9.5 The QR Method At the present time this is the most efficient and widely used general method for the calculation of all of the eigenvalues of a matrix. The method was first published in 1961 by J.G.F. Francis and it has since been the subject of intense investigation. The QR method is quite complex in both its theory and application, and we are able to give only an introduction to the theory of the method. For actual algorithms for both symmetric and nonsymmetric matrices, refer to those in EISPACK and Wilkinson-Reinsch (1971).

Given a matrix A, there is a factorization

$$A = QR$$

with R upper triangular and Q orthogonal. With A real, both Q and R can be chosen real; and their construction is given in section 9.3. We will assume A is real throughout this section. Let $A_1=A$, and define a sequence of matrices A_m, Q_m and R_m by

$$A_m = Q_m R_m, \qquad A_{m+1} = R_m Q_m, \qquad m=1,2,\ldots \qquad (9.5.1)$$

The sequence $\{A_m\}$ will converge to either a triangular matrix with the eigenvalues of A on its diagonal or to a near-triangular matrix from which the eigenvalues can be easily calculated. In this form the convergence is usually slow; and a technique known as *shifting* is used to accelerate the convergence. The technique of shifting will be introduced and illustrated later in the section.

Before illustrating (9.5.1) with an example, a few properties of it will be derived. From (9.5.1), $R_m=Q_m^T$, and thus

$$A_{m+1} = Q_m^T A_m Q_m. \qquad (9.5.2)$$

A_{m+1} is orthogonally similar to A_m, and thus by induction to $A_1 \equiv A$. From (9.5.2),

$$A_{m+1} = Q_m^T \cdots Q_1^T A_1 Q_1 \cdots Q_m. \qquad (9.5.3)$$

Introduce the matrices P_m and U_m by

$$P_m = Q_1 \cdots Q_m, \qquad U_m = R_m \cdots R_1. \qquad (9.5.4)$$

Then from (9.102)

$$A_{m+1} = P_m^T A_1 P_m, \qquad m \geq 1. \qquad (9.5.5)$$

The matrix P_m is orthogonal, and U_m is upper triangular.

For later use, we derive a further relation involving P_m and U_m.

$$P_m U_m = Q_1 \cdots Q_m R_m \cdots R_1$$

$$= Q_1 \cdots Q_{m-1} A_m R_{m-1} \cdots R_1.$$

From (9.5.3) with m replacing m+1,

$$Q_1 \cdots Q_{m-1} A_m = A_1 Q_1 \cdots Q_{m-1}. \qquad (9.5.6)$$

Using this,

$$P_m U_m = A_1 Q_1 \cdots Q_{m-1} R_{m-1} \cdots R_1 = A_1 P_{m-1} U_{m-1}.$$

Since $P_1 U_1 = Q_1 R_1 = A_1$, induction on the last statement implies

$$P_m U_m = A_1^m, \qquad m \geq 1. \qquad (9.5.7)$$

<u>Example</u>. Let

$$A_1 = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 3 & 1 \\ 0 & 1 & 4 \end{bmatrix}. \qquad (9.5.8)$$

The eigenvalues are

$$\lambda_1 = 3+\sqrt{3} \doteq 4.7321, \qquad \lambda_2 = 3.0, \qquad \lambda_3 = 3-\sqrt{3} \doteq 1.2679.$$

The iterates A_m do not converge rapidly, and only a few are given to indicate the qualitative behaviour of the convergence.

$$A_2 = \begin{bmatrix} 3.0000 & 1.0954 & 0 \\ 1.0954 & 3.0000 & -1.3416 \\ 0 & -1.3416 & 3.0000 \end{bmatrix}, \quad A_3 = \begin{bmatrix} 3.7059 & .9558 & 0 \\ .9558 & 3.5214 & .9738 \\ 0 & .9738 & 1.7727 \end{bmatrix},$$

$$A_7 = \begin{bmatrix} 4.6792 & .2979 & 0 \\ .2979 & 3.0524 & .0274 \\ 0 & .0274 & 1.2684 \end{bmatrix}, \quad A_8 = \begin{bmatrix} 4.7104 & .1924 & 0 \\ .1924 & 3.0216 & -.0115 \\ 0 & -.0115 & 1.2680 \end{bmatrix},$$

$$A_9 = \begin{bmatrix} 4.7233 & .1229 & 0 \\ .1229 & 3.0087 & .0048 \\ 0 & .0048 & 1.2680 \end{bmatrix}, \quad A_{10} = \begin{bmatrix} 4.7285 & .0781 & 0 \\ .0781 & 3.0035 & -.0020 \\ 0 & -.0020 & 1.2680 \end{bmatrix}.$$

The elements in the (1,2) position decrease geometrically with a ratio of about .64 per iterate, and those in the (2,3) position decrease with a ratio of about .42 per iterate. The value in the (3,3) position of A_{15} will be 1.2679, which is correct to five places.

