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CONVERGENCE OF THE TRIDIAGONAL QR ALGORITHM WITH SHIFTS FROM THE LOWER RIGHT 3×3 SUBMATRICES

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Abstract. The convergence results obtained by J. H. Wilkinson [Linear Algebra Appl. 1 (1968) 409–420] for the tridiagonal QR algorithm are further developed. We choose an eigenvalue of the 3×3 submatrix in the lower right corner of the iterating tridiagonal matrix as the shift and show that global convergence of the QR iteration can be established mathematically. Numerical testing on random tridiagonal matrices of order ≤ 40 also indicates that convergence on average is about 10% faster than that with the Wilkinson shift, measured in terms of the maximum number of iterations required to find an approximate eigenvalue.

Key words. QR algorithm; convergence analysis; shift strategy; symmetric tridiagonal matrices

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1. Introduction. A notable attainment in the development of the QR algorithm was Wilkinson's mathematical proof of *global* convergence of the QR iteration for real, symmetric tridiagonal matrices with the efficient shift strategy he proposed [11], in which an eigenvalue from the lower right 2×2 submatrix is chosen as the shift. Since then, a number of different proofs and extensions have been given [1, 2, 4–10]. In this paper we make a further extension to Wilkinson's shift, with emphasis placed on the analysis of global convergence. The main results are described as follows.

Given a real symmetric tridiagonal matrix

$$T := \begin{bmatrix} \alpha_1 & \beta_1 & & & & \\ \beta_1 & \alpha_2 & \beta_2 & & & \\ & \beta_2 & \ddots & \ddots & & \\ & & \ddots & \alpha_{n-2} & \beta_{n-2} & \\ & & & \beta_{n-2} & \alpha_{n-1} & \beta_{n-1} \\ & & & & \beta_{n-1} & \alpha_n \end{bmatrix} \tag{1.1}$$

of order $n \geq 4$ with *positive* off-diagonal elements $\{\beta_i\}_{i=1}^{n-1}$, let $\left\{T^{(k)}\right\}$ be a sequence of tridiagonal QR iterates generated by

$$T^{(1)} := T$$

$$\text{for } k = 1, 2, 3, \cdots$$

$$T^{(k)} - \lambda^{(k)} I =: Q^{(k)} R^{(k)}, \tag{1.2}$$

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

where $\lambda^{(k)}$ is the *shift* selected as an eigenvalue of the lower right 3×3 submatrix of $T^{(k)}$, which is closest to, but not equal to, $\alpha_n^{(k)}$ and satisfies the condition $|\lambda^{(k)} - \alpha_n^{(k)}| \leq$

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$|\lambda^{(k)} - \alpha_{n-2}^{(k)}|$. (Such a choice for $\lambda^{(k)}$ is always feasible.) Then

$$\beta_{n-1}^{(k)} \to 0 \quad \text{as} \quad k \to \infty,$$

and $\alpha_n^{(k)}$ can be taken as an (approximate) eigenvalue of T; the asymptotic rate of convergence is

$$\beta_{n-1}^{(k+1)} = O(\beta_{n-1}^{(k)3}\beta_{n-2}^{(k)2}\beta_{n-3}^{(k)2}) \quad \text{if} \quad \beta_{n-2}^{(k)} \to 0 \quad \text{and} \quad \beta_{n-3}^{(k)} \to 0.$$

In practice, numerical convergence is about 10% faster than that with the Wilkinson shift, measured in terms of the maximam number of iterations required to get an eigenvalue, for random tridiagonal matrices of size $n \leq 40$.

Our analysis is based on the employment of the three-term recurrence relation associated with $T^{(k)}$ and a parametric representation of the orthogonal factor $Q^{(k)}$, both of which, together with the notation used, are introduced in §2. With the rule for determining the shift $\lambda^{(k)}$ explained in §3, an intriguing monotonic property of $\beta_{n-1}^{(k)}\beta_{n-2}^{(k)2}\beta_{n-3}^{(k)}$ in the iteration is obtained; this property provides the foundation for the proof of global convergence $\beta_{n-1}^{(k)} \to 0$. Details of the analysis, as well as an estimation on the rate of convergence, constitute §4. A simple numerical testing is conducted in §5, and finally some concluding remarks are given in §6.

