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THE RELATION BETWEEN THE QR AND LR ALGORITHMS*

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Abstract. For an Hermitian matrix the QR transform is diagonally similar to two steps of the LR transforms. Even for non-Hermitian matrices the QR transform may be written in rational form.

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1. Summary.

In this section we assume that the reader is familiar with LR and QR. The transformations are presented in the next section. A slight variation of the LR algorithm that is suitable for positive definite Hermitian matrices is the Cholesky (LR) algorithm: $A = CC^*$ is mapped into $\hat{A} = C^*C$.

In the positive definite Hermitian case, two steps of Cholesky yield the same matrix as one step of QR. At first glance this is surprising (how can LR produce a unitary similarity?) and the proof is sometimes given as an exercise in textbooks; see [4], [1], and [9]. Students are often left with the (false) impression that positive definiteness is essential.

In recent years understanding of these algorithms has improved. Both the LR and QR algorithms are instances of GR algorithms [10]. For all such algorithms k steps applied to A are equivalent to a similarity driven by a factorization of A^k:

$$A^k = G_k R_k, \qquad A \to G_k^{-1} A G_k. \tag{1.1}$$

Consequently, two steps of LR on A is equivalent to a similarity driven by $A^2 : A^2 = LU, A \to L^{-1}AL$. On the other hand, one step of QR on A is equivalent (up to a diagonal similarity) to a similarity driven by A^*A:

$$A = QR, \qquad A^*A = R^*R (= LD^2L^*), \qquad A \to Q^*AQ = RAR^{-1}.$$

If A is Hermitian, then $A^*A = A^2$ and two steps of LR must be equivalent to one of QR. Despite these remarks it is still interesting to see the equivalence in detail, and that is the topic of section 2.

The catch is that LR can break down so the more careful statement is that two LR steps (if they exist) are equivalent to one QR step (which always exists). What is of more than passing interest is that LR is entirely rational in operation whereas QR requires square roots and is not rational. The remarks made above show that these square roots in QR are somehow not essential; QR may be better thought of as LR driven by A^*A. It is this viewpoint that leads to the various root-free QR algorithms that have been so successful for symmetric tridiagonal matrices. Four versions are described in [6] and an even faster one appeared recently in [3].

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For non-Hermitian matrices there is a similar rational version of QR and it is described in section 3.

We follow Householder conventions for notation except for denoting the conjugate transpose of F by F^* instead of F^H. We ignore shifts because they complicate the analysis and add nothing to a theoretical paper.

2. Connection of QR to LR. Two algorithms that play an important role in matrix eigenvalue computations are the LR and QR algorithms. The former was discovered by Rutishauser in 1958 [7] and the latter developed by Francis in 1959–1960 [2]. A formal derivation of QR was given in [5]. Both algorithms have been widely studied and good references are [9], [8], and [6].

Recall the basic decompositions.

Triangular factorization (LU). If and only if $B \in \mathbf{C}^{n\times n}$ has nonzero leading principal minors of orders $1, 2, \ldots, n-1$, then B has a unique decomposition

$$B = LDU,$$

where L is unit lower triangular, D is diagonal, and U is unit upper triangular.

Gram-Schmidt factorization (QR). All $B \in \mathbf{C}^{n\times n}$ may be written

$$B = QR,$$

where $Q^* = Q^{-1}$ and R is upper triangular with nonnegative diagonal entries. The factorization is unique if and only if the columns of B are linearly independent.

From the basic factorizations come the basic transforms.

LR transform. If $B = LDU$, then its LR transform is defined by

$$\overset{\circ}{B} = DUL = L^{-1}BL = (DU)B(DU)^{-1}.$$

Here is the irritating ambiguity in LR; the definition $\overset{\circ}{B} = ULD$ would be equally legitimate. For theoretical purposes one could consider the equivalence class of all diagonal similarities on a given matrix.

QR Transform. If $B = QR$ (uniquely), then its QR transform is defined by

$$\hat{B} = RQ = Q^*BQ = RBR^{-1}.$$

Remark 1. If A is Hermitian and positive definite, then $A = LD^2L^*$ and its *Cholesky transform* is given by $A' = DL^*LD$. Note that

$$A' = D^{-1} \overset{\circ}{A} D$$

is a diagonal similarity transformation but uses square roots. LR destroys the Hermitian property but only by a diagonal similarity.

Denote the Cholesky transform of A' by A'' and the LR transform of $\overset{\circ}{A}$ by $\overset{\circ\circ}{A}$. If A is Hermitian and positive definite, then $A'' = \hat{A}$: two steps of Cholesky equal one of QR. However, the positive definite property is not essential as the following result shows.

All L's are unit lower triangular and all D's are diagonal and real. For completeness we include all the diagonal matrices.

