

LINEAR MODEL NOTES

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1. MATRIX ALGEBRA

1.1. Column and Null Space.

Exercise 1.1. Let $X \in \mathcal{M}_{m,n}$. Then $\mathcal{N}(X) = \mathcal{N}(X^T X)$.

Proof. Let $a \in \mathcal{N}(X)$. Then $Xa = 0$. So $X^T Xa = 0$. Thus $a \in \mathcal{N}(X^T X)$. Conversely, suppose that $a \in \mathcal{N}(X^T X)$. Then $X^T Xa = 0$. So

$$\begin{aligned} 0 &= a^T X^T Xa \\ &= (Xa)^T (Xa) \\ &= \|Xa\|^2 \end{aligned}$$

Hence $Xa = 0$ and $a \in \mathcal{N}(X)$. □

Exercise 1.2. Let $X \in \mathcal{M}_{m,n}$. Then $\mathcal{C}(X^T) = \mathcal{C}(X^T X)$.

Proof.

$$\begin{aligned}\mathcal{C}(X^T) &= \mathcal{N}(X)^\perp \\ &= \mathcal{N}(X^T X)^\perp \\ &= \mathcal{C}(X^T X)\end{aligned}$$

□

Exercise 1.3. Let $X \in \mathcal{M}_{m,n}$. If $X^T X = 0$, then $X = 0$.

Proof. Suppose that $X^T X = 0$. Then

$$\begin{aligned}\text{rank}(X^T) &= \dim \mathcal{C}(X^T) \\ &= \dim \mathcal{C}(X^T X) \\ &= \text{rank}(X^T X) \\ &= 0\end{aligned}$$

So $X^T = X = 0$.

□

Exercise 1.4. Let $X \in \mathcal{M}_{m,n}$ and $A, B \in \mathcal{M}_{n,p}$. Then $X^T X A = X^T X B$ iff $X A = X B$.

Proof. Clearly if $X A = X B$, then $X^T X A = X^T X B$. Conversely, suppose that $X^T X A = X^T X B$. Then $X^T X (A - B) = 0$. So for each $i = 1, \dots, p$, $X^T X (A - B)e_i = 0$. Thus for each $i = 1, \dots, p$ $X(A - B)e_i \in \mathcal{N}(X^T) \cap \mathcal{C}(X) = \{0\}$. Hence $X(A - B) = 0$ and $X A = X B$. □

Theorem 1.5. Let $X \in \mathcal{M}_{m,n}$. Then

$$\text{nullity}(X) + \text{rank}(X) = n$$

.

Exercise 1.6. Let $X \in \mathcal{M}_{m,n}$. Then

$$\text{rank}(X^T) = \text{rank}(X)$$

Proof. We have that

$$\begin{aligned}\text{rank}(X^T) &= \text{rank}(X^T X) \\ &= n - \text{nullity}(X^T X) \\ &= n - \text{nullity}(X) \\ &= \text{rank}(X)\end{aligned}$$

□

Definition 1.7. Let $X \in \mathcal{M}_{m,n}$. Then X is said to have **full column rank** if $\text{rank}(X) = n$

Exercise 1.8. Let $X \in \mathcal{M}_{m,n}$. If X has full column rank, then

$$\mathcal{N}(X) = \{0\}$$

Proof. Suppose that X has full column rank. Then $\text{rank}(X) = n$ Hence $\text{nullity}(X) = 0$ and $\mathcal{N}(X) = \{0\}$. □

1.2. Generalized Inverses.

Definition 1.9. Let $A \in \mathcal{M}_{m,n}$ and $G \in \mathcal{M}_{n,m}$. Then G is said to be a **generalized inverse** of A if $AGA = A$.

Theorem 1.10. Let $A \in \mathcal{M}_{m,n}$. Suppose that $\text{rank}(A) = r$. Then there exists $P \in \mathcal{M}_{m,m}$, $Q \in \mathcal{M}_{n,n}$, $C \in \mathcal{M}_{r,r}$ such that P, Q, C are non-singular, $\text{rank}(C) = r$ and

$$A = P \begin{pmatrix} C & 0 \\ 0 & 0 \end{pmatrix} Q$$

Exercise 1.11. Let

$$A = P \begin{pmatrix} C & 0 \\ 0 & 0 \end{pmatrix} Q$$

as in the previous theorem and $D \in \mathcal{M}_{r,m-r}$, $E \in \mathcal{M}_{n-r,r}$, $F \in \mathcal{M}_{n-r,m-r}$. Put

$$G = Q^{-1} \begin{pmatrix} C^{-1} & D \\ E & F \end{pmatrix} P^{-1}$$

Then G is a generalized inverse of A .

Proof.

$$\begin{aligned} AGA &= \left[P \begin{pmatrix} C & 0 \\ 0 & 0 \end{pmatrix} Q \right] \left[Q^{-1} \begin{pmatrix} C^{-1} & D \\ E & F \end{pmatrix} P^{-1} \right] \left[P \begin{pmatrix} C & 0 \\ 0 & 0 \end{pmatrix} Q \right] \\ &= P \begin{pmatrix} C & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} C^{-1} & D \\ E & F \end{pmatrix} \begin{pmatrix} C & 0 \\ 0 & 0 \end{pmatrix} Q \\ &= P \begin{pmatrix} I & CD \\ 0 & 0 \end{pmatrix} \begin{pmatrix} C & 0 \\ 0 & 0 \end{pmatrix} Q \\ &= P \begin{pmatrix} C & 0 \\ 0 & 0 \end{pmatrix} Q \\ &= A \end{aligned}$$

□

Note 1.12. The previous exercise and theorem guarantee the existence of a generalized inverse for all matrices. We will take $G = A^-$ to mean that G is a generalized inverse of A . Unless otherwise specified, A^- will refer to a generic generalized inverse of A , that is, unless otherwise specified, any statement about A^- will apply to all generalized inverses of A .

Theorem 1.13. Let $A \in \mathcal{M}_{m,n}$. Suppose that $\text{rank}(A) = r$. Let $P \in \mathcal{M}_{m,m}$, $Q \in \mathcal{M}_{n,n}$ permutation matrices and $C \in \mathcal{M}_{r,r}$. Suppose that $\text{rank}(C) = r$ and $PAQ = \begin{pmatrix} C & D \\ E & F \end{pmatrix}$. Then

$$Q \begin{pmatrix} C^{-1} & 0 \\ 0 & 0 \end{pmatrix} P = A^-.$$

Exercise 1.14. Let $X \in \mathcal{M}_{m,n}$. Then $(X^T)^- = (X^-)^T$.

Proof.

$$\begin{aligned} X^T(X^-)^T X^T &= (X X^- X)^T \\ &= X^T \end{aligned}$$

□

Exercise 1.15. Let $X \in \mathcal{M}_{m,n}$. Then $\mathcal{C}(XX^-) = \mathcal{C}(X)$.

Proof. Clearly $\mathcal{C}(XX^-) \subset \mathcal{C}(X)$. Let $b \in \mathcal{C}(X)$. Then there exists $a \in \mathbb{R}^n$ such that $Xa = b$. Then

$$\begin{aligned} XX^-b &= XX^-Xa \\ &= Xa \\ &= b \end{aligned}$$

So $b \in \mathcal{C}(XX^-)$. Thus $\mathcal{C}(X) \subset \mathcal{C}(XX^-)$ and $\mathcal{C}(X) = \mathcal{C}(XX^-)$ □

Exercise 1.16. Let $X \in \mathcal{M}_{m,n}$. Then $\mathcal{N}(X) = \mathcal{N}(X^-X)$

Proof. From the previous exercise, we have that

$$\begin{aligned} \mathcal{N}(X) &= \mathcal{C}(X^T)^\perp \\ &= \mathcal{C}(X^T(X^T)^-)^\perp \\ &= \mathcal{C}(X^T(X^-)^T)^\perp \\ &= \mathcal{C}((X^-X)^T)^\perp \\ &= \mathcal{N}(X^-X) \end{aligned}$$

□

Exercise 1.17. Let $X \in \mathcal{M}_{m,n}$. Then $X^- = (X^T X)^- X^T$.

Proof. By definition, $X^T X (X^T X)^- X^T X = X^T X$. A previous exercise implies that $X(X^T X)^- X^T X = X$. Thus $X^- = (X^T X)^- X^T$. □

1.3. Projections.

Definition 1.18. Let $A \in \mathcal{M}_{m,m}$. Then A is said to be **idempotent** if $A^2 = A$.

Exercise 1.19. Let $X \in \mathcal{M}_{m,n}$. Then XX^- and X^-X are idempotent

Proof.

$$\begin{aligned} (XX^-)(XX^-) &= (XX^-X)X^- \\ &= XX^- \end{aligned}$$

The case is similar for X^-X . □

Exercise 1.20. Let $A \in \mathcal{M}_{m,m}$. If A is idempotent, then $I - A$ is idempotent.

