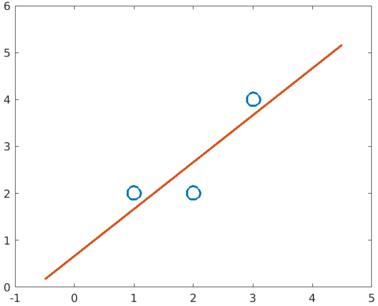
Week 11: Best Approximation and Least Squares

Dr Niall Madden

15 and 18 November, 2022



These slides are adapted (slightly) from ones by Tobias Rossmann.

Outline

For more details,

- Section 6.3 (Best Approximation) and 6.6 (Least Squares) in Lay et al: https://nuigalway-primo.hosted.exlibrisgroup.com/permalink/f/1pmb9lf/353GAL_ALMA_DS5192067630003626
- Chapters 10 and 11 of *Linear Algebra for Data Science* https://shainarace.github.io/LinearAlgebra/leastsquares.html

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PART 1: Announcements and Preview of Week 11

Assignment 5

Assignment 5 opened on Thursday 10 Nov). Deadline is 5pm, Friday, 25th of November.

Communication Skills : Next steps...

- Instructions at https://www.niallmadden.ie/2223-MA313/22_23_Communication_Skills.pdf have been updated.
- Deadline is 5pm Friday, 18 November.
- Presentations will be during the week 21–25 November:
  - Monday at 12.00 in AC204 (i.e., MA335 class time)
  - Tuesday at 13.00 in AC202 (i.e., MA313 class time)
  - Thursday at 12.00 in IT206 (i.e., MA313 tutorial time)

Next week

- Tuesday's and Thursdays classes will be used for presentations.
- Friday's class will be used to review the module and preview the exam.
- I'll also provide some sample exam-type questions, with solutions, and video.

The big ideas from this week will be solving Least Squares Problems.

- Why it is that the orthogonal projection is the best solution.
- How to find it.

These are the essential ideas from recent lectures that you need for this week.

- The **INNER PRODUCT** of vectors u and v in $\mathbb{R}^n$ is the real number given by

$$u \cdot v = u^T v = u_1 v_1 + u_2 v_2 + \cdots + u_n v_n.$$

- The **LENGTH** (or "Euclidian norm") of a vector $v \in \mathbb{R}^n$ is $\|v\| := \sqrt{v \cdot v} = \sqrt{v_1^2 + \cdots + v_n^2}$. If $\|u\| = 0$ that means all the entries in u are zero.
- The **distance** between vectors $u, v \in \mathbb{R}^n$ is $\|u - v\| = u \cdot v = u^\top v$
- $u, v \in \mathbb{R}^n$ are **orthogonal** if $u \cdot v = 0$. We may write this as $u \perp v$.
- **Pythagorean Theorem:** If $u \perp v$, then $\|u + v\|^2 = \|u\|^2 + \|v\|^2$.

- Given a subspace, W, of $\mathbb{R}^n$, the vector $z \in \mathbb{R}^n$ is **orthogonal** to W if $z \perp w$ for all $w \in W$.

- In particular, given a matrix A, if z is orthogonal to $\operatorname{Col} A$, then $a_j \perp z$ for a_j is column j of A. That is $a_j^\top z = 0$. Since this is true of any j, in fact $A^\top z = 0$.

- Every vector $v \in \mathbb{R}^n$ has a **unique representation**

$$v = \hat{v} + z \qquad \text{for } \hat{v} \in W, \qquad \text{and } z \perp W.$$

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PART 2: Orthogonal Matrices

This is actually left over from last week... I'll skim through it.

Definition: ORTHONORMAL

The vectors $u_1, \ldots, u_p \in \mathbb{R}^n$ are **orthonormal** if they are orthogonal unit vectors. That is:

- $u_i \perp u_j$ for all $i \neq j$. Equivalently, $u_i \cdot u_j = 0$ for all $i \neq j$.
- $\|u_i\| = 1$ for all i.

Note: If $u_1, \ldots, u_p$ are orthogonal and all non-zero, then $\frac{1}{\|u_1\|}u_1, \ldots, \frac{1}{\|u_p\|}u_p$ are orthonormal.

