

### QR Decomposition

Every finite set of linearly independent vectors  $\{X_1, X_2, \dots, X_n\}$  may be associated with an orthonormal set of nonzero vectors  $\{Q_1, Q_2, \dots, Q_n\}$  with respect to a specific inner product  $\langle \cdot, \cdot \rangle$ ; each vector  $Q_k$  ( $k = 1, 2, \dots, n$ ) is a linear combination of  $X_j$  through  $X_{j-1}$ . The following algorithm for producing the vectors  $Q_j$  is called the *Gram-Schmidt orthonormalization process*.

Step 1.1: Set  $r_{11} = \sqrt{\langle X_1, X_1 \rangle}$ .

Step 1.2: Let  $Q_1$  be the Normalized  $X_1$  (i.e.,  $Q_1 = \frac{1}{r_{11}}X_1$ ) and  $j = 1$ .

Step 2.1: If  $j = n$ , stop; the algorithm is complete; otherwise, increase  $j$  by 1 and continue.

Step 3.1: Calculate  $r_{ij} = \langle Q_i, X_j \rangle$  for  $i = 1, 2, \dots, j - 1$ .

Step 3.2: Calculate

$$Y_j = X_j - \sum_{i=1}^{j-1} r_{ij}Q_i.$$

Step 3.3: Set  $r_{jj} = \sqrt{\langle X_j, X_j \rangle}$ .

Step 3.4:  $Q_j = \frac{1}{r_{jj}}Y_j$ .

Step 4.1: Return to Step 2.

Every  $m \times n$  matrix  $A$  ( $m \geq n$ ) can be factored into the product of a matrix  $Q$  having orthonormal vectors for its columns, and an upper (right) triangular matrix  $R$ . The product

$$A = QR$$

is the **QR decomposition** of  $A$ . If  $A$  is square, then  $Q$  is unitary (i.e.,  $QQ^* = I_n$ ).

By modifying a little the Gram-Schmidt algorithm, we obtain the following algorithm which may be used in the **QR decomposition process**.

Step 1: Set  $r_{kk} = \sqrt{\langle X_k, X_k \rangle}$  and  $Q_k = \frac{1}{r_{kk}}X_k$

Step 2: For  $j = k + 1, k + 2, \dots, n$ , set  $r_{kj} = \langle Q_k, X_j \rangle$ .

Step 3: For  $j = k + 1, k + 2, \dots, n$ , replace  $X_j$  by  $X_j - r_{kj}Q_k$ .

**Example 1.** Let

$$A = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} = [A_1, A_2, A_3, A_4].$$

**First iteration:**

$$\begin{aligned} r_{11} &= \|A_1\|_2 = \sqrt{3} \\ Q_1 &= \frac{1}{r_{11}}A_1 = \frac{1}{\sqrt{3}}[0, 1, 1, 1]^T \\ r_{12} &= \langle Q_1, A_2 \rangle = \frac{2}{\sqrt{3}} \\ r_{13} &= \langle Q_1, A_3 \rangle = \frac{2}{\sqrt{3}} \\ r_{14} &= \langle Q_1, A_4 \rangle = \frac{2}{\sqrt{3}} \\ A_2 &:= A_2 - r_{12}Q_1 = \frac{1}{3}[3, -2, 1, 1]^T \\ A_3 &:= A_3 - r_{13}Q_1 = \frac{1}{3}[3, 1, -2, 1]^T \\ A_4 &:= A_4 - r_{14}Q_1 = \frac{1}{3}[3, 1, 1, -2]^T. \end{aligned}$$

**Second iteration:**

$$\begin{aligned} r_{22} &= \|A_2\|_2 = \frac{\sqrt{15}}{3} \\ Q_2 &= \frac{1}{r_{22}}A_2 = \frac{1}{\sqrt{15}}[3, -2, 1, 1]^T \\ r_{23} &= \langle Q_2, A_3 \rangle = \frac{1}{\sqrt{15}} \\ r_{24} &= \langle Q_2, A_4 \rangle = \frac{2}{\sqrt{15}} \\ A_3 &:= A_3 - r_{23}Q_2 = \frac{1}{5}[3, 3, -4, 1]^T \\ A_4 &:= A_4 - r_{24}Q_2 = \frac{1}{5}[3, 3, 1, -4]^T. \end{aligned}$$

