

Linear Algebra

Week 10

Last time we saw:

$$x^* = \operatorname{argmin}_{x \in \mathbb{R}^n} \|Ax - b\|^2 \iff \frac{A^T A x^* = A^T b}{\text{normal equations}}$$

Single choice (only one option is correct):

- $b - Ax^*$ is orthogonal to the row space of A
- $b - Ax^*$ is orthogonal to the column space of A
- x^* is in the null space of A
- the solution x^* does not always exist

Let $A \in \mathbb{R}^{m \times n}$, $\operatorname{rank}(A) = n$:

$$\implies A^T A \in \mathbb{R}^{n \times n}, \operatorname{rank}(A^T A) = n$$

(see exercise 7.2, from $C(AT) = C(A^T A)$ we can also follow that $A^T A x = A^T b$ always has a solution)

Hence $A^T A$ is invertible. This allows us to write:

$$A^T A x = A^T b$$

$$\iff x = (A^T A)^{-1} A^T b$$

$$\iff Ax = A (A^T A)^{-1} A^T b$$

Ax is the orthogonal projection of b onto $C(A)$.

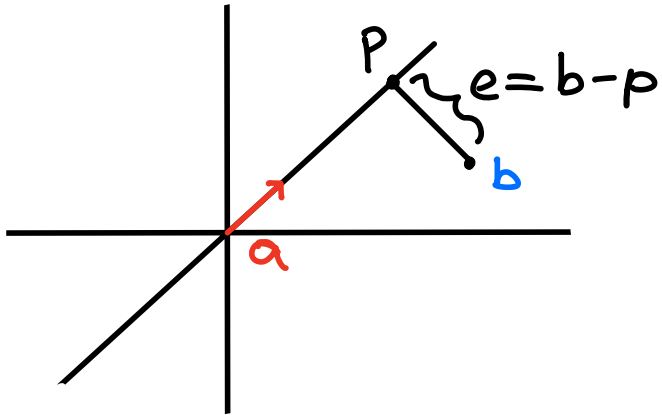
The projection matrix to project onto $C(A)$ is given by

$$P = A (A^T A)^{-1} A^T$$

Applying this formula for $A = a \in \mathbb{R}^n$, $a \neq 0$ gives us:

$$Pb = \operatorname{proj}_{\operatorname{span}(a)}(b) = a (a^T a)^{-1} a^T b = \frac{a^T b}{a^T a} a = \frac{a a^T}{a^T a} b$$

Alternatively, we could derive this similarly to how we derived the normal equations:



$$\begin{aligned} & b-p \perp a \\ \Rightarrow & a^T(b-p) = 0 \\ \Leftrightarrow & a^T b = a^T p \\ \Leftrightarrow & a^T b = a^T x a \\ \Leftrightarrow & x = \frac{a^T b}{a^T a} \\ \Leftrightarrow & a x = a \frac{a^T b}{a^T a} \end{aligned}$$

Recommendation: Compare this to the geometric definition of the dot product from week two.

Orthonormality

We call a set of vectors $\{q_1, \dots, q_n\}$ **orthonormal** if each vector in the set has length one and is orthogonal to all others in the set. We can express this as:

$$q_i^T q_j = \begin{cases} 0, & i \neq j \\ 1, & i = j \end{cases} = \delta_{ij}$$

- 1) Can you give an example of such a set?
- 2) Is any such set linearly independent?

1) An example of such a set is the canonical basis of \mathbb{R}^3 ,
 $\left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\} \rightarrow$ good baseline for finding (counter) examples

2) Yes! If $q_i \neq 0$ for all $i \in \{1, \dots, n\}$ (no vectors in the set are zero) and $q_i^T q_j = 0$ if $i \neq j$ (vectors are pairwise orthogonal)

Why are orthonormal vectors useful?

\rightarrow They make projections easier (see section on QR decomposition)
(there's also other answers to this,)
change of basis

Exercise If q_1 and q_2 are orthonormal vectors in \mathbb{R}^5 , what combination $\alpha q_1 + \beta q_2$ is closest to a given vector b ?

