The QR Transformation

A Unitary Analogue to the LR Transformation—Part 1

By J. G. F. Francis*

The LR transformation, due to Rutishauser, has proved to be a powerful method for finding the eigenvalues of symmetric band matrices. Little attention, however, has been paid to its application to the more difficult problem of finding eigenvalues of general unsymmetric matrices. If the matrices are large two important difficulties are likely to occur. Firstly, triangular decomposition, which is the basis of the method, is by no means always numerically stable, and secondly, the amount of computation required by the method is likely to be very great. This paper describes an algorithm similar to the LR transformation except that the transformations involved in it are all unitary and can thus be expected to be numerically stable. It is then shown that there are various advantages in first converting the matrix to almost-triangular form; in particular, the amount of work involved in the algorithm can then be greatly reduced.

Part 1 of the paper† is largely concerned with proof of convergence, and the theoretical aspect. Part 2, to be published in January, discusses practical computation and gives results of experiments.

1. Introduction

There is a wide-spread belief that the similarity transformation of matrices by unitary transformations should show particular numerical stability when used in computing their eigenvalues. A sense in which this is true has recently been proved by Fike (1959). It may well be that, in practice, if we can replace 2×2 unitary matrices in a calculation by elementary transformations (including permutations of rows and columns), we should do so and expect equally good results for much less work. However, the attraction of unitary transformations and rotations remains, based partly on the success of their application to finding eigenvalues of symmetric matrices and partly on their suitability for mathematical analysis.

Whenever it is possible, a valuable way of regarding many methods for finding eigenvalues is to consider the similarity transformation on the matrix implied by the method. This transformation often causes a concentration of information about the eigenvalues by a process involving elimination of elements in the matrix. When the LR transformation developed by Rutishauser (1958) is looked at in this way, we see it as a series of similarity transformations on the matrix, each of which consists of the pre-multiplication by a matrix which eliminates the subdiagonal elements, and the post-multiplication by its inverse.

The transformation matrices used by Rutishauser are triangular. In this paper it is proved that the transformations can be unitary, and the *QR transformation*, as I have (somewhat arbitrarily) named this modification of Rutishauser's algorithm, is shown to be particularly suitable for unsymmetric matrices which are first reduced to almost-triangular form.

In the present part of the paper we are concerned with QR transformation from a theoretical point of view; in Part 2 I shall outline a practical program and give experimental results.

Statement of the LR Transformation

Rutishauser (1958, and in other papers) has described an iterative procedure for finding the eigenvalues of a wide class of matrices. The method consists of forming a sequence of matrices $A^{(k)}$ where $A^{(1)} = A$ the original matrix, and $A^{(k+1)}$ is derived from $A^{(k)}$ by decomposing it into lower and upper triangular matrices, $L^{(k)}$ and $R^{(k)}$, and forming the product of these in the reversed order. Thus:

$$A^{(k)} = L^{(k)}R^{(k)}$$
$$A^{(k+1)} = R^{(k)}L^{(k)}.$$

It can readily be seen that the process consists of a series of similarity transformations on the original matrix:

$$A^{(k+1)} = L^{(k)-1}A^{(k)}L^{(k)}$$
$$= L^{(k)-1}L^{(k-1)-1} \ldots L^{(1)-1}A\,L^{(1)}L^{(2)} \ldots L^{(k)}.$$

Rutishauser shows that if certain conditions are fulfilled then, as $k \to \infty$, so $A^{(k)}$ tends to an upper triangular matrix of which the diagonal elements are the eigenvalues in order of modulus, the first being the largest.

The Unitary-Triangular or QR Transformation

It is well known that the triangular decomposition $A = LR$ can lead to gross inaccuracies when a pivotal element r_{ii} of the upper triangular matrix R is small (which can happen even though the determinant of A is not small). Moreover, automatic fixed-point computation of the decomposition is difficult to program as numbers of any magnitude can be generated; also, if a

* Formerly of the National Research Development Corporation.

† Part 1 was originally received on 29 October 1959 and re-submitted, with Part 2, on 6 June 1961.

pivotal element is actually zero then the process breaks down. The conditions for convergence given by Rutishauser (1958, theorem 3) are irrelevant to these difficulties in the early stages of the LR transformation; for example, the conditions can be fulfilled and yet the first element of A may be zero, making triangular decomposition altogether impossible.

Now one way of obtaining the matrix $R = L^{-1}A$ is by elementary transformations which eliminate the sub-diagonal elements of A in turn. This is reminiscent of methods for the triangular reduction of a matrix in inversion or the solution of simultaneous equation; thus we might ask the question whether a more stable method of triangulation can be built into a similar algorithm to the LR transformation. In particular, can we form R from A by either Gaussian elimination with interchange of rows (to select the largest pivot), or else by elimination with unitary transformations? Both these methods [for the first, see Wilkinson (1959*a*)] involve exceptionally little (perhaps minimal) loss of accuracy, and are easy to program in fixed-point arithmetic.

Here we shall confine discussion to the method of unitary transformations. The suggested algorithm is as follows.

The matrix $A^{(k)}$ is decomposed into the product of a unitary matrix $Q^{(k)}$ and an upper triangular matrix $R^{(k)}$. This can be done by pre-multiplying $A^{(k)}$ by a unitary matrix $Q^{(k)*} = (Q^{(k)})^{-1}$ chosen so as to reduce $A^{(k)}$ to an upper triangle. $A^{(k+1)}$ is formed by post-multiplying $R^{(k)}$ by $Q^{(k)}$. Thus

$$A^{(1)} = A$$
$$A^{(k)} = Q^{(k)}R^{(k)}, \quad A^{(k+1)} = R^{(k)}Q^{(k)}, \quad k = 1, 2, \ldots \quad (1)$$

The matrix $Q^{(k)}$ may be found explicitly or may only exist as a product of simple factors.

As in the LR transformation we can also write the algorithm as a similarity transformation:

$$A^{(k+1)} = Q^{(k)*}Q^{(k-1)*} \ldots Q^{(1)*}AQ^{(1)}Q^{(2)} \ldots Q^{(k)}. \quad (2)$$

The unitary-triangular decomposition of any square matrix exists. The diagonal elements of the triangular matrix can always be made real and positive, and if this is so, and the matrix is non-singular, then the decomposition is unique. We shall prove this in theorem 1.

