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1. Approximate Solutions to Inconsistent Systems

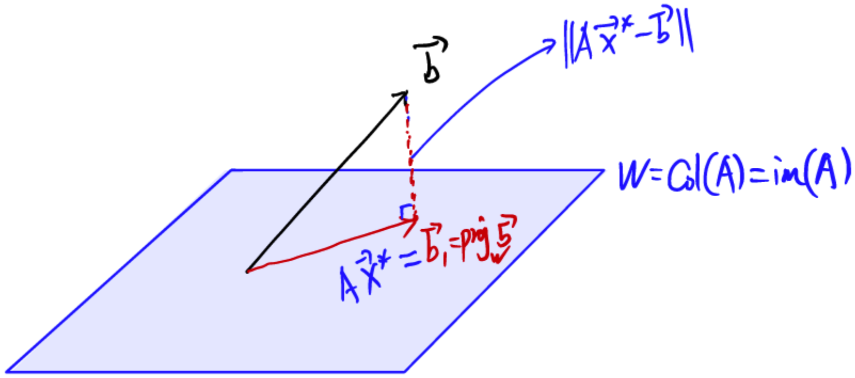
- Let A be an $n \times m$ matrix and let $\vec{b}$ be an n-dimensional vector such that the system
$$A\vec{x} = \vec{b}$$
is inconsistent (no solution). (if and only if $\vec{b} \notin \operatorname{Col} A = \operatorname{im} A = \operatorname{Span}(\vec{a}_1, \cdots, \vec{a}_m)$).

- In this case a natural question to ask is which m-dimensional vector(s) $\vec{x}^*$ has/have the property that $A\vec{x}^*$ is closest to $\vec{b}$. Here "closeness" of $A\vec{x}^*$ to $\vec{b}$ is measured by the smallness of
$$||A\vec{x}^* - \vec{b}||$$

[Least-Squares Problem/Solutions]

For an $n \times m$ matrix A and an inconsistent system $A\vec{x} = \vec{b}$, find the vector(s) $\vec{x}^* \in \mathbb{R}^m$ such that
$$||A\vec{x}^* - \vec{b}|| \leq ||A\vec{x} - \vec{b}||$$
for all $x \in \mathbb{R}^m$.

$||A\vec{x}^* - \vec{b}||$ is the least squares **error**.



- To find the Least Square solution(s) $\vec{x}^*$ of an inconsistent system $A\vec{x} = \vec{b}$, we replace the system by the consistent system $A\vec{x} = \vec{b}_1$ with $\vec{b}_1$ the closest vector in $\operatorname{Col} A$ to $\vec{b}$, namely $\vec{b}_1 = \operatorname{proj}_{\operatorname{Col} A}(\vec{b})$.

Theorem. [Solution to the Least-Squares Problem]

Let A be an $n \times m$ matrix. Let $\vec{b} \in \mathbb{R}^n$ and $\vec{b}_1 = \operatorname{proj}_{\operatorname{Col} A}(\vec{b})$. Then, any solutions $\vec{x}^*$ of the consistent system $A\vec{x} = \vec{b}_1$ is a least-squares solution.

Example 1. Find the least-squares solutions for the system $A\vec{x} = \vec{b}$, where $A = \begin{bmatrix} -1 & 4 \\ 1 & 8 \\ -1 & 4 \end{bmatrix}$ and $\begin{bmatrix} 14 \\ -4 \\ 0 \end{bmatrix}$

$\{\vec{a}_1, \vec{a}_2\}$ is an orthogonal basis for $Col(A)$. since $\vec{a}_1 \cdot \vec{a}_2 = 0$

Step1: $\vec{b}_1 = proj_{Col A}(\vec{b}) = \dfrac{\vec{b}\cdot\vec{a}_1}{\vec{a}_1\cdot\vec{a}_1}\vec{a}_1 + \dfrac{\vec{b}\cdot\vec{a}_2}{\vec{a}_2\cdot\vec{a}_2}\vec{a}_2$

$= -\frac{18}{3}\vec{a}_1 + \frac{24}{96}\vec{a}_2 = -6\vec{a}_1 + \frac{1}{4}\vec{a}_2 = \begin{bmatrix} 7 \\ -4 \\ 7 \end{bmatrix}$

Step2: Solve $A\vec{x} = \vec{b}_1$

$[\vec{a}_1 \ \vec{a}_2]\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \vec{b}_1$

$x_1\vec{a}_1 + x_2\vec{a}_2 = \vec{b}_1$

So $\vec{x} = \begin{bmatrix} -6 \\ \frac{1}{4} \end{bmatrix}$ is a least squares solution

Theorem. (Normal Equation)

The set of Least-Square solutions of the inconsistent system $A\vec{x} = \vec{b}$ coincides with the solution set of the consistent system of **normal equations**

