$$(2m-1)!! = 1\cdot 3\cdot 5 \cdots (2m-1), \qquad m > 0,$$
$$= 1 \qquad m = 0.$$

These expansions agree with those of Thompson [1] except that the factor of $\pi^{1/2}$ has been inadvertently omitted in his paper and there is a sign error in his expansion for I_1. (Apparently the author intended to include a factor $\pi^{-1/2}$ in defining the integrals, as the reciprocal factor is otherwise necessary in all the other expressions for the integrals in the paper. There are also other minor misprints in Eq. (2), the equation preceding it, and in the first, second, third, and fifth equations following Eq. (1).)

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Singular and Invariant Matrices Under the *QR* Transformation*

By Beresford Parlett

0. Introduction. The above two classes of matrix are usually ignored in discussions of the QR algorithm [1], [3], [4]. Some familiarity with the algorithm is assumed.

There are good reasons for this neglect. Firstly the algorithm is not well defined for singular matrices and thus its behavior is difficult to describe. Secondly the problem of describing all matrices which are left invariant under the QR transformation is in general rather difficult.

The purpose of this note is to point out that with a preliminary reduction to Hessenberg form both difficulties disappear. We show first that singular matrices reveal their zero eigenvalues, one per iteration. Secondly we describe all matrices which are invariant.

A given square matrix A (real or complex) may be reduced to Hessenberg form A_1 ($a_{ij} = 0$, $i > j + 1$) in a variety of ways. If any subdiagonal elements $a_{i+1,i}$ vanish then A_1 is said to be reduced and may be partitioned appropriately as

$$(1) \qquad A_1 = \begin{pmatrix} H_1 & H_{12} & \cdot & H_{1m} \\ 0 & H_2 & \cdot & H_{2m} \\ \cdot & \cdot & \cdot & \cdot \\ & & & H_m \end{pmatrix}$$

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where the $H_i \in$ UHM, the class of *unreduced Hessenberg matrices.* We include 1×1 matrices in UHM. The QR algorithm acts independently on each H_i, $i = 1, \cdots, m$. If all the H_i are 1×1 then H is upper triangular and the algorithm terminates immediately.

We denote the jth column of a matrix M by m_j.

1. Singular Matrices. If A_1 is singular then at least one H_i must be singular. Let us consider a singular $n \times n$ matrix $H \in$ UHM.

Any matrix A can be factorized into a product QR where Q is unitary and R is upper triangular with nonnegative diagonal elements. The jth column of Q, q_j, is of unit length and in the direction of the orthogonal perpendicular from a_j onto Span $(a_1, \cdots, a_{j-1})$. Let $H = QR$.

Because $H \in$ UHM the first $(n - 1)$ columns of H are linearly independent. Since $h_j = \sum_{\nu=1}^{j} q_\nu r_{\nu j}$ we have

$$(2) \qquad r_{jj} = \left\| h_j - \sum_{\nu=1}^{j-1} q_\nu r_{\nu j} \right\|_2 > 0, \qquad j = 1, \cdots, n-1$$

and

$$(3) \qquad q_{j+1,j} = r_{jj}^{-1} h_{j+1,j} \neq 0, \qquad j = 1, \cdots, n-1.$$

Since R is singular $r_{nn} = 0$. However q_n must be in the direction of the normal to the hyperspace Span $(h_1, \cdots, h_{n-1})$. Apart from the sign of q_n, which may be fixed by requiring det $(Q) > 0$, we have a unique factorization, QR, whether or not H be singular.

One QR transformation yields $\bar{H} = RQ$ and

$$(4) \qquad \bar{h}_{j,j-1} = r_{jj} q_{j,j-1} \neq 0, \qquad j = 2, \cdots, n-1,$$

$$(5) \qquad \bar{h}_{n,n-1} = r_{nn} q_{n,n-1} = 0, \qquad \bar{h}_{nn} = r_{nn} q_{nn} = 0.$$

Thus after one transformation a zero eigenvalue is revealed and by (4) the leading principal $(n - 1)$-submatrix, $\bar{H}_{n-1} \in$ UHM. Either $\bar{H}_{n-1}$ is nonsingular or else another QR transform will yield another zero eigenvalue of H. If the algebraic multiplicity of the zero eigenvalue is m then exactly m QR transformations will reveal them and either terminate the algorithm (if $m \geqq n - 1$) or leave a nonsingular matrix $\bar{H}_{n-m} \in$ UHM.

3. Invariant Matrices. The algorithm produces from A a sequence $\{A_s\}$ where

$$(6) \qquad A_s = Q_s R_s, \qquad A_{s+1} = R_s Q_s = P_s^* A P_s, \qquad P_s = Q_1 Q_2 \cdots Q_s,$$

and P_s is the unitary factor of A^s. Here we assume that A is nonsingular. It is desired that A_s tend to upper triangular form as $s \to \infty$.

Certainly if A is upper triangular with positive diagonal then $A_s = A$ for all s. Even if the diagonal is not positive the elements of A_s vary only in signum and the form remains triangular. Thus triangular A are invariant in a trivial sense which we exclude by saying that the algorithm terminates immediately if A_s is triangular.

We are concerned with invariant matrices which do not reveal their eigenvalues. From (6) we see that the convergence of P_s implies the convergence of A_s. The converse is not true however. If A is unitary then $P_s = A^s$, which need not converge, although $A_s = A$ and so $\{A_s\}$ converges (but not to triangular form). What we want is that P_s converge (at least to within post multiplication by a diagonal unitary matrix). By (6) $P_s = P_{s-1}Q_s$, and if $P_s \to P_\infty$ then det $(P_\infty) = \pm 1$ and $Q_s \to I$ as $s \to \infty$. Thus $A_s \sim R_s$, the desired triangular form.

