

# 250A Linear Statistical Models A Review

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## 1 Span

- Given a vector space  $V$  over a field  $K$ , the span of  $S \subseteq V$  can be defined as the set of all finite linear combinations of elements of  $S$ :

$$\text{span}(S) = \left\{ \sum_{i=1}^k \lambda_i \mathbf{v}_i \mid \mathbf{v}_i \in S, \lambda_i \in K \right\},$$

which is a subspace of  $V$ . Clearly,  $S \subset \text{span}(S)$ . We say  $S$  spans  $V$ .

## 2 Basis

- If  $\mathbf{x}$  can be expressed as a linear combination:  $\mathbf{x} = \sum_{i=1}^n \alpha_i \mathbf{v}_i$ , then  $\{\mathbf{v}_1, \dots, \mathbf{v}_n\}$  is called a basis. A basis is not unique. For example, the followings both are a basis of  $V = \mathbb{R}^3$ .

$$\left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}, \quad \left\{ \begin{pmatrix} 3 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 4 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}$$

- If  $x_1, \dots, x_k$  ( $k < n$ ) are linearly independent vectors, then they can be extended to form a basis for the  $n$ -dimensional vector space of  $V$ .

## 3 Subspace

- If  $S$  and  $T$  are subspaces of  $V$ , then  $S \cap T$  (intersection) and  $S + T = \{s + t \mid s \in S, t \in T\}$  are also subspaces of  $V$ . However,  $S \cup T = \{s \text{ or } t \mid s \in S, t \in T\}$  (union) is not always a subspace of  $V$ .
- $S^\perp = \{\mathbf{v} \in V \mid (\mathbf{v}, \mathbf{s}) = 0, \forall \mathbf{s} \in S\}$  is a vector space (subspace). *Proof:* Let  $\mathbf{v}_1, \mathbf{v}_2 \in S^\perp$  and  $\alpha \in \mathbb{R}$ ,

$$\begin{aligned} (\alpha \mathbf{v}_1 + \mathbf{v}_2, \mathbf{s}) &= \alpha(\mathbf{v}_1, \mathbf{s}) + (\mathbf{v}_2, \mathbf{s}) = 0 \Rightarrow \alpha \mathbf{v}_1 + \mathbf{v}_2 \in S^\perp, \\ \mathbf{0}, \mathbf{s} &\Rightarrow \mathbf{0} \in S^\perp. \end{aligned}$$

- $N(\mathbf{A})$  is a vector space (subspace). *Proof:* Let  $\mathbf{x}, \mathbf{y} \in N(\mathbf{A})$  and  $\alpha \in \mathbb{R}$ , then  $\mathbf{A}(\alpha \mathbf{x} + \mathbf{y}) = 0 \Rightarrow \alpha \mathbf{x} + \mathbf{y} \in N(\mathbf{A})$  and  $\mathbf{A}\mathbf{0} = \mathbf{0} \Rightarrow \mathbf{0} \in N(\mathbf{A})$ .

## 4 Inner product

- A vector space  $V$  is an *inner product space* if it is endowed with an inner product defined as  $V \times V \rightarrow \mathbb{R}$ , and has the following properties: For  $x, y, z \in V$  and  $\alpha, \beta \in \mathbb{R}$ ,

(i) Symmetry:  $(x, y) = (y, x)$

(ii) Linearity:  $(\alpha x + \beta y, z) = \alpha(x, z) + \beta(y, z)$

(iii) Non-negative:  $(x, x) \geq 0$  with equality if and only if  $x = 0$ .

- If  $x_1, \dots, x_n$  are orthogonal vectors in  $V$  with an inner product  $(\cdot, \cdot)$ , then they are linearly independent.

*Proof:* Suppose  $\sum_{i=1}^n \alpha_i x_i = 0$ . Then

$$0 = (0, x_j) = \left( \sum_{i=1}^n \alpha_i x_i, x_j \right) = \alpha_j \|x_j\|^2 \Rightarrow \alpha_j = 0, \quad j = 1, \dots, n.$$

- Even if  $x$  and  $y$  are orthogonal, they are not always linearly independent as either one can be zero.

- **Cauchy–Schwarz inequality:**  $(x, y)^2 \leq \|x\|^2 \|y\|^2 \Leftrightarrow |(x, y)| \leq \|x\| \|y\|$  with equality iff  $x = 0$  or  $y = 0$ . *Proof:* Set  $w_1 = x/\|x\|$  and  $w_2 = y/\|y\|$ .  $0 \leq (w_1 - w_2, w_1 - w_2) = 2(1 - (w_1, w_2)) \Rightarrow (w_1, w_2) \leq 1$ .

Example: Applying  $x_i = \sqrt{a_i}$  and  $y_i = 1/\sqrt{a_i}$  yields

$$\left(\sum_{i=1}^n 1\right)^2 \leq \sum_{i=1}^n a_i \sum_{i=1}^n 1/a_i \Rightarrow \frac{n}{\sum_{i=1}^n 1/a_i} \leq \frac{\sum_{i=1}^n a_i}{n},$$

meaning that Harmonic mean  $\leq$  Arithmetic mean ( $\leq$  Geometric mean).

## 5 Some useful results for Matrices

- Let  $c_i$  be a vector with 1 for the  $i$ th element and 0 elsewhere.
- If  $Ax = 0$  for  $\forall x$ , then  $x = 0$ : Setting  $x = c_i$  leads to  $Ax = a_i = 0$ , where  $a_i$  is the  $i$ th column of  $A$ .
- If  $A$  is symmetric and  $x'Ax = 0$  for  $\forall x$ , then  $A = 0$ : Setting  $x = c_i$  leads to  $x'Ax = a_{ii} = 0$ . Further, setting  $x = c_i + c_j$  ( $i \neq j$ ) leads to  $x'Ax = a_{ii} + 2a_{ij} + a_{jj} = 0 \Rightarrow a_{ij} = 0$ .
- If  $A$  is *not* symmetric, however, this is FALSE. Although  $a_{ii} = 0$  still satisfies, we have  $a_{ij} + a_{ji} = 0$  instead of  $2a_{ij} = 0$ . The counterexample is like this:

$$A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \Rightarrow (x_1 \ x_2) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 0 \quad \forall x.$$

- If  $A$  is symmetric and nonsingular (usually variance-covariance matrix), then

$$\beta' A \beta - 2b' \beta = (\beta - A^{-1}b)' A (\beta - A^{-1}b) - b' A^{-1}b.$$

## 6 Trace and Eigenvalues

- Given a *square* matrix  $A$ , consider  $Ax = \lambda x \Leftrightarrow (A - \lambda I)x = 0$ , where  $x \neq 0$ . Then  $A - \lambda I$  is always singular because otherwise (if nonsingular)  $x = 0$ , which contradicts the assumption. Thus, solving  $|A - \lambda I| = 0$  obtains  $\lambda$  (eigenvalue) and the corresponding  $x$  (eigenvector).
- If  $A$  is an  $n \times n$  symmetric with eigenvalues  $\lambda_i$  ( $i = 1, \dots, n$ ),
  - $\text{tr}(A) = \sum_{i=1}^n \lambda_i$  and  $\det(A) = |A| = \prod_{i=1}^n \lambda_i$  by expanding  $|\lambda I_n - A|$ .
  - $\text{tr}(A^k) = \text{tr}[(T \Lambda T')^k] = \text{tr}(T \Lambda^k T') = \text{tr}(\Lambda^k) = \sum_{i=1}^n \lambda_i^k$  by the SD and the trace property.

## 7 Fundamental subspaces

- The space spanned by the *columns* of  $A$ , called the column space of  $A$ , is denoted by  $\mathcal{C}(A)$ .
- Let  $A \in \mathbb{R}^{n \times p}$ .

$$\text{Column space of } A = \mathcal{C}(A) = \{Ax \mid x \in \mathbb{R}^p\},$$

$$\text{Row space of } A = \mathcal{R}(A) = \{A'x \mid x \in \mathbb{R}^n\} = \mathcal{C}(A'),$$

$$\text{Null space of } A = \mathcal{N}(A) = \{x \in \mathbb{R}^p \mid Ax = 0\},$$

$$\text{Left null space of } A = \mathcal{N}(A') = \{x \in \mathbb{R}^n \mid A'x = 0\}.$$

- $\mathcal{N}(A) = \mathcal{C}(A')^\perp$ . *Proof:* If  $x \in \mathcal{N}(A)$ , then  $Ax = 0 \Rightarrow b'Ax = 0, \forall b \Rightarrow x'(A'b) = 0 \Rightarrow x \in \mathcal{C}(A')^\perp$ . Conversely, if  $x \in \mathcal{C}(A')^\perp$ , then  $x'y = x'(A'b) = 0, \forall b \Rightarrow b'Ax = 0, \forall b \Rightarrow Ax = 0 \Rightarrow x \in \mathcal{N}(A)$ .

- $(\Omega_1 \cap \Omega_2)^\perp = \Omega_1^\perp + \Omega_2^\perp$ . Let  $\Omega_i = \mathcal{N}(A_i)$  ( $i = 1, 2$ ). Then

$$\begin{aligned}\Omega_1 \cap \Omega_2 &= \mathcal{N}(A_1) \cap \mathcal{N}(A_2) = \mathcal{N}\begin{pmatrix} A_1 \\ A_2 \end{pmatrix} \\ \Rightarrow (\Omega_1 \cap \Omega_2)^\perp &= \mathcal{N}\begin{pmatrix} A_1 \\ A_2 \end{pmatrix}^\perp = \mathcal{C}(A_1' \mid A_2') = \mathcal{C}(A_1') + \mathcal{C}(A_2') = \Omega_1^\perp + \Omega_2^\perp.\end{aligned}$$

- (HW1) If  $\mathcal{C}(A) \subseteq \mathcal{C}(B)$ , show there exists  $C$  s.t.  $A = BC$ . What is  $\text{rank}(C)$  if  $A$  has full column rank?  
*Solution* Let  $a_i$  be the  $i$ th column of  $A$  ( $i = 1, \dots, m$ ), then since  $a_i \in \mathcal{C}(A) \subseteq \mathcal{C}(B)$ , there exists  $c_i$  such that  $a_i = Bc_i$ , so that  $A = BC$ . Then  $m = \text{rank}(A) = \text{rank}(BC) \leq \text{rank}(C) \leq m$  follows  $\text{rank}(C) = \text{rank}(A)$ .

## 8 Rank

- $\text{rank}(A)$  is equivalent to the maximum number of linearly independent rows or columns.
- $\text{rank}(AB) \leq \min(\text{rank}(A), \text{rank}(B))$  since the rows of  $AB$  are linear combinations of the rows of  $B$  and the columns of  $AB$  are linear combinations of the columns of  $A$ .
- If  $X$  is  $n \times p$  of rank  $p$  and  $B$  is  $p \times q$  of rank  $q$ , then  $\text{rank}(XB) = q$ .

*Proof 1:*  $XBa = X(Ba) = 0 \Rightarrow Ba = 0 \Rightarrow a = 0$ . So,  $XB$  also has linearly independent columns.

*Proof 2:*  $q = \text{rank}(B) = \text{rank}[(X'X)^{-1}X'XB] \leq \text{rank}(XB) \leq \text{rank}(B) = q$ .

- If  $A$  is any matrix and  $P$  and  $Q$  are any comfortable nonsingular matrices, then  $\text{rank}(PAQ) = \text{rank}(A)$ .

*Proof:*  $\text{rank}(A) \leq \text{rank}(PAQ) \leq \text{rank}(P^{-1}PAQQ^{-1}) = \text{rank}(A)$ .

- (HW1) Suppose the columns of a comfortable matrix  $C$  are added to columns of  $A$  to form the augmented matrix  $(A \mid C)$ . Then  $\text{rank}(A \mid C) \geq \text{rank}(A)$ .

*Solution:* Use the monotonicity of dimension. Let  $\mathbf{A} = (\mathbf{a}_1 \cdots \mathbf{a}_p)$  and  $\mathbf{C} = (\mathbf{c}_1 \cdots \mathbf{c}_q)$ . Then

$$C(\mathbf{A}) = \text{span}\{\mathbf{a}_1, \dots, \mathbf{a}_p\} \subseteq \text{span}\{\mathbf{a}_1, \dots, \mathbf{a}_p, \mathbf{c}_1, \dots, \mathbf{c}_q\} = C(\mathbf{A} \mid \mathbf{C}).$$

Hence,  $\dim(C(\mathbf{A})) \leq \dim(C(\mathbf{A} \mid \mathbf{C}))$ , or equivalently,  $\text{rank}(\mathbf{A}) \leq \text{rank}(\mathbf{A} \mid \mathbf{C})$ .

- By the above and the SD,  $\text{rank}(A) = \text{rank}(T'AT) = \text{rank}(\Lambda)$ , i.e.,  $\text{rank}(A) = \text{No. of nonzero eigenvalues}$ .
- Any  $n \times n$  symmetric matrix  $\mathbf{A}$  has a set of  $n$  orthogonal eigenvectors and  $C(\mathbf{A})$  is the space spanned by those eigenvectors corresponding to nonzero eigenvalues.

*Proof:* Suppose  $\lambda_{r+1} = \dots = \lambda_n = 0$ . Since  $\mathbf{A} = \mathbf{T}\mathbf{\Lambda}\mathbf{T}' = \sum_{i=1}^r \lambda_i \mathbf{t}_i \mathbf{t}_i'$ ,

$$\mathbf{A}\mathbf{x} = \sum_{i=1}^r \lambda_i \mathbf{t}_i \mathbf{t}_i' \mathbf{x} = \sum_{i=1}^r \lambda_i (\mathbf{t}_i' \mathbf{x}) \mathbf{t}_i, \quad \exists \mathbf{x},$$

which means that  $C(\mathbf{A})$  is spanned by  $\mathbf{t}_1, \dots, \mathbf{t}_r$ .

- Let  $\mathbf{X}$  be a  $n \times p$  matrix of rank  $r < p$  and  $\mathbf{X}$  partitions  $(\mathbf{X}_1 \mid \mathbf{X}_2)$ , where  $\mathbf{X}_1 \in \mathbb{R}^{n \times r}$  and  $\mathbf{X}_2 \in \mathbb{R}^{n \times (p-r)}$ , then show that  $\mathbf{X} = \mathbf{X}_1 \mathbf{L}$  where  $\mathbf{L}$  is  $r \times p$  of rank  $r$ . *Proof:* there exists  $\mathbf{H}$  s.t.  $\mathbf{X}_2 = \mathbf{X}_1 \mathbf{H}$ , so that

$$\mathbf{X} = (\mathbf{X}_1 \mid \mathbf{X}_1 \mathbf{H}) = \mathbf{X}_1 (\mathbf{I}_r \mid \mathbf{H}) := \mathbf{X}_1 \mathbf{L} \Rightarrow r = \text{rank}(\mathbf{I}_r) \leq \text{rank}(\mathbf{I}_r \mid \mathbf{H}) = \text{rank}(\mathbf{L}) \leq \min(r, p) = r.$$

- If  $\mathbf{A} \in \mathbb{R}^{n \times p}$  is of full column rank,  $\mathbf{A}\mathbf{x} = 0 \Rightarrow \mathbf{x} = 0$  ( $\mathbf{A}\mathbf{x} = 0 \Leftrightarrow \mathbf{x} = 0$ ) since

$$(\mathbf{a}_1, \dots, \mathbf{a}_p) \begin{pmatrix} x_1 \\ \vdots \\ x_p \end{pmatrix} = \sum_{j=1}^p x_j \mathbf{a}_j = 0.$$

- Then  $\mathbf{A}'\mathbf{A}$  is non-singular (invertible).

*Proof 1:* Consider  $\mathbf{A}'\mathbf{A}\mathbf{x} = 0$ . If  $\mathbf{A}'\mathbf{A}$  is not invertible, there must be a nonzero  $\mathbf{x}$  such that  $\mathbf{A}\mathbf{x} = 0$ , which contradicts the fact that  $\mathbf{A}$  has full column rank.

*Proof 2:*  $\mathbf{x}'\mathbf{A}'\mathbf{A}\mathbf{x} = \|\mathbf{A}\mathbf{x}\|^2 \geq 0$ . Since  $\mathbf{A}\mathbf{x} = \mathbf{0}$  holds iff  $\mathbf{x} = 0$ ,  $\mathbf{A}'\mathbf{A} \succ \mathbf{0} \Rightarrow \mathbf{A}'\mathbf{A}$  is nonsingular/invertible.

- Likewise, if  $\mathbf{A} \in \mathbb{R}^{n \times p}$  is of full row rank,  $\mathbf{A}'\mathbf{x} = 0 \Rightarrow \mathbf{x} = 0$ .
- (HW1) Show the product of two full row rank matrices always full row rank.

*Solution:* Let  $\mathbf{A}$  and  $\mathbf{B}$  be of full row rank. Then  $(\mathbf{B}\mathbf{C})'\mathbf{x} = \mathbf{C}'(\mathbf{B}'\mathbf{x}) = \mathbf{0} \Rightarrow \mathbf{B}'\mathbf{x} = \mathbf{0} \Rightarrow \mathbf{x} = \mathbf{0}$ .

- **Rank-nullity theorem:** If a matrix  $A \in \mathbb{R}^{n \times p}$  with  $\text{rank}(A) = r$

$$\dim C(A) + \dim \mathcal{N}(A) = p \quad \text{or} \quad \text{rank}(A) + \text{nullity}(A) = p.$$

*Proof:* Let  $s = \dim \mathcal{N}(A)$  and  $\alpha_1, \dots, \alpha_s$  be a basis for  $\mathcal{N}(A) \in \mathbb{R}^p$ . Add  $(p - s)$  linearly independent vectors  $\beta_1, \dots, \beta_{p-s}$  so that  $\{\alpha_1, \dots, \alpha_s, \beta_1, \dots, \beta_{p-s}\}$  is a basis for  $\mathbb{R}^p$ . Then  $x$  can be written as:

$$x = \sum_{i=1}^s c_i \alpha_i + \sum_{j=1}^{p-s} d_j \beta_j \Rightarrow Ax = \sum_{j=1}^{p-s} d_j (A\beta_j) \quad \because A\alpha_i = 0,$$

which means that any vector in  $C(A)$  is spanned by  $A\beta_1, \dots, A\beta_{p-s}$ . Next, we want to show that there are linearly independent vectors: Suppose

$$\sum_{j=1}^{p-s} \gamma_j (A\beta_j) = A \sum_{j=1}^{p-s} \gamma_j \beta_j = 0 \Rightarrow \sum_{j=1}^{p-s} \gamma_j \beta_j \in N(A),$$

leading to

$$\sum_{j=1}^{p-s} \gamma_j \beta_j = \sum_{i=1}^s \delta_i \alpha_i \Rightarrow \sum_{j=1}^{p-s} \gamma_j \beta_j - \sum_{i=1}^s \delta_i \alpha_i = 0.$$

Since  $\{\alpha_1, \dots, \alpha_s, \beta_1, \dots, \beta_{p-s}\}$  is a basis for  $\mathbb{R}^p$ ,  $\gamma_j (= \delta_i) = 0, \forall i, j$ . That is,  $A\beta_1, \dots, A\beta_{p-s}$  are linearly independent, or equivalently,  $\{A\beta_1, \dots, A\beta_{p-s}\}$  is a basis for  $C(A)$  so that  $p - s = \dim C(A) = \text{rank}(A) = r$ .

- $\text{rank}(X'X) = \text{rank}(X) = \text{rank}(XX') = \text{rank}(X')$ .

*Proof:* Show  $N(X'X) = N(X)$ .  $a \in N(X) \Rightarrow Xa = 0 \Rightarrow X'Xa = 0 \Rightarrow a \in N(X'X) \Rightarrow N(X) \subseteq N(X'X)$ . Conversely,  $a \in N(X'X) \Rightarrow X'Xa = 0 \Rightarrow \|Xa\|^2 = 0 \Rightarrow Xa = 0 \Rightarrow a \in N(X) \Rightarrow N(X'X) \subseteq N(X)$ . Next

$$N(X'X) = N(X) \Rightarrow \dim N(X'X) = \dim N(X)$$

Since both  $X'X$  and  $X$  have the same  $p$  columns, by the rank-nullity theorem,

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

In a similar way,  $\text{rank}(XX') = \text{rank}(X')$ . Since  $\text{rank}(X'X) = \text{rank}(XX')$ , we show the lemma.

- Also,  $\text{rank}(X^+X) = \text{rank}(X) = \text{rank}(XX^+) = \text{rank}(X^+)$  holds, where  $X^+$  is the Moore Penrose inverse (Midterm).
- $C(X'X) = C(X')$ . *Proof:*  $a \in C(X'X) \Rightarrow a = X'Xb = X'c, \exists c = Xb \Rightarrow a \in C(X')$ , so  $C(X'X) \subseteq C(X')$ . However,  $\dim(C(X'X)) = \dim(C(X'))$  by the above lemma, leading to  $C(X'X) = C(X')$ . This implies that we can always find one or more solutions to  $X'X\beta = X'y$ .

## 9 Symmetric and idempotent

- If  $A$  is symmetric, i.e.,  $A' = A$ , then  $A^n$  is also symmetric.
- Symmetric matrices have only real eigenvalues:

*Proof 1:*  $\lambda\|x\|^2 = (\lambda x, x) = (Ax, x) = (x, A'x) = (x, Ax) = \lambda^*\|x\|^2 \Rightarrow \lambda^* = \lambda$ .

*Proof 2:* Let  $\mathbf{Ax} = \lambda\mathbf{x} = (\alpha + i\beta)\mathbf{x}$  ( $\mathbf{x} \neq 0$ ). Define  $\mathbf{B} = (\mathbf{A} - (\alpha - i\beta)\mathbf{I})'(\mathbf{A} - (\alpha + i\beta)\mathbf{I})$ . Then

$$\mathbf{B} = \mathbf{A}^2 - 2\alpha\mathbf{A} + \alpha^2\mathbf{I} + \beta^2\mathbf{I} = (\mathbf{A} - \alpha\mathbf{I})^2 + \beta^2\mathbf{I} \quad \because \mathbf{A}' = \mathbf{A}.$$

Since  $\mathbf{Bx} = (\mathbf{A} - (\alpha - i\beta)\mathbf{I})'(\mathbf{Ax} - (\alpha + i\beta)\mathbf{x}) = \mathbf{0}$  by the assumption,

$$0 = \mathbf{x}'\mathbf{Bx} = \mathbf{x}'(\mathbf{A} - \alpha\mathbf{I})^2\mathbf{x} + \beta^2\mathbf{x}'\mathbf{x} = \|(\mathbf{A} - \alpha\mathbf{I})\mathbf{x}\|^2 + \beta^2\|\mathbf{x}\|^2 \quad \because (\mathbf{A} - \alpha\mathbf{I})' = (\mathbf{A} - \alpha\mathbf{I}).$$

The last two terms are both nonnegative, so  $\beta = 0$ .

- The eigenvectors corresponding to distinct eigenvalues are orthogonal to each other.

*Proof:* Let  $\mathbf{Ax} = \lambda_1\mathbf{x}$  and  $\mathbf{Ay} = \lambda_2\mathbf{y}$  ( $\lambda_1 \neq \lambda_2$ ). Then

$$\lambda_1(\mathbf{x}, \mathbf{y}) = (\lambda_1\mathbf{x}, \mathbf{y}) = (\mathbf{Ax}, \mathbf{y}) = (\mathbf{x}, \mathbf{A}'\mathbf{y}) = (\mathbf{x}, \mathbf{Ay}) = (\mathbf{x}, \lambda_2\mathbf{y}) = \lambda_2(\mathbf{x}, \mathbf{y}) \Rightarrow (\mathbf{x}, \mathbf{y}) = 0.$$

- If  $A^2 = A$ ,  $A$  is said to be idempotent. **A symmetric and idempotent matrix is called a *projection matrix***, whose eigenvalues are 0 or 1 as  $\lambda^2x = \lambda(Ax) = A^2x = Ax = \lambda x \Rightarrow \lambda$ .
  - $X^+X$  is a projection matrix, where  $X^+$  is the Moore-Penrose inverse (Midterm):  $(X^+X)' = X^+X$  and  $(X^+X)(X^+X) = X^+X$ . So does  $XX^+$ .
- If  $A$  is *symmetric* and orthogonal, i.e.,  $A'A = AA' = I$ , then row and columns of  $A$  are orthogonal each other. Also,  $\det(A'A) = |A|^2 = 1 \Rightarrow |A| \pm 1$ , which does *not* mean eigenvalues are  $\pm 1$  (e.g.,  $\pm 0.5, \pm 2$ ).
- If  $A \in \mathbb{R}^{n \times n}$  with rank  $r < n$  is (symmetric) and idempotent, by above and the spectral decomposition,

$$T'AT = \Lambda = \begin{pmatrix} I_r & O \\ O & O \end{pmatrix} \Rightarrow A = T\Lambda T' = \underbrace{(T_1}_{n \times r} | T_2) \begin{pmatrix} I_r & O \\ O & O \end{pmatrix} \begin{pmatrix} T_1' \\ T_2' \end{pmatrix} = T_1 T_1',$$

where  $AT_1 = T_1$  ( $\lambda_1 = \dots = \lambda_r = 1$ ) and  $AT_2 = O$  ( $\lambda_{r+1} = \dots = \lambda_n = 0$ ). Note that

–  $t_1, \dots, t_r \in C(A) = R(A)$ , while  $t_{r+1}, \dots, t_n \in N(A)$ ,  $i = r+1, \dots, n$ .

– Note: Unlike  $T$ ,  $T_1$  and  $T_2$  are *not* orthogonal as they are not square. Since  $T_1$  has orthogonal columns, however,  $T_1' T_1 = I_r$ .

