Sandia technical report 96-0913J: How the QR algorithm fails to converge and how to fix it *

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Abstract

In certain cases the shifted QR algorithm for real matrices converges slowly, if at all, when implemented in finite precision arithmetic. These obstacles are traced to a family of orthgonal similarity classes for which certain QR algorithms fail to converge on an open subset of a given orthogonal similarity class. A modification to the QR algorithm is recommended with which the resulting algorithm has only strongly repelling fixed points over $R^{4\times 4}$ in the family of orthogonal similarity classes considered in this work. It is also shown that the multi-shift QR algorithm fails.

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Contents

1 Introduction And Summary

QR iteration is the method of choice for computing the eigenvalues of Hessenberg (i.e. $H = (h_{i,j})$ such that $h_{i,j} = 0$ for $i > j+1$) matrices [9, 13, 7, 2]. There is no convergence proof. Until recently examples of failure were known in exact arithmetic only [3]. These results only apply to certain shift strategy (to be discussed). Our results are first to show that QR iteration with any previously published shift strategy may converge unacceptably slowly, if at all, when implemented in finite precision arithmetic, and second to propose a new shift strategy for which convergence is rapid in all cases known to the author.

Finite precision computation in this work refers to double precision arithmetic with machine epsilon $\epsilon \approx 2.2\mathrm{e}-16$.

The EISPACK subroutine HQR (see [13]) is an implementation of the algorithm described in [9], though an improved Exceptional shift is employed. The current implementations of HQR limit the number of iterations for an n−by−n without a decoupling to $30n$. In double precision arithmetic these versions of HQR fail for

$$H(\eta) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & \eta & 0 \\ 0 & -\eta & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{1}$$

such that $10^{-6} \geq \eta \geq 2 \times 10^{-14}$. This was observed by J. Demmel, and is the first example of failure of HQR in finite precision arithmetic known to us. If no restriction is placed on the number of iterations, then in finite precision arithmetic HQR is slowly (i.e. in 10^4 iterations) convergent for all $H(\eta)$. In this case the accuracy of the computed eigenvalues is unacceptably poor. In this article we assume that there is no restriction on the number of iterations.

For HQR with the EISPACK exceptional shift strategy a matrix is given for which HQR still has not converged after 10^8 iterations.

For HQR with the original shift strategy, the exceptional shifts suffice to map the iterates out of the basin of non-convergence, but for η sufficiently small, the convergence is slow (i.e. over 10^5 iterations for $\eta = 10^{-7}$). In such cases the accuracy of any computed eigenvalues is unacceptably poor.

In §3 a family of orthogonal similarity classes is identified on which certain QR algorithms fail to converge on an open subset of a given orthogonal similarity class.

In §5 a modification is recommended with which the maximum number of QR iterations to decouple any matrix known to us is 36. This algorithm has only strongly repelling fixed points over $R^{4\times 4}$ in the family of orthogonal similarity classes considered in this work.

In §6 a family of matrices related to $H(\eta)$ (see equation (1)) but of arbitrary order n for which multi-shift QR does not converge in $30n$ steps for $n = 70$, 80, and 90 in finite precision arithmetic.

2 QR Iterations

QR iteration determines a sequence $\{H^{(i)}\}_{i\geq 0}$ of orthogonally similar Hessenberg matrices which hopefully converge to a block upper triangular matrix. A general QR iteration passes from $H^{(i)}$ to $H^{(i+1)}$ by

$$\begin{cases} p(H^{(i)}) = Q_i R_i \\ H^{(i+1)} = Q_i^T H^{(i)} Q_i \end{cases} \tag{2}$$

$Q_i R_i$ is a factorization of $p(H^{(i)})$ as orthogonal times upper triangular. If $H^{(i)}$ is Hessenberg then $H^{(i+1)}$ is Hessenberg [7]. Algorithms differ only in the definition of the monic polynomial $p(.)$, called the *shift polynomial*. The term shift applies because a first degree monic polynomial is a translation or shift.

HQR is the composite algorithm

$$\begin{cases} QRF & \text{Iteration} \notin \{11, 21\} \\ EX & \text{Iteration} \in \{11, 21\} \end{cases} \tag{3}$$

QRF selects the characteristic polynomial of the 2−by−2 South East (SE) submatrix of H as the shift polynomial at each step.

QRF is not globally convergent [11, 9]. This is relieved in HQR by adding the *Exceptional shift* [9], denoted EX above.

Throughout this paper we shall use the notational conventions of [7].

2.1 Properties Of QR Algorithms

In this section we summarize the properties of Hessenberg QR algorithms used in later sections.

H is *unreduced* if no $(k+1, k)$ entry vanishes. If H is reduced, the eigenvalue problem decouples. The QR iteration, (2), is applied to unreduced submatrices of H. The purpose of a shift strategy is to compute iterates that deflate in as few iterations as possible.

Certain properties of unreduced Hessenberg matrices are listed below.

1. If $p(H^{(i)})$ is singular then $H^{(i)}$ is reduced [7].
2. Diagonal entries of R are uniquely determined only up their sign [7].
3. $H^{(i)}$ is determined to within a diagonal similarity by a real diagonal matrix D with ± 1's along the diagonal [7].
4. $H^{(i+1)} = DH^{(i)}D^{-1}$ for a D as above iff $p(H^{(i)}) = \text{scalar} \times \text{orthogonal}$ [11].
5. A sequence of QR steps with shift polynomials $(p_k(.))$ is equivalent to a single iteration with polynomial

$$\prod_k p_k(.).$$

Property (1) shows that an ideal shift is a polynomial that annihilates an eigenvalue of H. Towards this end, $p(.)$ is usually the characteristic polynomial of a South East (SE) submatrix of H at each step. This is called a generalized Rayleigh quotient shift [1]. The Rayleigh quotient shift, translation by the SE element of H, is never a complex number and thus a poor shift for nonsymmetric matrices. QRF (see equation 3) uses the next most simple shift, the generalized Rayleigh quotient shift for the 2−by−2 SE submatrix.

The exceptional shift polynomial was originally defined to be $p(\zeta) = \zeta^2 - \frac{3}{2}\beta\zeta + \beta^2$ where $\beta = |h_{n,n-1}| + |h_{n-1,n-2}|$ in [9]. Here $H = (h_{i,j})$. The EISPACK implementation of HQR uses an improved exceptional shift polynomial $p(\zeta - h_{n,n})$ [13]. The results of this paper hold for either $p(\zeta)$ or $p(\zeta - h_{n,n})$ [13].

Property (2) is given to motivate the 3rd property, and the 3rd is given to explain the presence of D in the 4th. Property 4 describes the most simple failure mode for QR. The known examples of the failure of QRF involve H and $p(.)$ such that $p(H)/||p(H)||$ is orthogonal [11, 9, 3].

Practical implementations of QR are efficient because $p(H)$ and R are not computed, but this makes orthogonal $p(H)/||p(H)||$ undetectable.

By property (5) if several consecutive QR iterations do not decouple the QR iterates, a shift polynomial of large degree is implicitly employed. *As the degree of the shift polynomial increases* it may become possible for $p(H)/||p(H)||$ to be orthogonal. For example a cycle of period 2 in QRF indicates that $p_i(H^{(i)})p_{i+1}(H^{(i)})$ is a multiple of an orthogonal matrix.

2.2 Representation Of Hessenberg Matrices

Any real n−by−n matrix H has a Schur decomposition $H = Q^T SQ$ such that $Q^T Q = I$. The real Schur form S is real block upper triangular with 1−by−1 diagonal blocks for real eigenvalues, and 2−by−2 diagonal blocks for complex conjugate pairs of eigenvalues. Given a unit n-vector q, we can form the matrix whose columns are the orbit of q under S and compute its QR decomposition,

$$[q, Sq, \cdots, S^{n-1}q] = QR, \tag{4}$$

and form the Hessenberg matrix $H = Q^T SQ$. This construction defines a map

$$(S, q) \longrightarrow H$$

from the set of unit vectors to the set of Hessenberg matrices orthogonally similar to S [7]. This result is known as the Implicit Q theorem. $(S, q) \longrightarrow H$ is onto, but not one to one. The inconvenient lack of injectivity is surmounted by working with the equivalence class, $\{q\}$, of all unit n−vectors q that correspond to the same Hessenberg matrix, H.

A QR iteration is equivalent to the power method in the sense that the following diagram commutes:

$$\begin{array}{ccc} H & \xrightarrow{\text{QR}} & \hat{H} \\ \downarrow & & \uparrow \\ \{q\} & \xrightarrow{p(S)q} & \{\hat{q}\} \end{array}$$

See [12, 3]. Here $p(.)$ is the shift polynomial that corresponds to H under an arbitrary shift strategy, and

$$\hat{q} = \frac{p(S)q}{||p(S)q||}.$$

3 Francis' QR Iteration

In this section we explain why Francis' QR iteration fails. Our technique is to apply the equivalence of QRF to the power method (see §2.1). In §3.1 we determine the orthogonal similarity class to analyze. The shift polynomial, $p(.)$, is determined as a function of the power method starting vector, q, in §3.2. In §3.2 we give a simple geometric characterization of the set of Hessenberg matrices in a certain family of orthogonal similarity classes that are invariant under the QRF. In §3.3 it is shown that along a portion of the invariant set, the fixed points are attracting within the orthogonal similar class. This implies that QRF fails on an open set within the orthogonal similarity class. In §3.4 we show that certain fixed points are not strongly repelling in $R^{4\times 4}$; this implies that at best QRF converges extremely slowly on an open set in $R^{4\times 4}$.

