Chapter 10

$QR$-Decomposition for Arbitrary Matrices

10.1 Orthogonal Reflections

Orthogonal symmetries are a very important example of isometries. First let us review the definition of a (linear) projection.

Given a vector space $E$, let $F$ and $G$ be subspaces of $E$ that form a direct sum $E = F \oplus G$.

Since every $u \in E$ can be written uniquely as $u = v + w$, where $v \in F$ and $w \in G$, we can define the two projections $p_F : E \to F$ and $p_G : E \to G$, such that

\[ p_F(u) = v \quad \text{and} \quad p_G(u) = w. \]
It is immediately verified that $p_G$ and $p_F$ are linear maps, and that $p_F^2 = p_F$, $p_G^2 = p_G$, $p_F \circ p_G = p_G \circ p_F = 0$, and $p_F + p_G = \text{id}$.

**Definition 10.1.** Given a vector space $E$, for any two subspaces $F$ and $G$ that form a direct sum $E = F \oplus G$, the *symmetry with respect to $F$ and parallel to $G$, or reflection about $F$* is the linear map $s : E \rightarrow E$, defined such that

$$s(u) = 2p_F(u) - u,$$

for every $u \in E$.

Because $p_F + p_G = \text{id}$, note that we also have

$$s(u) = p_F(u) - p_G(u)$$

and

$$s(u) = u - 2p_G(u),$$

$s^2 = \text{id}$, $s$ is the identity on $F$, and $s = -\text{id}$ on $G$. 

We now assume that $E$ is a Euclidean space of finite dimension.

**Definition 10.2.** Let $E$ be a Euclidean space of finite dimension $n$. For any two subspaces $F$ and $G$, if $F$ and $G$ form a direct sum $E = F \oplus G$ and $F$ and $G$ are orthogonal, i.e. $F = G^\perp$, the *orthogonal symmetry with respect to $F$ and parallel to $G$, or orthogonal reflection about $F$* is the linear map $s : E \to E$, defined such that

$$s(u) = 2p_F(u) - u,$$

for every $u \in E$.

When $F$ is a hyperplane, we call $s$ an *hyperplane symmetry with respect to $F$ or reflection about $F*, and when $G$ is a plane, we call $s$ a *flip about $F*.

It is easy to show that $s$ is an isometry.
Using Proposition 9.8, it is possible to find an orthonormal basis \((e_1, \ldots, e_n)\) of \(E\) consisting of an orthonormal basis of \(F\) and an orthonormal basis of \(G\).

Assume that \(F\) has dimension \(p\), so that \(G\) has dimension \(n - p\).

With respect to the orthonormal basis \((e_1, \ldots, e_n)\), the symmetry \(s\) has a matrix of the form

\[
\begin{pmatrix}
I_p & 0 \\
0 & -I_{n-p}
\end{pmatrix}
\]
Thus, \( \det(s) = (-1)^{n-p} \), and \( s \) is a rotation iff \( n - p \) is even.

In particular, when \( F \) is a hyperplane \( H \), we have \( p = n - 1 \), and \( n - p = 1 \), so that \( s \) is an improper orthogonal transformation.

When \( F = \{0\} \), we have \( s = -\text{id} \), which is called the symmetry with respect to the origin. The symmetry with respect to the origin is a rotation iff \( n \) is even, and an improper orthogonal transformation iff \( n \) is odd.

When \( n \) is odd, we observe that every improper orthogonal transformation is the composition of a rotation with the symmetry with respect to the origin.
When $G$ is a plane, $p = n - 2$, and $\det(s) = (-1)^2 = 1$, so that a flip about $F$ is a rotation.

In particular, when $n = 3$, $F$ is a line, and a flip about the line $F$ is indeed a rotation of measure $\pi$.

When $F = H$ is a hyperplane, we can give an explicit formula for $s(u)$ in terms of any nonnull vector $w$ orthogonal to $H$.

We get

$$s(u) = u - 2 \frac{(u \cdot w)}{\|w\|^2} w.$$

Such reflections are represented by matrices called *Householder matrices*, and they play an important role in numerical matrix analysis. Householder matrices are symmetric and orthogonal.
Over an orthonormal basis \((e_1, \ldots, e_n)\), a hyperplane reflection about a hyperplane \(H\) orthogonal to a nonnull vector \(w\) is represented by the matrix

\[
H = I_n - 2 \frac{WW^\top}{\|W\|^2} = I_n - 2 \frac{WW^\top}{W^\top W},
\]

where \(W\) is the column vector of the coordinates of \(w\).

Since

\[
p_G(u) = \frac{(u \cdot w)}{\|w\|^2} w,
\]

the matrix representing \(p_G\) is

\[
\frac{WW^\top}{W^\top W},
\]

and since \(p_H + p_G = \text{id}\), the matrix representing \(p_H\) is

\[
I_n - \frac{WW^\top}{W^\top W}.
\]
The following fact is the key to the proof that every isometry can be decomposed as a product of reflections.

**Proposition 10.1.** Let $E$ be any nontrivial Euclidean space. For any two vectors $u, v \in E$, if $\|u\| = \|v\|$, then there is an hyperplane $H$ such that the reflection $s$ about $H$ maps $u$ to $v$, and if $u \neq v$, then this reflection is unique.