<u>The preliminary reduction of A to simpler form</u> The QR method (9.100) can be relatively expensive because the QR factorization is time consuming when repeated many times. To decrease the expense the matrix is prepared for the QR method by reducing it to a simpler form, one for which the QR factorization is much less expensive.

If A is symmetric, it is reduced to a similar symmetric tridiagonal matrix exactly as described in §9.3. If A is nonsymmetric, it is reduced to a similar *Hessenberg matrix*. A matrix B is Hessenberg if

$$b_{ij} = 0, \qquad \text{for all } i>j+1. \tag{9.5.4}$$

It is upper triangular except for a single nonzero subdiagonal. The matrix A is reduced to Hessenberg form using the same algorithm as was used for reducing symmetric matrices to tridiagonal form.

With A tridiagonal or Hessenberg, the Householder matrices of §9.3 take a simple form when calculating the QR factorization. But generally the plane rotations (9.3.28) are used in place of the Householder matrices because they are more efficient to compute and apply in this situation. Having produced $A_1=Q_1R_1$ and $A_2=R_1Q_1$, we need to know that the form of A_2 is the same as that of A_1 in order to continue using the less expensive form of QR factorization.

Suppose A_1 is in the Hessenberg form. From §9.3 the factorization $A_1=Q_1R_1$ has the following value of Q_1:

$$Q_1 = H_1 \dots H_{n-1}, \qquad (9.5.10)$$

with each H_k a Householder matrix (9.3.12):

$$H_k = I-2w^{(k)}w^{(k)T}, \qquad 1 \le k \le n-1. \qquad (9.5.11)$$

Because the matrix A_1 is of Hessenberg form, the vectors $w^{(k)}$ can be shown to have the special form

$$w_i^{(k)}=0 \text{ for } i<k \text{ and } i>k+1. \qquad (9.5.12)$$

This can be shown from the equations for the components of $w^{(k)}$, and in particular (9.3.10). From (9.5.12), the matrix H_k will differ from the identity in only the four elements in positions (k,k), $(k,k+1)$, $(k+1,k)$, and $(k+1,k+1)$. And from this it is a fairly straightforward computation to show that Q_1 must be Hessenberg in form. Another necessary lemma is that the product of an upper triangular matrix and a Hessenberg matrix is again

Hessenberg. Just multiply the two forms of matrices, observing the respective patterns of zeros, in order to prove this lemma. Combining these results, observing that R_1 is upper triangular, we have that $A_2=R_1Q_1$ must be in Hessenberg form.

If A_1 is symmetric and tridiagonal, then it is trivially Hessenberg. From the preceding result, A_2 must also be Hessenberg. But A_2 is symmetric since

$$A_2^T = (Q_1^T A_1 Q_1)^T = Q_1^T A_1^T Q_1 = Q_1^T A_1 Q_1 = A_2.$$

Since any symmetric Hessenberg matrix is tridiagonal, we have shown that A_2 is tridiagonal. Note that the iterates in the example (9.5.8) illustrate this result.

A convergence result for the QR method A convergence result is given for a large class of matrices, symmetric and nonsymmetric. Part of the proof will show the factor which determines the speed of convergence of the method. For a more general discussion of the method, see Golub-Van Loan (1983, §7.5, §8.2), Parlett (1968), Parlett (1980, Chap. 8), and Wilkinson (1965, Chap. 8).

Theorem 9.6 Let A be a real matrix of order n, and let its eigenvalues $\{\lambda_i\}$ satisfy

$$|\lambda_1| > |\lambda_2| > \dots > |\lambda_n| > 0. \qquad (9.5.13)$$

Then the iterates A_m of the QR method, defined in (9.5.1), will converge to an upper triangular matrix which contains the eigenvalues $\{\lambda_i\}$ in the diagonal positions. If A is symmetric, the sequence $\{A_m\}$ converges to a diagonal matrix.

Proof. The proof is fairly lengthy and involved, and the reader may wish to skip it and go onto the discussion following the proof. The main factor in determining the speed of convergence is contained in (9.5.19), and it is illustrated following the proof. This proof follows closely that of Wilkinson (1965. pp. 517-519).