2. Basic relations in the QR transformation. In this preliminary section we follow the treatment as presented in [8] and [9], and consider one step of the QR iteration $T \to \widehat{T}$. Given a tridiagonal T with spectrum $\lambda(T)$ and a real number λ, we form the orthogonal-triangular factorization

$$T - \lambda I =: QR\,, \tag{2.1}$$

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 [4, 7], and hence Q is upper Hessenberg. With Q we define $\widehat{T}$, the QR transform of T, by $\widehat{T} := Q^{\mathrm{T}}TQ$, where Q^{T} is the transpose of Q. It is easy to check that

$$\widehat{T} - \lambda I = RQ\,, \tag{2.2}$$

and that $\widehat{T}$ is also symmetric tridiagonal. Let $\{\widehat{\beta}_i\}_{i=1}^{n-1}$ and $\{\sigma_i\}_{i=1}^{n-1}$ be the subdiagonal elements of $\widehat{T}$ and Q, and let $\{\rho_i\}_{i=1}^{n}$ be the diagonal elements of R; these quantities are all *positive* if $\lambda \notin \lambda(T)$. This fact is easily seen by equating the corresponding subdiagonal entries on each side of the matrix equations (2.1) and (2.2), respectively:

$$\beta_j = \sigma_j\rho_j\,, \tag{2.3}$$

$$\widehat{\beta}_j = \sigma_j\rho_{j+1}, \qquad 1 \leq j < n. \tag{2.4}$$

Observe that, for each QR transformation $T \to \widehat{T}$ with shift λ,

$$\lambda \in \lambda(T) \Longleftrightarrow \rho_n = 0 \Longleftrightarrow \widehat{\beta}_{n-1} = 0 \Longrightarrow \widehat{\alpha}_n := \mathbf{e}_n^{\mathrm{T}}\widehat{T}\mathbf{e}_n = \lambda.$$

Since Q is orthogonal and upper Hessenberg with positive subdiagonal elements $\{\sigma_i\}_{i=1}^{n-1}$, it can be uniquely factorized as a product of n elementary orthogonal matrices [2, 3]:

$$Q =: Q(\gamma_1, \gamma_2, \cdots, \gamma_n) =: G_1(\gamma_1)G_2(\gamma_2)\cdots G_n(\gamma_n), \tag{2.5}$$

where

$$G_j(\gamma_j) := \operatorname{diag}\left(I_{j-1}, \begin{bmatrix} -\gamma_j & \sigma_j \\ \sigma_j & \gamma_j \end{bmatrix}, I_{n-j-1}\right), \quad |\gamma_j|^2 + \sigma_j^2 = 1, \quad 1 \le j < n, \quad (2.6)$$

$$G_n(\gamma_n) := \operatorname{diag}(I_{n-1}, -\gamma_n), \qquad |\gamma_n| = 1.$$

Here I_j is the identity matrix of order j and $\{\gamma_i\}_{i=1}^n$ are usually termed as the *Schur parameters* of Q [3]. In numerical linear algebra, this is exactly how Q is constructed in the triangularization of $T - \lambda I$ [7]; for convenience, reflectors, rather than rotators, are used here. We refer to (2.5) as the Schur parametric representation of Q [3].

Let T_j, Q_j, and R_j be the successive leading principal submatrices of T, Q, and R, respectively, for $j = 1, 2, \cdots, n$. We have, by the triangularity of R,

$$T_j - \lambda I_j = Q_j R_j, \qquad 1 \le j \le n.$$

Let χ_j denote the characteristic polynomial of T_j. Then, with Q in its parametric form $Q(\gamma_1, \gamma_2, \cdots, \gamma_n)$, each χ_j can be expressed as a product of γ_j (observe that $\det Q_j = (-1)^j \gamma_j$) and the leading diagonal elements $\rho_1, \rho_2, \cdots, \rho_j$ of R [9]:

$$\chi_j = \chi_j(\lambda) := \det(\lambda I_j - T_j) = \rho_1 \rho_2 \cdots \rho_j \gamma_j, \quad 1 \le j \le n. \quad (2.7)$$

And it is well known that these polynomials satisfy a three-term recurrence relation [7]: $\chi_{-1} := 0$, $\chi_0 := 1$,

$$\chi_j = (\lambda - \alpha_j)\chi_{j-1} - \beta_{j-1}^2 \chi_{j-2}, \qquad 1 \le j \le n. \quad (2.8)$$