We shall prove below that, if certain conditions are fulfilled, the matrix $A^{(k)}$ tends to an upper triangular matrix as $k \to \infty$, the diagonal elements of which are the eigenvalues of A. We know, *a priori*, by a theorem due to Schur, that any matrix can be reduced to a triangular matrix by a similarity transformation using a suitable unitary matrix.

2. Notation

Small Greek letters denote scalars. Capital letters represent matrices generally with complex elements.

Lower-case letters in bold-face type denote column vectors or the columns of matrices. They usually have a suffix giving their position in an array. The elements of a column or vector appear in light-face type with one more suffix.

If we write a bar over a square matrix we mean the rectangular matrix obtained by omitting its first column. A bar over a vector indicates that we omit its first element.

The conjugate transpose of the matrix A is written A^*; by $\bar{A}^*$ we mean $(\bar{A})^*$. Row vectors always have an asterisk.

The modulus of the scalar λ is written $|\lambda|$ and its complex conjugate $\bar{\lambda}$. The length of the vector $\boldsymbol{a}$, $(\boldsymbol{a}^*\boldsymbol{a})^{\frac{1}{2}}$, is written $||\boldsymbol{a}||$.

The determinant of the matrix A is written $|A|$.

The unit matrix, written I (or I_m if we wish to express its order), has columns $\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_m$. Normally the dimensions of a matrix will be implicit in the context.

If a matrix has a suffix or superfix in brackets the same affix usually appears in brackets with its columns and elements. Thus, for example,

$$A^{(k)} = [\boldsymbol{a}_1^{(k)}, \boldsymbol{a}_2^{(k)}, \ldots] = [a_{ij}^{(k)}]$$
$$\bar{\boldsymbol{B}}_i = [\boldsymbol{b}_{(i)2}, \boldsymbol{b}_{(i)3}, \ldots]$$
and $$\bar{\boldsymbol{c}}_i^{(k)*} = [\bar{c}_{2i}^{(k)}, \bar{c}_{3i}^{(k)}, \ldots].$$

3. Unitary-Triangular Decomposition; the Fundamental LR/QR Theorem

Lemma. For any vector $\boldsymbol{b}$ with say m elements (in general complex) a unitary matrix M exists such that $M^*\boldsymbol{b} = ||\boldsymbol{b}||\boldsymbol{e}_1$. (This implies $\bar{M}^*\boldsymbol{b} = 0$, $\boldsymbol{m}_1^*\boldsymbol{b} = ||\boldsymbol{b}||$.)

When $\boldsymbol{b}$ is zero, M can be any unitary matrix. We will consider $\boldsymbol{b} \neq \boldsymbol{0}$, in which case the first column of M is uniquely determined.

We mean by an elementary unitary matrix one that differs from the unit matrix at most in one principal 2×2 submatrix. This submatrix (say of the matrix T) has the general form:

$$\begin{bmatrix} t_{ii} & t_{ij} \\ t_{ji} & t_{jj} \end{bmatrix} = \begin{bmatrix} e^{i\alpha}\cos\theta & -e^{i\beta}\sin\theta \\ e^{i\gamma}\sin\theta & e^{i\delta}\cos\theta \end{bmatrix}$$

where α, β, γ, δ and θ are real and $\alpha - \beta - \gamma + \delta \equiv 0 \pmod{2\pi}$.

A unitary matrix M^*, such that $M^*\boldsymbol{b} = ||\boldsymbol{b}||\boldsymbol{e}_1$, can conveniently be constructed out of a series of elementary unitary matrices, $M^* = T_m T_{m-1} \ldots T_1$. If $\boldsymbol{b}$ is multiplied in turn by the T_r, then T_1 makes the first element b_1 of $\boldsymbol{b}$ real and non-negative, and the other transformations eliminate in turn the remaining elements b_r $(r = 2, 3, \ldots, m)$.

We define $T_r = I$ if $b_p = 0$ for all $p \leqslant r$. Otherwise the elements of T_r are given by $t_{ij}^{(r)} = \delta_{ij}$, except for $t_{r1}^{(r)}$, $t_{1r}^{(r)}$, $t_{11}^{(r)}$ and $t_{rr}^{(r)}$.

For $r = 1$, $t_{11}^{(1)} = \dfrac{\bar{b}_1}{|b_1|}$ (T_1 is a diagonal matrix);

for $r = 2, 3, \ldots, m$, $\quad t_{11}^{(r)} = t_{rr}^{(r)} = \left(1 - \dfrac{|b_r|^2}{\sum_{p \leqslant r} |b_p|^2}\right)^{\frac{1}{2}}$

$$t_{r1}^{(r)} = -\,\bar{t}_{1r}^{(r)} = \frac{-b_r}{(\sum_{p \leqslant r} |b_p|^2)^{\frac{1}{2}}}.$$

(Expressed in the general form above, the non-trivial submatrices of the $\boldsymbol{T}_r$ each have $\alpha = \delta = 0$ and $-\pi/2 \leqslant \theta \leqslant \pi/2$ with the exception of $\boldsymbol{T}_1$ for which α is not necessarily zero.)

The first column, $\boldsymbol{m}_1$, of $\boldsymbol{M}$ is unique for since

$$\boldsymbol{M}^*\boldsymbol{b} = ||\boldsymbol{b}||\boldsymbol{e}_1$$

we have $\qquad \boldsymbol{M}\boldsymbol{e}_1 = \boldsymbol{m}_1 = \dfrac{1}{||\boldsymbol{b}||}\,.\,\boldsymbol{b}.$

Later we will refer to the above procedure for forming $\boldsymbol{M}$, but for complete generality, $\overline{\boldsymbol{M}}$, the rectangular matrix consisting of all but the first column of $\boldsymbol{M}$, can be replaced by $\overline{\boldsymbol{M}}\boldsymbol{G}$, where $\boldsymbol{G}$ is any unitary matrix of order $m - 1$.

