Numerical Analysis MATH50003 (2025–26) Problem Sheet 6

We explore simple rotations, reflections, and the properties of orthogonal/unitary matrices. We also see how reflections can be used to introduce zeros into a matrix. This leads to an algorithm for computing the QR factorisation of a matrix.

We begin with some simple examples of 2×2 rotations:

Problem 1 What simple rotation matrices $Q_1, Q_2 \in SO(2)$ have the property that:

$$Q_1 \begin{bmatrix} 1 \\ 2 \end{bmatrix} = \begin{bmatrix} \sqrt{5} \\ 0 \end{bmatrix}, Q_2 \begin{bmatrix} \sqrt{5} \\ 2 \end{bmatrix} = \begin{bmatrix} 3 \\ 0 \end{bmatrix}$$

SOLUTION

The rotation that takes $[x, y]$ to the x-axis is

$$\frac{1}{\sqrt{x^2+y^2}} \begin{bmatrix} x & y \\ -y & x \end{bmatrix}.$$

Hence we get

$$Q_1 = \frac{1}{\sqrt{5}} \begin{bmatrix} 1 & 2 \\ -2 & 1 \end{bmatrix}$$
$$Q_2 = \frac{1}{3} \begin{bmatrix} \sqrt{5} & 2 \\ -2 & \sqrt{5} \end{bmatrix}$$

END

We now look for specific examples of Householder reflections. These have the important property that they introduce zeros below the top entry, a feature that will be used in the development of an algorithm for the QR factorisation:

Problem 2 Consider the vectors

$$\boldsymbol{a} = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} \qquad \text{and} \qquad \boldsymbol{b} = \begin{bmatrix} 1 \\ 2\mathrm{i} \\ 2 \end{bmatrix}.$$

Use reflections to determine the entries of orthogonal/unitary matrices Q_1, Q_2, Q_3 such that

$$Q_1 \boldsymbol{a} = \begin{bmatrix} 3 \\ 0 \\ 0 \end{bmatrix}, Q_2 \boldsymbol{a} = \begin{bmatrix} -3 \\ 0 \\ 0 \end{bmatrix}, Q_3 \boldsymbol{b} = \begin{bmatrix} -3 \\ 0 \\ 0 \end{bmatrix}$$

SOLUTION

For Q_1: we have

$$
\begin{aligned}
\boldsymbol{y} &= \boldsymbol{a} - \|\boldsymbol{a}\|\boldsymbol{e}_1 = \begin{bmatrix} -2 \\ 2 \\ 2 \end{bmatrix} \\
\boldsymbol{w} &= \frac{\boldsymbol{y}}{\|\boldsymbol{y}\|} = \frac{1}{\sqrt{3}} \begin{bmatrix} -1 \\ 1 \\ 1 \end{bmatrix} \\
Q_1 = Q_{\boldsymbol{w}} &= I - \frac{2}{3} \begin{bmatrix} -1 \\ 1 \\ 1 \end{bmatrix} [-1 \ 1 \ 1] = I - \frac{2}{3} \begin{bmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{bmatrix} \\
&= \frac{1}{3} \begin{bmatrix} 1 & 2 & 2 \\ 2 & 1 & -2 \\ 2 & -2 & 1 \end{bmatrix}
\end{aligned}
$$

For Q_2: we have

$$
\begin{aligned}
\boldsymbol{y} &= \boldsymbol{a} + \|\boldsymbol{a}\|\boldsymbol{e}_1 = \begin{bmatrix} 4 \\ 2 \\ 2 \end{bmatrix} \\
\boldsymbol{w} &= \frac{\boldsymbol{y}}{\|\boldsymbol{y}\|} = \frac{1}{\sqrt{6}} \begin{bmatrix} 2 \\ 1 \\ 1 \end{bmatrix} \\
Q_2 = Q_{\boldsymbol{w}} &= I - \frac{1}{3} \begin{bmatrix} 2 \\ 1 \\ 1 \end{bmatrix} [2 \ 1 \ 1] = I - \frac{1}{3} \begin{bmatrix} 4 & 2 & 2 \\ 2 & 1 & 1 \\ 2 & 1 & 1 \end{bmatrix} \\
&= \frac{1}{3} \begin{bmatrix} -1 & -2 & -2 \\ -2 & 2 & -1 \\ -2 & -1 & 2 \end{bmatrix}
\end{aligned}
$$

