

# Gram-Schmidt orthogonalization

## System of linear equations

We consider a system of linear equations of the form  $\mathbf{A} \cdot \mathbf{x} = \mathbf{y}$ , where the coefficient matrix has the form

$$\mathbf{A} = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 4 \\ 3 & 4 & 4 \end{pmatrix}$$

and the right-hand side is given by the column vector

$$\mathbf{y} = \begin{pmatrix} 1 \\ 1 \\ 2 \end{pmatrix}$$

## Solution par orthogonalization Gram-Schmidt

Construct an orthogonal matrix  $\mathbf{Q}$ , with  $\mathbf{Q}^T \cdot \mathbf{Q} = \mathbf{1}$ , such that

$$\mathbf{Q} = \mathbf{A} \cdot \mathbf{R},$$

where  $\mathbf{R}$  is *upper triangular*.

Start from the three column vectors of  $\mathbf{A}$ ,

$$\mathbf{a}_1 = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}, \quad \mathbf{a}_2 = \begin{pmatrix} 2 \\ 3 \\ 4 \end{pmatrix}, \quad \mathbf{a}_3 = \begin{pmatrix} 3 \\ 4 \\ 4 \end{pmatrix}$$

which are not orthogonal,

$$\mathbf{A}^T \cdot \mathbf{A} = \begin{pmatrix} 14 & 20 & 23 \\ 20 & 29 & 34 \\ 23 & 34 & 41 \end{pmatrix} \neq \mathbf{1}.$$

### Step 1

Take  $\mathbf{u}_1 = \mathbf{a}_1$  as first unnormalized column vector of a basis  $\{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3\}$  fulfilling  $\mathbf{u}_i^T \cdot \mathbf{u}_j = \|\mathbf{u}_i\| \|\mathbf{u}_j\| \delta_{ij}$ ,

$$\mathbf{u}_1 = \mathbf{a}_1 = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$$

Normalize this column vector and write

$$\mathbf{q}_1 = \begin{pmatrix} \frac{1}{\sqrt{14}} \\ \sqrt{\frac{2}{7}} \\ \frac{3}{\sqrt{14}} \end{pmatrix} = R_{11}\mathbf{a}_1, \text{ where } R_{11} = \frac{1}{\|\mathbf{u}_1\|} = \frac{1}{\sqrt{14}}$$

## Step 2

Construct the second unnormalized basis vector

$$\mathbf{u}_2 = \mathbf{a}_2 - (\mathbf{q}_1^T \cdot \mathbf{a}_2) \mathbf{q}_1 = \begin{pmatrix} \frac{4}{7} \\ \frac{1}{7} \\ -\frac{2}{7} \end{pmatrix}$$

and normalize,

$$\mathbf{q}_2 = \begin{pmatrix} \frac{4}{\sqrt{21}} \\ \frac{1}{\sqrt{21}} \\ -\frac{2}{\sqrt{21}} \end{pmatrix}$$

Write

$$\mathbf{q}_2 = \frac{1}{\|\mathbf{u}_2\|} (\mathbf{a}_2 - (\mathbf{q}_1^T \cdot \mathbf{a}_2) \mathbf{q}_1) = \frac{1}{\|\mathbf{u}_2\|} (\mathbf{a}_2 - (\mathbf{q}_1^T \cdot \mathbf{a}_2) (R_{11} \mathbf{a}_1)) = R_{12} \mathbf{a}_1 + R_{22} \mathbf{a}_2$$

where

$$R_{12} = -\frac{10}{\sqrt{21}}, \quad R_{22} = \sqrt{\frac{7}{3}}$$

## Step 3

Construct the third and last unnormalized basis vector

$$\mathbf{u}_3 = \mathbf{a}_3 - (\mathbf{q}_1^T \cdot \mathbf{a}_3) \mathbf{q}_1 - (\mathbf{q}_2^T \cdot \mathbf{a}_3) \mathbf{q}_2 = \begin{pmatrix} -\frac{1}{6} \\ \frac{1}{3} \\ -\frac{1}{6} \end{pmatrix}$$

and normalize,

$$\mathbf{q}_3 = \begin{pmatrix} -\frac{1}{\sqrt{6}} \\ \sqrt{\frac{2}{3}} \\ -\frac{1}{\sqrt{6}} \end{pmatrix}.$$

