

QR in two dimensions

Autor(en): **Kreyszig, Erwin / Todd, John**

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QR in Two Dimensions

The *QR* process is one of the most efficient ways of determining the characteristic values of a matrix. It is a unitary analog of the *LR* process of RUTISHAUSER [1]. However even the best proofs available are unfit for beginners' consumption and the later developments of the process are not yet fully understood. We present here a discussion of the two-dimensional case, in its simplest form. The formal description of the process will be given in the n -dimensional case.

Let A be a complex $n \times n$ matrix. It is well-known that A can be written in the form

$$A = QR \tag{1}$$

where Q is unitary and R upper triangular. This is essentially the result of the Gram-Schmidt orthogonalization process. Moreover, if we require the diagonal elements of R to be positive, then the representation (1) is unique.

The *QR*-algorithm consists in deriving sequences of matrices $\{A_n\}$, $\{Q_n\}$, $\{R_n\}$ from $A = A_1$ by repeated use of (1). Given $A_n = Q_n R_n$ we form the reversed product $A_{n+1} = R_n Q_n$ and factorize this as $A_{n+1} = Q_{n+1} R_{n+1}$. Since

$$A_{n+1} = R_n Q_n = (Q_n^* Q_n) R_n Q_n = Q_n^* (Q_n R_n) Q_n = Q_n^* A_n Q_n \tag{2}$$

the matrices $\{A_n\}$ are all (unitarily) similar to A and have the same characteristic values as A . The basic fact is that, in certain circumstances, the sequence $\{A_n\}$ converges geometrically to an upper triangular matrix, which has the characteristic values of A on the diagonal. For discussions of this result see the original papers of H. RUTISHAUSER [1], J. G. F. FRANCIS [2], V. N. KUBLANOWSKAJA [3] and more recent work of B. PARLETT [4, 5, 6], A. S. HOUSEHOLDER [7], G. W. STEWART [8] and J. H. WILKINSON [9].

In practice, appropriate “shifts” are introduced and quadratic convergence can be obtained.

For simplicity we discuss the real two dimensional case. Let

$$A = \begin{bmatrix} a & \beta \\ \gamma & \delta \end{bmatrix}$$

be real and unimodular, $\det A = 1$. We compute the QR decomposition. If, where $c = \cos \theta$, $s = \sin \theta$,

$$A = A_1 = \begin{bmatrix} a & \beta \\ \gamma & \delta \end{bmatrix} = \begin{bmatrix} c & s \\ s & -c \end{bmatrix} \begin{bmatrix} \xi & \eta \\ 0 & \zeta \end{bmatrix}$$

then

$$c = a(a^2 + \gamma^2)^{-1/2}, s = \gamma(a^2 + \gamma^2)^{-1/2}.$$

Next

$$A_2 = \begin{bmatrix} c & s \\ s & -c \end{bmatrix} \begin{bmatrix} a & \beta \\ \gamma & \delta \end{bmatrix} \begin{bmatrix} c & s \\ s & -c \end{bmatrix} = \begin{bmatrix} (a + \delta - (a/(a^2 + \gamma^2))) & \gamma - \beta - (\gamma/(a^2 + \gamma^2)) \\ -\gamma/(a^2 + \gamma^2) & a/(a^2 + \gamma^2) \end{bmatrix}.$$

If we write

$$A_n = \begin{bmatrix} a_n & \beta_n \\ \gamma_n & \delta_n \end{bmatrix}$$

then the recurrence relations determining a_{n+1}, γ_{n+1} are

$$\begin{cases} a_{n+1} = (a_1 + \delta_1) - (a_n/(a_n^2 + \gamma_n^2)), \\ \gamma_{n+1} = -\gamma_n/(a_n^2 + \gamma_n^2), \end{cases} \quad n = 1, 2, \dots \quad (3)$$

What we have to prove from (3) is that, in certain circumstances

$$a_n \rightarrow \lambda, \gamma_n \rightarrow 0$$

where λ is an appropriate characteristic value of A . The solution to non-linear systems of difference equations such as (3) is not usually easy.

