

HOMEWORK-2

1. To prove Gauss-Markov Theorem,

Assume a linear model;

$$y = X\beta + \varepsilon$$

$$y \in \mathbb{R}^{n \times 1}$$

$$X \in \mathbb{R}^{n \times p}$$

$$\beta \in \mathbb{R}^{p \times 1}$$

$\varepsilon \in \mathbb{R}^{n \times 1}$  vectors of errors

$$E[\varepsilon] = 0$$

$$\text{var}(\varepsilon) = \sigma^2$$

↳ Least squares estimate  $\hat{\beta}$  is given by,

$$\hat{\beta} = (X^T X)^{-1} X^T y$$

Unbiasedness of  $\hat{\beta}$   $[E[\hat{\beta}]] = \beta$ .

$$E[\hat{\beta}] = E[(X^T X)^{-1} X^T y]$$

$$= (X^T X)^{-1} X^T E[y] = (X^T X)^{-1} X^T y = \beta$$

$\Rightarrow \hat{\beta}$  is unbiased.

↳ Any other linear Unbiased Estimator.

If  $C^T y$  is any other linear Unbiased estimator of  $\alpha^T \beta$

$$E[\alpha^T C^T y] = \alpha^T \beta$$

$$y = X\beta + \varepsilon$$

$$\therefore E[C^T y] = C^T E[X\beta + \varepsilon] = C^T X\beta$$

Given it is unbiased; comparing  $C^T X\beta = \alpha^T \beta$

$$\text{we get, } C^T X = \alpha^T$$

Since  $C^T x = a^T$  & any other estimator, it could potentially have additional components & can be written as,  $C^T = a^T \hat{\beta} + b^T$

$$C^T y = a^T \hat{\beta} + b^T y$$

i.e  $C^T$  includes a component that projects  $y$  onto  $x$  to capture  $a^T \beta \Rightarrow (a^T (x^T x)^{-1} x^T)$  which multiplied by  $y$  gives estimate  $a^T \hat{\beta}$ , where  $\hat{\beta} = (x^T x)^{-1} x^T y$ . plus another component  $b^T$ .

where,  $b^T x = 0$  {null space of  $x$ }

$$\therefore E[C^T y] = a^T E[\hat{\beta}] + b^T E[y] = a^T \beta$$

$$\frac{\text{Variance of } \hat{\beta}}{\text{Var}(\hat{\beta})} = \text{Var}((x^T x)^{-1} x^T y) = (x^T x)^{-1} x^T \underbrace{\text{Var}(y)}_{= \sigma^2} x (x^T x)^{-1}$$

$$\therefore \text{Var}[b^T x] = b^T \text{Var}[x] b$$

$$\therefore \text{Var}(\hat{\beta}) = \sigma^2 (x^T x)^{-1} \underbrace{x^T x}_{I} (x^T x)^{-1}$$

$$\therefore \text{Var}(\hat{\beta}) = \sigma^2 (x^T x)^{-1} \Rightarrow \text{Var}(a^T \hat{\beta}) = \sigma^2 a^T (x^T x)^{-1} a$$

$$\therefore \text{Var}(\hat{\beta}) = \sigma^2 (x^T x)^{-1} \Rightarrow \text{Var}(\hat{\beta}) = \sigma^2 a^T (x^T x)^{-1} a$$

Variance of  $C^T y$

$$\begin{aligned} \text{Var}(C^T y) &= \text{Var}(a^T \hat{\beta} + b^T y) \\ &= \text{Var}(a^T \hat{\beta}) + \text{Var}(b^T y) \\ &= a^T \text{Var}(\hat{\beta}) a + \sigma^2 b^T b \\ &= \underline{\sigma^2 a^T (x^T x)^{-1} a} + \sigma^2 b^T b \end{aligned}$$

also,  $b^T b \geq 0$

$$\therefore \text{Var}(C^T y) \geq \sigma^2 a^T (x^T x)^{-1} a$$

$$\boxed{\text{i.e. } \text{Var}(C^T y) \geq \text{Var}(a^T \hat{\beta})}$$

Another method. [From discussion class reference]

