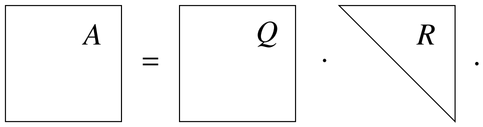
2.3.6 QR Decomposition

Each real symmetric $N \times N$ matrix A can be decomposed into

$$A = Q \cdot R \, , \tag{2.98}$$

where Q is an orthonormal $N{\times}N$ matrix ($Q{\cdot}Q^{\mathrm{T}} = \mathbb{1}$) and where R is an (upper) triangular matrix,



The matrix Q can be obtained either from the Gram-Schmidt orthogonization procedure applied to the columns of A, or it can be obtained via a sequence of Householder transformations that successively remove the column entries below the diagonal of A.

In index representation, the equation $A = Q \cdot R$ reads

$$a_{ij} = \sum_{k=1}^{j} q_{ik} r_{kj} \, . \tag{2.99}$$

Seeing the $A = (\vec{a}_1, \vec{a}_2, \ldots, \vec{a}_N)$ and $Q = (\vec{q}_1, \vec{q}_2, \ldots, \vec{q}_N)$ as matrices composed of column vectors, then the vectors $\vec{a}_i = (a_{i1}, \ldots, a_{iN})^{\mathrm{T}}$ can be seen as linear combination of the vectors $\vec{q}_i = (q_{i1}, \ldots, q_{iN})^{\mathrm{T}}$, and vice versa.

The desired similarity transformation becomes

$$A \quad \longrightarrow Q^{-1} \cdot A \cdot Q = Q^{\mathrm{T}} \cdot A \cdot Q = R \cdot Q \, , \tag{2.100}$$

where we have used $Q^{-1} = Q^{\mathrm{T}}$ (Q is orthogonal) for the first step, and $R = Q^{\mathrm{T}} \cdot A$ in the second. From (2.46) we conclude that this mapping leaves the eigenvalues unchanged.

The transformation (2.100) can be repeated several times to transform the matrix A into the desired form. In many cases, the sequence

$$A_s = Q_s \cdot R_s \longrightarrow A_{s+1} = R_s \cdot Q_s = Q_s^{\mathrm{T}} \cdot A_s \cdot Q_s$$

converges to an upper triangular matrix (Schur form of A). Then we can simply read off the eigenvalues on the diagonal.

Note, are all eigenvalues of A different (non-degenerate) then the sequence A_{s+1} converges to an upper triangular matrix. Are some eigenvalues equal (their absolute value), then there remains a block of order M on the diagonal, where M is the degree of degeneracy of the eigenvalue.

The effort is

$\boldsymbol{N^3}$ for general matrices,

$\boldsymbol{N^2}$ for matrices in Hessenberg form (2.97),

$\boldsymbol{N}$ for tridiagonal matrices. This is the reason, why the QR method is often combined with the Householder transformation.

The overall procedure is a follows:

First, one calculates the QR decomposition $A = Q \cdot R$.

Then, one does the RQ transformation $A' = R \cdot Q = Q^{\mathrm{T}} \cdot A \cdot Q$.

Because R is (◹), A' can simply be obtained by back-substitution.

The remaining question is how to do the first step in this procedure, how to calculate the QR decomposition. As mentioned before, this can be achieved either by Gram-Schmidt orthogonalization, or by a Householder transformation.

Calculation with the Gram-Schmidt method:

As discussed in Section 2.3.1, we can always obtain an orthogonal set of column vectors for a quadratic matrix of full rank with the help of the Gram-Schmidt orthogonalization method.

