The QR algorithm for real symmetric matrices with multiple eigenvalues

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The success of the QR algorithm depends critically on the choice of the shifts of origin. This paper describes a method of choosing this shift which ultimately gives cubic convergence to the root of smallest modulus whatever its multiplicity.

In the practical application of the QR algorithm for the computation of the eigenvalues of a matrix A_1, sequences of matrices A_s, Q_s and R_s are derived which are defined by the relations

$$A_s - k_sI = Q_sR_s, \qquad R_sQ_s + k_sI = A_{s+1}, \tag{1}$$

where the Q_s are unitary and the R_s are upper-triangular. The quantities k_s are chosen so as to accelerate the convergence of the A_s to upper-triangular form. In this paper we are concerned with the case when A_1 is real and symmetric; these properties are then shared by all A_s.

If we take $k_s = 0$ for all s it has been shown (by Francis, 1961) that, provided $|\lambda_i| = |\lambda_j|$ only when $\lambda_i = \lambda_j$, the A_s tend to upper-triangular form, and since we are assuming that A_1 and hence all A_s are real and symmetric, this means that our A_s tend to *diagonal* form. Apart from exceptional cases (disorder of eigenvalues) the λ_i occur in order of decreasing modulus down the diagonal of the limiting A_s. We shall consider the case when A_1 has eigenvalues λ_i such that

$$\lambda_{n-r+1} = \lambda_{n-r+2} = \dots = \lambda_n \tag{2}$$

$$|\lambda_1| \geqslant |\lambda_2| \geqslant \dots \geqslant |\lambda_{n-r}| > |\lambda_{n-r+1}| \tag{3}$$

so that the eigenvalue of smallest modulus is of multiplicity r. We show that in this case there is ultimately a simple method of choosing the k_s which gives cubic convergence to λ_n of the last r diagonal elements of A_s.

Ultimate form of the A_s

For any real symmetric matrix A_1 with eigenvalues λ_i there exists an orthogonal matrix Q such that

$$A_1 = Q^T \operatorname{diag}(\lambda_i) Q \tag{4}$$

where the λ_i may be taken in order of decreasing absolute magnitude. Hence

$$A_1 - \lambda_n I = Q^T \operatorname{diag}(\lambda_i - \lambda_n) Q \tag{5}$$

and if λ_n is an eigenvalue of multiplicity r the matrix $\operatorname{diag}(\lambda_i - \lambda_n)$ has r zero diagonal elements and is therefore of rank $n - r$. Since Q^T and Q are of rank n the rank of $A_1 - \lambda_n I$ is also $n - r$.

Consider now the sequence of matrices A_s obtained from A_1 by the QR algorithm with $k_s = 0$. Each of the A_s has an eigenvalue λ_n of multiplicity r and hence $A_s - \lambda_n I$ is of rank $n - r$. If we write

$$A_s = \left[\begin{array}{c:c} F_s & G_s \\ \hdashline G_s^T & \underbrace{H_s}_{r} \end{array}\right]\}r, \tag{6}$$

then from the general theory of the convergence of the QR algorithm we know that $G_s \to 0$, $F_s \to \operatorname{diag}(\lambda_i)$ $(i = 1, \dots, n - r)$ and $H_s \to \lambda_n I_r$. Hence for sufficiently large s the matrix $F_s \to \lambda_n I_{n-r}$ is of rank $n - r$, since its eigenvalues are tending to $\lambda_i - \lambda_n$ $(i = 1, \dots, n-r)$; $F_s - \lambda_n I_{n-r}$ is therefore ultimately non-singular. If we define B_s by the relation

$$B_s = \left[\begin{array}{c:c} I_{n-r} & 0 \\ \hdashline -G_s^T(F_s - \lambda_n I_{n-r})^{-1} & I_r \end{array}\right] \left[\begin{array}{c:c} F_s - \lambda_n I_{n-r} & G_s \\ \hdashline G_s^T & H_s - \lambda_n I_r \end{array}\right], \tag{7}$$

then B_s is of the same rank as $A_s - \lambda_n I$, that is $n - r$. But we have

$$B_s = \left[\begin{array}{c:c} F_s - \lambda_n I_{n-r} & G_s \\ \hdashline 0 & H_s - \lambda_n I_r - G_s^T(F_s - \lambda_n I_{n-r})^{-1} G_s \end{array}\right] \tag{8}$$

and hence we must have

$$H_s - \lambda_n I_r - G_s^T(F_s - \lambda_n I_{n-r})^{-1} G_s = 0, \tag{9}$$

or B_s would be of rank greater than $n - r$.

Choice of k_s

In order to achieve a high rate of convergence it is well known that k_s should be chosen to be as close as possible to λ_n. We show that the choice $k_s = (A_s)_{nn}$ ultimately gives cubic convergence. For the purpose of

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our analysis we shall use the 2-norm of a matrix defined by

$$||X||_2 = \max_{x \neq 0} ||Xx||_2/||x||_2 \qquad (10)$$

where $||x||_2$ is the Euclidean length of the vector x. Notice that we do not require X to be square. It follows from this definition that if the eigenvalues of X^HX are σ_i^2, where $\sigma_1^2 \geqslant \sigma_2^2 \geqslant \ldots \geqslant \sigma_n^2 \geqslant 0$, then

$$||X||_2 = \sigma_1. \qquad (11)$$

When X is a real symmetric matrix $\sigma_1 = |\lambda_1|$ where λ_1 is the eigenvalue of X of maximum modulus.