Definition: ORTHONORMAL BASIS

An **orthonormal basis** of a subspace W of $\mathbb{R}^n$ is a basis of W that consists of orthonormal vectors.

Example: The standard basis of $\mathbb{R}^n$ is orthonormal.

Theorem

Let A be an $n \times n$ matrix. Then the following are equivalent:

(a) The columns of A form an orthonormal basis of $\mathbb{R}^n$.

(b) $A^\top A = I_n = AA^\top$. (That is, A is invertible and $A^{-1} = A^\top$.)

(c) $Ax \cdot Ay = x \cdot y$ for all $x, y \in \mathbb{R}^n$.

(d) $\|Ax\| = \|x\|$ for all $x \in \mathbb{R}^n$

Definition: ORTHOGONAL MATRIX

An $n \times n$ matrix A is **orthogonal** if $A^\top A = I_n$ (in which case also $AA^\top = I_n$).

Example

- Reflections: e.g. $\begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$.
- Rotations: $\begin{bmatrix} \cos\vartheta & -\sin\vartheta \\ \sin\vartheta & \cos\vartheta \end{bmatrix}$ for $\vartheta \in \mathbb{R}$, e.g. $\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$ or $\begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$.

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PART 3: Best Approximation

What are orthogonal projections used for?

Part 3: Best Approximation

Let W by a subspace of $\mathbb{R}^n$.

The **orthogonal projection** of a vector $v \in \mathbb{R}^n$ is denoted $\hat{v} = \mathrm{proj}_W v$.

It has the property that $(v - \hat{v}) \perp W$.

Question

What are orthogonal projections good for?

Hint: take W to be a one-dimensional subspace of R^2.

Part 3: Best Approximation

Best Approximation Theorem

Let W be a subspace of $\mathbb{R}^n$. Let

$$\mathrm{proj}_W \colon \mathbb{R}^n \to W, \quad v \mapsto \hat{v}$$

be the orthogonal projection onto W. Then for any $v \in \mathbb{R}^n$,

$$\|v - \hat{v}\| \leqslant \|v - w\| \qquad \text{for any } w \in W,$$

with equality if and only if $w = \hat{v}$.
Hence: $\hat{v}$ is the unique vector in W which minimises the distance from v.

Proof

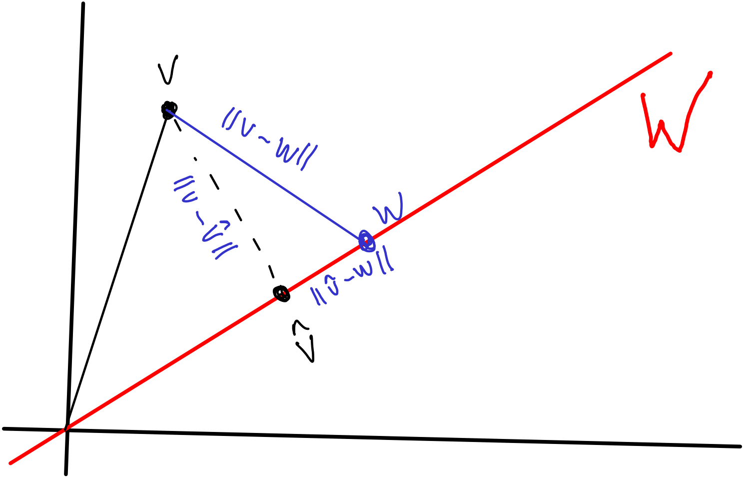
- We want to show that $\|v - \hat{v}\| \leqslant \|v - w\|$. for any $w \in W$.
- Since $\hat{v}$ is the orthogonal projection of v onto W, we know that $(v - \hat{v}) \perp W$.
- Also, both $\hat{v}$ and w are in W, so $\hat{v} - w \in W$.
- It follows that $(v - \hat{v}) \perp (\hat{v} - w)$.
- So we can apply Pythagoras' Theorem:

$$\|(v - \hat{v}) + (\hat{v} - w)\|^2 = \|v - \hat{v}\|^2 + \|\hat{v} - w\|^2.$$

- That gives $\|v - w\|^2 = \|v - \hat{v}\|^2 + \|\hat{v} - w\|^2$.
- But $\|\hat{v} - w\| \geq 0$, so we can conclude $\|v - w\|^2 \geq \|v - \hat{v}\|^2$.