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

Proof: Let $V = \text{im}\, A$.
$\vec{x}_*$ is a least-squares solution for $A\vec{x} = \vec{b} \iff A\vec{x}_* = \text{proj}_V \vec{b}$

$\iff \vec{b} - A\vec{x}_* = \vec{b}^\perp \in (\text{im}\, A)^\perp = \ker A^T$

$\iff A^T(\vec{b} - A\vec{x}_*) = \vec{0}$

$\iff A^T\vec{b} - A^T A\vec{x}_* = \vec{0}$

$\iff A^T A\vec{x}_* = A^T\vec{b}$

Example 2. Find the least-squares solutions for the system $A\vec{x} = \vec{b}$, where $A = \begin{bmatrix} -1 & 4 \\ 1 & 8 \\ -1 & 4 \end{bmatrix}$ and $\vec{b} = \begin{bmatrix} 14 \\ -4 \\ 0 \end{bmatrix}$

$$A^TA = \begin{bmatrix} -1 & 1 & -1 \\ 4 & 8 & 4 \end{bmatrix} \begin{bmatrix} -1 & 4 \\ 1 & 8 \\ -1 & 4 \end{bmatrix} = \begin{bmatrix} 3 & 0 \\ 0 & 96 \end{bmatrix}$$

$$A^T\vec{b} = \begin{bmatrix} -1 & 1 & -1 \\ 4 & 8 & 4 \end{bmatrix} \begin{bmatrix} 14 \\ -4 \\ 0 \end{bmatrix} = \begin{bmatrix} -18 \\ 24 \end{bmatrix}$$

Solve the normal equation $A^TA\vec{x} = A^T\vec{b}$

$$\left[\begin{array}{cc|c} 3 & 0 & -18 \\ 0 & 96 & 24 \end{array}\right] \to \left[\begin{array}{cc|c} 1 & 0 & -6 \\ 0 & 1 & 1/4 \end{array}\right]$$

So $\vec{x} = \begin{bmatrix} -6 \\ 1/4 \end{bmatrix}$ is the least-squares solution

(2) The image $\text{im}(A)$ is a plane in $\mathbb{R}^3$ passing the origin. Find the distance from the vector $\vec{b}$ (or the point $(14, -4, 0)$) to the plane $\text{im}(A)$. (Hint: Use the geometric meaning of the least-squares solution in (1))

The distance is given be the norm of $\vec{b}^{\perp} = \vec{b} - \text{proj}_{\text{im}(A)} \vec{b}$.

We know that $\text{proj}_{\text{im}(A)} \vec{b} = Ax^* = \begin{bmatrix} -1 & 4 \\ 1 & 8 \\ -1 & 4 \end{bmatrix} \begin{bmatrix} -6 \\ 1/4 \end{bmatrix} = \begin{bmatrix} 7 \\ -4 \\ 7 \end{bmatrix}$.

So, $\vec{b}^{\perp} = \begin{bmatrix} 14 \\ -4 \\ 0 \end{bmatrix} - \begin{bmatrix} 7 \\ -4 \\ 7 \end{bmatrix} = \begin{bmatrix} 7 \\ 0 \\ -7 \end{bmatrix}$. So the distance is $||\vec{b}^{\perp}|| = 7\sqrt{2}$.

Example 3. Find the least-squares solutions for the system $A\vec{x} = \vec{b}$, where $A = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix}$

and $\vec{b} = \begin{bmatrix} 1 \\ 3 \\ 2 \\ 4 \end{bmatrix}$

Step 1. Construct the normal equation $A^TA\vec{x} = A^T\vec{b}$

$$A^TA = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}\begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 4 & 2 & 2 \\ 2 & 2 & 0 \\ 2 & 0 & 2 \end{bmatrix}$$

$$A^T\vec{b} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}\begin{bmatrix} 1 \\ 3 \\ 2 \\ 4 \end{bmatrix} = \begin{bmatrix} 10 \\ 4 \\ 6 \end{bmatrix}$$

Solve the normal equation

$$\left[\begin{array}{ccc|c} 4 & 2 & 2 & 10 \\ 2 & 2 & 0 & 4 \\ 2 & 0 & 2 & 6 \end{array}\right] \to \cdots \to \text{rref} = \left[\begin{array}{ccc|c} 1 & 0 & 1 & 3 \\ 0 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 \end{array}\right]$$

$x_1 = 3 - x_3$
$x_2 = -1 + x_3$
x_3 free

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 - x_3 \\ -1 + x_3 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ -1 \\ 0 \end{bmatrix} + x_3\begin{bmatrix} -1 \\ 1 \\ 1 \end{bmatrix}$$

A technical property:

Proposition.

Let A be an $n \times m$ matrix.

- $\ker(A) = \ker(A^TA)$
- If $\ker(A) = \{0\}$, then A^TA is an invertible matrix.