We define δ by the relation

$$\delta = \min | \lambda_i - \lambda_n| \qquad (i = 1, \ldots, n - r), \qquad (12)$$

and consider first of all iteration with $k_s = 0$. If we denote the eigenvalues of F_s by λ_i' $(i = 1, \ldots, n - r)$ and those of H_s by λ_i'' $(i = n - r + 1, \ldots, n)$ then

$$\lambda_i' \to \lambda_i \quad (i = 1, \ldots, n - r),$$
$$\lambda_i'' \to \lambda_n \quad (i = n - r + 1, \ldots, n). \qquad (13)$$

Hence given any positive ϵ there exists an s such that

$$||G_s||_2 = ||G_s^T||_2 \leqslant \epsilon, \text{ and } |\lambda_i' - \lambda_n| > \frac{2}{3}\delta. \qquad (14)$$

We assume further that

$$\epsilon < \frac{1}{3}\delta. \qquad (15)$$

If s satisfies conditions (14) the matrix $F_s - \lambda_n I$ is certainly non-singular and hence from (9)

$$H_s = \lambda_n I_r + G_s^T(F_s - \lambda_n I_{n-r})^{-1}G_s$$
$$= \lambda_n I_r + M_s, \qquad (16)$$

where $\quad M_s = G_s^T(F_s - \lambda_n I_{n-r})^{-1}G_s, \qquad (17)$

and hence $||M_s||_2 \leqslant ||G_s^T||_2 \, ||(F_s - \lambda_n I_{n-r})^{-1} \, ||_2||G_s||_2$

$$\leqslant \epsilon^2 \max |(\lambda_i' - \lambda_n)^{-1}|$$
$$< 3\epsilon^2/2\delta < \frac{1}{6}\delta. \qquad (18)$$

Relations (16) and (18) show that the convergence of A_s takes place in rather a special way. When $||G_s|| \leqslant \epsilon$ the matrix H_s differs from $\lambda_n I_r$ by a matrix with elements which are of order ϵ^2. Immediate consequences of relations (16) and (18) are

$$|a_{nn}^{(s)} - \lambda_n| < 3\epsilon^2/2\delta < \frac{1}{6}\delta \qquad (19)$$

and

$$|\lambda_i'' - \lambda_n| < 3\epsilon^2/2\delta. \qquad (20)$$

Hence

$$|\lambda_i'' - a_{nn}^{(s)}| \leqslant |\lambda_i'' - \lambda_n| + |\lambda_n - a_{nn}^{(s)}|$$
$$\leqslant 3\epsilon^2/2\delta + 3\epsilon^2/2\delta = 3\epsilon^2/\delta \qquad (21)$$

and

$$|\lambda_i' - a_{nn}^{(s)}| > |\lambda_i' - \lambda_n| - |a_{nn}^{(s)} - \lambda_n|$$
$$> \frac{2}{3}\delta - \frac{1}{6}\delta = \frac{1}{2}\delta. \qquad (22)$$

The last of these relationships shows that $F_s - a_{nn}^{(s)}I$ is non-singular.

Consider now a step of the QR algorithm with $k_s = a_{nn}^{(s)}$. If we write

$$A_s - a_{nn}^{(s)}I = Q_sR_s$$

then $\quad Q_s^T(A_s - a_{nn}^{(s)}I) = R_s \qquad (23)$

and Q_s^T is itself an orthogonal matrix. We write

$$Q_s^T = \begin{bmatrix} P & Q \\ R & S \end{bmatrix}, \quad R_s = \begin{bmatrix} X & Y \\ 0 & Z \end{bmatrix}, \qquad (24)$$

where the partitioning is conformal with that of A_s in (6) Equation (23) therefore gives

$$\begin{bmatrix} P & Q \\ R & S \end{bmatrix} \begin{bmatrix} F_s - a_{nn}^{(s)}I & G_s \\ G_s^T & H_s - a_{nn}^{(s)}I \end{bmatrix} = \begin{bmatrix} X & Y \\ 0 & Z \end{bmatrix} \qquad (25)$$

and hence

$$R(F_s - a_{nn}^{(s)}I) + SG_s^T = 0, \qquad (26)$$
$$RG_s + S(H_s - a_{nn}^{(s)}I) = Z. \qquad (27)$$