(Note: see diagram on next slide).

Part 3: Best Approximation



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PART 4: Least Squares Problems

Part 4: Least Squares Problems

Motivation

Suppose that some *mathematical model* of a phenomenon predicts that it can be described by the equation of a line: $y = u_1 + u_2 x$ for some unknown coefficients $u_1, u_2 \in \mathbb{R}$.

By taking **measurements**, we find points $\begin{bmatrix} x_1 \\ y_1 \end{bmatrix}, \ldots, \begin{bmatrix} x_N \\ y_N \end{bmatrix}$ that the line should fit. Due to measurement errors, there might not be any pair u_1, u_2 with $u_1 + u_2 x_i = y_i$ for all $i = 1, \ldots, N$. The system is usually **over determined**, meaning there are too many equations to be satisfied at the same time.

There is no solution for works for all equations, so we try to find the *best approximation*.

Part 4: Least Squares Problems

Example

Suppose we wanted to find the line, $y = u_1 + u_2 x$ that best fits the data $(1, 2)$, $(2, 2)$, and $(3, 4)$. Write down a matrix-vector equation for this problem.

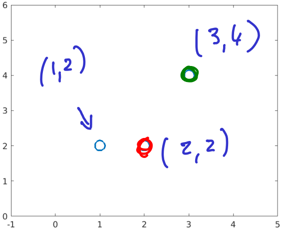
Equation is

$u_1 + u_2 x = y$.

$u_1 + u_2(1) = 2$

$u_1 + u_2(2) = 2$

$u_1 + u_2(3) = 4$



$$\begin{array}{ccc} A & u & b. \\ \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} & \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} & \begin{bmatrix} 2 \\ 2 \\ 4 \end{bmatrix} \end{array}$$

Part 4: Least Squares Problems

We would like to solve a problem $Ax = b$, meaning that we try to find x. If we could, then $\|b - Ax\| = 0$.

But there is no solution. So we try to find the $\hat{x}$ that makes $A\hat{x} - b$ as small as possible.

Defn: LINEAR LEAST-SQUARES PROBLEM

Given an $m \times n$ matrix A and a vector $b \in \mathbb{R}^m$, the associated **linear least-squares problem** is to minimise the length of the **residual** (also called "approximation error"), $\|A\hat{x} - b\|$, to an exact solution "$Ax = b$" among all vectors $x \in \mathbb{R}^n$.

More formally: A **least-squares solution** of the system "$Ax = b$" is any $\hat{x} \in \mathbb{R}^n$ such that $\|A\hat{x} - b\| \leqslant \|Ax - b\|$ for all $x \in \mathbb{R}^n$.

Part 4: Least Squares Problems

Questions

1. Is there always a choice of $\hat{x}$ which minimises $\|A\hat{x} - b\|$?
2. If so, how can we find it? [Normal Equation(s)]
3. Why is this called "least-squares"?

1 Yes: it is the best approximation problem again (but what is W?).

3. We are trying to minimize $\|Ax - b\|$

If $z = Ax - b$, this is

$$\sqrt{z_1^2 + z_2^2 + \dots + z_n^2}.$$

Part 4: Least Squares Problems

Finished here Tuesday.

Let's explain this problem in terms of the terminology we've developed recently:

1. Solving $Ax = b$ means we are trying to find the coefficients in x that allow us to express b as a linear combination of the columns of A.
2. If $b \notin \operatorname{Col} A$, then there is no solution.
3. But $\operatorname{Col} A$ is a subspace of $\mathbb{R}^n$, so we can look at the orthogonal projection of b onto $\operatorname{Col} A$. That is...

We wish to find $\hat{x} \in \mathbb{R}^n$ such that $A\hat{x}$ is the closest point to b within all of $\operatorname{Col} A$. By the Best Approximation Theorem, this means that

$$A\hat{x} = \operatorname{proj}_{\operatorname{Col} A}(b).$$

It follows that such an $\hat{x}$ exists. But how can we find it?