \alpha_{n-1} & \beta_n \\
& & & \beta_n & \alpha_n
\end{bmatrix} \]

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with positive subdiagonal elements \( \{ \beta_k \}_{k=1}^{n-1} \) and a real shift parameter \( \lambda \), consider the orthogonal-triangular factorization of

\[
T - \lambda I = QR,
\]

where \( Q \) is orthogonal and \( R \) is upper triangular with nonnegative diagonal elements. This factorization is the matrix formulation of the Gram–Schmidt orthonormalizing process applied to the columns of \( T - \lambda I \) from left to right, and hence \( Q \) is upper Hessenberg. The factorization is unique if \( \lambda \) is not an eigenvalue of \( T \), and this is the case we usually assume. From \( Q \) we define \( b \), the \( QR \) transform of \( T \), by \( b = QTQ^T \). It is easy to check that

\[
b - \lambda I = DRQ,
\]

and that \( b \) is also symmetric tridiagonal. Let \( \{ \hat{\beta}_k \}_{k=1}^{n-1} \) and \( \{ \sigma_k \}_{k=1}^{n-1} \) be the subdiagonal elements of \( b \) and \( Q \), respectively and let \( \{ \alpha_k \}_{k=1}^{n} \) be the diagonal elements of \( R \); these quantities are all positive if \( \lambda \notin \lambda(T) \), where \( \lambda(T) \) denotes the set of eigenvalues of \( T \). This fact is easily seen by equating the corresponding subdiagonal entries on each side of the matrix equations (1.1) and (1.2), respectively:

\[
\beta_k = \sigma_k \rho_k, \quad \text{for } 1 \leq k < n.
\]

Observe that

\[
\lambda \in \lambda(T) \iff \rho_n = 0 \iff \hat{\beta}_{n-1} = 0 \iff \alpha_n := e_n^T \hat{T} e_n = \lambda.
\]

To avoid triviality in later analysis, the order of \( T \) is assumed at least 3. The tridiagonal \( QR \) algorithm iterates the \( QR \) transformation \( T \rightarrow \hat{T} \), with an appropriate shift \( \lambda \) selected at each step:

\[
T^{(1)} := T
\]

for \( k = 1, 2, 3, \ldots \)

\[
T^{(k)} - \lambda^{(k)} I := Q^{(k)} R^{(k)},
\]

\[
T^{(k+1)} := R^{(k)} Q^{(k)} + \lambda^{(k)} I,
\]

and a sequence of unreduced (i.e., \( \beta_j^{(k)} > 0 \), \( 1 \leq j < n \), as conveniently defined in this paper) tridiagonal matrices \( \{ T^{(k)} \} \) is produced if \( \lambda_j^{(k)} \notin \lambda(T) \). The remarkable fact is that, with the shift strategy properly devised \[13\], \( \beta_{n-1}^{(k)} \rightarrow 0 \) rapidly as \( k \rightarrow \infty \). Numerically, as soon as \( \beta_{n-1}^{(k)} \) becomes negligible to working accuracy, the last diagonal entry \( \sigma_n^{(k)} \) of \( T^{(k)} \) is accepted as an approximate eigenvalue of \( T \) and the computation proceeds on the submatrix obtained by deleting the last row and column; sequentially all the eigenvalues are computed and come out in turn \[8,12\]. Here we consider three basic types of shift strategy. Their defining rules and resulting properties are outlined as follows:
(1) Rayleigh shift (R-shift) [7,8,13]. \( \lambda^{(k)} := \alpha^{(k)}_n \), the last diagonal element of \( T^{(k)} \).
- Monotonic decrease of the residual: \( \rho^{(k+1)}_{n-1} \leq \rho^{(k)}_{n-1} \).
- Cubic rate, if convergence occurs: \( \rho^{(k+1)}_{n-1} = O(\beta^{(k)}_{n-1}) \) if \( \beta^{(k)}_{n-1} \to 0 \).
- Only linear rate of \( \rho^{(k)}_{n-1} \to 0 \) if \( \beta^{(k)}_{n-1} \to \beta > 0 \).

(2) Wilkinson shift (W-shift) [8,13]. The shift \( \lambda^{(k)} \) is taken as the eigenvalue of
\[
\begin{bmatrix}
\alpha^{(k)}_{n-1} & \beta^{(k)}_{n-1} \\
\beta^{(k)}_{n-1} & \alpha^{(k)}_n
\end{bmatrix},
\]
which is closer to \( \alpha^{(k)}_n \), that is, \( \lambda^{(k)} \) is chosen to satisfy the following characteristic relations:
\[
(\alpha^{(k)}_{n-1} - \lambda^{(k)})(\alpha^{(k)}_n - \lambda^{(k)}) = \beta^{(k)}_{n-1}^2,
\]
\[
\left| \alpha^{(k)}_n - \lambda^{(k)} \right| \leq \beta^{(k)}_{n-1} \leq \left| \alpha^{(k)}_{n-1} - \lambda^{(k)} \right|.
\] (1.5) (1.6)
- Global convergence always guaranteed: \( \rho^{(k)}_{n-1} \to 0 \).
- Quadratic rate of convergence: \( \beta^{(k+1)}_{n-1} = O(\beta^{(k)}_{n-1})^2 \).
- Implemented in current software packages.

(3) Jiang–Zhang shift (JZ-shift) [6]. The shift \( \lambda^{(k)} \) is taken as
\[
\begin{align*}
\text{the R-shift if} & \quad \beta^{(k)}_{n-2} \geq \sqrt{2}\beta^{(k)}_{n-1}^2, \\
\text{the W-shift if} & \quad \beta^{(k)}_{n-2} < \sqrt{2}\beta^{(k)}_{n-1}.
\end{align*}
\]
- Monotonic decrease of the residual: \( \rho^{(k+1)}_{n-1} \leq \rho^{(k)}_{n-1} \).
- Global convergence guaranteed: \( \rho^{(k)}_{n-1} \to 0 \).
- Cubic rate of convergence: \( \beta^{(k+1)}_{n-1} = O(\beta^{(k)}_{n-1})^3 \).

