# 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:

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

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

#### 2 Basis

• If **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 following 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  $x_1, \ldots, x_k$  (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  $\alpha \in \mathbb{R}$ ,

$$(\alpha \mathbf{v}_1 + \mathbf{v}_2, \mathbf{s}) = \alpha(\mathbf{v}_1, \mathbf{s}) + (\mathbf{v}_2, \mathbf{s}) = 0 \implies \alpha \mathbf{v}_1 + \mathbf{v}_2 \in S^{\perp},$$

$$(\mathbf{0}, \mathbf{s}) = 0 \implies \mathbf{0} \in S^{\perp}.$$

•  $N(\mathbf{A})$  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  $\mathbf{A0} = \mathbf{0} \Rightarrow \mathbf{0} \in N(\mathbf{A})$ .

# 4 Inner product

- A vector space V is an *inner product space* if it is endowed with an inner product defined as  $V \times V \to \mathbb{R}$ , 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) > 0 with equality if and only if x = 0.
- If  $x_1, \ldots, x_n$  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

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

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

• Cauchy-Schwarz inequality:  $(x, y)^2 \le ||x||^2 ||y||^2 \Leftrightarrow |(x, y)| \le ||x|| ||y||$  with equality iff x = 0 or y = 0. Proof: Set  $w_1 = x/||x||$  and  $w_2 = y/||y||$ .  $0 \le (w_1 - w_2, w_1 - w_2) = 2(1 - (w_1, w_2)) \Rightarrow (w_1, w_2) \le 1$ . Example: Applying  $x_i = \sqrt{a_i}$  and  $y_i = 1/\sqrt{a_i}$  yields

$$\left(\sum_{i=1}^{n} 1\right)^{2} \le \sum_{i=1}^{n} a_{i} \sum_{i=1}^{n} 1/a_{i} \quad \Rightarrow \quad \frac{n}{\sum_{i=1}^{n} 1/a_{i}} \le \frac{\sum_{i=1}^{n} a_{i}}{n},$$

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 A = 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 = O: 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:

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

• 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, ..., n,
  - $-\operatorname{tr}(A) = \sum_{i=1}^{n} \lambda_i$  and  $\det(A) = |A| = \prod_{i=1}^{n} \lambda_i$  by expanding  $|\lambda I_n A|$ .
  - $-\operatorname{tr}(A^k) = \operatorname{tr}[(T\Lambda T')^k] = \operatorname{tr}(T\Lambda^k T') = \operatorname{tr}(\Lambda^k) = \sum_{i=1}^n \lambda_i^k$  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  $A \in \mathbb{R}^{n \times p}$ .

Column space of 
$$A = \mathcal{C}(A) = \{Ax \mid x \in \mathbb{R}^p\}$$
,  
Row space of  $A = \mathcal{R}(A) = \{A'x \mid x \in \mathbb{R}^n\} = \mathcal{C}(A')$ ,  
Null space of  $A = \mathcal{N}(A) = \{x \in \mathbb{R}^p \mid Ax = 0\}$ ,  
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  $x \in N(A)$ , then  $Ax = 0 \Rightarrow b'Ax = 0, \forall b \Rightarrow x'(A'b) = 0 \Rightarrow x \in C(A')^{\perp}$ . 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

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

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

#### 8 Rank

- rank(A) is equivalent to the maximum number of linearly independent rows or columns.
- $\operatorname{rank}(AB) \leq \min(\operatorname{rank}(A), \operatorname{rank}(B))$  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  $\operatorname{rank}(XB) = q$ . Proof 1:  $XBa = X(Ba) = 0 \Rightarrow Ba = 0 \Rightarrow a = 0$ . So, XB also has linearly independent columns. Proof 2:  $q = \operatorname{rank}(B) = \operatorname{rank}[(X'X)^{-1}X'XB] \leq \operatorname{rank}(XB) \leq \operatorname{rank}(B) = q$ .
- If A is any matrix and P and Q are any comfortable nonsingular matrices, then  $\operatorname{rank}(PAQ) = \operatorname{rank}(A)$ .  $\operatorname{Proof}: \operatorname{rank}(A) \leq \operatorname{rank}(PAQ) \leq \operatorname{rank}(P^{-1}PAQQ^{-1}) = \operatorname{rank}(A)$ .
- (HW1) Suppose the columns of a comfortable matrix C are added to columns of A to form the augmented matrix  $(A \mid C)$ . Then  $\operatorname{rank}(A \mid C) \geq \operatorname{rank}(A)$ .