Proof. Suppose that A is idempotent. Then

$$\begin{aligned} (I - A)(I - A) &= I^2 - IA - AI + A^2 \\ &= I - 2A + A \\ &= I - A \end{aligned}$$

□

Theorem 1.21. Let $A \in \mathcal{M}_{m,m}$. If A is idempotent, then $\text{rank}(A) = \text{tr}(A)$.

Definition 1.22. Let $P \in \mathcal{M}_{m,m}$ and $S \subset \mathbb{R}^m$ a subspace. Then P is said to be a **projection matrix** onto S if

- (1) P is idempotent
- (2) $\mathcal{C}(P) \subset S$
- (3) for each $x \in S$, $Px = x$

Note 1.23. In the previous definition, (2) and (3) imply that $\mathcal{C}(X) = S$, so to say that X projects “onto” S is accurate.

Exercise 1.24. Let $S \subset \mathbb{R}^m$ and P, Q projection matrices onto S . Then $PQ = Q$.

Proof. Let $x \in \mathbb{R}^m$. Then $Qx \in \mathcal{C}(Q) = S$. So $PQx = Qx$. Thus $PQ = Q$. □

Exercise 1.25. Let $X \in \mathcal{M}_{m,n}$. Then XX^{-} is a projection onto $\mathcal{C}(X)$.

Proof. A previous exercises tells us that XX^{-} is idempotent. Another previous exercise tells us that $\mathcal{C}(XX^{-}) = \mathcal{C}(X)$. Let $b \in \mathcal{C}(X)$. Then there exists $a \in \mathbb{R}^n$ such that $Xa = b$. So

$$\begin{aligned} XX^{-}b &= XX^{-}Xa \\ &= Xa \\ &= b \end{aligned}$$

□

Exercise 1.26. Let $X \in \mathcal{M}_{m,n}$. Then $I - X^{-}X$ is a projection onto $\mathcal{N}(X)$

Proof. Since $X^{-}X$ is idempotent, so is $I - X^{-}X$. Let $b \in \mathcal{C}(I - X^{-}X)$. Then there exists $a \in \mathbb{R}^n$ such that $(I - X^{-}X)a = b$. Then

$$\begin{aligned} Xb &= X(I - X^{-}X)a \\ &= (X - XX^{-}X)a \\ &= (X - X)a \\ &= 0a \\ &= 0 \end{aligned}$$

So $\mathcal{C}(I - X^{-}X) \subset \mathcal{N}(X)$. Let $a \in \mathcal{N}(X)$. Then $Xa = 0$ and

$$\begin{aligned} (I - X^{-}X)a &= a - X^{-}Xa \\ &= a \end{aligned}$$

So for each $a \in \mathcal{N}(X)$, $(I - X^{-}X)a = a$. □

Exercise 1.27. Let $S \subset \mathbb{R}^m$ be a subspace and $P \in \mathcal{M}_{m,m}$ be a symmetric projection matrix onto S . Then P is unique.

Proof. Let $Q \in \mathcal{M}_{m,m}$ be a symmetric projection matrix onto S . Then

$$\begin{aligned} (P - Q)^T(P - Q) &= P^T P - P^T Q - Q^T P + Q^T Q \\ &= P^2 - PQ - QP + Q^2 \\ &= P - Q - P + Q \\ &= 0 \end{aligned}$$

Thus $P - Q = 0$ and $P = Q$. □

Definition 1.28. Let $X \in \mathcal{M}_{m,n}$. We define P_X by

$$P_X = X(X^T X)^- X^T$$

Exercise 1.29. Let $X \in \mathcal{M}_{m,n}$. Then P_X is well defined, that is, P_X is independent of the choice of $(X^T X)^-$.

Proof. Suppose that G, H are generalized inverses of $X^T X$. By definition, we have

$$\begin{aligned} X^T X G X^T X &= X^T X H X^T X \Rightarrow X G X^T X = X H X^T X \\ &\Rightarrow X^T X G^T X^T = X^T X H X^T \\ &\Rightarrow X G^T X^T = X H X^T \\ &\Rightarrow X G X^T = X H X^T = P_X \end{aligned}$$

□

Note 1.30. Recall that $X^- = (X^T X)^- X^T$. So that $P_X = X X^-$ is indeed a projection onto $\mathcal{C}(X)$. Recall that $[(X^T X)^-]^T$ is a generalized inverse of $(X^T X)^T = (X^T X)$. Hence $P_X^T = X[(X^T X)^-]^T X^T = P_X$. Since P_X is symmetric, it is the unique symmetric projection onto $\mathcal{C}(X)$.

Exercise 1.31. Let $X \in \mathcal{M}_{m,n}$. Then $(X^T)^- = X(X^T X)^-$.

Proof. We know that $P_X X = X$. Transposing both sides, we get that

$$\begin{aligned} X^T &= X^T P_X \\ &= X^T X (X^T X)^- X^T \end{aligned}$$

So

$$(X^T)^- = X(X^T X)^-$$

□

Note 1.32. Recall that $(X^T)^- = X(X^T X)^-$. So that $P_X = (X^T)^- X^T$. A previous exercises tells us that $I - P_X$ is a projection on $\mathcal{N}(X^T)$. Since $I - P_X$ is symmetric, it is the unique symmetric projection onto $\mathcal{N}(X^T)$.

Exercise 1.33. Let $X_1, X_2 \in \mathcal{M}_{m,n}$. Suppose that $\mathcal{C}(X_1) = \mathcal{C}(X_2)^\perp$. Then $P_{X_1} P_{X_2} = P_{X_2} P_{X_1} = 0$.

Proof. Since $I - P_{X_1}$ is the unique symmetric projection onto $\mathcal{N}(X_1^T) = \mathcal{C}(X_1)^\perp = \mathcal{C}(X_2)$, we have that $I - P_{X_1} = P_{X_2}$. Thus $P_{X_1} P_{X_2} = P_{X_1} (I - P_{X_1}) = 0$. Similarly, $P_{X_2} P_{X_1} = 0$. □

Exercise 1.34. Let $X \in \mathcal{M}_{m,n}$. For each $z \in \mathcal{N}(X^T)$, $P_X z = 0$.

Proof. Let $z \in \mathcal{N}(X^T)$. Then $P_X z = X(X^T X)^- (X^T z) = 0$. □

Exercise 1.35. Let $X_1, X_2 \in \mathcal{M}_{m,n}$. If $\mathcal{C}(X_1) \subset \mathcal{C}(X_2)$, then $P_{X_2} - P_{X_1}$ is the unique projection onto $\mathcal{C}((I - P_{X_1})X_2)$.

Proof. Clearly $P_{X_2} - P_{X_1}$ is symmetric. Since $\mathcal{C}(X_1) \subset \mathcal{C}(X_2)$, we have that $P_{X_2} P_{X_1} = P_{X_1}$. Also, by symmetry,

$$\begin{aligned} (P_{X_1} P_{X_2})^T &= P_{X_2}^T P_{X_1}^T \\ &= P_{X_2} P_{X_1} \\ &= P_{X_1} \end{aligned}$$

So $P_{X_1}P_{X_2} = P_{X_1}^T = P_{X_1}$. Now we have that

(1)

$$\begin{aligned} (P_{X_2} - P_{X_1})^2 &= (P_{X_2} - P_{X_1})(P_{X_2} - P_{X_1}) \\ &= P_{X_2}^2 + P_{X_1}^2 - P_{X_2}P_{X_1} - P_{X_1}P_{X_2} \\ &= P_{X_2} + P_{X_1} - P_{X_1} - P_{X_1} \\ &= P_{X_2} - P_{X_1} \end{aligned}$$

So $P_{X_2} - P_{X_1}$ is idempotent.

(2) Let $x \in \mathbb{R}^m$. Then there exist unique $y \in \mathcal{C}(X_2)$ and $z \in \mathcal{C}(X_2)^\perp = \mathcal{N}(X_2^T)$ such that $x = y + z$. So there exists $e \in \mathbb{R}^n$ such that $y = X_2e$. Since $z \in \mathcal{N}(X_2^T)$, $P_{X_2}z = 0$. Then

$$\begin{aligned} (P_{X_2} - P_{X_1})x &= P_{X_2}x - P_{X_1}x \\ &= P_{X_2}x - P_{X_1}P_{X_2}x \\ &= y - P_{X_1}y \\ &= X_2e - P_{X_1}X_2e \\ &= (I - P_{X_1})X_2e \\ &\in \mathcal{C}((I - P_{X_1})X_2) \end{aligned}$$

(3) Let $x \in \mathcal{C}((I - P_{X_1})X_2)$. Then there exists $e \in \mathbb{R}^n$ such that $x = (I - P_{X_1})X_2e$. So

$$\begin{aligned} (P_{X_2} - P_{X_1})x &= P_{X_2}(I - P_{X_1})x \\ &= P_{X_2}(I - P_{X_1})(I - P_{X_1})X_2e \\ &= P_{X_2}(I - P_{X_1})X_2e \\ &= (P_{X_2} - P_{X_1})X_2e \\ &= P_{X_2}X_2e - P_{X_1}X_2e \\ &= X_2e - P_{X_1}X_2e \\ &= (I - P_{X_1})X_2e \\ &= x \end{aligned}$$

□

1.4. Solving Linear Equations.

Definition 1.36. Let $A \in \mathcal{M}_{m,n}$ and $b \in \mathbb{R}^m$. Then the system $Ax = b$ is said to be **consistent** if $b \in \mathcal{C}(A)$.