The global convergence of tridiagonal QR (i.e., \( \rho^{(k)}_{n-1} \to 0 \)) with the W-shift was first proved by Wilkinson [13] using a plane rotation argument. The proof is based on the monotonic decrease of \( \beta^{(k)}_{n-2}\beta^{(k)}_{n-1} \). The result was then generalized by Dekker and Traub [1] to Hermitian matrices. Later Hoffmann and Parlett [4] used a residual estimate to obtain a constructive proof by exploiting the relation of QR to inverse iteration. The convergence analysis simplifies because we can show the monotonic decline of \( \beta^{(k)}_{n-2}\beta^{(k)}_{n-1} \) (instead of \( \beta^{(k)}_{n-2}\beta^{(k)}_{n-1} \) to zero, and this approach is presented in Parlett’s book [8]. Using a similar approach, Jiang and Zhang [6] proposed a mixed type of the R- and W-shift with global convergence and cubic rate. In this paper, sharper bounds on the related (products of) subdiagonal elements are obtained through the use of the three-term recurrence relation (for the characteristic polynomials of the leading principal submatrices of \( T^{(k)} \)), and a constructive proof of \( \rho^{(k)}_{n-1} \to 0 \) with the W-shift is given by showing that \( \rho^{(k+2)}_{n-1} < \sqrt{\omega}\rho^{(k)}_{n-1} \), where \( \omega \) is a positive number \( < 0.675 \). We further illustrate that, with the W-shift, the rate of convergence is essentially cubic, in the sense that the extreme case \( |\alpha^{(k)}_{n-1} - \alpha^{(k)}_n| \to 0 \),
while \( \beta_n^{(k)} \rightarrow 0 \) in which only quadratic rate can be guaranteed is asymptotically unstable and cannot happen in practice. We also generalize the JZ-shift [6] and present a parametric mixed shift strategy with global convergence and cubic rate (see Theorem 3.3), in which the JZ-shift is a special case with parameter \( \theta = 1/\sqrt{2} \).

2. Basic relations

2.1. Schur parameterization of \( Q \)

Any unitary upper Hessenberg matrix \( Q \in \mathbb{C}^{n \times n} \) with positive subdiagonal elements \( \sigma_k := e_{k+1}^* Q e_k, \) \( 1 \leq k < n, \) can be uniquely factorized as a product of \( n \) elementary unitary matrices [2,3]:

\[
Q = Q(\gamma_1, \gamma_2, \ldots, \gamma_n) =: G_1(\gamma_1)G_2(\gamma_2) \cdots G_n(\gamma_n),
\]

(2.1)

where

\[
G_k(\gamma_k) := \text{diag}\left( I_{k-1}, \begin{bmatrix} -\gamma_k & \sigma_k \\ \sigma_k & F_k \end{bmatrix}, I_{n-k-1} \right),
\]

\(|\gamma_k|^2 + \sigma_k^2 = 1, \ 1 \leq k < n, \)

\[
G_n(\gamma_n) := \text{diag}(I_{n-1}, -\gamma_n), \ |\gamma_n| = 1.
\]

Here \( I_j \) is the identity matrix of order \( j \) and \( \{\gamma_k\}_k^n \) are usually termed as the Schur parameters of \( Q \) [3]. These parameters can be read off from the top row and the subdiagonal of \( Q \):

\[
\gamma_1 = -e_1^* Q e_1, \\
\gamma_k = -e_k^* Q e_k / \sigma_1 \sigma_2 \cdots \sigma_{k-1}, \ 2 \leq k \leq n.
\]

To see this, simply multiply out the product \( G_1(\gamma_1)G_2(\gamma_2) \cdots G_n(\gamma_n) \) and get

\[
Q = \begin{bmatrix}
-\gamma_0 \gamma_1 & -\gamma_0 \sigma_1 \gamma_2 & \cdots & -\gamma_0 \sigma_1 \sigma_2 \cdots \sigma_{k-1} \gamma_k & \cdots & -\gamma_0 \sigma_1 \sigma_2 \cdots \sigma_{n-1} \gamma_n \\
\sigma_1 & -\gamma_1 \gamma_2 & \cdots & -\gamma_1 \sigma_2 \cdots \sigma_{k-1} \gamma_k & \cdots & -\gamma_1 \sigma_2 \cdots \sigma_{n-1} \gamma_n \\
& \ddots & \ddots & \ddots & \ddots & \ddots \\
& & \ddots & -\gamma_{k-1} \gamma_k & \cdots & -\gamma_{k-1} \sigma_k \cdots \sigma_{n-1} \gamma_n \\
& & & \ddots & \ddots & \ddots \\
& & & & \ddots & -\gamma_{n-1} \gamma_n \\
& & & & & \sigma_k \\
& & & & & \cdots \\
& & & & & \cdots \\
& & & & & \cdots
\end{bmatrix},
\]

(2.3)

where \( \gamma_0 := 1 \). We refer to the representation (2.3) as the Schur parametric form of \( Q \).
2.2. Characteristic relations in \( T \)

Consider the factorization \( T - \lambda I = QR \). Let \( T_k, Q_k \) and \( R_k \) be the successive leading principal submatrices of \( T, Q \) and \( R \), respectively for \( k = 1, 2, \ldots, n \). We have, by the triangularity of \( R \),

\[
T_k - \lambda I_k = Q_k R_k, \quad 1 \leq k \leq n.
\]

Let \( \chi_k \) be the characteristic polynomial of \( T_k \). Then, with \( Q \) in its Schur parametric form \( Q(\gamma_1, \gamma_2, \ldots, \gamma_n) \), each \( \chi_k \) can be expressed as a product of the Schur parameter \( \gamma_k \) of \( Q \) (observe that \( \det Q_k = (-1)^k \gamma_k \)) and diagonal elements \( \rho_1, \rho_2, \ldots, \rho_k \) of \( R \) [11]:

\[
\chi_k = \chi_k(\lambda) := \det(\lambda I_k - T_k) = \rho_1 \rho_2 \cdots \rho_k \gamma_k, \quad 1 \leq k \leq n.
\]  

(2.4)

Also it is well known that these polynomials \( \{\chi_k\} \) satisfy a three-term recurrence relation [8]:

\[
\begin{align*}
\chi_{k-1} & := 0, \quad \chi_0 := 1, \\
\chi_k = (\lambda - \alpha_k) \chi_{k-1} - \beta_{k-1}^2 \chi_{k-2}, & \quad 1 \leq k \leq n.
\end{align*}
\]  

(2.5)

2.3. Rate estimate of \( \beta_{n-1} \)

To estimate the order of convergence of \( \beta_{n-1}^{(k)} \) to zero, a relation between \( \beta_{n-1} \) and \( \hat{\beta}_{n-1} \) is needed for one \( QR \) step. Based on Lemma 2 of [6], we have

\[
\hat{\beta}_{n-1} = \frac{\rho_1 \rho_2 \cdots \rho_{n-2} |\chi_n(\lambda)|}{\left(\rho_1 \rho_2 \cdots \rho_{n-2} \beta_{n-1}\right)^2 + |\chi_{n-1}(\lambda)|^2} \beta_{n-1}.
\]  

(2.6)

This relation is an identity and can be easily checked through the use of (1.3), (1.4), (2.2), and (2.4). Note that the same relation holds for a Hessenberg \( QR \) step; for details, see [11].

2.4. Properties related to convergence of \( QR \)

We develop relations among the asymptotic behaviors of some key elements for the convergence of tridiagonal \( QR \). A further generalization for normal Hessenberg matrices was given in [10], and a related subject was discussed in [5, 6]. In the following, sometimes to represent an expression \( |\psi^{(k)} - \phi^{(k)}| \to 0 \) as \( k \to \infty \), we use the notation \( \psi^{(k)} \leftrightarrow \phi^{(k)} \).