We start with the matrix $A = (\vec{a}_1, \vec{a}_2, \ldots, \vec{a}_N)$ with the column vectors

$$\vec{a}_1 = \begin{pmatrix} a_{11} \\ a_{12} \\ \vdots \\ a_{1N} \end{pmatrix} \qquad \vec{a}_2 = \begin{pmatrix} a_{21} \\ a_{22} \\ \vdots \\ a_{2N} \end{pmatrix} \qquad \ldots \qquad \vec{a}_N = \begin{pmatrix} a_{N1} \\ a_{N2} \\ \vdots \\ a_{NN} \end{pmatrix} ,$$

and recall the projection operator (2.36),

$$\mathrm{Proj}_{\vec{e}}\,\vec{v} = \frac{\langle \vec{e}, \vec{v} \rangle}{\langle \vec{e}, \vec{e} \rangle}\vec{e} \quad \text{with} \quad \langle \vec{e}, \vec{a} \rangle = \vec{e}^{\,\mathrm{T}} \cdot \vec{a} = \sum_{i}^{N} e_i \, a_i \, . \tag{2.101}$$

With that, we can define a new orthogonal base:

$$
\begin{aligned}
\vec{u}_1 &= \vec{a}_1 & \& \qquad \vec{e}_1 &= \frac{\vec{u}_1}{||\vec{u}_1||} \\
\vec{u}_2 &= \vec{a}_2 - \mathrm{Proj}_{\vec{e}_1} \vec{a}_2 & \& \qquad \vec{e}_2 &= \frac{\vec{u}_2}{||\vec{u}_2||} \\
\vec{u}_3 &= \vec{a}_3 - \mathrm{Proj}_{\vec{e}_1} \vec{a}_3 - \mathrm{Proj}_{\vec{e}_2} \vec{a}_3 & \& \qquad \vec{e}_3 &= \frac{\vec{u}_3}{||\vec{u}_3||} \\
& & \vdots & \\
\vec{u}_i &= \vec{a}_i - \sum_{j=1}^{i-1} \mathrm{Proj}_{\vec{e}_j} \vec{a}_i & \& \qquad \vec{e}_i &= \frac{\vec{u}_i}{||\vec{u}_i||}
\end{aligned}
$$

Resorting gives us

$$
\begin{aligned}
\vec{a}_1 &= ||\vec{u}_1||\, \vec{e}_1 \\
\vec{a}_2 &= ||\vec{u}_2||\, \vec{e}_2 + \mathrm{Proj}_{\vec{e}_1} \vec{a}_2 \\
\vec{a}_3 &= ||\vec{u}_3||\, \vec{e}_3 + \mathrm{Proj}_{\vec{e}_1} \vec{a}_2 + \mathrm{Proj}_{\vec{e}_2} \vec{a}_3 \\
&\vdots \\
\vec{a}_i &= ||\vec{u}_i||\, \vec{e}_3 + \sum_{j=1}^{i-1} \mathrm{Proj}_{\vec{e}_j} \vec{a}_i \,,
\end{aligned}
$$

or more elegantly from $\langle \vec{e}_i, \vec{e}_j \rangle = \delta_{ij}$,

$$
\begin{array}{rcllllll}
\vec{a}_1 &=& \vec{e}_1\, ||\vec{u}_1|| & & & & \\
\vec{a}_2 &=& \vec{e}_1 \langle \vec{e}_1, \vec{a}_2 \rangle & + \vec{e}_2\, ||\vec{u}_2|| & & & \\
\vec{a}_3 &=& \vec{e}_1 \langle \vec{e}_1, \vec{a}_3 \rangle & + \vec{e}_2 \langle \vec{e}_2, \vec{a}_3 \rangle & + \vec{e}_3\, ||\vec{u}_3|| & & \\
\vec{a}_4 &=& \vec{e}_1 \langle \vec{e}_1, \vec{a}_4 \rangle & + \vec{e}_2 \langle \vec{e}_2, \vec{a}_4 \rangle & + \vec{e}_3 \langle \vec{e}_3, \vec{a}_4 \rangle & + \vec{e}_4\, ||\vec{u}_4|| & \\
\vdots & & & & & & \\
\vec{a}_N &=& \vec{e}_1 \langle \vec{e}_1, \vec{a}_N \rangle & + \vec{e}_2 \langle \vec{e}_2, \vec{a}_N \rangle & + \vec{e}_3 \langle \vec{e}_3, \vec{a}_N \rangle & + \quad \ldots & + \vec{e}_N\, ||\vec{u}_N|| \,.
\end{array}
$$