Notation: $A \oplus B =$

$$\begin{bmatrix} A & 0 \\ 0 & B \end{bmatrix}.$$

Let $Q = [q_1, q_2, \ldots]$ denote the columns of the matrix Q.

3.1 A Schur-Hamiltonian Orthogonal Similarity Class

Property (4) of §2 applied to the matrix $H(\eta)$ defined in equation (1) states that $H(\eta)$ is a fixed point for QR if and only if

$$p(H(\eta))/\|p(H(\eta))\|$$

is orthogonal. We shall now see that $H(\eta)$ is not a fixed point. For θ such that $\eta = 2\sin(\theta)$, $H(\eta)$ has a real Schur form

$$\tilde{S}(\theta) = \begin{bmatrix} R(\theta) & X(\theta)\Delta \\ 0 & -R^T(\theta) \end{bmatrix}$$

for

$$R(\theta) = \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix}, \qquad \Delta = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Since $H(\eta)$ and $\tilde{S}(\theta)$ are orthogonally similar, the matrix $p(H(\eta))/\|p(H(\eta))\|$ is orthogonal iff $p(\tilde{S}(\theta))/\|p(\tilde{S}(\theta))\|$ is orthogonal, which is the case iff $R(\theta)$ commutes with $X(\theta)$. This is not so, but $X(\theta)$ is *near* the commutator of $R(\theta)$, namely the set of matrices of the form $\kappa R(\omega)$. That is, the right family of orthogonal similarity classes to analyze is

$$S(\theta, \omega, \kappa) = \begin{bmatrix} R(\theta) & \kappa R(\omega)\Delta \\ 0 & -R^T(\theta) \end{bmatrix}. \tag{5}$$

This work concerns shift strategies for QR iteration in the family of orthogonal similarity classes $S(\theta, \omega, \kappa)$. The squared matrix,

$$S^2(\theta, \omega, \kappa) = I\cos(2\theta) + (R(\frac{\pi}{2}) \oplus R(-\frac{\pi}{2}))\sin(2\theta), \tag{6}$$

has a single complex conjugate pair of eigenvalues and is orthogonal. This implies that $S^2(\theta, \omega, \kappa) + \delta I$ is a scalar multiple of an orthogonal matrix for each δ. If H is orthogonally similar to $S(\theta, \omega, \kappa)$ and $p(\zeta) = \zeta^2 - \tau\zeta + \delta$ is the shift polynomial, then H is invariant under QR if and only if $\tau = 0$ since $p(S(\theta, \omega, \kappa))$ must be block diagonal. The locus of $\tau = 0$ will determined using the Theorem below in §3.2.

The following notation will be used though out this work. Define $-\pi \le \alpha, \beta < \pi$ and $0 \le \gamma \le \pi/2$ by

$$q = \begin{bmatrix} R(-\alpha)e_1\cos(\gamma) \\ R(-\beta)e_1\sin(\gamma) \end{bmatrix} = \begin{bmatrix} \cos(\gamma)\cos(\alpha) \\ \cos(\gamma)\sin(\alpha) \\ \sin(\gamma)\cos(\beta) \\ \sin(\gamma)\sin(\beta) \end{bmatrix}. \tag{7}$$

As we shall now see, without loss of generality one may select a representative q from the equivalence class $\{q\}$ for which $\beta = 0$. Because $S(\theta, \omega, \kappa)$ commutes with

$$\Sigma_\eta \stackrel{\text{def}}{=} R(\eta) \oplus R(-\eta)$$

for each η, the equivalence class of all unit vectors that q correspond to a given Hessenberg H (see §2.1) is the set such that γ and $\alpha + \beta$ are constant.

Theorem. Unreduced Hessenberg matrices orthogonally similar to $S(\theta, \omega, \kappa)$ defined in equation (5) are J-symmetric for

$$J = \begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}.$$

Remark. In [10] the term "Schur-Hamiltonian" form is proposed for Schur forms such as $S(\theta, \omega, \kappa)$.

Proof. In the following θ, ω and κ are constant and we simply write S for $S(\theta, \omega, \kappa)$. S is J-symmetric, that is

$$JS = \begin{bmatrix} 0 & R(\frac{\pi}{2} - \theta) \\ R^T(\frac{\pi}{2} - \theta) & -\kappa R(\frac{\pi}{2} + \omega)\Delta \end{bmatrix}$$

is symmetric.

An unreduced Hessenberg matrix orthogonally similar to S is of the form $H = Q^T S Q$ for an orthogonal matrix Q defined by

$$[q, Sq, S^2q, S^3q] = QR.$$

Here q is a unit vector and R is upper triangular. For any Hessenberg H with Schur form S there is at least one q such that $H = Q^T S Q$ (see §2.1).

We will show how to select a representative q corresponding to a given H such that Q is J-orthogonal (i.e. $Q^T J Q = J$).

Σ_η has two more relevant properties, namely

$$J\Sigma_\eta = \Sigma_{-\eta} J$$

and, like J, $J\Sigma_\eta$ is skew-symmetric,

$$\begin{aligned} (J\Sigma_\eta)^T &= \Sigma_\eta^T J^T \\ &= -\Sigma_{-\eta} J \\ &= -J\Sigma_\eta. \end{aligned}$$

Thus, for each q and η, $q^T J \Sigma_{2\eta} q = 0$ and

$$\begin{aligned} (\Sigma_{\frac{\pi}{2}} q)^T \ J\Sigma_{2\eta} q &= q^T \Sigma_{-\frac{\pi}{2}} J \Sigma_{2\eta} q \\ &= q^T J \Sigma_{\frac{\pi}{2}+2\eta} q = 0. \end{aligned}$$

To appreciate the significance of all this, bear in mind that equation (6) implies that $S^2 q$ may be replaced by $\Sigma_{\frac{\pi}{2}} q$ in the definition of Q. Thus $J\Sigma_{2\eta} q = \pm q_4$ for η such that $(Sq)^T \ J\Sigma_{2\eta} q = 0$.

We now show that such an η does exist. The identity $\Delta R(-\beta) = R(\beta)\Delta$ is helpful in the algebraic manipulations required to derive that for each η,

$$(Sq)^T \ J\Sigma_{2\eta} q = -\sin(\gamma)(2\cos(\gamma)\sin(\theta + \beta - \alpha + 2\eta) + \kappa \sin(\gamma)\sin(2\beta + \omega + 2\eta)).$$

If $\theta + \beta - \alpha \equiv 2\beta + \omega \mod \pi$, then choose η such that $\sin(2\beta + \omega + 2\eta) = 0$. Otherwise choose η such that

$$\frac{\sin(\theta + \beta - \alpha + 2\eta)}{\sin(2\beta + \omega + 2\eta)} = \frac{\kappa}{2}\tan(\gamma). \tag{8}$$

By a similar argument one can show that $J\Sigma_{2\eta}q_2 = \pm q_3$. Of course we are free to scale q_3 and q_4 by -1 to obtain the desired sign. Given q determine η so that equation (8) holds. The the initial vector $\Sigma_\eta q$ corresponds to the orthogonal and J-orthogonal matrix $\Sigma_\eta Q$. Therefore

$$HJ = (\Sigma_\eta Q)^T S(\Sigma_\eta Q)J = (\Sigma_\eta Q)^T SJ(\Sigma_\eta Q)$$

is symmetric $\Box$
Corollary Unreduced Hessenberg matrices, H, orthogonally similar to $S(\theta)$ are of the form

$$H = \begin{bmatrix} h_{1,1} & h_{1,2} & h_{1,3} & h_{1,4} \\ h_{2,1} & h_{2,2} & h_{2,3} & -h_{1,3} \\ 0 & h_{3,2} & -h_{2,2} & h_{1,2} \\ 0 & 0 & h_{2,1} & -h_{1,1} \end{bmatrix}. \tag{9}$$

3.2 QRF Invariant Matrices

In this section we determine a closed form expression for the QRF shift polynomial, $p(\zeta)$, as a function of $S(\theta,\omega,\kappa)$ and q. Using the Corollary $p(\zeta)$ may be determined from $H(1:2,1:2)$. The QRF-invariant set is then determined in terms of either q or H.

For clarity we introduce intermediate quantities ν, σ, ρ, and μ defined in the table below.