- Positive definite and semi-positive definite are defined only to symmetric matrices.
  - If  $\mathbf{A}$  is p.d.  $\Rightarrow |\mathbf{A}| > 0 \Rightarrow \mathbf{A}$  is non-singular.
  - If  $\mathbf{A}$  is idempotent, then  $\text{rank}(\mathbf{A}) = \text{tr}(\mathbf{A}) =$  the number of eigenvalues 1.

## 10 Projections on Subspaces

- Let  $P_\Omega$  and  $P_\omega$  be the projection matrix onto  $\Omega = C(X)$  and  $\omega \subseteq \Omega$ .
- $P_\Omega(I - P_\Omega) = O \Rightarrow I - P_\Omega = P_{\Omega^\perp}$ , that is,  $I - P_\Omega$  projects onto  $\Omega^\perp$ .
- Since  $P_\omega P_\Omega = P_\Omega P_\omega = P_\omega$ , we have  $P_\omega(P_\Omega - P_\omega) = O$ , meaning that  $P_\Omega - P_\omega$  projects onto  $\omega^\perp \cap \Omega$ .
- $(I - P_\Omega)(P_\Omega - P_\omega) = (P_\Omega - P_\omega) - P_\Omega(P_\Omega - P_\omega) = O \Rightarrow I - P_\Omega \perp P_\Omega - P_\omega$ .

- If  $A_1$  is any matrix such that  $\omega = \mathcal{N}(A_1) \cap \Omega$ , then  $\omega^\perp \cap \Omega = \mathcal{C}(P_\Omega A'_1)$ .

*Proof:* Since  $\omega^\perp = (\mathcal{N}(A_1) \cap \Omega)^\perp = \mathcal{C}(A'_1) + \Omega^\perp$ , if  $x \in \omega^\perp \cap \Omega$ , then  $x = P_\Omega x = P_\Omega[A'_1 \alpha + (I - P_\Omega)\beta] = P_\Omega A'_1 \alpha \in \mathcal{C}(P_\Omega A'_1) \Rightarrow \omega^\perp \cap \Omega \subseteq \mathcal{C}(P_\Omega A'_1)$ . Conversely, if  $x \in \mathcal{C}(P_\Omega A'_1)$ , then  $x \in \mathcal{C}(P_\Omega) = \Omega$ . Also, if  $z \in \omega = \mathcal{N}(A_1) \cap \Omega$ , then  $x'z = \alpha' A_1 P_\Omega z = \alpha' A_1 z = 0$ , so that  $x \in \omega^\perp \cap \Omega \Rightarrow \mathcal{C}(P_\Omega A'_1) \subseteq \omega^\perp \cap \Omega$ .

- If  $A_1$  is a  $q \times n$  matrix of rank  $q$ , then  $\text{rank}(P_\Omega A'_1) = q$  if and only if  $\mathcal{C}(A'_1) \cap \Omega^\perp = 0$ .

*Proof:* We have  $\text{rank}(\mathbf{P}_\Omega \mathbf{A}'_1) \leq \text{rank}(\mathbf{A}_1) = q$ . Let  $\mathbf{A}'_1 = (\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_q) \in \mathbb{R}^{n \times q}$  and suppose  $\text{rank}(\mathbf{P}_\Omega \mathbf{A}'_1) < q$ . Then there exists nonzero  $\sum_i c_i \mathbf{a}_i \in \mathcal{C}(\mathbf{A}'_1)$  such that  $\mathbf{P}_\Omega \mathbf{A}'_1 \mathbf{c} = \sum_i c_i \mathbf{P}_\Omega \mathbf{a}_i = 0$  that is perpendicular to  $\Omega$ . Hence,  $\mathcal{C}(\mathbf{A}'_1) \cap \Omega^\perp \neq 0$ , which is a contradiction.

## 11 Positive (semi-) Definite

- $\mathbf{A}$  is positive definite iff  $\mathbf{x}' \mathbf{A} \mathbf{x} > 0$ ,  $\forall \mathbf{x} \neq \mathbf{0}$  or iff all leading minors have positive determinant. If  $\mathbf{A}$  is positive definite,  $\mathbf{A}$  is clearly non-singular.
- $\mathbf{A}$  is positive semi-definite if  $\mathbf{x}' \mathbf{A} \mathbf{x} \geq 0$ ,  $\forall \mathbf{x} \neq 0$ .
- The diagonal elements of a p.d. matrix are all positive: Setting  $\mathbf{x} = \mathbf{e}_i$  leads to  $\mathbf{x}' \mathbf{A} \mathbf{x} = a_{ii} > 0$ ,  $\forall i$ .
- If  $\mathbf{A}$  is p.d., there exists the non-singular and symmetric matrix  $\mathbf{A}^{\frac{1}{2}}$  such that  $\mathbf{A}^{\frac{1}{2}} \mathbf{A}^{\frac{1}{2}} = \mathbf{A}$ .

*Proof:* Since  $\mathbf{A}$  is symmetric and has only positive eigenvalues, by spectral decomposition,

$$\mathbf{A} = \mathbf{T} \mathbf{\Lambda} \mathbf{T}' = \mathbf{T} \mathbf{\Lambda}^{\frac{1}{2}} \mathbf{\Lambda}^{\frac{1}{2}} \mathbf{T}' = (\mathbf{T} \mathbf{\Lambda}^{\frac{1}{2}} \mathbf{T}') (\mathbf{T} \mathbf{\Lambda}^{\frac{1}{2}} \mathbf{T}') = \mathbf{A}^{\frac{1}{2}} \mathbf{A}^{\frac{1}{2}} \quad \text{since } \mathbf{T}' \mathbf{T} = \mathbf{I}.$$

- If  $\mathbf{A}$  is p.s.d., we also have  $\mathbf{A}$  s.t.  $\mathbf{A}^{\frac{1}{2}} \mathbf{A}^{\frac{1}{2}} = \mathbf{A}$ , but  $\mathbf{A}$  is singular ( $|\mathbf{A}| = 0$ ).
  - If  $\mathbf{A}$  is p.s.d., then  $\mathbf{X}' \mathbf{A} \mathbf{X} = \mathbf{O} \Rightarrow \mathbf{A} \mathbf{X} = \mathbf{O}$ . Note  $\mathbf{A}$  is singular so that  $\mathbf{A}^{-1}$  and  $\mathbf{A}^{-1/2}$  does not exist.
- Proof:* For  $\forall \mathbf{a}$ ,  $\mathbf{a}' \mathbf{X}' \mathbf{A} \mathbf{X} \mathbf{a} = \|\mathbf{A}^{1/2} \mathbf{X} \mathbf{a}\|^2 = 0 \Rightarrow \mathbf{A}^{1/2} \mathbf{X} \mathbf{a} = \mathbf{0} \Rightarrow \mathbf{A} \mathbf{X} \mathbf{a} = \mathbf{0}$  (not  $\mathbf{X} \mathbf{a} = \mathbf{0}$ ), so  $\mathbf{A} \mathbf{X} = \mathbf{O}$ .
- **Simultaneous diagonalization:** If  $\mathbf{A} \succ \mathbf{O}$  and  $\mathbf{B} \succeq \mathbf{O}$ , then there exists  $\mathbf{U}$  ( $|\mathbf{U}| \neq 0$ ) s.t.

$$\mathbf{U}' \mathbf{A} \mathbf{U} = \mathbf{I}, \quad \mathbf{U}' \mathbf{B} \mathbf{U} = \mathbf{D} = \text{diag}(d_1, \dots, d_n).$$

*Proof:* By definition of positive definite, we can assume  $\mathbf{A}$  and  $\mathbf{B}$  are symmetric. Also,  $\mathbf{A} \succ \mathbf{O}$  implies that  $\mathbf{A}^{1/2}$  exists, so that  $\mathbf{A}^{-\frac{1}{2}} \mathbf{B} \mathbf{A}^{-\frac{1}{2}}$  is symmetric. By the spectral decomposition,

$$\mathbf{T}' \mathbf{A}^{-\frac{1}{2}} \mathbf{B} \mathbf{A}^{-\frac{1}{2}} \mathbf{T} = (\mathbf{A}^{-\frac{1}{2}} \mathbf{T})' \mathbf{B} (\mathbf{A}^{-\frac{1}{2}} \mathbf{T}) = \mathbf{U}' \mathbf{B} \mathbf{U} = \mathbf{D} \succeq \mathbf{O},$$

where  $\mathbf{U} = \mathbf{A}^{-\frac{1}{2}} \mathbf{T}$ . Then  $\mathbf{U}' \mathbf{A} \mathbf{U} = \mathbf{T}' \mathbf{A}^{-\frac{1}{2}} \mathbf{A} \mathbf{A}^{-\frac{1}{2}} \mathbf{T} = \mathbf{T}' \mathbf{T} = \mathbf{I}$  as  $\mathbf{T}$  is orthogonal.

– If  $\mathbf{A} \succ \mathbf{O}$  and  $\mathbf{B} \succ \mathbf{O}$  and  $\mathbf{A} \succ \mathbf{B}$ , then 1)  $|\mathbf{A}| > |\mathbf{B}|$  and 2)  $\mathbf{B}^{-1} - \mathbf{A}^{-1} \succ \mathbf{O}$ .

*Proof of (1):* Since  $\mathbf{U}$  is nonsingular,  $\mathbf{I} - \mathbf{D} = \mathbf{U}'(\mathbf{A} - \mathbf{B})\mathbf{U} \succ \mathbf{O}$ . Hence,  $d_i < 1$  for  $\forall i$ . Hence,

$$0 < |\mathbf{I}| - |\mathbf{D}| = |\mathbf{U}'|(|\mathbf{A}| - |\mathbf{B}|)|\mathbf{U}| = (|\mathbf{A}| - |\mathbf{B}|)|\mathbf{U}'\mathbf{U}| = (|\mathbf{A}| - |\mathbf{B}|)|\mathbf{A}|^{-1} \Rightarrow |\mathbf{A}| - |\mathbf{B}| > 0.$$

*Proof of (2):* We have  $\mathbf{A}^{-1} \mathbf{U} \mathbf{U}'$  and  $\mathbf{B}^{-1} = \mathbf{U} \mathbf{D}^{-1} \mathbf{U}'$ , so that

$$\mathbf{B}^{-1} - \mathbf{A}^{-1} = \mathbf{U}(\mathbf{D}^{-1} - \mathbf{I})\mathbf{U}' \succ \mathbf{O} \quad \because \mathbf{D}^{-1} - \mathbf{I} \succ \mathbf{O}.$$

- If  $\mathbf{A}$  is an  $n \times n$  p.d. and  $\mathbf{B}$  is an  $n \times n$  symmetric matrix, then  $\mathbf{A} - t\mathbf{B}$  is p.d. for  $|t|$  sufficiently small. *Brief proof:* The  $i$ th leading minor determinant of  $\mathbf{A} - t\mathbf{B}$  is a function of  $t$ , which is positive when  $t = 0$ . Since the function is continuous, it will be positive for  $|t| < \delta_i$  for  $\delta_i$  sufficiently small. Let  $\delta = \min(\delta_1, \dots, \delta_n)$ , then all the leading minor determinants will be positive for  $|t| < \delta$ .



- If  $L$  is positive definite then for any  $b$ ,

$$\max_{h^n h \neq 0} \left[ \frac{(h'b)^2}{h' L h} \right] = b' L^{-1} b.$$

*Proof:* Use Cauchy–Schwarz inequality:  $(u'v)^2 \leq \|u\|^2 \|v\|^2$ . Suppose  $u \neq 0$ , then we have

$$\frac{(u'v)^2}{\|u\|^2} \leq \|v\|^2$$

Further let  $u = L^{1/2}h$  ( $h \neq 0$ ) and  $v = L^{-1/2}b$  as  $L \succ O$ , then

$$\frac{(h'b)^2}{h' L h} \leq b' L^{-1} b$$

with the equality holds when  $L^{1/2}h = cL^{-1/2}b \Rightarrow cb = Lh$ , where  $c$  is a scalar.

## 12 Eigenvalue Application

- Let  $A$  be an  $n \times n$  symmetric matrix, then

$$\max_{x: x \neq 0} \left( \frac{x' A x}{x' x} \right) = \lambda_{\text{MAX}}, \quad \min_{x: x \neq 0} \left( \frac{x' A x}{x' x} \right) = \lambda_{\text{MIN}}$$

and these values occur when  $x$  is the eigenvector corresponding to the  $\lambda_{\text{MAX}}$  and  $\lambda_{\text{MIN}}$ , respectively.

*Proof:* Suppose  $\lambda_1 \geq \dots \geq \lambda_n$ . By the spectral decomposition,  $T' A T = \Lambda$ . Setting  $x = T y$  leads to

$$\frac{x' A x}{x' x} = \frac{y' T' A T y}{y' T' T y} = \frac{y' \Lambda y}{y' y} = \frac{\sum_{i=1}^n \lambda_i y_i^2}{\sum_{i=1}^n y_i^2} \leq \lambda_1$$

with equality when  $y = e_1 \Rightarrow x = T e_1 = t_1$ . Also,

$$\frac{x' A x}{x' x} = \frac{y' T' A T y}{y' T' T y} = \frac{y' \Lambda y}{y' y} = \frac{\sum_{i=1}^n \lambda_i y_i^2}{\sum_{i=1}^n y_i^2} \geq \lambda_n$$

with equality when  $y = e_n \Rightarrow x = T e_n = t_n$ .

- (HW1) Show the minimum and maximum eigenvalues of

$$B = \frac{2b}{2b-1} I_n - \frac{1_n 1_n'}{2b-1}, \quad b > \frac{1}{2}.$$

*Solution:* For  $x \neq 0$ ,

$$\frac{x' B x}{x' x} = \frac{2b}{2b-1} - \frac{1}{2b-1} \frac{(1_n' x)^2}{x' x}.$$

By Cauchy–Schwarz inequality,

$$\frac{x' B x}{x' x} \geq \frac{2b}{2b-1} - \frac{1}{2b-1} \frac{\|1_n\|^2 \|x\|^2}{x' x} = \frac{2b}{2b-1} - \frac{n}{2b-1} = \frac{2b-n}{2b-1} = \lambda_{\text{MIN}}$$

with equality iff  $x = c 1_n$ . Also,

$$\frac{x' B x}{x' x} \leq \frac{2b}{2b-1} = \lambda_{\text{MAX}}$$

with equality iff  $1_n' x = 0$ , i.e.,  $1_n \perp x$ .

## 13 Partitioned Matrix

- Basic determinant properties

$$\left| \begin{pmatrix} I & B \\ O & I \end{pmatrix} \right| = \left| \begin{pmatrix} I & O \\ C & I \end{pmatrix} \right| = |I| = 1, \quad \left| \begin{pmatrix} A_{11} & O \\ O & I \end{pmatrix} \right| = |A_{11}|, \quad \left| \begin{pmatrix} I & O \\ O & A_{22} \end{pmatrix} \right| = |A_{22}|$$

follow

$$\begin{aligned} \left| \begin{pmatrix} I & O \\ A_{21} & A_{22} \end{pmatrix} \right| &= \left| \begin{pmatrix} I & O \\ O & A_{22} \end{pmatrix} \right| \left| \begin{pmatrix} I & O \\ A_{22}^{-1}A_{21} & I \end{pmatrix} \right| = |A_{22}|, \\ \left| \begin{pmatrix} A_{11} & O \\ A_{21} & A_{22} \end{pmatrix} \right| &= \left| \begin{pmatrix} A_{11} & O \\ O & I \end{pmatrix} \right| \left| \begin{pmatrix} I & O \\ A_{21} & A_{22} \end{pmatrix} \right| = |A_{11}||A_{22}|. \end{aligned}$$

- Let  $A_{11.2} = A_{11} - A_{12}A_{22}^{-1}A_{21}$  (Schur complement), then  $|A| = |A_{22}||A_{11.2}| = |A_{11}||A_{22.1}|$  since

$$|A| = \left| 1 \cdot \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \cdot 1 \right| = \left| \begin{pmatrix} I & -A_{12}A_{22}^{-1} \\ O & I \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} I & O \\ -A_{22}^{-1}A_{21} & I \end{pmatrix} \right| = \left| \begin{pmatrix} A_{11.2} & O \\ O & A_{22} \end{pmatrix} \right|.$$

- (HW2) Let  $A \in \mathbb{R}^{n \times m}$  and  $B \in \mathbb{R}^{m \times n}$  then  $|I_n + AB| = |I_m + BA|$ . *Proof:*

$$|I_m + AB| = \begin{vmatrix} I_m + AB & O \\ B & I_n \end{vmatrix} = \begin{vmatrix} I_m & A \\ O & I_n \end{vmatrix} \begin{vmatrix} I_m & -A \\ B & I_n \end{vmatrix} = \begin{vmatrix} I_m & -A \\ B & I_n \end{vmatrix} \begin{vmatrix} I_m & A \\ O & I_n \end{vmatrix} = \begin{vmatrix} I_m & O \\ B & I_n + BA \end{vmatrix} = |I_n + BA|.$$

- (HW3) If a partition matrix

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \succeq O,$$

then  $N(A_{22}) \subset N(A_{12})$  and  $C(A_{21}) \subset C(A_{22})$ .

*Proof:* Let  $x' = (x'_1 \ \alpha x'_2)$ , where  $x_2 \in N(A_{22})$  and  $\alpha \in \mathbb{R}$ .

$$\begin{aligned} 0 \leq x'Ax &= x'_1A_{11}x_1 + \alpha x'_2A_{21}x_1 + \alpha x'_1A_{12}x_2 + \alpha^2 x'_2A_{22}x_2 \\ &= x'_1A_{11}x_1 + 2\alpha x'_1A_{12}x_2 \quad \text{since } A'_{21} = A_{12}, \ A_{22}x_2 = 0. \end{aligned}$$

To satisfy that  $\text{RHS} \geq 0$  for  $\forall \alpha$ ,  $x'_1A_{12}x_2$  has to be zero for  $\forall x_1$ . Then,  $A_{12}x_2 = 0$ . Hence,  $N(A_{22}) \subset N(A_{12})$ . It follows from this relationship that

$$\begin{aligned} N(A_{22}) \subset N(A_{12}) &\Leftrightarrow C(A'_{22})^\perp \subset C(A'_{12})^\perp \\ &\Leftrightarrow C(A_{22})^\perp \subset C(A_{21})^\perp \quad \text{since } A'_{22} = A_{22}, \ A'_{12} = A_{21} \\ &\Leftrightarrow C(A_{21}) \subset C(A_{22}). \end{aligned}$$

## 14 Inverse Matrix

- Sherman-Morrison-Woodbury formula:** Let  $A$  and  $B$  be nonsingular  $m \times m$  and  $n \times n$  matrices, respectively, and let  $U$  be  $m \times n$  and  $V$  be  $n \times m$ . Then

$$\begin{aligned} (A + UBV)^{-1} &= A^{-1} - A^{-1}UB(B + BVA^{-1}UB)^{-1}BVA^{-1} \\ &= A^{-1} - A^{-1}U(B^{-1} + VA^{-1}U)^{-1}VA^{-1}. \end{aligned}$$

*Proof:* Pre- or post- multiply by  $A + UBV$  to get  $I_m$ .

- Setting  $B = 1$ ,  $U = \pm u \in \mathbb{R}^m$ , and  $V = v' \in \mathbb{R}^m$ , we have

$$(A \pm uv')^{-1} = A^{-1} \mp \frac{A^{-1}uv'A^{-1}}{1 \pm v'A^{-1}u}.$$

## 15 Generalized inverse

- Let  $\mathbf{A} \in \mathbb{R}^{n \times m}$  with rank of  $r < \min(n, m)$  (not full rank), then there exists  $\mathbf{A}^-$ , s.t. (i)  $\mathbf{A}\mathbf{A}^-\mathbf{A} = \mathbf{A}$ .
- Such a matrix always exists and is called a generalized inverse or g-inverse (HW1).

*Proof:* If  $\mathbf{A}$  is non-singular, then  $\mathbf{B} = \mathbf{A}^{-1}$  is unique.

If  $\mathbf{A}$  is singular, suppose  $\mathbf{A} \in \mathbb{R}^{m \times n}$  with  $\text{rank}(\mathbf{A}) = r$ . By the rank factorization, we obtain  $\mathbf{A} = \mathbf{C}\mathbf{R}$ , where  $\mathbf{C} \in \mathbb{R}^{m \times r}$  is full column rank and  $\mathbf{R} \in \mathbb{R}^{r \times n}$  is full row rank. Since  $\mathbf{A}\mathbf{B}\mathbf{A} = (\mathbf{C}\mathbf{R})\mathbf{B}(\mathbf{C}\mathbf{R}) = \mathbf{C}(\mathbf{R}\mathbf{B}\mathbf{C})\mathbf{R}$ , we want to find  $\mathbf{B}$  s.t.  $\mathbf{R}\mathbf{B}\mathbf{C} = \mathbf{I}$  so that  $\mathbf{A}\mathbf{B}\mathbf{A} = \mathbf{A}$ . As mentioned before,  $\mathbf{C}'\mathbf{C}$  and  $\mathbf{R}\mathbf{R}'$  are non-singular even though  $\mathbf{A}$  is singular. Hence, there always exists

$$\mathbf{B} = \mathbf{R}'(\mathbf{R}\mathbf{R}')^{-1}(\mathbf{C}'\mathbf{C})^{-1}\mathbf{C}'$$

such that  $\mathbf{R}\mathbf{B}\mathbf{C} = \mathbf{I}$ .

- $\mathbf{A}^-$  is not unique. There are several ways of getting it: If  $\mathbf{A}^-$  is a g-inverse, then
  - $\mathbf{G} = \mathbf{A}^- + (\mathbf{I} - \mathbf{A}^-\mathbf{A})\mathbf{W}$  ( $\mathbf{W} \neq \mathbf{O}$ ) is also a g-inverse since  $\mathbf{A}\mathbf{G}\mathbf{A} = \mathbf{A}(\mathbf{A}^- + (\mathbf{I} - \mathbf{A}^-\mathbf{A})\mathbf{W})\mathbf{A} = \mathbf{A}\mathbf{A}^-\mathbf{A} + (\mathbf{A} - \mathbf{A}\mathbf{A}^-\mathbf{A})\mathbf{W}\mathbf{A} = \mathbf{A}$ , or
  - $\mathbf{G} = \mathbf{A}^- + \mathbf{u}\mathbf{v}'$  ( $\mathbf{u}\mathbf{v}' \neq \mathbf{O}$ ) is also a g-inverse, where  $\mathbf{u} \in N(\mathbf{A})$  s.t.  $\mathbf{u} \neq \mathbf{0}$  or  $\mathbf{v} \in N(\mathbf{A}')$  s.t.  $\mathbf{v} \neq \mathbf{0}$ , since  $\mathbf{A}\mathbf{G}\mathbf{A} = \mathbf{A}\mathbf{A}^-\mathbf{A} + (\mathbf{A}\mathbf{u})\mathbf{v}'\mathbf{A} = \mathbf{A}$ .
- Taking transpose of the above property yields  $\mathbf{A}'(\mathbf{A}^-)'\mathbf{A}' = \mathbf{A}'$ , leading to  $(\mathbf{A}')^- = (\mathbf{A}^-)'$ .
- A solution(s) to  $\mathbf{A}\mathbf{x} = \mathbf{b}$  is  $\mathbf{x} = \mathbf{A}^-\mathbf{b}$ , which is not unique, as  $\mathbf{A}(\mathbf{A}^-\mathbf{b}) = \mathbf{A}\mathbf{A}^-\mathbf{A}\mathbf{x} = \mathbf{A}\mathbf{x} = \mathbf{b}$ .
- If  $\mathbf{A}^-$  also satisfies three more conditions: (ii)  $\mathbf{A}^-\mathbf{A}\mathbf{A}^- = \mathbf{A}^-$ , (iii)  $(\mathbf{A}\mathbf{A}^-)' = \mathbf{A}\mathbf{A}^-$ , and (iv)  $(\mathbf{A}^-\mathbf{A})' = \mathbf{A}^-\mathbf{A}$ , then  $\mathbf{A}^-$  is denoted by  $\mathbf{A}^+$ , which is called the **Moore-Penrose inverse**.
- Moore-Penrose inverse  $\mathbf{A}^+$  is unique. If  $\mathbf{B}^+$  is another Moore-Penrose inverse, then

$$\begin{aligned} \mathbf{B}^+ &= \mathbf{B}^+\mathbf{A}\mathbf{B}^+ = \mathbf{B}^+\mathbf{A}\mathbf{A}^+\mathbf{A}\mathbf{B}^+ = \mathbf{A}'(\mathbf{B}^+)'\mathbf{A}^+(\mathbf{B}^+)'\mathbf{A}' = \mathbf{A}'(\mathbf{A}^+)'\mathbf{A}'(\mathbf{B}^+)'\mathbf{A}^+(\mathbf{B}^+)'\mathbf{A}'(\mathbf{A}^+)'\mathbf{A}' \\ &= \mathbf{A}^+\mathbf{A}\mathbf{B}^+\mathbf{A}\mathbf{A}^+\mathbf{A}\mathbf{B}^+\mathbf{A}\mathbf{A}^+ = \mathbf{A}^+\mathbf{A}\mathbf{A}^+\mathbf{A}\mathbf{A}^+ = \mathbf{A}^+\mathbf{A}\mathbf{A}^+ = \mathbf{A}^+. \end{aligned}$$

- (HW5) Show  $\mathcal{C}(\mathbf{A}^+) = \mathcal{C}(\mathbf{A}')$ .