By the symmetric and *unreduced* Hessenberg structure of $T^{(k)}$ in the QR iteration with shift $\lambda^{(k)}$, the following three asymptotic conditions are equivalent:

$$\begin{array}{ll} (a) & |\chi_n(\lambda^{(k)})| \to 0, \\ (b) & |\lambda^{(k)} - \lambda_{j(k)}| \to 0 \text{ for some } \lambda_{j(k)} \in \lambda(T), \\ (c) & \rho_n^{(k)} \to 0, \end{array} \quad (2.9)$$

where $\rho_n^{(k)}$ measures the closeness of linear dependency of the last column of $T^{(k)} - \lambda^{(k)} I$ on the left $(n-1)$ columns, which always span an $(n-1)$-dimensional subspace, as we have

$$\mathbf{q}_n^{(k)\mathrm{T}}(T^{(k)} - \lambda^{(k)} I) = \rho_n^{(k)} \mathbf{e}_n^{\mathrm{T}}$$

by premultiplying (1.2) with the transpose of $\mathbf{q}_n^{(k)} := Q^{(k)} \mathbf{e}_n$.

For each QR step $T \to \widehat{T}$, the following identity (simplified from Lemma 2 in [6])

$$\widehat{\beta}_{n-1} = \left[\frac{\rho_1 \rho_2 \cdots \rho_{n-2} |\chi_n(\lambda)|}{(\rho_1 \rho_2 \cdots \rho_{n-2} \beta_{n-1})^2 + |\chi_{n-1}(\lambda)|^2}\right] \beta_{n-1} \quad (2.10)$$

can readily be checked through the use of (2.3), (2.4), (2.7), and (2.8). A relation of this type was used by Jiang and Zhang [6] to estimate the rate of convergence of $\beta_{n-1}^{(k)}$ for tridiagonal matrices. The same relation holds for a Hessenberg QR step; for details, see [9].

3. The cubic shift. Let $\widetilde{T}_3$ denote the lower right 3×3 submatrix of T. From the expression of T (see (1.1)) it is easy to check that the characteristic equation for $\widetilde{T}_3$ (i.e., $\det(\lambda I_3 - \widetilde{T}_3) = 0$) can be presented as

$$(\lambda - \alpha_{n-2})[(\lambda - \alpha_{n-1})(\lambda - \alpha_n) - \beta_{n-1}^2] = (\lambda - \alpha_n)\beta_{n-2}^2, \tag{3.1}$$

which, under the condition $\lambda \neq \alpha_{n-2}$, further leads to the modular equality

$$|(\lambda - \alpha_{n-1})(\lambda - \alpha_n) - \beta_{n-1}^2| = \left| \frac{\lambda - \alpha_n}{\lambda - \alpha_{n-2}} \right| \beta_{n-2}^2. \tag{3.2}$$

Let $\tau_1 < \tau_2 < \tau_3$ be the three roots of (3.1) on the real line which are strictly interlaced with the roots, say $\omega_1 < \omega_2$, of

$$(\lambda - \alpha_{n-1})(\lambda - \alpha_n) - \beta_{n-1}^2 = 0,$$

the characteristic equation for the lower right 2×2 submatrix. Note that α_n always sits in between ω_1 and ω_2, and no matter where α_{n-2} is located, it is clear that at least *one* of the roots $\{\tau_i\}_{i=1}^3$, say τ_j, satisfies the conditions

$$\tau_j \neq \alpha_n, \tag{3.3}$$

$$|\tau_j - \alpha_n| \leq |\tau_j - \alpha_{n-2}|, \tag{3.4}$$

that is, τ_j is closer to α_n than to α_{n-2} but not equal to α_n. If (the middle root) $\tau_2 = \alpha_n$, then *both* τ_1 and τ_3 satisfy (3.3), (3.4), with equality holds in (3.4); this special case happens only if $\alpha_n = \alpha_{n-2}$, as can be readily checked with (3.1). Hence it is always possible to choose the shift λ among $\{\tau_i\}_{i=1}^3$ which satisfies the requirements

$$\lambda \neq \alpha_n \tag{3.5}$$

and

$$|\lambda - \alpha_n| \leq |\lambda - \alpha_{n-2}| \tag{3.6}$$

with $|\lambda - \alpha_n|$ as small as possible; in case of a tie (when $\alpha_n = \alpha_{n-2}$) we can choose either τ_1 or τ_3. We hereby refer to the shift λ determined by this strategy as the *cubic shift*.