We can now prove:

THEOREM 1. *For any matrix $\boldsymbol{A}$ (of order n, say)† there exists a unitary matrix $\boldsymbol{Q}$ such that $\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{R}$ where $\boldsymbol{R}$ is an upper (right) triangular matrix which has real, non-negative, diagonal elements. Moreover, $\boldsymbol{Q}$ is unique if $\boldsymbol{A}$ is non-singular.*

PROOF. By the lemma we can transform $\boldsymbol{A}$ so as to eliminate the subdiagonal elements column by column starting on the left, and thus reduce it to a triangle.

We define $\boldsymbol{B}_1 = \boldsymbol{A}$ and form $\boldsymbol{B}_{i+1} = \overline{\boldsymbol{M}}_i^*\overline{\boldsymbol{B}}_i$ for $i = 1, 2, \ldots n - 1$ (the bars indicate omission of first row of $\boldsymbol{M}_i^*$ and column of $\boldsymbol{B}_i$). $\boldsymbol{M}_i$ is determined for $i = 1, 2, \ldots, n$ such that $\boldsymbol{M}_i^*\boldsymbol{b}_{(i)1} = ||\boldsymbol{b}_{(i)1}||\boldsymbol{e}_1$ (where $\boldsymbol{b}_{(i)1}$ is the first column of $\boldsymbol{B}_i$).

If $\boldsymbol{N}_i = \begin{bmatrix} \boldsymbol{I}_{i-1} & 0 \\ 0 & \boldsymbol{M}_i \end{bmatrix}$, where $\boldsymbol{M}_i$ is of order $n - i + 1$, then $\boldsymbol{N}_n^*\boldsymbol{N}_{n-1}^* \ldots \boldsymbol{N}_1^*\boldsymbol{A} = \boldsymbol{R}$, where $r_{ii} = ||\boldsymbol{b}_{(i)1}||$ and $r_{ij} = 0$ for $i > j$.

Thus, if $\boldsymbol{Q} = \boldsymbol{N}_1\boldsymbol{N}_2 \ldots \boldsymbol{N}_n$, we have $\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{R}$ as in the theorem.

Now suppose that we have two unitary-triangular decompositions $\boldsymbol{A} = \boldsymbol{Q}_1\boldsymbol{R}_1 = \boldsymbol{Q}_2\boldsymbol{R}_2$. If $\boldsymbol{A}$ is non-singular then so are $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$; we then have $\boldsymbol{R}_1\boldsymbol{R}_2^{-1} = \boldsymbol{Q}_1^*\boldsymbol{Q}_2$ and, as $\boldsymbol{Q}_1^*\boldsymbol{Q}_2$ is unitary, $(\boldsymbol{R}_1\boldsymbol{R}_2^{-1})^{-1} = (\boldsymbol{R}_1\boldsymbol{R}_2^{-1})^*$, which shows that $\boldsymbol{R}_1\boldsymbol{R}_2^{-1}$ is diagonal, since the left-hand side is upper-triangular and the right-hand side lower-triangular. Furthermore, if we consider the diagonal, $r_{(2)ii}/r_{(1)ii} = \bar{r}_{(1)ii}/\bar{r}_{(2)ii}$ and therefore, as the $r_{(1)ii}$ and $r_{(2)ii}$ are real and positive, $r_{(1)ii} = r_{(2)ii}$. Hence $\boldsymbol{R}_1\boldsymbol{R}_2^{-1} = \boldsymbol{I}$ and so $\boldsymbol{Q}_1 = \boldsymbol{Q}_2$ and $\boldsymbol{Q}$ is unique.

The above proof effectively gives a method for performing the first half of one step of the algorithm (1); the step would be completed by post-multiplying the triangular matrix $\boldsymbol{R}$ by the matrices $\boldsymbol{N}_1, \boldsymbol{N}_2, \ldots, \boldsymbol{N}_n$ in turn.

We now obtain a similar result to the fundamental theorem 1 of Rutishauser (1958).

Equation (2) gives $\boldsymbol{Q}^{(1)} \ldots \boldsymbol{Q}^{(k-1)}\boldsymbol{A}^{(k)} = \boldsymbol{A}\boldsymbol{Q}^{(1)} \ldots \boldsymbol{Q}^{(k-1)}$ and, as $\boldsymbol{A}^{(k)} = \boldsymbol{Q}^{(k)}\boldsymbol{R}^{(k)}$, we have

$$\boldsymbol{Q}^{(1)} \ldots \boldsymbol{Q}^{(k)}\boldsymbol{R}^{(k)} = \boldsymbol{A}\boldsymbol{Q}^{(1)} \ldots \boldsymbol{Q}^{(k-1)}$$
$$\boldsymbol{Q}^{(1)} \ldots \boldsymbol{Q}^{(k-1)}\boldsymbol{R}^{(k-1)} = \boldsymbol{A}\boldsymbol{Q}^{(1)} \ldots \boldsymbol{Q}^{(k-2)}$$

and so on.

If we write $\boldsymbol{P}^{(k)} = \boldsymbol{Q}^{(1)}\boldsymbol{Q}^{(2)} \ldots \boldsymbol{Q}^{(k)}$
and $\boldsymbol{S}^{(k)} = \boldsymbol{R}^{(k)}\boldsymbol{R}^{(k-1)} \ldots \boldsymbol{R}^{(1)}$
then
$$\begin{aligned}\boldsymbol{P}^{(k)}\boldsymbol{S}^{(k)} &= \boldsymbol{Q}^{(1)}\boldsymbol{Q}^{(2)} \ldots \boldsymbol{Q}^{(k)}\boldsymbol{R}^{(k)}\boldsymbol{R}^{(k-1)} \ldots \boldsymbol{R}^{(1)} \\ &= \boldsymbol{A}\boldsymbol{Q}^{(1)} \ldots \boldsymbol{Q}^{(k-1)}\boldsymbol{R}^{(k-1)} \ldots \boldsymbol{R}^{(1)} \\ &= \boldsymbol{A}^2\boldsymbol{Q}^{(1)} \ldots \boldsymbol{Q}^{(k-2)}\boldsymbol{R}^{(k-2)} \ldots \boldsymbol{R}^{(1)}\end{aligned}$$

and by repeated substitution we get $\boldsymbol{P}^{(k)}\boldsymbol{S}^{(k)} = \boldsymbol{A}^k$.