THEOREM 2.1. *If A is Hermitian, and permits triangular factorization, then $\overset{\circ\circ}{A}$ is diagonally similar to $\hat{A}$.*

Proof. By hypothesis $A = L_1 D_1 L_1^*$ and so

$$\overset{\circ}{A} = D_1 L_1^* L_1.$$

Since $L_1^* L_1$ is positive definite it permits triangular factorization

$$L_1^* L_1 = L_2 D_2^2 L_2^* \qquad (D_2 \text{ positive}). \tag{2.1}$$

Consequently, the triangular factorization of $\overset{\circ}{A}$ is

$$\overset{\circ}{A} = (D_1 L_2 D_1^{-1})(D_1 D_2^2) L_2^*.$$

Thus,

$$\begin{aligned} \overset{\circ\circ}{A} &= D_1 D_2^2 L_2^* D_1 L_2 D_1^{-1} \\ &= (D_1 D_2) M (D_1 D_2)^{-1}, \end{aligned}$$

where

$$M := D_2 L_2^* D_1 L_2 D_2.$$

It remains to show that M is similar to $\hat{A}$ with a diagonal unitary transformation. Rewrite (2.1) as

$$I = (L_1^{-*} L_2 D_2)(D_2 L_2^* L_1^{-1}).$$

Since D_2 is real

$$Q = L_1^{-*} L_2 D_2 \tag{2.2}$$

is unitary. Use $Q = Q^{-*}$ to obtain another triangular factorization of Q

$$Q = L_1 L_2^{-*} D_2^{-1}. \tag{2.3}$$

Now use Q to rewrite M as

$$\begin{aligned} M &= (D_2 L_2^* L_1^{-1})(L_1 D_1 L_1^*)(L_1^{-*} L_2 D_2) \\ &= Q^* A Q. \end{aligned} \tag{2.4}$$

Finally, using (2.3),

$$\begin{aligned} A &= L_1 D_1 L_1^* \\ &= (L_1 L_2^{-*} D_2^{-1})(D_2 L_2^* D_1 L_1^*) \\ &= Q \operatorname{sign}(D_1) \cdot \operatorname{sign}(D_1) D_2 L_2^* D_1 L_1^* \\ &= Q \operatorname{sign}(D_1) R \end{aligned}$$

reveals the QR factorization of A since R has nonnegative diagonal. By (2.4)

$$\begin{aligned} \hat{A} &= \operatorname{sign}(D_1) M \operatorname{sign}(D_1) \\ &= \operatorname{sign}(D_1)(D_1 D_2)^{-1} \overset{\circ\circ}{A} (D_1 D_2) \operatorname{sign}(D_1)^{-1}, \end{aligned}$$

as claimed. ∎

Remark 2. When the LR transform is to be applied to an Hermitian matrix it is possible to modify the algorithm so that the Hermitian property is restored after two steps. In the notation used above

$$\overset{\circ}{A} = D_1 L_1^* L_1 = D_1 (L_2 D_2)(L_2 D_2)^*$$

and one then redefines $\overset{\circ\circ}{A}$ by

$$\overset{\circ\circ}{A} := (L_2 D_2)^* D_1 (L_2 D_2) = M.$$

Such a modification forces a different mapping for odd and even steps and employs square roots.

The advantage of Theorem 2.1 over the explanation (1.1) mentioned in section 1 is that it reveals explicitly in (2.2) and (2.3) how the triangular factors L_1 and $L_2 D_2$ from LR yield the triangular factorization of Q from QR.

Remark 3. The QR transform does not require that A permit triangular factorization. In fact $\hat{A}$ cannot be derived from two steps of LR when, and only when, the orthogonal factor Q does not permit factorization as

$$Q = L_1 D_2^{-1} (D_2 L_2^{-*} D_2^{-1}).$$

In many cases, but not all, a well-chosen symmetric permutation $A \to \Pi A \Pi^t$ will give rise to a new Q that permits triangular factorization.

3. The non-Hermitian case. For general matrices the LR transform preserves band structure while the QR transform destroys the upper bandwidth. So the two procedures are not equivalent. Nevertheless it is legitimate to ask whether the QR transform can be represented in an alternative form related to triangular factorization.

The answer is yes. The key to extending the result of the previous section is to factor the given matrix B with a congruence transformation

$$B = FCF^*.$$

This appears to be a strange representation of a non-Hermitian matrix.

Suppose B permits triangular factorization

$$B = L_1 D_1 U_1.$$

Rewrite this as

$$B = L_1 (D_1 U_1 L_1^{-*}) L_1^*$$

and note that the middle factor is upper triangular instead of diagonal. Define, as earlier,

$$\overset{\circ}{B} = (D_1 U_1 L_1^{-*})(L_1^* L_1),$$

and use the Cholesky factorization

$$L_1^* L_1 = (L_2 D_2)(L_2 D_2)^*$$

to define

$$\begin{aligned}\overset{\circ\circ}{B} &= D_2 L_2^* (D_1 U_1 L_1^{-*}) L_2 D_2 \\ &= (D_2 L_2^* L_1^{-1})(L_1 D_1 U_1)(L_1^{-*} L_2 D_2) \\ &= Q^* B Q, \qquad \text{using (2.2).}\end{aligned}$$

Moreover,

$$\begin{aligned} B &= L_1 D_1 U_1 \\ &= (L_1 L_2^{-*} D_2^{-1})(D_2 L_2^* D_1 U_1) \\ &= Q \operatorname{sign}(D_1)(\overline{\operatorname{sign}(D_1)} D_2 L_2^* D_1 U_1) \end{aligned}$$

is the QR factorization of B.

Now, in general, $\operatorname{sign}(D_1) = \operatorname{diag}(\exp(i\varphi_1), \ldots, \exp(i\varphi_n))$.

Another way to interpret these expressions is to observe that, ignoring diagonal unitary matrices, the Q factor of B is the Q factor of its lower triangular factor L_1.

Note that $\overset{\circ}{B} = L_1^{-1} B L_1$, $\overset{\circ\circ}{B} = (D_2 L_2^*) \overset{\circ}{B} (D_2 L_2^*)^{-1}$, and so the nice unitary matrix Q is again split into its two triangular factors L_1 and $(D_2 L_2^*)^{-1}$.

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