The required conditions (3.5), (3.6) on λ will become natural later in the analysis of $|\chi_n(\lambda)|$ in which the left side of equation (3.2) appears as a critical factor that can be manipulated by selecting the proper shift among $\{\tau_i\}_{i=1}^3$.

Note that to guarantee the use of (3.2) from (3.1), we need $\lambda \neq \alpha_{n-2}$, which is equivalent to (3.5). Here we present an extreme example to illustrate that, if (3.5) is not satisfied, convergence of $\beta_{n-1}^{(k)}$ to zero will not take place. Let $\alpha_1 = \alpha_2 = \cdots = \alpha_n \equiv \alpha$ for the tridiagonal T in (1.1), where $n \equiv 2m$ is an even integer ≥ 4. Without the requirement $\lambda^{(k)} \neq \alpha_n^{(k)}$ in selecting the cubic shift, it can be shown that $\lambda^{(k)} = \alpha_n^{(k)} = \alpha_{n-1}^{(k)} = \cdots = \alpha_1^{(k)} \equiv \alpha$ for all $k = 1, 2, 3, \cdots$, and that $\beta_{2j-2}^{(k)} \to 0$ ($\beta_0^{(k)} \equiv 0$), but $\beta_{2j-1}^{(k)} \to \delta_j > 0$, $j = 1, 2, \cdots, m = n/2$, all with linear rates only, as the eigenvalues $\{\alpha \pm \delta_j\}_{j=1}^m$ of T are symmetrically located about the number α in m pairs.

4. Convergence of the QR iteration. Success in achieving global convergence usually hinges on whether a monotonically decreasing quantity containing the crucial element $\beta_{n-1}^{(k)}$ can be found in the iteration [11, 1, 4, 7, 6, 9, 10]; we investigate this likelihood in a QR step $T \to \widehat{T}$ through the use of the three-term recurrence relation associated with T and the Schur parametric representation of Q.

4.1. Monotonic decrease of $\boldsymbol{\beta}_{n-3}\boldsymbol{\beta}_{n-2}^2\boldsymbol{\beta}_{n-1}$. It is natural to start with $\chi_n(\lambda)$, the characteristic polynomial of T, and examine if a sharp enough upper bound for $|\chi_n(\lambda)|$ can be constructed by demanding that the shift λ satisfy certain specific conditions.

From the three-term recurrence relation (2.8) we know

$$\chi_{n-2} = (\lambda - \alpha_{n-2})\chi_{n-3} - \beta_{n-3}^2\chi_{n-4} \tag{4.1}$$

and

$$\begin{aligned}\chi_{n-1} &= (\lambda - \alpha_{n-1})\chi_{n-2} - \beta_{n-2}^2\chi_{n-3} \\ &= (\lambda - \alpha_{n-1})[(\lambda - \alpha_{n-2})\chi_{n-3} - \beta_{n-3}^2\chi_{n-4}] - \beta_{n-2}^2\chi_{n-3} \\ &= [(\lambda - \alpha_{n-1})(\lambda - \alpha_{n-2}) - \beta_{n-2}^2]\chi_{n-3} - (\lambda - \alpha_{n-1})\beta_{n-3}^2\chi_{n-4}. \end{aligned} \tag{4.2}$$

Now using (4.1) and (4.2) to replace the factors χ_{n-2} and χ_{n-1} in the relation

$$\chi_n = (\lambda - \alpha_n)\chi_{n-1} - \beta_{n-1}^2\chi_{n-2} \tag{4.3}$$

and expressing χ_n in terms of χ_{n-3} and χ_{n-4} as was just done with χ_{n-1} in (4.2), we obtain, after collecting like terms and simplification,