Item	Description
ν	$\nu = q^T S(\theta,\omega,\kappa)q = h_{1,1}$
ρ	$\rho \geq 0, \quad \rho^2 = \|\|S(\theta,\omega,\kappa)q\|\|^2 - \nu^2$
σ	$\sigma = \|\|S(\theta,\omega,\kappa)q\|\|^2 = \rho^2 + \nu^2$
μ	$\mu = q^T \Sigma_{\frac{\pi}{2}} S(\theta,\omega,\kappa)q$

The quantities ρ and ν relate q_2 and q by

$$q_2\rho = S(\theta,\omega,\kappa)q - q\nu. \tag{10}$$

$S(\theta,\omega,\kappa)$ has multiple eigenvalues if and only if θ is an integer multiple of $\pi/2$, and in this case any Hessenberg matrix orthogonally similar to $S(\theta,\omega,\kappa)$ is reduced. We will not discuss this case further. In the remainder of this work we assume that θ is not an integer multiple of $\pi/2$. The fact that $S(\theta,\omega,\kappa)$ has no real eigenvalues (since $\sin(\theta) \neq 0$) implies that $\rho > 0$.

Equation (10) expressed in matrix form is $[q, S(\theta,\omega,\kappa)q] = [q_1, q_2]R_2$ for R_2 defined by

$$R_2 = \begin{bmatrix} 1 & \nu \\ 0 & \rho \end{bmatrix}.$$

The submatrix $H(1:2,1:2)$ is determined from

$$\begin{aligned} H(1:2,1:2) &= [q_1,q_2]^T S(\theta,\omega,\kappa)[q_1,q_2] \\ &= R_2^{-T}[q, S(\theta,\omega,\kappa)q]^T S(\theta,\omega,\kappa)[q, S(\theta,\omega,\kappa)q]R_2^{-1}. \end{aligned}$$

For clarity we write S for $S(\theta,\omega,\kappa)$. Substitute equation (6) and then equation (10) to obtain

$$\begin{aligned} q^T S^T S^2 q &= q^T S^T (I\cos(2\theta) + \Sigma_{\frac{\pi}{2}}\sin(2\theta))q \\ &= \nu\cos(2\theta) - \mu\sin(2\theta), \end{aligned}$$

and

$$\begin{bmatrix} q^T S q & q^T S^2 q \\ q^T S^T S q & q^T S^T S^2 q \end{bmatrix} = \begin{bmatrix} \nu & \cos(2\theta) \\ \sigma & \nu\cos(2\theta) - \mu\sin(2\theta) \end{bmatrix}.$$

Thus

$$H(1:2,1:2) = \begin{bmatrix} 1 & 0 \\ -\nu/\rho & 1/\rho \end{bmatrix} \begin{bmatrix} \nu & \cos(2\theta) \\ \sigma & \nu\cos(2\theta)-\mu\sin(2\theta) \end{bmatrix} \begin{bmatrix} 1 & -\nu/\rho \\ 0 & 1/\rho \end{bmatrix}$$

$$= \begin{bmatrix} \nu & \cos(2\theta) \\ \rho & -\frac{\nu}{\rho}\sin(2\theta) \end{bmatrix} \begin{bmatrix} 1 & -\nu/\rho \\ 0 & 1/\rho \end{bmatrix}$$

$$= \begin{bmatrix} \nu & \frac{\cos(2\theta)-\nu^2}{\rho} \\ \rho & -\nu-\sin(2\theta)\frac{\mu}{\rho^2} \end{bmatrix}. \tag{11}$$

Now apply the Corollary to find that $p(\zeta) = \zeta^2 - \tau\zeta + \delta$ for

$$\tau = \sin(2\theta)\frac{\mu}{\rho^2}, \qquad \delta = -\cos(2\theta) - \nu\tau. \tag{12}$$

The following identities can be verified by direct calculation.

$$\nu = \cos(\theta)\cos(2\gamma) + \cos(\alpha+\beta+\omega)\sin(2\gamma)\kappa/2 \tag{13}$$

$$\sigma = 1 + \kappa\sin(2\gamma)\cos(\alpha+\beta+\omega-\theta) + \kappa^2\sin^2(\gamma)$$

$$\mu = -\sin(\theta)\cos(2\gamma) - \sin(\alpha+\beta+\omega)\sin(2\gamma)\kappa/2 \tag{14}$$

Note that α, β, ω such that $\alpha+\beta+\omega$ is constant; we are free to assume $\beta = \omega = 0$. The QRF-invariant set is the locus of $\mu = 0$ and $\sin(\theta) \neq 0$. For each $\alpha, \beta, \theta, \omega, \kappa$ there exists γ such that $\mu = 0$. For example if $\kappa = -2\sin(\theta)$, then the QRF invariant set is the locus of $\cot(2\gamma) = \sin(\alpha+\omega)$.

We select the representative q from the equivalence class, $\alpha+\beta$ constant, for which $\beta = 0$. That is,

$$q = \begin{bmatrix} \cos(\alpha)\cos(\gamma) \\ \sin(\alpha)\cos(\gamma) \\ \sin(\gamma) \\ 0 \end{bmatrix}.$$

The class of Hessenberg matrices orthogonally similar to $S(\theta,\omega,\kappa)$ is 2-dimensional and may be parameterized by the angles (α,γ).

A closed form expression for the QRF invariant matrices in the orthogonal similarity class of S will be required in §3.4. We derive this expression here. Because the orbit matrix may be expressed

$$[q, Sq, S^2q, S^3q] = [\ \ [q, Sq], \quad S^2[q, Sq]\ \ ],$$

$H = Q^TSQ$ for $Q_2 = [q_1, q_2]$ and Q defined in the QR decomposition $[Q_2, S^2Q_2] = QR$. Equation (6) and the hypothesis $\mu = 0$ imply

$$Q_2^TS^2Q_2 = I\cos(2\theta) + Q_2^T\Sigma_{\frac{\pi}{2}}Q_2 = I\cos(2\theta).$$

Using equation (6) again we have

$$[q_3, q_4] = (S^2Q_2 - Q_2\cos(2\theta)) \times \text{scalar} = \Sigma_{\frac{\pi}{2}}Q_2.$$

Since S and the skew matrix $\Sigma_{\frac{\pi}{2}}$ commute

$$H = \begin{bmatrix} Q_2^TSQ_2 & Q_2^TS\Sigma_{\frac{\pi}{2}}Q_2 \\ Q_2^T\Sigma_{\frac{\pi}{2}}^TSQ_2 & Q_2^T\Sigma_{\frac{\pi}{2}}^TS\Sigma_{\frac{\pi}{2}}Q_2 \end{bmatrix} = \begin{bmatrix} Q_2^TSQ_2 & -Q_2^T\Sigma_{\frac{\pi}{2}}^TSQ_2 \\ Q_2^T\Sigma_{\frac{\pi}{2}}^TSQ_2 & Q_2^TSQ_2 \end{bmatrix}. \tag{15}$$

Substitute equation (10), the hypothesis $\mu = 0$ and equation (6) to find

$$\begin{aligned} q^T \Sigma_{\frac{\pi}{2}}^T S q_2 &= \frac{1}{\rho} q^T \Sigma_{\frac{\pi}{2}}^T S(Sq - q\nu) \\ &= \frac{1}{\rho} q^T \Sigma_{\frac{\pi}{2}}^T S^2 q \\ &= \frac{\sin(2\theta)}{\rho} q^T \Sigma_{\frac{\pi}{2}}^T \Sigma_{\frac{\pi}{2}} q = \frac{\sin(2\theta)}{\rho}. \end{aligned}$$

Substitute this equation and equation (11) into equation (15) to obtain

$$H = \left[\begin{array}{cccc} \nu & \frac{\cos(2\theta)-\nu^2}{\rho} & 0 & -\frac{\sin(2\theta)}{\rho} \\ \rho & -\nu & 0 & 0 \\ 0 & \frac{\sin(2\theta)}{\rho} & \nu & \frac{\cos(2\theta)-\nu^2}{\rho} \\ 0 & 0 & \rho & -\nu \end{array} \right]. \tag{16}$$

Popular implementations of HQR fail or converge extremely slowly for certain matrices of this type discussed in §4.

3.3 QRF Dynamics

In this section we show that QRF fails to converge on an open set within certain orthogonal similarity classes $S = S(\theta, \omega, \kappa)$. QRF iteration in an orthogonal similarity class of $S = S(\theta, \omega, \kappa)$ is shown to be equivalent to a 2D vector field.

The following comments imply that a sufficient condition for an invariant curve within a smooth vector field to be attracting is that the Jacobian have spectrum $\{1, \lambda\}$ for $|\lambda| < 1$.

In the following we change from numerical linear algebra notation to mathematical analysis notation. Our hypotheses are that $F : \mathcal{D} \subset R^2 \to R^2$ is a smooth vector field with unique smooth invariant curve $g : \mathcal{D} \subset R \to R$; for each $x \in I$, $F(x, g(x)) = (x, g(x))$. Moreover $DF(x, g(x))$ has eigenvalues 1 and $\lambda(x)$ and there exists $x_0 \in I$ such that $|\lambda(x_0)| < 1$. We claim that for (x, y) sufficiently near to $(x_0, g(x_0))$, the iterates $F^{(k)}(x, y) \stackrel{k\to\infty}{\longrightarrow} (\hat{x}, g(\hat{x}))$ for some $\hat{x} \in I$.