**Theorem 2.1.** Let \( \{T^{(k)}\} \) be the \( QR \) iterates of \( T \) with either \( R \)- or \( W \)-shift \( \lambda^{(k)} \). Then, the following conditions (a)–(g) are equivalent:

(a) \( \rho_{0}^{(k)} \to 0 \);

(b) \( \beta_{n-1}^{(k)} \to 0 \);
(c) \( \lambda^{(k)} \to \lambda_n \) for some \( \lambda_n \in \lambda(T) \);

(d) \( \chi_n(\lambda^{(k)}) \to 0 \);

(e) \( \sigma_{n-1}^{(k)} \to 0 \);

(f) \( Q^{(k)} e_n \to \pm e_n \);

(g) \( \|R^{(k)} e_n\| \to 0 \);

and each of these further implies that:

(h) \( \rho_1^{(k)} \rho_2^{(k)} \cdots \rho_{n-1}^{(k)} \iff |\chi_{n-1}^{(k)}(\lambda^{(k)})| \geq \delta^{n-1} + O(\varepsilon) \) for some arbitrarily small number \( \varepsilon \), where \( \delta := \min_{j \neq k} |\lambda_j - \lambda_k| : \lambda_j, \lambda_k \in \lambda(T) \) > 0; that is, \( \{\rho_j^{(k)}\}_{j=1}^{n-1} \) and \( |\chi_{n-1}^{(k)}(\lambda^{(k)})| \) are all bounded away from zero.

**Proof.** (a) \( \Rightarrow \) (b): From (1.4) \( \beta_{n-1}^{(k)} = \sigma_{n-1}^{(k)} \rho_n^{(k)} \leq \rho_n^{(k)} \to 0 \).

(b) \( \Rightarrow \) (c): According to the tridiagonal structure of \( T^{(k)} \), \( \beta_{n-1}^{(k)} \to 0 \Rightarrow |\alpha_n^{(k)} - \lambda_n^{(k)}| \to 0 \) for some \( \lambda_n^{(k)} \in \lambda(T) \), which may depend on \( k \). For each \( QR \) transformation \( T \to \tilde{T} \) we have

\[
\begin{align*}
(\beta_{n-1}^{2} + |\alpha_n^{(k)} - \lambda_n^{(k)}|^{2})^{1/2} & = \|\tilde{e}_n^{(k)} (\tilde{T} - \lambda I)\| = \|e_n^{(k)} QR\| = \|e_n^{(k)} R\| = \rho_n \\
& \leq \|R e_n\| = \|Q R e_n\| = \|(T - \lambda I) e_n\| \\
& = (\beta_{n-1}^{2} + |\alpha_n^{(k)} - \lambda_n^{(k)}|^{2})^{1/2}.
\end{align*}
\]  

(2.7)

Hence \( |\alpha_n^{(k+1)} - \lambda^{(k)}| \to 0 \), because \( \beta_{n-1}^{(k)} \to 0 \) and

\[ |\alpha_n^{(k)} - \lambda^{(k)}| \begin{cases} 0 & \text{with the R-shift} \\ \leq \rho_{n-1}^{(k)} & \text{with the W-shift} \end{cases} \]  

(2.8)

Therefore, \( |\Delta_n^{(k+1)} - \Delta_n^{(k)}| \to 0 \) and, since the eigenvalues of \( T \) are distinct, the sequence \( \Delta_n^{(k)} \) converges to a fixed eigenvalue, say \( \lambda_n \), of \( T \). So does the shift sequence \( \lambda^{(k)} \); that is, \( \lambda^{(k)} \to \lambda_n \) for some \( \lambda_n \in \lambda(T) \).

(c) \( \Rightarrow \) (d): This implication is trivial.

(d) \( \Rightarrow \) (a): \( |\chi_n(\lambda^{(k)})| \to 0 \iff |\lambda^{(k)} - \lambda_j^{(k)}| \to 0 \) for some \( \lambda_j^{(k)} \in \lambda(T) \) \( \iff \|T^{(k)} - \lambda^{(k)} I\| Q^{(k)} e_n \equiv \rho_n^{(k)} \to 0 \), by the symmetric and unreduced tridiagonal structure of \( T^{(k)} \).

We have shown that conditions (a)–(d) are equivalent.

(b) \( \Rightarrow \) (h): Suppose \( \lambda^{(k)} \to \lambda_n \in \lambda(T) \) (since (b) \( \Rightarrow \) (c)); let \( \lambda_1, \lambda_2, \ldots, \lambda_{n-1} \) be the remaining distinct eigenvalues of \( T \) so that for real \( \lambda \)

\[
\chi_n(\lambda) = (\lambda - \lambda_n) \prod_{j=1}^{n-1} (\lambda - \lambda_j).
\]

Then, since \( \beta_{n-1}^{(k)} \to 0 \Rightarrow |\alpha_n^{(k)} - \lambda_n| \to 0 \), we know from the recurrence relation (2.5) that
Comparing (2.10) with (2.9) we have
\[
\beta_{n-1}^{(k)}(\lambda^{(k)}) = \prod_{j=1}^{n-1} (\lambda^{(k)} - \lambda_j),
\]
and therefore by (2.4), as \( \lambda^{(k)} \rightarrow \lambda_n \),
\[
\beta_{n-1}^{(k)}(\lambda^{(k)}) = \prod_{j=1}^{n-1} (\lambda^{(k)} - \lambda_j) > 0
\]
for some sufficiently small \( \epsilon \), where \( \delta := \min_{j \neq k} \{|\lambda_j - \lambda_k| : \lambda_j, \lambda_k \in \lambda(T)\} > 0 \); together with (e) (which will be shown next) we prove (h).

(b) \( \Leftrightarrow \) (e): \( \beta_{n-1}^{(k)} = \sigma_{n-1}^{(k)} \rho_{n-1}^{(k)} \rightarrow 0 \Leftrightarrow \sigma_{n-1}^{(k)} \rightarrow 0 \), since by (2.11) \( \rho_{n-1}^{(k)} \) is bounded away from zero.

(e) \( \Leftrightarrow \) (f): This is obvious from (2.3) and (2.2).

(b) \( \Leftrightarrow \) (g): Use the relations given in (2.7) and (2.8). \( \square \)

3. Convergence of the QR iteration
3.1. With the Rayleigh shift

The results given in this section for the R-shift are well known [13]; nevertheless, for the purpose of application to the mixed shift strategy, we derive them by use of recurrence formulas.

Lemma 3.1. Let \( \tilde{T} \) be the QR transform of \( T \) with the R-shift \( \lambda^{(k)} \). Then

(a) \( |\chi_n(\lambda)| = \beta_{n-1}^2 |\chi_{n-2}(\lambda)| \); 
(b) \( \tilde{\beta}_{n-1} = |\gamma_{n-2}|^{1/2} \beta_{n-1} < \beta_{n-1} \); 
(c) \( \tilde{\beta}_{n-2} \beta_{n-1} = |\gamma_{n-2}|^{1/2} \sigma_{n-2} \beta_{n-1}^2 \leq 1/2 \beta_{n-1}^2 \).

