Matrix methods – QR factorisation (1)

MATH 2740 – Mathematics of Data Science – Lecture 07

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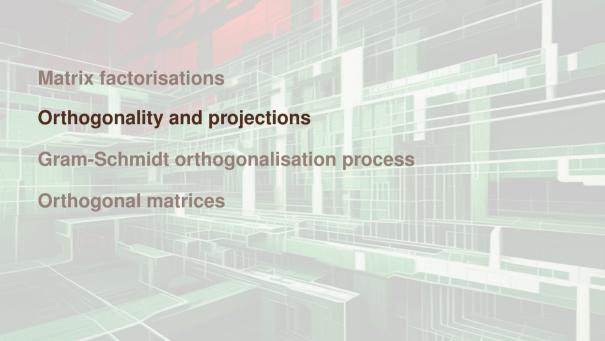
Outline

Matrix factorisations

Matrix factorisations are popular because they allow to perform some computations more easily

There are several different types of factorisations. Here, we study just the QR factorisation, which is useful for many least squares problems

Definition 1 (Orthogonal set of vectors)

The set of vectors $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k\} \in \mathbb{R}^n$ is an **orthogonal set** if

$$\forall i, j = 1, \ldots, k, \quad i \neq j \implies \boldsymbol{v}_i \bullet \boldsymbol{v}_j = 0$$

Theorem 2

$\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k\} \in \mathbb{R}^n$ with $\forall i, \boldsymbol{v}_i \neq \boldsymbol{0}$, orthogonal set $\implies \{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k\} \in \mathbb{R}^n$ linearly independent

Definition 3 (Orthogonal basis)

Let S be a basis of the subspace $W \subset \mathbb{R}^n$ composed of an orthogonal set of vectors. We say S is an **orthogonal basis** of W

Proof of Theorem 2

Assume $\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$ orthogonal set with $\mathbf{v}_i \neq \mathbf{0}$ for all $i = 1, \ldots, k$. Recall $\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$ is LI if

$$c_1 \mathbf{v}_1 + \cdots + c_k \mathbf{v}_k = \mathbf{0} \iff c_1 = \cdots = c_k = 0$$

So assume $c_1, \ldots, c_k \in \mathbb{R}$ are s.t. $c_1 \mathbf{v}_1 + \cdots + c_k \mathbf{v}_k = \mathbf{0}$. Recall that $\forall \mathbf{x} \in \mathbb{R}^k$, $\mathbf{0}_k \bullet \mathbf{x} = 0$. So for some $\mathbf{v}_i \in \{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$

$$
\begin{aligned}
0 &= \mathbf{0} \bullet \mathbf{v}_i \\
&= (c_1 \mathbf{v}_1 + \cdots + c_k \mathbf{v}_k) \bullet \mathbf{v}_i \\
&= c_1 \mathbf{v}_1 \bullet \mathbf{v}_i + \cdots + c_k \mathbf{v}_k \bullet \mathbf{v}_i
\end{aligned}
\tag{1}
$$

As $\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$ orthogonal, $\mathbf{v}_j \bullet \mathbf{v}_i = 0$ when $i \neq j$, (1) reduces to

$$c_i \mathbf{v}_i \bullet \mathbf{v}_i = 0 \iff c_i \|\mathbf{v}_i\|^2 = 0$$

As $\mathbf{v}_i \neq 0$ for all i, $\|\mathbf{v}_i\| \neq 0$ and so $c_i = 0$. This is true for all i, hence the result $\quad\square$

Example – Vectors of the standard basis of $\mathbb{R}^3$

For $\mathbb{R}^3$, we denote

$$\boldsymbol{i} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \boldsymbol{j} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \text{ and } \boldsymbol{k} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

($\mathbb{R}^k$ for $k > 3$, we denote them $\boldsymbol{e}_i$)

Clearly, $\{\boldsymbol{i}, \boldsymbol{j}\}$, $\{\boldsymbol{i}, \boldsymbol{k}\}$, $\{\boldsymbol{j}, \boldsymbol{k}\}$ and $\{\boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k}\}$ orthogonal sets. The standard basis vectors are also $\neq \boldsymbol{0}$, so the sets are LI. And

$$\{\boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k}\}$$

is an orthogonal basis of $\mathbb{R}^3$ since it spans $\mathbb{R}^3$ and is LI

$$c_1 \boldsymbol{i} + c_2 \boldsymbol{j} + c_3 \boldsymbol{k} = c_1 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + c_2 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + c_3 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

Orthonormal version of things

Definition 4 (Orthonormal set)

The set of vectors $\{v_1, \ldots, v_k\} \in \mathbb{R}^n$ is an **orthonormal set** if it is an orthogonal set and furthermore

$$\forall i = 1, \ldots, k, \quad \|v_i\| = 1$$

Definition 5 (Orthonormal basis)

A basis of the subspace $W \subset \mathbb{R}^n$ is an **orthonormal basis** if the vectors composing it are an orthonormal set

$\{v_1, \ldots, v_k\} \in \mathbb{R}^n$ is orthonormal if

$$v_i \bullet v_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

Projections

Definition 6 (Orthogonal projection onto a subspace)