The sketch of the proof follows. Without loss of generality $x_0 = 0$ and for each $x \in I$, $g(x) = 0$. The smoothness of $F = (f_1, f_2)$ implies that

$$\delta(x, y) = \begin{cases} f_2(x, y)/y & \text{if } y \neq 0 \\ \lambda(x) & \text{if } y = 0 \end{cases}$$

is also smooth, but we only use the fact that $\delta(x, y) = \lambda(x) + O(|x| + |y|)$. For this implies the existence of $c < 1$ such that for $|x| + |y|$ sufficiently small,

$$|f_2(x, y)| \quad \leq \quad c \quad |y|.$$

From this we see that $\{e_2^T F^k(x, y)\}_{k \geq 1}$ converges to zero geometricly while $\{e_1^T F^k(x, y)\}_{k \geq 1}$ remains bounded. The desired stability result now follows from the bound

$$||(x, y) - F(x, y)|| \quad = \quad ||(x, y) - (x, 0) + F(x, 0) - F(x, y)|| \quad \leq \quad |y| \quad \left(1 + ||\frac{\partial F}{\partial y}||\right).$$

In the remainder of this section we show determined the eigenvalues of the QRF Jacobian at a fixed point. An example of parameter values for which $0 < \lambda < 1$ is given in § 4.2.

Each point in the domain $\mathcal{D} = \{(\alpha, \gamma) : -\pi \le \alpha < \pi, 0 \le \gamma < \pi/2\}$ corresponds to a distinguished representative of an equivalence class of initial vectors

$$q = \begin{bmatrix} \cos(\alpha)\cos(\gamma) \\ \sin(\alpha)\cos(\gamma) \\ \sin(\gamma) \\ 0 \end{bmatrix}.$$

To each 4-vector $\mathbf{v} = (w, x, y, z)^T$ there corresponds a

$$g(\mathbf{v}) = (\tan^{-1}(x/w) + \tan^{-1}(z/y), \tan^{-1}\sqrt{(w^2+x^2)/(y^2+z^2)}\ ) \in \mathcal{D}.$$

The QRF vector iteration $q \mapsto p(S)q/||p(S)q||$ induces a vector field f on $\mathcal{D}$ which could be defined as $f(\alpha, \gamma) = g(p(S)q)$, but we derive a simpler characterization below. At a fixed point, $\mu = 0$, 1 is an eigenvalue of Df and we seek the other eigenvalue, λ, which reveals the dynamics of QRF near the invariant manifold.

Before taking any derivatives though we simplify $p(S)q$. The QRF shift polynomial is $p(\zeta) = \zeta^2 - \tau\zeta + \delta$ for τ and δ determined in equation (12). Substitute equation (6) below to find

$$\begin{aligned} p(S) &= S^2 - S\tau + I\delta \\ &= -S\tau + \Sigma_{\frac{\pi}{2}} \sin(2\theta) + I(\delta + \cos(2\theta)) \\ &= \Sigma_{\frac{\pi}{2}} \sin(2\theta) - (S + \nu I)\tau \\ &= \Sigma_{\frac{\pi}{2}}^T (I + \Sigma_{\frac{\pi}{2}}(S + \nu I)\frac{\mu}{\rho^2}) \sin(2\theta). \end{aligned}$$

We define $f(\alpha, \gamma) = g(\mathbf{v})$ for

$$\mathbf{v} = q + \Sigma_{\frac{\pi}{2}}(S + \nu I)q\frac{\mu}{\rho^2}. \tag{17}$$

Now for the derivative $D_a f = D_{\mathbf{v}} g\ D_a \mathbf{v}$ for $D_a = [D_\alpha, D_\gamma]$. In general,

$$D_v g = \begin{bmatrix} \frac{-x}{w^2+x^2} & \frac{w}{w^2+x^2} & \frac{-z}{y^2+z^2} & \frac{y}{y^2+z^2} \\ \frac{-w}{\mathbf{v}^T\mathbf{v}}\sqrt{\frac{y^2+z^2}{w^2+x^2}} & \frac{-x}{\mathbf{v}^T\mathbf{v}}\sqrt{\frac{y^2+z^2}{w^2+x^2}} & \frac{y}{\mathbf{v}^T\mathbf{v}}\sqrt{\frac{w^2+x^2}{y^2+z^2}} & \frac{z}{\mathbf{v}^T\mathbf{v}}\sqrt{\frac{w^2+x^2}{y^2+z^2}} \end{bmatrix},$$

but evaluated at $\mu = 0$ substitute $\mathbf{v} = q$ and there appears

$$D_{\mathbf{v}} g = \begin{bmatrix} \sec(\gamma)e_1^T R(\alpha + \frac{\pi}{2}) & \csc(\gamma)e_1^T R(\frac{\pi}{2}) \\ -\sin(\gamma)e_1^T R(\alpha) & \cos(\gamma)e_1^T \end{bmatrix}, \tag{18}$$

One may verify that $D_{\mathbf{v}} g\ \ D_a q = I$. Next differentiate equation (17) and substitute $\mu = 0$ to obtain

$$\begin{aligned} D_a \mathbf{v} &= D_a q + D_a \left(\Sigma_{\frac{\pi}{2}}(S + \nu I)q\frac{1}{\rho^2}\right)\mu + \left(\Sigma_{\frac{\pi}{2}}(S + \nu I)q\frac{1}{\rho^2}\right)\nabla\mu \\ &= D_a q + \Sigma_{\frac{\pi}{2}}(S + \nu I)q(D_a\mu)\rho^{-2}. \end{aligned}$$

Surprisingly $D_{\mathbf{v}} g \Sigma_{\frac{\pi}{2}} q = \mathbf{0}$. Multiplying equation (18) on the right by $\Sigma_{\frac{\pi}{2}}$ and substituting equation (5) we have $D_{\mathbf{v}} g \Sigma_{\frac{\pi}{2}} S q =$

$$\begin{bmatrix} -\sec(\gamma)e_1^T R(\alpha) & \csc(\gamma)e_1^T \\ -\sin(\gamma)e_1^T R(\alpha + \frac{\pi}{2}) & -\cos(\gamma)e_1^T R(\frac{\pi}{2}) \end{bmatrix} \begin{bmatrix} R(\theta - \alpha)e_1 \cos(\gamma) + \kappa R(\omega)e_1 \sin(\gamma) \\ -R(-\theta)e_1 \sin(\gamma) \end{bmatrix} =$$

$$\begin{bmatrix} -\kappa\cos(\alpha + \omega)\tan(\gamma) - 2\cos(\theta) \\ \kappa\sin(\alpha + \omega)\sin^2(\gamma) \end{bmatrix}.$$

Recall that γ becomes a dependent variable to to ensure $\mu = 0$. Equation (14) evaluated at $\beta = 0$ states that

$$\mu = -\sin(\theta)\cos(2\gamma) - \sin(\alpha+\omega)\sin(2\gamma)\kappa/2,$$

and thus

$$\nabla\mu = \left(-\frac{\kappa}{2}\cos(\alpha+\omega)\sin(2\gamma), -\kappa\sin(\alpha+\omega)\cos(2\gamma) + 2\sin(\theta)\sin(2\gamma)\right).$$

We have shown that

$$D_a f = I + (D_{\mathbf{v}} g)\Sigma_{\frac{\pi}{2}} Sq(\nabla\mu)\rho^{-2}.$$

A matrix of this form has eigenvalues 1 and

$$\lambda = 1 + \frac{\psi}{\rho^2} \tag{19}$$

for $\psi = (\nabla\mu)\ D_{\mathbf{v}} g\ \Sigma_{\frac{\pi}{2}} Sq$. Substitute $\nabla\mu$ and $D_{\mathbf{v}} g\ \Sigma_{\frac{\pi}{2}} Sq$ to find

$$\begin{aligned}\psi &= \frac{\kappa^2}{2}\cos^2(\alpha+\omega)\tan(\gamma)\sin(2\gamma) + \kappa\cos(\alpha+\omega)\sin(2\gamma)\cos(\theta) \\ &- \kappa^2\sin^2(\alpha+\omega)\sin^2(\gamma)\cos(2\gamma) + 2\kappa\sin(\alpha+\omega)\sin(2\gamma)\sin^2(\gamma)\sin(\theta).\end{aligned}$$

Collect terms with like powers of κ and expand $\sin(2\gamma)$ to eliminate $\tan(\gamma)$ and there appears

$$\begin{aligned}\psi = \kappa^2\sin^2(\gamma)\ \ (\cos^2(\alpha+\omega) - \sin^2(\alpha+\omega)\cos(2\gamma)\ \ ) \\ +\kappa\sin(2\gamma)\ \ (\cos(\alpha+\omega)\cos(\theta) + \sin(\alpha+\omega)2\sin^2(\gamma)\sin(\theta)\ \ ).\end{aligned} \tag{20}$$

3.4 Analysis Of The QRF Invariant Set In $R^{4\times 4}$

In exact arithmetic the eigenvalue λ defined in equation 19 governs the dynamics of QRF iteration:

$$\begin{aligned}|\lambda| < 1 &\Rightarrow \text{Locally attracting invariant set} \\ |\lambda| > 1 &\Rightarrow \text{Locally repelling invariant set.}\end{aligned}$$

QR iterates computed in finite precision arithmetic are approximately orthogonally similar (backward stability). But a QR iterate computed in finite precision arithmetic may differ substantially from the corresponding exact QR iterates. See [8] for a detailed discussion of this topic. Even if $|\lambda| < 1$, a QRF fixed point may ultimately be repelling in finite precision arithmetic. To understand this, one must consider QR iteration both as a map within an orthogonal similarity class and as a map over the space of n-by-n matrices, $R^{n\times n}$. This work is the only analysis of QR to consider dynamics over $R^{n\times n}$ known to the author.