If rank $A = m$, then A^TA is an $m \times m$ invertible matrix.

In this case, the normal equation $(A^TA)\vec{x} = A^T\vec{b}$ has a unique solution: $\vec{x} = (A^TA)^{-1}A^T\vec{b}$

2. Data Fitting.

Problem: Fitting a function of a certain type of data. We use the following three example to illustrate this application.

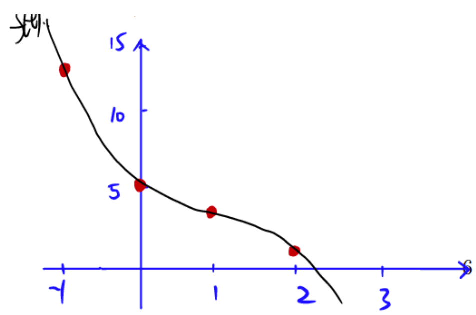
Example 4. Find a cubic polynomial $f(t) = c_0 + c_1 t + c_2 t^2 + c_3 t^3$ whose graph passes through the points $(0, 5)$, $(1, 3)$, $(-1, 13)$, $(2, 1)$

Solution:

We need to solve the linear system
$$\begin{cases} c_0 & = 5 \\ c_0 + c_1 + c_2 + c_3 & = 3 \\ c_0 - c_1 + c_2 - c_3 & = 13 \\ c_0 + 2c_1 + 4c_2 + 8c_3 & = 1 \end{cases}$$

$$[A|\vec{b}] = \begin{bmatrix} 1 & 0 & 0 & 0 & 5 \\ 1 & 1 & 1 & 1 & 3 \\ 1 & -1 & 1 & -1 & 13 \\ 1 & 2 & 4 & 8 & 1 \end{bmatrix} \to \cdots \to \textbf{rref}[A|\vec{b}] = \begin{bmatrix} 1 & 0 & 0 & 0 & 5 \\ 0 & 1 & 0 & 0 & -4 \\ 0 & 0 & 1 & 0 & 3 \\ 0 & 0 & 0 & 1 & -1 \end{bmatrix}$$

So, the linear system has the unique solution $\begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} 5 \\ -4 \\ 3 \\ -1 \end{bmatrix}$ So, the cubic polynomial is $f(t) = 5 - 4t + 3t^2 - t^3$.



perfect fit, but calculation is hard.

Example 5. Fit a quadratic function $g(t) = c_0 + c_1 t + c_2 t^2$ to the four data points $(0, 5)$, $(1, 3)$, $(-1, 13)$, $(2, 1)$

We need to solve the linear system

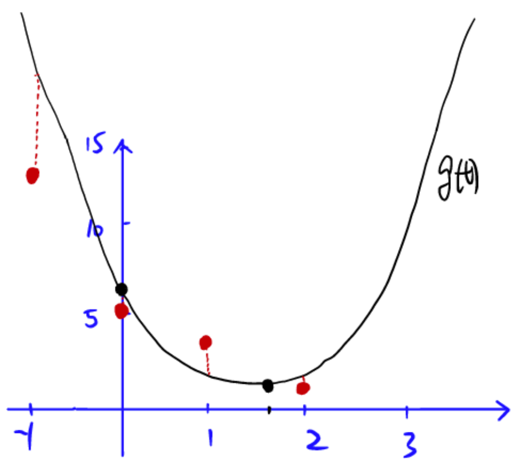
$$\begin{cases} c_0 & = 5 \\ c_0 + c_1 + c_2 & = 3 \\ c_0 - c_1 + c_2 & = 13 \\ c_0 + 2c_1 + 4c_2 & = 1 \end{cases}$$

As matrix equation $A\vec{x} = \vec{b}$, where $A = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 2 & 4 \end{bmatrix}$ and $\vec{b} = \begin{bmatrix} 5 \\ 3 \\ 13 \\ 1 \end{bmatrix}$

$A^T A = \begin{bmatrix} 4 & 2 & 6 \\ 2 & 6 & 8 \\ 6 & 8 & 18 \end{bmatrix}$ $\quad A^T \vec{b} = \begin{bmatrix} 22 \\ -8 \\ 20 \end{bmatrix}$

Solve the normal equation $A^T A \vec{x} = A^T \vec{b}$ $\quad \vec{x} = \begin{bmatrix} 5.9 \\ -5.3 \\ 1.5 \end{bmatrix} = \vec{c}^*$

So, the quadratic function $g(t) = 5.9 - 5.3t + 1.5t^2$



$A\vec{c}^* = \begin{bmatrix} g(a_1) \\ g(a_2) \\ g(a_3) \\ g(a_4) \end{bmatrix}$ $\quad \vec{b} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$

$\|\vec{b} - A\vec{c}^*\|^2 = (b_1 - g(a_1))^2 + (b_2 - g(a_2))^2 + (b_3 - g(a_3))^2 + (b_4 - g(a_4))^2$

The sum of the vertical distances between graph and data points is minimal.