Exercise 1.37. Let $A \in \mathcal{M}_{m,n}$ and $G \in \mathcal{M}_{n,m}$. Then $G = A^-$ iff for each $b \in \mathcal{C}(A)$, Gb solves $Ax = b$.

Proof. Suppose that $G = A^-$. Let $b \in \mathcal{C}(A)$. Then there exists $x^* \in \mathbb{R}^n$ such that $Ax^* = b$. So

$$\begin{aligned} A(Gb) &= AG(Ax^*) \\ &= (AGA)x^* \\ &= Ax^* \\ &= b \end{aligned}$$

So Gb solves $Ax = b$. Conversely, Suppose that for each $b \in \mathcal{C}(A)$, Gb solves $Ax = b$. Let $z \in \mathbb{R}^n$. So $Az \in \mathcal{C}(A)$. Then

$$\begin{aligned}(AGA)z &= A[G(Az)] \\ &= Az\end{aligned}$$

Since for each $z \in \mathbb{R}^n$ $AGAz = Az$, $AGA = A$ and $G = A^-$. □

Exercise 1.38. Let $b \in \mathcal{C}(A)$. Then

$$\{x \in \mathbb{R}^n : Ax = b\} = \{A^-b + (I - A^-A)z : z \in \mathbb{R}^n\}$$

.

Proof. Let $x \in \{A^-b + (I - A^-A)z : z \in \mathbb{R}^n\}$. Then there exists $z \in \mathbb{R}^n$ such that $x = A^-b + (I - A^-A)z$. Since $(I - A^-A)$ is a projection onto $\mathcal{N}(A)$,

$$\begin{aligned}Ax &= AA^-b \\ &= b\end{aligned}$$

So $x \in \{x \in \mathbb{R}^n : Ax = b\}$. Conversely, let $x \in \{x \in \mathbb{R}^n : Ax = b\}$. Then

$$\begin{aligned}x &= A^-(Ax) + (x - A^-Ax) \\ &= A^-(b) + (I - A^-A)x \\ &\in \{A^-b + (I - A^-A)z : z \in \mathbb{R}^n\}\end{aligned}$$

□

1.5. Moore-Penrose Pseudoinverse.

Theorem 1.39. Singular Value Decomposition:

Let $A \in \mathcal{M}_{m,n}$. Suppose that $\text{rank}(A) = r$. Then there exist $U \in \mathcal{M}_{m,m}$, $V \in \mathcal{M}_{n,n}$, and $D_0 \in \mathcal{M}_{r,r}$ such that

- (1) $A = U \begin{pmatrix} D_0 & 0 \\ 0 & 0 \end{pmatrix} V^T$
- (2) $U^T U = I$
- (3) $V^T V = I$
- (4) $D_0 = \text{diagonal}(d_1, d_2, \dots, d_r)$ with $d_1 \geq d_2 \geq \dots \geq d_r > 0$

Note 1.40. Put $D = \begin{pmatrix} D_0 & 0 \\ 0 & 0 \end{pmatrix} \in \mathcal{M}_{m,n}$

- (1) Since D_0 is symmetric, $D^T = \begin{pmatrix} D_0 & 0 \\ 0 & 0 \end{pmatrix} \in \mathcal{M}_{n,m}$
- (2) Since D_0 is diagonal, D_0^{-1} is also diagonal and symmetric

Definition 1.41. Let $A \in \mathcal{M}_{m,m}$ and $A^+ \in \mathcal{M}_{n,m}$. Then A^+ is said to be a **Moore-Penrose pseudoinverse** of A if

- (1) $AA^+A = A$
- (2) $A^+AA^+ = A^+$
- (3) AA^+ is symmetric
- (4) A^+A is symmetric

Note 1.42. We have that $P_X = XX^+ = X(X^T X)^- X^T$.

Exercise 1.43. Let $A \in \mathcal{M}_{m,n}$ and $S, T \in \mathcal{M}_{n,m}$. If S and T are m - p pseudoinverses of A , then $S = T$.

Proof. Suppose that S, T satisfy properties (1)-(4). Then

$$\begin{aligned}
 S &= SAS \\
 &= (SA)^T S \\
 &= A^T S^T S \\
 &= (ATA)^T S^T S \\
 &= A^T T^T A^T S^T S \\
 &= (TA)^T (SA)^T S \\
 &= (TA)(SA)S \\
 &= TA(SAS) \\
 &= TAS
 \end{aligned}$$

and

$$\begin{aligned}
 T &= TAT \\
 &= T(AT)^T \\
 &= TT^T A^T \\
 &= TT^T (ASA)^T \\
 &= TT^T A^T S^T A^T \\
 &= T(AT)^T (AS)^T \\
 &= T(AT)(AS) \\
 &= (TAT)AS \\
 &= TSA
 \end{aligned}$$

So $S = T$

□

Exercise 1.44. Let $A \in \mathcal{M}_{m,n}$ have singular value decomposition $A = UDV^T = U \begin{pmatrix} D_0 & 0 \\ 0 & 0 \end{pmatrix} V^T$.

Define $D^+ = \begin{pmatrix} D_0^{-1} & 0 \\ 0 & 0 \end{pmatrix} \in \mathcal{M}_{n,m}$. Then D^+ is the m - p pseudoinverse of D .

Proof.

(1)

$$\begin{aligned}
DD^+D &= \begin{pmatrix} D_0 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} D_0^{-1} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} D_0 & 0 \\ 0 & 0 \end{pmatrix} \\
&= \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} D_0 & 0 \\ 0 & 0 \end{pmatrix} \\
&= \begin{pmatrix} D_0 & 0 \\ 0 & 0 \end{pmatrix} \\
&= D
\end{aligned}$$

(2) Similar to (1).

(3)

$$\begin{aligned}
(DD^+)^T &= \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}^T \\
&= \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} \\
&= DD^+
\end{aligned}$$

(4) Similar to (3).

□

Exercise 1.45. Let $A \in \mathcal{M}_{m,n}$ have singular value decomposition $A = UDV^T$. So $A^T \in \mathcal{M}_{n,m}$ has singular value decomposition $A^T = VD^TU^T$. Then $(D^T)^+ = (D^+)^T$

Proof. Since $D^T = \begin{pmatrix} D_0 & 0 \\ 0 & 0 \end{pmatrix} \in \mathcal{M}_{n,m}$, we have that $(D^T)^+ = \begin{pmatrix} D_0^{-1} & 0 \\ 0 & 0 \end{pmatrix} = (D^+)^T$ □

Exercise 1.46. Let $A \in \mathcal{M}_{m,n}$ have singular value decomposition $A = UDV^T$. Define $A^+ = VD^+U^T$. Then A^+ is the m - p pseudoinverse of A .

Proof. (1)

$$\begin{aligned}
AA^+A &= (UDV^T)(VD^+U^T)(UDV^T) \\
&= UDD^+DV^T \\
&= UDV^T \\
&= A
\end{aligned}$$

(2) Similar to (1)

(3)

$$\begin{aligned}
(AA^+)^T &= [(UDV^T)(VD^+U^T)]^T \\
&= (UDD^+U^T)^T \\
&= U(DD^+)^TU^T \\
&= UDD^+U^T \\
&= (UDV^T)(VD^+U^T) \\
&= AA^+
\end{aligned}$$

(4) Similar to (3). □

Exercise 1.47. Let $A \in \mathcal{M}_{m,n}$ have singular value decomposition $A = UDV^T$. Then $(A^T)^+ = (A^+)^T$.

Proof.

$$\begin{aligned} (A^T)^+ &= [(UDV^T)^T]^+ \\ &= (VD^T U^T)^+ \\ &= U(D^T)^+ V^T \\ &= U(D^+)^T V^T \\ &= (VD^+ U^T)^T \\ &= (A^+)^T \end{aligned}$$

□

Exercise 1.48. Let $A \in \mathcal{M}_{m,n}$. Then there exists a unique matrix $A^+ \in \mathcal{M}_{n,m}$ such that A^+ is the m - p pseudoinverse of A .

Proof. The existence of and uniqueness of A^+ are shown in the previous exercises. □

Exercise 1.49. Let $A \in \mathcal{M}_{m,m}$. Then $(A^+)^+ = A$.

Proof. We observe that A satisfies properties (1)–(4) for A^+ . By uniqueness, $(A^+)^+ = A$. □

Exercise 1.50. Let $A \in \mathcal{M}_{m,n}$ and $b \in \mathcal{C}(A)$. Put $S = \{x \in \mathbb{R}^n : Ax = b\}$. Then

$$\|A^+b\| = \min_{x \in S} \|x\|$$

.