Since $\boldsymbol{P}^{(k)}$ is unitary and $\boldsymbol{S}^{(k)}$ is triangular, and the unitary-triangular decomposition of a non-singular matrix is unique (by theorem 1), we obtain:

THEOREM 2. *If $\boldsymbol{A}$ is non-singular, the matrix $\boldsymbol{P}^{(k)} = \boldsymbol{Q}^{(1)} \ldots \boldsymbol{Q}^{(k)}$, such that $\boldsymbol{A}^{(k+1)} = \boldsymbol{P}^{(k)*}\boldsymbol{A}\boldsymbol{P}^{(k)}$ can be derived from the unitary-triangular decomposition of $\boldsymbol{A}^k$, viz. $\boldsymbol{A}^k = \boldsymbol{P}^{(k)}\boldsymbol{S}^{(k)}$.*

The first step in the proof of the convergence of the method is an analysis of the triangulation of $\boldsymbol{A}^k$.

4. The Analysis of $\boldsymbol{A}^k = \boldsymbol{P}^{(k)}\boldsymbol{S}^{(k)}$, Convergence

We shall now assume that $\boldsymbol{A}$ is non-singular and that its eigenvalues have distinct moduli.

As in the proof of theorem 1, since $\boldsymbol{P}^{(k)*}$ triangulates $\boldsymbol{A}^k$, we can write $\boldsymbol{P}^{(k)} = \boldsymbol{N}_1^{(k)}\boldsymbol{N}_2^{(k)} \ldots \boldsymbol{N}_n^{(k)}$, where $\boldsymbol{N}_i^{(k)} = \begin{bmatrix} \boldsymbol{I}_{i-1} & 0 \\ 0 & \boldsymbol{M}_i^{(k)} \end{bmatrix}$ and the matrices $\boldsymbol{M}_i^{(k)}$ are given by the equations:

$$\begin{aligned}&\boldsymbol{M}_i^{(k)*}\boldsymbol{b}_{(i)1}^{(k)} = ||\boldsymbol{b}_{(i)1}^{(k)}||\boldsymbol{e}_1 \\ &\boldsymbol{B}_{i+1}^{(k)} = \overline{\boldsymbol{M}}_i^{(k)*}\overline{\boldsymbol{B}}_i^{(k)} \qquad \text{and } \boldsymbol{B}_1^{(k)} = \boldsymbol{A}^k.\end{aligned} \tag{3}$$

(Note that the superfix (k) gives the stage of the QR transformation and the suffix i the stage of the triangulation.)

Now let us assume that at some value of i

$$\boldsymbol{B}_i^{(k)} = \boldsymbol{Y}_i^{(k)}\boldsymbol{\Lambda}_i^k\boldsymbol{X}_i^* \tag{4}$$

where $\boldsymbol{Y}_i^{(k)}$ and $\boldsymbol{X}_i$ (which is independent of k) are non-singular matrices of order $m = n - i + 1$ and $\boldsymbol{\Lambda}_i$ is a diagonal matrix whose elements are some particular selection of m eigenvalues of $\boldsymbol{A}$. The ordering of the $\lambda_{(i)r}$, $\boldsymbol{x}_{(i)r}$ and $\boldsymbol{y}_{(i)r}^{(k)}$ is as yet undetermined.

Temporarily omitting the suffix i we have

$$\boldsymbol{B}^{(k)} = \boldsymbol{Y}^{(k)}\boldsymbol{\Lambda}^k\boldsymbol{X}^* = \sum_{r=1}^{m} \lambda_r^k\boldsymbol{y}_r^{(k)}\boldsymbol{x}_r^* \tag{5}$$

and therefore $\boldsymbol{b}_1^{(k)} = \sum_{r=1}^{m} \lambda_r^k\bar{x}_{1r}\boldsymbol{y}_r^{(k)}$.

† Subsequently we will assume that the matrix $\boldsymbol{A}$ has order n.

From (3), $\overline{M}^{(k)*}\ b_1^{(k)} = 0$

so that
$$\sum_{r=1}^{m} \lambda_r^k \bar{x}_{1r} \overline{M}^{(k)*} y_r^{(k)} = 0. \tag{6}$$

We now use the condition on the eigenvalues of A. Because of subsequent considerations of convergence we arrange the λ_r, x_r and $y_r^{(k)}$ so that λ_1 is the largest (in modulus) of the λ_r for which $x_{1r} \neq 0$ (we can certainly make this choice since X is non-singular).

Thus, from (6), we obtain:

$$\lambda_1^k \overline{M}^{(k)*} y_1^{(k)} = -\sum_{r=2}^{m} \lambda_r^k \frac{\bar{x}_{1r}}{\bar{x}_{11}} \overline{M}^{(k)*} y_r^{(k)}. \tag{7}$$

Defining $\bar{x}_r$ as the $(m-1)$-vector containing all but the first element of x_r we have, from (5),

$$\bar{B}^{(k)} = \sum_{r=1}^{m} \lambda_r^k y_r^{(k)} \bar{x}_r^* \quad \text{and} \quad \overline{M}^{(k)*} \bar{B}^{(k)} = \sum_{r=1}^{m} \lambda_r^k \overline{M}^{(k)*} y_r^{(k)} \bar{x}_r^*$$

which, with (7), gives

$$\overline{M}^{(k)*} \bar{B}^{(k)} = \sum_{r=2}^{m} \lambda_r^k \overline{M}^{(k)*} y_r^{(k)} \left[\bar{x}_r - \frac{x_{1r}}{x_{11}} \bar{x}_1 \right]^*.$$

Thus, since $B_{i+1}^{(k)} = \overline{M}_i^{(k)*} \bar{B}_i^{(k)}$ we can write

$$B_{i+1}^{(k)} = Y_{i+1}^{(k)} \Lambda_{i+1}^k X_{i+1}^* \tag{8}$$

where, for $r = 2, 3, \ldots, m$:

$$\left.\begin{aligned} x_{(i+1)r-1} &= \bar{x}_{(i)r} - \frac{x_{(i)1r}}{x_{(i)11}} \bar{x}_{(i)1} \\ y_{(i+1)r-1}^{(k)} &= \overline{M}_i^{(k)*} y_{(i)r}^{(k)} \\ \lambda_{(i+1)r-1} &= \lambda_{(i)r}. \end{aligned}\right\} \tag{9}$$

Hence $B_{i+1}^{(k)}$ has the same form as $B_i^{(k)}$. Neither X_{i+1} nor $Y_{i+1}^{(k)}$, which are square and of order $m-1$, can be singular since, in (8), $B_{i+1}^{(k)}$ and Λ_{i+1}^k are non-singular. This is clearly true because $|A^k| = |B_{i+1}^{(k)}| \cdot \prod_{r=1}^{i} ||b_{(r)1}^{(k)}||$ and $|A| \neq 0$.

