

The Orthogonal Projection Matrix onto $\mathcal{C}(\mathbf{X})$ and the Normal Equations

Theorem 2.1:

\mathbf{P}_X , the orthogonal projection matrix onto $\mathcal{C}(X)$, is equal to $X(X'X)^{-1}X'$.

The matrix $X(X'X)^{-1}X'$ satisfies

(a) $[X(X'X)^{-1}X'] [X(X'X)^{-1}X'] = [X(X'X)^{-1}X']$

(b) $X(X'X)^{-1}X'y \in \mathcal{C}(X) \forall y \in \mathbb{R}^n$

(c) $X(X'X)^{-1}X'x = x \forall x \in \mathcal{C}(X)$

(d) $X(X'X)^{-1}X' = [X(X'X)^{-1}X']'$

(e) $X(X'X)^{-1}X'$ is the same \forall GI of $X'X$.

It is useful to establish a few results before proving Theorem 2.1.

Show that if \mathbf{A} is a symmetric matrix and \mathbf{G} is a GI of \mathbf{A} , then \mathbf{G}' is also GI of \mathbf{A} .

Proof:

$$\begin{aligned}AGA = A &\Rightarrow (AGA)' = A' \\ &\Rightarrow A'G'A' = A' \\ &\Rightarrow AG'A = A \quad (\because A = A') \\ \therefore G' &\text{ is a GI of } A.\end{aligned}$$

□.

Result 2.4:

$$\mathbf{X}'\mathbf{X}\mathbf{A} = \mathbf{X}'\mathbf{X}\mathbf{B} \iff \mathbf{X}\mathbf{A} = \mathbf{X}\mathbf{B}.$$

One direction is obvious (\Leftarrow).

Can you prove the other (\Rightarrow)?

Proof (\implies):

$$\begin{aligned}(\mathbf{XA} - \mathbf{XB})'(\mathbf{XA} - \mathbf{XB}) &= (\mathbf{A}'\mathbf{X}' - \mathbf{B}'\mathbf{X}')(\mathbf{XA} - \mathbf{XB}) \\ &= \mathbf{A}'\mathbf{X}'\mathbf{XA} - \mathbf{A}'\mathbf{X}'\mathbf{XB} - \mathbf{B}'\mathbf{X}'\mathbf{XA} + \mathbf{B}'\mathbf{X}'\mathbf{XB} \\ &= \mathbf{A}'\mathbf{X}'\mathbf{XA} - \mathbf{A}'\mathbf{X}'\mathbf{XA} - \mathbf{B}'\mathbf{X}'\mathbf{XA} + \mathbf{B}'\mathbf{X}'\mathbf{XA} \\ &= \mathbf{0}.\end{aligned}$$

∴ by Lemma A1,

$$XA - XB = \mathbf{0} \Rightarrow XA = XB.$$



Result 2.5:

Suppose $(X'X)^-$ is any GI of $X'X$. Then $(X'X)^-X'$ is a GI of X , i.e.,

$$X(X'X)^-X'X = X.$$

Proof of Result 2.5

Since $(X'X)^-$ is a GI of $X'X$,

$$X'X(X'X)^-X'X = X'X.$$

By Result 2.4, the result follows.

(Take $A = (X'X)^-X'X$ and $B = I$. Then

$$XA = X(X'X)^-X'X = X = XB.)$$



Corollary to Result 2.5:

For $(X'X)^-$ any GI of $X'X$,

$$X'X(X'X)^-X' = X'.$$

Proof of Corollary:

Suppose $(X'X)^-$ is any GI of $X'X$.

$\therefore X'X$ is symmetric, $[(X'X)^-]'$ is also a GI of $X'X$.