Since A has distinct eigenvalues, there is a nonsingular matrix X for which

$$X^{-1}AX = D = \text{diag}[\lambda_1,\ldots,\lambda_n]. \qquad (9.5.14)$$

Then

$$A^m = XD^mX^{-1}. \qquad (9.5.15)$$

Since A is real and all of its eigenvalues are of distinct magnitude, it cannot have any complex roots, as they would have to occur in conjugate pairs of equal magnitude.

The next few paragraphs will derive some alternative forms for A^m, based on modifying (9.5.15). Assume X^{-1} has the decomposition

$$X^{-1} = LU. \qquad (9.5.16)$$

For the appropriate modification to use when this is not possible and pivoting must be used, see Wilkinson (1965, p. 519). Combining (9.5.15) and (9.5.16),

$$A^m = X(D^mLD^{-m})D^mU. \qquad (9.5.17)$$

Recall that in the derivation of the decomposition (9.5.16) in §8.1 of Chapter 8, the diagonal elements of L could be chosen to be 1. Then the matrix D^mLD^{-m} is lower triangular with diagonal elements equal to 1, and

$$(D^mLD^{-m})_{ij} = \left(\frac{\lambda_i}{\lambda_j}\right)^m L_{ij}, \qquad 1 \le j < i \le n. \qquad (9.5.18)$$

Define E_m implicitly by

$$D^m L D^{-m} = I + E_m.$$

E_m is a lower triangular matrix which converges to zero: using (9.5.18) and (9.5.13),

$$\|E_m\|_\infty \le c \cdot \underset{1 \le j \le n-1}{\text{Maximum}} \left| \frac{\lambda_{j+1}}{\lambda_j} \right|^m , \qquad m \ge 1, \qquad (9.5.19)$$

for some constant $c > 0$.

The matrix X can be factored.

$$X = QR,$$

for some orthogonal Q and nonsingular upper triangular R. Returning to (9.5.17), this leads to

$$\begin{aligned} A^m &= QR(I+E_m)D^m U \\ &= Q(I+RE_m R^{-1})RD^m U. \end{aligned} \qquad (9.5.20)$$

Using another QR factorization,

$$I+RE_m R^{-1} = \tilde{Q}_m \tilde{R}_m. \qquad (9.5.21)$$

We require the diagonal elements of R_m to be positive, which is possible from the construction for the factorization given in §8.3. Also see the discussion between (9.3.15) and (9.3.16), which shows that with this positivity assumption, the decomposition (9.5.21) is unique.

We can show that

$$\tilde{Q}_m, \tilde{R}_m \longrightarrow I \quad \text{as } m \to \infty. \qquad (9.5.22)$$

Using (9.5.21) and (9.5.19), it is straightforward to show that

$$\tilde{R}_m^T \tilde{R}_m - I \longrightarrow 0 \qquad \text{as } m \to \infty.$$

A detailed examination of the coefficients of $\tilde{R}_m^T \tilde{R}_m$ will then show that $\tilde{R}_m \to I$, using the positivity of the diagonal elements. Using this result in (9.5.21) will then show $\tilde{Q}_m \to I$.

Using (9.5.21) in (9.5.20),

$$A^m = (Q\tilde{Q}_m)(\tilde{R}_m R D^m U). \qquad (9.5.23)$$

Clearly $Q\tilde{Q}_m$ is orthogonal. And because $\tilde{R}_m$, R, U are upper triangular and D^m is diagonal, we have their product is upper triangular. Thus (9.5.23) is a QR factorization of A^m. Returning to (9.5.7), we have the second QR factorization

$$A^m = P_m U_m$$

Comparing these results and using the uniqueness of the QR factorization expressed in (9.3.15) and (9.3.16), we have

$$P_m = (Q\tilde{Q}_m)\tilde{D}_m, \qquad U_m = \tilde{D}_m(\tilde{R}_m R D^m U), \qquad (9.5.24)$$

for some diagonal matrix $\tilde{D}_m$ with

$$\tilde{D}_m^2 = I, \qquad m \geq 1. \qquad (9.5.25)$$

We now examine the behavior of the sequence $\{A_m\}$ as $m \to \infty$. From (9.5.5) and (9.5.24),

$$\begin{aligned} A_{m+1} &= P_m^T A P_m \\ &= \tilde{D}_m \tilde{Q}_m^T Q^T A Q \tilde{Q}_m \tilde{D}_m \end{aligned}$$