At this stage in the analysis we also define $\lambda_i = \lambda_{(i)1}$.

Now, as there are no equal eigenvalues, A may be diagonalized and $U^*AV = \Lambda$, where V and $U^* = V^{-1}$ are the matrices of right and left eigenvectors. We therefore put $B_1^{(k)} = A^k = V\Lambda^k U^*$, and define $Y_1^{(k)} = Y_1 = V$, $X_1 = U$ and $\Lambda_1 = \Lambda$, and thus have, by induction, an analysis of the triangulation of A^k.

In this analysis the order $\lambda_1, \lambda_2, \ldots, \lambda_n$; $u_1, u_2, \ldots, u_n$ and $v_1, v_2, \ldots, v_n$ has been determined by the nature of $X_1 = U$. It is quite easily verified that the order is such that, for each i, the minor

$$\rho_i = \begin{vmatrix} u_{11} & u_{12} \ldots u_{1i} \\ u_{21} & u_{22} \ldots u_{2i} \\ \cdot & \\ \cdot & \\ \cdot & \\ u_{i1} & u_{i2} \ldots u_{ii} \end{vmatrix}$$

is non-zero and λ_i is the largest in modulus of the λ_j, $j > i-1$, such that this is so.

The matrix X_{i+1} is derived from X_i thus:

$$X_i \begin{bmatrix} 1 & \eta_2 & \eta_3 & \ldots & \eta_m \\ & 1 & & & \\ & & 1 & & 0 \\ & & & \ddots & \\ & 0 & & & 1 \end{bmatrix} = \begin{bmatrix} x_{(i)11} & 0 \ldots 0 \\ x_{(i)21} & \\ \cdot & \\ \cdot & \quad X_{i+1} \\ \cdot & \\ x_{(i)m1} & \end{bmatrix}$$

where $\eta_r = -\dfrac{x_{(i)1r}}{x_{(i)11}}$, so we have $\rho_i = \prod_{r=1}^{i} x_{(i)11}$.

The Convergence of $Q^{(k)}$

Let us suppose that we have a set of matrices

$$N_i^{(k-1)} = \begin{bmatrix} I_{i-1} & 0 \\ 0 & M_i^{(k-1)} \end{bmatrix}$$

such that, if $P^{(k-1)} = N_1^{(k-1)} N_2^{(k-1)} \ldots N_n^{(k-1)}$, then $P^{(k-1)*} A^{k-1} = S^{(k-1)}$ is triangular. Thus, in the analysis of the decomposition of A^{k-1}, we know the matrices $Y_i^{(k-1)}$.

We shall first prove by induction that, in the analysis of the decomposition of A^k, the matrices $Y_i^{(k)}$ can be determined such that $Y_i^{(k)} \to Y_i^{(k-1)}$ as $k \to \infty$.

Let us assume that, for some value of i,

$$Y_i^{(k)} \to Y_i^{(k-1)}. \tag{10}$$

From (4), $b_{(i)1}^{(k)} = \sum_{r=1}^{m} \lambda_{(i)r}^k \bar{x}_{(i)1r} y_{(i)r}^{(k)}$

and so, since $\lambda_{(i)1}^k \bar{x}_{(i)11} y_{(i)1}^{(k)} = \lambda_i^k \bar{x}_{(i)11} y_{(i)1}^{(k)}$ is the dominant term in this sum ($y_{(i)1}^{(k)} \neq 0$ because $Y_i^{(k)}$ is non-singular) we have, as $k \to \infty$,

$$\frac{1}{|\lambda_i^k|} \cdot b_{(i)1}^{(k)} \to \frac{1}{|\lambda_i^k|} \cdot \lambda_i^k \bar{x}_{(i)11} y_{(i)1}^{(k)}$$

and similarly $\dfrac{1}{|\lambda_i^k|} \cdot b_{(i)1}^{(k-1)} \to \dfrac{1}{|\lambda_i^k|} \cdot \lambda_i^{k-1} \bar{x}_{(i)11} y_{(i)1}^{(k-1)}$.

Therefore, using (10) we obtain

$$\frac{1}{|\lambda_i^k|} \cdot b_{(i)1}^{(k)} \to \frac{\lambda_i}{|\lambda_i^k|} \cdot b_{(i)1}^{(k-1)}. \tag{11}$$

We now form $M_i^{(k)}$ by modifying $M_i^{(k-1)}$.

If $c_{(i)}^{(k)} = M_i^{(k-1)*} b_{(i)1}^{(k)}$, we construct a matrix $Z_i^{(k)} = T_m T_{m-1} \ldots T_1$ by the procedure used in the lemma in Section 3 such that $Z_i^{(k)} c_{(i)}^{(k)} = ||c_{(i)}^{(k)}|| e_1$. Since, from (11),

$$\frac{1}{|\lambda_i^k|} \cdot c_{(i)}^{(k)} = \frac{1}{|\lambda_i^k|} \cdot M_i^{(k-1)*} b_{(i)1}^{(k)} \to \frac{\lambda_i}{|\lambda_i^k|} \cdot M_i^{(k-1)*} b_{(i)1}^{(k-1)} = \frac{\lambda_i}{|\lambda_i^k|} \cdot ||b_{(i)1}^{(k-1)}|| e_1$$

it follows that, for $r > 1$, the $T_r \to I$ (because $t_{11}^{(r)} = t_{rr}^{(r)} \to 1$ and $t_{r1}^{(r)} = -\bar{t}_{1r}^{(r)} \to 0$). For $r = 1$ the element $t_{11}^{(1)}$ of T_1 is given by $t_{11}^{(1)} = \dfrac{\bar{c}_{(i)1}^{(k)}}{|c_{(i)1}^{(k)}|} \to \dfrac{\bar{\lambda}_i}{|\lambda_i|}$.