We assume that A has a dominant characteristic value λ . This means that A has distinct real characteristic values which are reciprocal, since A is unimodular. We may assume that λ is positive for otherwise we could deal with $-A$. Hence

$$\lambda + \lambda^{-1} = a + \delta = k, \text{ say, where } k > 2.$$

We discuss an example first. We normalize the matrix

$$\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$$

to a unimodular

$$A = A_1 = \begin{bmatrix} 2/\sqrt{3} & -1/\sqrt{3} \\ -1/\sqrt{3} & 2/\sqrt{3} \end{bmatrix},$$

with characteristic roots $\sqrt{3}, 1/\sqrt{3}$.

Application of the relations (3) gives

	$n=1$	$n=2$	$n=3$	$n=4$
$a_n/\sqrt{3} =$	2/3	14/15	122/123	1094/1095
$\gamma_n/\sqrt{3} =$	-1/3	1/5	-3/41	9/365

which indicates that $a_n \rightarrow \sqrt{3}, \gamma_n \rightarrow 0$. The general form of a_n, γ_n can be conjectured from the above table and established by induction. We find

$$\frac{a_n}{\sqrt{3}} = \frac{3 \times 9^{n-1} + 1}{3(9^{n-1} + 1)}, \quad \frac{(-1)^n \gamma_n}{\sqrt{3}} = \frac{2 \times 3^{n-1}}{3(9^{n-1} + 1)},$$

so that the convergence of $\{\gamma_n\}$ is ultimately geometric with common ratio $1/3 = \lambda^{-2}$ while that of $\{a_n\}$ is ultimately geometric with common ratio $1/9 = \lambda^{-4}$.

In the general real 2×2 case we can prove that

$$\begin{cases} a_{n+1} = \frac{p(a^2 + \gamma^2 + aq) - (a + q)}{(a + q)^2 + \gamma^2} \\ \gamma_{n+1} = (-1)^n \frac{\gamma(pq + 1)}{(a + q)^2 + \gamma^2} \end{cases} \quad (4)$$

where $v_n = \lambda^n - \lambda^{-n}, p = p_n = v_{n+1}/v_n, q = q_n = -v_{n-1}/v_n$. Since $p_n \sim \lambda, q_n \sim -\lambda^{-1}$ this gives $a_n \rightarrow \lambda, \gamma_n \rightarrow 0$.

In order to establish (4) we write $x_n = a_n, y_n = (-1)^n \gamma_n$ in (3) to get

$$x_{n+1} = k - (x_n/(x_n^2 + y_n^2)), y_{n+1} = y_n/(x_n^2 + y_n^2), \quad (5)$$

which we combine as $z_{n+1} = k - \bar{z}_n / (z_n \bar{z}_n)$, i.e.,

$$z_{n+1} = k - z_n^{-1}, \quad n = 1, 2, \dots, \quad (6)$$

where $z_r = x_r + iy_r$, $\bar{z}_r = x_r - iy_r$.

We have therefore reduced our problem to that of the iteration of the fractional linear transformation

$$w = \frac{kz - 1}{z}. \quad (7)$$

This is a well-known problem. An essentially geometric solution is given, e.g., by T. J. P. A. BROMWICH [10, p. 22, ex. 4]. This depends on the fact that (7) can be represented in the form

$$\frac{w - \lambda}{w - \lambda^{-1}} = \lambda^{-2} \left(\frac{z - \lambda}{z - \lambda^{-1}} \right) \quad (7')$$

which gives

$$\frac{z_{n+1} - \lambda}{z_{n+1} - \lambda^{-1}} = \lambda^{-2n} \left(\frac{z_1 - \lambda}{z_1 - \lambda^{-1}} \right),$$

so that $z_n \rightarrow \lambda$, as required. We can derive (7') using the fact that a fractional linear transformation with fixed points at $0, \infty$ is necessarily linear, or by using the cross-ratio property of fractional linear transformations. For details compare, e.g. CARATHÉODORY [11, p. 14] or KREYSZIG [12, p. 503].