Let  $\tilde{\beta} = Cy$  be another estimator  $\beta$

$$\text{where, } C = (x^T x)^{-1} x^T + D$$

where,  $D = \text{non-zero matrix.}$

$$\begin{aligned}\therefore E[\tilde{\beta}] &= E[Cy] \\ &= E[(x^T x)^{-1} x^T + D](x\beta + \varepsilon) \\ &= ((x^T x)^{-1} x^T + D)x\beta + ((x^T x)^{-1} x^T + D) \underbrace{E[\varepsilon]}_0 \\ &= ((x^T x)^{-1} x^T + D)x\beta \\ &= \underbrace{(x^T x)^{-1} x^T}_{I} x\beta + Dx\beta \\ &= (I + Dx)\beta\end{aligned}$$

$$\Rightarrow E[\tilde{\beta}] = \beta \quad \text{when } Dx = 0$$

so it is unbiased.

$$\begin{aligned}\text{Var}(\tilde{\beta}) &= \text{Var}(Cy) \\ &= C \text{Var}(y) C^T\end{aligned}$$

$$\begin{aligned}&= \sigma^2 C C^T \\ &= \sigma^2 ((x^T x)^{-1} x^T + D)(x(x^T x)^{-1} + D^T) \\ &= \sigma^2 ((x^T x)^{-1})^T x^T x (x^T x)^{-1} + ((x^T x)^{-1})^T x^T D^T + D x (x^T x)^{-1} + D D^T \\ &= \sigma^2 (x^T x)^{-1} + \sigma^2 (x^T x)^{-1} (Dx)^T + \sigma^2 D x (x^T x)^{-1} + \sigma^2 D D^T \\ &= \underbrace{\sigma^2 (x^T x)^{-1}}_{\text{Var}(\hat{\beta})} + \sigma^2 D D^T \\ &= \text{Var}(\hat{\beta}) + \sigma^2 D D^T\end{aligned}$$

$$\boxed{\Rightarrow \text{Var}(\tilde{\beta}) \geq \text{Var}(\hat{\beta})}$$

## 2. Linear Regression with Orthogonal Design.

Sol:  $x_0, \dots, x_p$  if  $x$  are orthogonal.

$\Rightarrow$  dot product = 0

i.e. for any two cols,  $x_0, \dots, x_p$ ;  $x_i \cdot x_j$  ( $i \neq j$ )  
we have

$$x_i^T x_j = 0$$

$\therefore$  in  $x$  matrix, all the elements of  $x$  will  
be zero, except diagonal elements.

Estimating  $\hat{\beta}$ .

we have,

$$\hat{\beta} = (x^T x)^{-1} x^T y$$

now since  $x$  is orthogonal matrix,

$$\begin{bmatrix} x_0 & x_1 & \dots & x_p \end{bmatrix}^T \begin{bmatrix} x_0 & x_1 & \dots & x_p \end{bmatrix} = x^T x$$

$$x^T x = \begin{bmatrix} x_0^T x_0 & 0 & 0 & \dots \\ 0 & x_1^T x_1 & & \\ \vdots & & \ddots & \\ & & & x_p^T x_p \end{bmatrix} = \text{diag}(x_0^T x_0, x_1^T x_1, \dots, x_p^T x_p) = D$$

$$\therefore (x^T x)^{-1} = D^{-1} = \begin{bmatrix} 1/x_0^T x_0 & & & \\ & 1/x_1^T x_1 & & \\ & & \ddots & \\ & & & 1/x_p^T x_p \end{bmatrix}$$

$$\therefore \hat{\beta} = D^{-1} X^T y$$

$$\Rightarrow \hat{\beta} = \begin{bmatrix} \frac{1}{x_0^T x_0} & & & \\ & \frac{1}{x_1^T x_0} & \cdots & 0 \\ 0 & & \ddots & \\ \vdots & & & \frac{1}{x_p^T x_0} \end{bmatrix} \begin{bmatrix} x_0 & x_1 & \cdots & x_p \end{bmatrix}^T y$$