Thus $\boldsymbol{M}_i^{(k)*} = \boldsymbol{Z}_i^{(k)}\boldsymbol{M}_i^{(k-1)*} \to \boldsymbol{T}_1\boldsymbol{M}_i^{(k-1)*}$, and so we can write $\overline{\boldsymbol{M}}_i^{(k)} \to \overline{\boldsymbol{M}}_i^{(k-1)}$ and $\boldsymbol{m}_{(i)1}^{(k)} \to \frac{\lambda_i}{|\lambda_i|}\boldsymbol{m}_{(i)1}^{(k-1)}$. This is combined with (10) to give $\overline{\boldsymbol{M}}_i^{(k)*}\overline{\boldsymbol{Y}}_i^{(k)} \to \overline{\boldsymbol{M}}_i^{(k-1)*}\overline{\boldsymbol{Y}}_i^{(k-1)}$ and therefore, since from (9) $\boldsymbol{Y}_{i+1}^{(k)} = \overline{\boldsymbol{M}}_i^{(k)*}\overline{\boldsymbol{Y}}_i^{(k)}$, we obtain $\boldsymbol{Y}_{i+1}^{(k)} \to \boldsymbol{Y}_{i+1}^{(k-1)}$, which is similar to our initial assumption.

When $i = 1$, $\boldsymbol{Y}_1^{(k)} = \boldsymbol{Y}_1^{(k-1)} = \boldsymbol{V}$, which completes the induction. We have simultaneously shown that, as $k \to \infty$, each $\overline{\boldsymbol{M}}_i^{(k)} \to \overline{\boldsymbol{M}}_i^{(k-1)}$ and each $\boldsymbol{m}_{(i)1}^{(k)} \to \frac{\lambda_i}{|\lambda_i|}\boldsymbol{m}_{(i)1}^{(k-1)}$.

Now the ith column of $\boldsymbol{P}^{(k)}$ is given by:

$$\boldsymbol{p}_i^{(k)} = \overline{\boldsymbol{M}}_1^{(k)}\overline{\boldsymbol{M}}_2^{(k)} \ldots \overline{\boldsymbol{M}}_{i-1}^{(k)}\boldsymbol{m}_{(i)1}^{(k)}$$

so we have proved that, as $k \to \infty$, $\boldsymbol{p}_i^{(k)} \to \frac{\lambda_i}{|\lambda_i|} \cdot \boldsymbol{p}_i^{(k-1)}$ and that this is true for whatever way in which the unitary-triangular decomposition of $\boldsymbol{A}^k$ is determined since, by theorem 1, the decomposition is unique. The method used above for forming $\boldsymbol{M}_1^{(k)}$, $\boldsymbol{M}_2^{(k)}$, ..., $\boldsymbol{M}_n^{(k)}$ is chosen for convenience in proving convergence.

Finally, since $\boldsymbol{Q}^{(k)} = \boldsymbol{P}^{(k-1)*}\boldsymbol{P}^{(k)}$ we have

$$q_{ij}^{(k)} = \boldsymbol{p}_i^{(k-1)*}\boldsymbol{p}_j^{(k)} \to \frac{\lambda_i}{|\lambda_i|} \cdot \delta_{ij}$$

and thus $\boldsymbol{Q}^{(\infty)} = \lim \boldsymbol{Q}^{(k)}$ exists and is a diagonal matrix, the ith element on the diagonal being $\frac{\lambda_i}{|\lambda_i|}$.

We can now prove:

THEOREM 3. *If any non-singular matrix $\boldsymbol{A}$ has eigenvalues of distinct modulus, then under the QR transformation the elements below the principal diagonal tend to zero, the moduli of those above the diagonal tend to fixed values, and the elements on the principal diagonal tend to the eigenvalues.*

PROOF. Since $\boldsymbol{A}^{(k)} = \boldsymbol{Q}^{(k)}\boldsymbol{R}^{(k)}$, and $\lim \boldsymbol{Q}^{(k)} = \boldsymbol{Q}^{(\infty)}$ exists and is diagonal with $q_{ii}^{(\infty)} = \frac{\lambda_i}{|\lambda_i|}$, we have

$$a_{ij}^{(k)} = \boldsymbol{e}_i^*\boldsymbol{Q}^{(k)}\boldsymbol{R}^{(k)}\boldsymbol{e}_j \to \boldsymbol{e}_i^*\boldsymbol{Q}^{(\infty)}\boldsymbol{R}^{(k)}\boldsymbol{e}_j = \frac{\lambda_i}{|\lambda_i|} \cdot r_{ij}^{(k)}.$$

Thus below the diagonal $\lim a_{ij}^{(k)} = 0$ because $\boldsymbol{R}^{(k)}$ is triangular. Also, since $\boldsymbol{Q}^{(k)}\boldsymbol{R}^{(k)} = \boldsymbol{R}^{(k-1)}\boldsymbol{Q}^{(k-1)}$, we have $\boldsymbol{Q}^{(\infty)}\boldsymbol{R}^{(k)} \to \boldsymbol{R}^{(k-1)}\boldsymbol{Q}^{(\infty)}$, and thus

$$\frac{\lambda_i}{|\lambda_i|} \cdot r_{ij}^{(k)} \to \frac{\lambda_j}{|\lambda_j|} \cdot r_{ij}^{(k-1)}, \quad \text{so that} \quad \lim|r_{ij}^{(k)}| = \lim|a_{ij}^{(k)}|$$

exists—in particular above the diagonal. The elements $a_{ij}^{(k)}$ clearly tend to the eigenvalues.

5. Eigenvalues of Equal Modulus

It is possible to show by a more general treatment than that given in Section 4 that, if the matrix $\boldsymbol{A}$ has some eigenvalues of equal modulus, then the matrix $\boldsymbol{A}^{(k)}$ becomes split into independent principal submatrices coupled only in so far as the eigenvectors are concerned. These submatrices are normally, but not always, each associated with groups of eigenvalues of the same modulus, a sufficient condition for this being that for any group, say all the λ_r for $p < r < q + 1$ such that $|\lambda_p| > |\lambda_r| > |\lambda_{q-1}|$,
the two minors

$$\begin{vmatrix} u_{11} & u_{12} \ldots u_{1p} \\ u_{21} & u_{22} \ldots u_{2p} \\ \cdot & \\ \cdot & \\ \cdot & \\ u_{p1} & u_{p2} \ldots u_{pp} \end{vmatrix}, \quad \begin{vmatrix} u_{11} & u_{12} \ldots u_{1q} \\ u_{21} & u_{22} \ldots u_{2q} \\ \cdot & \\ \cdot & \\ \cdot & \\ u_{q1} & u_{q2} \ldots u_{qq} \end{vmatrix}$$

should not be zero.