Proof. Let $x \in S$. A previous exercise tells us that there exists $z \in \mathbb{R}^n$ such that $x = A^+b + (I - A^+A)z$. Then

$$\begin{aligned} \|x\|^2 &= \|A^+b + (I - A^+A)z\|^2 \\ &= (A^+b + (I - A^+A)z)^T (A^+b + (I - A^+A)z) \\ &= \|A^+b\|^2 - 2z^T (I - A^+A)^T (A^+b) + \|(I - A^+A)z\|^2 \\ &= \|A^+b\|^2 - 2z^T (I - A^+A)A^+b + \|(I - A^+A)z\|^2 \\ &= \|A^+b\|^2 + \|(I - A^+A)z\|^2 \\ &\geq \|A^+b\|^2 \end{aligned}$$

□

1.6. Differentiation.

Definition 1.51. Let $Q : \mathbb{R}^n \rightarrow \mathbb{R}$ given by $b \mapsto Q(b)$. Suppose that $Q \in C^1(\mathbb{R}^n)$. We define

$$\frac{\partial Q}{\partial b} = \begin{pmatrix} \frac{\partial Q}{\partial b_1} \\ \vdots \\ \frac{\partial Q}{\partial b_n} \end{pmatrix}$$

Exercise 1.52. Let $a, b \in \mathbb{R}_n$ and $A \in \mathcal{M}_{n,n}$. Then

$$(1) \quad \frac{\partial a^T b}{\partial b} = a$$

$$(2) \quad \frac{\partial b^T A b}{\partial b} = (A + A^T)b$$

Proof.

(1) Since

$$a^T b = \sum_{i=1}^n a_i b_i$$

We have that

$$\frac{\partial a^T b}{\partial b_i} = a_i$$

and therefore

$$\frac{\partial a^T b}{\partial b} = a$$

(2) Since

$$\begin{aligned} b^T A b &= \sum_{i=1}^n b_i \sum_{j=1}^n A_{i,j} b_j \\ &= \sum_{i=1}^n \sum_{j=1}^n b_i A_{i,j} b_j \end{aligned}$$

The terms containing b_i are

$$A_{i,i} b_i^2 + \sum_{\substack{j=1 \\ j \neq i}}^n (A_{i,j} + A_{j,i}) b_i b_j$$

This implies that

$$\begin{aligned} \frac{\partial b^T A b}{\partial b_i} &= 2A_{i,i} b_i + \sum_{\substack{j=1 \\ j \neq i}}^n (A_{i,j} + A_{j,i}) b_j \\ &= \sum_{j=1}^n (A_{i,j} + A_{j,i}^T) b_j \\ &= [(A + A^T)b]_i \end{aligned}$$

So

$$\frac{\partial b^T A b}{\partial b} = (A + A^T)b$$

□

1.7. Quadratic Forms and Eigendecomposition.

Definition 1.53. Let $A \in \mathcal{M}_{n,n}$. Then A is said to be **positive semi-definite** if for each $x \in \mathbb{R}^n$,

$$x^T A x \geq 0$$

Definition 1.54. Let $A \in \mathcal{M}_{n,n}$. Then A is said to be **positive-definite** if for each $x \in \mathbb{R}^n$, $x \neq 0$ implies that

$$x^T A x > 0$$

Exercise 1.55. Let $A \in \mathcal{M}_{n,n}$. If A is positive-definite, then A is invertible.

Exercise 1.56. Let $A \in \mathcal{M}_{n,n}$. Then A is invertible iff for each eigenvalue λ of A , $\lambda \neq 0$.

Proof. Suppose that A is invertible. Let $x \in \mathbb{R}^n$. Suppose that $Ax = 0$. Then $x = 0$. So x is not an eigenvector of A . So 0 is not an eigenvalue of A . Conversely. Suppose that A is not invertible. Then there exists $x \in \ker A$ such that $x \neq 0$. Then $Ax = 0 = 0x$. So 0 is an eigenvalue of A . \square

Proof. Suppose that A is positive definite. Let $x \in \ker A$. Suppose that $x \neq 0$. Then $x^T A x = x^T 0 = 0$, which is a contradiction. Hence $\ker A = \{0\}$. So $\text{rank}(A) = n$ and A is invertible. \square

Exercise 1.57. Let $A \in \mathcal{M}_{n,n}$. If A is positive semi-definite (respectively positive definite), then the eigenvalues of A are nonnegative (respectively positive).

Proof. Let $\lambda \in \mathbb{C}$ be an eigenvalue of A and $x \in \mathbb{R}^n$ a corresponding eigenvector. Then $x \neq 0$. So $x^T x \geq 0$. If A is positive semi-definite, then

$$\begin{aligned} 0 &\leq x^T A x \\ &= \lambda x^T x \end{aligned}$$

Hence $\lambda \geq 0$. The case is similar for A positive definite. \square

Definition 1.58. Let $U \in \mathcal{M}_{n,n}$. Then U is said to be **orthogonal** if $U^T U = U U^T = I$

Theorem 1.59. Let $A \in \mathcal{M}_{n,n}$ be a symmetric matrix and $\lambda_1, \dots, \lambda_n$ the eigenvalues of A . Then

- (1) $\lambda_1, \dots, \lambda_n \in \mathbb{R}$
- (2) for $i, j \in \{1, \dots, n\}$ if $i \neq j$ and x_i, x_j are eigenvectors corresponding to λ_i, λ_j respectively, then $x_i^T x_j = 0$.
- (3) there exist $U, D \in \mathcal{M}_{n,n}$ such that U is orthogonal, $D = \text{diag}(\lambda_1, \dots, \lambda_n)$ and $A = U D U^T$.

Note 1.60. We will be dealing with covariance matrices which are positive semi-definite symmetric matrices and thus have nonnegative eigenvalues.

2. THE LINEAR MODEL

2.1. Model Description.

Definition 2.1. Given $y \in \mathbb{R}_m$ a vector of observed responses to the matrix $X \in \mathcal{M}_{m,n}$ of observed inputs, we will consider the model

$$y = Xb + e$$

where $b \in \mathbb{R}_n$ is a vector of unknown parameters and $e \in \mathbb{R}^m$ is a random vector of unobserved errors with zero mean.

Definition 2.2. For a parameter vector $b \in \mathbb{R}^n$, we have that $e = y - Xb$. For this reason, e is called the **residual vector** or simply the “residuals”.

Note 2.3. The goal will be to find a parameter vector $b \in \mathbb{R}^n$ that makes the residuals to be as small as possible.

2.2. Least Squares Optimization.

Definition 2.4. We define the **cost function**, $Q : \mathbb{R}^n \rightarrow \mathbb{R}$ by

$$\begin{aligned} Q(b) &= \|y - Xb\|^2 \\ &= (y - Xb)^T(y - Xb) \end{aligned}$$

Definition 2.5. Let $b \in \mathbb{R}^n$. Then b is said to be a **least squares solution** for the model if

$$Q(b) = \inf_{c \in \mathbb{R}^n} Q(c)$$

Exercise 2.6. If b is a least squares solution for the model, then $X^T Xb = X^T y$.

Proof. Suppose that b is a least squares solution for the model, then Q has a global minimum at b . Since Q is convex in b , this global minimum is also a local minimum. Thus

$$\frac{\partial Q}{\partial b}(b) = 0$$

By definition,

$$\begin{aligned} Q(b) &= y^T y - y^T Xb - b^T X^T y + b^T X^T Xb \\ &= y^T y - 2y^T Xb + b^T X^T Xb \end{aligned}$$

Thus

$$\begin{aligned} 0 &= \frac{\partial Q}{\partial b}(b) \\ &= -2X^T y + 2X^T Xb \end{aligned}$$

Hence $X^T Xb = X^T y$. □

Definition 2.7. For $y \in \mathbb{R}^m$ and $X \in \mathcal{M}_{m,n}$, we define the **normal equation** to be

$$X^T Xb = X^T y$$

Exercise 2.8. The normal equation is consistent.

Proof. We have that $X^T y \in \mathcal{C}(X^T) = \mathcal{C}(X^T X)$. □

Exercise 2.9. Let $b \in \mathbb{R}^n$. Then b is a least squares solution for the model iff b satisfies the normal equation.

Proof. The previous exercises tells us that if b is a least squares solution for the model, then b satisfies the normal equation. Conversely, suppose that b satisfies the normal equation.