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

$$C(\mathbf{A}) = \operatorname{span}\{\mathbf{a}_1, \dots, \mathbf{a}_n\} \subseteq \operatorname{span}\{\mathbf{a}_1, \dots, \mathbf{a}_n, \mathbf{c}_1, \dots, \mathbf{c}_n\} = C(\mathbf{A}|\mathbf{C}).$$

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

- By the above and the SD,  $rank(A) = rank(T'AT) = rank(\Lambda)$ , i.e., rank(A) = No. of nonzero eigenvalues.
- Any  $n \times n$  symmetric matrix **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  $\lambda_{r+1} = \cdots = \lambda_n = 0$ . 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 **X** be a  $n \times p$  matrix of rank r < p and **X** partitions  $(\mathbf{X}_1 \mid \mathbf{X}_2)$ , where  $X_1 \in \mathbb{R}^{n \times r}$  and  $X_2 \in \mathbb{R}^{n \times (p-r)}$ , then show that  $\mathbf{X} = \mathbf{X}_1 \mathbf{L}$  where **L** is  $r \times p$  of rank r. *Proof*: there exists **H** s.t.  $\mathbf{X}_2 = \mathbf{X}_1 \mathbf{H}$ , so that

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

• 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

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

• Then A'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:  $\mathbf{x}'\mathbf{A}'\mathbf{A}\mathbf{x} = \|\mathbf{A}\mathbf{x}\|^2 \ge 0$ . Since  $\mathbf{A}\mathbf{x} = \mathbf{0}$  holds iff  $\mathbf{x} = 0$ ,  $\mathbf{A}'\mathbf{A} \succ \mathbf{O} \Rightarrow \mathbf{A}'\mathbf{A}$  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 **A** and **B** be of full row rank. Then  $(\mathbf{BC})'\mathbf{x} = \mathbf{C}'(\mathbf{B}'\mathbf{x}) = \mathbf{0} \Rightarrow \mathbf{B}'\mathbf{x} = \mathbf{0} \Rightarrow \mathbf{x} = \mathbf{0}$ .
- Rank-nullity theorem: If a matrix  $A \in \mathbb{R}^{n \times p}$  with rank(A) = r

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

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

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

which means that any vector in C(A) is spanned by  $A\beta_1, \ldots, A\beta_{p-s}$ . They are linearly independent vectors since suppose

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

leading to

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

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

•  $\operatorname{rank}(X'X) = \operatorname{rank}(X) = \operatorname{rank}(XX') = \operatorname{rank}(X')$ .

*Proof*: First 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,  $a \in N(X'X) \Rightarrow X'Xa = 0 \Rightarrow \|Xa\|^2 = 0 \Rightarrow Xa = 0 \Rightarrow a \in N(X) \Rightarrow N(X'X) \subseteq N(X)$ . Then we have  $\dim N(X'X) = \dim N(X)$ . Since both X'X and X have the same p columns, by the rank-nullity theorem.

$$p - \operatorname{rank}(X'X) = p - \operatorname{rank}(X) \implies \operatorname{rank}(X'X) = \operatorname{rank}(X).$$