QR iteration maps $H = [h_{i,j}]$ to $Q^T HQ$ where $p(H) = QR$. In this section $J = D_H Q^T HQ$ is analyzed. Each column of J corresponds to a

$$\frac{\partial}{\partial h_{i,j}} Q^T HQ.$$

In §3.5.2 we determine that at a point on the QRF-invariant set the eigenvalues of J are $\{1_6, -1_6, \hat{\lambda}\}$ where subscripts indicate multiplicities and

$$\hat{\lambda} = 1 + \frac{\sigma - \cos(2\theta)}{\rho^2}. \tag{21}$$

The 2-by-2 Jacobian of the QRF map restricted to $S(\theta,\omega,\kappa)$ also has one non-constant eigenvalue λ, but $\lambda \neq \hat{\lambda}$.

This spectral information implies that for matrices near a QRF-invariant matrix with $\lambda < 1$ and $\hat{\lambda} < 1$, the QRF iterates change slowly. In the parlance of the dynamics community, the invariant set is either weakly repelling or weakly attracting. An example of parameter values for which $0 < \hat{\lambda} < 1$ is given in § 4.2.

In §3.4.1 we determine B, Q, and R such that $p(H) = B = QR$. Next in §3.4.2 we show given $\dot{B}$, that $\dot{Q} = QS$ for a certain skew matrix S (not to be confused with the symplectic family $S(\theta, \omega, \kappa)$).

3.4.1 Q And R Along The QRF Invariant Set

For H orthogonally similar to $S(\theta, \omega, \kappa)$ and along the QRF invariant curve $\tau = \mu = 0$, there is a surprisingly simple expression for Q. For the following values of A and E, equation (16) may be re-written

$$H = \begin{bmatrix} A & -E \\ E & A \end{bmatrix}, \quad A = \begin{bmatrix} \nu & \frac{\cos(2\theta) - \nu^2}{\rho} \\ \rho & \nu \end{bmatrix}, \quad E = \frac{\sin(2\theta)}{\rho} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}.$$

In this special case,

$$H^2 = \begin{bmatrix} C & -D \\ D & C \end{bmatrix}, \quad C = A^2 - E^2 = \cos(2\theta) I, \quad D = AE - EA = \sin(2\theta) I.$$

Remarkably, $\cos(2\theta) + \delta = 0$ on the QRF invariant set (see equation (12)). Thus $p(H) = Q \sin(2\theta)$ and

$$Q = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}.$$

3.4.2 Sensitivity Of QR

Let B be invertible; $B = QR$ for $Q^* = Q^{-1}$ and R upper triangular with positive diagonal entries. Suppose that B is a smooth function of a real parameter, t, with derivative $\dot{B} = D_t B(t)$.

$$\begin{aligned} Q^*Q = I \quad &\Rightarrow \quad Q^*\dot{Q} + \dot{Q}^*Q = 0 \\ &\Rightarrow \quad Q^*\dot{Q} \text{ is skew Hermitian.} \qquad (22) \\ B = QR \quad &\Rightarrow \quad \dot{B} = Q\dot{R} + \dot{Q}R \\ &\Rightarrow \quad F \stackrel{\text{def}}{=} Q^*\dot{B}R^{-1} = \dot{R}R^{-1} + Q^*\dot{Q}. \qquad (23) \end{aligned}$$

Split F as $F = L + D + U$ where L is strictly lower triangular and U is strictly upper triangular. Define

$$\tilde{R} \quad \stackrel{\text{def}}{=} \quad \dot{R}R^{-1} \quad = \quad \text{upper triangular with real diagonal.}$$

Equation (23) implies that

$$F + F^* = (L + U^*) + (D + \bar{D}) + (U + L^*) = \tilde{R} + \tilde{R}^*,$$

where the last equality is a consequence of equation (22). Thus

$$\tilde{R} = \frac{1}{2}(D + \bar{D}) + (U + L^*).$$

By equation (23),

$$\begin{aligned} Q^*\dot{Q} \quad = \quad F - \tilde{R} \quad &= \quad \frac{1}{2}(D - \bar{D}) + L - L^* \\ \Rightarrow \quad \dot{Q} &= Q[L + \sqrt{-1}\Im m D - L^*] \\ \Rightarrow \quad \dot{R} &= [\Re e D + U + L^*] R \end{aligned}$$

3.4.3 Eigen-Decomposition Of The QRF Jacobian Over $R^{4\times 4}$

To determine J recall from §3.5.2 that for $F = Q^T\dot{B}\csc(2\theta) =$

$$\left[\begin{array}{cc} 0 & I \\ -I & 0 \end{array}\right](e_i e_j^T H + H e_i e_j^T)\csc(2\theta).$$

L is the strict lower triangular part of F and $S = L - L^T$. By the product rule,

$$\begin{aligned} \frac{\partial}{\partial h_{i,j}} Q^T H Q &= \dot{Q}^T H Q + Q^T \dot{H} Q + Q^T H \dot{Q} \\ &= \dot{Q}^T H Q + Q^T H \dot{Q} + Q^T \dot{H} Q \\ &= S^T(Q^T H Q) + (Q^T H Q)S + Q^T \dot{H} Q \\ &= S^T H + H S + Q^T \dot{H} Q \\ &= HS - SH + Q^T e_i e_j^T Q. \end{aligned}$$

This matrix corresponds to a certain column of the Jacobian.

Similarly the H-derivative of the shift polynomial $p(\zeta) = \zeta^2 - \zeta\tau + \delta$ is

$$\left[\frac{\partial}{\partial h_{i,j}} p(\zeta)\right] = -T\zeta + \Delta, \quad T = \left[\begin{array}{cc} 0_2 & 0_2 \\ 0_2 & I_2 \end{array}\right], \quad \Delta = \left[\begin{array}{cc} 0_2 & 0_2 \\ 0_2 & -A^T \end{array}\right].$$

In this notation,

$$\frac{\partial}{\partial h_{i,j}} B = e_i e_j^T H + H e_i e_j^T - H e_i^T T e_j + I_4 e_i^T \Delta e_j \tag{24}$$

To save space we introduce the notation

$$\xi = \frac{\cos(2\theta) - \nu^2}{\rho}, \qquad \phi = \frac{\sin(2\theta)}{\rho}.$$

In this notation the QRF-invariant matrices orthogonally similar to $S(\theta)$ are of the form

$$H = \left[\begin{array}{cccc} \nu & \xi & & -\phi \\ \rho & -\nu & & \\ & \phi & \nu & \xi \\ & & \rho & -\nu \end{array}\right].$$

Expand equation (24) to find

$$\left[\frac{\partial}{\partial h_{i,j}} B\right]_{1\le i,j\le 4} =$$

$$\left[\begin{array}{cccccccccccccccc}
2\nu & \xi & & -\phi & \rho & & & & & \phi & 2\nu & \xi & & & \rho & \\
\rho & & & & & \rho & & & & & \rho & & & & & \rho \\
 & & & & & & & & & & & & & & & \\
 & & & & & & & & & & & & & & & \\
\xi & & & & & \xi & & & & & \xi & & & & & \xi \\
 & \xi & & -\phi & \rho & -2\nu & & & & \phi & & \xi & & & \rho & -2\nu \\
\phi & & & & & \phi & & & & & \phi & & & & & \phi \\
 & & & & & & & & & & & & & & & \\
 & & & & & & & & -2\nu & -\xi & -\xi & \phi & -\rho & & & \\
 & & & & & & & & -\phi & & & & & -\rho & & \\
2\nu & \xi & & -\phi & \rho & & & & & & & & & & & \\
\rho & & & & & \rho & & & & & & & & & & \\
-\phi & & & & & -\phi & & & -\xi & & -\phi & & & -\xi & & \\
 & & & & & & & & & -\xi & & & -\rho & -2\nu & & \\
\xi & & & & & \xi & & & & & & & & -\phi & & \\
 & \xi & & -\phi & \rho & -2\nu & & & & \phi & & & & & &
\end{array}\right].$$