For Q_3 we just need to be careful to conjugate:

$$
\begin{aligned}
\boldsymbol{y} &= \boldsymbol{b} + \|\boldsymbol{b}\|\boldsymbol{e}_1 = \begin{bmatrix} 4 \\ 2\mathrm{i} \\ 2 \end{bmatrix} \\
\boldsymbol{w} &= \frac{\boldsymbol{y}}{\|\boldsymbol{y}\|} = \frac{1}{\sqrt{6}} \begin{bmatrix} 2 \\ \mathrm{i} \\ 1 \end{bmatrix} \\
Q_3 = Q_{\boldsymbol{w}} &= I - \frac{1}{3} \begin{bmatrix} 2 \\ \mathrm{i} \\ 1 \end{bmatrix} [2 \ -\mathrm{i} \ 1] = I - \frac{1}{3} \begin{bmatrix} 4 & -2\mathrm{i} & 2 \\ 2\mathrm{i} & 1 & \mathrm{i} \\ 2 & -\mathrm{i} & 1 \end{bmatrix} \\
&= \frac{1}{3} \begin{bmatrix} -1 & 2\mathrm{i} & -2 \\ -2\mathrm{i} & 2 & -\mathrm{i} \\ -2 & \mathrm{i} & 2 \end{bmatrix}
\end{aligned}
$$

END

In the notes we discussed properties of orthogonal/unitary matrices. Here we prove these properties, which will be used in subsequent proofs. These problems also introduce an important concept of a normal matrix: one which commutes with its adjoint. Both symmetric and orthogonal/unitary matrices are normal. Note that normal matrices are diagonalisable via unitary matrices (an example of *the spectral theorem*).

Problem 3(a) Show for a unitary matrix $Q \in U(n)$ and a vector $\boldsymbol{x} \in \mathbb{C}^n$ that multiplication by Q preserve the 2-norm: $\|Q\boldsymbol{x}\| = \|\boldsymbol{x}\|$.

SOLUTION

$$\|Q\boldsymbol{x}\|^2 = (Q\boldsymbol{x})^\star Q\boldsymbol{x} = \boldsymbol{x}^\star Q^\star Q\boldsymbol{x} = \boldsymbol{x}^\star\boldsymbol{x} = \|\boldsymbol{x}\|^2$$

END

Problem 3(b) Show that the eigenvalues λ of a unitary matrix Q are on the unit circle: $|\lambda| = 1$. Hint: recall for any eigenvalue λ that there exists a unit eigenvector $\boldsymbol{v} \in \mathbb{C}^n$ (satisfying $\|\boldsymbol{v}\| = 1$).

SOLUTION Let $\boldsymbol{v}$ be a unit eigenvector corresponding to λ: $Q\boldsymbol{v} = \lambda\boldsymbol{v}$ with $\|\boldsymbol{v}\| = 1$. Then

$$1 = \|\boldsymbol{v}\| = \|Q\boldsymbol{v}\| = \|\lambda\boldsymbol{v}\| = |\lambda|.$$

END

Problem 3(c) Show for an orthogonal matrix $Q \in O(n)$ that $\det Q = \pm 1$. Give an example of $Q \in U(n)$ such that $\det Q \neq \pm 1$. Hint: recall for any real matrices A and B that $\det A = \det A^\top$ and $\det(AB) = \det A \det B$.

SOLUTION

$$(\det Q)^2 = (\det Q^\top)(\det Q) = \det Q^\top Q = \det I = 1.$$

An example would be a 1×1 complex-valued matrix $\exp(\mathrm{i})$.

END

Problem 3(d) A normal matrix commutes with its adjoint. Show that $Q \in U(n)$ is normal.

SOLUTION

$$QQ^\star = I = Q^\star Q$$

END

Problem 3(e) The spectral theorem states that any normal matrix is unitarily diagonalisable: if A is normal then $A = V\Lambda V^\star$ where $V \in U(n)$ and Λ is diagonal. Use this to show that $Q \in U(n)$ is equal to I if and only if all its eigenvalues are 1.

SOLUTION

Note that Q is normal and therefore by the spectral theorem for normal matrices we have

$$Q = V\Lambda V^\star = VV^\star = I$$

since V is unitary.

END

We now turn to QR factorisation beginning with an example that can be done by hand. (This example was very delicately chosen; so this problem is not examinable but does help to understand how the QR factorisation works and its relationship to the reduced QR factorisation.)

Problem 4 Use Householder reflections to compute QR and reduce QR factorisations of the matrix

$$A = \begin{bmatrix} -1 & 2 \\ 2 & 4 \\ 2 & 3 \end{bmatrix}.$$

SOLUTION Because the first entry has negative sign we have

$$\boldsymbol{y}_1 = \begin{pmatrix} -1 \\ 2 \\ 2 \end{pmatrix} - 3 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} -4 \\ 2 \\ 2 \end{pmatrix} \Rightarrow \boldsymbol{w}_1 = \frac{1}{\sqrt{6}} \begin{pmatrix} -2 \\ 1 \\ 1 \end{pmatrix}.$$

Hence

$$Q_1 = I - 2\boldsymbol{w}_1\boldsymbol{w}_1^\top = \begin{bmatrix} -1 & 2 & 2 \\ 2 & 2 & -1 \\ 2 & -1 & 2 \end{bmatrix} /3$$