**Third iteration:**

$$\begin{aligned} r_{33} &= \|A_3\|_2 = \frac{\sqrt{35}}{5} \\ Q_3 &= \frac{1}{r_{33}}A_3 = \frac{1}{\sqrt{35}}[3, 3, -4, 1]^T \\ r_{34} &= \langle Q_3, A_4 \rangle = \frac{2}{\sqrt{35}} \\ A_4 &:= A_4 - r_{34}Q_3 = \frac{3}{7}[1, 1, 1, -2]^T. \end{aligned}$$

**Fourth iteration:**

$$\begin{aligned} r_{44} &= \|A_4\|_2 = \frac{\sqrt{63}}{7} \\ Q_4 &= \frac{1}{r_{44}}A_4 = \frac{1}{\sqrt{7}}[1, 1, 1, -2]^T. \end{aligned}$$

Thus

$$\begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 3/\sqrt{15} & 3/\sqrt{35} & 1/\sqrt{7} \\ 1/\sqrt{3} & -2/\sqrt{15} & 3/\sqrt{35} & 1/\sqrt{7} \\ 1/\sqrt{3} & 1/\sqrt{15} & -4/\sqrt{35} & 1/\sqrt{7} \\ 1/\sqrt{3} & 1/\sqrt{15} & 1/\sqrt{35} & -2/\sqrt{7} \end{pmatrix} \begin{pmatrix} \sqrt{3} & 2/\sqrt{3} & 2/\sqrt{3} & 2/\sqrt{3} \\ 0 & \sqrt{15}/3 & 2/\sqrt{15} & 2/\sqrt{15} \\ 0 & 0 & \sqrt{35}/5 & 2/\sqrt{35} \\ 0 & 0 & 0 & \sqrt{63}/7 \end{pmatrix}.$$

**Eigenvalues.** By using the **QR** decomposition algorithm we may approximate the eigenvalues of an  $n \times n$  diagonalizable matrix  $A$  (i.e.,  $A$  has  $n$  linearly independent eigenvectors). We proceed as follows:

Let  $A = A^{(0)} = Q^{(0)}R^{(0)}$ . Define  $A^{(1)} = R^{(0)}Q^{(0)}$ .

Let  $A^{(1)} = Q^{(1)}R^{(1)}$ . Define  $A^{(2)} = R^{(1)}Q^{(1)}$ .

Continuing in this manner, we generate a sequence of matrices  $A^{(k)}$  where

$$\begin{aligned} A^{(0)} &= A \\ A^{(k)} &= Q^{(k)}R^{(k)} \text{ and } A^{(k+1)} = R^{(k)}Q^{(k)}. \end{aligned}$$

Clearly,

$$A^{(k+1)} = (Q^{(k)})^{-1}R^{(k)}Q^{(k)} \quad k = 0, 1, 2, \dots$$

The sequence finally converges to a diagonal matrix. When this occurs, the diagonal entries of the matrix  $A^{(k)}$  are approximations to the eigenvalues of  $A$ , and the approximations improve as we move on in the sequence. It is important to note that unlike the various power methods and deflation methods, *repeated eigenvalues* do not necessarily cause any particular problem.

**Example 2.** For the matrix  $A = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}$  some of the elements of the sequence are as follows:

$$\begin{aligned} A^{(1)} &= \begin{pmatrix} 3.666666 & 0.235702 & 0.408248 \\ 0.235702 & 0.833333 & -0.288675 \\ 0.408248 & -0.288675 & 0.500000 \end{pmatrix} \\ A^{(2)} &= \begin{pmatrix} 3.731707 & 0.005322 & 0.034080 \\ 0.005322 & 0.982578 & -0.111553 \\ 0.034080 & -0.111553 & 0.285714 \end{pmatrix} \end{aligned}$$

$$A^{(5)} = \begin{pmatrix} 3.732050 & 0.000000 & 0.000000 \\ 0.000000 & 0.999993 & -0.002199 \\ 0.000000 & -0.002200 & 0.267956 \end{pmatrix}$$

$$A^{(7)} = \begin{pmatrix} 3.732050 & 0.000000 & 0.000000 \\ 0.000000 & 1.000000 & -0.000158 \\ 0.000000 & -0.000158 & 0.267949 \end{pmatrix}$$

$$A^{(10)} = \begin{pmatrix} 3.732050 & 0.000000 & 0.000000 \\ 0.000000 & 1.000000 & -0.000003 \\ 0.000000 & -0.000003 & 0.267949 \end{pmatrix}$$