Thus Result 2.5 implies that

$$\begin{aligned}\mathbf{X}[(\mathbf{X}'\mathbf{X})^{-1}]'\mathbf{X}'\mathbf{X} &= \mathbf{X} \\ \Rightarrow [\mathbf{X}[(\mathbf{X}'\mathbf{X})^{-1}]'\mathbf{X}'\mathbf{X}]' &= [\mathbf{X}]' \\ \Rightarrow \mathbf{X}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}' &= \mathbf{X}'.\end{aligned}$$



Now we can prove Theorem 2.1:

First show $\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$ is idempotent.

$$\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}' = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}' \text{ by Result 2.5.}$$

Now show that

$$\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} \in \mathcal{C}(\mathbf{X}) \quad \forall \mathbf{y} \in \mathbb{R}^n.$$

$X(X'X)^{-1}X'y = Xz$, where $z = (X'X)^{-1}X'y$.

Thus, $X(X'X)^{-1}X'y \in \mathcal{C}(X)$.

Now show that

$$\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{z} = \mathbf{z} \quad \forall \mathbf{z} \in \mathcal{C}(\mathbf{X}).$$

If $\mathbf{z} \in \mathcal{C}(\mathbf{X})$, $\exists \mathbf{c} \ni \mathbf{z} = \mathbf{X}\mathbf{c}$. \therefore

$$\begin{aligned} \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{z} &= \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{X}\mathbf{c} \\ &= \mathbf{X}\mathbf{c} \text{ (By Result 2.5)} \\ &= \mathbf{z}. \end{aligned}$$

Thus, we have $\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{z} = \mathbf{z} \forall \mathbf{z} \in \mathcal{C}(\mathbf{X})$.

Now we know $X(X'X)^{-1}X'$ is a projection matrix onto $\mathcal{C}(X)$.

To be the unique projection matrix onto $\mathcal{C}(X)$, $X(X'X)^{-1}X'$ must be symmetric.

To show symmetry of $X(X'X)^-X'$, it will help to first show that

$$X(X'X)_1^-X' = X(X'X)_2^-X'$$

for any two GIs of $X'X$ denoted $(X'X)_1^-$ and $(X'X)_2^-$.

By the Corollary to Result 2.5

$$\mathbf{X}' = \mathbf{X}'\mathbf{X}(\mathbf{X}'\mathbf{X})_2^{-}\mathbf{X}'.$$

Therefore,

$$\begin{aligned}\mathbf{X}(\mathbf{X}'\mathbf{X})_1^{-}\mathbf{X}' &= \mathbf{X}(\mathbf{X}'\mathbf{X})_1^{-}\mathbf{X}'\mathbf{X}(\mathbf{X}'\mathbf{X})_2^{-}\mathbf{X}' \\ &= \mathbf{X}(\mathbf{X}'\mathbf{X})_2^{-}\mathbf{X}' \text{ by Result 2.5.}\end{aligned}$$

$\therefore \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'$ is the same regardless of which GI for $\mathbf{X}'\mathbf{X}$ is used.

Now show that $\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$ is symmetric.

$$\begin{aligned} [X(X'X)^{-1}X']' &= X[(X'X)^{-1}]'X' \\ &= X(X'X)^{-1}X' \end{aligned}$$

\therefore symmetry of $X'X$ implies that $[(X'X)^{-1}]'$ is a GI of $X'X$, and $X(X'X)^{-1}X'$ is the same regardless of choice of GI. \square

We have shown that $\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$ is the orthogonal projection matrix onto $\mathcal{C}(\mathbf{X})$.

We know that it is the only symmetric projection matrix onto $\mathcal{C}(\mathbf{X})$ by Result A.16.

Example:

Find the orthogonal projection matrix onto $\mathcal{C}(\mathbf{1}_{n \times 1})$.

Also, simplify $P_X y$ in this case.

$\mathbf{X}'\mathbf{X} = \mathbf{1}'\mathbf{1} = n$. Thus $(\mathbf{X}'\mathbf{X})^{-} = \frac{1}{n}$.

$$\begin{aligned}\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}' &= \mathbf{1} \begin{bmatrix} 1 \\ n \end{bmatrix} \mathbf{1}' \\ &= \frac{1}{n} \mathbf{1}\mathbf{1}'.\end{aligned}$$

Thus, when $X = \mathbf{1}$, P_X is an $n \times n$ matrix whose entries are each $\frac{1}{n}$.