We now show that Hyperplane reflections can be used to obtain another proof of the $QR$-decomposition.
10.2 QR-Decomposition Using Householder Matrices

First, we state the result geometrically. When translated in terms of Householder matrices, we obtain the fact advertised earlier that every matrix (not necessarily invertible) has a QR-decomposition.

**Proposition 10.2.** Let $E$ be a nontrivial Euclidean space of dimension $n$. Given any orthonormal basis $(e_1, \ldots, e_n)$, for any $n$-tuple of vectors $(v_1, \ldots, v_n)$, there is a sequence of $n$ isometries $h_1, \ldots, h_n$, such that $h_i$ is a hyperplane reflection or the identity, and if $(r_1, \ldots, r_n)$ are the vectors given by

$$r_j = h_n \circ \cdots \circ h_2 \circ h_1(v_j),$$

then every $r_j$ is a linear combination of the vectors $(e_1, \ldots, e_j)$, $(1 \leq j \leq n)$. Equivalently, the matrix $R$ whose columns are the components of the $r_j$ over the basis $(e_1, \ldots, e_n)$ is an upper triangular matrix. Furthermore, the $h_i$ can be chosen so that the diagonal entries of $R$ are nonnegative.
Remarks. (1) Since every $h_i$ is a hyperplane reflection or the identity, 

$$\rho = h_n \circ \cdots \circ h_2 \circ h_1$$

is an isometry.

(2) If we allow negative diagonal entries in $R$, the last isometry $h_n$ may be omitted.

(3) Instead of picking $r_{k,k} = \|u''_k\|$, which means that

$$w_k = r_{k,k} e_k - u''_k,$$

where $1 \leq k \leq n$, it might be preferable to pick $r_{k,k} = -\|u''_k\|$ if this makes $\|w_k\|^2$ larger, in which case

$$w_k = r_{k,k} e_k + u''_k.$$

Indeed, since the definition of $h_k$ involves division by $\|w_k\|^2$, it is desirable to avoid division by very small numbers.

Proposition 10.2 immediately yields the $QR$-decomposition in terms of Householder transformations.
Theorem 10.3. For every real $n \times n$-matrix $A$, there is a sequence $H_1, \ldots, H_n$ of matrices, where each $H_i$ is either a Householder matrix or the identity, and an upper triangular matrix $R$, such that

$$R = H_n \cdots H_2 H_1 A.$$  

As a corollary, there is a pair of matrices $Q, R$, where $Q$ is orthogonal and $R$ is upper triangular, such that $A = QR$ (a QR-decomposition of $A$). Furthermore, $R$ can be chosen so that its diagonal entries are non-negative.

Remarks. (1) Letting

$$A_{k+1} = H_k \cdots H_2 H_1 A,$$

with $A_1 = A$, $1 \leq k \leq n$, the proof of Proposition 10.2 can be interpreted in terms of the computation of the sequence of matrices $A_1, \ldots, A_{n+1} = R$. 
The matrix $A_{k+1}$ has the shape

$$A_{k+1} = \begin{pmatrix}
\times & \times & \times & \mathbf{u}_1^{k+1} & \times & \times & \times & \times \\
0 & \times & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & \times & \mathbf{u}_k^{k+1} & \times & \times & \times & \times \\
0 & 0 & 0 & \mathbf{u}_{k+1}^{k+1} & \times & \times & \times & \times \\
0 & 0 & 0 & \mathbf{u}_{k+2}^{k+1} & \times & \times & \times & \times \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \mathbf{u}_{n-1}^{k+1} & \times & \times & \times & \times \\
0 & 0 & 0 & \mathbf{u}_n^{k+1} & \times & \times & \times & \times 
\end{pmatrix}$$

where the $(k + 1)$th column of the matrix is the vector

$$\mathbf{u}_{k+1} = h_k \circ \cdots \circ h_2 \circ h_1(v_{k+1}),$$

and thus

$$\mathbf{u}'_{k+1} = (u_1^{k+1}, \ldots, u_k^{k+1}),$$

and

$$\mathbf{u}''_{k+1} = (u_{k+1}^{k+1}, u_{k+2}^{k+1}, \ldots, u_n^{k+1}).$$

If the last $n - k - 1$ entries in column $k + 1$ are all zero, there is nothing to do and we let $H_{k+1} = I$. 
Otherwise, we kill these $n - k - 1$ entries by multiplying $A_{k+1}$ on the left by the Householder matrix $H_{k+1}$ sending $(0, \ldots, 0, u_{k+1}^{k+1}, \ldots, u_n^{k+1})$ to $(0, \ldots, 0, r_{k+1,k+1}, 0, \ldots, 0)$, where
\[ r_{k+1,k+1} = \| (u_{k+1}^{k+1}, \ldots, u_n^{k+1}) \| . \]

(2) If we allow negative diagonal entries in $R$, the matrix $H_n$ may be omitted ($H_n = I$).

(3) If $A$ is invertible and the diagonal entries of $R$ are positive, it can be shown that $Q$ and $R$ are unique.
(4) The method allows the computation of the determinant of $A$. We have
\[
\det(A) = (-1)^m r_{1,1} \cdots r_{n,n},
\]
where $m$ is the number of Householder matrices (not the identity) among the $H_i$.

(5) The condition number of the matrix $A$ is preserved. This is very good for numerical stability.