Solution The projection of b onto $\text{span}(q_1, q_2)$:
 $\alpha = q_1 \cdot b, \beta = q_2 \cdot b.$

We call $Q \in \mathbb{R}^{n \times n}$ **orthogonal**

$$\text{if } Q^T Q = I.$$

Important: Q has to be a square matrix and have orthonormal columns. Orthogonal columns are not sufficient.

Properties:

1. $Q^{-1} = Q^T$
2. the columns and rows of Q form orthonormal bases of \mathbb{R}^n
3. they preserve lengths: $\|Qx\| = \|x\|$

1. $Q^T Q = I$ for $Q \in \mathbb{R}^{n \times n}$ implies $Q^{-1} = Q^T$ (cf. exercise 5)

2. $(Q^T Q)_{ij} = q_i^T q_j = \delta_{ij}$ where q_i for $1 \leq i \leq n$ is a column of Q .

Hence the columns of Q are orthonormal per definition of an orthonormal set. We can apply the same argument with $Q Q^T$ and the rows of Q . There is no proof stated here but orthonormal sets are always linearly independent (pairwise orthogonality is not enough to follow this, all vectors have to be non zero too!). n linearly independent vectors in \mathbb{R}^n form a basis.

$$\begin{aligned} 3. \|Qx\| &= \sqrt{\langle Qx, Qx \rangle} = \sqrt{(Qx)^T Qx} = \sqrt{x^T Q^T Q x} = \sqrt{x^T x} \\ &= \|x\| \end{aligned}$$

What kinds of linear transformations do orthogonal matrices correspond to?

- Rotations, reflections

With the length preserving property $\|Qx\| = \|x\|$ these two are the only options!

Given are orthogonal matrices $A, B \in \mathbb{R}^{n \times n}$:

Exercise

Which of the following is true?

~~a)~~ A^T is orthogonal Proof: $A^T(A^T)^T = A^T A = I$

b) $A+B$ is orthogonal Counterexample: $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix}$

c) $A+AT$ is orthogonal Counterexample: $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$

~~d)~~ AB^{-1} is orthogonal

Proof:
$$(AB^{-1})(AB^{-1})^T = AB^{-1}(B^{-1})^T A^T$$
$$= AB^T B A^T = AA^T = I$$

The Gram-Schmidt Algorithm

input: $\{a_1, \dots, a_n\}$, linearly independent

output: $\{u_1, \dots, u_n\}$, orthonormal

$\text{span}\{u_1, \dots, u_k\} = \text{span}\{a_1, \dots, a_k\}$ for all $1 \leq k \leq n$

Pseudocode

$$u_1 = \frac{a_1}{\|a_1\|}$$

for $k=2, \dots, n$

$$\tilde{u}_k = a_k - \underbrace{\sum_{i=1}^{k-1} \langle a_k, u_i \rangle u_i}_{\substack{\text{scalar} \\ \text{product}}}$$

$$u_k = \frac{\tilde{u}_k}{\|\tilde{u}_k\|}$$

projection of a_k onto $\text{span}(u_1, \dots, u_{k-1})$

Remember it in terms of this

Demo

<https://www.desmos.com/3d/ac00d3e14b>

Exercise

$$A = \begin{bmatrix} 1 & 2 & 4 \\ 0 & 0 & 5 \\ 0 & 3 & 6 \end{bmatrix}$$

Apply the Gram-Schmidt algorithm on the columns of A collecting them in a matrix Q . Then factorize A into $A=QR$.

Solution:

$$u_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

$$\tilde{u}_2 = a_2 - \langle a_2, u_1 \rangle u_1 = \begin{bmatrix} 2 \\ 0 \\ 3 \end{bmatrix} - \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \cdot 2 = \begin{bmatrix} 0 \\ 0 \\ 3 \end{bmatrix} \Rightarrow u_2 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

$$\tilde{u}_3 = a_3 - \langle a_3, u_2 \rangle u_2 - \langle a_3, u_1 \rangle u_1 = \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix} - 6 \cdot \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} - 4 \cdot \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 5 \\ 0 \end{bmatrix} \quad u_3 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 2 & 4 \\ 0 & 3 & 6 \\ 0 & 0 & 5 \end{bmatrix}$$

Assumptions:

- $A \in \mathbb{R}^{m \times n}$
- $\text{rank}(A) = n$

$$A = Q R \quad \text{decomposition}$$

\swarrow $m \times n$ \swarrow $n \times n$

- output from Gram-Schmidt
- orthonormal columns (not always orthogonal)

- $R = Q^T b$
- upper triangular
- invertible
- $(R)_{ij} = \langle u_i, a_j \rangle$ in Gram Schmidt

What is this good for?