Note that

$$Q_1\boldsymbol{a}_2 = \boldsymbol{a}_2 - \frac{1}{3}\begin{pmatrix} -2 \\ 1 \\ 1 \end{pmatrix}(-4+4+3) = \begin{pmatrix} 4 \\ 3 \\ 2 \end{pmatrix}.$$

thus

$$A = Q_1 \begin{pmatrix} 3 & 4 \\ & 3 \\ & 2 \end{pmatrix}$$

Continuing we have $A_2 = [3, 2]$ hence construct

$$\boldsymbol{y}_2 = \begin{pmatrix} 3 \\ 2 \end{pmatrix} + \sqrt{13}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 3+\sqrt{13} \\ 2 \end{pmatrix} \Rightarrow \boldsymbol{w}_2 = \frac{1}{\sqrt{26+6\sqrt{13}}}\begin{pmatrix} 3+\sqrt{13} \\ 2 \end{pmatrix}.$$

Hence

$$Q_2 = I - 2\boldsymbol{w}_2\boldsymbol{w}_2^\top = \begin{bmatrix} -9-3\sqrt{13} & -6-2\sqrt{13} \\ -6-2\sqrt{13} & 9+3\sqrt{13} \end{bmatrix} /(13+3\sqrt{13})$$

and we have

$$A = \underbrace{Q_1 \begin{bmatrix} 1 & \\ & Q_2 \end{bmatrix}}_{Q} \begin{bmatrix} 3 & 4 \\ & -\sqrt{13} \\ & 0 \end{bmatrix}$$

where

$$Q = \begin{bmatrix} -1 & -30-10\sqrt{13} & 6+2\sqrt{13} \\ 2 & -12-4\sqrt{13} & -21-7\sqrt{13} \\ 2 & -3-\sqrt{13} & 24+8\sqrt{13} \end{bmatrix} \begin{bmatrix} 1/3 & & \\ & 1/(3(13+3\sqrt{13})) & \\ & & 1/(3(13+3\sqrt{13})) \end{bmatrix}$$

The reduced QR factorisation comes from dropping the last column of Q and row of R:

$$A = \underbrace{\begin{bmatrix} -1 & -30-10\sqrt{13} \\ 2 & -12-4\sqrt{13} \\ 2 & -3-\sqrt{13} \end{bmatrix} \begin{bmatrix} 1/3 & \\ & 1/(3(13+3\sqrt{13})) \end{bmatrix}}_{\hat{Q}} \underbrace{\begin{bmatrix} 3 & 4 \\ & -\sqrt{13} \end{bmatrix}}_{\hat{R}}$$

END

Our last two problems concern the uniqueness of the QR factorisation.

Problem 5(a) Show that every matrix $A \in \mathbb{R}^{m\times n}$ has a QR factorisation such that the diagonal of R is non-negative. Make sure to include the case of more columns than rows (i.e. $m < n$).

SOLUTION

We first show for $m < n$ that a QR decomposition exists. Writing

$$A = [\boldsymbol{a}_1|\cdots|\boldsymbol{a}_n]$$

and taking the first m columns (so that it is square) we can write $[\boldsymbol{a}_1|\cdots|\boldsymbol{a}_m] = QR_m$. It follows that $R := Q^\star A$ is right-triangular.

We can write:

$$D = \begin{bmatrix} \operatorname{sign}(r_{11}) & & \\ & \ddots & \\ & & \operatorname{sign}(r_{pp}) \end{bmatrix}$$

where $p = \min(m, n)$ and we define $\operatorname{sign}(0) = 1$. Note that $D^\top D = I$. Thus we can write: $A = QR = QDDR$ where (QD) is orthogonal and DR is upper-triangular with positive entries.

END

Problem 5(b) Show that the QR factorisation of a square invertible matrix $A \in \mathbb{R}^{n\times n}$ is unique, provided that the diagonal of R is positive.

SOLUTION

Assume there is a second factorisation also with positive diagonal

$$A = QR = \tilde{Q}\tilde{R}$$

Then we know

$$Q^\top \tilde{Q} = R\tilde{R}^{-1}$$

Note $Q^\top \tilde{Q}$ is a product of orthogonal matrices so is also orthogonal. It's eigenvalues are the same as $R\tilde{R}^{-1}$, which is upper triangular. The eigenvalues of an upper triangular matrix are the diagonal entries, which in this case are all positive. Since all eigenvalues of an orthogonal matrix are on the unit circle (see Q1(b) above) we know all m eigenvalues of $Q^\top \tilde{Q}$ are 1. By Q1(e) above, this means that $Q^\top \tilde{Q} = I$. Hence

$$\tilde{Q} = (Q^\top)^{-1} = Q$$

and

$$\tilde{R} = (\tilde{Q})^{-1} A = R.$$

END