*Proof:* If  $\mathbf{x} \in \mathcal{C}(\mathbf{A}^+)$ , then  $\mathbf{x} = \mathbf{A}^+\mathbf{u} = \mathbf{A}^+\mathbf{A}\mathbf{A}^+\mathbf{u} = \mathbf{A}'(\mathbf{A}^+)'\mathbf{A}^+\mathbf{u} \in \mathcal{C}(\mathbf{A}')$  for some  $\mathbf{u}$ . If  $\mathbf{x} \in \mathcal{C}(\mathbf{A}')$ , then  $\mathbf{x} = \mathbf{A}'\mathbf{w} = (\mathbf{A}^+\mathbf{A})'\mathbf{A}'\mathbf{w} = \mathbf{A}^+\mathbf{A}\mathbf{A}'\mathbf{w} \in \mathcal{C}(\mathbf{A}^+)$  for some  $\mathbf{w}$ .

## 16 Decomposition

- Rank factorization:  $\underbrace{\mathbf{A}}_{n \times p} = \underbrace{\mathbf{C}}_{n \times r} \underbrace{\mathbf{R}}_{r \times p}$ , where  $\mathbf{C}$  has full column rank and  $\mathbf{R}$  has full row rank. Then  $(\mathbf{C}'\mathbf{C})^{-1}\mathbf{C}'\mathbf{C} = \mathbf{R}\mathbf{R}'(\mathbf{R}\mathbf{R}')^{-1} = \mathbf{I}_r$ .
- (HW1) If  $\mathbf{P}\mathbf{A}'\mathbf{A} = \mathbf{Q}\mathbf{A}'\mathbf{A}$ , then  $\mathbf{P}\mathbf{A}' = \mathbf{Q}\mathbf{A}'$  for any comfortable matrices  $\mathbf{P}$  and  $\mathbf{Q}$ .

*Solution:* If  $\mathbf{A}$  is non-singular, or  $\mathbf{A}^{-1}$  exists,  $\mathbf{P}\mathbf{A}'\mathbf{A} = \mathbf{Q}\mathbf{A}'\mathbf{A} \Rightarrow \mathbf{P}\mathbf{A}' = \mathbf{Q}\mathbf{A}'$ .

If  $\mathbf{A}$  is singular and  $\text{rank}(\mathbf{A}) = r$ , we have  $\mathbf{A} = \mathbf{C}\mathbf{R}$  by the rank factorization, where  $\mathbf{C} \in \mathbb{R}^{n \times r}$  is full column rank and  $\mathbf{R} \in \mathbb{R}^{r \times n}$  is full row rank. Then

$$\mathbf{P}\mathbf{A}'\mathbf{A} = \mathbf{Q}\mathbf{A}'\mathbf{A} \Rightarrow (\mathbf{P} - \mathbf{Q})\mathbf{A}'\mathbf{A} = \mathbf{O} \Rightarrow (\mathbf{P} - \mathbf{Q})\mathbf{R}'\mathbf{C}'\mathbf{C}\mathbf{R} = \mathbf{O}.$$

Note that the  $r \times r$  matrices  $\mathbf{C}'\mathbf{C}$  and  $\mathbf{R}\mathbf{R}'$  are non-singular or invertible because we have

$$\text{rank}(\mathbf{C}'\mathbf{C}) = \text{rank}(\mathbf{C}) = \text{rank}(\mathbf{R}\mathbf{R}') = \text{rank}(\mathbf{R}) = r \text{ (full rank)}$$

Thus, multiplying by  $\mathbf{R}'(\mathbf{R}\mathbf{R}')^{-1}(\mathbf{C}'\mathbf{C})^{-1}\mathbf{C}'$  (g-inverse of  $\mathbf{A}$ ), we obtain

$$(\mathbf{P} - \mathbf{Q})\mathbf{R}'\mathbf{C}'\mathbf{C}\mathbf{R}[\mathbf{R}'(\mathbf{R}\mathbf{R}')^{-1}(\mathbf{C}'\mathbf{C})^{-1}\mathbf{C}'] = \mathbf{O} \Rightarrow (\mathbf{P} - \mathbf{Q})\mathbf{R}'\mathbf{C}' = \mathbf{O} \Rightarrow (\mathbf{P} - \mathbf{Q})\mathbf{A}' = \mathbf{O}.$$

- QR factorization (Gram-Schmidt algorithm): Suppose  $\mathbf{A} \in \mathbb{R}^{n \times k}$  and  $\mathbf{Q} = (\mathbf{q}_1 \cdots \mathbf{q}_k)$ , where

$$\mathbf{q}_i = \frac{\mathbf{a}_i - \sum_{j=1}^{i-1} (\mathbf{a}_i, \mathbf{q}_j) \mathbf{q}_j}{\|\mathbf{a}_i - \sum_{j=1}^{i-1} (\mathbf{a}_i, \mathbf{q}_j) \mathbf{q}_j\|}, \quad 1 \leq i \leq k \quad (\text{orthonormal columns}).$$

Then  $\mathbf{A} = \mathbf{QR}$ , where  $\mathbf{R}$  is an upper triangle. QR decomposition is often used to solve the linear least squares problem.

*Application:* Consider normal equations:  $X'X\beta = X'y$ . Solving  $\hat{\beta} = (X'X)^{-1}X'y$  is computationally costly. If we obtain  $X = QR$ , then the normal equations become

$$R'Q'QR\beta = R'Q'y \Rightarrow R'R\beta = R'Q'y \Rightarrow (R')^{-1}R'R\beta = (R')^{-1}R'Q'y \Rightarrow R\beta = Q'y.$$

Since  $R$  is an upper triangular, it is easier to compute  $\beta$  by solving this from the last element of  $\beta$ .

- Spectral decomposition: If  $\mathbf{A}$  is a  $n \times n$  symmetric matrix, then  $\mathbf{A} = \mathbf{T}\mathbf{\Lambda}\mathbf{T}' = \sum_i \lambda_i \mathbf{t}_i \mathbf{t}_i'$ , or  $\mathbf{T}'\mathbf{A}\mathbf{T} = \mathbf{\Lambda}$ , where  $\mathbf{\Lambda} = \text{diag}(\lambda_1, \dots, \lambda_n)$  and  $\mathbf{T}$  is an orthogonal matrix (not symmetric in general) with eigenvectors. The columns of  $\mathbf{T}$  are eigenvectors, which form an orthogonal basis for  $\mathbb{R}^n$ .
  - $C(\mathbf{A})$  is spanned by its eigenvector:  $Ax = \sum_i \lambda_i \mathbf{t}_i \mathbf{t}_i' \mathbf{x} = \sum_i \lambda_i (\mathbf{t}_i' \mathbf{x}) \mathbf{t}_i \in C(\mathbf{A})$ .
- Singular value decomposition: Let  $\mathbf{A} \in \mathbb{R}^{n \times p}$  with rank of  $r$ ,

$$\begin{aligned} \underbrace{\mathbf{A}}_{n \times p} &= \underbrace{(\mathbf{S}_r \mid \mathbf{S}_{p-r})}_{n \times p} \begin{pmatrix} \mathbf{D}_r & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \end{pmatrix} \underbrace{\begin{pmatrix} \mathbf{T}_r' \\ \mathbf{T}_{p-r}' \end{pmatrix}}_{p \times p} \quad (\text{normal form}) \\ &= \underbrace{\mathbf{S}_r}_{n \times r} \mathbf{D}_r \underbrace{\mathbf{T}_r'}_{r \times p} \quad (\text{reduced form}) \\ &= \sum_{i=1}^r \sigma_i \mathbf{s}_i \mathbf{t}_i' \quad (\text{outer product form}), \end{aligned}$$

where  $\mathbf{D}_r = \text{diag}(\sigma_1, \dots, \sigma_r)$  for  $\sigma_1 \geq \dots \geq \sigma_r > 0$ .  $\mathbf{S}_r' \mathbf{S}_r = \mathbf{T}_r' \mathbf{T}_r = \mathbf{I}_r$  (Converse is not identity!).

- Solution 1: Find  $\sigma_i^2$  (eigenvalues) and  $\mathbf{t}_i$  (eigenvectors) by solving  $\mathbf{A}'\mathbf{A}\mathbf{t}_i = \sigma_i^2 \mathbf{t}_i$ . Then

$$\mathbf{s}_i = \frac{\mathbf{A}\mathbf{t}_i}{\sigma_i}, \quad i = 1, \dots, r,$$

where  $\mathbf{s}_i' \mathbf{s}_j = \mathbf{t}_i \mathbf{A}' \mathbf{A} \mathbf{t}_j / (\sigma_i \sigma_j) = (\sigma_j / \sigma_i) \mathbf{t}_i \mathbf{t}_j = \delta_{ij}$ , i.e.,  $\mathbf{S}_r$  is orthogonal as well as  $\mathbf{T}_r$ .

- Solution 2: Find  $\sigma_i^2$  and  $\mathbf{s}_i$  by solving  $\mathbf{A}\mathbf{A}'\mathbf{s}_i = \sigma_i^{-1} \mathbf{A}\mathbf{A}'\mathbf{A}\mathbf{t}_i = \sigma_i \mathbf{A}\mathbf{t}_i = \sigma_i^2 \mathbf{s}_i$ . Then

$$\mathbf{t}_i = \frac{\mathbf{A}'\mathbf{s}_i}{\sigma_i}, \quad i = 1, \dots, r.$$

- The Moore–Penrose inverse:  $\mathbf{A}^+ = \mathbf{T}\mathbf{D}_r^{-1}\mathbf{S}'$  that satisfies the following four properties: (i)  $\mathbf{A}\mathbf{A}^+\mathbf{A} = (\mathbf{S}\mathbf{D}_r\mathbf{T}')(\mathbf{T}\mathbf{D}_r^{-1}\mathbf{S}')(\mathbf{S}\mathbf{D}_r\mathbf{T}') = \mathbf{S}\mathbf{D}_r\mathbf{T}' = \mathbf{A}$ , (ii)  $\mathbf{A}^+\mathbf{A}\mathbf{A}^+ = \mathbf{T}\mathbf{D}_r^{-1}\mathbf{S}' = \mathbf{A}^+$ , (iv)  $(\mathbf{A}^+\mathbf{A})' = [(\mathbf{T}\mathbf{D}_r^{-1}\mathbf{S}')(\mathbf{S}\mathbf{D}_r\mathbf{T}')] = (\mathbf{T}\mathbf{T}')' = \mathbf{T}\mathbf{T}' = \mathbf{A}^+\mathbf{A}$ , and (iii)  $(\mathbf{A}\mathbf{A}^+)' = \mathbf{S}\mathbf{S}' = \mathbf{A}\mathbf{A}^+$ .
- (HW2) Find the SVD of  $\mathbf{X}$  whose first row is  $(1, 0, 0, 0)$  and the second row is  $(-1, 0, 0, 0)$ .

*Solution:*  $r = \text{rank}(\mathbf{X}) = 1$  and

$$\mathbf{X}'\mathbf{X} = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

implies that the eigenvector greater than 0 is  $\lambda = 2$ . Thus,  $\sigma_1 = \sqrt{2}$ . The corresponding eigenvector is

$$(2\mathbf{I} - \mathbf{X}'\mathbf{X})\mathbf{t}_1 = \mathbf{0} \Rightarrow \mathbf{t}_1 = (1, 0, 0, 0)'$$

Then,

$$\mathbf{s}_1 = \frac{\mathbf{X}\mathbf{t}_1}{\sigma_1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

Hence,

$$\begin{aligned} \mathbf{X} &= \mathbf{S}_r \mathbf{D}_r \mathbf{T}_r' = \mathbf{s}_1 \sigma_1 \mathbf{t}_1' = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} (\sqrt{2}) \begin{pmatrix} 1 & 0 & 0 & 0 \end{pmatrix} \quad (\text{reduced form}) \\ &= \mathbf{S} \mathbf{D} \mathbf{T}' = (\mathbf{s}_1 \ \mathbf{s}_2) \begin{pmatrix} \sigma_1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{t}_1' \\ \mathbf{t}_2' \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \sqrt{2} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad (\text{normal form}) \end{aligned}$$

In the normal form of SVD,  $\mathbf{s}_2$  and  $\mathbf{t}_2$  orthogonal to  $\mathbf{s}_1$  and  $\mathbf{t}_1$  were chosen, respectively.

- **Cholesky's decomposition:** If  $\mathbf{A}$  is p.d., there exists a *unique* upper triangular matrix  $\mathbf{R}$  with positive diagonal elements such that  $\mathbf{A} = \mathbf{R}'\mathbf{R}$ . This is useful for efficient numerical solutions, e.g., Monte Carlo simulations. The Cholesky decomposition is roughly twice as efficient as the LU decomposition for solving systems of linear equations.

## 17 Expectation and Variance-covariance

- For a random matrix  $\mathbf{Z}$  and comfortable matrices,  $E(\mathbf{AZB} + \mathbf{C}) = \mathbf{A}E(\mathbf{Z})\mathbf{B} + \mathbf{C}$ .
- $\text{Cov}(\mathbf{X}, \mathbf{Y}) = E[(\mathbf{X} - E(\mathbf{X}))(\mathbf{Y} - E(\mathbf{Y}))']$  and  $\text{Cov}(\mathbf{X}, \mathbf{X}) = \text{Var}(\mathbf{X})$ .
- $\text{Cov}(\mathbf{AX}, \mathbf{BY}) = \mathbf{A} \text{Cov}(\mathbf{X}, \mathbf{Y}) \mathbf{B}'$ .
- $\text{Var}(a\mathbf{X} + b\mathbf{Y}) = a^2 \text{Var}(\mathbf{X}) + ab[\text{Cov}(\mathbf{X}, \mathbf{Y}) + \text{Cov}(\mathbf{Y}, \mathbf{X})] + b^2 \text{Var}(\mathbf{Y})$ . Note  $\text{Cov}(\mathbf{X}, \mathbf{Y}) \neq \text{Cov}(\mathbf{Y}, \mathbf{X})$ .
- $E(\mathbf{x}'\mathbf{Ax}) = \text{tr}(\mathbf{A}\mathbf{\Sigma}) + \boldsymbol{\mu}'\mathbf{A}\boldsymbol{\mu}$ , where  $\mathbf{\Sigma} = \text{Var}(\mathbf{X})$ .
  - $E[(\mathbf{x} - \mathbf{b})'\mathbf{A}(\mathbf{x} - \mathbf{b})] = \text{tr}(\mathbf{A}\mathbf{\Sigma}) + (\boldsymbol{\mu} - \mathbf{b})'\mathbf{A}(\boldsymbol{\mu} - \mathbf{b})$  as  $\text{Var}(\mathbf{X} - \mathbf{b}) = \text{Var}(\mathbf{X})$ .
  - If  $\mathbf{\Sigma} = \sigma^2 \mathbf{I}_n$ ,  $E(\mathbf{x}'\mathbf{Ax}) = \sigma^2 \text{tr}(\mathbf{A}) + \boldsymbol{\mu}'\mathbf{A}\boldsymbol{\mu} = \sigma^2(\text{sum of the coefficient of } X_i^2) + (\mathbf{x}'\mathbf{Ax})_{\mathbf{x}=\boldsymbol{\mu}}$

## 18 Multivariate normal distribution

- If  $\mathbf{y} \sim N_p(\boldsymbol{\mu}, \mathbf{\Sigma})$ , the density is  $f(\mathbf{Y} | \boldsymbol{\mu}, \mathbf{\Sigma}) = C e^{-\frac{1}{2}(\mathbf{y}-\boldsymbol{\mu})'\mathbf{\Sigma}^{-1}(\mathbf{y}-\boldsymbol{\mu})}$ , where  $C = (2\pi)^{-p/2} |\mathbf{\Sigma}|^{-1/2}$ .

*Proof:* By SD,  $\mathbf{\Sigma} = \mathbf{T}\mathbf{\Lambda}\mathbf{T}'$ , where  $\mathbf{\Lambda} = (\lambda_1, \dots, \lambda_p)$  and let  $\mathbf{Z} = \mathbf{T}'(\mathbf{y} - \boldsymbol{\mu}) \Rightarrow \mathbf{y} = \mathbf{T}\mathbf{Z} + \boldsymbol{\mu}$ , then

$$1 = \int_{\mathbf{y} \in \mathbb{R}^p} C e^{-\frac{1}{2}(\mathbf{y}-\boldsymbol{\mu})'\mathbf{\Sigma}^{-1}(\mathbf{y}-\boldsymbol{\mu})} d\mathbf{y} = \int_{\mathbf{z} \in \mathbb{R}^p} C e^{-\frac{1}{2}\mathbf{z}'\mathbf{\Lambda}^{-1}\mathbf{z}} |J| d\mathbf{z} = \int_{\mathbf{z} \in \mathbb{R}^p} C e^{-\frac{1}{2} \sum_{i=1}^p z_i^2 / \lambda_i} d\mathbf{z}$$

since  $|J| = |\det(d\mathbf{y}/d\mathbf{x})| = |\det(\mathbf{T})| = |\pm 1| = 1$ . Further

$$\int_{\mathbf{z} \in \mathbb{R}^p} C e^{-\frac{1}{2} \sum_{i=1}^p z_i^2 / \lambda_i} d\mathbf{z} = C \prod_{i=1}^p \int_{-\infty}^{\infty} e^{-\frac{1}{2} z_i^2 / \lambda_i} dz_i = C \prod_{i=1}^p (\sqrt{2\pi\lambda_i}) = C(2\pi)^{p/2} |\mathbf{\Sigma}|^{1/2}.$$

- For the above,  $E(\mathbf{z}) = \mathbf{0} \Rightarrow E(\mathbf{y}) = \boldsymbol{\mu}$  and  $\text{Cov}(\mathbf{Y}) = \text{Cov}(\mathbf{T}\mathbf{Z} + \boldsymbol{\mu}) = \mathbf{T}\mathbf{\Lambda}\mathbf{T}' = \mathbf{\Sigma}$ .
- Mgf of  $\mathbf{y} \sim N_p(\boldsymbol{\mu}, \mathbf{\Sigma})$  is  $\psi_{\mathbf{Y}}(\mathbf{t}) = \exp(\boldsymbol{\mu}'\mathbf{t} + \frac{1}{2}\mathbf{t}'\mathbf{\Sigma}\mathbf{t})$ .

*Proof:* If  $\boldsymbol{\mu} = \mathbf{0}$ , the mgf of  $\mathbf{y}_0 \sim N_p(\mathbf{0}, \mathbf{\Sigma})$  is

$$E(e^{\mathbf{t}'\mathbf{y}_0}) = C \int e^{\mathbf{t}'\mathbf{y}_0} e^{-\frac{1}{2}\mathbf{y}_0'\mathbf{\Sigma}^{-1}\mathbf{y}_0} d\mathbf{y}_0 = C \int e^{-\frac{1}{2}[(\mathbf{y}_0 - \mathbf{\Sigma}\mathbf{t})'\mathbf{\Sigma}^{-1}(\mathbf{y}_0 - \mathbf{\Sigma}\mathbf{t}) - \mathbf{t}'\mathbf{\Sigma}\mathbf{t}]} d\mathbf{y}_0 = e^{\frac{1}{2}\mathbf{t}'\mathbf{\Sigma}\mathbf{t}},$$

so that  $E(e^{\mathbf{t}'\mathbf{y}}) = E(e^{\mathbf{t}'(\mathbf{y}_0 + \boldsymbol{\mu})}) = e^{\mathbf{t}'\boldsymbol{\mu}} E(e^{\mathbf{t}'\mathbf{y}_0}) = e^{\boldsymbol{\mu}'\mathbf{t} + \frac{1}{2}\mathbf{t}'\mathbf{\Sigma}\mathbf{t}}$ .

- Let  $\mathbf{y} \sim N_n(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ . If  $\mathbf{x} = \mathbf{A}\mathbf{y} + \mathbf{b}$ , where  $\mathbf{A} \in \mathbb{R}^{m \times n}$  with rank  $m$  (**full row rank**), then  $\mathbf{x} \sim N_m(\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}')$ . Note:  $\mathbf{A}$  must have full row rank to ensure  $\mathbf{A}\boldsymbol{\Sigma}\mathbf{A}' \succ \mathbf{O}$ ; otherwise  $\mathbf{x}\mathbf{A}\boldsymbol{\Sigma}\mathbf{A}'\mathbf{x}$  can be zero for nonzero  $\mathbf{x}$ .
- All subsets of  $\mathbf{y}$  are multivariate normal: Take  $\mathbf{A} = (\mathbf{I}_k \mid \mathbf{O}) \in \mathbb{R}^{k \times n}$ ,  $\mathbf{A}\mathbf{y} = (y_1, \dots, y_k) \sim N_k(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ .
- For  $\mathbf{a} \in \mathbb{R}^n \setminus \{\mathbf{0}\}$ ,  $\mathbf{a}'\mathbf{y} \sim N_1(\mathbf{a}'\boldsymbol{\mu}, \mathbf{a}'\boldsymbol{\Sigma}\mathbf{a})$ , i.e., a linear combination of  $y_i$ 's is univariate normal.
- Suppose  $\mathbb{E}(\mathbf{Y}) = \boldsymbol{\mu}$  and  $\text{Var}(\mathbf{Y}) = \boldsymbol{\Sigma}$ .  $\mathbf{Y} \sim N_n(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \Leftrightarrow \mathbf{a}'\mathbf{Y}$  has a univariate normal for all  $\mathbf{a}$ .  
*Proof:* ( $\Rightarrow$ ) See above. ( $\Leftarrow$ ) If  $\mathbf{t}'\mathbf{Y}$  has a univariate normal for all  $\mathbf{t}$ . By assumption,  $\mathbf{t}'\mathbf{Y} \sim N(\mathbf{t}'\boldsymbol{\mu}, \mathbf{t}'\boldsymbol{\Sigma}\mathbf{t})$  and hence the mgf of  $\mathbf{t}'\mathbf{Y}$  is  $M_{\mathbf{t}'\mathbf{Y}}(s) = \mathbb{E}[e^{s(\mathbf{t}'\mathbf{Y})}] = \exp[(\mathbf{t}'\boldsymbol{\mu})s + \mathbf{t}'\boldsymbol{\Sigma}\mathbf{t}s^2/2]$ . Putting  $s = 1$  yields  $M_{\mathbf{t}'\mathbf{Y}}(1) = \mathbb{E}(e^{\mathbf{t}'\mathbf{Y}}) = \exp[\mathbf{t}'\boldsymbol{\mu} + \mathbf{t}'\boldsymbol{\Sigma}\mathbf{t}/2] = M_{\mathbf{Y}}(\mathbf{t})$ , which means that  $\mathbf{Y} \sim N_n(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ .
- Yet, even though all marginals of  $\mathbf{X}$  are normal,  $\mathbf{X}$  may *not* be normally distributed (See 250A HW).
- Consider the joint density of  $X \in \mathbb{R}^p$  and  $Y \in \mathbb{R}^q$ :

$$\begin{pmatrix} X \\ Y \end{pmatrix} \sim N_{p+q} \left( \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix} \right),$$

then  $X \perp\!\!\!\perp Y \Leftrightarrow \Sigma_{12} = \Sigma'_{21} = \mathbf{O}_{p \times q}$  so that  $f_{X,Y}(x, y \mid \mu_1, \mu_2, \Sigma) = f_X(x \mid \mu_1, \Sigma_{11})f_Y(y \mid \mu_2, \Sigma_{22})$ .

*Proof:* Use MGF.  $\psi_{X,Y}(t) = e^{t'\mu + t'\Sigma t/2} = e^{t'_1\mu_1 + t'_1\Sigma_{11}t_1 + t'_2\mu_2 + t'_2\Sigma_{22}t_2} = \psi_X(t_1)\psi_Y(t_2)$ .

- In the above setting, the conditional density of  $X$  given  $Y = y$  is

$$X \mid Y = y \sim N_p(\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(y - \mu_2), \Sigma_{11.2})$$

The proof is below.

- Theorem 2.5: Let  $\mathbf{Y} \sim N_n(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ ,  $\mathbf{U} = \mathbf{A}\mathbf{Y}$  and  $\mathbf{V} = \mathbf{B}\mathbf{Y}$ . Then  $\mathbf{U} \perp \mathbf{V} \Leftrightarrow \text{Cov}[\mathbf{U}, \mathbf{V}] = \mathbf{A}\boldsymbol{\Sigma}\mathbf{B}' = \mathbf{0}$ .

## 19 Conditional multivariate normal distribution

- If  $\mathbf{A}_{22}$  is invertible and given that

$$\mathbf{X} = \begin{pmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{pmatrix} \in \mathbb{R}^{p+q}, \quad \mathbf{A} = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix} \in \mathbb{R}^{(p+q) \times (p+q)}.$$

Let  $\mathbb{E}(\mathbf{X}_1) = \boldsymbol{\mu}_1$  and  $\mathbb{E}(\mathbf{X}_2) = \boldsymbol{\mu}_2$ .