In this case the $q - p$ eigenvalues λ_r will be the limiting values of the roots of the submatrix $[a_{ij}^{(k)}]$, $p<(i,j)<q+1$; the elements not included in this submatrix with both $i > p$ and $j \leqslant q$ converge to zero.

If the above condition holds and a group of eigenvalues are all equal, then (so long as the matrix can be diagonalized) this group will be resolved as a strictly diagonal submatrix.

On the other hand, if there are no eigenvalues of equal modulus apart from equal eigenvalues (e.g. a positive definite matrix), and the matrix can be diagonalized, then one can show that no further conditions are required for all the eigenvalues to be resolved in the limit (cf. Rutishauser, 1958, theorem 4).

6. Normal, Hermitian and Band Matrices

The matrices of both left and right eigenvectors of a normal matrix are the conjugate transpositions of one another and are therefore unitary; thus $\boldsymbol{A} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^*$. (If $\boldsymbol{A}$ is hermitian $\boldsymbol{\Lambda}$ is real, and if also real $\boldsymbol{V}$ is orthogonal.) Hence it follows that if $\boldsymbol{A}$ is normal (hermitian or real symmetric) then so is $\boldsymbol{A}^{(k+1)} = \boldsymbol{P}^{(k)*}\boldsymbol{A}\boldsymbol{P}^{(k)}$ ($\boldsymbol{P}^{(k)}$ is orthogonal if $\boldsymbol{A}$ is real symmetric). In the limit $\boldsymbol{A}^{(k)}$ is diagonal because, since it is triangular and normal, we have

$$\sum_i |a_{ii}^{(k)}|^2 \to \sum |\lambda_i|^2 = \text{trace}\,(\boldsymbol{A}^{(k)*}\boldsymbol{A}^{(k)}) = \sum_i \sum_j |a_{ij}^{(k)}|^2.$$

We therefore obtain:

THEOREM 4. *Under the QR transformation a normal (hermitian or real symmetric) matrix remains normal (hermitian or real symmetric) and tends to a diagonal matrix if the eigenvalues are non-zero and have distinct moduli.*

If the matrix $\boldsymbol{A}$ has zeros in position (i,j) for all $i > j + d$, for some d the matrix $\boldsymbol{Q}$ has the same elements zero and therefore so does $\boldsymbol{RQ}$. Clearly, when $a_{ij} = \overline{a}_{ji}$, we have:

THEOREM 5. *If A is a hermitian band matrix then the matrices $A^{(k)}$ generated from it by the QR transformation are also band matrices of the same width.*

Notice that if A is not hermitian the band property is not retained.

There is also an interesting connection between the QR and the LR transformations when the matrix is hermitian. The LR transformation using hermitian Choleski decomposition gives

$$\underline{A}^{(k+1)} = \underline{R}^{(k)}\underline{R}^{(k)*} \text{ where } \underline{R}^{(k)*}\underline{R}^{(k)} = \underline{A}^{(k)} \text{ and } \underline{A}^{(1)} = A,$$

the underlining distinguishing the LR from the QR case. Thus if we write $\underline{A}^{(k+1)} = \underline{S}^{(k)}A\underline{S}^{(k)-1}$, where $\underline{S}^{(k)} = \underline{R}^{(k)}\underline{R}^{(k-1)}\ldots\underline{R}^{(1)}$ we have $A^k = \underline{S}^{(k)*}\underline{S}^{(k)}$.

Now we obtain $A^k = P^{(k)}S^{(k)}$ from the QR transformation and thus $A^{k*}A^k = A^{2k} = S^{(k)*}S^{(k)}$ as A is hermitian. Thus

$$A^{2k} = S^{(k)*}S^{(k)} = \underline{S}^{(2k)*}\underline{S}^{(2k)},$$

and since Choleski decomposition is unique we see that $S^{(k)} = \underline{S}^{(2k)}$ and $A^{(k+1)} = \underline{A}^{(2k+1)}$, which shows that the QR transformation generates alternate members of the series of matrices generated by the LR (Choleski) transformation.

We can also see why it is that, whereas the LR transformation requires a positive definite hermitian matrix for necessarily stable Choleski decomposition, the QR transformation can be applied safely to any matrix.

7. The Hessenberg Almost Triangular Form as Starting Matrix

It is not claimed that the QR transformation is likely to be useful for finding eigenvalues when the matrix involved is hermitian, because other very satisfactory methods involving less work exist for these matrices. We are thus mainly interested in the use of the QR algorithm for finding the eigenvalues of unsymmetric matrices. Now the amount of computation that the method involves in one iteration on a general matrix is rather large (proportional to n^3), but if the matrix is first reduced to "almost triangular" or Hessenberg form the amount can be considerably decreased (made proportional to n^2). We will show below that there are also other important advantages in using this form.

An almost triangular matrix has zeros in position (i, j) for $i > j + 1$. Perhaps the best method for reducing a matrix to this form is one which makes use of elementary similarity transformations (combined with permutations to keep all multiples less than one) to eliminate in turn the unwanted elements in the columns, starting on the left. This procedure has been described, for example, by Wilkinson (1959*b*). Alternatively, the elements can be eliminated in the same sequence by unitary transformations, though such methods (Givens, 1958; Wilkinson, 1960) involve more work. Each of these methods proves to be numerically stable.

We now give some of the relevant properties of the almost triangular matrix. We shall denote the subdiagonal elements $a_{i\,i-1}$ by α_i, $i = 2, 3, \ldots, n$.

We first notice that, if any element α_r is zero, then the matrix can be partitioned at this point, and the submatrices $[a_{ij}]$ with $(i, j) < r$ and with $(i, j) \geqslant r$ can be treated separately (in so far as the eigenvalues are concerned).

THEOREM 6. *The almost triangular form of a matrix is preserved under the QR transformation.*

This is because the matrices $Q^{(k)}$ in the algorithm are also almost triangular.