$$\Rightarrow \hat{\beta} = \begin{bmatrix} \frac{x_0^T}{x_0^T x_0} y \\ \frac{x_1^T}{x_1^T x_0} y \\ \frac{x_1^T}{x_1^T x_1} y \\ \vdots \\ \frac{x_p^T}{x_p^T x_0} y \end{bmatrix} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \vdots \\ \hat{\beta}_p \end{bmatrix}$$

$$\Rightarrow \hat{\beta}_j = \frac{x_j^T}{x_j^T x_j} y$$

3. Minimum Norm Solution:

When  $X^T X$  not invertible  $\rightarrow$  no unique solution.

$$D = (X \in \mathbb{R}^{n \times (p+1)}) \quad r = \text{rank of matrix}$$

$$\text{SVD of } X = U \Sigma V^T$$

$$U \in \mathbb{R}^{n \times (p+1)}$$

$$V \in \mathbb{R}^{(p+1) \times r}$$

$$\Sigma \in \mathbb{R}^{r \times (p+1)}$$

$$U^T U = I_n$$

$$V^T V = I_r$$

$$\Sigma = \text{diag}(\sigma_1, \dots, \sigma_r)$$

(a) To show  $\beta_{\min} = V \Sigma^{-1} U^T y$  is solution to normal eqn

normal equation is given by,

$$X^T X \beta = X^T y$$

$\therefore X^T X$  is not invertible, we need to make use of SVD

to show,  $\beta_{\text{min}} = V\Sigma^{-1}U^T y$  satisfies normal eq<sup>n</sup>, let's substitute  $\beta_{\text{min}}$  in normal equation,

$$x^T x \beta_{\text{min}} = x^T y$$

we need to prove after substitution, we get L.H.S = R.H.S

$$x^T x \underbrace{V\Sigma^{-1}U^T y}_{\beta_{\text{min}}} = x^T y$$

now substituting  $x = U\Sigma V^T$ ,

$$(U\Sigma V^T)^T (U\Sigma V^T) V\Sigma^{-1} U^T y = (U\Sigma V^T)^T y$$

$$= (\underbrace{U\Sigma U^T}_{I_d}) (\underbrace{U\Sigma V^T}_{}) V\Sigma^{-1} U^T y = V\Sigma U^T y$$

we have  $U^T U = I_d$

$$\therefore V\Sigma \underbrace{\Sigma^T}_{I_d} V\Sigma^{-1} U^T y = V\Sigma U^T y \quad | V^T V = I_d$$

$$V\Sigma \underbrace{\Sigma^T}_{I_d} \Sigma^{-1} U^T y = V\Sigma U^T y$$

$$\Rightarrow V\Sigma U^T y = V\Sigma U^T y = x^T y$$

∴  $\beta_{\text{min}}$  satisfies normal eq.

∴  $\beta_{\text{min}}$  ~~satisfies~~ satisfies normal eq.

(b) To show: for any other solution  $\beta$  to normal eq<sup>n</sup>  
 $\|\beta\| \geq \|\beta_{\text{min}}\|$

Prof:

Normal equation is given by,

$$x^T x \beta = x^T y \quad \text{where } \beta = \beta_{\text{min}}$$

When  $x = U\Sigma V^T$ ,

minimum norm solution is given by

$$\beta_{\text{min}} = V\Sigma^{-1}U^T y$$

Suppose,  $\beta$  is any solution to normal equation.

$$\Rightarrow x^T x \beta = x^T y$$

taking difference between  $\beta_{\text{true}}$  &  $\beta$ )

let,  $\beta - \beta_{\text{true}} = b$  for some vector  $b$ .