Consider the transformation

$$\begin{pmatrix} \mathbf{Y} \\ \mathbf{X}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{I}_p & -\mathbf{A}_{12}\mathbf{A}_{22}^{-1} \\ \mathbf{O} & \mathbf{I}_q \end{pmatrix} \begin{pmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{pmatrix}.$$

Since this is a linear transformation, the joint distribution is also multivariate normal with  $\mathbb{E}(\mathbf{Y}) = \boldsymbol{\mu}_1 - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\boldsymbol{\mu}_2$ ,  $\mathbb{E}(\mathbf{X}_2) = \boldsymbol{\mu}_2$ . and covariance matrix

$$\text{Var} \begin{pmatrix} \mathbf{Y} \\ \mathbf{X}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{I}_p & -\mathbf{A}_{12}\mathbf{A}_{22}^{-1} \\ \mathbf{O} & \mathbf{I}_q \end{pmatrix} \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{I}_p & -\mathbf{A}_{12}\mathbf{A}_{22}^{-1} \\ \mathbf{O} & \mathbf{I}_q \end{pmatrix}' = \begin{pmatrix} \mathbf{A}_{11.2} & \mathbf{O}' \\ \mathbf{O} & \mathbf{A}_{22} \end{pmatrix},$$

which implies that  $\mathbf{Y}$  and  $\mathbf{X}_2$  are uncorrelated and then independent. Thus, the conditional distribution of  $\mathbf{Y} \mid \mathbf{X}_2 = \mathbf{x}_2$  is the same as the marginal distribution of  $\mathbf{Y}$ :

$$\mathbf{Y} \mid \mathbf{X}_2 = \mathbf{x}_2 \sim N_p(\boldsymbol{\mu}_1 - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\boldsymbol{\mu}_2, \mathbf{A}_{11.2}).$$

Further, because of this independence,  $\mathbf{X}_1 = \mathbf{Y} + \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{X}_2$  given  $\mathbf{X}_2 = \mathbf{x}_2$  is distributed as

$$\begin{aligned} \mathbf{X}_1 \mid \mathbf{X}_2 = \mathbf{x}_2 &\sim N_p(\boldsymbol{\mu}_1 - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\boldsymbol{\mu}_2 + \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{x}_2, \mathbf{A}_{11.2}) \\ &\sim N_p(\boldsymbol{\mu}_1 + \mathbf{A}_{12}\mathbf{A}_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2), \mathbf{A}_{11.2}) \end{aligned}$$

- If  $\mathbf{A}_{22}$  is not invertible, consider the transformation with g-inverse of  $\mathbf{A}_{22}$

$$\begin{pmatrix} \mathbf{Y} \\ \mathbf{X}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{I}_p & -\mathbf{A}_{12}\mathbf{A}_{22}^- \\ \mathbf{O} & \mathbf{I}_q \end{pmatrix} \begin{pmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{pmatrix}.$$

Then, covariance matrix

$$\begin{aligned} \text{Var} \begin{pmatrix} \mathbf{Y} \\ \mathbf{X}_2 \end{pmatrix} &= \begin{pmatrix} \mathbf{I}_p & -\mathbf{A}_{12}\mathbf{A}_{22}^- \\ \mathbf{O} & \mathbf{I}_q \end{pmatrix} \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{I}_p & \mathbf{O}' \\ -\mathbf{A}_{22}^-\mathbf{A}_{21} & \mathbf{I}_q \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^-\mathbf{A}_{21} & \mathbf{A}_{12} - \mathbf{A}_{12}\mathbf{A}_{22}^-\mathbf{A}_{22} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{I}_p & \mathbf{O}' \\ -\mathbf{A}_{22}^-\mathbf{A}_{21} & \mathbf{I}_q \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{A}_{11.2} - (\mathbf{A}_{12} - \mathbf{A}_{12}\mathbf{A}_{22}^-\mathbf{A}_{22})\mathbf{A}_{22}^-\mathbf{A}_{21} & \mathbf{A}_{12} - \mathbf{A}_{12}\mathbf{A}_{22}^-\mathbf{A}_{22} \\ \mathbf{A}_{21} - \mathbf{A}_{22}\mathbf{A}_{22}^-\mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix}. \end{aligned}$$

For the top left,

$$\mathbf{A}_{11.2} - (\mathbf{A}_{12} - \mathbf{A}_{12}\mathbf{A}_{22}^-\mathbf{A}_{22})\mathbf{A}_{22}^-\mathbf{A}_{21} = \mathbf{A}_{11.2} - \mathbf{A}_{12}\mathbf{A}_{22}^-\mathbf{A}_{21} + \mathbf{A}_{12}\mathbf{A}_{22}^-\mathbf{A}_{22}\mathbf{A}_{22}^-\mathbf{A}_{21} = \mathbf{A}_{11.2}.$$

For the top right and bottom left,

$$\begin{aligned} \mathbf{A}_{12} - \mathbf{A}_{12}\mathbf{A}_{22}^-\mathbf{A}_{22} &= \mathbf{H}'\mathbf{A}_{22} - \mathbf{H}'\mathbf{A}_{22}\mathbf{A}_{22}^-\mathbf{A}_{22} = \mathbf{O} \\ \mathbf{A}_{21} - \mathbf{A}_{22}\mathbf{A}_{22}^-\mathbf{A}_{21} &= \mathbf{A}_{22}\mathbf{H} - \mathbf{A}_{22}\mathbf{A}_{22}^-\mathbf{A}_{22}\mathbf{H} = \mathbf{O}. \end{aligned}$$

since  $C(\mathbf{A}_{21}) \subseteq C(\mathbf{A}_{22})$  implies that there exists  $\mathbf{H}$  such that  $\mathbf{A}_{21} = \mathbf{A}_{22}\mathbf{H}$  and  $\mathbf{A}_{12} = \mathbf{H}'\mathbf{A}_{22}$ .

Therefore, as for the previous case,

$$\begin{aligned} \mathbf{Y} \mid \mathbf{X}_2 = \mathbf{x}_2 &\sim N_p(\boldsymbol{\mu}_1 - \mathbf{A}_{12}\mathbf{A}_{22}^-\boldsymbol{\mu}_2, \mathbf{A}_{11.2}) \\ \Rightarrow \mathbf{X}_1 \mid \mathbf{X}_2 = \mathbf{x}_2 &\sim N_p(\boldsymbol{\mu}_1 + \mathbf{A}_{12}\mathbf{A}_{22}^-(\mathbf{x}_2 - \boldsymbol{\mu}_2), \mathbf{A}_{11.2}) \end{aligned}$$

## 20 Multivariate T distribution

Let  $Y = (Y_1, Y_2, \dots, Y_p)'$  is said to have a multivariate  $t$  distribution if its PDF is given by

$$f(y) = \frac{\Gamma(\frac{1}{2}(\nu + n))}{(\pi\nu)^{n/2}\Gamma(\frac{1}{2}\nu)} |\Sigma|^{-1/2} \left[ 1 + \frac{(y - \mu)'\Sigma^{-1}(y - \mu)}{\nu} \right]^{-(p+\nu)/2},$$

where  $\Sigma \succ O$ . We say  $Y \sim t_p(\nu, \mu, \Sigma)$ . This distribution has the following properties:

- If  $\Sigma = (\sigma_{ij})$ , then  $(Y_i - \mu_i)/\sqrt{\sigma_{ii}} \sim t_\nu$ .
- $(Y - \mu)'\Sigma^{-1}(Y - \mu) \sim F_{n,\nu}$ .

## 21 Quadratic form

- Let  $X$  be a  $p$ -dimensional random variable with mean  $\mu$  and covariance  $\Sigma$  (not assumed normal yet). Consider the quadratic form  $Q = x'Ax$  for some comfortable  $A$ . Then  $\mathbb{E}(Q) = \text{tr}(A\Sigma) + \mu'A\mu$ . *Proof:*

$$\begin{aligned} \mathbb{E}(x'Ax) &= \mathbb{E}[\text{tr}(x'Ax)] = \mathbb{E}[\text{tr}(Axx')] = \mathbb{E}[\text{tr}(A(x - \mu)(x - \mu)' + A\mu\mu')] \\ &= \text{tr} A \mathbb{E}[(x - \mu)(x - \mu)'] + \text{tr}(A\mu\mu'). \end{aligned}$$

- Example: Consider the mean of a sample variance  $S^2 = \sum_{i=1}^n (x_i - \bar{x})^2 / (n - 1)$ , where  $x_i \sim N(\mu, \sigma^2)$ :

$$(n - 1)S^2 = \sum_{i=1}^n (x_i - \bar{x})^2 = x' \left( I_n - \frac{1_n 1_n'}{n} \right) x := x'Ax,$$

so that  $\mathbb{E}(n - 1)S^2 = \text{tr}(A\Sigma) + x'Ax|_{x=\mu} = \sigma^2 \text{tr}(A) + 0 = \sigma^2(n - 1) \Rightarrow \mathbb{E}S^2 = \sigma^2$ .

- Let  $y \sim N_p(0, \mathbf{I}_p)$  and let  $A$  be symmetric. Then  $Q = y' Ay \sim \chi_r^2(0) \Leftrightarrow A$  is idempotent of rank  $r$ :

*Proof:* ( $\Leftarrow$ ) Using the spectral decomposition of  $A$ ,

$$\begin{aligned} Q &= y' T \Lambda T' y = z' \Lambda z = \sum_{i=1}^r z_i^2 \sim \chi_r^2(0) \quad \because z = T' y \sim N_n(0, T' T = I_n) \\ &= y' T_1 T_1' y = z_r' z_r = \sum_{i=1}^r z_i^2 \sim \chi_r^2(0) \quad \because z_r = T_1' y \sim N_r(0, T_1' T_1 = I_r) \end{aligned}$$

( $\Rightarrow$ ) Express the MGF of  $Q = y' Ay \sim \chi_r^2$  with  $A$ , which is known. For  $t < 1/2$ ,

$$\frac{1}{(1-2t)^{r/2}} = E(e^{Qt}) = \int (2\pi)^{-p/2} \exp \left[ -\frac{y'(I-2tA)y}{2} \right] dy = \frac{1}{|I-2tA|^{1/2}} = \prod_{i=1}^p \frac{1}{(1-2t\lambda_i)^{1/2}}$$

by SD. It follows that  $r$  of  $p$  eigenvalues have to be 1 and the others 0 so that  $A$  is idempotent.

- If  $y \sim N_p(0, \Sigma)$ , then  $Q = y' Ay \sim \chi_r^2(0) \Leftrightarrow A\Sigma$  is idempotent of rank  $r$ , or equivalently,  $A\Sigma A = A$ .

*Proof:* Let  $x = \Sigma^{-1/2} y \sim N(0, I_p) \Rightarrow y = \Sigma^{1/2} x$ , then  $Q = x' \Sigma^{1/2} A \Sigma^{1/2} x$ . By the above theorem,

$$\begin{aligned} Q = x' \Sigma^{1/2} A \Sigma^{1/2} x \sim \chi_r^2 &\Leftrightarrow x' \Sigma^{1/2} A \Sigma^{1/2} x \text{ is idempotent of rank } r \\ &\Leftrightarrow (\Sigma^{1/2} A \Sigma^{1/2})(\Sigma^{1/2} A \Sigma^{1/2}) = \Sigma^{1/2} A \Sigma^{1/2} \\ &\Leftrightarrow A \Sigma A = A \quad \Leftrightarrow A \Sigma A \Sigma = A \Sigma \end{aligned}$$

with  $r = \text{rank}(\Sigma^{1/2} A \Sigma^{1/2}) = \text{tr}(\Sigma^{1/2} A \Sigma^{1/2}) = \text{tr}(A \Sigma) = \text{rank}(A \Sigma)$ .

*Another solution:*  $r = \text{rank}(A) = \text{rank}(A \Sigma A) \leq \text{rank}(A \Sigma) \leq \text{rank}(A)$  and Mgf of  $Q = \mathbf{y}' \mathbf{A} \mathbf{y}$  is

$$E(e^{Qt}) = \frac{1}{(2\pi)^{\frac{p}{2}} |\Sigma|^{\frac{1}{2}}} \int e^{-\frac{1}{2} \mathbf{y}' (\Sigma^{-1} - 2t\mathbf{A}) \mathbf{y}} d\mathbf{y} = \frac{1}{|\Sigma^{-1} - 2t\mathbf{A}|^{\frac{1}{2}} |\Sigma|^{\frac{1}{2}}} = \frac{1}{|\mathbf{I} - 2t\mathbf{A}\Sigma|^{\frac{1}{2}}}.$$

provided that  $|t|$  is small enough. Note that if  $\Sigma \succ O$  and  $A' = A$ , then  $\Sigma + tA$  is also p.d. for small  $|t|$ .

- Let  $y \sim N_p(0, \mathbf{I}_p)$ ,  $A_i$  is symmetric and  $Q_i = y' A_i y \sim \chi_{r_i}^2$  for  $i = 1, 2$ . Then  $Q_1 \perp Q_2 \Leftrightarrow A_1 A_2 = O$ .

*Proof:* ( $\Rightarrow$ )  $Q_1 \perp Q_2 \Rightarrow Q_1 + Q_2 = y'(A_1 + A_2)y \sim \chi_{r_1+r_2}^2 \Rightarrow A_1 + A_2$  is idempotent by above, that is,

$$(A_1 + A_2)^2 = A_1 + A_2 \quad \Rightarrow \quad A_1 A_2 + A_2 A_1 = O.$$

**Left and right multiplications by  $A_1$**  yield  $A_1 A_2 + A_1 A_2 A_1 = A_1 A_2 A_1 + A_2 A_1 \Rightarrow A_1 A_2 = A_2 A_1 = O$ .

( $\Leftarrow$ ) Suppose  $A_1 A_2 = O$ . Find the Mgf of  $Q_1$  and  $Q_2$ :

$$\begin{aligned} \psi_{Q_1, Q_2}(t_1, t_2) &= E(e^{t_1 Q_1 + t_2 Q_2}) = \int (2\pi)^{-p/2} \exp \left[ -\frac{1}{2} y'(I - 2t_1 A_1 - 2t_2 A_2) y \right] dy \\ &= \frac{1}{|I - 2t_1 A_1 - 2t_2 A_2|^{1/2}} \\ &= \frac{1}{|I - 2t_1 A_1|^{\frac{1}{2}} |I - 2t_2 A_2|^{\frac{1}{2}}} \quad \because A_1 A_2 = O \\ &= \psi_{Q_1}(t_1) \psi_{Q_2}(t_2), \end{aligned}$$

meaning that  $Q_1 \perp Q_2$ .

- If  $y \sim N_p(0, \Sigma)$ ,  $A_i$  is symmetric and  $Q_i = y' A_i y \sim \chi_{r_i}^2$  for  $i = 1, 2$ . Then  $Q_1 \perp Q_2 \Leftrightarrow A_1 \Sigma A_2 = O$ .

*Proof 1:* Same process as the above: ( $\Rightarrow$ )  $Q_1 \perp Q_2 \Rightarrow (A_1 + A_2)\Sigma$  is idempotent by above, that is,

$$(A_1 + A_2)\Sigma(A_1 + A_2) = A_1 + A_2 \quad \Rightarrow \quad A_1 \Sigma A_2 + A_2 \Sigma A_1 = O \quad \Rightarrow \quad A_1 \Sigma A_2 = A_2 \Sigma A_1 = O.$$



( $\Leftarrow$ ) Suppose  $A_1 \Sigma A_2 = 0$ ,  $E(e^{t_1 Q_1 + t_2 Q_2}) = |\Sigma|^{-\frac{1}{2}} |\Sigma^{-1} - 2tA_1 - 2tA_2|^{-\frac{1}{2}} = |I - 2tA_1 \Sigma|^{-\frac{1}{2}} |I - 2tA_2 \Sigma|^{-\frac{1}{2}}$ .

*Proof 2:* Let  $x = \Sigma^{-\frac{1}{2}} y \sim N_p(0, \mathbf{I}_p)$ , then  $Q_i = x' \Sigma^{\frac{1}{2}} A_i \Sigma^{\frac{1}{2}} x$ . Hence, by the above theorem,

$$Q_1 \perp Q_2 \Leftrightarrow \Sigma^{\frac{1}{2}} A_1 \Sigma^{\frac{1}{2}} \Sigma^{\frac{1}{2}} A_2 \Sigma^{\frac{1}{2}} = O \Leftrightarrow A_1 \Sigma A_2 = O.$$

- Let  $y \sim N_p(0, I_p)$ . If  $Q_1 - Q_2 \geq 0$  and  $Q_i = y' A_i y \sim \chi_{r_i}^2$  for  $i = 1, 2$  then

$$Q_1 - Q_2 \perp\!\!\!\perp Q_2, \quad Q_1 - Q_2 \sim \chi_{r_1 - r_2}^2.$$

*Proof:* Since  $Q_1 - Q_2 = y'(A_1 - A_2)y \geq 0, \forall y \in \mathbb{R}^p$ , take  $z \in N(A_1)$  to obtain

$$0 \leq z'(A_1 - A_2)z = -z'A_2 z \leq 0 \quad \because A_2 \succeq O$$

so that  $z'A_2 z = z'A_2^2 z = \|A_2 z\|^2 = 0 \Rightarrow A_2 z = 0 \Rightarrow z \in N(A_2)$ . So we have  $N(A_1) \subseteq N(A_2)$ . Specifically,  $(I_p - A_1)y \in N(A_1)$  since  $A_1(I_p - A_1)y = (A_1 - A_1^2)y = 0$ . It follows that

$$A_2(I_p - A_1)y = 0, \forall y \Rightarrow A_2 - A_2 A_1 = O \quad \text{and} \quad A_2 - A_1 A_2 = O \quad \because A_1' = A_1, A_2' = A_2.$$

Using the equation to get  $(A_1 - A_2)A_2 = A_1 A_2 - A_2^2 = A_1 A_2 - A_2 = O \Rightarrow Q_1 - Q_2 \perp\!\!\!\perp Q_2$  and

$$\begin{aligned} (A_1 - A_2)^2 &= A_1 - A_1 A_2 - A_2 A_1 + A_2 = A_1 - A_2, \\ \text{rank}(A_1 - A_2) &= \text{tr}(A_1 - A_2) = \text{tr}(A_1) - \text{tr}(A_2) = r_1 - r_2, \end{aligned}$$

which shows  $Q_1 - Q_2 \sim \chi_{r_1 - r_2}^2(0)$ .

- If  $\mathbf{y} \sim N_p(\mathbf{m}, \mathbf{I}_p)$  and  $\mathbf{A}$  is **idempotent** of rank  $k$ . Then  $(\mathbf{y} - \mathbf{a})' \mathbf{A} (\mathbf{y} - \mathbf{a}) \sim \chi_k^2((\mathbf{m} - \mathbf{a})' \mathbf{A} (\mathbf{m} - \mathbf{a}))$ .

*Proof:* Let  $\mathbf{z} = \mathbf{y} - \mathbf{a}$ , then  $\mathbf{z} \sim N_p(\mathbf{m} - \mathbf{a}, \mathbf{I}_p)$ . By the spectral decomposition, we obtain

$$\mathbf{A} = \mathbf{T} \mathbf{\Lambda} \mathbf{T}' = \mathbf{T}_1 \mathbf{T}_1',$$

where  $\mathbf{T}$  is orthogonal,  $\mathbf{T}_1$  has  $k$  column eigenvectors corresponding to eigenvalues 1 ( $\mathbf{A} \mathbf{T}_1 = \mathbf{T}_1$ ), and  $\mathbf{T}_2$  consists of  $p - k$  column eigenvectors corresponding to eigenvalues 0 ( $\mathbf{A} \mathbf{T}_2 = \mathbf{O}$ ). Then

$$\mathbf{z}' \mathbf{A} \mathbf{z} = (\mathbf{T}_1' \mathbf{z})' \mathbf{T}_1' \mathbf{z} \sim \chi_k^2(\|\mathbf{T}_1' (\mathbf{m} - \mathbf{a})\|^2) \sim \chi_k^2((\mathbf{m} - \mathbf{a})' \mathbf{A} (\mathbf{m} - \mathbf{a}))$$

since  $\mathbf{T}_1' \mathbf{z} \sim N_k(\mathbf{T}_1' (\mathbf{m} - \mathbf{a}), \mathbf{I}_k)$  and  $\|\mathbf{T}_1' (\mathbf{m} - \mathbf{a})\|^2 = (\mathbf{m} - \mathbf{a})' \mathbf{A} (\mathbf{m} - \mathbf{a})$ .

- **Important!** In general, what if  $y \sim N_p(\mu, \Sigma)$ ? We can write

$$Q = y' A y = y' \Sigma^{-1/2} T (T' \Sigma^{1/2} A \Sigma^{1/2} T) T' \Sigma^{-1/2} y,$$

where  $T$  is orthogonal such that  $T'(\Sigma^{1/2} A \Sigma^{1/2})T = D = (\lambda_1, \dots, \lambda_p)$  by spectral decomposition of  $\Sigma^{1/2} A \Sigma^{1/2}$ . Note that  $\text{rank}(D) = \text{rank}(\Sigma^{1/2} A \Sigma^{1/2}) = \text{rank}(A)$ . Further let  $z = T' \Sigma^{-1/2} y \sim N_p(T' \Sigma^{-1/2} \mu, \mathbf{I}_p)$ , so that

$$Q = z' D z = \sum_{i=1}^p \lambda_i z_i^2, \quad \text{where} \quad z_i \sim N(t_i' \Sigma^{-1/2} \mu, 1) \Rightarrow z_i^2 \sim \chi_1^2((t_i' \Sigma^{-1/2} \mu)^2 = \mu').$$

Hence,  $Q = y' A y$  is a weighted linear combination of independent noncentral  $\chi^2$  r.v.s with one degree of freedom and noncentrality parameters  $\theta_i = (t_i' \Sigma^{-1/2} \mu)^2$ .

The weights are non-zero eigenvalues of  $\Sigma^{1/2} A \Sigma^{1/2}$ , or equivalently, eigenvalues of  $A \Sigma$  or  $\Sigma A$  because

$$|\Sigma^{1/2} A \Sigma^{1/2} - \lambda I_p| = |\Sigma^{1/2} \|A \Sigma - \lambda I_p\| \Sigma^{-1/2}| = |A \Sigma - \lambda I_p| = |\Sigma A - \lambda I_p|.$$

- Ex.1: Special case: When  $A = \Sigma^{-1}$ , then  $\Sigma^{1/2} A \Sigma^{1/2} = I_p$ , so that  $D = I_p$  and  $Q = z' z \sim \chi_p^2(\theta)$ , where

$$\theta = \mu' \Sigma^{-1/2} \left( \sum_{i=1}^p t_i t_i' \right) \Sigma^{-1/2} \mu = \mu' \Sigma^{-1} \mu.$$

- Ex.2: Common case: When  $\Sigma = I_p$  and  $A$  is idempotent with  $\text{rank}(A) = r \leq p$ , then

$$Q = \sum_{i=1}^r z_i^2 \sim \chi_r^2(\theta), \quad \text{where} \quad z_i^2 \sim \chi_1^2(\theta_i = \mu' t_i t_i' \mu)$$

with the noncentral parameter

$$\theta = \sum_{i=1}^p \theta_i = \sum_{i=1}^r \mu' t_i t_i' \mu = \mu' \left( \sum_{i=1}^r t_i t_i' \right) \mu = \mu' A \mu.$$

- Ex.3: When  $\Sigma^{1/2} A \Sigma^{1/2}$  is idempotent, or equivalently  $A \Sigma$  is idempotent, in other word,  $A \Sigma A = A$  with  $\text{rank}(A \Sigma) = r \leq p$ , then  $D = I_r$  so that

$$Q = \sum_{i=1}^r z_i^2 \sim \chi_r^2(\theta), \quad \text{where} \quad z_i^2 \sim \chi_1^2(\theta_i = \mu' \Sigma^{-1/2} t_i t_i' \Sigma^{-1/2} \mu)$$

with the noncentral parameter

$$\theta = \sum_{i=1}^p \theta_i = \sum_{i=1}^r \mu' \Sigma^{-1/2} t_i t_i' \Sigma^{-1/2} \mu = \mu' \Sigma^{-1/2} \left( \sum_{i=1}^r t_i t_i' \right) \Sigma^{-1/2} \mu = \mu' A \mu.$$

## 22 Non-central chi-square distribution

- Define: Let  $X_i \stackrel{\text{ind}}{\sim} N(\mu_i, 1)$ ,  $i = 1, \dots, n$  and  $\mu = (\mu_1, \dots, \mu_n)'$ , then  $Y = \sum_{i=1}^n X_i^2$  is said to have a noncentral  $\chi^2$  distribution with  $n$  degrees of freedom and non-centrality parameter  $\delta = \sum_{i=1}^n \mu_i^2 = \|\mu\|^2$ , or  $Y \sim \chi_n^2(\|\mu\|^2)$ . Why does the distribution of  $Y$  depend only on  $n$  and  $\|\mu\|^2$ .
- This  $Y$  can be expressed as the sum of a noncentral  $\chi^2$  with 1 df and a central  $\chi^2$  with  $n - 1$  dfs.

*Proof:* Let  $a_1 = \mu / \|\mu\|$  so that  $a_1' a_1 = (\mu' \mu) / \|\mu\|^2 = 1$ . Construct  $A$  with linearly independent rows:

$$A = \begin{pmatrix} a_1' \\ a_2' \\ \vdots \\ a_n' \end{pmatrix} \quad \text{s.t.} \quad A' A = A A' = I_n \quad (a_i' a_j = \delta_{ij}).$$

Then we have

$$W = AX \sim N_n \left( \begin{pmatrix} \|\mu\| \\ \mathbf{0} \end{pmatrix}, I_n \right)$$

as  $a_1' \mu = \|\mu\|$ ,  $a_i' \mu = a_i' (a_1 \|\mu\|) = 0$ ,  $i = 2, \dots, n$ , and  $\text{Cov}(W) = A \text{Cov}(X) A' = A A' = I_n$ . Hence,

$$Y = \sum_{i=1}^n X_i^2 = X' X = X' A' A X = W' W = W_1^2 + \sum_{i=2}^n W_i^2,$$

where  $W_1 \sim N(\|\mu\|, 1) \Rightarrow W_1^2 \sim \chi_1^2(\|\mu\|^2)$  and  $W_i \sim N(0, 1)$ ,  $i > 1 \Rightarrow \sum_{i=2}^n W_i^2 \sim \chi_{n-1}^2(0)$ .

- Let  $\delta = \|\mu\|^2$ , then the mean of  $Y$  is

$$E(Y) = E(W_1^2) + E \left( \sum_{i=2}^n W_i^2 \right) = E((W_1 - \delta)^2 + \delta) + n - 1 = \text{Var}(W_1) + \delta + n - 1 = n + \delta,$$

while the variance of  $Y$ ,  $2n + 4\delta$ , would be hard to obtain from this property.