Then

$$\begin{aligned}
 Q(c) &= (y - Xc)^T(y - Xc) \\
 &= (y - Xb + Xb - Xc)^T(y - Xb + Xb - Xc) \\
 &= (y - Xb)^T(y - Xb) - (y - Xb)^T(X(b - c)) - (b - c)^T X^T(y - Xb) + (b - c)^T X^T(X(b - c)) \\
 &= Q(b) - 2(b - c)^T X^T(y - Xb) + \|X(b - c)\|^2 \\
 &= Q(b) + \|X(b - c)\|^2
 \end{aligned}$$

Thus b minimizes Q . □

Exercise 2.10. Let $b \in \mathbb{R}^n$ be a least squares solution for the model. Then $\|y\|^2 = \|Xb\|^2 + \|e\|^2$

Proof. Since b satisfies the normal equation, we have that $X^T(y - Xb) = 0$. Thus

$$\begin{aligned}
 Xb \cdot e &= b^T X^T e \\
 &= b^T X^T(y - Xb) \\
 &= b^T 0 \\
 &= 0
 \end{aligned}$$

So Xb and e are orthogonal. Therefore

$$\begin{aligned}
 \|y\|^2 &= \|Xb + e\|^2 \\
 &= \|Xb\|^2 + \|e\|^2
 \end{aligned}$$

□

2.3. Estimation.

Note 2.11. In what follows we are considering the model $y = Xb + e$ with $y, e \in \mathbb{R}^n$, $b \in \mathbb{R}^p$, $X \in \mathcal{M}_{n,p}$ and $\mathbb{E}[e] = 0$.

Definition 2.12. Let Then $\lambda \in \mathbb{R}^p$. The function $t(y)$ is said to be a linear unbiased estimator for the function $f(b) = \lambda^T b$ if there exists $a \in \mathbb{R}^n$, $c \in \mathbb{R}$ such that $t(y) = c + a^T y$ and for each $b \in \mathbb{R}^p$, $\mathbb{E}[t(y)] = \lambda^T b$.

Exercise 2.13. Let Then $\lambda \in \mathbb{R}^p$ and $a \in \mathbb{R}^n$, $c \in \mathbb{R}$. Suppose that $t(y) = c + a^T y$ is an unbiased linear estimator for $f(b) = \lambda^T b$. Then $c = 0$ and $\lambda = X^T a$.

Proof. We have that for each $b \in \mathbb{R}^p$,

$$\begin{aligned}
 \lambda^T b &= \mathbb{E}[c + a^T y] \\
 &= c + a^T \mathbb{E}[y] \\
 &= c + a^T Xb
 \end{aligned}$$

Taking $b = 0$, we get that $c = 0$. So for each $b \in \mathbb{R}^p$, $\lambda^T b = a^T Xb$. This implies that $\lambda^T = a^T X$ and $\lambda = X^T a$. □

Definition 2.14. Let $\lambda \in \mathbb{R}^p$. Then the function $f(b) = \lambda^T b$ is said to be **linearly estimable** if there exists a linear, unbiased estimator for $f(b)$. Equivalently, $f(b) = \lambda^T b$ is linearly estimable if there exists $a \in \mathbb{R}^n$ such that for each $b \in \mathbb{R}^p$ $\mathbb{E}[a^T y] = \lambda^T b$

Exercise 2.15. Let $\lambda \in \mathbb{R}^p$. Then the following are equivalent:

- (1) $f(b) = \lambda^T b$ is linearly estimable
- (2) $\lambda \in \mathcal{C}(X^T)$
- (3) for each $G \in X^-$ of X , $\lambda^T = \lambda^T G X$
- (4) there exists $G \in X^-$ of X such that $\lambda^T = \lambda^T G X$

$f(b) = \lambda^T b$ is linearly estimable iff $\lambda \in \mathcal{C}(X^T)$.

Proof. (1) \Rightarrow (2)

Suppose that $f(b)$ is linearly estimable. Then there exists $a \in \mathbb{R}^n$ such that for each $b \in \mathbb{R}^p$ $\mathbb{E}[a^T y] = \lambda^T b$. Then for each $b \in \mathbb{R}^p$,

$$\lambda^T b = a^T \mathbb{E}[y] = a^T X b$$

Hence $\lambda^T = a^T X$ and $X^T a = \lambda$. So $\lambda \in \mathcal{C}(X^T)$.

(2) \Rightarrow (3)

Suppose that $\lambda \in \mathcal{C}(X^T)$. Let $G \in X^-$. Then $G^T \in (X^T)^-$. Since $\lambda \in \mathcal{C}(X^T)$, there exists $a \in \mathbb{R}^n$ such that $X^T a = \lambda$. A previous exercise tells us that there exists $z \in \mathbb{R}^n$ such that

$$a = G^T \lambda + (I - G^T X^T) z$$

So

$$\begin{aligned} \lambda &= X^T a \\ &= X^T [G^T \lambda + (I - G^T X^T) z] \\ &= X^T G^T \lambda \end{aligned}$$

Hence $\lambda^T = \lambda^T G X$.

(3) \Rightarrow (4)

Trivial.

(4) \Rightarrow (1)

Suppose that there exists $G \in X^-$ such that $\lambda^T = \lambda^T G X$. Choose $a = G^T \lambda \in \mathbb{R}^n$. Let $b \in \mathbb{R}^p$. Then

$$\begin{aligned} \mathbb{E}[a^T y] &= a^T \mathbb{E}[y] \\ &= \lambda^T G \mathbb{E}[y] \\ &= \lambda^T G X b \\ &= \lambda^T b \end{aligned}$$

So $f(b) = \lambda^T b$ is linearly estimable. □

Definition 2.16. Let $\hat{b} \in \mathbb{R}^p$ be a least squares solution and $\lambda \in \mathbb{R}^n$. Then $\hat{f} = \lambda^T \hat{b}$ is said to be a least squares estimator of $f(b) = \lambda^T b$.

Exercise 2.17. Let $\hat{b} \in \mathbb{R}^p$ be a least squares solution and $\lambda \in \mathbb{R}^n$. Then $\hat{f} = \lambda^T \hat{b}$ is the unique least squares estimator of $f(b) = \lambda^T b$ iff $f(b)$ is linearly estimable.

Proof. Suppose that $f(b) = \lambda^T b$ is linearly estimable. Then $\lambda \in \mathcal{C}(X^T)$. So there exists $a \in \mathbb{R}^n$ such that $\lambda^T = a^T X$. Let b' be a least squares solution. Then there exists $z \in \mathbb{R}^p$ such that

$$b' = (X^T X)^- X^T y + (I - (X^T X)^- (X^T X))z$$

Then

$$\begin{aligned} \lambda^T b' &= \lambda^T \left[(X^T X)^- X^T y + (I - (X^T X)^- (X^T X))z \right] \\ &= a^T X (X^T X)^- X^T y + a^T X (I - (X^T X)^- X^T X)z \\ &= a^T P_X y + a^T (X - P_X X)z \\ &= a^T P_X y \end{aligned}$$

In particular, $\lambda^T b' = a^T P_X y = \lambda^T \hat{b}$.

Conversely, suppose that $\hat{f} = \lambda^T \hat{b}$ is the unique least squares estimator of $f(b) = \lambda^T b$. Then for each $z \in \mathbb{R}^p$,

$$\lambda^T \hat{b} = \lambda^T (X^T X)^- X^T y + \lambda^T (I - (X^T X)^- X^T X)z$$

So for each $z \in \mathbb{R}^p$,

$$\lambda^T (X^T X)^- X^T y + \lambda^T (I - (X^T X)^- X^T X)z = 0$$

and thus

$$\lambda^T (I - (X^T X)^- X^T X) = 0$$

Therefore

$$\lambda^T = \lambda^T (X^T X)^- X^T X$$

Transposing both sides, we obtain that

$$\lambda = X^T X [(X^T X)^-]^T \lambda \in \mathcal{C}(X^T)$$

So $f(b) = \lambda^T b$ is linearly estimable □

Exercise 2.18. Let $\lambda \in \mathbb{R}^p$ and $\hat{b} \in \mathbb{R}^p$ a least squares solution. If $f(b) = \lambda^T b$ is linearly estimable, then the unique least squares estimator $\hat{f} = \lambda^T \hat{b}$ of $f(b)$ is a linear unbiased estimator of $f(b)$.

Proof. Suppose that $f(b) = \lambda^T b$ is linearly estimable. Then there exists $a \in \mathbb{R}^n$ such that $\lambda^T = a^T X$. The previous exercise tells us that

$$\lambda^T \hat{b} = \lambda^T (X^T X)^- X^T y$$

Thus for each $b \in \mathbb{R}^p$,

$$\begin{aligned} \mathbb{E}[\lambda^T \hat{b}] &= \mathbb{E}[\lambda^T (X^T X)^- X^T y] \\ &= \lambda^T (X^T X)^- X^T \mathbb{E}[y] \\ &= \lambda^T (X^T X)^- X^T X b \\ &= a^T X (X^T X)^- X^T X b \\ &= a^T P_X X b \\ &= a^T X b \\ &= \lambda^T b \end{aligned}$$

□

2.4. Imposing Restrictions for a Unique Solution.

Definition 2.19. Let $X \in \mathcal{M}_{n,p}$ with $\text{rank}(X) = r$, let $s = p - r$ and $C \in \mathcal{M}_{s,p}$ with $\text{rank}(C) = s$ and $\mathcal{C}(X^T) \cap \mathcal{C}(C^T) = \{0\}$ and let $y \in \mathbb{R}^n$. We consider the system

$$\begin{pmatrix} X^T X \\ C \end{pmatrix} b = \begin{pmatrix} X^T y \\ 0 \end{pmatrix}$$

or equivalently the system

$$\begin{pmatrix} X \\ C \end{pmatrix} b = \begin{pmatrix} P_X y \\ 0 \end{pmatrix}$$

These systems are the **restricted normal equations with restrictions C** .