Completing the QR transformation we have

$$A_{s+1} = \begin{bmatrix} F_{s+1} & G_{s+1} \\ G_{s+1}^T & H_{s+1} \end{bmatrix}$$
$$= \begin{bmatrix} X & Y \\ 0 & Z \end{bmatrix} \begin{bmatrix} P^T & R^T \\ Q^T & S^T \end{bmatrix} + a_{nn}^{(s)}I, \qquad (28)$$

giving

$$G_{s+1}^T = ZQ^T. \qquad (29)$$

Proof of cubic convergence

We shall prove that $||G_{s+1}||_2$ is of order ϵ^3 showing that the process is cubically convergent. We shall need two simple results for the norms of the submatrices of Q_s^T. Since from the definition of the 2-norm the norm of any submatrix is not greater than that of the matrix itself, we have

$$||P||_2 \leqslant ||Q_s^T||_2 = 1 \qquad (30)$$
$$||S||_2 \leqslant ||Q_s^T||_2 = 1, \qquad (31)$$

the equalities coming from the relation $Q_sQ_s^T = I$. We have also

$$PP^T + QQ^T = I \qquad (32)$$

and $\quad P^TP + R^TR = I, \qquad (33)$

and since the eigenvalues of PP^T and P^TP are the same this implies that

$$||R||_2 = ||Q||_2. \qquad (34)$$

Equation (26) gives

$$R = -SG_s^T(F_s - a_{nn}^{(s)}I)^{-1}, \qquad (35)$$

$$||R||_2 \leqslant ||S||_2||G_s^T||_2 \; ||(F_s - a_{nn}^{(s)}I)^{-1}||_2$$
$$\leqslant \epsilon \max | \lambda_i' - a_{nn}^{(s)} |^{-1}$$
$$< 2\epsilon/\delta \text{ from (22).} \qquad (36)$$

Hence from equation (27)

$$||Z||_2 \leqslant ||R||_2 \; ||G_s||_2 + ||S||_2 \; ||H_s - (a_{nn}^{(s)})I||$$
$$\leqslant 2\epsilon^2/\delta + \max | \lambda_i'' - a_{nn}^{(s)} |$$
$$< 2\epsilon^2/\delta + 3\epsilon^2/\delta$$
$$= 5\epsilon^2/\delta. \qquad (37)$$

Finally from equation (29)

$$||G_{s+1}^T||_2 \leqslant ||Z||_2||Q^T||_2 = ||Z||_2||R||_2 < 10\epsilon^3/\delta^2. \quad (38)$$

In connexion with the symmetric LL^T algorithm for positive definite matrices Rutishauser (1960) has described a method of choosing k_s which gives cubic convergence to the smallest eigenvalue. The proof we have just given may be modified to show that Rutishauser's technique gives cubic convergence whatever the multiplicity of the smallest eigenvalue. However, when this eigenvalue is of multiplicity r Rutishauser's technique requires the solution of an eigenvalue problem of order r and is therefore not quite so convenient as the process we have just described.

Numerical example

In **Table 1** we exhibit a matrix A_s of order four with the eigenvalues 6, 4, 2, 2, at a late stage in the iterative process. The 2×2 matrix G_s^T is such that $||G_s^T||_2$ is of the order of 0·04. Since $\delta = 2$ the condition $\epsilon < \frac{1}{3}\delta$ is certainly satisfied so that $H_s - 2I$ must certainly be small; in fact it will be seen that it is of the order of 0·0004. One iteration was performed using $k_s = a_{44}^{(s)}$ and the resulting A_{s+1} is displayed. It will be seen that $||G_{s+1}^T||_2 < 0{\cdot}000002$, while $H_{s+1} = 2I$ to working accuracy.

Table 1

Lower triangle of A_s

5·81522 813			
0·57853 605	4·18421 247		
−0·03866 598	−0·00586 326	2·00039 187	
−0·00506 679	−0·01912 924	0·00005 135	2·00016 753

Lower triangle of A_{s+1}

5·95048 519			
0·31076 986	4·04951 481		
−0·00000 168	0·00000 026	2·00000 000	
−0·00000 022	−0·00000 145	0·00000 000	2·00000 000

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Book Reviews

Mathematical Theory of Automata, edited by Jerome Fox, 1964; 640 pages. (London and New York: *John Wiley and Sons.*, 75s.).

This book is the proceedings of a symposium held in New York in April, 1962. The thirty-three papers are almost all reports of research done by the authors and not reviews or expository papers; they are therefore at a high level of specialization. This is not a book for the general reader, but it contains a number of interesting papers for reference by experts in this field. No formal grouping into subjects has been made though the papers divide into fairly clear-cut sections: theorem proving, computability, finite-state machines and self-organizing systems. Those who work in these areas will wish to have access to the book; it is unlikely to be useful to others.

A few of the papers can be read by the non-specialist with little prior knowledge. A review paper by Davis gives a short and lucid account of some of the classic unsolvable problems showing the reasons why the problems arose and their importance. Gelernter describes the methods used in his heuristic Geometry Theorem Machine to set up theorems and sub-theorems for the machine to prove. A method of pattern recognition is described by Unger which uses a two-dimensional grid of combinational cells to recognize features of patterns such as concavity to the right or the presence of holes.

The papers on finite-state machines are made difficult to read by the absence of a unified system of notation. A number of mathematical disciplines have contributed to this subject; the theory of groups and of semi groups, lattice theory, graph theory and the theory of computability to mention some examples, and the result seems to have been that authors have invented cumbersome notations which are difficult to read and remember.

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