We saw previously the special case $\begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix}$.

$$\begin{aligned} P_{xy} &= \frac{1}{n} \mathbf{1} \mathbf{1}' \mathbf{y} \\ &= \frac{1}{n} \mathbf{1} \sum_{i=1}^n y_i = \mathbf{1} \frac{1}{n} \sum_{i=1}^n y_i \\ &= \mathbf{1} \bar{y} = \begin{bmatrix} \bar{y} \\ \bar{y} \\ \vdots \\ \bar{y} \end{bmatrix}. \end{aligned}$$

By Corollary A.4 to Result A.16, we know that

$$\mathbf{I} - \mathbf{P}_X = \mathbf{I} - \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$$

is the orthogonal projection matrix onto $\mathcal{C}(\mathbf{X})^\perp = \mathcal{N}(\mathbf{X}')$.

This is Result 2.6.

Fitted Values and Residuals

By Result A.4, any $\mathbf{y} \in \mathbb{R}^n$ may be written as

$$\mathbf{y} = \mathbf{s} + \mathbf{t},$$

where $\mathbf{s} \in \mathcal{C}(\mathbf{X})$ and $\mathbf{t} \in \mathcal{C}(\mathbf{X})^\perp = \mathcal{N}(\mathbf{X}')$.

Furthermore, the vectors $\mathbf{s} \in \mathcal{C}(\mathbf{X})$ and $\mathbf{t} \in \mathcal{C}(\mathbf{X})^\perp$ are unique.

Fitted Values and Residuals

Because

$$y = P_X y + (I - P_X)y$$

$$P_X y \in \mathcal{C}(X) \text{ and } (I - P_X)y \in \mathcal{C}(X)^\perp,$$

we get $s = P_X y$ and $t = (I - P_X)y$.

Moreover,

$$\hat{y} \equiv P_X y = \text{the vector of fitted values}$$

$$\hat{\varepsilon} \equiv (I - P_X)y = y - \hat{y} = \text{the vector of residuals.}$$

Let P_W and P_X denote the orthogonal projection matrices onto $\mathcal{C}(W)$ and $\mathcal{C}(X)$, respectively.

Suppose $\mathcal{C}(W) \subseteq \mathcal{C}(X)$. Show that

$$P_W P_X = P_X P_W = P_W.$$

Proof:

$$\mathcal{C}(W) \subseteq \mathcal{C}(X) \Rightarrow \exists B \ni XB = W.$$

$$\begin{aligned} \therefore P_X P_W &= X(X'X)^{-1}X'W(W'W)^{-1}W' \\ &= X(X'X)^{-1}X'XB(W'W)^{-1}W' \\ &= \quad \quad \quad XB(W'W)^{-1}W' \\ &= \quad \quad \quad W(W'W)^{-1}W' \\ &= \quad \quad \quad P_W. \end{aligned}$$

Now

$$\begin{aligned}P_X P_W = P_W &\Rightarrow (P_X P_W)' = P_W' \\&\Rightarrow P_W' P_X' = P_W' \\&\Rightarrow P_W P_X = P_W.\end{aligned}$$



Theorem 2.2:

If $\mathcal{C}(\mathbf{W}) \subseteq \mathcal{C}(\mathbf{X})$, then $\mathbf{P}_X - \mathbf{P}_W$ is the orthogonal projection matrix onto $\mathcal{C}((\mathbf{I} - \mathbf{P}_W)\mathbf{X})$.