Example 6. Fit a linear function $h(t) = c_0 + c_1 t$ to the four data points $(0, 5)$, $(1, 3)$, $(-1, 13)$, $(2, 1)$

We need to solve the linear system

$$\begin{cases} c_0 &= 5 \\ c_0 + c_1 &= 3 \\ c_0 - c_1 &= 13 \\ c_0 + 2c_1 &= 1 \end{cases}$$

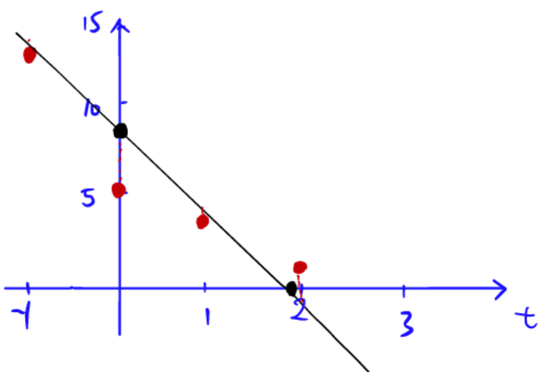
As matrix equation $A\vec{x} = \vec{b}$, where $A = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & -1 \\ 1 & 2 \end{bmatrix}$ and $\vec{b} = \begin{bmatrix} 5 \\ 3 \\ 13 \\ 1 \end{bmatrix}$

$$A^TA = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & -1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & -1 \\ 1 & 2 \end{bmatrix} = \begin{bmatrix} 4 & 2 \\ 2 & 6 \end{bmatrix}$$

$$A^T\vec{b} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & -1 & 2 \end{bmatrix} \begin{bmatrix} 5 \\ 3 \\ 13 \\ 1 \end{bmatrix} = \begin{bmatrix} 22 \\ -8 \end{bmatrix}$$

Solve the normal equation $A^TA\vec{x} = A^T\vec{b}$ $\vec{x} = \begin{bmatrix} 7.4 \\ -3.8 \end{bmatrix}$

So the linear function is $h(t) = 7.4 - 3.8t$



Remark: More generally, we can consider n-points $(a_1, b_1), (a_2, b_2), \ldots, (a_n, b_n)$.

- Find a linear function $h(t) = c_0 + c_1 t$ fits the data by the least squares.

More generally, the following question is very standard in statistics.

Example 7. Consider the data with n points (a_1, b_1), (a_2, b_2), $\ldots$, (a_n, b_n). Find a linear function $h(t) = c_0 + c_1 t$ fits the data by the least squares. (Suppose $a_1 \neq a_2$)

We need to solve the least-squares problem for $A\vec{x} = \vec{b}$, for $A = \begin{bmatrix} 1 & a_1 \\ 1 & a_2 \\ \vdots & \\ 1 & a_n \end{bmatrix}$ and $\vec{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$

$$A^T A = \begin{bmatrix} 1 & a_1 \\ 1 & a_2 \\ \vdots & \\ 1 & a_n \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 \\ a_1 & a_2 & \cdots & a_n \end{bmatrix} = \begin{bmatrix} n & \sum_{i=1}^n a_i \\ \sum_{i=1}^n a_i & \sum_{i=1}^n a_i^2 \end{bmatrix}$$

$$A^T b = \begin{bmatrix} 1 & a_1 \\ 1 & a_2 \\ \vdots & \\ 1 & a_n \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^n b_i \\ \sum_{i=1}^n a_i a_i \end{bmatrix}$$

Since $a_1 \neq a_2$, we know that rank $A = 2$.
The normal equation $A^T A\vec{x} = A^T\vec{b}$ has a unique solution

$$\vec{x}_* = (A^T A)^{-1} A^T \vec{b} = \frac{1}{n\sum_{i=1}^n a_i^2 - (\sum_{i=1}^n a_i)^2} \begin{bmatrix} \sum_{i=1}^n a_i^2 & -\sum_{i=1}^n a_i \\ -\sum_{i=1}^n a_i & n \end{bmatrix} \begin{bmatrix} \sum_{i=1}^n b_i \\ \sum_{i=1}^n a_i a_i \end{bmatrix}$$

$$= \frac{1}{n\sum_{i=1}^n a_i^2 - (\sum_{i=1}^n a_i)^2} \begin{bmatrix} (\sum_{i=1}^n a_i^2)(\sum_{i=1}^n b_i) - (\sum_{i=1}^n a_i)(\sum_{i=1}^n a_i a_i) \\ -(\sum_{i=1}^n a_i)(\sum_{i=1}^n b_i) + n\sum_{i=1}^n a_i a_i \end{bmatrix}$$