- The pdf of  $Y$  is given by

$$f_Y(y; n, \delta) = \sum_{i=0}^{\infty} \frac{e^{-\delta/2} (\delta/2)^i}{i!} f_{X_{n+2i}}(y), \quad X_{n+2i} \sim \chi_{n+2i}^2(0),$$

which is a Poisson-weighted mixture of *central* chi-square distributions (See 250A HW).

- (HW8 in 250B). Equivalently, we say that, if  $V \mid K \sim \chi_{p+2k}^2(0)$  and  $K \sim \text{Pois}(\alpha'\alpha/2)$ , then  $V \sim \chi_p^2(\alpha'\alpha)$ . In addition, if  $U \sim N_p(\alpha, I_p)$ , then since  $U'U \sim \chi_p^2(\alpha'\alpha)$

$$E\left(\frac{1}{U'U}\right) = E\left[E\left(\frac{1}{U'U} \mid K\right)\right] = E\left(\frac{1}{p+2K-2}\right).$$

- The MGF is given by

$$M_Y(t) = \exp\left(\frac{\delta t}{1-2t}\right) \frac{1}{(1-2t)^{n/2}}, \quad t < \frac{1}{2}.$$

Using  $\psi(t) = \log M_Y(t) = \delta t/(1-2t) - (n/2) \log(1-2t)$ , the mean and variance are

$$E(Y) = \psi'(0) = \frac{\delta}{(1-2t)^2} + \frac{n}{1-2t} \Big|_{t=0} = n + \delta,$$

$$\text{Var}(Y) = \psi''(0) = \frac{4\delta}{(1-2t)^3} + \frac{2n}{(1-2t)^2} \Big|_{t=0} = 2n + 4\delta.$$

## 23 Non-central T distribution

- Suppose  $X \sim N(\theta, 1)$ ,  $V \sim \chi_\nu^2(0)$ , and  $X \perp\!\!\!\perp V$ , then  $T = X/\sqrt{V/\nu}$  has a noncentral  $t$  distribution with noncentrality parameter  $\theta$ ,  $T \sim t_\nu(\theta)$ . The pdf of  $T$  is complicated. Mgf pf  $T$  does not exist.
- Using the above expression, the mean of  $T$  is

$$E(T) = E(X)\sqrt{\nu}E(V^{-1/2}) = \theta \sqrt{\frac{\nu}{2}} \frac{\Gamma((\nu-1)/2)}{\Gamma(\nu/2)}, \quad \nu > 1;$$

otherwise, it does not exist.

- Example 1: Let  $X_i \sim N(\mu, \sigma^2)$  and  $S^2 = \sum_{i=1}^n (x_i - \bar{x})^2 / (n-1)$ . What is the dist. of  $\sqrt{n}(\bar{X} - a)/S$ ?

$$\frac{\sqrt{n}(\bar{X} - a)}{\sigma} \sim N\left(\frac{\sqrt{n}(\mu - a)}{\sigma}, 1\right), \quad \frac{(n-1)S^2}{\sigma^2} \sim \chi_{n-1}^2(0).$$

It follows that

$$T = \frac{\sqrt{n}(\bar{X} - a)/\sigma}{\sqrt{(n-1)S^2/(\sigma^2(n-1))}} = \frac{\sqrt{n}(\bar{X} - a)}{S} \sim t_{n-1}\left(\theta = \frac{\sqrt{n}(\mu - a)}{\sigma}\right).$$

- Example 2: Let  $Y_i \stackrel{iid}{\sim} N(\mu, \sigma^2)$ ,  $i = 1, 2, 3, 4$ . Find  $k$  such that

$$T = k \frac{(\bar{Y} - \mu_0)}{\sqrt{(y_1 - y_2)^2 + (y_1 + y_2 - 2y_3)^2/3 + (y_1 + y_2 + y_3 - 3y_4)^2/6}}$$

has a noncentral density. Note that  $n = 4$ . Since  $\bar{Y} \sim N(\mu, \sigma^2/4)$

$$X = \frac{2(\bar{Y} - \mu_0)}{\sigma} \sim N\left(\theta = \frac{2(\mu - \mu_0)}{\sigma}, 1\right).$$

Want to have the quadratic form for the denominator. Suppose

$$A = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 1/\sqrt{3} & 1/\sqrt{3} & -2/\sqrt{3} & 0 \\ 1/\sqrt{6} & 1/\sqrt{6} & 1/\sqrt{6} & -3/\sqrt{6} \end{pmatrix} \in \mathbb{R}^{3 \times 4}$$

Then

$$W = Ay = \begin{bmatrix} y_1 - y_2 \\ (y_1 + y_2 - 2y_3)/\sqrt{3} \\ (y_1 + y_2 + y_3 - 3y_4)/\sqrt{6} \end{bmatrix} \sim N_3(A\mu = 0, \sigma^2 AA' = 2\sigma^2 I_3),$$

so that we have  $W'W/(2\sigma^2) \sim \chi_3^2(0)$ . Therefore,

$$T = \frac{X}{\sqrt{W'W/(2\sigma^2 \times 3)}} = \frac{2\sqrt{6}(\bar{Y} - \mu_0)}{\sqrt{W'W}} \sim t_3(\theta) \Rightarrow k = 2\sqrt{6}.$$

- Let  $(X_i, Y_i)$ ,  $i = 1, \dots, n$  be a random sample from the bivariate normal distribution with parameters  $m_1, m_2, v_1^2, v_2^2$ , and correlation  $r$ . If  $d$  is a fixed constant, find a constant  $k$  so that

$$T = \frac{k(\bar{X} - \bar{Y} - d)}{\sqrt{\sum_{i=1}^n (X_i - Y_i - \bar{X} + \bar{Y})^2}}.$$

*Proof:* Let  $Z_i = X_i - Y_i$ ,  $\bar{Z} = \bar{X} - \bar{Y}$  and  $\mathbf{A} = (1 \ -1)$ . Then

$$Z_i = \mathbf{A} \begin{pmatrix} X_i \\ Y_i \end{pmatrix} \sim N(\mathbf{A}\mathbf{m} = m_1 - m_2, \mathbf{A}\Sigma\mathbf{A}' = \nu^2),$$

where  $\nu^2 = v_1^2 - 2rv_1v_2 + v_2^2$ . It follows that

$$W := \frac{\sqrt{n}(\bar{Z} - d)}{\nu} \sim N\left(\frac{\sqrt{n}(m_1 - m_2 - d)}{\nu}, 1\right), \quad V := \frac{\sum_{i=1}^n (Z_i - \bar{Z})^2}{\nu^2} \sim \chi_{n-1}^2(0)$$

Since  $\bar{Z} \perp \sum_{i=1}^n (Z_i - \bar{Z})^2$  and hence  $W \perp V$  even though  $r \neq 0$ . Thus,

$$\frac{W}{\sqrt{\frac{V}{n-1}}} = \frac{\sqrt{n}(\bar{Z} - d)/\nu}{\sqrt{\frac{\sum_{i=1}^n (Z_i - \bar{Z})^2/\nu^2}{n-1}}} = \frac{\sqrt{n(n-1)}(\bar{Z} - d)}{\{\sum_{i=1}^n (Z_i - \bar{Z})^2\}^{1/2}} \sim t_{n-1}\left(\frac{\sqrt{n}(m_1 - m_2 - d)}{\nu}\right),$$

which is equivalent to  $T$  if  $k = \sqrt{n(n-1)}$ .

## 24 Non-central F distribution

- Suppose  $X \sim \chi_n^2(\theta)$ ,  $Y \sim \chi_m^2(0)$ , and  $V \perp W$ , then  $F = (X/n)/(Y/m)$  has a noncentral  $F$  distribution with noncentrality parameter  $\theta$ ,  $F \sim F_{n,m}(\theta)$ . The pdf of  $F$  is complicated. Mgf of  $F$  does not exist.
- Using the above expression, the mean of  $T$  is

$$E(F) = \frac{m}{n} E(X) E(V^{-1}) = \frac{m}{n} \frac{n + \theta}{m - 2}, \quad m > 2;$$

otherwise, it does not exist. Also, the variance of  $F$  is

$$\begin{aligned} \text{Var}(F) &= \left(\frac{m}{n}\right)^2 \text{Var}\left(\frac{X}{Y}\right) = \left(\frac{m}{n}\right)^2 [E(X^2)E(Y^{-2}) - E(X)^2E(Y^{-1})^2] \\ &= \left(\frac{m}{n}\right)^2 \left[ \frac{2n + 4\theta + (n + \theta)^2}{(m-2)(m-4)} - \frac{(n + \theta)^2}{(m-2)^2} \right] \\ &= 2 \frac{(n + 2\theta)(m-2) + (n + \theta)^2}{(m-2)^2(m-4)} \left(\frac{m}{n}\right)^2, \quad m > 4. \end{aligned}$$

- (Final) Let  $x_1 = (1, 1, 1, 1, 1)'$  and  $x_2 = (1, 1, 0, 0, 0)'$ ,  $\theta = (6, 6, 2, 2, 2)'$ , and  $Y \sim N_5(\theta, I_5)$ . Let  $V = \mathcal{L}(x_1, x_2)$  and let  $\hat{Y}$  be the orthogonal projection of  $Y$  onto  $V$ . Find a constant  $K$  so that

$$F = \frac{K \|\hat{Y}\|^2}{\|Y - \hat{Y}\|^2}.$$

*Solution:* We have  $\|\hat{Y}\| = Y'PY \sim \chi_2^2(\theta'P\theta)$  and  $\|Y - \hat{Y}\|^2 = Y'QY \sim \chi_3^2(\theta'Q\theta)$ . Since  $P_V\theta = \theta$  (need to calculate),  $\theta'P\theta = \|\theta\|^2 = 84$  and  $\theta'Q\theta = 0$ . Hence,  $F \sim F_{2,3}(84)$  with  $K = 1.5$ .

## 25 Independence theorem and lemma

- Let  $y_p \sim N_p(0, I_p)$ ,  $u = Ay$  and  $v = By$ . If  $\text{Cov}(u, v) = AB' = O$ , then  $u \perp v$  and  $u'u \perp v'v$ .
- Further let

$$A = \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} \in \mathbb{R}^{k \times p}, \quad B = \begin{pmatrix} B_1 \\ B_2 \end{pmatrix} \in \mathbb{R}^{l \times p}$$

and  $A_1 \in \mathbb{R}^{k_1 \times p}$  and  $B_1 \in \mathbb{R}^{l_1 \times p}$  have linearly independent rows. Then

$$C = \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \in \mathbb{R}^{(k_1+l_1) \times p}$$

is of full row rank since

$$C'x = (A_1' \mid B_1') \begin{pmatrix} x_{k_1} \\ x_{l_1} \end{pmatrix} = 0 \quad \Rightarrow \quad A_1'x_{k_1} = B_1'x_{l_1} = 0 \quad \Rightarrow \quad x = 0.$$

Let  $u_1 = A_1y$  and  $v_1 = B_1y$ , then  $u \perp v \Rightarrow u_1 \perp v_1$  since

$$u = Ay = \begin{pmatrix} A_1y \\ A_2y \end{pmatrix} = \begin{pmatrix} A_1y \\ HA_1y \end{pmatrix} = \begin{pmatrix} I_{k_1} \\ H_1 \end{pmatrix} u_1, \quad v = \begin{pmatrix} I_{l_1} \\ H_2 \end{pmatrix} v_1.$$

- **Craig's theorem:** If  $y \sim N_p(0, \Sigma)$  and  $Q_i = y'A_iy$ . Then  $Q_i \perp Q_j \Leftrightarrow A_i\Sigma A_j = O$ .  
*Proof:*  $\Leftarrow$  is derived from joint mgf of  $Q_i$  and  $Q_j$ , i.e.,  $E(e^{t_1Q_1+t_2Q_2})$ . The other direction is difficult.
  - This also holds in the general case:  $y \sim N_p(m, \Sigma)$  (see HW5).
  - Especially, if  $\Sigma = I$ , then  $Q_i \perp Q_j \Leftrightarrow A_iA_j = O$ .

- **Loynes' lemma.** If  $M^2 = M = M'$ ,  $P = P' \succeq O$ , and  $I - M - P \succeq O$ , then  $MP = PM = O$ .

*Proof:* Let  $x \in \mathbb{R}^n$  and  $y = Mx$  then  $y'y = y'Mx = y'MMx = y'My$ . By assumption,

$$0 \leq y'(I - M - P)y = -y'Py \leq 0 \quad \because P \succeq O.$$

Hence,  $y'Py = 0 \Rightarrow \|Py\| = 0 \Rightarrow Py = PMx = 0$  for  $\forall x \Rightarrow PM = O$  and  $(PM)' = MP = O$ .

- **Marsaglia-Garaybill's Lemma.** If  $D_1, D_2, \dots, D_q$  are symmetric  $n \times n$  matrices, then **any of two** of the following statements imply the third:

- $D_1, D_2, \dots, D_q$  are idempotent;
- $D_iD_j = O$ ,  $\forall i \neq j$ .
- $D = D_1 + D_2 + \dots + D_q$  is idempotent;

*Proof:*

$$- (i) + (ii) \rightarrow (iii): D^2 = (\sum_{i=1}^q D_i)^2 = \sum_{i=1}^q D_i^2 + \sum_{i \neq j} D_iD_j = \sum_{i=1}^q D_i = D.$$

– (i) + (iii)  $\rightarrow$  (ii): Consider

$$\mathbf{I} - \mathbf{D}_i - \mathbf{D}_j = (\mathbf{I} - \mathbf{D}) + (\mathbf{D} - \mathbf{D}_i - \mathbf{D}_j).$$

$\mathbf{I} - \mathbf{D} \succeq \mathbf{O}$  by (iii) and  $\mathbf{D} - \mathbf{D}_i - \mathbf{D}_j = \sum_{k \neq i, j} \mathbf{D}_k \succeq \mathbf{O}$  by (i), so that  $\mathbf{I} - \mathbf{D}_i - \mathbf{D}_j \succeq \mathbf{O} \Rightarrow \mathbf{D}_i \mathbf{D}_j = \mathbf{O}$  by Loynes' lemma.

– (ii) + (iii)  $\rightarrow$  (i): Let  $\mathbf{D}_i \mathbf{x} = \lambda_i \mathbf{x}$  for  $\mathbf{x} \neq \mathbf{0}$ . If  $\lambda \neq 0$ , then, by (ii),

$$\mathbf{D} \mathbf{x} = \frac{\mathbf{D} \mathbf{D}_i \mathbf{x}}{\lambda_i} = \frac{\mathbf{D}_i^2 \mathbf{x}}{\lambda_i} = \mathbf{D}_i \mathbf{x},$$

which implies that  $\mathbf{D}_i$  has the same nonzero eigenvalues of  $\mathbf{D}$ . By (iii),  $\lambda_i = 1$ .

- **Cochran's theorem.** Let  $\mathbf{y} \sim N_p(\mathbf{0}, \mathbf{I}_p)$  and  $\mathbf{y}'\mathbf{y} = \sum_{i=1}^k Q_i = \sum_{i=1}^k \mathbf{y}'\mathbf{A}_i\mathbf{y}$ , where  $\text{rank}(\mathbf{A}_i) = r_i$ ,  $i = 1, \dots, k$ . Then the following statements are equivalent:

- (i)  $Q_i \perp Q_j$  for  $1 \leq i \neq j \leq k$ ;
- (ii)  $Q_i \sim \chi_{r_i}^2(0)$ ,  $i = 1, \dots, k$ ;
- (iii)  $\sum_{i=1}^k r_i = p$ .

*Proof:*

– (i)  $\rightarrow$  (ii):  $Q_i \perp Q_j \Rightarrow \mathbf{A}_i \mathbf{A}_j = \mathbf{O}$  by Craig, and  $\mathbf{I} = \sum_{i=1}^k \mathbf{A}_i$  is idempotent. By **MG lemma**,  $\mathbf{A}_i$  is idempotent, so that  $Q_i \sim \chi_{r_i}^2(0)$ .

(Another solution)  $Q_i \perp Q_j \Rightarrow Q_1 \perp Q_2 + \dots + Q_k \Rightarrow \mathbf{A}_1(\mathbf{A}_2 + \dots + \mathbf{A}_k) = \mathbf{O}$  by Craig  $\Rightarrow \mathbf{A}_1(\mathbf{I} - \mathbf{A}_1) = \mathbf{O} \Rightarrow \mathbf{A}_1$  is idempotent.

– (ii)  $\rightarrow$  (iii): Since  $\mathbf{I} = \sum_{i=1}^k \mathbf{A}_i$ , and  $\mathbf{A}_i$  is idempotent,

$$\sum_{i=1}^k r_i = \sum_{i=1}^k \text{tr}(\mathbf{A}_i) = \text{tr} \left( \sum_{i=1}^k \mathbf{A}_i \right) = \text{tr}(\mathbf{I}_p) = p.$$

– (iii)  $\rightarrow$  (i): Let  $\alpha_1, \dots, \alpha_{r_i}$  be eigenvalues of  $\mathbf{A}_i$  and  $\mathbf{T}$  be an orthogonal matrix such that  $\mathbf{T}'\mathbf{A}_i\mathbf{T} = \text{diag}(\alpha_1, \dots, \alpha_{r_i}, 0, \dots, 0)$  by the spectral decomposition. Then we can write

$$\mathbf{I} = \mathbf{T}'\mathbf{T} = \mathbf{T}'\mathbf{A}_i\mathbf{T} + \mathbf{T}'\mathbf{A}_{(-i)}\mathbf{T},$$

where  $\mathbf{A}_{(-i)} = \sum_{j \neq i}^k \mathbf{A}_j$ , meaning that  $\mathbf{T}'\mathbf{A}_{(-i)}\mathbf{T}$  also has to be orthogonal. Suppose  $\mathbf{T}'\mathbf{A}_{(-i)}\mathbf{T} = \text{diag}(\beta_1, \dots, \beta_p)$ . Then

$$\mathbf{I} = \text{diag}(\alpha_1 + \beta_1, \dots, \alpha_{r_i} + \beta_{r_i}, \beta_{r_i+1}, \dots, \beta_p)$$

yields  $\beta_{r_i+1} = \dots = \beta_p = 1$ . Hence,  $\text{rank}(\mathbf{T}'\mathbf{A}_{(-i)}\mathbf{T}) \geq p - r_i$ . **However,**

$$\text{rank}(\mathbf{T}'\mathbf{A}_{(-i)}\mathbf{T}) = \text{rank}(\mathbf{A}_{(-i)}) = \text{rank} \left( \sum_{j \neq i}^k \mathbf{A}_j \right) \leq \sum_{j \neq i}^k \text{rank}(\mathbf{A}_j) = p - r_i.$$

leading to  $\text{rank}(\mathbf{T}'\mathbf{A}_{(-i)}\mathbf{T}) = p - r_i \Rightarrow \beta_1 = \dots = \beta_{r_i} = 0 \Rightarrow \alpha_1 = \dots = \alpha_{r_i} = 1 \Rightarrow \mathbf{A}_i$  is (symmetric and) idempotent for  $i = 1, \dots, k$ . This result and the fact that  $\mathbf{I} = \sum_{i=1}^k \mathbf{A}_i$  is idempotent follow  $\mathbf{A}_i \mathbf{A}_j = \mathbf{O}$  by **MG lemma** and hence  $Q_i \perp Q_j$  by Craig's theorem if  $\Sigma = \mathbf{I}$ .

## 26 Orthogonal Projection

- Let  $\Omega \subseteq V = \mathbb{R}^n$ . Any  $y \in V$  can be written *uniquely* as  $y = u + v$ , where  $u \in \Omega$ ,  $v \in \Omega^\perp$ .

*Proof:* Suppose  $\dim(\Omega) = r$ . Let  $\{x_1, \dots, x_r\}$  be an **orthogonal basis** for  $\Omega$ . **Expand this to an orthogonal basis for  $V$  by adding  $\{x_{r+1}, \dots, x_k\}$ .** Then  $y \in V$  is expressed as

$$y = \sum_{i=1}^r \alpha_i x_i + \sum_{i=r+1}^k \alpha_i x_i = u + v.$$

If there are  $u_1, u_2, v_1, v_2$  such that  $u_i \in \Omega$  and  $v_i \in \Omega^\perp$ ,  $i = 1, 2$ . Then we have  $u_1 + v_1 = u_2 + v_2 \Rightarrow u_1 - u_2 = v_2 - v_1 \in \Omega \cap \Omega^\perp = \{0\} \Rightarrow u_1 = u_2$  and  $v_1 = v_2$ , which shows the uniqueness.

- Orthogonal projection of  $y$  on  $\Omega$  is  $u$ , and then  $y - u \in \Omega^\perp$  (residual).  $P_\Omega$  such that  $P_\Omega y = u \in \Omega$  is called the orthogonal projection matrix (orthogonal projector) of  $y$  on  $\Omega$ .
  - Let  $\mathbf{P}_\Omega \mathbf{y} = \mathbf{u} \in \Omega$ , then  $\mathbf{y} - \mathbf{u} = (\mathbf{I} - \mathbf{P}_\Omega) \mathbf{y} = \mathbf{v} \in \Omega^\perp$
  - **Claim:**  $P_\Omega$  is unique. *Proof:* If there are two such matrices  $P_\Omega$  and  $\widetilde{P}_\Omega$ , then  $P_\Omega y = u = \widetilde{P}_\Omega y \Rightarrow (P_\Omega - \widetilde{P}_\Omega)y = 0$  for  $\forall y \in \mathbb{R}^n \Rightarrow \widetilde{P}_\Omega = P_\Omega$ .
- How to find  $P_\Omega$ : Again, let  $\dim(\Omega) = r$  and  $\{x_1, \dots, x_r, x_{r+1}, \dots, x_k\}$  be an orthogonal basis for  $V = \mathbb{R}^n$ . WLOG, assume that  $\{x_1, \dots, x_r\}$  is an orthogonal basis for  $\Omega$ . Then, if  $y \in V$ , we can write

$$y = \sum_{i=1}^r \alpha_i x_i + \sum_{i=r+1}^k \alpha_i x_i = u + v, \quad u \in \Omega, \quad v \in \Omega^\perp.$$

If  $\ell = 1, \dots, r$ , then  $(x_\ell, y) = x'_\ell y = \alpha_\ell$ . Hence, the orthogonal projection  $u$  is given by

$$u = \sum_{i=1}^r \alpha_i x_i = \sum_{i=1}^r (x'_i y) x_i = (x_1, \dots, x_r) \begin{pmatrix} x'_1 y \\ \vdots \\ x'_r y \end{pmatrix} = TT' y = P_\Omega y.$$

Note that  $T$  has orthogonal columns but is not an orthogonal matrix as  $T$  is not symmetric.

- **Very importantly** (again), we can write  $P = TT'$ , where  $T$  has **orthogonal columns** (not symmetric), i.e.,  $T'T = I_r$ .  $T$  is *not* unique as there are an infinite number of orthogonal basis; but,  $P$  is unique.
- From above,  $P$  is the orthogonal projection matrix if and only if  $P$  is **symmetric and idempotent**.
 

*Proof:* ( $\Rightarrow$ ) If  $P = TT'$ , then  $P$  is obviously symmetric and idempotent. ( $\Leftarrow$ ) If  $P$  is symmetric and idempotent,  $P = U\Lambda U' = U_1 U_1'$ , where  $U = (U_1 \mid U_2)$  and  $U_1$  has  $r$  orthogonal columns.
- Hence, we can write  $y = P_\Omega y + (I_p - P_\Omega)y = u + v$ , where  $u \in \Omega$  and  $v \in \Omega^\perp$ .
- $\mathbf{P}_\Omega = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'$  is the orthogonal projector onto  $\Omega = C(\mathbf{X})$ :

- Symmetric:  $(\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}')' = \mathbf{X}[(\mathbf{X}'\mathbf{X})^{-}]'\mathbf{X}' = \mathbf{X}[(\mathbf{X}'\mathbf{X})^{-}]\mathbf{X}' = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'$  since  $\mathbf{A}\mathbf{A}^{-}\mathbf{A} = \mathbf{A} \Rightarrow \mathbf{A}'(\mathbf{A}^{-})'\mathbf{A}' = \mathbf{A}' = \mathbf{A}'(\mathbf{A}')^{-}\mathbf{A}' \Rightarrow (\mathbf{A}^{-})' = (\mathbf{A}')^{-}$  if  $\mathbf{A}$  is symmetric.
- Idempotent: We want to show  $\mathbf{P}_\Omega^2 = \mathbf{P}_\Omega$  or  $(\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}')(\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}') = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'$ , but we **cannot use the second property of the Moore-Penrose inverse**.

*Proof:* By the property of a g-inverse:  $\mathbf{A}\mathbf{A}^{-}\mathbf{A} = \mathbf{A}$ ,

$$\begin{aligned} \mathbf{X}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{X} &= \mathbf{X}'\mathbf{X} \Rightarrow (\mathbf{X}^+)' \mathbf{X}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{X} = (\mathbf{X}^+)' \mathbf{X}'\mathbf{X} \\ &\Rightarrow (\mathbf{X}\mathbf{X}^+)' \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{X} = (\mathbf{X}\mathbf{X}^+)' \mathbf{X} \\ &\Rightarrow \mathbf{X}\mathbf{X}^+ \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{X} = \mathbf{X}\mathbf{X}^+ \mathbf{X} \\ &\Rightarrow \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{X} = \mathbf{X} \\ &\Rightarrow \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}' = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}' \\ &\Rightarrow \mathbf{P}_\Omega^2 = \mathbf{P}_\Omega. \end{aligned}$$

- If  $\omega$  is a subspace of  $\Omega$  (i.e.,  $\omega \subseteq \Omega$ ),  $P_\omega P_\Omega = P_\Omega P_\omega = P_\omega$ . *Proof:* Let  $y \in V$ , then  $P_\omega y \in \omega \subseteq \Omega$ . Then  $P_\Omega(P_\omega y) = P_\omega y \Rightarrow (P_\Omega P_\omega - P_\omega)y = 0, \forall y$ , so  $P_\Omega P_\omega = P_\omega$ . Take transpose to get  $P_\omega P_\Omega = P_\omega$ .
- Consider  $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon} \in \mathbb{R}^n$ , where  $\mathbf{X}$  is not full rank and  $E(\boldsymbol{\epsilon}) = \mathbf{0}$  and  $\text{Cov}(\boldsymbol{\epsilon}) = \sigma^2 \mathbf{I}_n$ . Then solving normal equations yields fitted vector  $\hat{\boldsymbol{\theta}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{y} = \mathbf{P}_\Omega \mathbf{y}$ , which is always UNIQUE even though  $\mathbf{X}$  is *not* full column rank, in other words,  $(\mathbf{X}'\mathbf{X})^{-}$  and  $\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{y}$  are *not* unique.