Proof of Theorem 2.2:

$$(\mathbf{P}_X - \mathbf{P}_W)' = \mathbf{P}'_X - \mathbf{P}'_W = \mathbf{P}_X - \mathbf{P}_W.$$

$\therefore \mathbf{P}_X - \mathbf{P}_W$ is symmetric.

$$\begin{aligned}(\mathbf{P}_X - \mathbf{P}_W)(\mathbf{P}_X - \mathbf{P}_W) &= \mathbf{P}_X\mathbf{P}_X - \mathbf{P}_W\mathbf{P}_X - \mathbf{P}_X\mathbf{P}_W + \mathbf{P}_W\mathbf{P}_W \\ &= \mathbf{P}_X - \mathbf{P}_W - \mathbf{P}_W + \mathbf{P}_W \\ &= \mathbf{P}_X - \mathbf{P}_W.\end{aligned}$$

$\therefore \mathbf{P}_X - \mathbf{P}_W$ is idempotent.

Is $(P_X - P_W)y \in \mathcal{C}((I - P_W)X) \forall y$?

$$\begin{aligned}(P_X - P_W)y &= (P_X - P_W P_X)y \\ &= (I - P_W)P_X y \\ &= (I - P_W)X(X'X)^{-1}X'y \\ &\in \mathcal{C}((I - P_W)X).\end{aligned}$$

Is $(P_X - P_W)z = z$ $z \in \mathcal{C}((I - P_W)X)$?

$$\begin{aligned}(P_X - P_W)(I - P_W)X &= P_X(I - P_W)X - P_W(I - P_W)X \\ &= (P_X - P_X P_W)X - (P_W - P_W P_W)X \\ &= (P_X - P_W)X - (P_W - P_W)X \\ &= (P_X - P_W P_X)X \\ &= (I - P_W)P_X X \\ &= (I - P_W)X.\end{aligned}$$

Now $\mathbf{z} \in \mathcal{C}((\mathbf{I} - \mathbf{P}_W)\mathbf{X})$.

$\Rightarrow \mathbf{z} = (\mathbf{I} - \mathbf{P}_W)\mathbf{X}\mathbf{c}$ for some \mathbf{c} . Therefore,

$$\begin{aligned}(\mathbf{P}_X - \mathbf{P}_W)\mathbf{z} &= (\mathbf{P}_X - \mathbf{P}_W)(\mathbf{I} - \mathbf{P}_W)\mathbf{X}\mathbf{c} \\ &= (\mathbf{I} - \mathbf{P}_W)\mathbf{X}\mathbf{c} \\ &= \mathbf{z}.\end{aligned}$$



We have previously seen that

$$\begin{aligned} Q(\mathbf{b}) &= (\mathbf{y} - \mathbf{X}\mathbf{b})'(\mathbf{y} - \mathbf{X}\mathbf{b}) \\ &= \|\mathbf{y} - \mathbf{X}\mathbf{b}\|^2 \geq \|\mathbf{y} - \mathbf{P}_X\mathbf{y}\|^2 \end{aligned}$$

$\forall \mathbf{b} \in \mathbb{R}^p$ with equality iff $\mathbf{X}\mathbf{b} = \mathbf{P}_X\mathbf{y}$.

Now we know that $P_X = X(X'X)^{-1}X'$.

Thus, $\hat{\beta}$ minimizes $Q(\mathbf{b})$ iff $X\hat{\beta} = X(X'X)^{-1}X'y$.

By Result 2.4, this equation is equivalent to

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

Because $X'X(X'X)^{-1}X' = X'$, $X'X\hat{\beta} = X'X(X'X)^{-1}X'y$ is equivalent to

$$X'X\hat{\beta} = X'y.$$

This system of linear equations is known as the Normal Equations (NE).

We have established Result 2.3:

$\hat{\beta}$ is a solution to the NE ($X'X\mathbf{b} = X'\mathbf{y}$) iff $\hat{\beta}$ minimizes $Q(\mathbf{b})$.

Corollary 2.1:

The NE are consistent.

Proof of Corollary 2.1:

NE are $X'Xb = X'y$.