Using  $\beta_{\text{true}} = \beta + b$  in normal eqn)

$$x^T x (\beta_{\text{true}} + b) = x^T y$$

$$x^T x \beta_{\text{true}} + x^T x b = x^T y$$

$\therefore$  previously proved,  
 $x^T x \beta_{\text{true}} = x^T y$

$$x^T y + x^T x b = x^T y$$

$$\Rightarrow x^T x b = 0$$

$\Rightarrow b$  lies in null space of  $x^T x$

$$\Rightarrow \beta = \beta_{\text{true}} + b \quad \text{(i)}$$

$\because$  any general solution to normal equation can be written as sum of minimum norm solution and any vector in null space of  $x^T x$

$\therefore$  to show,  $\|\beta\| \geq \|\beta_{\text{true}}\|$

norm of  $\beta$  can be written as:

$$\|\beta\| = \|\beta_{\text{true}} + b\|$$

$\therefore x^T x b = 0$  i.e.  $b$  is  $\perp$   $\beta_{\text{true}}$ ,

$$\|\beta\|^2 = \|\beta_{\text{true}} + b\|^2 = \|\beta_{\text{true}}\|^2 + \|b\|^2$$

by Pythagorean theorem

$$\Rightarrow \|\beta\|^2 \geq \|\beta_{\text{true}}\|^2.$$

$$\Rightarrow \|\beta\| \geq \|\beta_{\text{true}}\|$$

(e)  $\sqrt{\Sigma}^{-1} U^T \rightarrow$  to check if this the Pseudo-inverse of  $X$ .

Penrose properties for pseudo-inverse is given by:

$$1. X X^+ X = X$$

$$2. X^+ X X^+ = X^+$$

$$3. (X X^+)^T = X X^+$$

$$4. (X^+ X)^T = X^+ X$$

$$X^+ = \sqrt{\Sigma}^{-1} U^T \quad \{ \text{to check}\}$$

Property 1:  $X X^+ X = X$

$$X X^+ X = (\sqrt{\Sigma} \sqrt{\Sigma}^T) (\sqrt{\Sigma}^{-1} U^T) (\sqrt{\Sigma} \sqrt{\Sigma}^T)$$

$$= U \Sigma \frac{\sqrt{\Sigma}^T}{\Sigma} \sqrt{\Sigma}^{-1} \frac{U^T}{\Sigma} U \Sigma \sqrt{\Sigma}^T$$

$$= U \Sigma \Sigma^{-1} \Sigma^T$$

$$= U \Sigma V^T = X$$

Property 2:

$$X^+ X X^+ = X^+$$

$$\underbrace{(V\Sigma^{-1}U^T)}_I (V\Sigma V^T) \underbrace{(V\Sigma^{-1}U^T)}_I$$

$$= V \underbrace{\Sigma^{-1}}_I \underbrace{\Sigma}_I V^T V \Sigma^{-1} U^T$$

$$V \Sigma^{-1} \cancel{U^T}$$

$$= X^+$$

Property 3:  $(X X^+)^T = \underbrace{X^+ X X^+}_I$

$$\underbrace{(V\Sigma V^T V\Sigma^{-1}U^T)}_I^T$$

$$= \dots$$

$$= (V U^T)^T$$

$$= V U^T \quad \text{---(i)}$$

$$X X^+ = V \underbrace{\Sigma V^T}_I V \Sigma^{-1} U^T$$

$$= V U^T \quad \text{---(ii)}$$

$$(i) = (ii)$$

Property 4:  $(X^+ X)^T = X^+ X$

$$\begin{aligned} (X^+ X)^T &= \left( \underbrace{(V\Sigma^{-1}U^T)}_I (V\Sigma V^T) \right)^T \\ &= (V U^T)^T = V V^T \quad \text{---(i)} \end{aligned}$$

$$X^+ X = V \Sigma^{-1} U^T V \Sigma V^T = V V^T \quad \text{---(ii)}$$

$$\Rightarrow (i) = (ii)$$

Since all four Penrose properties are satisfied,

$\Sigma^{-1} U^T$  is pseudo-inverse of  $X$ .