$$\begin{aligned}\chi_n &= \{(\lambda - \alpha_n)[(\lambda - \alpha_{n-1})(\lambda - \alpha_{n-2}) - \beta_{n-2}^2] - (\lambda - \alpha_{n-2})\beta_{n-1}^2\}\chi_{n-3} \\ &\quad -[(\lambda - \alpha_n)(\lambda - \alpha_{n-1})\beta_{n-3}^2 - \beta_{n-1}^2\beta_{n-3}^2]\chi_{n-4} \\ &= -[(\lambda - \alpha_n)(\lambda - \alpha_{n-1}) - \beta_{n-1}^2]\beta_{n-3}^2\chi_{n-4}, \end{aligned} \tag{4.4}$$

where, for the last equality to hold, we choose λ to satisfy (3.1), the characteristic equation for $\widetilde{T}_3$, to make the term containing χ_{n-3} vanish. Since there are three (distinct) roots for the cubic equation, there is leeway to select the one that results in an easier-to-handle upper bound on $|\chi_n(\lambda)|$. From (4.4) we have

$$|\chi_n| = |(\lambda - \alpha_n)(\lambda - \alpha_{n-1}) - \beta_{n-1}^2|\beta_{n-3}^2|\chi_{n-4}|$$

which, according to (3.2), is equivalent to

$$|\chi_n| = \left|\frac{\lambda - \alpha_n}{\lambda - \alpha_{n-2}}\right|\beta_{n-2}^2\beta_{n-3}^2|\chi_{n-4}| \tag{4.5}$$

if $\lambda \neq \alpha_{n-2}$; and we obtain

$$|\chi_n| \leq \beta_{n-2}^2\beta_{n-3}^2|\chi_{n-4}| \tag{4.6}$$

if we choose λ to be the cubic root that further satisfies condition (3.6); if there is more than one root to reach (4.6), select the one which is closer to α_n (to make the factor $|\lambda - \alpha_n|/|\lambda - \alpha_{n-2}|$ in (4.5) smaller).

Now applying the relations (2.7), (2.3) to (4.6) we obtain, after eliminating the nonzero common factor $\rho_1\rho_2\cdots\rho_{n-2}$ on each side,

$$\rho_{n-1}\rho_n \leq |\gamma_{n-4}|\sigma_{n-3}^2\sigma_{n-2}^2\rho_{n-3}\rho_{n-2}. \tag{4.7}$$

Using the identities $\beta_j = \sigma_j\rho_j$, $\widehat{\beta}_j = \sigma_j\rho_{j+1}$ (see (2.3) and (2.4)), it is easy to verify that the following inequality

$$\widehat{\beta}_{n-3}\widehat{\beta}_{n-2}^2\widehat{\beta}_{n-1} \leq |\gamma_{n-4}|\sigma_{n-3}^2\sigma_{n-2}^2\beta_{n-3}\beta_{n-2}^2\beta_{n-1} \tag{4.8}$$

is equivalent to (4.7), which is further equivalent to (4.6), as we have just shown. Since the factors σ_j, γ_j (sines and cosines) in (4.8) are all bounded by 1, the monotonicity of $\beta_{n-3}\beta_{n-2}^2\beta_{n-1}$ through each QR step is proven. In a similar way, it can readily be checked that

$$\widehat{\beta}_{n-1}\beta_{n-1}^2 \le |\gamma_{n-4}|\sigma_{n-3}\sigma_{n-2}\sigma_{n-1}^2\beta_{n-3}\beta_{n-2}\beta_{n-1} \tag{4.9}$$

is also equivalent to (4.7).

4.2. Global convergence $\boldsymbol{\beta_{n-1}^{(k)} \to 0}$. From (4.8) we know that in the QR iteration, $\beta_{n-3}^{(k)}\beta_{n-2}^{(k)2}\beta_{n-1}^{(k)}$ form a bounded, monotonically decreasing sequence which has a limit, say β. We claim that $\beta = 0$. Suppose $\beta > 0$; then it would follow from (4.8) that

$$|\gamma_{n-4}^{(k)}|\sigma_{n-3}^{(k)2}\sigma_{n-2}^{(k)2} \to 1 \quad \text{as} \quad k \to \infty,$$

which, according to the identity $|\gamma_j|^2 + \sigma_j^2 = 1$, implies that

$$|\gamma_{n-4}^{(k)}| \to 1, \quad |\gamma_{n-3}^{(k)}| \to 0, \quad \text{and} \quad |\gamma_{n-2}^{(k)}| \to 0 \quad \text{as} \quad k \to \infty. \tag{4.10}$$