A second method is simply to establish, by induction,

$$z_{n+1} = \frac{pz_1 + 1}{z_1 + q} \quad (8)$$

where $z_1 = a - iy$ and $p = p_n$, $q = q_n$ are as defined above. Taking the real and imaginary parts of (8) gives (4).

Our third method, preferable in the matrix context, follows. We begin by recalling that if

$$W = \frac{aw + \beta}{\gamma w + \delta}, \quad w = \frac{az + b}{cz + d}$$

then

$$W = \frac{Az + B}{Cz + D} \quad \text{where} \quad \begin{bmatrix} A & B \\ C & D \end{bmatrix} = \begin{bmatrix} a & \beta \\ \gamma & \delta \end{bmatrix} \begin{bmatrix} a & b \\ c & d \end{bmatrix}.$$

Thus the iteration of a fractional linear transformation is equivalent to the powering of a matrix.

We use the following result.

Lemma. If M is a 2×2 matrix with distinct characteristic values λ, μ then

$$M^n = \begin{bmatrix} ad\lambda^n - bc\mu^n & -ab(\lambda^n - \mu^n) \\ cd(\lambda^n - \mu^n) & -bc\lambda^n + ad\mu^n \end{bmatrix} \quad (9)$$

where

$$T = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

is a unimodular matrix which diagonalizes M .

Proof. Either by induction or let $D = \text{diag} [\lambda, \mu]$ so that $T^{-1}MT = D$, $M = TDT^{-1}$ and

$$\begin{aligned} M^n &= \{TDT^{-1}\} \{TDT^{-1}\} \dots \{TDT^{-1}\} \\ &= TD^nT^{-1} \\ &= \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} \lambda^n & 0 \\ 0 & \mu^n \end{bmatrix} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix} \end{aligned}$$

which gives (9), on multiplying out.

We now observe that when $A = \begin{bmatrix} k & -1 \\ 1 & 0 \end{bmatrix}$ then

$$T = (\lambda - \lambda^{-1})^{-1/2} \begin{bmatrix} \lambda & \lambda^{-1} \\ 1 & 1 \end{bmatrix},$$

where λ is as already defined. The rest of the discussion is a matter of elementary algebra.

Writing as before, $v_n = \lambda^n - \lambda^{-n}$, we find from (9)

$$z_{n+1} \equiv x_{n+1} + iy_{n+1} = \frac{v_{n+1}(x_1 + iy_1) - v_n}{v_n(x_1 + iy_1) - v_{n-1}}.$$

Multiplying above and below on the right by $v_n(x_1 - iy_1) - v_{n-1}$ and equating real and imaginary parts shows that

$$\begin{cases} x_{n+1} = \{v_n v_{n+1}(x_1^2 + y_1^2) + v_n v_{n-1} - x_1(v_n^2 + v_{n+1}v_{n-1})\}/D, \\ y_{n+1} = (v_n^2 - v_{n+1}v_{n-1})y_1/D, \end{cases}$$

where

$$D = v_n^2(x_1^2 + y_1^2) - 2v_{n-1}v_n x_1 + v_{n-1}^2.$$

This is another form of (4). We find that, as $n \rightarrow \infty$,

$$\begin{cases} x_{n+1} - \lambda = [2(\lambda - \lambda^{-1})\{a^2 + \gamma^2 + 1 - ka\} + O(\lambda^{-2n})]/D, \\ y_{n+1} = (\lambda - \lambda^{-1})^2 \gamma / D, \end{cases} \quad (10)$$

where

$$D = [(a - \lambda^{-1})^2 + \gamma^2] \lambda^{2n} + O(1) = O(\lambda^{2n}).$$

The relations (10) establish the convergence of the *QR*-process.

Note that when the matrix A is symmetric, as well as unimodular, we have $a\delta - \gamma^2 = 1$, i. e., $a(k - a) - \gamma^2 = 1$, i. e. $a^2 + \gamma^2 + 1 = ka$ so that (10) gives $x_n - \lambda = O(\lambda^{-4n})$, $y_n = O(\lambda^{-2n})$, in agreement with the numerical results in the special case.

Erwin Kreyszig (University of Windsor, Canada) and
John Todd (California Institute of Technology, Pasadena, USA)

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