Proof. Part (a) is immediate from the recurrence relation (2.5) with \( k = n \). The equalities in (b) and (c) are obtained by using (2.4), (1.3), and (1.4) in (a). The inequalities are from the fact that \( |\gamma_j| + \sigma_j^2 \geq 1 \) and \( \sigma_j > 0 \) for \( 1 \leq j < n \). \( \square \)

Theorem 3.1. Let \( \{T^{(k)}\} \) be the QR iterates of \( T \) with the R-shift \( \lambda^{(k)} \) applied exclusively. Then, either \( \beta_{n-1}^{(k)} \rightarrow 0 \) with \( \beta_{n-1}^{(k+1)} = O(\beta_{n-1}^{(k)}) \), or \( \beta_{n-2}^{(k)} \rightarrow 0 \) with \( \beta_{n-2}^{(k+1)} = O(\beta_{n-2}^{(k)}) \) if \( \beta_{n-1}^{(k)} \rightarrow 0 \).

Proof. From Lemma 3.1(b), \( \beta_{n-1}^{(k)} \) form a bounded decreasing sequence which has a limit, say \( \beta \). If \( \beta = 0 \), then \( \beta_{n-1}^{(k)} \rightarrow 0 \) and from (2.6) and Lemma 3.1(a) we see, for each QR step, that
\[
\tilde{\beta}_{n-1} = \left[ \frac{\rho_1 \rho_2 \cdots \rho_{n-2} |x_{n-2}|}{(\rho_1 \rho_2 \cdots \rho_{n-2} \tilde{\beta}_{n-1})^2 + |x_{n-1}|^2} \right] \tilde{\beta}_{n-1}^3.
\]

Therefore, by Theorem 2.1(b) and (h), \( \tilde{\beta}_{n-1}^{(k+1)} = O(\tilde{\beta}_{n-1}^{(k)}) \) as \( \tilde{\beta}_{n-1}^{(k)} \to 0 \). If \( \tilde{\beta}_{n-1}^{(k)} \to \beta > 0 \), then from Lemma 3.1(b)
\[
|\gamma_{n-2}^{(k)}| = \frac{\beta_{n-1}^{(k)}}{\rho_{n-1}^{(k)}} \tilde{\beta}_{n-1}^{(k)} \to 1.
\]
Hence \( |\gamma_{n-2}^{(k)}| \to 1 \), \( \sigma_{n-1}^{(k)} \to 1 \), since both factors are bounded above by unity. So \( \rho_{n-2}^{(k)} = \sigma_{n-2}^{(k)} \rho_{n-2}^{(k)} \to 0 \), because \( \sigma_{n-2}^{(k)} \to 0 \) and \( \rho_{n-2}^{(k)} \) is bounded. From Theorem 2.1(b) and (d) we infer that \( |x_{n-1}^{(k)}(\tilde{\lambda}_{n}^{(k)})| = \rho_{1}^{(k)} \rho_{2}^{(k)} \cdots \rho_{n}^{(k)} \) is bounded away from zero, so are \( \rho_{j}^{(k)} \) \( \forall j \). Therefore \( \rho_{n-2}^{(k)} = O(\rho_{n-2}^{(k)}) \) because \( \tilde{\beta}_{n-2}^{(k)} = (\rho_{n-1}^{(k)} / \rho_{n-2}^{(k)}) \tilde{\beta}_{n-2}^{(k)} \) for each QR step. \( \square \)

**Remark 3.1.** If, with the R-shift \( \alpha_{n}^{(k)}, \rho_{n-2}^{(k)} \to 0 \) (while \( \beta_{n-1}^{(k)} \to \beta > 0 \)), then, from the recurrence relation (2.5),
\[
|x_{n-1}^{(k)}| = |\alpha_{n}^{(k)} - \alpha_{n-1}^{(k)}| |x_{n-2}^{(k)}| \to 0.
\] (3.1)

We also have (shown in the proof of the last theorem) \( \alpha_{n}^{(k)} \to 0, \sigma_{n-1}^{(k)} \to 1 \), and \( \rho_{1}^{(k)} \rho_{2}^{(k)} \cdots \rho_{n}^{(k)} \) is bounded below from zero. These conditions together with (2.4) imply that \( |x_{n-1}^{(k)}(\tilde{\lambda}_{n}^{(k)})| \to 0 \) while \( |x_{n-2}^{(k)}(\tilde{\lambda}_{n}^{(k)})| \) is bounded away from zero; so with (3.1) we conclude that \( |\alpha_{n}^{(k)} - \alpha_{n-1}^{(k)}| \to 0 \) and, as \( \beta_{n-2}^{(k)} \to 0 \) linearly, a 2-by-2 limiting matrix of the form
\[
S_2 := \begin{bmatrix} \alpha & \beta \\ \beta & \alpha \end{bmatrix}
\] (3.2)
is decoupled from \( T^{(k)} \) in its lower-right corner, where \( \alpha \) is the limit of both \( \alpha_{n}^{(k)} \) and \( \sigma_{n-1}^{(k)} \equiv \tilde{\lambda}_{n}^{(k)} \). However, this situation \( \beta_{n-1}^{(k)} \to \beta > 0 \) is unstable in the sense that one QR step with any slight perturbation \( \varepsilon \) in the shift \( \lambda \) from \( \alpha \) will drive the subdiagonal limit \( \beta \) down to a value \( \tilde{\beta} < \beta \); that is, with \( \lambda = \alpha + \varepsilon \),
\[
S_2 = \begin{bmatrix} \alpha - 2 \tilde{\varepsilon} & \tilde{\beta} \\ \tilde{\beta} & \alpha + 2 \tilde{\varepsilon} \end{bmatrix},
\] (3.3)
where
\[
\tilde{\varepsilon} = \frac{\beta^2}{\beta^2 + \varepsilon^2}, \quad \tilde{\beta} = \frac{\beta^2 - \varepsilon^2}{\beta^2 + \varepsilon^2} \beta < \beta.
\] (3.4)
In other words, \( \beta \) is not a stable lower bound for the monotonically decreasing \( \beta_{n-1}^{(k)} \).