Note 2.20. Requiring $\text{rank}(C) = s$ means that the rows of C (i.e. the restrictions) are linearly independent. To have a unique solution to

$$\begin{pmatrix} X \\ C \end{pmatrix} b = \begin{pmatrix} P_X y \\ 0 \end{pmatrix}$$

we must have

$$\mathcal{N}\left(\begin{pmatrix} X \\ C \end{pmatrix}\right) = \{0\}$$

or equivalently,

$$\mathcal{C}\left(\begin{pmatrix} X^T & C^T \end{pmatrix}\right) = \mathbb{R}^p$$

Since $\text{rank}(X^T) = \text{rank}(X) = r$, we have that $\mathcal{C}\left(\begin{pmatrix} X^T & C^T \end{pmatrix}\right) = \mathbb{R}^p$ iff $\mathcal{C}(X^T) \cap \mathcal{C}(C^T) = \{0\}$.

Exercise 2.21. Under the assumptions for the restricted normal equations, the following systems are equivalent:

(1)

$$\begin{pmatrix} X^T X \\ C \end{pmatrix} b = \begin{pmatrix} X^T y \\ 0 \end{pmatrix}$$

(2)

$$\begin{pmatrix} X^T X \\ C^T C \end{pmatrix} b = \begin{pmatrix} X^T y \\ 0 \end{pmatrix}$$

(3)

$$(X^T X + C^T C)b = X^T y$$

Proof. (1) \Rightarrow (2) We need to show that for each $b \in \mathbb{R}^p$ $Cb = 0$ implies that $C^T Cb = 0$. This is immediate since $\mathcal{N}(C^T C) = \mathcal{N}(C)$.

(2) \Rightarrow (3) Let $b \in \mathbb{R}^p$ be a solution to system (1). Then we have that

$$(X^T X + C^T C)b = X^T Xb + C^T Cb = X^T y + 0 = X^T y$$

(3) \Rightarrow (1) Suppose that $(X^T X + C^T C)b = X^T y$. This implies that $C^T Cb = X^T(y - Xb)$. So

$$C^T Cb \in \mathcal{C}(C^T C) \cap \mathcal{C}(X^T) = \mathcal{C}(C^T) \cap \mathcal{C}(X^T) = \{0\}$$

Hence $b \in \mathcal{N}(C^T C) = \mathcal{N}(C)$. So $Cb = 0$ and $X^T Xb = (X^T X + C^T C)b = X^T y$, orquivalently,

$$\begin{pmatrix} X^T X \\ C \end{pmatrix} b = \begin{pmatrix} X^T y \\ 0 \end{pmatrix}$$

□

Exercise 2.22. Under the assumptions for the restricted normal equations, we have the following:

- (1) $X^T X + C^T C$ is invertible
- (2) $(X^T X + C^T C)^{-1} X^T y$ is the unique solution to $X^T Xb = X^T y$ and $Cb = 0$.
- (3) $(X^T X + C^T C)^{-1}$ is a generalized inverse of $X^T X$
- (4) $C(X^T X + C^T C)^{-1} X^T = 0$
- (5) $C(X^T X + C^T C)^{-1} C^T = I$

Proof.

(1)

$$\begin{aligned} \mathbb{R}^p &= \mathcal{C} \left(\begin{pmatrix} X^T & C^T \end{pmatrix} \right) \\ &= \mathcal{C} \left(\begin{pmatrix} X^T & C^T \end{pmatrix} \begin{pmatrix} X \\ C \end{pmatrix} \right) \\ &= \mathcal{C}(X^T X + C^T C) \end{aligned}$$

Since $X^T X + C^T C \in \mathcal{M}_{p,p}$ and $\text{rank}(X^T X + C^T C) = p$, we have that $X^T X + C^T C$ is invertible.

- (2) Put $b = (X^T X + C^T C)^{-1} X^T y$. Then $(X^T X + C^T C)b = X^T y$. A previous exercise tells us that b is a solution to the system

$$\begin{pmatrix} X^T X \\ C \end{pmatrix} b = \begin{pmatrix} X^T y \\ 0 \end{pmatrix}$$

which implies that $X^T Xb = X^T y$ and $Cb = 0$.

- (3) From (2), we know that

$$X^T X [(X^T X + C^T C)^{-1} X^T y] = X^T y$$

Since $y \in \mathbb{R}^n$ is arbitrary, we have

$$X^T X (X^T X + C^T C)^{-1} X^T = X^T$$

Multiplying both sides on the right by X tells us that $(X^T X + C^T C)^{-1}$ is a generalized inverse of $X^T X$.

- (4) From (2), we know that

$$C(X^T X + C^T C)^{-1} X^T y = 0$$

Since $y \in \mathbb{R}^n$ is arbitrary,

$$C(X^T X + C^T C)^{-1} X^T = 0$$

(5)

□

2.5. Constrained Parameter Space.

Definition 2.23. Let $P \in \mathcal{M}_{p,q}$ and $\delta \in \mathbb{R}^q$. Suppose that P has full column rank. We define the **constrained parameter space** $\mathcal{T} = \{b \in \mathbb{R}^p : P^T b = \delta\}$.

Note 2.24. Since P has full column rank, $\mathcal{C}(P^T) = \mathbb{R}^q$ and for each $\delta \in \mathbb{R}^q$, $P^T b = \delta$ is consistent. We now fix P, δ so that \mathcal{T} is fixed.

Definition 2.25. Let $\lambda \in \mathbb{R}^p$. The function $t(y)$ is said to be a **linear unbiased estimator in \mathcal{T}** for $f(b) = \lambda^T b$ if there exists $a \in \mathbb{R}^n$, $c \in \mathbb{R}$ such that $t(y) = c + a^T y$ and for each $b \in \mathcal{T}$, $\mathbb{E}[t(y)] = \lambda^T b$.

Definition 2.26. Let $\lambda \in \mathbb{R}^p$. The function $f(b) = \lambda^T b$ is said to be **linearly estimable in \mathcal{T}** if there exists a linear unbiased estimator in \mathcal{T} for $f(b) = \lambda^T b$. Equivalently $\lambda^T b$ is linearly estimable in \mathcal{T} if there exist $a \in \mathbb{R}^n$, $c \in \mathbb{R}$ such that for each $b \in \mathcal{T}$, $\mathbb{E}[c + a^T y] = \lambda^T b$.

Theorem 2.27. Let $\lambda \in \mathbb{R}^p$ and $a \in \mathbb{R}^n$. Then $t(y) = c + a^T y$ is a linear unbiased estimator for $f(b) = \lambda^T b$ iff if there exists $d \in \mathbb{R}^q$ such that $\lambda = X^T a + P d$ and $c = d^T \delta$.

Definition 2.28. We define the **normal equations with restrictions \mathcal{T}** to be

$$\begin{pmatrix} X^T X & P \\ P^T & 0 \end{pmatrix} \begin{pmatrix} b \\ \theta \end{pmatrix} = \begin{pmatrix} X^T y \\ \delta \end{pmatrix}$$

Theorem 2.29. We have the following:

- (1) The restricted normal equations are consistent.
- (2) Let \hat{b} be the first component of a solution to the restricted normal equations. Then $Q(\hat{b}) = \min_{b \in \mathcal{T}} Q(b)$.
- (3) Let \hat{b} be the first component of a solution to the restricted normal equations and $b \in \mathcal{T}$. Then $Q(b) = Q(\hat{b})$ iff b is the first component of a solution of to the restricted normal equations.

2.6. The Gauss-Markov Model.

Definition 2.30. Let $X \in \mathcal{M}_{n,p}$, $y \in \mathbb{R}^n$. We consider the model $y = Xb + e$ where $\mathbb{E}[e] = 0$, $\text{Var}(e) = \sigma^2 I_n$. This model is called the **Gauss-Markov model**. Note that $\mathbb{E}[y] = Xb$ and $\text{Var}(y) = \sigma^2 I$.

Theorem 2.31. Let $a, c \in \mathbb{R}^n$, $A \in \mathcal{M}_{p,n}$ and y a random vector in \mathbb{R}^n . Then

- (1) $\mathbb{E}[a^T y] = a^T \mathbb{E}[y]$
- (2) $\text{Var}(a^T y) = a^T \text{Var}(y) a$
- (3) $\text{Cov}(a^T y, c^T y) = a^T \text{Var}(y) c$
- (4) $\text{Var}(Ay) = A^T \text{Var}(y) A$

Exercise 2.32. Let $\lambda^T \in \mathbb{R}^p$ and $\hat{b} \in \mathbb{R}^p$ a least squares solution. Suppose that $f(b) = \lambda^T b$ is linearly estimable. Then the unique least squares estimator $\hat{f} = \lambda^T \hat{b}$ satisfies

$$\text{Var}(\hat{f}) = \sigma^2 \lambda^T (X^T X)^{-} \lambda$$

Proof. Uniqueness of \hat{f} tells us that $\hat{f} = \lambda^T (X^T X)^{-} X^T y$. A previous exercise tells us that for each gen. inv. X^- of X , $\lambda^T = \lambda^T X^- X$. Recall that $(X^T X)^{-} X^T$ is a gen. inv. of X .