For $S^{(i,j)}$ defined by

$$\frac{\partial}{\partial h_{i,j}} Q = Q S^{(i,j)},$$

apply the result of §3.5.1 to obtain

$$\rho\phi\left[S^{(i,j)}\right] =$$

$$\begin{bmatrix}
 & & 2\nu & \rho & & & \rho & & & & & & & & & \\
 & & \xi & & & & & \rho & & & & \phi & & & & \\
-2\nu & -\xi & & & -\rho & & & & & & -\phi & & \rho & & & \\
-\rho & & & & & -\rho & & & & & & -\rho & & & & \\
 & & \xi & & & & & \rho & & & & & & & & \\
 & & & \xi & & & \xi & -2\nu & & & & \phi & & & & \\
-\xi & & & & & -\xi & & & & & & & & & & \rho \\
 & -\xi & & & -\rho & 2\nu & & & & -\phi & & & & & -\rho & \\
 & -\rho & & & & & & & & & -2\nu & -\rho & & & -\rho & \\
\rho & & & & & & & & & & -\xi & & & & & -\rho \\
 & & & & & & & & 2\nu & \xi & & & \rho & & & \\
 & & & & & & & & \rho & & & & & \rho & & \\
 & & -\phi & & & -\rho & & & & & -\xi & & & & & -\rho \\
 & & & & \rho & & -\phi & & & & & -\xi & & & -\xi & 2\nu \\
\phi & & & & & \phi & & & \xi & & & & & \xi & & \\
 & & & & & & & & & \xi & & & \rho & -2\nu & &
\end{bmatrix}$$

Due to the preservation of Hessenberg form under QR iteration the $(3,1)$, $(4,1)$ and $(4,2)$ 4-by-4 blocks are not shown below. By equation (24),

$$\rho\phi\left[\frac{\partial}{\partial h_{i,j}} Q^T H Q\right]_{1\le i\le 4,\quad 1\le j\le 2} =$$

$$\begin{bmatrix}
\rho\phi & -2\nu\phi & \xi^2-\rho^2 & 2\nu(\rho-\xi) & & & & \\
 & -\xi\phi & 2\nu(\rho-\xi) & \rho^2-\xi^2 & & & & \\
 & & (\xi+\rho)\phi & -2\nu\phi & & & & \rho\phi \\
 & & & -\rho\phi & & & & \\
 & & & & \rho\phi & -2\nu\phi & \xi^2-\rho^2 & 2\nu(\rho-\xi) \\
 & & & & & -\xi\phi & 2\nu(\rho-\xi) & \rho^2-\xi^2 \\
 & & & & & & \xi\phi & -2\nu\phi \\
 & & \rho\phi & & & & & \\
 & & & & & & & -\rho\phi \\
 & & & & & & & \\
 & & & & & & & \\
 & & & & & & & \\
 & & & & & & & \\
 & & & & & & & \\
 & & & & & & & \\
 & & & & & & &
\end{bmatrix}$$

and

$$\rho\phi\left[\frac{\partial}{\partial h_{i,j}} Q^T H Q\right]_{1\le i\le 4,\quad 3\le j\le 4} =$$

$$
\begin{bmatrix}
 & & \xi\phi+\rho\phi & & & & & \\
 & -\phi^2 & -2\nu\phi & -\xi\phi & & & & \\
 & -2\nu\phi & -\phi^2-\rho^2-\rho\xi & 2\rho\nu & & -\rho\phi & & \\
 & & 2\rho\nu & \rho^2+\rho\xi & & & & \\
 & \phi^2 & & \xi\phi & & & \rho\phi & \\
 & & -\rho\phi & & & & & \\
 & -\xi\phi & & \phi^2 & & & -\rho^2-\rho\xi & 2\rho\nu \\
 & & & & & & 2\rho\nu & \rho^2+\rho\xi \\
 & 2\nu\phi & \rho^2-\xi^2 & 2\nu(\xi-\rho) & & \rho\phi & & \\
 & \xi\phi & 2\nu(\xi-\rho) & \xi^2-\rho^2 & & & & \\
 & & -\xi\phi & 2\nu\phi & & & & \\
 & & & \rho\phi & & & & \\
 & & & & -\rho\phi & 2\nu\phi & \rho^2-\xi^2 & 2\nu(\xi-\rho) \\
\rho\phi & & & & & (\xi+\rho)\phi & 2\nu(\xi-\rho) & \xi^2-\rho^2 \\
 & & & & & & -\xi\phi & 2\nu\phi \\
 & & & & & & & \rho\phi
\end{bmatrix}
$$

This matrix is assembled into J using a map from the indices of entries of H to $\{1, ..., 13\}$. For the map defined schematically by the matrix

$$
\begin{bmatrix}
1 & 10 & 5 & 9 \\
12 & 2 & 7 & 6 \\
 & 8 & 3 & 11 \\
 & & 13 & 4
\end{bmatrix},
$$

J is block upper triangular with block diagonal

$$
J_6 \oplus -1 \oplus \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \oplus \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \oplus \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}
$$

for

$$
\rho\phi J_6 =
$$

$$
\begin{bmatrix}
\rho\phi & -\xi\phi & (\xi+\rho)\phi & -\rho\phi & \xi^2-\rho^2 & \rho^2-\xi^2 \\
\rho\phi & \xi\phi & \xi\phi & & \xi^2-\rho^2 & \rho^2-\xi^2 \\
 & -\xi\phi & -\xi\phi & \rho\phi & \rho^2-\xi^2 & \xi^2-\rho^2 \\
-\rho\phi & (\xi+\rho)\phi & -\xi\rho & \rho\phi & \rho^2-\xi^2 & \xi^2-\rho^2 \\
 & -\phi^2 & -\phi^2-\rho^2-\rho\xi & \rho(\xi+\rho) & \phi(\xi+\rho) & -\xi\phi \\
 & -\phi^2 & -\phi^2-\rho^2-\rho\xi & -\rho(\xi+\rho) & \rho(\xi+\rho) & \rho\phi
\end{bmatrix}.
$$

Next for

$$
L_4 = \begin{bmatrix}
1 & & & \\
-1 & 1 & & \\
1 & & 1 & \\
1 & & & 1
\end{bmatrix},
$$

there holds $\mathrm{diag}(L_4, I_2) J_6 \mathrm{diag}(L_4^{-1}, I_2) =$

$$
\begin{bmatrix}
1-2\frac{\xi}{\rho} & -\frac{\xi}{\rho} & \frac{\xi+\rho}{\rho} & -1 & \frac{\xi^2-\rho^2}{\rho\phi} & \frac{\rho^2-\xi^2}{\rho\phi} \\
 & & -1 & 1 & & \\
 & & 1 & & & \\
 & 1 & 1 & & & \\
-2\frac{\phi}{\rho}-2\frac{\xi+\rho}{\phi} & -\frac{\phi}{\rho} & \frac{\phi^2+\rho^2+\rho\xi}{\rho\phi} & \frac{\xi+\rho}{\phi} & \frac{\xi+\rho}{\rho} & -\frac{\xi}{\rho} \\
-2\frac{\xi+\rho}{\phi} & & -\frac{\xi+\rho}{\phi} & \frac{\xi+\rho}{\phi} & 1 &
\end{bmatrix}.
$$

Transpose rows and columns 2 and 5, then 3 and 6 to obtain a block upper triangular matrix block diagonal

$$J_3 \oplus \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \oplus 1$$

where

$$J_3 = \begin{bmatrix} 1 - 2\frac{\xi}{\rho} & \frac{\xi^2-\rho^2}{\rho\phi} & \frac{\rho^2-\xi^2}{\rho\phi} \\ -2\frac{\xi+\rho}{\phi} - 2\frac{\phi}{\rho} & \frac{\xi+\rho}{\rho} & -\frac{\xi}{\rho} \\ -2\frac{\xi+\rho}{\phi} & 1 & \end{bmatrix},$$

Lastly for

$$U_2 = \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix},$$

$\mathrm{diag}(1, U_2) J_3 \mathrm{diag}(1, U_2^{-1})$ is block lower triangular with block diagonal

$$\begin{bmatrix} 1 - 2\frac{\xi}{\rho} & \frac{\xi^2-\rho^2}{\rho\phi} \\ -2\frac{\phi}{\rho} & \frac{\xi}{\rho} \end{bmatrix} \oplus 1.$$

The 2-by-2 matrix has eigenvalues $\lambda = 2 - \xi/\rho$ and -1.

4 Exceptional QR Shifts

Matrices invariant under QRF are known (see [11]) and examples of QRF attracting fixed points within an orthogonal similarity class have been given for 3-by-3 matrices in [3]. HQR remains efficient in these cases in part because QR iterations 11 and 21 use an exceptional shift instead of QRF (see §2 or [9]. The EISPACK HQR implementation uses a modified exceptional shift. We are indebted to W. Kahan who recalled that the HQR shift strategy was actually to use EX shifts every 10 iterations, but this was not implemented because in 1970 no one thought that more than 30 QR iterations would ever be necessary. We discuss four versions of HQR, with original or EISPACK exceptional shifts and with exceptional shifts at only steps 11 and 21 or at every 10th iteration. The table below summarizes the worst case behavior known to the author in finite (double) precision arithmetic;

Iterations	11,21	Every 10th
Original	$> 10^6$	$> 10^4$
EISPACK	$> 10^8$	318

We define these strategies and demonstrate poor convergence behavior in an orthogonal similarity class $S(\theta, \omega, \kappa)$ for each.

One fix to HQR is to use EISPACK exceptional shifts every 10 iterations, and substantially increase the maximum number of allowed QR iterations. See §5 for more effective remedies.