In the language of Rayleigh quotient iteration, this phenomenon is well-known and has long been investigated; see, for example, [8, pp. 75–85, 159–161] and the references therein. Here, we exhibit an interesting type of \( T \) such that, in exact arithmetic, the QR sequence \( \{T^{(k)}\} \) with the R-shift is not stationary in \( \beta_{n-1}^{(k)} \) and has the prop-
Consider the following unreduced symmetric tridiagonal matrix $T_\alpha$ of even order, say $n = 2m$:

$$
T_\alpha := \begin{bmatrix}
\alpha & \beta_1 & 0 & \cdots & 0 \\
\beta_1 & \alpha & \beta_2 & \cdots & 0 \\
0 & \beta_2 & \alpha & \cdots & 0 \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & 0 & \cdots & \beta_{2m-1}
\end{bmatrix}.
$$

It can be shown that, with the R-shift $\alpha$, the whole diagonal of each $T^{(k)}_\alpha$, $k = 1, 2, 3, \ldots$, is constant at $\alpha$ and invariant under $QR$, i.e., $\alpha^{(k)}_i = \alpha$, for $i = 1, 2, \ldots, 2m$, and that $\beta_{2j-1}^{(k)} \to \beta_{2j-1}^{(\infty)} > 0$, $\beta_{2j}^{(k)} \to 0$ ($\beta_{2m}^{(k)} \equiv 0$) linearly, for $j = 1, 2, \ldots, m$; therefore $T^{(k)}_\alpha$ converges to the limiting matrix

$$
T^{(\infty)}_\alpha = \text{diag}\left(\begin{bmatrix} \alpha & \beta_1^{(\infty)} \\ \beta_1^{(\infty)} & \alpha \end{bmatrix}, \begin{bmatrix} \alpha & \beta_3^{(\infty)} \\ \beta_3^{(\infty)} & \alpha \end{bmatrix}, \ldots, \begin{bmatrix} \alpha & \beta_{2m-1}^{(\infty)} \\ \beta_{2m-1}^{(\infty)} & \alpha \end{bmatrix}\right)
$$

with eigenvalues $\{\alpha \pm \beta_{2j-1}^{(\infty)}\}^m_{j=1}$ located symmetrically about the number $\alpha$. The crucial observation in this exceptional case is that the shift $\lambda^{(k)} \equiv \alpha$ is invariant throughout; this phenomenal situation can be created numerically if an explicit R-shift scheme is used in $QR$, because there is no perturbation in the shift from $\alpha$ at all, not even any rounding errors in “computing” the R-shift and the diagonal of $T_\alpha - \alpha I$. Note that, however, the slightest numerical perturbation in the shift from $\alpha$ will lead to $\beta_{n-1}^{(k)} \to 0$ ultimately.

### 3.2. With the Wilkinson shift

We start with a technical lemma which will readily lead to the proof of global convergence of $\beta_{n-1}^{(k)}$.

**Lemma 3.2.** Let $\tilde{T}$ be the $QR$ transform of $T$ and let $\tilde{\tilde{T}}$ be the $QR$ transform of $\tilde{T}$, each with the W-shift. Then $\tilde{\beta}_{n-1}^{(2)} < \omega \beta_{n-1}^{(2)}$, where $\omega$ is a positive number $< 0.675$.

**Proof.** Substituting $\chi_k = \rho_1 \rho_2 \cdots \rho_k \gamma_k$ into the recurrence relation $\chi_n = (\lambda - \alpha_n) \chi_{n-1} - \beta_{n-1}^2 \chi_{n-2}$, we obtain, after eliminating the common factor $\rho_1 \rho_2 \cdots \rho_{n-1}$ and noting that $\beta_{n-1} = \sigma_{n-1} \rho_{n-1}$,

$$
\rho_n \gamma_n = (\lambda - \alpha_n) \gamma_{n-1} - \beta_{n-1}^2 \gamma_{n-2}.
$$

Applying the triangle inequality, we have
Proof. By Lemma 3.2, 

$$\beta_{n-1}^{(k+2)} < \sqrt{\omega \beta_{n-1}^{(k)}}$$, where $0 < \omega < 0.675$; both $\beta_{n-1}^{(2j-1)} \to 0$ and $\beta_{n-1}^{(2j)} \to 0$. \(\square\)

**Theorem 3.2.** Let \{T^{(k)}\} be the QR iterates with the W-shift. Then $\beta_{n-1}^{(k)} \to 0$.

**Proof.** By Lemma 3.2, $\beta_{n-1}^{(k+2)} < \sqrt{\omega \beta_{n-1}^{(k)}}$, where $0 < \omega < 0.675$; both $\beta_{n-1}^{(2j-1)} \to 0$ and $\beta_{n-1}^{(2j)} \to 0$. \(\square\)

---

It is quite elementary to calculate upper bounds for the factors containing parameters $\gamma_k$, $\sigma_k$ on the right-hand side of inequalities in (3.9) and (3.11). To avoid digression, this is done in Appendix A.
Remark 3.2. Consider the asymptotic behavior of $\beta^{(k)}_{n-1} \to 0$ with the W-shift. As pointed out by Wilkinson [13] the rate of convergence is at least quadratic though we expect it to be cubic in general. Indeed, as $\beta^{(k)}_{n-1} \to 0$, the shift $\lambda^{(k)}$ converges to some eigenvalue of $T$, say $\lambda_n$. If $\beta^{(k)}_{n-2} \to 0$ as well, then $|\alpha^{(k)}_{n-1} - \lambda^{(k)}_{n-1}| \to 0$, where $\lambda^{(k)}$ is an eigenvalue distinct from $\lambda_n$. So $|\alpha^{(k)}_{n-1} - \lambda^{(k)}| \geq \delta + O(\varepsilon)$ for small enough $\varepsilon$, where $\delta$ is defined in Theorem 2.1(h), and from (1.5)

$$|\alpha^{(k)}_{n-1} - \lambda^{(k)}| = \frac{\beta^{(k)2}_{n-1}}{|\lambda^{(k)}|}$$

$$= O(\beta^{(k)^2}_{n-1}) \text{ as } \beta^{(k)}_{n-1} \to 0 \text{ (and } \beta^{(k)}_{n-2} \to 0).$$

Since $\lambda_n = \beta^{(k)2}_{n-1}(\alpha^{(k)}_{n-1}) = \lambda^{(k)}_{n-3}$, as shown in (3.6), we know with (3.12) that $|\lambda^{(k)}_{n-1}| = O(\beta^{(k)^2}_{n-2})$, and from (2.6) and Theorem 2.1(h) that

$$\rho^{(k)1}_{n-1} = \left[\frac{\rho^{(k)}_1 \rho^{(k)}_2 \cdots \rho^{(k)}_n}{(\rho^{(k)}_1 \rho^{(k)}_2 \cdots \rho^{(k)}_{n-2})^2 + |\lambda^{(k)}_{n-1}|^2}\right] \beta^{(k)1}_{n-1}$$

$$= O(\beta^{(k)^2}_{n-2}) \rho^{(k)3}_{n-1}$$

as $\beta^{(k)}_{n-1} \to 0$ and $\beta^{(k)}_{n-2} \to 0$. Clearly the conclusion of cubic order of $\rho^{(k)}_{n-1} \to 0$ can be reached under the extra condition that $|\alpha^{(k)}_{n-1} - \lambda^{(k)}|$ is bounded away from zero. Let us take a closer look at what the asymptotic form of $T^{(k)}$ would be if, on the contrary, there is a subsequence

$$|\alpha^{(j)}_{n-1} - \lambda^{(j)}| \to 0.$$  

Similar with the argument used in (2.7), we have, for each $QR$ step $T \to \tilde{T}$,

