QR Factorization and Householder Matrices

The QR factorization is the decomposition $A = QR$, where $Q$ is an orthogonal matrix ($Q^{-1} = Q^T$) and $R$ is a right (i.e., upper) triangular matrix. We could use Gram-Schmidt to factor $A = QR$, but using Householder matrices is more robust and faster.

The Householder matrix for a reflection about the hyper-plane perpendicular to a vector $u$ is

$$H = I - \frac{2uu^T}{||u||^2} = I - 2\hat{u}\hat{u}^T$$

where $\hat{u}$ is a unit vector. Note that $H$ is symmetric ($H^T = H$) and orthogonal ($H^{-1} = H^T H = H^2 = I$).

$H$ is used to change the columns of $A$ into the columns of $R$. If $a = [a_1 \ a_2 \ \cdots \ a_n]^T$ and $r = [||a|| \ 0 \ \cdots \ 0]^T$, then $Ha = r$ for $u = a - r$:

$$Ha = \left( I - \frac{2uu^T}{||u||^2} \right) a = a - (a - r) \frac{2(a - r)^T a}{(a - r)^T (a - r)} = a - (a - r) = r$$

since $||a|| = ||r||$. $H_1$ changes $A$ to $H_1A$ where the first column of $H_1A$ is the first column of $R$.

For the second column of $R$, $H_2$ is applied to $H_1A$ by setting $a = [0 \ a_2 \ \cdots \ a_n]^T = $ second column of $H_1A$ with 0 above the diagonal element and $r = [0 \ ||a|| \ 0 \ \cdots \ 0]^T$; then form $u = a - r$ and $H_2 = I - 2uu^T/||u||^2$. The first row and first column of $H_1A$ are unchanged in $H_2H_1A$ because the first element of $u$ is 0.

Applying this transformation to each of the first $n-1$ columns of $A$ gives

$$H_{n-1} \cdots H_1A = R, \quad A = (H_1 \cdots H_{n-1})R = QR$$

since $H_i^{-1} = H_i^T = H_i$.

Example:

$$A = \begin{bmatrix} 3 & 4 \\ 4 & 0 \end{bmatrix}, \quad a = \begin{bmatrix} 3 \\ 4 \end{bmatrix}, \quad r = \begin{bmatrix} 5 \\ 0 \end{bmatrix}, \quad u = a - r = \begin{bmatrix} -2 \\ 4 \end{bmatrix}$$
\[
H = \begin{bmatrix}
1 & 0 \\
0 & 1 \\
\end{bmatrix} - \frac{2}{20} \begin{bmatrix}
4 & -8 \\
-8 & 16 \\
\end{bmatrix} = \begin{bmatrix}
0.6 & 0.8 \\
0.8 & -0.6 \\
\end{bmatrix}, \quad HA = \begin{bmatrix}
5 & 2.4 \\
0 & 3.2 \\
\end{bmatrix} = R
\]

Note that \(H^T = H\) and that \(H^{-1} = H\).

In the QR.m and QRsteps.m codes,
\[
H = I - \rho uu^T, \quad \rho = \frac{2}{||u||^2}.
\]

The Householder reflection that zeros all but the \(k\)th component of \(x\) is constructed by
\[
\sigma = \pm ||x|| \\
u = x + \sigma e_k \\
\rho = \frac{2}{||u||^2} = \frac{1}{\sigma u_k} \\
H = I - \rho uu^T.
\]

Either sign for \(\sigma = \pm ||x||\) would work in exact arithmetic, but with roundoff error it is best to choose \(\text{sign}\{\sigma\} = \text{sign}\{x_k\}\), so that \(x_k + \sigma\) is actually an addition rather than a subtraction.