*Proof* (again): Set  $\mathbf{P}_\Omega$  and  $\tilde{\mathbf{P}}_\Omega$ , where  $\mathbf{P}_\Omega \mathbf{y} = \mathbf{u} = \tilde{\mathbf{P}}_\Omega \mathbf{y} \Rightarrow (\mathbf{P}_\Omega - \tilde{\mathbf{P}}_\Omega)\mathbf{y} = \mathbf{0}$  for  $\forall \mathbf{y} \Rightarrow \mathbf{P}_\Omega = \tilde{\mathbf{P}}_\Omega$ .

## 27 Gauss Markov's theorem

- Consider  $E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta} = \boldsymbol{\theta} \in C(\mathbf{X})$ , where  $\mathbf{X}$  has full column rank and  $\boldsymbol{\epsilon} \sim N_n(\mathbf{0}, \sigma^2 \mathbf{I}_n)$ . If  $\hat{\boldsymbol{\beta}}$  is an ordinary least square (OLS) estimate of  $\boldsymbol{\beta}$ , i.e.,  $\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$ , then  $\hat{\boldsymbol{\theta}} = \mathbf{X}\hat{\boldsymbol{\beta}}$  has the property that  $\mathbf{c}'\mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{c}'\hat{\boldsymbol{\theta}}$  is the best linear unbiased estimator (BLUE) of  $\mathbf{c}'\mathbf{X}\boldsymbol{\beta} = \mathbf{c}'\boldsymbol{\theta}$ ,  $\forall \mathbf{c}$ .

*Proof:* Suppose  $a'y$  (linear combination of  $y = (y_1, \dots, y_n)'$ ) is a linear unbiased estimator of  $c'\boldsymbol{\theta}$ , i.e.,  $E(a'y) = c'\boldsymbol{\theta}$ . Since  $E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta} = \boldsymbol{\theta}$ ,  $a'\mathbf{X}\boldsymbol{\beta} = c'\boldsymbol{\theta}$ ,  $\forall \boldsymbol{\beta} \Rightarrow a'\mathbf{X} = c'\mathbf{X}$ . Also,

$$\text{Var}(a'y) = \sigma^2 a'a, \quad \text{Var}(c'\hat{\boldsymbol{\theta}}) = \sigma^2 c' \text{Var}(\mathbf{X}\hat{\boldsymbol{\beta}})c = \sigma^2 c'(\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}')c = \sigma^2 a'P_{C(\mathbf{X})}a,$$

so that  $\text{Var}(a'y) - \text{Var}(c'\hat{\boldsymbol{\theta}}) = \sigma^2 a'(I_n - P_X)a \succeq 0 \Rightarrow \text{Var}(a'y) \succeq \text{Var}(c'\hat{\boldsymbol{\theta}})$ , which is minimum variance.

- Similarly,  $c'\hat{\boldsymbol{\theta}}$  is BLUE for  $c'\boldsymbol{\beta}$ : Suppose  $a'y$  is a linear unbiased estimator of  $c'\boldsymbol{\beta}$ , then  $a'\mathbf{X}\boldsymbol{\beta} = c'\boldsymbol{\beta}$ ,  $\forall \boldsymbol{\beta} \Rightarrow a'\mathbf{X} = c'$ . Then  $\text{Var}(a'y) - \text{Var}(c'\hat{\boldsymbol{\theta}}) = \sigma^2 a'a - \sigma^2 c'(\mathbf{X}'\mathbf{X})^{-1}c = \sigma^2 a'(I_n - P_X)a \succeq 0$ .

## 28 Estimability

- Consider  $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon} \in \mathbb{R}^n$ , where  $\text{rank}(\mathbf{X}) = r < p$  (**not full rank**) and  $\text{Cov}(\boldsymbol{\epsilon}) = \sigma^2 \mathbf{I}_n$  and  $\boldsymbol{\beta} : p \times 1$ .
- In a less-than-full-rank model,  $\hat{\boldsymbol{\beta}}$  is not unique so that  $\boldsymbol{\beta}$  is **not estimable**, that is, there is *no* linear unbiased estimate for  $\boldsymbol{\beta}$ . Proof can be done by contradiction.

*Proof:* If there is a linear unbiased estimator for  $\boldsymbol{\beta}$ , we have  $E(a'_i y) = \beta_i$ ,  $i = 1, \dots, p$ . Setting  $A' = (a'_1, \dots, a'_p)$  leads to  $E(Ay) = \boldsymbol{\beta} \Rightarrow AX\boldsymbol{\beta} = \boldsymbol{\beta}$ ,  $\forall \boldsymbol{\beta} \Rightarrow AX = I_p$ . However,  $p = \text{rank}(I_p) = \text{rank}(AX) \leq \text{rank}(X) = r$ , which contradicts with  $r < p$ .

- However  $\hat{\boldsymbol{\theta}} = \hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}}$  is unique, so each element  $\theta_i$  of  $\boldsymbol{\theta} = \mathbf{X}\boldsymbol{\beta}$  can be estimated as  $\hat{\theta}_i = x'_i \hat{\boldsymbol{\beta}}$ .
- Definition: The parametric function  $a'\boldsymbol{\beta}$  is said to be estimable if it has a linear unbiased estimate,  $b'Y$ .
- By the discussion in Gauss Markov theorem, a  $a'\boldsymbol{\beta}$  is estimable if there exists a vector  $b$  such that  $E(b'Y) = a'\boldsymbol{\beta} \Rightarrow b'X\boldsymbol{\beta} = a'\boldsymbol{\beta}, \forall \boldsymbol{\beta} \Rightarrow X'b = a \in C(X')$  or  $a' = b'X$ .

- **Theorem:**  $a'\boldsymbol{\beta}$  is estimable if and only if  $a' = a'(X'X)^{-}X'X$ .

*Proof:* ( $\Leftarrow$ )  $a'(X'X)^{-}X'X = a' \Rightarrow a = X'X(X'X)^{-}a \in C(X')$ . ( $\Rightarrow$ ) If  $a'\boldsymbol{\beta}$  is estimable, then  $a' = b'X \Rightarrow a'(X'X)^{-}X'X = b'X(X'X)^{-}X'X = b'P_X X = b'X = a'$ .

- $a'\boldsymbol{\beta}$  is estimable  $\Leftrightarrow a \in C(X')$ :  $a'\boldsymbol{\beta} = E(b'Y) = b'X\boldsymbol{\beta}$ ,  $\forall \boldsymbol{\beta}$ , so that  $a' = b'X$  or  $a = X'b$ .
- By the above,  $\text{Var}[a'\boldsymbol{\beta}] = a' \text{Var}[(X'X)^{-}X'y]a = \sigma^2 a'[(X'X)^{-}X'X(X'X)^{-}]a = \sigma^2 a'(X'X)^{-}a$ .
- If  $a'\boldsymbol{\beta}$  is estimable,  $a'\hat{\boldsymbol{\beta}}$  is unique. *Proof*  $a' = b'X \Rightarrow a'\boldsymbol{\beta} = b'X\boldsymbol{\beta} = b'\boldsymbol{\theta}$ . Similarly,  $a'\hat{\boldsymbol{\beta}} = b'X\hat{\boldsymbol{\beta}} = b'\hat{\boldsymbol{\theta}}$ , **which is unique**. By theorem for BLUE,  $b'\hat{\boldsymbol{\theta}}$  is the BLUE of  $b'\boldsymbol{\theta}$ , so that  $a'\hat{\boldsymbol{\theta}}$  is the BLUE of  $a'\boldsymbol{\theta}$ .

- Since the GLS estimate is simply the OLS for a transformed model,  $a'\hat{\boldsymbol{\beta}}_W$  is the BLUE of  $a'\boldsymbol{\beta}$ . This implies that the OLS estimate  $a'\hat{\boldsymbol{\beta}}$  is not BLUE in a less-than-full-rank model, although this still be unbiased. That is  $E(a'\hat{\boldsymbol{\beta}}) = E(a'\hat{\boldsymbol{\beta}}_w) = a'\boldsymbol{\beta}$ , but  $\text{var}[b'Y] \geq \text{var}[a'\hat{\boldsymbol{\beta}}] \geq \text{var}[a'\hat{\boldsymbol{\beta}}_W]$ .



- $a'\widehat{\mathbb{E}}(\widehat{\beta})$  is an estimable function of  $\beta$ . *Proof:*  $a'\widehat{\mathbb{E}}(\widehat{\beta}) = a'\mathbb{E}[(X'X)^-X'Y] = a'(X'X)^-X'X\beta = c'\beta$ , where  $c = X'X(X'X)^-a \in C(X')$ .
  - If  $a'\widehat{\beta}$  is **invariant** with respect to  $\widehat{\beta}$ ,  $a'\beta$  is estimable. See HW.
  - Suppose that  $E(Y) = X\beta$  and  $\text{Var}(Y) = \sigma^2 I_n$ .  $a'Y$  is the linear unbiased estimate of  $E(a'Y)$  with minimum variance iff  $\text{cov}(a'Y, b'Y) = 0$  for all  $b$  such that  $E(b'Y) = 0$  (i.e.,  $b'X = 0'$ ).
- Proof:* Suppose  $c'Y = (a + b)'Y$ . Then  $E(c'Y) = \textcolor{red}{c}'X\beta = \textcolor{red}{a}'X\beta = E(a'Y)$  for  $\forall b$  s.t.  $E(b'Y) = 0$ .  $\text{var}(c'Y) = \text{var}(a'Y) + \text{var}(b'Y) + \text{cov}(a'Y, b'Y) \geq \text{var}(a'Y) + \text{var}(b'Y)$  with equality iff  $\text{cov}(a'Y, b'Y) = 0$ .
- **Example:** Consider a one-way ANOVA,  $y_{ij} = \mu + \tau_i + \epsilon_{ij}$ ,  $i = 1, \dots, a$  (No. of group),  $j = 1, \dots, n_i$  (No. of obs in the  $i$ th group). Let  $n = \sum_{i=1}^a n_i$ . Then the model can be written as

$$\mathbb{E}(y) = X\beta \in \mathbb{R}^n$$

$$\mathbb{E} \begin{pmatrix} y_{11} \\ \vdots \\ y_{1n_1} \\ \vdots \\ y_{a1} \\ \vdots \\ y_{an_a} \end{pmatrix} = \underbrace{\begin{pmatrix} 1_{n_1} & 1_{n_1} & 0 & \cdots & 0 \\ 1_{n_2} & 0 & 1_{n_2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 1_{n_a} & 0 & 0 & \cdots & 1_{n_a} \end{pmatrix}}_{n \times (a+1)} \underbrace{\begin{pmatrix} \mu \\ \tau_1 \\ \vdots \\ \tau_a \end{pmatrix}}_{(a+1) \times 1},$$

where  $X$  has less than full rank as  $\text{rank}(X) = a < (a+1)$ . Calculate  $(X'X)^-X'X$ :

$$X'X = \underbrace{\begin{pmatrix} n & n_1 & \cdots & n_a \\ n_1 & n_1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ n_a & 0 & \cdots & n_a \end{pmatrix}}_{(a+1) \times (a+1)} \Rightarrow \textcolor{red}{(X'X)^-} = \textcolor{red}{\begin{pmatrix} 0 & 0 & \cdots & 0 \\ 0 & n_1^{-1} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & n_a^{-1} \end{pmatrix}}.$$

Hence, the condition for  $c'\beta$  to be estimable is  $c' = c'(X'X)^-X'X$ :

$$\begin{aligned} (c_0, c_1, \dots, c_a) &= (c_0, c_1, \dots, c_a) \begin{pmatrix} 0 & 0 & \cdots & 0 \\ 0 & n_1^{-1} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & n_a^{-1} \end{pmatrix} \begin{pmatrix} n & n_1 & \cdots & n_a \\ n_1 & n_1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ n_a & 0 & \cdots & n_a \end{pmatrix} \\ &= \left( \sum_{i=1}^a c_i, c_1, \dots, c_a \right) \Rightarrow c_0 = \sum_{i=1}^a c_i. \end{aligned}$$

E.g.,  $(0, 1, -1, 0, \dots, 0)\beta = \tau_1 - \tau_2$  is estimable, but  $(1, -1, 0, 0, \dots, 0)\beta = \mu - \tau_1$  is *not* estimable.

## 29 Distribution theory

- Consider  $y = X\beta + \epsilon \sim N_n(X\beta, \sigma^2 I_n)$ , where  $X : n \times p$ ,  $\text{rank}(X) = p$ , and  $\beta : p \times 1$ .  $Q_X = I_n - P_X$ .
- $\widehat{\beta} \sim N_p(\beta, \sigma^2(X'X)^{-1})$ . So, the pdf is

$$f(\widehat{\beta} \mid \beta, \sigma^2) = (2\pi\sigma^2)^{-p/2} |(X'X)|^{-1/2} \exp \left[ -\frac{(\widehat{\beta} - \beta)' X'X (\widehat{\beta} - \beta)}{2\sigma^2} \right].$$

- $(\widehat{\beta} - \beta)' \textcolor{red}{X}'X (\widehat{\beta} - \beta) / \sigma^2 \sim \chi_p^2(0)$  by above.

- $\hat{\beta} \perp y - \hat{y}$  since  $\text{Cov}(\hat{\beta}, y - \hat{y}) = \text{Cov}((X'X)^{-1}X'y, Q_X y) = (X'X)^{-1}X'(\sigma^2 I_n)Q_X' = 0$ .
- $\hat{\beta} \perp S^2 = (y - \hat{y})'(y - \hat{y})/(n - p) = y'Q_X y/(n - p)$  by above.
- $\text{SSE}/\sigma^2 = (n - p)S^2/\sigma^2 = y'Q_X y/\sigma^2 \sim \chi_r^2(0)$ , where  $r = \text{rank}(Q_X) = n - p$ .

*Proof:*  $y'Q_X y = (y - X\beta)'Q_X(y - X\beta) = \epsilon'Q_X\epsilon$  and  $Q_X$  is symmetric and idempotent of rank  $n - p$ .

$$- E(\text{SSE}/\sigma^2) = n - p \Rightarrow E(\text{SSE}/(n - p)) = \sigma^2.$$

$$- \text{Another solution: } E(y'Q_X y) = \text{tr}(Q_X \sigma^2 I_n) + \mu Q_X \mu = \sigma^2(n - p).$$

- MLE of  $\beta$  coincides with the least square estimate for  $\beta$ :  $\hat{\beta} = (X'X)^{-1}X'y$ .
- MLE of  $\sigma^2$  is  $\hat{\sigma}_{\text{MLE}}^2 = \text{SSE}/n = \|y - X\hat{\beta}\|^2/n$ , which is biased, while  $\hat{\sigma}^2 = \text{SSE}/(n - p)$  is unbiased.
- The information matrix is given by

$$I = -E\left(\frac{\partial^2 \ell}{\partial \theta \partial \theta'}\right) = \text{Var}\left[\frac{\partial \ell}{\partial \theta}\right] = \begin{bmatrix} -E\left(\frac{\partial^2 \ell}{\partial \beta \partial \beta'}\right) & -E\left(\frac{\partial^2 \ell}{\partial \beta \partial \sigma^2}\right) \\ -E\left(\frac{\partial^2 \ell}{\partial \sigma^2 \partial \beta'}\right) & -E\left(\frac{\partial^2 \ell}{(\partial \sigma^2)^2}\right) \end{bmatrix} = \begin{pmatrix} \frac{X'X}{\sigma^2} & 0 \\ 0' & \frac{n}{2\sigma^4} \end{pmatrix},$$

which gives us the multivariate Cramer-Rao lower bound for unbiased estimates of  $(\beta, \sigma^2)$ , namely,

$$I^{-1} = \begin{pmatrix} \sigma^2(X'X)^{-1} & 0 \\ 0 & 2\sigma^4/n \end{pmatrix}.$$

Since  $\text{Var}(\hat{\beta}) = \sigma^2(X'X)^{-1}$ , which attains the lower bound,  $\hat{\beta}$  is said to be the minimum variance unbiased estimate (**MVUE**) of  $\beta$ .

- If columns in  $X$  are orthogonal each other, i.e.,  $X = (x_1, \dots, x_p)$  and  $x_i \perp x_j$ ,  $i \neq j$ . Then since  $X'X = \text{diag}(x_1'x_1, \dots, x_p'x_p)$ , the OLS estimate is given by

$$\hat{\beta} = (X'X)^{-1}X'Y = \begin{pmatrix} (x_1'x_1)^{-1} & & 0 \\ & \ddots & \\ 0 & & (x_p'x_p)^{-1} \end{pmatrix} \begin{pmatrix} x_1'Y \\ \vdots \\ x_p'Y \end{pmatrix} \Rightarrow \hat{\beta}_j = (x_j'x_j)^{-1}x_j'Y,$$

meaning that the OLS estimate of  $\beta_j$ ,  $\hat{\beta}_j$ , is unchanged if any of the other  $\beta_k$  ( $k \neq j$ ) equals zero. Also,

$$\text{SSE} = Y'Y - Y'P_X Y = Y'Y - \hat{\beta}'X'X\hat{\beta} = Y'Y - \sum_{j=1}^p \hat{\beta}_j^2 \|x_j\|^2,$$

which implies that if  $\beta_j = 0$ , the only change in the SSE is the *addition* of the term  $\hat{\beta}_j x_j'Y$  or  $\hat{\beta}_j \|x_j\|^2$ .

- Example: Suppose  $x_{ij}$  are standardized so that for  $j = 1, \dots, p$ , the sample mean is  $\sum_i x_{ij} = 0$  and the sample variance  $\sum_i x_{ij}^2 = c$ . We now show that  $(1/p) \sum_{j=1}^p \text{var}(\hat{\beta}_j)$  is minimized when the column of  $X$  are mutually orthogonal.

*Proof:* Since the first column of  $X$  is unity, we have

$$\begin{aligned} X'X &= \begin{pmatrix} n & 0' \\ 0 & C \end{pmatrix} \Rightarrow (X'X)^{-1} = \begin{pmatrix} n^{-1} & 0' \\ 0 & C^{-1} \end{pmatrix}. \\ \Rightarrow \sum_{j=1}^p \text{var}(\hat{\beta}_j) &= \text{tr}[\text{Var}(\hat{\beta})] = \sigma^2 \text{tr}[(X'X)^{-1}] = \sigma^2 [\text{tr}(C^{-1}) + n^{-1}] = \sigma^2 \sum_{j=1}^p \lambda_j^{-1}, \end{aligned}$$

where  $\lambda_1 = n$  and  $\lambda_j$  ( $j \geq 2$ ) are eigenvalues of  $C$ .  $\text{tr}(C) = c(p - 1) = \sum_j \lambda_j$  gives  $\lambda_j = c$ . So, there exists an orthogonal matrix  $T$  s.t.  $C = T\Lambda T' = cI_p$ , so that the column of  $X$  must be mutually orthogonal.

### 30 MLE for Multivariate Normal without vector/matrix derivative

- Suppose  $y_1, \dots, y_n$  be a random sample from  $N_p(\mu, V)$ .
- Let  $A = \sum_{i=1}^n (y_i - \bar{y})(y_i - \bar{y})' \succ O$ , then log-likelihood is

$$\begin{aligned}\ell(\mu, V) &= C - \frac{n}{2} \log |V| - \frac{1}{2} \sum_{i=1}^n (y_i - \mu)' V^{-1} (y_i - \mu) \\ &= C - \frac{n}{2} \log |V| - \frac{1}{2} \sum_{i=1}^n (y_i - \bar{y})' V^{-1} (y_i - \bar{y}) - \frac{1}{2} \sum_{i=1}^n (\bar{y} - \mu)' V^{-1} (\bar{y} - \mu) \\ &\leq C - \frac{n}{2} \log |V| - \frac{1}{2} \text{tr}(V^{-1} A)\end{aligned}$$

with equality (maximum) when  $\mu = \hat{\mu} = \bar{y}$ .

- Further let  $\lambda_1, \dots, \lambda_n$  be eigenvalues of  $A^{1/2} V^{-1} A^{1/2}$ ,

$$\begin{aligned}\ell(\hat{\mu}, V) &= C - \frac{n}{2} \log |V| - \frac{1}{2} \text{tr}(V^{-1} A) \\ &= C + \frac{n}{2} \log |V^{-1}| - \frac{1}{2} \text{tr}(V^{-1} A) + \frac{n}{2} \log |A| - \frac{n}{2} \log |A| \\ &= \tilde{C} - \frac{n}{2} \log |V^{-1} A| - \frac{1}{2} \text{tr}(V^{-1} A) \\ &= \tilde{C} - \frac{n}{2} \log |A^{1/2} V^{-1} A^{1/2}| - \frac{1}{2} \text{tr}(A^{1/2} V^{-1} A^{1/2}) \\ &= \tilde{C} - \frac{n}{2} \log \prod_{i=1}^n \lambda_i - \frac{1}{2} \sum_{i=1}^n \lambda_i \\ &= \tilde{C} - \frac{1}{2} \sum_{i=1}^n (n \log \lambda_i - \lambda_i).\end{aligned}$$

Hence  $\partial \ell / \partial \lambda_i = 0 \Rightarrow \hat{\lambda}_i = n \Rightarrow A^{1/2} \hat{V}^{-1} A^{1/2} = n I_n \Rightarrow \hat{V}^{-1} = n A^{-1} \Rightarrow \hat{V} = A/n$ . Note  $\partial^2 \ell / \partial \lambda_i^2 < 0$ .

### 31 Generalized Least Square Estimate

- Consider  $y = X\beta + \epsilon$ , where  $\text{Cov}(\epsilon) = \sigma^2 V$ . Let  $\tilde{*} = V^{-1/2}*$ , then  $\tilde{y} = \tilde{X}\beta + \tilde{\epsilon}$  and  $\text{Cov}(\tilde{\epsilon}) = \sigma^2 I_n$ , so

$$\hat{\beta}_W = (\tilde{X}' \tilde{X})^{-1} \tilde{X}' \tilde{y} = (X' V^{-1} X)^{-1} X' V^{-1} y,$$

which is said to be the *generalized* least square (GLS) estimate. If  $V$  is diagonal (not identity), then this can be called *weighted* least square (WLS) estimate.

- SSE (or RSS, residual sum of squares) is

$$\text{SSE} = (\tilde{Y} - \tilde{X} \hat{\beta}_W)' (\tilde{Y} - \tilde{X} \hat{\beta}_W) = (Y - X \hat{\beta}_W)' V^{-1} (Y - X \hat{\beta}_W)$$

- Let  $P_{\tilde{X}}$  be the orthogonal projection such that  $P_{\tilde{X}} y = \tilde{X} \hat{\beta}_W$ , then

$$\begin{aligned}\text{SSE} &= (\tilde{Y} - \tilde{X} \hat{\beta}_W)' (\tilde{Y} - \tilde{X} \hat{\beta}_W) = \tilde{Y}' (I - P_{\tilde{X}}) \tilde{Y} = (\tilde{Y} - \tilde{X} \hat{\beta}_W)' (I - P_{\tilde{X}}) (\tilde{Y} - \tilde{X} \hat{\beta}_W) = \tilde{\epsilon}' (I - P_{\tilde{X}}) \tilde{\epsilon} \\ &\Rightarrow \frac{\text{SSE}}{\sigma^2} = \frac{(Y - X \hat{\beta}_W)' V^{-1} (Y - X \hat{\beta}_W)}{\sigma^2} = \frac{\tilde{\epsilon}' (I - P_{\tilde{X}}) \tilde{\epsilon}}{\sigma^2} \sim \chi_{n-p}^2(0)\end{aligned}$$

as  $\tilde{\epsilon} \sim N(0, \sigma^2 I_n)$  and  $\text{rank}(I_n - P_{\tilde{X}}) = \text{tr}(I_n - P_{\tilde{X}}) = n - p$ .

- If  $\epsilon \sim N_n(0, \sigma^2 V)$ , then  $\hat{\beta}_W \sim N_p(\beta, \sigma^2(X'V^{-1}X)^{-1})$
- Suppose  $V = \text{diag}(\omega_1, \dots, \omega_n)$ , where  $\omega_i = \text{Var}(y_i)$ . If  $\omega_i$  depends only on the values of  $X$ , then errors are heteroscedastic.
- (Important) Let  $\hat{\beta}$  be OLS estimate.  $\hat{\beta}_W = \hat{\beta} \Leftrightarrow C(V^{-1}X) = C(X) \Leftrightarrow C(VX) = C(X)$ .

