QR Decomposition

Every finite set of linearly independent vectors $\{X_1, X_2, \cdots, X_n\}$ may be associated with an orthonormal set of nonzero vectors $\{Q_1, Q_2, \cdots, Q_n\}$ with respect to a specific inner product $< \, , \, >$; each vector Q_k $(k = 1, 2, \cdots, n)$ 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 $r_{11} = \sqrt{< X_1, X_1 >}$.
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 $r_{ij} =< Q_i, X_j >$ for $i = 1, 2, \cdots j - 1$.
Step 3.2: Calculate

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

Step 3.3: Set $r_{jj} = \sqrt{< X_j, X_j >}$.
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 $r_{kk} = \sqrt{< X_k, X_k >}$ and $Q_k = \frac{1}{r_{kk}} X_k)$
Step 2: For $j = k + 1, k + 2, \cdots, n$, set $r_{kj} =< Q_k, X_j >$.
Step 3: For $j = k + 1, k + 2, \cdots, n$, 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:

$$
\begin{aligned}
r_{11} = ||A_1||_2 = \sqrt{3} \\
Q_1 = \frac{1}{r11}A_1 = \frac{1}{\sqrt{3}}[0,1,1,1]^T \\
r_{12} =< Q_1, A_2 >= \frac{2}{\sqrt{3}} \\
r_{13} =< Q_1, A_3 >= \frac{2}{\sqrt{3}} \\
r_{14} =< Q_1, A_4 >= \frac{2}{\sqrt{3}} \\
A_2 := A_2 - r_{12}Q_1 = \frac{1}{3}[3,-2,1,1]^T \\
A_3 := A_3 - r_{13}Q_1 = \frac{1}{3}[3,1,-2,1]^T \\
A_4 := A_4 - r_{14}Q_1 = \frac{1}{3}[3,1,1,-2]^T.
\end{aligned}
$$

Second iteration:

$$
\begin{aligned}
r_{22} = ||A_2||_2 = \frac{\sqrt{15}}{3} \\
Q_2 = \frac{1}{r22}A_2 = \frac{1}{\sqrt{15}}[3,-2,1,1]^T \\
r_{23} =< Q_2, A_3 >= \frac{1}{\sqrt{15}} \\
r_{24} =< Q_2, A_4 >= \frac{2}{\sqrt{15}} \\
A_3 := A_3 - r_{23}Q_2 = \frac{1}{5}[3,3,-4,1]^T \\
A_4 := A_4 - r_{24}Q_2 = \frac{1}{5}[3,3,1,-4]^T.
\end{aligned}
$$

Third iteration:

$$
\begin{aligned}
r_{33} = ||A_3||_2 = \frac{\sqrt{35}}{5} \\
Q_3 = \frac{1}{r33}A_3 = \frac{1}{\sqrt{35}}[3,3,-4,1]^T \\
r_{34} =< Q_3, A_4 >= \frac{2}{\sqrt{35}} \\
A_4 := A_4 - r_{24}Q_3 = \frac{3}{7}[1,1,1,-2]^T.
\end{aligned}
$$

Fourth iteration:

$$
\begin{aligned}
r_{44} = ||A_4||_2 = \frac{\sqrt{63}}{7} \\
Q_4 = \frac{1}{r44}A_4 = \frac{1}{\sqrt{7}}[1,1,1,-2]^T.
\end{aligned}
$$

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

$$A^{(0)} = A$$

$$A^{(k)} = Q^{(k)}R^{(k)} \text{ and } A^{(k+1)} = R^{(k)}Q^{(k)}.$$

Clearly,

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

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:

$$A^{(1)} = \begin{pmatrix} 3.666666 & 0.235702 & 0.408248 \\ 0.235702 & 0.833333 & -0.288675 \\ 0.408248 & -0.288675 & 0.500000 \end{pmatrix}$$

$$A^{(2)} = \begin{pmatrix} 3.731707 & 0.005322 & 0.034080 \\ 0.005322 & 0.982578 & -0.111553 \\ 0.034080 & -0.111553 & 0.285714 \end{pmatrix}$$

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

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

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

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 $A^{(3)}$.