Then

$$\begin{aligned}
 \text{Var}(\hat{f}) &= \text{Var}(\lambda^T (X^T X)^{-} X^T y) \\
 &= \lambda^T (X^T X)^{-} X^T \text{Var}(y) (\lambda^T (X^T X)^{-} X^T)^T \\
 &= \sigma^2 \lambda^T (X^T X)^{-} X^T (\lambda^T (X^T X)^{-} X^T)^T \\
 &= \sigma^2 \lambda^T (X^T X)^{-} \left(\lambda^T (X^T X)^{-} X^T X \right)^T \\
 &= \sigma^2 \lambda^T (X^T X)^{-} (\lambda^T)^T \\
 &= \sigma^2 \lambda^T (X^T X)^{-} \lambda
 \end{aligned}$$

□

Exercise 2.33. Let $\lambda \in \mathbb{R}^p$. Suppose that $f(b) = \lambda^T b$ is linearly estimable. Then $\hat{f} = \lambda^T \hat{b}$ is the minimum variance linear unbiased estimator for $f(b)$.

Proof. Let $t(y) = c + a^T y$ be a linear unbiased estimator for $f(b) = \lambda^T b$. Recall that $c = 0$ and $\lambda = X^T a$, $\hat{f} = \lambda^T (X^T X)^{-} X^T y$ and for each generalized inverse X^- of X , $\lambda^T X^- X = \lambda^T$. Then

$$\begin{aligned}
 \text{Var}(t(y)) &= \text{Var}(a^T y) \\
 &= \text{Var}(\hat{f} + (a^T y - \hat{f})) \\
 &= \text{Var}(\hat{f}) + \text{Var}(a^T y - \hat{f}) + 2\text{Cov}(\hat{f}, a^T y - \hat{f})
 \end{aligned}$$

Now

$$\begin{aligned}
 \text{Cov}(\hat{f}, a^T y - \hat{f}) &= \text{Cov}(\lambda^T (X^T X)^{-} X^T y, a^T y - \lambda^T (X^T X)^{-} X^T y) \\
 &= \lambda^T (X^T X)^{-} X^T \text{Var}(y) \left[a^T - \lambda^T (X^T X)^{-} X^T \right]^T \\
 &= \sigma^2 \lambda^T (X^T X)^{-} X^T \left[a^T - \lambda^T (X^T X)^{-} X^T \right]^T \\
 &= \sigma^2 \lambda^T (X^T X)^{-} \left[a^T X - \lambda^T (X^T X)^{-} X^T X \right]^T \\
 &= \sigma^2 \lambda^T (X^T X)^{-} \left[a^T X - \lambda^T (X^T X)^{-} X^T X \right]^T \\
 &= \sigma^2 \lambda^T (X^T X)^{-} \left[a^T X - \lambda^T \right]^T \\
 &= \sigma^2 \lambda^T (X^T X)^{-} (X^T a - \lambda) \\
 &= 0
 \end{aligned}$$

Hence $\text{Var}(t(y)) = \text{Var}(\hat{f}) + \text{Var}(a^T y - \hat{f}) \geq \text{Var}(\hat{f})$

□

Theorem 2.34.

- (1) For each $A, B \in \mathcal{M}_{n,n}$ and $\alpha \in \mathbb{R}$, $\text{tr}(\alpha A + B) = \alpha \text{tr}(A) + \text{tr}(B)$.
- (2) For each $A \in \mathcal{M}_{n,p}$ and $B \in \mathcal{M}_{p,n}$, $\text{tr}(AB) = \text{tr}(BA)$.
- (3) For each random matrix $Z \in \mathcal{M}_{n,n}$, $\mathbb{E}[\text{tr}(Z)] = \text{tr}(\mathbb{E}[Z])$.

Exercise 2.35. Let $z \in \mathbb{R}^p$ be a random vector. Suppose that $\mathbb{E}[z] = \mu$ and $\text{Var}(z) = \Sigma$. Then for each $A \in \mathcal{M}_{p,p}$,

$$\mathbb{E}[z^T A z] = \mu^T A \mu + \text{tr}(A \Sigma)$$

Proof. Note that

$$\mathbb{E}[z^T A z] = \mathbb{E}[(z - \mu)^T A (z - \mu)] + \mathbb{E}[\mu^T A (z - \mu)] + \mathbb{E}[z^T A \mu]$$

Observe that

$$\begin{aligned} \mathbb{E}[(z - \mu)^T A (z - \mu)] &= \mathbb{E}[\text{tr}((z - \mu)^T A (z - \mu))] \\ &= \mathbb{E}[\text{tr}((A(z - \mu)(z - \mu)^T))] \\ &= \text{tr}(\mathbb{E}[(A(z - \mu)(z - \mu)^T)]) \\ &= \text{tr}(A \mathbb{E}[(z - \mu)(z - \mu)^T]) \\ &= \text{tr}(A \Sigma) \end{aligned}$$

and that

$$\begin{aligned} \mathbb{E}[\mu^T A (z - \mu)] &= \mathbb{E}[\mu^T A (z - \mu)] \\ &= \mu^T A \mathbb{E}[z - \mu] \\ &= 0 \end{aligned}$$

and that

$$\begin{aligned} \mathbb{E}[z^T A \mu] &= \mathbb{E}[z^T] A \mu \\ &= \mu^T A \mu \end{aligned}$$

Thus $\mathbb{E}[z^T A z] = \mu^T A \mu + \text{tr}(A \Sigma)$. □

Definition 2.36. Put $\hat{e} = y - \hat{y} = (I - P_X)y$. Then the **sum of squares error**, SSE , is defined to be $SSE = \hat{e}^T \hat{e} = y^T (I - P_X)y$.

Exercise 2.37. Let $r = \text{rank}(X)$. Define

$$\hat{\sigma}^2 = \frac{SSE}{n - r}$$

Then $\hat{\sigma}^2$ is an unbiased estimator for σ^2 .

Proof. The previous exercise tells us that

$$\begin{aligned} \mathbb{E}[SSE] &= \mathbb{E}[y^T (I - P_X)y] \\ &= b^T X^T (I - P_X) X b + \sigma^2 \text{tr}(I - P_X) \\ &= \sigma^2 \text{tr}(I - P_X) \\ &= \sigma^2 \text{rank}(I - P_X) \\ &= \sigma^2 \text{nullity}(X^T) \\ &= \sigma^2 (n - r) \end{aligned}$$

So $\mathbb{E}[\hat{\sigma}^2] = \sigma^2$. □

2.7. The Aitken Model.

Definition 2.38. Let $X \in \mathcal{M}_{n,p}$, $y \in \mathbb{R}^n$ and $V \in \mathcal{M}_{n,n}$. We consider the model $y = Xb + e$ where $\mathbb{E}[e] = 0$, $\text{Var}(e) = \sigma^2 V$. This model is called the **Aitken model**. Note that $\mathbb{E}[y] = Xb$ and $\text{Var}(y) = \sigma^2 V$.

Definition 2.39. Let $R \in \mathcal{M}_{n,n}$. Suppose that R is invertible and $RV R^T = I$ or equivalently, $V = (R^T R)^{-1}$. We define the **transformed Aitken model** by $z = Ry$, $U = RX$, $f = Re$ so that

$$z = Ub + f$$

Note that

$$\mathbb{E}[z] = RXb = Ub$$

and

$$\text{Var}(f) = R\text{Var}(e)R^T = \sigma^2 RV R^T = \sigma^2 I$$

Definition 2.40. Under the transformed Aitken model, we can look for solutions $b \in \mathbb{R}^p$ to the normal equations

$$U^T U b = U^T z$$

When we transform back to the Aitken model, we have the **Aitken equations**

$$X^T V^{-1} X b = X^T V^{-1} y$$

We denote a solution to the Aitken equations by \hat{b}_{GLS} and a solution to the normal equations by \hat{b}_{OLS}

3. DISTRIBUTION THEORY

3.1. Introduction.

Definition 3.1. Let $x \in \mathbb{R}^p$ be a random vector. Define $m_x : \mathbb{R}^p \rightarrow [0, \infty]$ by

$$m_x(t) = \mathbb{E}[e^{t^T x}]$$

We call m_x the **moment generating function of X** .

Theorem 3.2. Let $x_1, x_2 \in \mathbb{R}^p$ be random vectors. Then $F_{x_1} = F_{x_2}$ iff $m_{x_1} = m_{x_2}$.