4.1 The Original Exceptional Shift Strategy

The original exceptional shift polynomial proposed in [9] is

$$p(\zeta) = \zeta^2 - \frac{3}{2}\beta\zeta + \beta^2$$

where

$$\beta = |h_{n,n-1}| + |h_{n-1,n-2}|. \tag{25}$$

In the family of orthogonal similarity classes, $S(\theta,\omega,\kappa)$, investigated in this work, *no* unreduced Hessenberg matrices are exactly invariant under this exceptional shift strategy. To see this, simply recall that in an orthogonal similarity class, $S(\theta,\omega,\kappa)$, the QR fixed points are the unreduced Hessenberg matrices for which the coefficient of ζ in $p(\zeta)$ vanishes, and observe that $\beta > 0$ if H is uncoupled.

Nonetheless this version of the HQR algorithm does converge slowly for certain matrices. See the table below. Our example of slow convergence assumes $\kappa = -2\sin(\theta)$. In this case equation (14) reduces to ($\beta = \omega = 0$)

$$\mu = \sin(\theta)(-\cos(2\gamma) + \sin(\alpha)\sin(2\gamma)).$$

Solve for $\mu = 0$ to find that the QRF invariant set is the locus of $\cot(2\gamma) = \sin(\alpha)$.

We choose $(\alpha,\gamma) = (\pi/2, \pi/8)$ in our example for the following reason. The original exceptional shift polynomial factors as

$$\zeta^2 - \frac{3}{2}\beta\zeta + \beta^2 = (\zeta - \beta e^{\sqrt{-1}\psi}) \quad (\zeta - \beta e^{\sqrt{-1}\psi}),$$

for $e^{\sqrt{-1}\psi} = (3+\sqrt{-7})/4$. Thus this shift favors eigenvalues with positive real part. For matrices in an orthogonal similarity class $S(\theta,\omega,\kappa)$, this exceptional shift tends to cause convergence to the eigen-pair in the right half plane. The corresponding vector q rotates towards $\gamma = 0$. For this reason convergence is delayed for the matrix in the orthogonal similarity class, $S(\theta, 0, -2\sin(2\theta))$, for which γ is maximal, namely $(\alpha,\gamma) = (\pi/2, \pi/8)$.

Table 1 below displays the number of QR iterations required to decouple the Hessenberg matrix that corresponds to $(\alpha,\gamma) = (\pi/2, \pi/8)$ for three implementations of the QR algorithm, each using the original exceptional shift. First we apply the entire shift strategy proposed in [9]: QRF at each step save 11 and 21, which are Exceptional. In column 3 iteration counts for the case in which exceptional shifts are taken at steps 10, 20, 30, $\cdots$ until convergence are given. Column 4 shows the iteration count when QRF is modified as defined in §5; we call the algorithm that results QRW.

QR Iteration Count with Original Exceptional Shift

θ	HQR: EX at steps 11,21	HQR: EX every 10 steps	QRW
$1e-1$	17	17	3
$1e-2$	26	26	3
$1e-3$	78	44	2
$1e-4$	5124	98	2
$1e-5$	$> 10^5$	242	2
$1e-6$	$> 10^6$	611	2
$1e-7$	$> 10^5$	1547	2
$1e-8$	$> 10^5$	3909	1
$1e-9$	$> 10^6$	9858	2
$1e-10$	$> 10^5$	$> 10^4$	2

4.2 The EISPACK Exceptional Shift

The EISPACK implementation of HQR uses the exceptional shift polynomial

$$p(\zeta - h_{n,n}) = \zeta^2 - (2h_{n,n} + \frac{3}{2}\beta)\zeta + (h_{n,n}+\beta)^2 - h_{n,n}\beta/2.$$

We claim that for μ, ν, ρ, σ given in equations (14) and (13), the Hessenberg matrix that corresponds to any given values of θ, κ, α, γ is given by

$$H = \begin{bmatrix} \nu & \frac{\cos(2\theta)-\nu^2}{\rho} & \frac{\mu}{\rho}\frac{\cos(2\theta)-\nu^2+\rho^2}{\sqrt{\rho^2-\mu^2}} & \frac{-2\mu\nu-\sin(2\theta)}{\sqrt{\rho^2-\mu^2}} \\ \rho & -\nu-\sin(2\theta)\frac{\mu}{\rho^2} & -\frac{\mu}{\rho^2}\frac{\mu\sin(2\theta)+2\nu\rho^2}{\sqrt{\rho^2-\mu^2}} & -\frac{\mu}{\rho}\frac{\cos(2\theta)-\nu^2+\rho^2}{\sqrt{\rho^2-\mu^2}} \\ 0 & \sin(2\theta)\frac{\sqrt{\rho^2-\mu^2}}{\rho^2} & \nu+\sin(2\theta)\frac{\mu}{\rho^2} & \frac{\cos(2\theta)-\nu^2}{\rho} \\ 0 & 0 & \rho & -\nu \end{bmatrix}. \tag{26}$$

This identity will not be derived here, but is included to allow the reader to determine the Hessenberg that corresponds to given values of θ, κ, α, γ.

We consider the H that corresponds to

$$\theta = .111866322512629152$$

$$\kappa = 1.08867072154101741$$

$$\alpha = .338146383137297168$$

$$\gamma = -.313987810419091240$$

H is (approximately) invariant under both QRF and the EISPACK Exceptional shift. H corresponds to an attracting fixed point within the orthogonal similarity class, $\lambda \approx 7/10$, and over $R^{4\times4}$ there holds $\hat{\lambda} \approx 8/10$. HQR with EISPACK Exceptional shift at iterations 11 and 21 does not converge after up to 10^8 QR iterations. But with EISPACK Exceptional shifts every 10th iteration, the number of QR iterations for convergence is 318, which is still much larger than the maximum allowed number of iterations.

5 How To Fix QR

In general Francis' double shift is the shift of lowest degree that well approximates complex eigenvalues without introducing complex arithmetic. To recover convergence in all known cases we selectively shift by the eigenvalue, w, of the SE 2−by−2 sub-matrix nearest the SE element. We refer to this shift strategy as a Wilkinson shift, because this is the shift strategy Wilkinson developed for the Hermitian QR algorithm. In contrast to QRF, we denote by QRW the QR algorithm with this shift.

The term *root* refers exclusively to a root of a shift polynomial. There are two viable options as to when to use QRW instead of QRF:

Option 1. Use QRW if $h_{n,n-1}h_{n-1,n} > 0$,

Option 2. Use QRW if $p(.)$ has real roots.

We will discuss the following QR iterations in the family of orthogonal similarity classes $S(\theta, \omega, \kappa)$.

QRF	Francis' shift
QRW	double Wilkinson shift
QR1	QRF or QRW as in Option 1
QR2	QRF or QRW as in Option 2
QR1E, QR2E	Use EISPACK Exceptional shifts
QR1O, QR2O	Use Original Exceptional shifts

We prove that in the family of orthogonal similarity classes $S(\theta, \omega, \kappa)$, QR1E and QR1O possess only strongly repelling ($\hat{\lambda} \geq 2$) fixed points over $R^{4\times4}$. This explains why QR1E and QR1O are observed to converge in finite precision arithmetic for matrices in the family of orthogonal similarity classes $S(\theta, \omega, \kappa)$. Next we outline the argument that QR2O is also convergent in finite precision arithmetic and give an example in which QR2E does not appear to converge.

We claim that Option 1 is contrived so that QR1 has only strongly repelling fixed points over $R^{4\times 4}$ in the family of orthogonal similarity classes $S(\theta, \omega, \kappa)$. Recall that the QRF shift polynomial is $p(\zeta) = \zeta^2 - \tau\zeta + \delta$ (see equation (12)). First we discuss the case in which the iteration is QRW. On the invariant set is a subset of the locus of $\delta = 0$;

$$0 = \delta = -\cos(2\theta) - \nu\tau \quad \Rightarrow \quad \cos(2\theta) = -\nu\tau.$$

The equation $\delta = 0$ also implies that the roots of $p(.)$ are 0 and τ. Recall from equation (16) that $h_{4,4} = -\nu$. Thus

$$\cos(2\theta) > 0 \quad \Rightarrow \quad w = \tau \neq 0.$$

Observe also from equation (16) that

$$h_{4,3}h_{3,4} = \cos(2\theta) - \nu^2.$$

Thus

$$h_{4,3}h_{3,4} > 0 \quad \Rightarrow \quad \cos(2\theta) > 0,$$

which implies that there are no QRW fixed points. Second we discuss the case in which the iteration is QRF. Only the QRF fixed points at which there holds $\cos(2\theta) - \nu^2 \leq 0$ remain fixed points under Option 1, Note that equation (10) implies that $\sigma = \rho^2 + \nu^2$; Substitute this equation into equation (21) to find, as desired, that

$$\hat{\lambda} = 1 + \frac{\sigma - \cos(2\theta)}{\rho^2} = 1 + \frac{\rho^2 + \nu^2 - \cos(2\theta)}{\rho^2} \geq 2.$$

Option 2 is natural, but the convergence properties of this family of algorithms depends on the choice of Exceptional shift, original or EISPACK. The matrix specified by the parameter values

$$\alpha = 2.187, \quad \gamma = .3613369902224367, \quad \theta = 1.1576, \quad \kappa = -4.356990028259095$$

is (approximately) invariant under QR2E; the Hessenberg appears invariant in finite precision arithmetic after as many as 40000 HQR iterations with EISPACK Exceptional shifts every 10 iterations. The Hessenberg that corresponds to any set of parameter values is given in equation (16).