$W \subset \mathbb{R}^n$ a subspace and $\{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_k\}$ an orthogonal basis of W. $\forall \boldsymbol{v} \in \mathbb{R}^n$, the **orthogonal projection** of $\boldsymbol{v}$ **onto** W is

$$\text{proj}_W(\boldsymbol{v}) = \frac{\boldsymbol{u}_1 \bullet \boldsymbol{v}}{\|\boldsymbol{u}_1\|^2} \boldsymbol{u}_1 + \cdots + \frac{\boldsymbol{u}_k \bullet \boldsymbol{v}}{\|\boldsymbol{u}_k\|^2} \boldsymbol{u}_k$$

Definition 7 (Component orthogonal to a subspace)

$W \subset \mathbb{R}^n$ a subspace and $\{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_k\}$ an orthogonal basis of W. $\forall \boldsymbol{v} \in \mathbb{R}^n$, the **component** of $\boldsymbol{v}$ **orthogonal to** W is

$$\text{perp}_W(\boldsymbol{v}) = \boldsymbol{v} - \text{proj}_W(\boldsymbol{v})$$

What this aims to do is to construct an orthogonal basis for a subspace $W \subset \mathbb{R}^n$

To do this, we use the *Gram-Schmidt orthogonalisation process*, which turn s a basis of W into an orthogonal basis of W

Gram-Schmidt process

Theorem 8

$W \subset \mathbb{R}^n$ *a subset and* $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k\}$ *a basis of W. Let*

$$\boldsymbol{v}_1 = \boldsymbol{x}_1$$

$$\boldsymbol{v}_2 = \boldsymbol{x}_2 - \frac{\boldsymbol{v}_1 \bullet \boldsymbol{x}_2}{\|\boldsymbol{v}_1\|^2} \boldsymbol{v}_1$$

$$\boldsymbol{v}_3 = \boldsymbol{x}_3 - \frac{\boldsymbol{v}_1 \bullet \boldsymbol{x}_3}{\|\boldsymbol{v}_1\|^2} \boldsymbol{v}_1 - \frac{\boldsymbol{v}_2 \bullet \boldsymbol{x}_3}{\|\boldsymbol{v}_2\|^2} \boldsymbol{v}_2$$

$$\vdots$$

$$\boldsymbol{v}_k = \boldsymbol{x}_k - \frac{\boldsymbol{v}_1 \bullet \boldsymbol{x}_k}{\|\boldsymbol{v}_1\|^2} \boldsymbol{v}_1 - \cdots - \frac{\boldsymbol{v}_{k-1} \bullet \boldsymbol{x}_k}{\|\boldsymbol{v}_{k-1}\|^2} \boldsymbol{v}_{k-1}$$

and

$$W_1 = \text{span}(\boldsymbol{x}_1), W_2 = \text{span}(\boldsymbol{x}_1, \boldsymbol{x}_2), \ldots, W_k = \text{span}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k)$$

Then $\forall i = 1, \ldots, k$, $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_i\}$ *orthogonal basis for* W_i

Theorem 9

Let $Q \in \mathcal{M}_{mn}$. The columns of Q form an orthonormal set if and only if

$$Q^T Q = \mathbb{I}_n$$

Definition 10 (Orthogonal matrix)

$Q \in \mathcal{M}_n$ is an **orthogonal matrix** if its columns form an orthonormal set

So $Q \in \mathcal{M}_n$ orthogonal if $Q^T Q = \mathbb{I}$, i.e., $Q^T = Q^{-1}$

Theorem 11 (NSC for orthogonality)

$Q \in \mathcal{M}_n$ *orthogonal* $\iff Q^{-1} = Q^T$

Theorem 12 (Orthogonal matrices "encode" isometries)

Let $Q \in \mathcal{M}_n$. TFAE

1. *Q orthogonal*
2. $\forall \boldsymbol{x} \in \mathbb{R}^n,\ \|Q\boldsymbol{x}\| = \|\boldsymbol{x}\|$
3. $\forall \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n,\ Q\boldsymbol{x} \bullet Q\boldsymbol{y} = \boldsymbol{x} \bullet \boldsymbol{y}$

Theorem 13

Let $Q \in \mathcal{M}_n$ be orthogonal. Then

1. *The rows of Q form an orthonormal set*
2. *Q^{-1} orthogonal*
3. $\det Q = \pm 1$
4. $\forall \lambda \in \sigma(Q),\ |\lambda| = 1$
5. *If $Q_2 \in \mathcal{M}_n$ also orthogonal, then QQ_2 orthogonal*

Proof of 4 in Theorem 13

All statements in Theorem 13 are easy, but let's focus on 4

Let λ be an eigenvalue of $Q \in \mathcal{M}_n$ orthogonal, i.e., $\exists \mathbb{R}^n \ni \boldsymbol{x} \neq \boldsymbol{0}$ s.t.

$$Q\boldsymbol{x} = \lambda\boldsymbol{x}$$

Take the norm on both sides

$$\|Q\boldsymbol{x}\| = \|\lambda\boldsymbol{x}\|$$

From 2 in Theorem 12, $\|Q\boldsymbol{x}\| = \|\boldsymbol{x}\|$ and from the properties of norms, $\|\lambda\boldsymbol{x}\| = |\lambda|\,\|\boldsymbol{x}\|$, so we have

$$\|Q\boldsymbol{x}\| = \|\lambda\boldsymbol{x}\| \iff \|\boldsymbol{x}\| = |\lambda|\,\|\boldsymbol{x}\| \iff 1 = |\lambda|$$

(we can divide by $\|\boldsymbol{x}\|$ since $\boldsymbol{x} \neq \boldsymbol{0}$ as an eigenvector) $\qquad\qquad\square$