

Linear Algebra Recitation

Week 7

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Best approximation (Least squares)

- Let $A = \begin{bmatrix} 1 & -1 \\ -1 & 2 \\ -1 & 0 \end{bmatrix}$ and $b = \begin{bmatrix} 3 \\ 4 \\ 5 \end{bmatrix}$ Does $Ax = b$ have a solution

$x \in \mathbb{R}^2$?

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$\left[\begin{array}{cc|c} 1 & -1 & 3 \\ -1 & 2 & 4 \\ -1 & 0 & 5 \end{array} \right] \sim \left[\begin{array}{cc|c} 1 & -1 & 3 \\ 0 & 1 & 7 \\ 0 & -1 & 8 \end{array} \right] \sim \left[\begin{array}{cc|c} 1 & -1 & 3 \\ 0 & 1 & 7 \\ 0 & 0 & 15 \end{array} \right]$$

$\underbrace{\quad}_A \quad \underbrace{\quad}_b$

$$\Rightarrow x_1 - x_2 = 3$$

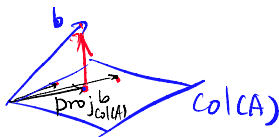
$$\begin{matrix} x_2 = 7 \\ x_2 = -8 \end{matrix} \quad \left. \begin{matrix} \\ \end{matrix} \right) (\downarrow)$$

Best approximation (Least squares)

- For a system $Ax = b$, a least squares solution, or the best approximation, gives the vector in $\text{col}(A)$ that is closest to b (i.e. minimizes $\|b - Ax\|_2$). Thus, in geometric terms, the least squares solution denoted by \hat{x} is the coordinates in terms of the basis of $\text{col}(A)$ that gives the projection vector of b , namely $A\hat{x} = \text{Proj}_{\text{col}(A)} b$.

$$Ax = \text{proj}_{\text{col}(A)} b = \hat{b}$$

$Ax = b$



$$b - A\hat{x} \in \text{col}(A)^\perp$$

- How to find \hat{x} : If \hat{x} is the least squares solution, the residual $r = b - A\hat{x}$ must be orthogonal to every vector in $\text{col}(A)$. In particular, the following must hold:

$$A^T = \begin{bmatrix} c_1^T \\ \vdots \\ c_n^T \end{bmatrix}$$

$$\begin{aligned} & \begin{bmatrix} c_1^T(b - A\hat{x}) \\ \vdots \\ c_n^T(b - A\hat{x}) \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix} \\ & \underline{A^T(b - A\hat{x}) = A^T b - A^T A\hat{x} = 0.} \end{aligned}$$

- Thus, we can solve the new system of equations $A^T A\hat{x} = A^T b$ to find \hat{x} .

Best approximation (Least squares) $Ax=b$

- Does $A^T A \hat{x} = A^T b$ (a.k.a. normal equation) have a solution? Notice that the right hand side is $A^T b \in \text{col}(A^T)$

- If $\text{col}(A^T) = \text{col}(A^T A) \implies$ there will be at least one solution!

Indeed, $A^T A v = A^T w$ $\text{rank}(A^T) = \text{rank}(A^T A)$
 $\text{col}(A^T A) \subset \text{col}(A^T)$ $\implies \text{col}(A^T A) = \text{col}(A^T)$

- If $A^T A$ has full rank, it is invertible and the least squares solution is

$\text{Proj}_{\text{col}(A)} b = A \hat{x}$ $\hat{x} = (A^T A)^{-1} A^T b$ *unique*
 $= A(A^T A)^{-1} A^T b$

- What if $A^T A$ is not full rank?: The solution \hat{x} is not unique. How do we find a least squares solution \hat{x} in this case?

\implies not a part of this course, but we use the concept of "pseudoinverses".