Theorem 3.3. Let $x_1 \in \mathbb{R}^{p_1}, \dots, x_n \in \mathbb{R}^{p_n}$ be random vectors. Put $p = \sum_{i=1}^n p_i$. For $t \in \mathbb{R}^p$, we can partition t as $t = (t_1^T, \dots, t_n^T)^T$ where $t_1 \in \mathbb{R}^{p_1}, \dots, t_n \in \mathbb{R}^{p_n}$. Put $x = (x_1^T, \dots, x_n^T)^T$. Then x_1, \dots, x_n are independent iff for each $t \in \mathbb{R}^p$, $m_x(t) = \prod_{i=1}^n m_{x_i}(t_i)$.

3.2. Multivariate Normal.

Definition 3.4. Let $x \in \mathbb{R}^p$ be a random vector, $\mu \in \mathbb{R}^p$ and $V \in \mathcal{M}_{p,p}$ be symmetric and positive semi-definite. Then x is said to have a **multivariate normal distribution with mean μ and covariance matrix V** , denoted $x \sim N_p(\mu, V)$, if for each $t \in \mathbb{R}^p$, $m_x(t) = e^{t^T \mu + \frac{1}{2} t^T V t}$.

Exercise 3.5. Let $x \sim N_p(\mu, V)$, $a \in \mathbb{R}^q$ and $B \in \mathcal{M}_{q,p}$. Define the random vector $y \in \mathbb{R}^q$ by $y = a + Bx$. Then $y \sim N_q(a + B\mu, BV B^T)$.

Proof. for $t \in \mathbb{R}^q$, we have that

$$\begin{aligned}
m_y(t) &= E[e^{t^T y}] \\
&= E[e^{t^T(a+Bx)}] \\
&= E[e^{t^T a} + t^T Bx] \\
&= e^{t^T a} E[e^{t^T Bx}] \\
&= e^{t^T a} m_x(B^T t) \\
&= e^{t^T a} e^{t^T B\mu + \frac{1}{2} t^T BVB^T t} \\
&= e^{t^T a + t^T B\mu + \frac{1}{2} t^T BVB^T t} \\
&= e^{t^T(a+B\mu) + \frac{1}{2} t^T BVB^T t}
\end{aligned}$$

So $y \sim N_q(a + B\mu, BVB^T)$. □

Exercise 3.6. Let $x \in \mathbb{R}^p$ be a multivariate normal random vector. Then any subvector of x is a multivariate normal random vector.

Proof. Let $x = (x_1, \dots, x_p)^T$. Suppose that $x \sim N_p(\mu, V)$. Let $x' = (x_{i_1}, \dots, x_{i_k})$ be a subvector of x . So $i_1 < \dots < i_k$ and $i_1, \dots, i_k \in \{1, \dots, p\}$. Choose a matrix $B \in \mathcal{M}_{q,p}$ such that $x' = Bx$. Then $x' \sim N_q(B\mu, BVB^T)$. □

Theorem 3.7. Let $x = (x_1^T, \dots, x_n^T)^T$, $\mu = (\mu_1^T, \dots, \mu_n^T)^T \in \mathbb{R}^p$ and $V = \begin{pmatrix} V_{1,1} & \cdots & V_{1,n} \\ & \ddots & \\ V_{n,1} & \cdots & V_{n,n} \end{pmatrix} \in$

$\mathcal{M}_{p,p}$ where $x_i, \mu_i \in \mathbb{R}^{p_i}$, $V_{i,j} \in \mathcal{M}_{p_i, p_j}$ and $\sum_{i=1}^n p_i = p$. If $x \sim N_p(\mu, V)$ then x_1, \dots, x_n are independent iff for each $i, j \in \{1, \dots, n\}$, $i \neq j$ implies that $V_{i,j} = 0$.

Exercise 3.8. Let $z = (z_1, \dots, z_p) \in \mathbb{R}^p$ be a random vector. Then $z \sim N_p(0, I)$ iff for each $i = 1, \dots, p$, $z_i \sim N_1(0, 1)$ and z_1, \dots, z_n are independent.

Proof. Suppose that $z \sim N_p(0, I)$. Since $z_i = e_i^T z$, the previous results tells us that for each $i = 1, \dots, p$, $z_i \sim N_1(0, 1)$ and z_1, \dots, z_n are independent. Conversely, suppose that for each $i = 1, \dots, p$, $z_i \sim N_1(0, 1)$ and z_1, \dots, z_n are independent. Then for each $t \in \mathbb{R}^p$,

$$\begin{aligned}
m_z(t) &= \prod_{i=1}^p m_{z_i}(t_i) \\
&= \prod_{i=1}^p e^{\frac{1}{2} t_i^2} \\
&= e^{\frac{1}{2} t^T t}
\end{aligned}$$

Thus $z \sim N_p(0, I)$. □

Exercise 3.9. Let $x \sim N_p(\mu, V)$, $a_1, a_2 \in \mathbb{R}^q$, $B_1, B_2 \in \mathcal{M}_{q,p}$, $y_1 = a_1 + B_1 x$ and $y_2 = a_2 + B_2 x$. Then y_1, y_2 are independent iff $B_1 V B_2^T = 0$.

Proof. Put $y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$, $a = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$ and $B = \begin{pmatrix} B_1 \\ B_2 \end{pmatrix}$. Since $y = a + Bx$ We know that $y \sim N_{2q}(a + B\mu, BV B^T)$. Observe that $BV B^T = \begin{pmatrix} B_1 V B_1^T & B_1 V B_2^T \\ B_2 V B_1^T & B_2 V B_2^T \end{pmatrix}$ A previous result tells us that y_1, y_2 are independent iff $B_1 V B_2^T = 0$ \square

3.3. Chi-Square.

Definition 3.10. Let u be a random variable, $p \in \mathbb{N}$ and $\phi \geq 0$. Then u is said to have a χ^2 **distribution with p degrees of freedom and noncentrality parameter ϕ** , denoted $u \sim \chi_p^2(\phi)$, if for each $t \in \mathbb{R}$,

$$m_u(t) = (1 - 2t)^{p/2} e^{2\phi t/(1-2t)}$$

If $\phi = 0$, we say that u has a (central) chi-square distribution with p degrees of freedom, denoted $u \sim \chi_p^2$.

Exercise 3.11. Let $z \sim N_p(0, I)$. Then $z^T z \sim \chi_p^2$.

Proof. One can show that $m_{z_i^2}(t) = (1 - 2t)^{1/2}$. By independence

$$m_{z^T z}(t) = m_{\sum_{i=1}^p z_i^2}(t) = (1 - 2t)^{p/2}$$

\square

Exercise 3.12. Let $u_1 \sim \chi_{p_1}^2(\phi_1), \dots, u_n \sim \chi_{p_n}^2(\phi_n)$. Put $u = \sum_{i=1}^n u_i$, $p = \sum_{i=1}^n p_i$ and $\phi = \sum_{i=1}^n \phi_i$. If u_1, \dots, u_n are independent, then $u \sim \chi_p^2(\phi)$.

Proof. By independence, we have that for each $t \in \mathbb{R}$,

$$\begin{aligned} m_u(t) &= \prod_{i=1}^n m_{u_i}(t) \\ &= \prod_{i=1}^n (1 - 2t)^{p_i/2} e^{2\phi_i t/(1-2t)} \\ &= (1 - 2t)^{p/2} e^{2\phi t/(1-2t)} \end{aligned}$$

\square

Theorem 3.13. Let $x \in \mathbb{R}^p$ be a random vector, $\mu \in \mathbb{R}^p$ and $V \in \mathcal{M}_{p,p}$ positive definite. If $x \sim N_p(\mu, V)$, then

$$x^T V^{-1} x \sim \chi_p^2(\mu^T V^{-1} \mu/2)$$

Definition 3.14. Let $p_1, p_2 \in \mathbb{N}$, $\phi \geq 0$, $u_1 \sim \chi_{p_1}^2(\phi)$ and $u_2 \sim \chi_{p_2}^2$. Then $\frac{u_1/p_1}{u_2/p_2}$ is said to have a F **distribution with noncentrality parameter ϕ and p_1, p_2 degrees of freedom**, denoted $\frac{u_1/p_1}{u_2/p_2} \sim F_{p_1, p_2}(\phi)$.

Definition 3.15. Let $\mu \in \mathbb{R}$, $k \in \mathbb{N}$, $u \sim N_1(\mu, 1)$ and $v \sim \chi_k^2$. Then $u/\sqrt{v/k}$ is said to have a t **distribution with noncentrality parameter μ and k degrees of freedom**, denoted $u/\sqrt{v/k} \sim t_k(\mu)$.

3.4. Quadratic Forms.

Exercise 3.16. *Let $\mu \in \mathbb{R}^p$ and $A, V \in \mathcal{M}_{p,p}$. Suppose that A is symmetric, V is nonsingular, AV is idempotent and $\text{rank}(AV) = s$. Let $x \sim N_p(\mu, V)$. Then $x^T A x \sim \chi_s^2(\mu A \mu^T / 2)$*

Exercise 3.17.