In practice however only A_s is available and its invariance is not distinguished by current programs from slow convergence. This has caused some computer programs based on the QR algorithm to fail unnecessarily.

Remark. All members of UHM are nonderogatory. The minor of the $(1, n)$ element of $H - zI$ vanishes for no value of z. Here n is the order of H.

Theorem 1. *Let $H \in UHM$. Then H is invariant under the basic QR algorithm if and only if H is a scalar multiple of a unitary matrix.*

Proof. We have just shown that unique factors Q and R exist such that $H = QR$. Now if H is invariant then $H = RQ$ and thus

$$HQ = QRQ = QH. \tag{7}$$

Yet (7), together with H being nonderogatory, implies (see [2]) that

$$Q = \phi(H), \qquad \phi(\xi) \equiv \sum_{\nu=0}^{d} \phi_\nu \xi^\nu, \qquad \phi_d \neq 0. \tag{8}$$

By the Hamilton-Cayley theorem we may take $d < n$. Since $H \in$ UHM the $(d + 1, 1)$ element of $\phi(H)$ is

$$\phi_d \prod_{i=1}^{d} h_{i+1,i} \neq 0.$$

Since $Q \in$ UHM, by (3), we must have $d = 1$ and

$$Q = \phi_0 I + \phi_1 H. \tag{9}$$

On comparing first columns on each side of $H = QR$ we find

$$r_{11}^{-1} h_{11} = \phi_0 + \phi_1 h_{11},$$

$$r_{11}^{-1} h_{21} = \phi_1 h_{21},$$

whence $\phi_0 = 0$, $\phi_1 = r_{11}^{-1}$. Thus $H = r_{11}Q$. Conversely if $\alpha^{-1}H$ is unitary then $Q = \alpha^{-1} H$, $R = \alpha I$, and H is invariant. Q.E.D.

Now consider a general Hessenberg matrix in form (1). The eigenvalues are determined solely by the diagonal blocks H_i. The H_{ij}, $i > j$, play no role in the algorithm. We begin with H_m and test for invariance ($H_m^* H_m = \alpha I$, $\alpha > 0$). If it is invariant some special treatment must be used (possibly the QR algorithm on $H_m - \alpha^{1/2} I$). If it is not invariant we proceed with the algorithm. On completing H_m we consider H_{m-1}, and so on, until all the H_i have been resolved.

3. Shifts of Origin. In practice Francis uses an extension of the basic algorithm which employs origin shifts to improve the convergence rate (when the basic algorithm does converge). We now restrict ourselves to real matrices in UHM and ask when they are invariant under this extended algorithm. We have for one double step

$$\bar{H} = Q^*HQ,$$
$$QR = H^2 - \sigma H + \rho I,$$

where σ and ρ are parameters depending only on the choice of origin shift.

Now Q may happen to be derogatory although H still is not. By [2] if $\bar{H} = H$ then Q is a polynomial in H. Proceeding as in the proof of Theorem 1 we find that first

$$Q = \phi_0 I + \phi_1 H + \phi_2 H^2$$

and then

$$r_{11}Q = \rho I - \sigma H + H^2. \tag{10}$$

Initially Francis puts $\sigma = \rho = 0$. Thus $H^2 = r_{11}Q$ and therefore $H = \alpha Q_1$, Q_1 orthogonal.

A fortiori the elements $h_{n-1,n-1}$, $h_{n-1,n}$, $h_{n,n-1}$, and h_{nn} do not change after one step. On the second step according to his strategy, Francis would put

$$\begin{aligned} \sigma &= h_{n-1,n-1} + h_{nn}, \\ \rho &= h_{n-1,n-1}h_{nn} - h_{n,n-1}h_{n-1,n}. \end{aligned} \tag{11}$$

By (10) we shall not have invariance unless $\rho I - \sigma H + H^2 = \beta Q_2$, Q_2 orthogonal. Being nonderogatory and normal H has distinct eigenvalues. We take $n \geqq 3$ and it follows that the mapping $\xi \rightarrow \phi(\xi) = \rho - \sigma\xi + \xi^2$ must take the whole circle of radius α, center the origin, into the concentric circle of radius β. Consideration of the cases $\xi = \pm\alpha, \pm i\alpha$ shows that

$$\sigma = \rho = 0. \tag{12}$$

What does this decree for the last two rows of H? We have

(i) $h_{n,n-1} = \alpha\gamma \neq 0$, γ to be determined,

(ii) $\alpha^2\gamma^2 + |h_{nn}|^2 = \alpha^2$, since $\alpha^{-1}H$ is orthogonal,

(iii) both eigenvalues of

$$\begin{pmatrix} h_{n-1,n-1} & h_{n-1,n} \\ h_{n,n-1} & h_{nn} \end{pmatrix}$$

vanish,

(iv) row $(n - 1)$ is orthogonal to row n.

It may be verified that conditions (i)–(iv) imply $\gamma = 1$. We have proved the following

THEOREM 2. *A real Hessenberg matrix of the form* (1) *is invariant under the extended algorithm of Francis if and only if each* H_i, $i = 1, \cdots, m$ *is a scalar multiple of an orthogonal matrix whose last two rows are of the form*

$$\begin{pmatrix} 0 & \cdots & 0 & 1 & 0 & 0 \\ 0 & \cdots & 0 & 0 & 1 & 0 \end{pmatrix}.$$

For those strategies which shift by (11) at each step, including the first, we have invariance whenever, for each H_i, $i = 1, \cdots, m$,

$$H_i^2 - \sigma H_i + \rho I$$

is a multiple of an orthogonal matrix.

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