Best approximation (Least squares)

Back to the example problem:

- Let $A = \begin{bmatrix} 1 & -1 \\ -1 & 2 \\ -1 & 0 \end{bmatrix}$ and $b = \begin{bmatrix} 3 \\ 4 \\ 5 \end{bmatrix}$ Find the least squares solution:
namely, find \hat{x} that minimizes $\|b - Ax\|_2$.

$$(A^T A) \hat{x} = A^T b$$

$$A^T = \begin{bmatrix} 1 & -1 & -1 \\ -1 & 2 & 0 \end{bmatrix}$$

$$A^T A = \begin{bmatrix} 3 & -3 \\ -3 & 5 \end{bmatrix}$$

$$A^T b = \begin{bmatrix} -6 \\ 5 \end{bmatrix}$$

$$\begin{bmatrix} 3 & -3 \\ -3 & 5 \end{bmatrix} x = \begin{bmatrix} -6 \\ 5 \end{bmatrix}$$

$$\begin{bmatrix} 3 & -3 & -6 \\ 0 & 2 & -1 \end{bmatrix} \sim \begin{bmatrix} 1 & -1 & -2 \\ 0 & 1 & -1/2 \end{bmatrix}$$

$$\begin{aligned} x_1 - x_2 &= -2 \\ x_2 &= -1/2 \end{aligned}$$

$$x_1 = -5/2$$

$$\hat{x} = \begin{bmatrix} -5/2 \\ -1/2 \end{bmatrix}$$

Uniqueness of least squares solution

- The least squares solution is unique when $A^T A x = A^T b$ has a unique solution $\iff N(A^T A) = \{\vec{0}\}$ (trivial)

- When is $N(A^T A)$ trivial? (How is it related to $N(A)$)?

$$\textcircled{1} v \in N(A^T A) \Rightarrow A^T A v = 0 \Rightarrow v^T A^T A v = 0 \Rightarrow \|A v\|^2 = 0 \Rightarrow A v = 0 \\ \Rightarrow v \in N(A) \Rightarrow N(A^T A) \subset N(A)$$

$$\textcircled{2} u \in N(A) \Rightarrow A u = 0 \Rightarrow A^T A u = 0 \Rightarrow u \in N(A^T A) \Rightarrow N(A) \subset N(A^T A)$$

- What happens if the normal equation has infinitely many solutions?

In particular, does the value Ax change among the solutions x of the normal equation?

x, y be least squares solutions $A^T A x = A^T b = A^T A y$
is $Ax = Ay$? $x^* = x + x_N$, $x_N \in N(A^T A) = N(A)$

$Ax^* = Ax + Ax_N = Ax$ so $\text{proj}_{\text{Col}(A)}^b$ is unique
even though x^* is not unique.

$$\begin{bmatrix} 1 & 0 \\ -1 & 0 \\ -1 & 0 \end{bmatrix} X = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

A b

$$\begin{bmatrix} 3 & 0 \\ 0 & 0 \end{bmatrix} X = \begin{bmatrix} -4 \\ 0 \end{bmatrix}$$

$A^T A$ $A^T b$

$$3x_1 = -4 \Rightarrow x_1 = -\frac{4}{3}$$

$$0x_2 = 0$$

$$x_N \in N(A^T A)$$

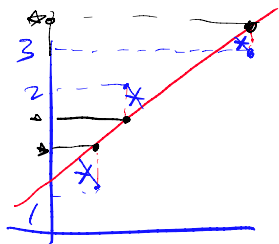
$$\begin{aligned} X &= x_p + x_N \\ &= \begin{bmatrix} -4/3 \\ 0 \end{bmatrix} + x_N \end{aligned}$$

infinitely many Least squares solutions -

Application of least squares:

Fitting a line through data.

- Suppose we want to find the line that best fits (in terms of euclidean distance) three data points $(1,1)$, $(2,2)$, $(4,3)$ in \mathbb{R}^2 . How to find this line using least squares?
- *If* there is a line $y = ax + b$ that interpolates these points exactly, what would this line do?



$$\begin{aligned}f(1) &= a + b = 1 \\f(2) &= 2a + b = 2 \\f(4) &= 4a + b = 3\end{aligned}$$
$$\begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 4 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

Application of least squares:

$$\begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 4 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

$$\begin{bmatrix} 2 & 7 \\ 7 & 3 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 17 \\ 6 \end{bmatrix}, \quad \left[\begin{array}{cc|c} 7 & 3 & 6 \\ 2 & 7 & 17 \end{array} \right] \sim \left[\begin{array}{cc|c} 7 & 3 & 6 \\ 0 & -2 & -1 \end{array} \right]$$

$$7a + 3b = 6 \quad b = 1/2$$

$$a = \frac{1}{7} \left(\frac{9}{2} \right) = 9/14$$

$$y = \frac{9}{14}x + 1/2$$