- Like LU decomposition for least squares

$$\begin{aligned}
 & A^T A x = A^T b \\
 \Leftrightarrow & (QR)^T Q R x = (QR)^T b && (A = QR) \\
 \Leftrightarrow & R^T Q^T Q R x = R^T Q^T b && ((AB)^T = B^T A^T) \\
 \Leftrightarrow & R^T R x = R^T Q^T b && (Q^T Q = I) \\
 \Leftrightarrow & R x = Q^T b && (\text{multiplying with } (R^T)^{-1} \text{ from left})
 \end{aligned}$$

/ solve efficiently via backward substitution

- Makes projections easier

$$\begin{aligned}
 \text{proj}_{\text{Col}(A)}(b) &= A (A^T A)^{-1} A^T b \\
 &= QR (QR)^T Q R)^{-1} (QR)^T b && (A = QR) \\
 &= QR (R^T Q^T Q R)^{-1} R^T Q^T b && ((AB)^T = B^T A^T) \\
 &= QR (R^T R)^{-1} R^T Q^T b && (Q^T Q = I) \\
 &= QR R^{-1} (R^T)^{-1} R^T Q^T b && (AB)^{-1} = B^{-1} A^{-1} \\
 &= Q Q^T b
 \end{aligned}$$

Exercise

Prove $Qx=0 \Rightarrow x=0$ when Q has orthogonal columns without saying the word linear independence.

Solution: We multiply with Q^T from the left:

$$Qx=0 \Leftrightarrow Q^T Q x = Q^T 0 = 0 \\ \Leftrightarrow x=0$$

Pseudoinverses

If there's no inverse, can we find something as close to it as possible? $\rightarrow A^+$

Let $A \in \mathbb{R}^{m \times n}$:

left inverse if full column rank: $A^+A = I$

$$A^+ = \underbrace{(A^T A)^{-1}}_{\text{invertible } n \times n \text{ matrix if rank}(A)=n} A^T \quad (1)$$

invertible $n \times n$ matrix if $\text{rank}(A)=n$

right inverse if full row rank: $AA^+ = I$

$$A^+ = A^T \underbrace{(A A^T)^{-1}}_{\text{invertible } m \times m \text{ matrix if rank}(A)=m} \quad (2)$$

invertible $m \times m$ matrix if $\text{rank}(A)=m$

General case: $\text{rank}(A)=r$

$$A^+ = R^+ C^+ \quad A = C R, \quad C \in \mathbb{R}^{m \times r}, \quad R \in \mathbb{R}^{r \times n}$$

first independent columns $r = \text{rank}(A)$ without zero rows

(holds for any full rank decomposition)

$$\begin{aligned}
A^{\dagger} &= R^{\dagger} C^{\dagger} \\
&= R^T (R R^T)^{-1} (C^T C)^{-1} C^T \quad ((1), (2) \text{ for } C, R) \\
&= R^T (C^T C R R^T)^{-1} C^T \quad ((AB)^{-1} = B^{-1} A^{-1}) \\
&= R^T (C^T A R^T)^{-1} C^T \quad (A = CR)
\end{aligned}$$

Examples

$$A_1 = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \quad A_2 = \begin{bmatrix} 2 & 0 \\ 0 & 4 \\ 0 & 0 \end{bmatrix} \quad A_3 = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 4 & 0 \end{bmatrix}$$

We apply the formula $A^{\dagger} = R^T (C^T A R^T)^{-1} C^T$ and get:

$$A_1^{\dagger} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \frac{1}{4} [1 \quad 1] = \frac{1}{4} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \quad A_2^{\dagger} = \begin{bmatrix} 1/2 & 0 & 0 \\ 0 & 1/4 & 0 \end{bmatrix}$$

$$A_3^{\dagger} = \begin{bmatrix} 1/2 & 0 \\ 0 & 1/4 \\ 0 & 0 \end{bmatrix}$$

References:

Last years course

<https://github.com/mitmath/1806>