*Solution:* We can write  $Y = Y_1 + Y_2$ , where  $Y_1 \in \mathcal{C}(X)$  and  $Y_2 \in \mathcal{C}(X)^\perp$ . First, since  $Y_1 \in \mathcal{C}(X)$ , we write  $Y_1 = Xa$ ,  $\exists a$ . Hence,

$$(X'V^{-1}X)^{-1}X'V^{-1}Y_1 = (X'V^{-1}X)^{-1}X'V^{-1}Xa = a = (X'X)^{-1}X'Y_1.$$

Hence, need to show  $(X'V^{-1}X)^{-1}X'V^{-1}Y_2 = (X'X)^{-1}X'Y_2$ . Since  $Y_2 \in \mathcal{C}(X)^\perp = \mathcal{N}(X')$ , we have

$$(X'V^{-1}X)^{-1}X'V^{-1}Y_2 = 0 \Leftrightarrow X'V^{-1}Y_2 = 0.$$

This holds iff  $Y_2 \in \mathcal{N}(X'V^{-1}) = \mathcal{C}(V^{-1}X)^\perp$ . Thus,  $\mathcal{C}(V^{-1}X)^\perp \subseteq \mathcal{C}(X)^\perp \Leftrightarrow \mathcal{C}(V^{-1}X) \supseteq \mathcal{C}(X)$ . However, by  $\text{rank}(V^{-1}X) = \text{rank}(X)$  and the rank-nullity theorem,  $\mathcal{C}(V^{-1}X) = \mathcal{C}(X)$ . Finally,

$$\mathcal{C}(V^{-1}X) = \mathcal{C}(X) \Leftrightarrow V^{-1}X = XW \Leftrightarrow X = VXW \Leftrightarrow \mathcal{C}(X) = \mathcal{C}(VX),$$

where  $W$  is a **nonsingular** matrix.

## 32 Add Regressions to a Model

- Assume that  $\mathbb{E}(y) = X\beta$ , where  $\text{Var}(\epsilon) = \sigma^2 I$  and then  $\hat{\beta} = (X'X)^{-1}X'y$ .
- Consider another model  $G: \mathbb{E}(y) = X\beta + Z\gamma$ , where the columns of  $X$  and  $Z$  are linearly independent.
- We can write the model G as

$$\mathbb{E}(y) = (X \ Z) \begin{pmatrix} \beta \\ \gamma \end{pmatrix} = W\delta.$$

- In a special case, if  $X'Z = O$ , i.e., they have columns that are orthogonal to one each other, then

$$\hat{\delta}_G = \begin{pmatrix} \hat{\beta}_G \\ \hat{\gamma}_G \end{pmatrix} = (W'W)^{-1}W'y = \begin{pmatrix} X'X & O \\ O & Z'Z \end{pmatrix}^{-1} \begin{pmatrix} X' \\ Z' \end{pmatrix} y = \begin{pmatrix} (X'X)^{-1}X'y \\ (Z'Z)^{-1}Z'y \end{pmatrix}, \Rightarrow \hat{\beta}_G = \hat{\beta}.$$

- In the general case, let  $P_X = X(X'X)^{-1}X'$  and  $Q_X = I - P_X$ . Then we can write G model as

$$\begin{aligned} \mathbb{E}(y) &= X\beta + P_X Z\gamma + Q_X Z\gamma \\ &= X[\beta + (X'X)^{-1}X'Z\gamma] + Q_X Z\gamma \\ &= X\alpha + Q_X Z\gamma. \end{aligned}$$

Since  $XQ_X' = XQ_X = O$ , as for the specific case,

$$\begin{aligned} \hat{\alpha} &= (X'X)^{-1}X'y = \hat{\beta}_G + (X'X)^{-1}X'Z\hat{\gamma}_G = \hat{\beta}_G + L\hat{\gamma}_G, \\ \hat{\gamma}_G &= (Z'Q_X'Q_X Z)^{-1}Z'Q_X y = (Z'Q_X Z)^{-1}Z'Q_X y = MZ'Q_X y, \\ \hat{\beta}_G &= (X'X)^{-1}X'(y - Z\hat{\gamma}_G) = \hat{\beta} - L\hat{\gamma}_G, \end{aligned}$$

where  $L = (X'X)^{-1}X'Z$  and  $M = (Z'Q_X Z)^{-1}$ .

Check that  $Z'Q_X Z$  is nonsingular: Suppose  $Z'Q_X Za = 0$ . Then

$$a'Z'Q_X Za = \|Q_X Za\|^2 = 0 \Rightarrow Q_X Za = 0 \Rightarrow Za = P_X Za = X(X'X)^{-1}X'Za \in \mathcal{C}(X).$$

However, we have  $X \perp Z \Rightarrow \mathcal{C}(Z) \cap \mathcal{C}(X) = \{0\}$ , so that  $a = 0$ , meaning that  $Z'Q_X Z$  is invertible.

- Variance-covariance matrix is a bit complicated.

$$\begin{aligned}
\text{Var}(\hat{\gamma}_G) &= \sigma^2 M Z' Q_X Z M = \sigma^2 M \\
\text{Cov}(\hat{\beta}, \hat{\gamma}_G) &= \text{Cov}((X'X)^{-1} X' y, M Z' Q_X y) = \sigma^2 (X'X)^{-1} X' Q_X Z M = O \\
\text{Var}(\hat{\beta}_G) &= \text{Var}(\hat{\beta} - L \hat{\gamma}_G) = \text{Var}(\hat{\beta}) + L \text{Var}(\hat{\gamma}_G) L' = \sigma^2 [(X'X)^{-1} + L M L'], \\
\text{Cov}(\hat{\beta}_G, \hat{\gamma}_G) &= \text{Cov}(\hat{\beta} - L \hat{\gamma}_G, \hat{\gamma}_G) = O - L \text{Var}(\hat{\gamma}_G) = -\sigma^2 L M.
\end{aligned}$$

To summarize,

$$\text{Cov} \begin{pmatrix} \hat{\beta}_G \\ \hat{\gamma}_G \end{pmatrix} = \sigma^2 \begin{pmatrix} (X'X)^{-1} + L M L' & -L M \\ -M L' & M \end{pmatrix}.$$

We also see that  $\text{Var}(\hat{\beta}_G) = \sigma^2 [(X'X)^{-1} + L M L'] \succeq \sigma^2 (X'X)^{-1} = \text{Var}(\hat{\beta})$  because

$$a' L M L' a = \|M^{1/2} L' a\|^2 \geq 0 \quad \Rightarrow \quad L M L' \succeq O,$$

which means that **adding regressors does not decrease the variance-covariance of  $\beta$  estimate**.

- Let  $P_W$  be the orthogonal projection matrix on  $C(W)$ .

$$\begin{aligned}
\hat{y}_{C(W)} &= P_W y = X \hat{\beta}_G + Z \hat{\gamma}_G \\
&= X(\hat{\beta} - L \hat{\gamma}_G) + Z \hat{\gamma}_G \\
&= P_X y + Q_X Z \hat{\gamma}_G \quad \because X L = P_X Z \\
&= (P_X + Q_X Z M Z' Q_X) y, \quad \forall y.
\end{aligned}$$

It follows that  $P_W = P_X + Q_X Z (Z' Q_X Z)^{-1} Z' Q_X$ .

- Using this, SSE in G model is given by

$$\begin{aligned}
\text{SSE}_G &= y'(I - P_W)y = y'(I - P_X - Q_X Z (Z' Q_X Z)^{-1} Z' Q_X)y \\
&= \text{SSE} - y' Q_X Z M Z' Q_X y \preceq \text{SSE}
\end{aligned}$$

since  $y' Q_X Z M Z' Q_X y = \|M^{1/2} Z' Q_X y\|^2 \geq 0 \Rightarrow Q_X Z M Z' Q_X \succcurlyeq O$ , meaning that adding regressors does not increase SSE.

### 33 Estimate under linear constraints

- Consider  $y = X\beta + \epsilon$ , where  $\mathbb{E}(\epsilon) = 0$  and  $\text{Cov}(\epsilon) = \sigma^2 I_n$ . Assume  $X : n \times p$  and  $\beta : p \times 1$ .
- First, suppose  $\text{rank}(X) = p$  (full column rank).
- Want to estimate  $\beta$  such that  $A\beta = c$ , where  $A : q \times p$  and  $c : q \times 1$ .
- The first method uses **Lagrange multiplier**:  $f(\beta) = \|y - X\beta\|^2 + \lambda'(A\beta - c)$ , where  $\lambda \in \mathbb{R}^q$ .

$$\frac{\partial f(\beta)}{\partial \beta} = -2X'(y - X\beta) + A'\lambda, \quad \frac{\partial f(\beta)}{\partial \lambda} = A\beta - c.$$

Both derivatives equal to zero gives

$$\hat{\beta}_H = \hat{\beta} - (X'X)^{-1} A' \hat{\lambda}_H / 2 \quad \Rightarrow \quad A \hat{\beta}_H = A \hat{\beta} - A (X'X)^{-1} A' \hat{\lambda}_H / 2 = c$$

so that  $\lambda_H / 2 = [A(X'X)^{-1} A']^{-1} (A \hat{\beta} - c)$  and hence

$$\hat{\beta}_H = \hat{\beta} - (X'X)^{-1} A' \hat{\lambda}_H / 2 = \hat{\beta} - (X'X)^{-1} A' [A(X'X)^{-1} A']^{-1} (A \hat{\beta} - c).$$

- Second approach assumes **there exists  $\beta_0$  s.t.  $A\beta_0 = c$** . Then

$$\tilde{y} = y - X\beta_0 = X(\beta - \beta_0) + \epsilon := X\gamma + \epsilon.$$

Let  $\theta = X\gamma \in C(X)$  and  $A_1 = A(X'X)^{-1}X'$ . Then

$$A_1\theta = A(X'X)^{-1}X'X\gamma = A(\beta - \beta_0) = 0 \quad \Rightarrow \quad \theta \in N(A_1).$$

Thus,  $\theta = C(X) \cap N(A_1) = \Omega \cap N(A_1) \equiv \omega \subseteq \Omega$ . It follows that  $\hat{\theta} = P_\omega \tilde{y}$ .

- **Lemma 1:** If  $\omega \subseteq \Omega$ , then  $P_\omega = P_\Omega - P_{\omega^\perp \cap \Omega}$ .

*Proof:*  $\omega \subseteq \Omega \Rightarrow P_\omega P_\Omega = P_\omega$ . So,  $(P_\omega y)'(P_\Omega - P_\omega)y = y'P_\omega(P_\Omega - P_\omega)y = 0$ , leading to

$$P_\omega \perp P_\Omega - P_\omega \quad \Rightarrow \quad P_\Omega - P_\omega = P_{\omega^\perp \cap \Omega}.$$

- **Lemma 2:**  $\omega^\perp \cap \Omega = C(P_\Omega A'_1)$ .

*Proof:* Show that  $\omega^\perp \cap \Omega \subseteq C(P_\Omega A'_1)$  and  $C(P_\Omega A'_1) \subseteq \omega^\perp \cap \Omega$ . We use

$$\omega^\perp \cap \Omega = (\Omega \cap N(A_1))^\perp \cap \Omega = (\Omega^\perp + C(A'_1)) \cap \Omega.$$

First, if  $x \in \omega^\perp \cap \Omega = (\Omega^\perp + C(A'_1)) \cap \Omega$ , then

$$x = P_\Omega[A'_1\alpha + (I - P_\Omega)\beta] = P_\Omega A'_1\alpha \in C(P_\Omega A'_1) \quad \Rightarrow \quad \omega^\perp \cap \Omega \subseteq C(P_\Omega A'_1).$$

Conversely, if  $z \in C(P_\Omega A'_1)$  and set  $x \in \omega = \Omega \cap N(A_1)$ , then  $\exists b$

$$z'x = (P_\Omega A'_1 b)'x = b'A_1 P_\Omega x = b'A_1 x = 0 \quad \Rightarrow \quad z \in \omega^\perp = \omega^\perp \cap \Omega \quad \Rightarrow \quad C(P_\Omega A'_1) \subseteq \omega^\perp \cap \Omega.$$

- Therefore, the estimate of  $\theta = X(\beta - \beta_0)$  is

$$\begin{aligned} \hat{\theta}_H &= P_\omega \tilde{y} = (P_\Omega - P_{\omega^\perp \cap \Omega})\tilde{y} \quad \text{by lemma 1} \\ &= (P_\Omega - P_{C(P_\Omega A'_1)})\tilde{y} \quad \text{by lemma 2} \\ &= (P_\Omega - P_\Omega A'_1(A_1 P_\Omega A'_1)^{-1}A_1 P_\Omega)(y - X\beta_0) \\ &= P_\Omega(y - X\beta_0) - P_\Omega A'_1(A_1 P_\Omega A'_1)^{-1}A_1 P_\Omega(y - X\beta_0) \\ &= X(\hat{\beta} - \beta_0) - P_\Omega A'_1(A_1 P_\Omega A'_1)^{-1}A_1 X(\hat{\beta} - \beta_0) \\ &= X(\hat{\beta} - \beta_0) - X(X'X)^{-1}A'(A(X'X)^{-1}A)^{-1}A(\hat{\beta} - \beta_0) \quad \because P_\Omega A'_1 = X(X'X)^{-1}A' \\ &= X(\hat{\beta} - \beta_0) - X(X'X)^{-1}A'(A(X'X)^{-1}A)^{-1}(A\hat{\beta} - c). \end{aligned}$$

Since we can write  $\hat{\theta}_H = X(\hat{\beta}_H - \beta_0)$ ,

$$\begin{aligned} X\hat{\beta}_H &= X\hat{\beta} - X(X'X)^{-1}A'(A(X'X)^{-1}A)^{-1}(A\hat{\beta} - c) \\ \Rightarrow \quad \hat{\beta}_H &= \hat{\beta} - (X'X)^{-1}A'[A(X'X)^{-1}A]^{-1}(A\hat{\beta} - c) \quad \because \text{premultiply by } (X'X)^{-1}X' \end{aligned}$$

Indeed,  $A\hat{\beta}_H = A\hat{\beta} - (A\hat{\beta} - c) = c$ . We can use  $(X'X)^-$ , which is more complicated as shown in the next section.

- $\text{var}(\hat{\beta}_{Hj}) \leq \text{var}(\hat{\beta}_j)$  as

$$\begin{aligned} \text{Var}(\hat{\beta}_H) &= \text{Var}[(I - (X'X)^{-1}A'[A(X'X)^{-1}A]^{-1}A)\hat{\beta}] \\ &= \sigma^2[(X'X)^{-1} - (X'X)^{-1}A'[A(X'X)^{-1}A]^{-1}A(X'X)^{-1}] \\ &\preceq \sigma^2(X'X)^{-1} = \text{Var}(\hat{\beta}). \end{aligned}$$

- Show  $\|Y - \hat{Y}_H\|^2 = \|Y - \hat{Y}\|^2 + \|\hat{Y} - \hat{Y}_H\|^2$  wisely.

*Proof:* Need to show  $(Y - \hat{Y})'(\hat{Y} - \hat{Y}_H) = 0$ . Let  $P_\omega$  be the projection matrix onto  $\omega = N(A_1) \cap \Omega$ . Since  $P_\Omega P_\omega = P_\omega P_\Omega = P_\omega$ ,

$$(Y - \hat{Y})'(\hat{Y} - \hat{Y}_H) = Y'(I - P_\Omega)(P_\Omega - P_\omega)Y = Y'(P_\Omega - P_\omega - P_\Omega + P_\Omega P_\omega)Y = 0.$$

### 34 Design matrix of less than full rank

- Consider the randomized block design with two treatments and two blocks:  $Y_{ij} = \mu + \alpha_i + \gamma_j + \epsilon_{ij}$ ,  $i, j = 1, 2$ . Then the model is

$$E(Y) = \begin{pmatrix} Y_{11} \\ Y_{12} \\ Y_{21} \\ Y_{22} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mu \\ \alpha_1 \\ \alpha_2 \\ \gamma_1 \\ \gamma_2 \end{pmatrix} = X\beta,$$

where the columns  $X$  are linearly *dependent* ( $\text{rank}(X) = 3$ ).

- We have two options for  $X$  to be of full rank. First, set  $\alpha_2 = 0$  and  $\gamma_2 = 0$ , i.e, regard them as reference:

$$E(Y) = \begin{pmatrix} Y_{11} \\ Y_{12} \\ Y_{21} \\ Y_{22} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \mu \\ \alpha_1 \\ \gamma_1 \end{pmatrix}$$

and the second is that we use two identifiability constraints,  $H\beta = 0$  or  $\sum_i \alpha_i = 0$  and  $\sum_j \gamma_j = 0$ :

$$\begin{pmatrix} \theta \\ 0 \end{pmatrix} = \begin{pmatrix} X \\ H \end{pmatrix} \beta = \begin{pmatrix} 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \\ 0 & \mathbf{1} & \mathbf{1} & 0 & 0 \\ 0 & 0 & 0 & \mathbf{1} & \mathbf{1} \end{pmatrix} \begin{pmatrix} \mu \\ \alpha_1 \\ \alpha_2 \\ \gamma_1 \\ \gamma_2 \end{pmatrix},$$

where the augmented matrix now has linearly *independent* columns. Thus **given  $\theta$ ,  $\beta$  becomes unique**,

- Suppose  $\text{rank}(X) = r < p$  and still  $A\beta = c \in \mathbb{R}^q$ , where  $A$  (full row rank) with  $a'_i$  in rows and  $c$  are known. If each of  $a'_i\beta$  is estimable for  $i = 1, \dots, q$ , then  $\forall m_i$ , such that  $\mathbb{E}(m'_i y) = a'_i\beta \Rightarrow m'_i X = a'_i$ . Hence, we have  $\mathbf{A} = \mathbf{M}\mathbf{X}$ , where  $M = (m_1, \dots, m_q)' \in \mathbb{R}^{q \times n}$  with rank  $q$  as  $q = \text{rank}(A) = \text{rank}(MX) \leq \text{rank}(M) \leq q$ .
- Recall that we consider  $\mathbb{E}(\tilde{y}) = X\gamma = \theta \in \Omega = C(X)$ . Then  $\mathbf{M}\theta = MX\gamma = A(\beta - \beta_0) = 0$ , so that  $\theta \in N(M) \cap \Omega := \omega \subseteq \Omega$ . Using this, we form  $X\hat{\gamma}_H = \hat{\theta}_H = P_\omega \tilde{y} = (P_\Omega - P_{C(P_\Omega M')})\tilde{y}$ . Since  $P_\Omega M' = X(X'X)^- X'M' = X(X'X)^- A'$  and  $MP_\Omega M' = A(X'X)^- A'$ , we also get the same formula:

$$\begin{aligned} X(\hat{\beta}_H - \beta_0) &= (P_\Omega - P_{C(P_\Omega M')})\tilde{y} \\ &= (P_\Omega - P_\Omega M'(MP_\Omega M')^- MP_\Omega)(y - X\beta_0) \\ &= (\mathbf{I}_n - P_\Omega M'(MP_\Omega M')^- M)(P_\Omega y - P_\Omega X\beta_0) \\ &= (I_n - P_\Omega M'(MP_\Omega M')^- M)X(\hat{\beta} - \beta_0) \\ &= X(\hat{\beta} - \beta_0) - P_\Omega M'(MP_\Omega M')^- MX(\hat{\beta} - \beta_0) \\ &= X(\hat{\beta} - \beta_0) - X(X'X)^- A'(A(X'X)^- A')^- A(\hat{\beta} - \beta_0) \end{aligned}$$

and similarly to full rank  $X$ ,

$$\begin{aligned} X\hat{\beta}_H &= X\hat{\beta} - X(X'X)^- A'(A(X'X)^- A')^- A(\hat{\beta} - \beta_0) \\ \Rightarrow X'X\hat{\beta}_H &= X'X\hat{\beta} - X'X(X'X)^- A'(A(X'X)^- A')^- A(\hat{\beta} - \beta_0) \\ \Rightarrow X'X\hat{\beta}_H &= X'X\hat{\beta} - \mathbf{A}'(A(X'X)^- A')^- A(\hat{\beta} - \beta_0) \end{aligned}$$

since  $X'X(X'X)^- A' = X'X(X'X)^- X'M' = \mathbf{X}'P_\Omega M' = \mathbf{X}'M' = A'$ .

Moreover, importantly, if  $A\beta = c$ , where  $A$  is of less than full rank, then  $\beta = A^-c$  is a solution (but not unique) as  $A\beta = A(A^-c) = AA^-A\beta = A\beta = c$ . Using this fact, we also have

$$\begin{aligned}\widehat{\beta}_H &= (X'X)^-X'X\widehat{\beta} - (X'X)^-A'(A(X'X)^-A')^-A(\widehat{\beta} - \beta_0) \\ &= (X'X)^-X'y - (X'X)^-A'(A(X'X)^-A')^-A(\widehat{\beta} - \beta_0) \\ &= \widehat{\beta} - (X'X)^-A'(A(X'X)^-A')^-(A\widehat{\beta} - c).\end{aligned}$$

- Claim that  $A(X'X)^-A'$  is invertible (nonsingular), i.e.,  $[A(X'X)^-A']^- = [A(X'X)^-A']^{-1}$ . Since  $A(X'X)^-A' = MP_\Omega M' = MP_\Omega P_\Omega M'$ , enough to show  $P_\Omega M'$  has full column rank ( $\text{rank}(P_\Omega M') = q$ ).

**Lemma 3:**  $P_\Omega M'$  has full column rank  $\Leftrightarrow \Omega^\perp \cap C(M') = \{0\}$ . *Proof:*

- ( $\Rightarrow$ ) Suppose  $\text{rank}(P_\Omega M') = q$  and set  $z \in \Omega^\perp \cap C(M')$ . First  $z \in C(M')$  leads to  $z = M'a$ ,  $\exists a$ . Further, since  $z \in \Omega^\perp = C(X)^\perp = N(X')$ ,  $0 = X'z = X'M'a = A'a \Rightarrow a = 0$  since  $A$  has full row rank. Hence  $z = 0 \Rightarrow \Omega^\perp \cap C(M') = \{0\}$ .
- ( $\Leftarrow$ ) Show the contraposition:  $\text{rank}(P_\Omega M') < q \Rightarrow \Omega^\perp \cap C(M') \neq \{0\}$ . Suppose  $\text{rank}(P_\Omega M') < q$ . For  $\exists \alpha \in \mathbb{R}^q \setminus \{0\}$  s.t.  $\sum_{i=1}^q \alpha_i (P_\Omega m_i) = P_\Omega \sum_{i=1}^q \alpha_i m_i = 0$ , so that  $\sum_{i=1}^q \alpha_i m_i \in \Omega^\perp \cap C(M') \setminus \{0\}$ .

In conclusion, if  $\Omega^\perp \cap C(M') = \{0\}$  or equivalently,  $\text{rank}(P_\Omega M') = q$  (full column rank),  $A(X'X)^-A'$  is invertible, so that  $A\widehat{\beta}_H = A\widehat{\beta} - A(\widehat{\beta} - \beta_0) = c$  even if  $X$  has less than full column rank.

## 35 Hypothesis testing under linear constraints

- Go back to the condition where  $X$  has full column rank and then the constrained estimate of  $\beta$  is

$$\widehat{\beta}_H = \widehat{\beta} - (X'X)^{-1}A'[A(X'X)^{-1}A']^{-1}(A\widehat{\beta} - c). \quad (*)$$

- Want to test  $H : A\beta = c$  vs  $H_A : A\beta \neq c$ , where  $A$  (full row rank) and  $c$  are known.
- Under  $H$ , the sum of square errors is given by

$$\text{SSE}_H = \|y - X\widehat{\beta}_H\|^2 = \|y - X\widehat{\beta} + X\widehat{\beta} - X\widehat{\beta}_H\|^2 = \text{SSE} + (\widehat{\beta}_H - \widehat{\beta})'X'X(\widehat{\beta}_H - \widehat{\beta})$$

Substituting (\*) into  $\widehat{\beta}_H$  provides

$$\text{SSE}_H - \text{SSE} = \|\widehat{Y} - \widehat{Y}_H\|^2 = (A\widehat{\beta} - c)'[A(X'X)^{-1}A']^{-1}(A\widehat{\beta} - c).$$

Here  $\widehat{\beta} \sim N_p(\beta, \sigma^2(X'X)^{-1}) \Rightarrow A\widehat{\beta} - c \sim N_q(0, \sigma^2 A(X'X)^{-1}A')$  under  $H_0$ , leading to

$$\frac{\text{SSE}_H - \text{SSE}}{\sigma^2} = (A\widehat{\beta} - c)'[\sigma^2 A(X'X)^{-1}A']^{-1}(A\widehat{\beta} - c) \sim \chi_q^2(0).$$

- Note that *without* restrictions, what is the expectation of the difference in SSE? We have

$$A\widehat{\beta} - c \sim N_p(A\beta - c, \sigma^2 A(X'X)^{-1}A).$$

Hence, let  $Z = A\widehat{\beta} - c$  and  $B = A(X'X)^{-1}A$ ,

$$\begin{aligned}\mathbb{E}[\text{SSE}_H - \text{SSE}] &= \mathbb{E}[Z'B^{-1}Z] = \text{tr}(B^{-1}(\sigma^2 B)) + (A\beta - c)'B^{-1}(A\beta - c) \\ &= \sigma^2 q + (A\beta - c)'[A(X'X)^{-1}A]^{-1}(A\beta - c) \\ &= \sigma^2 q + (\text{SSE}_H - \text{SSE})_{\widehat{\beta}=\beta}.\end{aligned}$$

implying that without restriction  $(\text{SSE}_H - \text{SSE})/\sigma^2 \sim \chi_q^2(\delta)$ , where  $\delta = (A\beta - c)'B^{-1}(A\beta - c)$ .



- We also have  $\text{SSE}/\sigma^2 = y'Q_X y/\sigma^2 \sim \chi_{n-p}^2(0)$ . Therefore, the  $F$  statistic for testing  $H_0$  is

$$F = \frac{(\text{SSE}_H - \text{SSE})/q}{\text{SSE}/(n-p)} = \frac{n-p}{q} \frac{\text{SSE}_H - \text{SSE}}{\text{SSE}} \sim F_{q, n-p}(0) \quad \text{under } H_0.$$

This is not enough! Need to show  $\text{SSE}_H - \text{SSE} \perp\!\!\!\perp \text{SSE}$ .