$$\beta^{(k)2}_{n-2} + 2|\alpha^{(k)}_{n-1} - \lambda^{2} + 2|\alpha^{(k)}_{n-1} - \lambda^{2}|^2$$

$$= \|e^{(k)^2}_{n-1}(\tilde{T} - \lambda I)\|^2 + \|e^{(k)}_{n-1}(\tilde{T} - \lambda I)\|^2 = \|e^{(k)}_{n-1} R\|^2 + \|e^{(k)}_{n} R\|^2$$

$$\leq \|Re^{(k)}_{n-1}\|^2 + \|Re^{(k)}_{n}\|^2 = \|(T - \lambda I)e^{(k)}_{n-1}\|^2 + \|(T - \lambda I)e^{(k)}_{n}\|^2$$

$$= \beta^{(k)2}_{n-2} + |\alpha^{(k)}_{n-1} - \lambda^{2} + 2|\alpha^{(k)}_{n-1} - \lambda^{2}|^2$$

$$\leq \frac{2}{\beta^{(k)2}_{n-2}} + |\alpha^{(k)}_{n-1} - \lambda^{2} + 2|\alpha^{(k)}_{n-1} - \lambda^{2}|^2.$$  

From (3.14), that $0 < \beta^{(k)}_{n-1} \to 0$ and $\lambda^{(k)} \to \lambda_n \in \lambda(T)$ for the W-shift $\lambda^{(k)}$, we infer, under hypothesis (3.14), that

$$0 < \beta^{(j+1)}_{n-2} < \beta^{(j)}_{n-2} + \varepsilon^{(j)}$$

where $\varepsilon^{(j)} \to 0.$

from (3.15). Note that $\beta \neq 0$; otherwise we would have $|\alpha^{(j)}_{n-1} - \lambda^{(j)}_{n-1}| \to 0$ for some eigenvalue $\lambda^{(j)}_{n-1}$ distinct from $\lambda_n$, to which the shift sequence $\lambda^{(j)}$ converges by Theorem 2.1(c), and a contradiction would be reached, since by (3.14) $|\alpha^{(j)}_{n-1} - \lambda^{(j)}| \to 0$. Also, from the recurrence relation (2.5) we have, under (3.14),
Using (2.4), (1.3), (1.4) and Theorem 2.1(e), (h) this asymptotic behavior is equivalent to

\[ |x_{n-1}^{(j)} - \beta_{n-2}^{(j)}x_{n-3}^{(j)}| \to 0, \]

which and (3.16) imply \( \sigma_{n-2}^{(j)} \to 1, \sigma_{n-3}^{(j)} \to 0, \) and by (1.3)

\[ \rho_{n-3}^{(j)} \to 0, \quad (3.17) \]

since all the quantities we discuss are bounded above. Again, applying (2.5) and (2.4) we know, with (3.17), that

\[ |x_{n-2}^{(j)} - |\lambda^{(j)} - \alpha_{n-2}^{(j)}|x_{n-3}^{(j)}| \to 0, \]

where \( |x_{n-2}^{(j)}| \to 0 \) (because \( \sigma_{n-2}^{(j)} \to 1 \)), and \( |x_{n-3}^{(j)}| \to \rho_{n-2}^{(j)} \rho_{n-3}^{(j)} \cdots \rho_{n-3}^{(j)} \) which is bounded away from zero (because Theorem 2.1(h) holds and \( \sigma_{n-3}^{(j)} \to 0 \)). Therefore, we infer that

\[ |\alpha_{n-2}^{(j)} - \lambda^{(j)}| \to 0. \quad (3.18) \]

Hence, under hypothesis (3.14) and the subsequent asymptotic behaviors of the elements in (3.16), (3.17) and (3.18), a limit submatrix

\[ S_3 := \begin{bmatrix} \lambda_n & \beta & 0 \\ \beta & \lambda_n & 0 \\ 0 & 0 & \lambda_n \end{bmatrix} \quad (3.19) \]

of order 3 would ultimately be generated in the bottom-right corner of \( T^{(k)} \) in exact arithmetic, though numerically \( |\alpha_n^{(k)} - \lambda_n| \leq \beta_{n-1}^{(k)} \to 0 \) should be much faster than \( |\alpha_{n-1}^{(k)} - \lambda_n| \to 0, \beta_{n-2}^{(k)} \to \beta \) and \( |\alpha_{n-2}^{(k)} - \lambda_n| \to 0, \beta_{n-3}^{(k)} \to 0 \). In this situation three eigenvalues of \( T \), namely \( \lambda_n \) and \( \lambda_n \pm \beta \), would emerge, and this type of spectral distribution is exactly the one considered in [14] to be excluded from \( T \) in order to guarantee an at least cubic rate (see also [8, p. 171]). Again, as we have seen in Remark 3.1, a limit matrix of the form (3.19) is unstable in that, for one QR step \( S_3 \to S_3 \), any slight difference between the shift \( \lambda \) and the constant diagonal \( \lambda_n \) (in the converging process this difference, in exact arithmetic, always exists for the W-shift \( \lambda^{(k)} \)) unless \( \beta_{n-1}^{(k)} \equiv 0 \) will drive the subdiagonal \( \beta \) to a smaller value \( \hat{\beta} \), as illustrated previously in (3.4), and \( \beta \) cannot be a stable limit for the asymptotically decreasing \( \beta_{n-2}^{(j)} \) (cf. (3.16)). Eventually \( \beta_{n-2}^{(j)} \searrow 0 \), and this contradicts the hypothesis \( |\alpha_{n-1}^{(j)} - \lambda^{(j)}| \to 0 \) in (3.14), which in practice will not hold; therefore, from (3.13) the asymptotic rate of \( \beta_{n-1}^{(k)} \to 0 \) is at least cubic.
3.3. With the mixed shift

We further propose a general mixed shift strategy with which the iterates $\beta_{n-1}^{(k)}$ have global convergence and a cubic rate. A special case of this general strategy (with parameter $\theta = 1/\sqrt{2}$) was given by Jiang and Zhang [6]. Analogous results for unitary matrices were obtained in [2,11]. Here we begin with a lemma which may be viewed as a weaker form of Theorem 3.2.

Lemma 3.3. Let $\{T^{(k)}\}$ be the QR iterates of $T$ with either R- or W-shift at each step. If W-shift is used infinitely many times, then $\beta_{n-1}^{(k)} \to 0$.

Proof. We have shown $\beta_{n-1}^{(k)} \to 0$ in Theorem 3.2 if W-shift is used exclusively. If not, there is no loss of generality in assuming that in the QR iteration R-shift is applied first. Then $\beta_{n-1}^{(k)}$ can be viewed as a sequence consisting only of the following three basic types of steps, distinct by the shifts applied:

- [a] $\beta_{n-1}^{(k)} \xrightarrow{R} \beta_{n-1}^{(k+1)}$,
- [b] $\beta_{n-1}^{(k)} \xrightarrow{R} \beta_{n-1}^{(k+1)} \xrightarrow{W} \beta_{n-1}^{(k+2)}$,
- [c] $\beta_{n-1}^{(k)} \xrightarrow{W} \beta_{n-1}^{(k+1)} \xrightarrow{W} \beta_{n-1}^{(k+2)}$,

where the letter (R or W) over the arrow represents the shift used in that QR step.

