

lecture 16. Orthogonality and least Squares Problems

$u, v \in \mathbb{R}^m$, $u \perp v$ if $u^T v = 0$.

In this case, $\|u+v\|^2 = \|u\|^2 + \|v\|^2$.

Two subspaces S and T . $S \perp T$ if

$\forall s \in S$, and $\forall t \in T$, $s^T t = 0$, i.e., $S \perp T$.

Four subspaces associated with $A \in \mathbb{R}^{m \times n}$

1. If $S \perp T$, then $S \cap T = \{0\}$

The formula $\dim(S+T) + \dim(S \cap T) = \dim(S) + \dim(T)$

implies $\dim(S) + \dim(T) = \dim(S+T) \leq m$.

So two planes in \mathbb{R}^3 can't be orth. to each other

2. when $S \perp T$, and $\dim(S) + \dim(T) = m$.

then T is called the orthogonal complement of S

denoted by $S^\perp = T$, Versi versa, $T^\perp = S$.

and $(S^\perp)^\perp = S$.

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

3. $C(A)^\perp = N(A^T)$, $\forall x \in \mathbb{R}^m$.

Example
 $A^T A x = 0 \Rightarrow A x = 0$
 $A x \in N(A^T) \cap C(A) \Rightarrow A x = 0$

$x = x_c + x_n$, with $x_c \in C(A)$, and $x_n \in N(A^T)$

and $x_c \perp x_n$. $Ax = 0 \Leftrightarrow \begin{pmatrix} A_1^T x \\ \vdots \\ A_m^T x \end{pmatrix} = 0$

$C(A^T)^\perp = N(A)$, $\forall y \in \mathbb{R}^n$

$y = y_c + y_n$. $y_c \in C(A^T)$, $y_n \in N(A)$. $y_c \perp y_n$

Example. Assume $Ax = b$ has solution, find the

solution with minimal length $\| \cdot \|$. Any solution

$x = a + b$, with $a \in C(A^T)$, $b \in N(A)$

$\|x\|^2 = \|a\|^2 + \|b\|^2$, set $b = 0$.

Example $S \subset \mathbb{R}^3$, and $S = \{0\}$, $S^\perp = ?$

$$\text{If } S = \text{span}\left\{\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}\right\}, \quad S^\perp = \text{span}\left\{\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}\right\}$$

$$S = \text{span}\left\{\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}\right\}, \quad S^\perp = \text{span}\left\{\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}\right\}$$

Example. $a \perp \text{span}\{v_1, \dots, v_k\}$ iff. $a \perp v_i, i=1, \dots, k$

Proof. " \Rightarrow " since $v_i \in \text{span}\{v_1, \dots, v_k\} \Rightarrow a \perp v_i$.

" \Leftarrow " $\forall x \in \text{span}\{v_1, \dots, v_k\}, x = \sum_{i=1}^k \alpha_i v_i$

$$a^T x = \sum_{i=1}^k \alpha_i \underbrace{a^T v_i}_{=0} = 0$$

least squares problems. $A \in \mathbb{R}^{m \times n}$

We have considered $Ax=b$, when $b \in C(A)$, there might be one or many solutions. But if $b \notin C(A)$, we can ask for an approximate solution in the sense of making $r = b - Ax$ small but not exactly zero, r is the so-called

residual of an approximate sol x .

least squares is one approach of quantifying the size of "smallness" of r , in terms of its

ℓ_2 -norm $\|r\|^2 = r_1^2 + r_2^2 + \dots + r_m^2$, $r = \begin{pmatrix} r_1 \\ \vdots \\ r_m \end{pmatrix}$

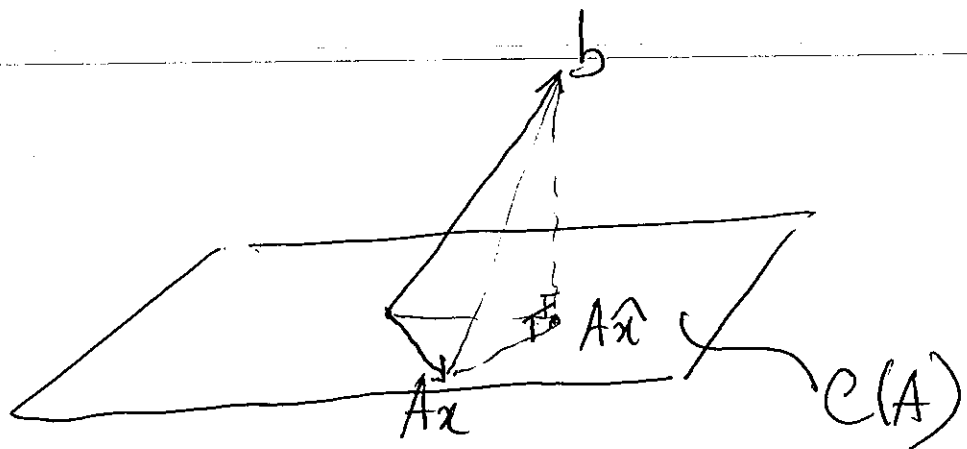
Other possibilities exist, e.g. $r_i = (b_i - A_i x)^2$

$\|r\|_1 = |r_1| + |r_2| + \dots + |r_m|$ $A = \begin{pmatrix} A_1 \\ \vdots \\ A_m \end{pmatrix}$

So we want find an $x \in \mathbb{R}^n$, s.t.

$$\min \|r\|^2 = \min_{x \in \mathbb{R}^n} \|b - Ax\|^2$$

This is to say we find $A\hat{x} \in C(A)$ s.t. the residue $\|b - A\hat{x}\|$ is the smallest in $\|\cdot\|_2$



Orthogonality principle: $\|r\|^2$ is minimized iff.

$$r \perp C(A) \Leftrightarrow a_i \perp r, \quad \forall i=1, \dots, n.$$

where $A = (a_1, \dots, a_n) \in \mathbb{R}^{m \times n}$

From $\begin{pmatrix} a_1^T r \\ a_2^T r \\ \vdots \\ a_n^T r \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$ we obtain

$$A^T r = 0 \quad A^T (b - A\hat{x}) = 0$$

Normal Eq $A^T A \hat{x} = A^T b$, this is an $n \times n$ linear

system. Since $\text{rank}[A^T A, A^T b] = \text{rank}(A^T A)$

it always has a solution, no matter what b is.