Then instead of constructing \(H\), \(Hx\) is computed as
\[
\tau = \rho u^T x \quad Hx = x - \tau u.
\]

**QR Algorithm for Eigenvalues**

See QR.m for an example. The QR Algorithm for computing the eigenvalues of \(A\) is
- Factor \(A = QR\)
- Set \(A_1 = RQ\)
- Factor \(A_1 = Q_1 R_1\)
- Set \(A_2 = R_1 Q_1\)
- Factor \(A_2 = Q_2 R_2\)
• Set $A_3 = R_2Q_2$

until $A_k$ is upper triangular (to a certain precision) and the eigenvalues of $A$ (to the same precision) are on the diagonal of $A_k$. The algorithm preserves the eigenvalues of $A$ since $A_1 = RQ = Q^{-1}AQ$ has the same eigenvalues as $A$ (similar matrices have the same eigenvalues).

Shifting $A$ to $A - sI$ can greatly speed up the convergence of $A$ to upper triangular form:

$$A - sI = QR, \quad A_1 \equiv RQ + sI, \ldots$$

$A_1$ has the same eigenvalues as $A$ since $A_1 = RQ + sI = Q^{-1}(A - sI)Q + sI = Q^{-1}AQ$.

*Example of Convergence of the QR Method (Strang):* First note that if $A$ is symmetric, $A_k \to$ a diagonal matrix.

Next note that if $Av = \lambda v, A/c = (\lambda/c)v$ for any $c \neq 0$.

We will now scale $A$ for the QR calculation of the eigenvalues of $A$. Consider the scaled matrix $A$ where $|\theta| \ll 1$, so that $|\sin \theta| \ll 1$ and $|\cos \theta| \approx 1$:

$$A = \begin{bmatrix} \cos \theta & \sin \theta \\ \sin \theta & 0 \end{bmatrix} = \begin{bmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{bmatrix} \begin{bmatrix} 1 & \cos \theta \sin \theta \\ 0 & \sin^2 \theta \end{bmatrix} = QR.$$  

Then

$$A_1 = RQ = \begin{bmatrix} (1 + \sin^2 \theta) \cos \theta & \sin^3 \theta \\ \sin^3 \theta & -(\cos \theta \sin^2 \theta) \end{bmatrix}$$

and the off-diagonal entries of $A_k$ will rapidly go to zero.

**Householder Matrices and Hessenberg Form**

Before the QR algorithm is begun for finding the eigenvalues of $A$, usually $A$ is first transformed to Hessenberg form (upper triangular plus one subdiagonal) through Householder reflections, speeding up the convergence to upper triangular form with the eigenvalues on the diagonal.

We will consider symmetric matrices $A$, where first $A$ is transformed to tridiagonal form; then the QR algorithm transforms the tridiagonal matrix to
just the main diagonal and the superdiagonal, with the eigenvalues on the diagonal.

A symmetric matrix can be made tridiagonal through Householder transformations:

\[ A \rightarrow A_1 = H_1 A H_1 \rightarrow A_2 = H_2 A_1 H_2 \rightarrow \ldots \rightarrow A_{n-2} = H_{n-2} A_1 H_{n-2}. \]

These transformations preserve the eigenvalues of \( A \) since they are similarity transformations (\( H_i^{-1} = H_i \)). Here \( H_1 \) takes \( a = [A_{11} \cdots A_{n1}]^T \) into \( r = [A_{11} \alpha 0 \cdots 0]^T \), where \( \alpha = \sqrt{A_{21}^2 + \cdots + A_{n1}^2} \).

Example:

\[
A = \begin{bmatrix}
1 & 0 & 1 \\
0 & 1 & 2 \\
1 & 2 & 0
\end{bmatrix}, \quad a = \begin{bmatrix}
1 \\
0 \\
1
\end{bmatrix}, \quad r = \begin{bmatrix}
1 \\
1 \\
0
\end{bmatrix}, \quad u = a - r = \begin{bmatrix}
0 \\
-1 \\
1
\end{bmatrix}
\]

\[
H_1 = \begin{bmatrix}
1 & 0 & 0 \\
0 & 0 & 1 \\
0 & 1 & 0
\end{bmatrix}, \quad A_1 = H_1 A H_1 = \begin{bmatrix}
1 & 1 & 0 \\
1 & 2 & 0 \\
0 & 1 & 1
\end{bmatrix}
\]