THEOREM 7. *If all the elements α_i are non-zero and the matrix can be diagonalized (i.e. has no non-linear elementary divisors) then it can have no repeated eigenvalues.*

This well-known result follows from the fact that the rank of $A - \lambda I$ is never less than $n - 1$ for any value of λ since the product of the elements α_i forms a non-zero minor of order $n - 1$.

Conversely, if an almost triangular matrix with linear elementary divisors has groups of repeated eigenvalues, and if there are p members in the largest group, then, however it may have been formed, there will be at least $p - 1$ zero α_i.

THEOREM 8. *If all the elements α_i are non-zero and the matrix can be diagonalized then none of the minors of order i in the first i columns of U^*, the matrix of row eigenvectors, can be zero for any value of i.*

PROOF. Let D be the $i \times n$ matrix of any i rows of U^* and let $1 \leqslant i < n$ (the case when $i = n$ is trivial). Then for some r the rth column of D is linearly dependent on the previous $r - 1$ columns. Consequently there is a vector x such that $Dx = O$ for which $x_r \neq 0$ and $x_q = 0$ for $q > r$. Now since $U^*A = \Lambda U^*$ we can write $DA = \Lambda_i D$, where Λ_i is a principal submatrix of Λ of order i. Thus $DAx = O$ and if we put $y = Ax$ we see that $y_{r-1} = \alpha_r x_r \neq 0$ and $y_q = 0$ for $q > r + 1$. Therefore, since $Dy = O$ the $(r + 1)$th column of D can be expressed as a linear combination of the previous r columns. Continuing this argument we obtain the result that all the remaining columns of D are dependent on the first $r - 1$. Now the i rows of D are linearly independent, being eigenvectors, and it must be possible to choose i independent columns. Hence we cannot have $r \leqslant i$ and we see that the first i columns of D must be linearly independent so that the leading minor of order i is not zero. This is the theorem.

Combining this theorem with the results in Section 4 and statements in Section 5 we obtain:

THEOREM 9. *If an almost triangular matrix A is non-singular, can be diagonalized, and has non-zero elements α_i, then under the QR transformation the principal diagonal elements of $A^{(k)}$ converge to the eigenvalues in order of size if their moduli are unequal. A group of $q - p$ eigenvalues of equal modulus and modulus less than that of p other eigenvalues becomes identified with the eigenvalues of the almost triangular submatrix $[a_{ij}^{(k)}]$ in which $p < (i, j) < q + 1$.*

8. Rate of Convergence and its Acceleration

In the simple case when the eigenvalues of A have distinct moduli and the matrix U is such that the eigenvalues appear on the diagonal of $A^{(k)}$ in order of modulus (which is usually true), one can show that normally the element $a_{ij}^{(k)}$ below the main diagonal of $A^{(k)}$ converges to zero like $\left(\frac{\lambda_i}{\lambda_j}\right)^k$ (in rare circumstances the convergence is faster).

This is the same rate of convergence as that obtained in the LR algorithm and, as Rutishauser states, it is unsatisfactorily slow in many cases. The difference of $a_{nn}^{(k)}$ from λ_n, say ε, is multiplied by roughly $\frac{\lambda_n}{\lambda_{n-1}}$ with each iteration of the QR algorithm. If the origin of the eigenvalues is shifted close to λ_n, say by $\zeta^{(k)}$, before an iteration and shifted back again afterwards, the difference is multiplied by roughly $\frac{\lambda_n - \zeta^{(k)}}{\lambda_{n-1} - \zeta^{(k)}}$ and thus we have an improved rate of convergence (for $\zeta^{(k)}$ sufficiently close to λ_n). Hence, if we base our choice of $\zeta^{(k+1)}$ on the element $a_{nn}^{(k)}$ in some way, we should be able to achieve a second-order rate of convergence to λ_n. The transformation becomes†

$$A^{(k)} - \zeta^{(k)}I = Q^{(k)}R^{(k)}$$
$$A^{(k+1)} = R^{(k)}Q^{(k)} + \zeta^{(k)}I.$$

Or, alternatively:

$$A^{(k+1)} = Q^{(k)*}A^{(k)}Q^{(k)},$$

where
$$Q^{(k)*}(A^{(k)} - \zeta^{(k)}I) = R^{(k)}. \tag{12}$$

We shall refer to this as the *generalized QR transformation*. Methods for choosing the origin shifts $\zeta^{(k)}$ will be given in Part 2 of the paper and we shall discuss there the adaptation of the algorithm to the more difficult, but important, problem that arises when there are eigenvalues of the same modulus—in particular conjugate complex pairs.

In the simple case, when λ_n has been found to sufficient accuracy, we can clearly reduce the order of the matrix by one by omitting its last row and column, and proceed to find λ_{n-1}. We may reasonably expect to find the eigenvalues roughly in order of size starting with the smallest, for while $a_{nn}^{(k)}$ is converging to λ_n, $a_{n-1\,n-1}^{(k)}$ will be tending to the eigenvalue closest to λ_n.

† Rutishauser (1958) suggests a similar algorithm when the LR transformation is applied to band matrices.

References

FIKE, C. T. (1959). "Note on the Practical Computation of Proper Values," *J. Ass. Comput. Mach.*, Vol. 6, p. 360.

GIVENS, W. (1958). "Computation of Plane Unitary Rotations Transforming a General Matrix to Triangular Form," *J. Soc. Indust. Appl. Math.*, Vol. 6, p. 26.

RUTISHAUSER, H. (1958). "Solution of Eigenvalue Problems with the LR-transformation," *Nat. Bur. Standards Appl. Math. Ser.*, No. 49, p. 47.

WILKINSON, J. H. (1959). "Rounding Errors in Algebraic Processes," Proc. International Conference on Information Processing, Paris, June 1959, London: Butterworths.

WILKINSON, J. H. (1959). "Stability of the Reduction of a Matrix to Almost Triangular and Triangular Forms by Elementary Similarity Transformations," *J. Ass. Comput. Mach.*, Vol. 6, p. 336.

WILKINSON, J. H. (1960). "Householder's Method for the Solution of the Algebraic Eigenproblem," *The Computer Journal*, Vol. 3, p. 23.