It has a unique solution $\hat{x} = (A^T A)^{-1} A^T b$

when A has full col rank, i.e., $r(A) = n \leq m$.

Now $p = A\hat{x} = A(A^T A)^{-1} A^T b = P_A b$

P_A is a projection matrix. $P = P^T$, $P^2 = P$.

Will discuss $r(A) < n$ later!

$$\text{Now } b = P_A b + (I - P_A)b$$

Since $P_A b \perp (I - P_A)b$. for arbitrary $x \in \mathbb{R}^n$

$$\|b - Ax\|^2 = \|(P_A b - Ax) + (I - P_A)b\|^2$$

Now $Ax \in C(A)$, $Ax \perp (I - P_A)b$.

$$= \|P_A b - Ax\|^2 + \|(I - P_A)b\|^2$$

The residual is minimized iff $Ax = P_A b$.

Given two lines:

$$P = (x, x, x), \quad x \in \mathbb{R}.$$

$$Q = (y, 3y, -1), \quad y \in \mathbb{R}.$$

Do the two lines meet at some point?

We can formulate the above as a LS problem.

$$\begin{aligned} \min_{P, Q} \|P - Q\|^2 &= \min_{x, y} \left\| \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} x - \begin{pmatrix} 1 \\ 3 \\ 0 \end{pmatrix} y - \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix} \right\|^2 \\ &= \left\| \begin{pmatrix} 1 & 1 \\ 1 & 3 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} - \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix} \right\|^2. \end{aligned}$$

Example. Fitting a straight line

$$f(t) = c + dt$$

to a set of points (t_i, b_i) , $i=1, \dots, m$.

The linear system is

$$c + dt_1 = b_1$$

$$c + dt_2 = b_2$$

$$\vdots$$

$$c + dt_m = b_m$$

$Ax = b$, with

$$A = \begin{pmatrix} 1 & t_1 \\ \vdots & \vdots \\ 1 & t_m \end{pmatrix}$$

$$b = \begin{pmatrix} b_1 \\ \vdots \\ b_m \end{pmatrix}$$

$$A^T A = \begin{pmatrix} m & \sum t_i \\ \sum t_i & \sum t_i^2 \end{pmatrix}, \quad A^T b = \begin{pmatrix} \sum b_i \\ \sum t_i b_i \end{pmatrix}$$

$$\hat{x} = (A^T A)^{-1} A^T b = \frac{1}{m \sum t_i^2 - (\sum t_i)^2} \begin{pmatrix} \sum t_i^2 - \sum t_i \\ -\sum t_i \quad m \end{pmatrix} \begin{pmatrix} \sum b_i \\ \sum t_i b_i \end{pmatrix}$$
$$= \frac{\begin{pmatrix} (\sum t_i^2)(\sum b_i) - (\sum t_i)(\sum t_i b_i) \\ m(\sum t_i b_i) - (\sum t_i)(\sum b_i) \end{pmatrix}}{m \sum t_i^2 - (\sum t_i)^2}$$

← This can be easily generalized to fitting a polynomial to a set of data, or supervised learning.

Supervised learning.

let. $g_1(x), \dots, g_n(x)$ be a set of basis functions, e.g., $1, x, \dots, x^{n-1}$, $x \in \mathbb{R}$, but in general $x \in \mathbb{R}^d$, multi-dimensional.

We are given a set of data points (x_i, y_i)

We want find a linear combination of the g_i 's

$$g(x) = \alpha_1 g_1(x) + \dots + \alpha_n g_n(x)$$

s.t. $g(x_i) \approx y_i$, $i=1, \dots, m$. If we

minimize $\sum_{i=1}^m (y_i - g(x_i))^2$, we have the

LS problem $\|Ax - b\|^2$, where

$$A = \begin{pmatrix} g_1(x_1) & \dots & g_n(x_1) \\ \vdots & & \vdots \\ g_1(x_m) & \dots & g_n(x_m) \end{pmatrix}, \quad x = \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix}, \quad b = \begin{pmatrix} y_1 \\ \vdots \\ y_m \end{pmatrix}.$$

Th. Let $C(A)$ denote the col space of A .

~~Th~~ If $C(A)$ is a subspace of $C(B)$, ^{then} $r(A) \leq r(B)$.

Let's prove the following $r(A+B) \leq r([A, B])$

Proof. $A = [a_1, \dots, a_n]$, $B = [b_1, \dots, b_n]$.

$$a_i \in C([A, B]), \quad b_i \in C([A, B])$$

hence $a_i + b_i \in C([A, B])$, which implies

$$C(A+B) \subseteq C([A, B]) \Rightarrow r(A+B) \leq r([A, B])$$

Corollary. $r(A+B) \leq r(A) + r(B)$

Corollary $|r(A) - r(B)| \leq r(A-B)$

$A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{n \times p}$ if $AB=0$, then

$$r(A) + r(B) \leq n.$$

Proof. $AB=0 \Rightarrow C(B) \subseteq N(A) \Rightarrow r(B) \leq \dim(N(A)) = n - r(A)$
 $= n - r(A)$