For type [a],

$$\beta_{n-1}^{(k)} > \beta_{n-1}^{(k+1)} \quad (3.20)$$

from Lemma 3.1(b). For type [b],

$$\frac{\omega}{2} \beta_{n-1}^{(k+1)^2} \geq \omega \beta_{n-2}^{(k+1)} \beta_{n-1}^{(k+1)} > \beta_{n-1}^{(k+2)^2} \quad (3.21)$$

by Lemma 3.1(c) and (3.9). For type [c],

$$\omega \beta_{n-1}^{(k)^2} > \beta_{n-1}^{(k+2)^2} \quad (3.22)$$

from Lemma 3.2. Note that for the sequence $\beta_{n-1}^{(k)}$ at least one of the types [b] and [c] is performed perpetually, since by assumption W-shift is used infinitely many times in the process. From (3.21) and (3.22) we know at least

$$\sqrt{\omega} \beta_{n-1}^{(k)} > \beta_{n-1}^{(k+2)} \quad (3.23)$$

holds for both [b] and [c], where $\omega$ was given in (3.10). Since decreases of $\beta_{n-1}^{(k)}$ consist of steps of (3.20) and infinitely many steps of (3.23), convergence of $\beta_{n-1}^{(k)}$ to zero is clear. □

Corollary 3.1. Let $\{T^{(k)}\}$ be the QR iterates of $T$ with R- and W-shift applied in alternating order. Then $\beta_{n-1}^{(k)} \to 0$. 

Proof. As presented in the proof of the preceding lemma, type [b] is performed throughout the iterative process with $\beta_{n-1}^{(k+2)} < \sqrt{\frac{\sigma_n}{\sigma_{n-1}}} \beta_{n-1}^{(k)}$ from (3.21).

**Theorem 3.3.** Let $\theta$ be a positive real number and let $\{T^{(k)}\}$ be the QR iterates of $T$ with the following shift strategy:

\[
\begin{align*}
\text{if } \theta \beta_{n-2}^{(k)} &\geq \beta_{n-1}^{(k)}, & \text{use the R-shift,} \\
\text{if } \theta \beta_{n-2}^{(k)} &< \beta_{n-1}^{(k)}, & \text{use the W-shift.}
\end{align*}
\]

(3.24)

Then $\beta_{n-1}^{(k)} \to 0$ and $\beta_{n-1}^{(k+1)} = O(\beta_{n-1}^{(k)})$. In particular:

(a) $\beta_{n-1}^{(k)} < \beta_{n-1}^{(k+1)}$ if $\omega \leq \theta$, where $\omega$ is defined in (3.10), $0 < \omega < 0.675$.

(b) $\beta_{n-1}^{(k)}$ can be majorized by a sequence which is at least geometrically convergent to zero if $\theta < 3\sqrt{3}/2$.

Proof. To show $\beta_{n-1}^{(k)} \to 0$, we consider two situations: If W-shift is applied infinitely many times, then $\beta_{n-1}^{(k)} \to 0$ by Lemma 3.3. If not, then ultimately R-shift is used and from Theorem 3.1 either $\beta_{n-1}^{(k)} \to 0$ or $\beta_{n-2}^{(k)} \to 0$; the latter also implies that $\theta \beta_{n-2}^{(k)} \geq \beta_{n-1}^{(k)} \to 0$.

For the asymptotic rate of $\beta_{n-1}^{(k)} \to 0$, with the R-shift we have $\beta_{n-1}^{(k+1)} = O(\beta_{n-1}^{(k)})$ from Theorem 3.1; with the W-shift we obtain $\beta_{n-1}^{(k+1)} = O(\beta_{n-2}^{(k)} \beta_{n-1}^{(k)}) = O(\beta_{n-1}^{(k)})$ by (3.13) and $\theta \beta_{n-2}^{(k)} < \beta_{n-1}^{(k)} \to 0$.

(a) Consider one QR step $T \to \widehat{T}$. For the R-shift, $\widehat{\beta}_{n-1}^{(k)} < \beta_{n-1}^{(k)}$ always holds by Lemma 3.1(b). For the W-shift,

\[
\beta_{n-1}^{(k)} \leq 0 \text{ if } \theta \beta_{n-2}^{(k)} \beta_{n-1}^{(k)} < \left(\frac{\omega}{\theta}\right) \beta_{n-1}^{(k)}, \quad \text{by (3.9),}
\]

\[
< \left(\frac{\omega}{\theta}\right) \beta_{n-1}^{(k)}, \quad \text{since } \theta \beta_{n-2}^{(k)} < \beta_{n-1}^{(k)} \text{ if W-shift is applied,}
\]

\[
\leq \beta_{n-1}^{(k)}, \quad \text{if } \omega \leq \theta.
\]

Hence $\beta_{n-1}^{(k)} \to 0$ monotonically if $\omega \leq \theta$.

(b) Again consider one QR step. First we show $\beta_{n-2}^{(k)} \beta_{n-1}^{(k)}$ decreases at least linearly after each step. With the R-shift we have

\[
\beta_{n-2}^{(k)} \beta_{n-1}^{(k)} = |\gamma_{n-2}|^2 \sigma_{n-2} \sigma_{n-1} \beta_{n-1}^{(k)}, \quad \text{from Lemma 3.1(c) and (b),}
\]

\[
\leq \left(\frac{2}{3\sqrt{3}}\right) \beta_{n-1}^{(k)}, \quad \text{because } |\gamma_{n-2}|^2 \sigma_{n-2} \leq \frac{2}{3\sqrt{3}} \text{ and } \sigma_{n-1} \leq 1,
\]

\[
\leq \left(\frac{20}{3\sqrt{3}}\right) \beta_{n-2}^{(k)} \beta_{n-1}^{(k)}, \quad \text{since } \theta \beta_{n-2} \geq \beta_{n-1}^{(k)} \text{ if R-shift is used.}
\]
With the W-shift we have
\[ \hat{\beta}_{n-2} \hat{\beta}_{n-1} = \sigma_n - 2\sigma_{n-1} \beta_{n-1} \rho_n^2, \]
where \( \sigma_n \) is defined in (1.3) and (1.4),
\[ \leq |\gamma_{n-3}| \sigma_n^2 - 2\sigma_{n-1}^2 (|\gamma_{n-1}| + |\gamma_{n-2}| \sigma_{n-1}) \beta_{n-2} \beta_{n-1} \]
\[ < \left( \frac{32}{25\sqrt{3}} \right) \beta_{n-2} \beta_{n-1}, \]
an upper-bound calculation given by (A.3) in Appendix A. \( \square \) (3.25)

Therefore, with either shift,
\[ \hat{\beta}_{n-2} \hat{\beta}_{n-1} \leq \mu \beta_{n-2} \beta_{n-1}, \]
where \( \mu = \max \left\{ \frac{2\theta}{3\sqrt{3}}, \frac{32}{25\sqrt{3}} \right\} \).