If we take $\hat{\beta} = (X'X)^{-1}X'y$, then

$$\begin{aligned}X'X\hat{\beta} &= X'X(X'X)^{-1}X'y \\ &= X'y.\end{aligned}$$



By Result A.13, $\hat{\beta}$ is a solution to $X'Xb = X'y$ iff

$$\hat{\beta} = (X'X)^{-1}X'y + [I - (X'X)^{-1}X'X]z$$

for some $z \in \mathbb{R}^p$.

Corollary 2.3:

$X\hat{\beta}$ is invariant to the choice of a solution $\hat{\beta}$ to the NE, i.e., if $\hat{\beta}_1$ and $\hat{\beta}_2$ are any two solutions to the NE, then $X\hat{\beta}_1 = X\hat{\beta}_2$.

Proof of Corollary 2.3:

$$\begin{aligned} X'X\hat{\beta}_1 &= X'X\hat{\beta}_2 (= X'y) \\ \Rightarrow X\hat{\beta}_1 &= X\hat{\beta}_2 \text{ by Result 2.4.} \end{aligned}$$



We will finish this set of notes with some other results from Section 2.2 of the text.

Lemma 2.1: $\mathcal{N}(\mathbf{X}'\mathbf{X}) = \mathcal{N}(\mathbf{X})$.

Result 2.2: $\mathcal{C}(\mathbf{X}'\mathbf{X}) = \mathcal{C}(\mathbf{X}')$.

Corollary 2.2: $\text{rank}(\mathbf{X}'\mathbf{X}) = \text{rank}(\mathbf{X})$.

Proof of Lemma 2.1:

$$\mathbf{Xc} = \mathbf{0} \Rightarrow \mathbf{X}'\mathbf{Xc} = \mathbf{0}$$

$$\therefore \mathcal{N}(\mathbf{X}) \subseteq \mathcal{N}(\mathbf{X}'\mathbf{X}).$$

$$\mathbf{X}'\mathbf{Xc} = \mathbf{0} \Rightarrow \mathbf{c}'\mathbf{X}'\mathbf{Xc} = 0$$

$$\Rightarrow \mathbf{Xc} = \mathbf{0}$$

$$\therefore \mathcal{N}(\mathbf{X}'\mathbf{X}) \subseteq \mathcal{N}(\mathbf{X}).$$

Thus, $\mathcal{N}(\mathbf{X}'\mathbf{X}) = \mathcal{N}(\mathbf{X})$.

□

Proof of Result 2.2:

$$\mathbf{X}'\mathbf{X}\mathbf{c} = \mathbf{X}'(\mathbf{X}\mathbf{c}) \Rightarrow \mathcal{C}(\mathbf{X}'\mathbf{X}) \subseteq \mathcal{C}(\mathbf{X}').$$

$$\begin{aligned}\mathbf{X}'\mathbf{c} &= \mathbf{X}'\mathbf{P}_X\mathbf{c} = \mathbf{X}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{c} \\ &= \mathbf{X}'\mathbf{X}[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{c}] \\ &\Rightarrow \mathcal{C}(\mathbf{X}') \subseteq \mathcal{C}(\mathbf{X}'\mathbf{X}).\end{aligned}$$

Thus, $\mathcal{C}(\mathbf{X}'\mathbf{X}) = \mathcal{C}(\mathbf{X}')$.

□

Proof of Corollary 2.2:

$$\mathcal{C}(\mathbf{X}'\mathbf{X}) = \mathcal{C}(\mathbf{X}')$$

$$\Rightarrow \dim(\mathcal{C}(\mathbf{X}'\mathbf{X})) = \dim(\mathcal{C}(\mathbf{X}'))$$

$$\Rightarrow \text{rank}(\mathbf{X}'\mathbf{X}) = \text{rank}(\mathbf{X}')$$

$$\Rightarrow \text{rank}(\mathbf{X}'\mathbf{X}) = \text{rank}(\mathbf{X}).$$



(Can facilitate finding $(\mathbf{X}'\mathbf{X})^{-}$ needed for $\hat{\beta}$ and \mathbf{P}_X .)