These results seem to indicate that the sequence is converging to a diagonal matrix with diagonal entries 3.732050, 1, 0.267949. Since all the matrices in the sequence are similar, these three numbers should be approximations to the eigenvalues of  $A$ . In fact, it is not difficult to show that the eigenvalues of  $A$  are  $2+\sqrt{3}$ , 1, and  $2-\sqrt{3}$ , so the “approximations” are correct to six decimal places.

**Accelerating convergence.** Convergence of the **QR** algorithm is markedly accelerated by a shift at each iteration. We denote the (n,n) entry of  $A^{(k-1)}$  by  $s_{k-1}$ . We use the **QR** decomposition for the shifted matrix  $A^{(k-1)} - s_{k-1}I_n$ . The following example illustrates the method.

**Example 3.** Let  $A = \begin{pmatrix} 3 & 1 \\ 1 & 5 \end{pmatrix}$ .

$$A^{(0)} - 5I_2 = \begin{pmatrix} -2 & 1 \\ 1 & 0 \end{pmatrix} = Q^{(0)}R^{(0)} = \begin{pmatrix} -0.894427 & 0.447214 \\ 0.447214 & 0.894427 \end{pmatrix} \begin{pmatrix} 2.236068 & -0.894427 \\ 0 & 0.447124 \end{pmatrix}$$

$$A^{(1)} = R^{(0)}Q^{(0)} + 5I_2 = \begin{pmatrix} 2.236068 & -0.894427 \\ 0 & 0.447124 \end{pmatrix} \begin{pmatrix} -0.894427 & 0.447214 \\ 0.447214 & 0.894427 \end{pmatrix} + 5 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 2.6 & 0.2 \\ 0.2 & 5.4 \end{pmatrix}$$

$$A^{(1)} - 5.4I_2 = \begin{pmatrix} -2.8 & 0.2 \\ 0.2 & 0 \end{pmatrix} = Q^{(1)}R^{(1)} = \begin{pmatrix} -0.997459 & 0.071247 \\ 0.071247 & 0.997459 \end{pmatrix} \begin{pmatrix} 2.807134 & -0.199492 \\ 0 & 0.014249 \end{pmatrix}$$

$$\begin{aligned} A^{(2)} &= R^{(1)}Q^{(1)} + 5.4I_2 = \begin{pmatrix} 2.807134 & -0.199492 \\ 0 & 0.014249 \end{pmatrix} \begin{pmatrix} -0.997459 & 0.071247 \\ 0.071247 & 0.997459 \end{pmatrix} + 5.4 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 2.585787 & 0.001015 \\ 0.001015 & 5.414213 \end{pmatrix} \end{aligned}$$

$$\begin{aligned} A^{(2)} - 5.414213I_2 &= \begin{pmatrix} -2.828426 & 0.001015 \\ 0.001015 & 0 \end{pmatrix} = Q^{(2)}R^{(2)} \\ &= \begin{pmatrix} -1.000000 & 0.000359 \\ 0.000359 & 1.000000 \end{pmatrix} \begin{pmatrix} 2.828427 & -0.1001015 \\ 0 & 0.000000 \end{pmatrix} \end{aligned}$$

$$\begin{aligned} A^{(3)} &= R^{(2)}Q^{(2)} + 5.414214I_2 = \begin{pmatrix} 2.828427 & -0.1001015 \\ 0 & 0.000000 \end{pmatrix} \begin{pmatrix} -1.000000 & 0.000359 \\ 0.000359 & 1.000000 \end{pmatrix} + 5.414213 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 2.585786 & -0.000000 \\ 0.000000 & 5.414213 \end{pmatrix} \end{aligned}$$

It follows that the eigenvalues of  $A$  are the diagonal entries of the diagonal matrix  $A^{(3)}$ .