If \( \theta < (3\sqrt{3})/2 \), then \( \mu < 1 \) is guaranteed and \( \beta_{n-2}^{(k)} \hat{\beta}_{n-1}^{(k)} \leq 0 \) at least geometrically.

Next we show that \( \hat{\beta}_{n-1}^{(3)} \) is dominated by a constant multiple of \( \beta_{n-2} \beta_{n-1} \):

- for the R-shift, \( \hat{\beta}_{n-1}^{(3)} \leq \theta \beta_{n-2}^2 \beta_{n-1} \), since \( \beta_{n-1} \leq \theta \beta_{n-2} \);
- for the W-shift, \( \hat{\beta}_{n-1}^{(3)} = \sigma_{n-1}^3 : \rho_n \cdot \rho_n^2 \), since \( \hat{\beta}_{n-1} = \sigma_{n-1} \rho_n \),
\[ \leq |\gamma_{n-3}| \sigma_{n-2}^2 (|\gamma_{n-1}| + |\gamma_{n-2}| \sigma_{n-1})^2 \beta_{n-2} \beta_{n-1}, \]
from (3.5) and (3.8),
\[ < \beta_{n-2} \beta_{n-1} \], from (A.4) in Appendix A. \( \square \) (3.26)

**Remark 3.3.** To show \( \beta_{n-1}^{(k)} \to 0 \) with the W-shift, we managed to capture the essential pattern of \( \beta_{n-1}^{(k)} \) by itself in two consecutive steps, namely \( \beta_{n-1}^{(k+2)} = \sqrt{\theta} \beta_{n-1}^{(k)} \) in Lemma 3.2; we could also have followed the technique used by [1, Lemma 7.4] or [8, Theorem 8.10.1], as illustrated by (3.25) and (3.26) in the proof of Theorem 3.3(b); here the convergence factor \( 32/(25\sqrt{3}) \) \( \approx 0.572 \) obtained to ensure \( \beta_{n-2} \beta_{n-1} \leq 0 \) is smaller than the factor \( 1/(\sqrt{2}) \) \( \approx 0.707 \) used in [1] or [8].

**Remark 3.4.** Though the mixed shift strategy (with \( 0 < \theta < \infty \)) in (3.24) guarantees cubic convergence, in normal usage it is less efficient than the W-shift; as \( \hat{\beta}_{n-1}^{(k)} \to 0 \) almost always faster than \( \beta_{n-2}^{(k)} \to 0 \), strategy (3.24) ultimately uses R-shift, not W-shift, which is numerically faster [9]. Generally speaking, the smaller the \( \theta \) value assigned (i.e., the closer to the exclusive use of W-shift), the faster the practical convergence observed, as numerical testing indicates. The samples we chose are thousands of tridiagonal matrices with entries \( \alpha_k \) and \( \beta_k \), produced, on \([-1, 1]\) and \([0, 10]\), respectively, by a pseudo-random number generator on the computer. For example, with \( \theta = 1/(\sqrt{2}) \) and \( n = 20 \), the mixed shift is about 5% slower than the W-shift, measured with the average number of iterations per eigenvalue. However, there are circumstances (e.g., \( \theta = 10^{-6} \), \( n = 20 \cdot 30 \) and beyond) under which the mixed shift is *slightly* yet consistently, faster (less than 0.1%, which is quite insignificant). The asymptotic analysis for the W-shift (cf. (3.13), which
exhibits better-than-cubic rate if $\beta_{n-2}^{(k)} \to 0$, together with the unstable nature of the extreme case $\beta_{n-2}^{(k)} \to \beta > 0$ (cf. (3.19)), as discussed in Remark 3.2, explains the reason why the W-shift is asymptotically more efficient than the R-shift, as has long been observed in numerical experiments.

Appendix A. Upper-bound computations

In the preceding section, suprema or upper bounds of certain elementary continuous functions of parameters $\gamma_k$, $\sigma_k(|\gamma_k|^2 + \sigma_k^2 = 1$, $\sigma_k > 0$, $1 \leq k < n$, $|\gamma_n| = 1$) are needed in order to analyze decreases in the products of the subdiagonal elements $\beta_k$ in one QR step. They are collected and formulated in this appendix. For simplicity, the bounds presented here may not be very sharp. In the following, we set $x := \sigma_{n-2}$, $y := \sigma_{n-1}$, where $0 < x \leq 1$, $0 < y \leq 1$. (Observe, however, that in the real QR process $\sigma_k|_{k=1}^{|n-1}$ are interrelated and not fully independent from each other.)

\begin{align}
|\gamma_n-3|\sigma_{n-2}\sigma_{n-1}^3(|\gamma_{n-1}| + |\gamma_{n-2}|\sigma_{n-1}) \\
< \sigma_{n-2}\sigma_{n-1}^3(|\gamma_{n-1}| + |\gamma_{n-2}|\sigma_{n-1}) \\
=: xy(\sqrt{1 - y^2 + \sqrt{1 - x^2}y}) \\
< y^3\sqrt{1 - y^2 + \frac{1}{2}y^4} \\
=: f(y) \\
\leq f\left(\frac{9}{10}\right) = \frac{27}{40} = 0.675. \quad (A.1)
\end{align}

\begin{align}
\sigma_{n-2}(|\gamma_{n-1}| + |\gamma_{n-2}|\sigma_{n-1}) \\
\leq \sigma_{n-2}|\gamma_{n-1}| + |\gamma_{n-2}|\sigma_{n-1} \\
=: x\sqrt{1 - y^2 + y\sqrt{1 - x^2}} \\
=: g(x, y) \\
\leq g\left(x, \sqrt{1 - x^2}\right) = 1. \quad (A.2)
\end{align}

\begin{align}
|\gamma_n-3|\sigma_{n-2}\sigma_{n-1}^2(|\gamma_{n-1}| + |\gamma_{n-2}|\sigma_{n-1}) \\
< \sigma_{n-2}\sigma_{n-1}^2(|\gamma_{n-1}| + |\gamma_{n-2}|\sigma_{n-1}) \\
=: x^2y^2\left(\sqrt{1 - y^2 + \sqrt{1 - x^2}}\right) \\
=: h(x^2, y^2) \\
\leq h\left(\frac{4}{5}, \frac{4}{5}\right) = \frac{32}{25\sqrt{5}} < 0.573. \quad (A.3)
\end{align}
jγn−3|σn−2σn−1|jγn−1| + jγn−2|σn−1|2
< σn−2σn−1(|jγn−1| + jγn−2|σn−1|2
:= xy4\left(\sqrt{1 - y^2} + \sqrt{1 - x^2y}\right)^2 < 1. \quad (A.4)

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References