Write

$$\begin{aligned} \mathbf{q}_3 &= \frac{1}{\|\mathbf{u}_3\|} (\mathbf{a}_3 - (\mathbf{q}_1^T \cdot \mathbf{a}_3) \mathbf{q}_1 - (\mathbf{q}_2^T \cdot \mathbf{a}_3) \mathbf{q}_2) = \\ &= \frac{1}{\|\mathbf{u}_3\|} (\mathbf{a}_3 - (\mathbf{q}_1^T \cdot \mathbf{a}_3) (R_{11} \mathbf{a}_1) - (\mathbf{q}_2^T \cdot \mathbf{a}_3) (R_{12} \mathbf{a}_1 + R_{22} \mathbf{a}_2)) = R_{13} \mathbf{a}_1 + R_{23} \mathbf{a}_2 + R_{33} \mathbf{a}_3. \end{aligned}$$

where

$$R_{13} = \frac{13}{\sqrt{6}}, \quad R_{23} = -8 \sqrt{\frac{2}{3}}, \quad R_{33} = \sqrt{6}$$

This is the final matrix  $\mathbf{Q}$ ,

$$\mathbf{Q} = \begin{pmatrix} \frac{1}{\sqrt{14}} & \frac{4}{\sqrt{21}} & -\frac{1}{\sqrt{6}} \\ \sqrt{\frac{2}{7}} & \frac{1}{\sqrt{21}} & \sqrt{\frac{2}{3}} \\ \frac{3}{\sqrt{14}} & -\frac{2}{\sqrt{21}} & -\frac{1}{\sqrt{6}} \end{pmatrix},$$

and this is the final matrix  $\mathbf{R}$ ,

$$\mathbf{R} = \begin{pmatrix} \frac{1}{\sqrt{14}} & -\frac{10}{\sqrt{21}} & \frac{13}{\sqrt{6}} \\ 0 & \sqrt{\frac{7}{3}} & -8 \sqrt{\frac{2}{3}} \\ 0 & 0 & \sqrt{6} \end{pmatrix}.$$

Check that  $\mathbf{Q} = \mathbf{A} \cdot \mathbf{R}$  and that  $\mathbf{Q}^T \cdot \mathbf{Q} = \mathbf{Q} \cdot \mathbf{Q}^T = \mathbf{1}$ :

$$\mathbf{Q} - \mathbf{A} \cdot \mathbf{R} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

$$\mathbf{Q}^T \cdot \mathbf{Q} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

$$\mathbf{Q} \cdot \mathbf{Q}^T = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

## Inverse of $\mathbf{A}$ and solution of $\mathbf{A} \cdot \mathbf{x} = \mathbf{y}$

Since  $\mathbf{Q} = \mathbf{A} \cdot \mathbf{R}$  and  $\mathbf{Q} \cdot \mathbf{Q}^T = \mathbf{1}$  it follows that  $\mathbf{A} \cdot \mathbf{R} \cdot \mathbf{Q}^T = \mathbf{1}$ , i.e. that

$$\mathbf{A}^{-1} = \mathbf{R} \cdot \mathbf{Q}^T.$$

Check

$$\mathbf{A} \cdot \mathbf{R} \cdot \mathbf{Q}^T = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Solve

$$\mathbf{x} = \mathbf{A}^{-1} \cdot \mathbf{y} = \mathbf{R} \cdot \mathbf{Q}^T \cdot \mathbf{y} = \begin{pmatrix} -2 \\ 3 \\ -1 \end{pmatrix}.$$

Check

$$\mathbf{A} \cdot \mathbf{x} - \mathbf{y} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$