From earlier X=QR, and

$$Q = XR^{-1}$$

$$Q^T = Q^{-1} = RX^{-1}.$$

Substituting above,

$$\begin{aligned} A_{m+1} &= \tilde{D}_m^T \tilde{Q}_m^T R X^{-1} A X R^{-1} \tilde{Q}_m \tilde{D}_m \\ &= \tilde{D}_m^T \tilde{Q}_m^T R D R^{-1} \tilde{Q}_m \tilde{D}_m \end{aligned} \qquad (9.5.26)$$

Consider just the diagonal elements of A_{m+1} since they are the main point of interest. The matrix RDR^{-1} is upper triangular and its diagonal elements are just $\{\lambda_1, \ldots, \lambda_n\}$. Using (9.5.22) and (9.5.25), that $\tilde{Q}_m \to I$ and $\tilde{D}_m^2 = I$, we will then have the diagonal elements of A_{m+1} will converge to the eigenvalues of A, ordered from largest to smallest in magnitude. In addition, since RDR^{-1} is upper triangular, the elements below the diagonal in A_{m+1} will converge to zero. The speed of convergence will depend completely on the speed of convergence of $\tilde{Q}_m$ to I; and this depends on the bound in (9.5.19).

If A is symmetric, then the iterates A_m are also symmetric. Since the lower triangular part of A_m converges to zero, the same is true of the part above the diagonal. This proves that for a symmetric matrix satisfying (9.5.13), A_m converges to a diagonal matrix. This completes the proof. ■

As pointed out in the proof, the critical factor in determining the speed of convergence are the ratios λ_{j+1}/λ_j, $1 \le j \le n-1$. Thus there is a geometric rate of convergence, and this can be very slow. In the example (9.5.8), the ratios of successive eigenvalues are

$$\frac{\lambda_2}{\lambda_1} \doteq 0.63, \qquad \frac{\lambda_3}{\lambda_2} \doteq 0.42.$$

And if the off-diagonal elements are observed, we see that they decrease with about these ratios.

For matrices whose eigenvalues do not satisfy (9.5.13), the iterates A_m may not converge to a triangular matrix. For A symmetric, the sequence $\{A_m\}$ will converge to a block diagonal matrix

$$A_m \longrightarrow D = \begin{bmatrix} B_1 & & & 0 \\ & B_2 & & \\ & & \ddots & \\ 0 & & & B_r \end{bmatrix}, \tag{9.5.27}$$

in which all blocks B_i have order 1 or 2. Thus the eigenvalues of A can be easily computed from those of D. If A is real and nonsymmetric, the situation is more complicated, but acceptable. For a discussion, see Wilkinson (1965, Chap. 8) and Parlett (1968).

To see that $\{A_m\}$ does not always converge to a diagonal matrix, consider the simple symmetric example

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

Its eigenvalues are $\lambda=\pm1$. Since A is orthogonal, we have

$$A = Q_1R_1 \qquad \text{with } Q_1 = A, \quad R_1 = I.$$

And thus

$$A_2 = R_1Q_1 = A,$$

and all iterates $A_m=A$. The sequence $\{A_m\}$ does not converge to a diagonal matrix.

<u>The QR method with shift</u> The QR algorithm is generally applied with a shift of origin for the eigenvalues in order to increase the speed of convergence. For a sequence of constants $\{c_m\}$, define $A_1=A$ and

$$\begin{aligned} A_m-c_mI &= Q_mR_m, \\ A_{m+1} &= c_mI + R_mQ_m, \qquad m=1,2,\ldots \end{aligned} \tag{9.5.28}$$

The matrices A_m are similar to A_1, since

$$R_m = Q_m^T(A_m - c_m I)$$

$$A_{m+1} = c_m I + Q_m^T(A_m - c_m I)Q_m$$

$$= c_m I + Q_m^T A_m Q_m - c_m I,$$

$$A_{m+1} = Q_m^T A_m Q_m, \qquad m \geq 1. \tag{9.5.29}$$

The eigenvalues of A_{m+1} are the same as those of A_m, and thence the same as those of A.