QR2O appears to yield a convergent algorithm in finite precision arithmetic over the family of orthogonal similarity classes $S(\theta, \omega, \kappa)$. We sketch the proof of convergence. The QRF invariant set, $\mu = 0$, and unreal roots arise only if

$$\delta = -\cos(2\theta) > 0 \quad \Rightarrow \quad \cos(2\theta) < 0.$$

In this case the QRF fixed points are repelling over $R^{4\times 4}$ as above. The analysis of the QRW invariant set is divided into two cases. In the first case, $\sin(2\theta)$ is bounded away from 0; this implies that β is "not small" and hence that the original Exceptional shift is effective. In the second case, $\sin(2\theta)$ is near 0, the QRW map within an orthogonal similarity classes $S(\theta, \omega, \kappa)$ has eigenvalues 1 and $\tilde{\lambda}$ on the invariant set such that

$$\lim_{|\frac{\pi}{2}| \to 0} \tilde{\lambda} = -\infty.$$

In words the QRW invariant set for $\sin(2\theta)$ is near 0 is repelling within a given orthogonal similarity class. Instead of a detailed proof we illustrate the ideas sketched with an example. For this algorithm the maximum number of QR iterations observed in finite precision arithmetic is 36 (with either 2 or 3 Exceptional shifts) for the Hessenberg matrix that corresponds to the parameter values

$$\alpha = 2.692793703076966, \quad \gamma = 3.203401609348687e-08,$$

$$\theta = 1.57079406646549, \quad \omega = 0, \quad \kappa = -7.194809726354949e+07$$

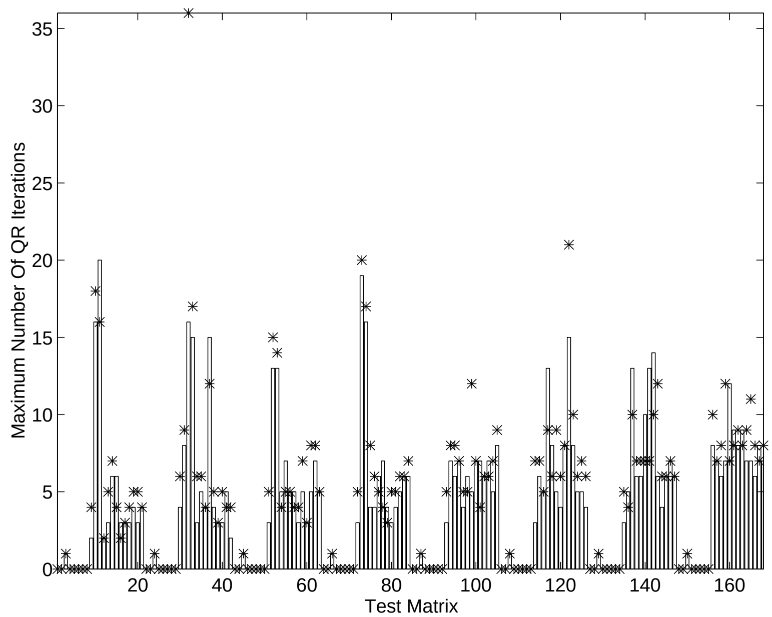

Figure 1: HQR (*) and QR2O (bar) Iterations for LAPACK Test Suite

In this case β defined in equation (25) is sufficiently large, $\beta \approx .0037$, that the first original Exceptional shift perturbs the matrix from the invariant set. On the other hand the invariant set is already sufficiently repelling that QR2 converges in 32 iterations without Exceptional shifts.

In tests on matrices from the LAPACK test suite HQR required a maximum of 36 iterations to decouple a sub-matrix, compared to a maximum of 20 iterations for QR2O. Overall QR2O is slightly faster than HQR. The performance of QR1E and QR1O is similar. The figure below shows the maximum number of QR iterations to decouple a submatrix for the 21 matrices in the LAPACK test suite; matrices of 8 different orders ranging from 4 to 64 were used.

QR2O may be implemented in LAPACK by adding fifteen lines to the subroutine SLAHQR. After the lines

```
*
*              Prepare to use Francis' double shift
*
            H44 = H( I , I )
            H33 = H( I-1, I-1 )
            H43H34 = H( I , I-1 )*H( I-1, I )
            S = H( I-1, I-2 )*H( I-1, I-2 )
```

add the lines

```
            DISC = (H33 - H44) * HALF
            DISC = DISC * DISC + H43H34
            IF( DISC.GT.ZERO )THEN
*
*              Real roots:  use Wilkinson's shift twice
*
              DISC = sqrt( DISC )
              AVE = HALF * ( H33 + H44 )
              IF( ABS(H33) - ABS(H44) .GT. ZERO )THEN
                H33 = H33 * H44 - H43H34
```

```
      H44 = H33/( SIGN( DISC, AVE ) + AVE )
   ELSE
      H44 = SIGN( DISC, AVE ) + AVE
   END IF
   H33 = H44
   H43H34 = ZERO
END If
```

6 Multishift QR Fails

We take as the definition of multishift QR the subroutine HSEQR from version 2.0 of LAPACK [1, 2]. To compute shifts HSEQR uses the LAPACK implementation of QR, LAHQR. In the examples at hand LAHQR frequently terminates without computing eigenvalues. For this reason we substituted our version of LAHQR modified as described in the next section to converge in all known cases.

HSEQR terminates without computing the eigenvalues of certain n−by−n unreduced Hessenberg matrices of the form $H_n + \eta E_n$ for H and E defined as follows.

$$H_n = \mathrm{diag}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

$E_n(2k+1, 2k) = 1$ for $1 \leq k < n/2$, $E_n(1, n) = 1$, and the other elements of E_n vanish.

The characteristic polynomial of $H_n + \eta E_n$ is $\phi^k - \eta^k$ for $k = n/2$ and $\phi(\zeta) = \zeta^2 - 1$. From the identity

$$\phi(H_n + \eta E_n) - \phi(H_n) = \eta(H_n E_n + E_n H_n) + \eta^2 E_n^2$$

and the observations $\phi(H_n) = 0$, $E_n^2 = 0$, and that $H_n E_n + E_n H_n$ is a permutation, we have that

$$\frac{1}{\eta}\phi(H_n + \eta E_n) = H_n E_n + E_n H_n$$

is orthogonal. We expect HSEQR to fail in the orthogonal similarity class of $H_n + \eta E_n$ because, as QR converges, the computed shift polynomials approximate powers of ϕ. Known values of n and η for which the double precision implementation DHSEQR fails are x-ed in the table below.

n	$\eta = 10^{-9}$	$\eta = 10^{-10}$	$\eta = 10^{-11}$	$\eta = 10^{-12}$
70			x	
80	x		x	x
90		x	x	

In each x-ed case DHSEQR terminates after $30n$ iterations without decoupling. This is easy to fix; if multi-shift QR, HSEQR, fails then use double shift QR, LAHQR.

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References

[1] Z. Bai and J. Demmel (1989). On a block implementation of the Hessenberg multishift QR iteration, *Int. J. High-speed Comp. 1,* 97-112.

[2] E. Anderson, Z. Bai, C. Bischof, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, S. Ostrouchov, D. Sorensen (1994). *LAPACK User's Guide*, SIAM, Philadelphia.

[3] S. Batterson (1990). Convergence of the shifted QR algorithm on 3×3 normal matrices, *Num. Math. 58*, 341-352.

[4] S. Batterson and D. Day (1992). Linear convergence in the shifted QR algorithm *Math. Comp. 59*, 141-152.

[5] A. Dubrulle and G. Golub (1993). A multishift QR iteration without computation of the shifts, Numerical Analysis Project Manuscript NA-93-04, Computer Science Department, Stanford University, Stanford California 94305.

[6] G. Francis (1961-2). The QR transformation, Parts I and II, *Comp. J. 4*, 265-272 and 332-345.

[7] G. Golub and C. Van Loan (1989). *Matrix Computations*, 2nd ed., Johns Hopkins Univ. Press, Baltimore.

[8] R. Lehoucq (1995). Analysis and implementation of an implicitly restarted Arnoldi iteration, PhD Thesis Rice University, Houston, Texas.

[9] R. Martin, G. Peters, and J. Wilkinson (1970). The QR algorithm for real Hessenberg matrices. *Num. Math. 14*, 219-231.

[10] C. Paige and C. Van Loan (1981). A Schur decomposition for Hamiltonian matrices, *Lin. Alg. Appl. 41*, 11-32.

[11] B. Parlett (1966). Singular and invariant matrices under the QR transformation, *Math. Comp. 20*, 611-615.

[12] B. Parlett and W. Kahan (1969). On the convergence of a practical QR algorithm, In: *Information Processing 68*, A. Morrell, editor, 114-118.

[13] B.T. Smith, J.M. Boyle, J.J. Dongarra, B.S. Garbow, Y. Ikebe, V. Klema, and C. Moler (1974). *Matrix Eigensystem Routines-Eispack Guide*, Lecture Notes in Computer Science, vol 6, Springer-Verlag.