However, substituting the identity $\chi_j = \rho_1\rho_2\cdots\rho_j\gamma_j$ into the recurrence relation (4.1) and canceling the common factor $\rho_1\rho_2\cdots\rho_{n-4}$ on each side, we obtain

$$\rho_{n-3}\rho_{n-2}\gamma_{n-2} = (\lambda - \alpha_{n-2})\rho_{n-3}\gamma_{n-3} - \beta_{n-3}^2\gamma_{n-4}.$$

If the asymptotic condition (4.10) were true, then from the above relation it would follow that

$$\beta_{n-3}^{(k)} \to 0 \quad \text{as} \quad k \to \infty.$$

But this contradicts the initial assumption that $\beta_{n-3}^{(k)}\beta_{n-2}^{(k)2}\beta_{n-1}^{(k)} \searrow \beta > 0$, as all elements involved in the iteration are bounded. Therefore, we infer that

$$\beta_{n-3}^{(k)}\beta_{n-2}^{(k)2}\beta_{n-1}^{(k)} \searrow 0,$$

which further implies, through (4.9), that

$$\beta_{n-1}^{(k+1)}\beta_{n-1}^{(k)} \to 0,$$

again because all these elements are bounded in the process. At this stage, there remains the possibility that a subsequence of $\{\beta_{n-1}^{(k)}\}$ could be bounded away from 0, and we show next that this is not possible. Suppose there is a number $\delta > 0$ such that

$$\beta_{n-1}^{(k_j)} \to 0, \tag{4.11}$$

but

$$\beta_{n-1}^{(k_j+1)} \ge \delta \quad \text{as } j \to \infty, \tag{4.12}$$

where $\{k_j\}$ represents a subsequence of $\{k\}$. Then from (4.12) and $\beta_{n-1}^{(k+1)} = \sigma_{n-1}^{(k)}\rho_n^{(k)}$ we would have

$$\rho_n^{(k_j)} \ge \sigma_{n-1}^{(k_j)}\rho_n^{(k_j)} \ge \delta, \tag{4.13}$$

and from (4.11) and $\beta_{n-1}^{(k)} = \sigma_{n-1}^{(k)}\rho_{n-1}^{(k)}$ we would infer that

$$\rho_{n-1}^{(k_j)} \to 0 \tag{4.14}$$

because if (4.13) were true, $\sigma_{n-1}^{(k_j)}$ would also be bounded away from 0 as $j \to \infty$. However, condition (4.14) further implies that

$$|\chi_n(\lambda^{(k_j)})| = \rho_1^{(k_j)}\rho_2^{(k_j)}\cdots\rho_{n-1}^{(k_j)}\rho_n^{(k_j)} \to 0,$$

which, by (2.9), is equivalent to $\rho_n^{(k_j)} \to 0$, a contradiction to (4.13). This completes the proof of $\beta_{n-1}^{(k)} \to 0$.

4.3. The rate of convergence. With the cubic shift, an asymptotic rate of $\beta_{n-1}^{(k)} \to 0$ better than *cubic* is guaranteed under the additional assumption that

$$\beta_{n-2}^{(k)} \to 0 \text{ and } \beta_{n-3}^{(k)} \to 0, \tag{4.15}$$

which in practice seems always to take place though at much slower rates. In such circumstances, each of $\alpha_n^{(k)}$, $\alpha_{n-1}^{(k)}$, and $\alpha_{n-2}^{(k)}$ approaches a distinct eigenvalue of T with

$$|\lambda^{(k)} - \alpha_n^{(k)}| \to 0, \quad |\lambda^{(k)} - \alpha_{n-1}^{(k)}| \geq \delta_1, \quad \text{and} \quad |\lambda^{(k)} - \alpha_{n-2}^{(k)}| \geq \delta_2 \tag{4.16}$$

as $k \to \infty$ for some positive numbers δ_1, δ_2. Note that another modular form of the characteristic equation (3.1) can be put as

$$\left|\frac{\lambda - \alpha_n}{\lambda - \alpha_{n-2}}\right| = \frac{\beta_{n-1}^2}{|(\lambda - \alpha_{n-1})(\lambda - \alpha_{n-2}) - \beta_{n-2}^2|} \tag{4.17}$$