*Proof:* Since  $X'Q_X = X'(I_n - P_X) = O$ ,  $X'y \perp\!\!\!\perp Q_X y$  by Craig's theorem, leading to

$$X'y \perp\!\!\!\perp Q_X y \Rightarrow (X'X)^{-1}X'y \perp\!\!\!\perp y'Q_X y \Rightarrow \hat{\beta} \perp\!\!\!\perp \text{SSE} \Rightarrow \text{SSE}_H - \text{SSE} \perp\!\!\!\perp \text{SSE}$$

as  $\text{SSE}_H - \text{SSE}$  is a function of  $\hat{\beta}$ .

- Let  $S_H^2 = (\text{SSE}_H - \text{SSE})/q$  and  $S^2 = \text{SSE}/(n-p)$ . From above,  $\mathbb{E}[S_H^2] = \sigma^2 + \delta$ , where  $\delta \geq 0$  as  $A(X'X)^{-1}A \succ O$  and  $E(S^2) = \sigma^2$ . When  $H : A\beta = c$  is true,  $\delta = 0$  so that  $E(S_H^2)$  is also unbiased for  $\sigma^2$ , that is,  $F = S_H^2/S^2 \approx 1$ . When  $H$  is false,  $\delta > 0$  and by  $E(S_H^2) > E(S^2)$  and  $S_H^2 \perp\!\!\!\perp S$ ,

$$E(F) = E\left[\frac{S_H^2}{S^2}\right] = E[S_H^2]E\left[\frac{1}{S^2}\right] > \frac{E[S_H^2]}{E[S^2]} > 1.$$

Thus, we reject  $H$  if  $F$  is significantly large ( $\Lambda$  is small).

- Exercise: If  $H : A\beta = c$  is true,

$$F = \frac{n-p}{q} \frac{\text{SSE}_H - \text{SSE}}{\text{SSE}} = \frac{n-p}{q} \frac{\epsilon'(P - P_H)\epsilon}{\epsilon'(I_n - P)\epsilon},$$

where  $P_H = P - X(X'X)^{-1}A'B^{-1}A(X'X)^{-1}X'$  is symmetric and idempotent.

*Proof:* The denominator is obvious. Show that  $\text{SSE}_H - \text{SSE} = \|\hat{Y} - \hat{Y}_H\|^2 = \epsilon'(P - P_H)\epsilon$ . We have

$$\begin{aligned} \text{SSE}_H - \text{SSE} &= (A\hat{\beta} - c)'[A(X'X)^{-1}A']^{-1}(A\hat{\beta} - c) \\ &= (\hat{\beta} - \beta)'A'[A(X'X)^{-1}A']^{-1}A(\hat{\beta} - \beta) \\ &= (Y - X\beta)'X(X'X)^{-1}A'B^{-1}A(X'X)^{-1}X'(Y - X\beta) \\ &= \epsilon'(P - P_H)\epsilon. \end{aligned}$$

- Example (The Straight Line). Let  $Y_i = \beta_0 + \beta_1 x_i + \epsilon_i$ ,  $i = 1, \dots, n$  or  $E(Y) = X\beta$ , where  $X = (1, x)$  and  $\beta = (\beta_0, \beta_1)$ . Then we have

$$\begin{aligned} X'X &= \begin{pmatrix} n & 1'x \\ 1'x & x'x \end{pmatrix} = \begin{pmatrix} n & n\bar{x} \\ n\bar{x} & \sum_i x_i^2 \end{pmatrix} \\ \Rightarrow (X'X)^{-1} &= \frac{1}{n \sum_i (x_i - \bar{x})^2} \begin{pmatrix} \sum_i x_i^2 & -n\bar{x} \\ -n\bar{x} & n \end{pmatrix} = \frac{1}{\sum_i (x_i - \bar{x})^2} \begin{pmatrix} \frac{1}{n} \sum_i x_i^2 & -\bar{x} \\ -\bar{x} & 1 \end{pmatrix} \end{aligned}$$

and so  $\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{x}$  and  $\hat{\beta}_1 = \sum_i (Y_i - \bar{Y})(x_i - \bar{x}) / \sum_i (x_i - \bar{x})^2$ . Note that since  $\text{Var}(\hat{\beta}) = \sigma^2(X'X)^{-1}$ , the correlation coefficient of  $\hat{\beta}_0$  and  $\hat{\beta}_1$ ,  $\rho$ , is

$$\rho = \frac{\text{cov}(\hat{\beta}_0, \hat{\beta}_1)}{\sqrt{\text{var}(\hat{\beta}_0) \text{var}(\hat{\beta}_1)}} = \frac{-n\bar{x}}{\sqrt{n \sum_i x_i^2}}.$$

$F$  statistics for testing

–  $H : \beta_1 = c$  is

$$F = \frac{(A\hat{\beta} - c)'[A(X'X)^{-1}A']^{-1}(A\hat{\beta} - c)/q}{\text{SSE}/(n-2)} = \frac{(\hat{\beta}_1 - c)^2}{S^2 / \sum_i (x_i - \bar{x})^2} \sim F_{1, n-2}.$$

–  $H : \beta_0 = c$  is

$$F = \frac{(\hat{\beta}_0 - c)^2}{S^2 \sum_i x_i^2 / [n \sum_i (x_i - \bar{x})^2]} \sim F_{1, n-2}.$$

Also, the fitted value is given by  $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i = \bar{Y} + \hat{\beta}_1 (x_i - \bar{x})$  and hence

$$\begin{aligned} \text{SSE} &= \sum_i (Y_i - \hat{Y}_i)^2 = \sum_i [Y_i - \bar{Y} - \hat{\beta}_1 (x_i - \bar{x})]^2 \\ &= \sum_i (Y_i - \bar{Y})^2 - 2\hat{\beta}_1 \sum_i (Y_i - \bar{Y})(x_i - \bar{x}) + \hat{\beta}_1^2 \sum_i (x_i - \bar{x})^2 \\ &= \sum_i (Y_i - \bar{Y})^2 - \hat{\beta}_1^2 \sum_i (x_i - \bar{x})^2 \\ &= \sum_i (Y_i - \bar{Y})^2 - \sum_i (\hat{Y}_i - \bar{Y})^2. \end{aligned}$$

so that  $\sum_i (Y_i - \bar{Y})^2 = \sum_i (Y_i - \hat{Y}_i)^2 + \sum_i (\hat{Y}_i - \bar{Y})^2 = \sum_i (Y_i - \hat{Y}_i)^2 + r^2 \sum_i (Y_i - \bar{Y})^2$ , where

$$r^2 = \frac{\text{SSReg}}{\text{SSTO}} = \frac{\sum_i (\hat{Y}_i - \bar{Y})^2}{\sum_i (Y_i - \bar{Y})^2} = \frac{\hat{\beta}_1^2 \sum_i (x_i - \bar{x})^2}{\sum_i (Y_i - \bar{Y})^2} = \frac{[\sum_i (Y_i - \bar{Y})(x_i - \bar{x})]^2}{\sum_i (Y_i - \bar{Y})^2 \sum_i (x_i - \bar{x})^2},$$

which is the square of the *sample correlation* between  $Y$  and  $x$ . We can write

$$(1 - r^2) \sum_i (Y_i - \bar{Y})^2 = \sum_i (Y_i - \hat{Y}_i)^2 = \text{SSE}.$$

Using SSE and  $r$ , the F statistic for testing

–  $H : \beta_1 = 0$  is

$$F = \frac{\hat{\beta}_1^2 \sum_i (x_i - \bar{x})^2}{\text{SSE}/(n-2)} = \frac{\hat{\beta}_1^2 \sum_i (x_i - \bar{x})^2 (n-2)}{(1-r^2) \sum_i (Y_i - \bar{Y})^2} = \frac{r^2 (n-2)}{1-r^2}.$$

–  $H : \beta_0 = 0$  is

$$F = \frac{n\hat{\beta}_0^2 \sum_i (x_i - \bar{x})^2}{\sum_i x_i^2 \text{SSE}/(n-2)} = \frac{n\bar{Y}^2 \sum_i (x_i - \bar{x})^2}{(1-r^2) \sum_i (Y_i - \bar{Y})^2 \sum_i x_i^2}.$$

## 36 Exercise under linear constraints (1)

- Consider the standard linear model:  $y = X\beta + \epsilon \in \mathbb{R}^n$ , where  $X : n \times p$ ,  $\beta : p \times 1$  and  $\epsilon \sim N_n(0, \sigma^2 I_n)$ .
- Here, set  $n = 10$  and  $p = 3$  and suppose  $X$  has *orthonormal* columns.
- We also have  $X'y = (1, 2, 3)'$  and  $y'y = 20$ .
- Set  $H : A\beta = c \in \mathbb{R}^q$ , in particular,  $\beta_1 + \beta_2 + \beta_3 = 2$  ( $q = 1$ )  $\Rightarrow A = (1, 1, 1)$  and  $c = 2$ .
- (a) Find  $\hat{\beta}_H$ . First  $\hat{\beta} = (X'X)^{-1}X'y = I_3(1, 2, 3) = (1, 2, 3)$ . Hence,

$$\begin{aligned} \hat{\beta}_H &= \hat{\beta} - (X'X)^{-1}A'[A(X'X)^{-1}A']^{-1}(A\hat{\beta} - c) \\ &= \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} - \frac{4}{3} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \frac{1}{3} \begin{pmatrix} -1 \\ 2 \\ 5 \end{pmatrix}. \end{aligned}$$

- (b) Determine  $\text{Cov}(\hat{\beta}_H)$ .

$$\begin{aligned}\text{Cov}(\hat{\beta}_H) &= \text{Cov}[(I_3 - (X'X)^{-1}A'[A(X'X)^{-1}A']^{-1}A)\hat{\beta}] \\ &= \text{Cov}[(I_3 - 3^{-1}1'_31_3)\hat{\beta}] \\ &= \sigma^2(I_3 - 3^{-1}1'_31_3)^2 \preceq \sigma^2 I_3 = \text{Cov}(\hat{\beta}),\end{aligned}$$

which implies that  $\hat{\beta}_H$  is biased but has lower variance than  $\hat{\beta}$ , which is unbiased without this constraint.

- (c) Calculate  $F$  test statistics. First, we have  $P_X = X(X'X)^{-1}X' = XX' \neq I_n$  and then

$$\text{SSE} = yQy = y'y - y'Py = 20 - \|X'y\|^2 = 20 - 14 = 6.$$

For the numerator,

$$\text{SSE}_H - \text{SSE} = (A\hat{\beta} - c)'[A(X'X)^{-1}A']^{-1}(A\hat{\beta} - c) = \frac{16}{3}.$$

Therefore,

$$F = \frac{(\text{SSE}_H - \text{SSE})/q}{\text{SSE}/(n-p)} = \frac{(16/3)/1}{6/(10-3)} = \frac{56}{9} = 6.22 \sim F_{1,7}.$$

Since  $F_{1,7,0.95} = 5.59$ , we reject  $H : \beta_1 + \beta_2 + \beta_3 = 2$ .

### 37 Exercise under linear constraints (2)

- Given  $Y = \theta + \epsilon$ , where  $\epsilon \sim N_4(0, \sigma^2 I_4)$  and  $1'_4 \theta = 0$ , show the F-statistic for testing  $H : \theta_1 = \theta_3$ .
- First, using the Lagrange multiplier, that is, from  $f(\theta) = \|Y - \theta\|^2 - \lambda(1'\theta)$ , we have

$$\hat{Y}_i = \hat{\theta}_i = Y_i - \bar{Y} \Leftrightarrow \hat{Y} = \hat{\theta} = (I_4 - 11'/4)Y$$

so that the denominator of the F-statistic is

$$S^2 = \frac{\text{SSE}}{n-p} = \frac{\|Y - \hat{Y}\|^2}{4-3} = 4\bar{Y}^2 = \frac{(1'Y)^2}{4}.$$

- For the numerator, we have two solutions, but  $X'X$  is  $3 \times 3$ , so the calculation of  $A(X'X)^{-1}A'$  would not be wise. Hence, use the Lagrange multiplier again. Set  $\theta_1 = \theta_3$  then

$$f(\theta) = (Y_1 - \theta_1)^2 + (Y_2 - \theta_2)^2 + (Y_3 - \theta_1)^2 + (Y_4 - \theta_4)^2 - \lambda(2\theta_1 + \theta_2 + \theta_4).$$

Solving the above, we have

$$\hat{Y}_{1H} = \hat{Y}_{3H} = \frac{Y_1 + Y_3}{2} - \bar{Y}, \quad \hat{Y}_{2H} = \hat{Y}_2, \quad \hat{Y}_{4H} = \hat{Y}_4.$$

Then the numerator of the  $F$  is

$$\frac{\text{SSE}_H - \text{SSE}}{q} = \frac{\|\hat{Y}_H - \hat{Y}\|^2}{1} = (\hat{Y}_{1H} - \hat{Y}_1)^2 + (\hat{Y}_{3H} - \hat{Y}_3)^2 = 2 \left( \frac{Y_1 - Y_3}{2} \right)^2 = \frac{(Y_1 - Y_3)^2}{2}$$

- Therefore, the  $F$  statistic is

$$F = \frac{(Y_1 - Y_3)^2/2}{(1'Y)^2/4} = \frac{2(Y_1 - Y_3)^2}{(Y_1 + Y_2 + Y_3 + Y_4)^2} \sim F_{1,1}(0).$$

## 38 Likelihood Ratio Test

- Let  $\Theta_0$  and  $\Theta$  be the null space and the whole space, respectively, and  $\hat{\theta}_0$  and  $\hat{\theta}$  be MLEs of  $\theta$  for each space. Then LRT statistic and its asymptotic distribution are

$$-2 \ln \Lambda = -2 \ln \frac{\max_{\theta \in \Theta_0} f(x|\theta)}{\max_{\theta \in \Theta} f(x|\theta)} = -2 \log \frac{L_{H_0}(\hat{\theta}_0)}{L_{H_A}(\hat{\theta})} \xrightarrow{D} \chi_r^2(0),$$

where  $r = \dim(\Theta) - \dim(\Theta_0)$ , i.e., difference in the number of parameters.

- If  $y \sim N_n(\beta, \sigma^2)$ . Then

$$\hat{\sigma}_H^2 = \frac{(y - X\hat{\beta}_0)'(y - X\hat{\beta}_0)}{n}, \quad \hat{\sigma}^2 = \frac{(y - X\hat{\beta})'(y - X\hat{\beta})}{n},$$

so that

$$L_{H_0}(\hat{\beta}_H, \hat{\sigma}_H^2) = (2\pi\hat{\sigma}_0^2)^{-n/2} e^{-n/2}, \quad L_{H_A}(\hat{\beta}, \hat{\sigma}^2) = (2\pi\hat{\sigma}^2)^{-n/2} e^{-n/2},$$

leading to

$$\Lambda = \frac{L_{H_0}(\hat{\beta}_0, \hat{\theta}_0)}{L_{H_A}(\hat{\beta}, \hat{\theta})} = \left( \frac{\hat{\sigma}_0^2}{\hat{\sigma}^2} \right)^{-n/2}, \quad -2 \log \Lambda = n(\log \hat{\sigma}_0^2 - \log \hat{\sigma}^2).$$

We reject  $H$  if  $\Lambda < c$ .  $\Lambda$  is not a convenient test statistic.

- Instead, using this notation, we have

$$F = \frac{(\text{SSE}_H - \text{SSE})/q}{\text{SSE}/(n-p)} = \frac{n-p}{q} \left( \frac{\text{SSE}_H}{\text{SSE}} - 1 \right) = \frac{n-p}{q} \left( \frac{\hat{\sigma}_0^2}{\hat{\sigma}^2} - 1 \right) = \frac{n-p}{q} (\Lambda^{-2/n} - 1).$$

We reject  $H$  when  $F > F_{q, n-p, 1-\alpha}$ .

## 39 Jensen's Inequality

- The direction of the inequality depends on the sign of  $f''(X)$ . How to remember?
- We know that  $\text{Var}(X) = E(X^2) - E(X)^2 \geq 0 \Rightarrow E(X^2) \geq E(X)^2$ . So if  $f(x) = x^2$ , then  $E(f(X)) \geq f(E(X))$ . This implies that

$$\begin{aligned} f(x) \text{ is a convex function } (f''(x) > 0) &\Rightarrow E(f(X)) \geq f(E(X)) \\ f(x) \text{ is a concave function } (f''(x) < 0) &\Rightarrow E(f(X)) \leq f(E(X)). \end{aligned}$$

If  $f(x) = x^{-1}, x > 0$ , since  $f''(x) = 2x^{-3} > 0$  ( $x > 0$ ),  $E(f(X)) \geq f(E(X)) \Rightarrow E(X^{-1}) \geq (E(X))^{-1}$ .

## 40 Iterative Algorithms

- Consider a model with log-likelihood  $\ell(\gamma)$ . Want to find  $\hat{\gamma}$ , the MLE of  $\gamma$ , by the iterative process.
- Fisher's method of scoring:

$$\begin{aligned} \gamma^{(m+1)} &= \gamma^{(m)} - \left\{ \mathbb{E} \left( \frac{\partial^2 \ell}{\partial \gamma \partial \gamma'} \right) \right\}_{\gamma^{(m)}}^{-1} \left( \frac{\partial \ell}{\partial \gamma} \right)_{\gamma^{(m)}} \\ &= \gamma^{(m)} + \left\{ \mathbb{E} \left( \frac{\partial \ell}{\partial \gamma} \frac{\partial \ell}{\partial \gamma'} \right) \right\}_{\gamma^{(m)}}^{-1} \left( \frac{\partial \ell}{\partial \gamma} \right)_{\gamma^{(m)}} \\ &= \gamma^{(m)} + I(\gamma^{(m)})^{-1} \ell'(\gamma^{(m)}), \end{aligned}$$

i.e.,  $\gamma$  is updated by adding the product of the *inverse Fisher* information and the **score** function.

- Newton method:

$$\begin{aligned}\gamma^{(m+1)} &= \gamma^{(m)} - \left( \frac{\partial^2 \ell}{\partial \gamma \partial \gamma'} \right)^{-1}_{\gamma^{(m)}} \left( \frac{\partial \ell}{\partial \gamma} \right)_{\gamma^{(m)}} \\ &= \gamma^{(m)} - H(\gamma^{(m)})^{-1} \ell'(\gamma^{(m)}),\end{aligned}$$

i.e.,  $\gamma$  is updated by subtracting the product of the inverse Hessian and the score function.

- Derivation (from 250B HW4): First, find the MLE of  $\theta$ , say  $\hat{\theta}$ , such that

$$\mathbf{u}(\hat{\theta}) = \frac{\partial \ell(\hat{\theta}, \mathbf{y})}{\partial \theta} = \mathbf{0}.$$

Taylor expansion of  $\mathbf{u}(\hat{\theta})$  around an initial value  $\theta_0$  up to the first order gives

$$\mathbf{u}(\hat{\theta}) \approx \mathbf{u}(\theta_0) + \frac{\partial \mathbf{u}(\theta_0)}{\partial \theta} (\hat{\theta} - \theta_0) = \mathbf{u}(\theta_0) + \mathbf{H}(\theta_0) (\hat{\theta} - \theta_0) = \mathbf{0} \Rightarrow \hat{\theta} = \theta_0 - \mathbf{H}^{-1}(\theta_0) \mathbf{u}(\theta_0).$$

## 41 Miscellaneous Exercises

- (Midterm) True or False: For any linear models, it is always true that the sum of residuals equals 0.

*Solution.* False; the sum of residuals is  $1'e = 1'(I - P)Y = 0$  only if  $1'P = 1'$  that is  $1_n \in C(P)$ .

- (Midterm) True or False. Let  $S$  be a  $n \times p$  matrix and  $T$  be a  $n \times q$  matrix and both have full column rank. Let  $P_S$  be the orthogonal projector onto  $C(S)$  and assume further that columns in  $S$  are linearly independent of those in  $T$ . Then  $T'(I - P_S)T$  is nonsingular.

*Solution:* Let  $Q_S = I - P_S$ . For  $a \in \mathbb{R}^q$ , suppose  $a'T'Q_S Ta = 0$ . Since  $a'T'Q_S Ta = \|Q_S^{1/2}Ta\|^2$ ,

$$a'T'Q_S Ta = 0 \Leftrightarrow \|Q_S^{1/2}Ta\|^2 = 0 \Leftrightarrow Q_S Ta = \mathbf{0} \Leftrightarrow Ta = S(S'S)^{-1}S'Ta \Leftrightarrow a = \mathbf{0}$$

as  $S \perp T$  implies  $C(S) \cap C(T) = \{\mathbf{0}\}$ .

- Given the predictor  $\hat{Y} = x\hat{\beta} \in \mathbb{R}$ , where  $X = (1, x_1, \dots, x_{p-1})$ . Show that  $\hat{Y}$  has a minimum variance of  $\sigma^2/n$  at the  $x$  point  $x_j = \bar{x}_{.j}$  ( $j = 1, 2, \dots, p-1$ ).

*Solution:* We know that  $Y_i = x'_i \beta$ , where  $x_i = (1, x_{i1}, \dots, x_{i,p-1})$ , and  $Y_i = \tilde{x}'_i \beta$ , where  $\tilde{x}_i = (1, x_{i1} - \bar{x}_{.1}, \dots, x_{i,p-1} - \bar{x}_{.p-1})$  (after scaling) have the same  $\hat{\beta}_j$ ,  $j = 1, \dots, p-1$  with a different  $\hat{\beta}_0$ . Then

$$\begin{aligned}\text{Var}(\hat{\beta}) &= \sigma^2 \begin{pmatrix} n & 0' \\ 0 & C \end{pmatrix}^{-1} = \sigma^2 \begin{pmatrix} 1/n & 0' \\ 0 & C^{-1} \end{pmatrix} \\ \Rightarrow \text{var}(\hat{Y}) &= \sigma^2 x' \begin{pmatrix} 1/n & 0' \\ 0 & C^{-1} \end{pmatrix} x = \sigma^2 \left( \frac{1}{n} + v' C^{-1} v \right) \geq \frac{\sigma^2}{n} \quad \because C \succ O\end{aligned}$$

with equality iff  $v = 0 \Leftrightarrow x_j = \bar{x}_{.j}$  ( $j = 1, 2, \dots, p-1$ ).

- (HW2) Show that  $\|x\| = \|y\|$  iff there exists an orthogonal matrix  $T$  such that  $Tx = y$  using the householder transformation matrix  $H$ , which is symmetric and orthogonal.

*Proof:* If  $Tx = y$ , then  $y'y = x'T'Tx = x'x \Rightarrow \|x\| = \|y\|$  since L2 norm is always positive.

If  $\|x\| = \|y\|$ , then  $\|x\|e_1 = \|y\|e_1 \Rightarrow H_1 x = H_2 y \Rightarrow H_2 H_1 x = y$ , where  $T = H_2 H_1$  is orthogonal.

- (HW4) Let  $X_1, \dots, X_{n_1}$  and  $Y_1, \dots, Y_{n_2}$  be independent random samples from  $N(\mu_1, v_1^2)$  and  $N(\mu_2, v_2^2)$ , and let  $S_1^2$  and  $S_2^2$  denote the sample variances. Then what is the distribution of

$$\frac{k(X_1 + X_2)}{|Y_1 - Y_2|} \quad \text{and} \quad \frac{k[(X_1 - c)^2 + (X_2 - c)^2]}{S_2^2}.$$

*Solution:* First,  $X_1 \perp X_2$  and  $Y_1 \perp Y_2$  follow

$$\frac{X_1 + X_2}{\sqrt{2}\nu_1} \sim N\left(\frac{\sqrt{2}\mu_1}{\nu_1}, 1\right), \quad \frac{Y_1 - Y_2}{\sqrt{2}\nu_2} \sim N(0, 1) \Rightarrow \frac{(Y_1 - Y_2)^2}{2\nu_2^2} \sim \chi_1^2(0),$$

respectively. Further, since  $(X_1 + X_2) \perp (Y_1 - Y_2)$ , we have

$$\frac{(X_1 + X_2)/(\sqrt{2}\nu_1)}{\sqrt{(Y_1 - Y_2)^2/(2\nu_2^2)}} = \frac{\nu_2}{\nu_1} \frac{X_1 + X_2}{|Y_1 - Y_2|} \sim t_1\left(\frac{\sqrt{2}\mu_1}{\nu_1}\right),$$

which is the given statistic if  $k = \nu_2/\nu_1$ . Secondly,  $X_1 \perp X_2$  leads to

$$\frac{(X_i - c)^2}{\nu_1^2} \sim \chi_1^2\left(\left(\frac{\mu_1 - c}{\nu_1}\right)^2\right) \Rightarrow \frac{(X_1 - c)^2 + (X_2 - c)^2}{\nu_1^2} \sim \chi_2^2\left(2\left(\frac{\mu_1 - c}{\nu_1}\right)^2\right)$$

and we know  $(n_2 - 1)S_2^2/\nu_2^2 \sim \chi_{n_2-1}^2(0)$ . Since  $X_i \perp S_2^2$  that is a function of  $Y_i$ ,

$$\frac{\frac{[(X_1 - c)^2 + (X_2 - c)^2]/\nu_1^2}{\frac{(n_2 - 1)S_2^2/\nu_2^2}{n_2 - 1}}}{\frac{(n_2 - 1)S_2^2/\nu_2^2}{n_2 - 1}} = \frac{\nu_2^2}{2\nu_1^2} \frac{(X_1 - c)^2 + (X_2 - c)^2}{S_2^2} \sim F_{2, n_2 - 1}\left(2\left(\frac{\mu_1 - c}{\nu_1}\right)^2\right),$$

which is the given statistic if  $k = \nu_2^2/(2\nu_1^2)$ .