To be more specific on the choice of shifts $\{c_m\}$, we will consider only a symmetric tridiagonal matrix A. For A_m, let

$$A_m = \begin{bmatrix} \alpha_1^{(m)} & \beta_1^{(m)} & 0 & \cdots & 0 \\ \beta_1^{(m)} & \alpha_2^{(m)} & \beta_2^{(m)} & & \vdots \\ 0 & & \ddots & & \\ \vdots & & & \ddots & \beta_{n-1}^{(m)} \\ 0 & \cdots & \cdots & \beta_{n-1}^{(m)} & \alpha_n^{(m)} \end{bmatrix} \tag{9.5.30}$$

There are two methods by which $\{c_m\}$ is chosen: (1) Let $c_m = \alpha_n^{(m)}$; and (2) let c_m be the eigenvalue of

$$\begin{bmatrix} \alpha_{n-1}^{(m)} & \beta_{n-1}^{(m)} \\ \beta_{n-1}^{(m)} & \alpha_n^{(m)} \end{bmatrix} \tag{9.5.31}$$

which is closest to $\alpha_n^{(m)}$. The second strategy is preferred; but in either case the matrices A_m converge to a block diagonal matrix in which the blocks have order 1 or 2, as in (9.5.27). It can be shown that either choice of $\{c_m\}$ ensures

$$\beta_{n-1}^{(m)}\beta_{n-2}^{(m)} \longrightarrow 0 \quad \text{as } n \to \infty, \tag{9.5.32}$$

generally at a much more rapid rate than with the original QR method (9.5.1).

From (9.5.29),

$$\|A_{m+1}\|_2 = \|Q_m^T A_m Q_m\|_2 = \|A_m\|_2.$$

using the operator matrix norm (7.3.19) and problem 27(c) of Chapter 7. The matrices $\{A_m\}$ are uniformly bounded, and consequently the same is true of their elements. From (9.5.32) and the uniform boundedness of $\{\beta_{n-1}^{(m)}\}$ and $\{\beta_{n-2}^{(m)}\}$, we have either $\beta_{n-1}^{(m)}\to 0$ or $\beta_{n-2}^{(m)}\to 0$ as $m\to\infty$. In the former case, $\alpha_n^{(m)}$ converges to an eigenvalue of A. And in the latter case, two eigenvalues can easily be extracted from the limit of the submatrix (9.5.31).

Once one or two eigenvalues have been obtained due to $\beta_{n-1}^{(m)}$ or $\beta_{n-2}^{(m)}$ being essentially zero, the matrix A_m can be reduced in order by one or two rows, respectively. Following this, the QR method with shift can be applied to the reduced matrix. The choice of shifts is designed to make the convergence to zero be more rapid for $\beta_{n-1}^{(m)}\beta_{n-2}^{(m)}$ than for the remaining off-diagonal elements of the matrix. In this way, the QR method becomes a rapid general purpose method, faster than any other method at the present time. For a proof of convergence of the QR method with shift, see Wilkinson (1968). For a much more complete discussion of the QR method, including the choice of a shift, see Parlett (1980, Chap. 8)

<u>Example</u>. Use the previous example (9.5.8), and use the first method of choosing the shift, $c_m=\alpha_n^{(m)}$. The iterates are

$$A_1 = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 3 & 1 \\ 0 & 1 & 4 \end{bmatrix}, \qquad A_2 = \begin{bmatrix} 1.4000 & .4899 & \\ .4899 & 3.2667 & .7454 \\ 0 & .7454 & 4.3333 \end{bmatrix}$$

$$A_3 = \begin{bmatrix} 1.2915 & .2017 & 0 \\ .2017 & 3.0202 & .2724 \\ 0 & .2724 & 4.6884 \end{bmatrix}, \qquad A_4 = \begin{bmatrix} 1.2737 & .0993 & 0 \\ .0993 & 2.9943 & .0072 \\ 0 & .0072 & 4.7320 \end{bmatrix}$$

$$A_5 = \begin{bmatrix} 1.2694 & .0498 & 0 \\ .0498 & 2.9986 & 0 \\ 0 & 0 & 4.7321 \end{bmatrix}.$$

The element $\beta_2^{(m)}$ converges to zero extremely rapidly, but the element $\beta_1^{(m)}$ converges to zero geometrically with a ratio of only about 0.5.

Mention should be made of the antecedent to the QR method, motivating much of it. In 1958, H. Rutishauser introduced an LR method based on the Gaussian elimination decomposition of a matrix into a lower triangular matrix times an upper triangular matrix. Define

$$A_m = L_m R_m, \qquad A_{m+1} = R_m L_m = L_m^{-1} A_m L_m$$

with L_m lower triangular, R_m upper triangular. When applicable, this method will generally be more efficient than the QR method. But the non-orthogonal similarity transformations can cause a deterioration of the conditioning of the eigenvalues of some non-symmetric matrices. And generally it is a more complicated algorithm to implement in an automatic program. A complete discussion is given in Wilkinson (1965, Chap. 8).