if $\lambda \neq \alpha_{n-2}$. Replacing the factor $|\lambda - \alpha_n|/|\lambda - \alpha_{n-2}|$ in the expression (4.5) of $|\chi_n|$ by (4.17) we obtain

$$|\chi_n| = \frac{\beta_{n-1}^2\beta_{n-2}^2\beta_{n-3}^2|\chi_{n-4}|}{|(\lambda - \alpha_{n-1})(\lambda - \alpha_{n-2}) - \beta_{n-2}^2|}, \tag{4.18}$$

from which we know

$$|\chi_n(\lambda^{(k)})| = O(\beta_{n-1}^{(k)2}\beta_{n-2}^{(k)2}\beta_{n-3}^{(k)2}) \text{ as } k \to \infty, \tag{4.19}$$

because, under condition (4.15) and hence (4.16), the denominator on the right side of (4.18) is bounded away from zero in the iteration. Finally, imbedding this asymptotic property (4.19) of $|\chi_n|$ into the relation (2.10) between $\widehat{\beta}_{n-1}$ and β_{n-1} leads to the conclusion that

$$\beta_{n-1}^{(k+1)} = O(\beta_{n-1}^{(k)3}\beta_{n-2}^{(k)2}\beta_{n-3}^{(k)2}) \text{ as } k \to \infty,$$

because all elements involved in the iteration are bounded and in particular, the term $|\chi_{n-1}|^2$ in the denominator in (2.10) is bounded below from zero; to see this, note that as $\beta_{n-1}^{(k)} \to 0$, we have from (4.3)

$$|\chi_n(\lambda^{(k)}) - (\lambda^{(k)} - \alpha_n^{(k)})\chi_{n-1}^{(k)}(\lambda^{(k)})| \to 0,$$

in which both $\chi_n(\lambda^{(k)}) \to 0$ and $|\lambda^{(k)} - \alpha_n^{(k)}| \to 0$, yet we know that $\chi_n(\lambda) = 0$ has only simple roots.

5. Numerical testing. We test the effectiveness of this cubic shift by incorporating the scheme into a Pal–Walker–Kahn version [7] of the tridiagonal QR algorithm, and comparing the numerical results with those from employing the Wilkinson shift, as well as some other shift strategies considered in the literature. Computation was done in double-precision Fortran on an IBM compatible PC with unit roundoff $\varepsilon \approx 10^{-19}$, and the testing was focused on determining the numbers of iterations required for $\beta_j^{(k)}$, $j = n-1, n-2, \cdots, 1$, to become negligible under the traditional criterion $\beta_j^{(k)} \le \varepsilon(|\alpha_j^{(k)}| + |\alpha_{j+1}^{(k)}|)$.

The following contractions are used to describe the various shift schemes incorporated in the QR iteration:

R	the Rayleigh-quotient shift [11, 7];
W	the Wilkinson shift [11, 7];
RW	a mixed shift strategy devised by Jiang and Zhang [6];
C	the cubic shift analyzed in this paper.

For a tridiagonal matrix T of size n, let **itmax** denote the *maximum* number of QR iterations required to get an approximate eigenvalue of T. We measure and list in the following table the numerical averages of **itmax** over 10,000 tridiagonal matrices with entries $\{\alpha_i\}_{i=1}^{n}$ and $\{\beta_i\}_{i=1}^{n-1}$ produced by a random-number generator with a uniform distribution on the intervals $(-1, 1)$ and $(0, 1)$, respectively.

itmax	$n = 10$	$n = 20$	$n = 30$	$n = 40$
R	5.70	6.19	6.50	6.73
W	4.27	4.48	4.59	4.65
RW	4.48	4.76	4.86	4.94
C	3.82	4.04	4.14	4.19

These preliminary data indicate that numerical convergence with the cubic shift is about 10% faster than that with the Wilkinson shift for matrices of order ≤ 40.

6. Concluding remarks. It seems reasonable to expect that, in constructing the shift, the more information we take from the lower right corner of the matrix, the less the average number of iterations is needed to deflate the matrix. Employing a technique different from that of Wilkinson [11], we demonstrate in this paper *how* to choose a higher order shift so that *global* convergence with a *faster* asymptotic rate can be achieved.

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