This means, that the right-hand side of (2.98) is

$$
Q \cdot R = (\vec{e}_1, \vec{e}_2, \ldots, \vec{e}_N) \cdot \begin{pmatrix} ||\vec{u}_1|| & \langle \vec{e}_1, \vec{a}_2 \rangle & \langle \vec{e}_1, \vec{a}_3 \rangle & \ldots & \langle \vec{e}_1, \vec{a}_N \rangle \\ & ||\vec{u}_2|| & \langle \vec{e}_2, \vec{a}_3 \rangle & \ldots & \langle \vec{e}_2, \vec{a}_N \rangle \\ & & ||\vec{u}_3|| & \ldots & \langle \vec{e}_3, \vec{a}_N \rangle \\ & & & \ddots & \vdots \\ & & & & ||\vec{u}_N|| \end{pmatrix} . \tag{2.102}
$$

Because of $\langle \vec{e}_i, \vec{a}_i \rangle = \|\vec{u}_i\|$ and $\langle \vec{e}_i, \vec{a}_j \rangle = 0$ for $i > j$ we get the simple expression

$$R = Q^{\mathrm{T}} \cdot A \;=\; \begin{pmatrix} \langle \vec{e}_1, \vec{a}_1 \rangle & \langle \vec{e}_1, \vec{a}_2 \rangle & \langle \vec{e}_1, \vec{a}_3 \rangle & \dots & \langle \vec{e}_1, \vec{a}_N \rangle \\ & \langle \vec{e}_2, \vec{a}_2 \rangle & \langle \vec{e}_2, \vec{a}_3 \rangle & \dots & \langle \vec{e}_2, \vec{a}_N \rangle \\ & & \langle \vec{e}_3, \vec{a}_3 \rangle & \dots & \langle \vec{e}_3, \vec{a}_N \rangle \\ & & & \ddots & \vdots \\ & & & & \langle \vec{e}_N, \vec{a}_N \rangle \end{pmatrix} . \tag{2.103}$$

Calculation of the matrices Q and R with the Householder method:

Recall from Section 2.3.5 the projection matrix (2.86),

$$P = \mathbb{1} - 2\,\vec{w} \cdot \vec{w}^{\mathrm{T}} \quad \text{with} \quad \vec{w} = \frac{\vec{x} - \|\vec{x}\|\vec{e}_1}{\|\vec{x} - \|\vec{x}\|\vec{e}_1\|} .$$

For the $N \times N$ matrix $A = (\vec{x}_1, \vec{a}_2, \dots, \vec{x}_N)$ and $\vec{x} = \vec{a}_1$ we have after the first step

$$P_1 \cdot A \;=\; \left(\begin{array}{c|cccc} \|\vec{a}_1\| & * & * & \dots & * \\ \hline 0 & & & & \\ 0 & & & & \\ \vdots & & A' & & \\ 0 & & & & \end{array}\right) . \tag{2.104}$$

The second Householder step give us

$$P_2 \cdot (P_1\, A) \;=\; \left(\begin{array}{c|c|ccc} \|\vec{a}_1\| & * & * & \dots & * \\ \hline 0 & \|\vec{a}_2\| & * & \dots & * \\ \cline{2-5} 0 & 0 & & & \\ \vdots & \vdots & & A'' & \\ 0 & 0 & & & \end{array}\right) . \tag{2.105}$$

The upper triangular matrix R is then simply the result of the sequence

$$R = P_N\, P_{N-1}\, \dots\, P_2\, P_1\, A\,, \tag{2.106}$$

while the orthogonal matrix Q follows as

$$Q = P_1^{\mathrm{T}}\, P_2^{\mathrm{T}}\, \dots\, P_{N-1}^{\mathrm{T}}\, P_N^{\mathrm{T}} . \tag{2.107}$$

From $P_i^{\mathrm{T}}\, P_i = \mathbb{1}$ it immediately follows that $Q \cdot R = A$.