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

- $\operatorname{rank}(X^+X) = \operatorname{rank}(X) = \operatorname{rank}(XX^+) = \operatorname{rank}(X^+)$  holds, where  $X^+$  is the Moore Penrose inverse.
- 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 
$$\mathbf{A}\mathbf{x} = \lambda \mathbf{x} = (\alpha + i\beta)\mathbf{x} \ (\mathbf{x} \neq 0)$$
. Define  $\mathbf{B} = (\mathbf{A} - (\alpha - i\beta)\mathbf{I})'(\mathbf{A} - (\alpha + i\beta)\mathbf{I})$ . Then

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

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

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

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

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

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

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

- 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  $\lambda^2 x = \lambda(Ax) = A^2 x = \lambda x \Rightarrow \lambda$ .
  - $-X^+X$  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,  $\det(A'A) = |A|^2 = 1 \implies |A| \pm 1$ , 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,

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

where  $AT_1 = T_1$  ( $\lambda_1 = \cdots = \lambda_r = 1$ ) and  $AT_2 = O$  ( $\lambda_{r+1} = \cdots = \lambda_n = 0$ ). 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,  $T_1T_1'$  is not identity as  $T_1$  not square. But  $T_1$  has orthogonal columns,  $T_1'T_1 = I_r$ .
- Positive definite and semi-positive definite are defined only to symmetric matrices.
  - If **A** is p.d.  $\Rightarrow$  |**A**| > 0  $\Rightarrow$  **A** is non-singular. The converse is not true.
  - If **A** is idempotent, then  $rank(\mathbf{A}) = tr(\mathbf{A}) = the number of eigenvalues 1.$

# 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  $P_{\Omega}-P_{\omega}=P_{\omega}^{\perp}\cap\Omega$ .
- $(I P_{\Omega})(P_{\Omega} P_{\omega}) = (P_{\Omega} P_{\omega}) P_{\Omega}(P_{\Omega} P_{\omega}) = O \Rightarrow I P_{\Omega} \perp \!\!\!\perp P_{\Omega} P_{\omega}.$
- If  $A_1$  is any matrix such that  $\omega = \mathcal{N}(A_1) \cap \Omega$ , then  $\omega^{\perp} \cap \Omega = \mathcal{C}(P_{\Omega}A_1)$ .

 $\begin{aligned} & \textit{Proof} \colon \text{Since } \omega^{\perp} = (\mathcal{N}(A_1) \cap \Omega)^{\perp} = \mathcal{C}(A_1') + \Omega^{\perp}, \text{ if } x \in \omega^{\perp} \cap \Omega, \text{ then } x = P_{\Omega}x = P_{\Omega}[A_1'\alpha + (I - P_{\Omega})\beta] = \\ & P_{\Omega}A_1'\alpha \in \mathcal{C}(P_{\Omega}A_1') \Rightarrow \omega^{\perp} \cap \Omega \subseteq C(P_{\Omega}A_1'). \text{ Conversely, if } x \in C(P_{\Omega}A_1'), \text{ then } x \in C(P_{\Omega}) = \Omega. \text{ Also, if } \\ & z \in \omega = \mathcal{N}(A_1) \cap \Omega, \text{ then } x'z = \alpha'A_1P_{\Omega}z = \alpha'A_1z = 0, \text{ so that } x \in \omega^{\perp} \cap \Omega \Rightarrow C(P_{\Omega}A_1') \subseteq \omega^{\perp} \cap \Omega. \end{aligned}$ 

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

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

#### 11 Positive (semi-) Definite

- **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 **A** is positive definite, **A** is clearly non-singular.
- **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  $x = c_i$  leads to  $x'Ax = a_{ii} > 0$ ,  $\forall i$ .
- If **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 A is symmetric and has only positive eigenvalues, by spectral decomposition,

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

- If **A** is p.s.d., we also have **A** s.t.  $\mathbf{A}^{\frac{1}{2}}\mathbf{A}^{\frac{1}{2}} = \mathbf{A}$ , but **A** is singular so that  $\mathbf{A}^{-1/2}$  does not exist.
  - Hence, if **A** is p.s.d., then  $\mathbf{X}'\mathbf{A}\mathbf{X} = \mathbf{O} \Rightarrow \mathbf{A}\mathbf{X} = \mathbf{O}$ . *Proof* below:

For 
$$\forall \mathbf{a}, \mathbf{a}' \mathbf{X}' \mathbf{A} \mathbf{X} \mathbf{a} = \|\mathbf{A}^{1/2} \mathbf{X} \mathbf{a}\|^2 = 0 \Rightarrow \mathbf{A}^{1/2} \mathbf{X} \mathbf{a} = \mathbf{0} \Rightarrow \mathbf{A} \mathbf{X} \mathbf{a} = \mathbf{0} \text{ (not } \mathbf{X} \mathbf{a} = \mathbf{0}), \text{ so } \mathbf{A} \mathbf{X} = \mathbf{0}.$$

• Simultaneous diagonalization: If  $A \succ O$  and  $B \succeq O$ , then there exists  $U(|U| \neq 0)$  s.t.

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

*Proof*: By definition of positive definite, we can assume **A** and **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 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 **A** is an  $n \times n$  p.d. and **B** is an  $n \times n$  symmetric matrix, then  $\mathbf{A} t\mathbf{B} \succ \mathbf{O}$  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  $\delta = \min(\delta_1, \ldots, \delta_n)$ , then all the leading minor determinants will be positive for  $|t| < \delta$ .
- If L is positive definite then for any b,

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

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

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

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

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

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

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

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

*Proof*: Suppose  $\lambda_1 \geq \cdots \geq \lambda_n$ . By the spectral decomposition,  $T'AT = \Lambda$ . Setting x = Ty leads to

$$\frac{x'Ax}{x'x} = \frac{y'T'ATy}{y'T'Ty} = \frac{y'\Lambda y}{y'y} = \frac{\sum_{i=1}^n \lambda_i y_i^2}{\sum_{i=1}^n y_i^2} \le \lambda_1$$

with equality when  $y = e_1 \Rightarrow x = Te_1 = t_1$ . Also,

$$\frac{x'Ax}{x'x} = \frac{y'T'ATy}{y'T'Ty} = \frac{y'\Lambda y}{y'y} = \frac{\sum_{i=1}^{n} \lambda_{i} y_{i}^{2}}{\sum_{i=1}^{n} y_{i}^{2}} \ge \lambda_{n}$$

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

• (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  $x \neq 0$ ,

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

By Cauchy-Schwarz inequality,

$$\frac{x'Bx}{x'x} \ge \frac{2b}{2b-1} - \frac{1}{2b-1} \frac{\|1_n\|^2 \|x\|^2}{x'x} = \frac{2b}{2b-1} - \frac{\mathbf{n}}{2b-1} = \frac{2b-n}{2b-1} = \lambda_{\text{MIN}}$$

with equality iff  $x = c1_n$ . Also,

$$\frac{x'Bx}{x'x} \le \frac{2b}{2b-1} = \lambda_{\text{MAX}}$$

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

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

• 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:

$$|\mathbf{I}_m + \mathbf{A}\mathbf{B}| = \begin{vmatrix} \mathbf{I}_m + \mathbf{A}\mathbf{B} & \mathbf{O} \\ \mathbf{B} & \mathbf{I}_n \end{vmatrix} = \begin{vmatrix} \mathbf{I}_m & \mathbf{A} \\ \mathbf{O} & \mathbf{I}_n \end{vmatrix} \begin{vmatrix} \mathbf{I}_m & -\mathbf{A} \\ \mathbf{B} & \mathbf{I}_n \end{vmatrix} = \begin{vmatrix} \mathbf{I}_m & \mathbf{A} \\ \mathbf{D} & \mathbf{I}_n \end{vmatrix} = \begin{vmatrix} \mathbf{I}_m & \mathbf{O} \\ \mathbf{B} & \mathbf{I}_n + \mathbf{B}\mathbf{A} \end{vmatrix} = |\mathbf{I}_n + \mathbf{B}\mathbf{A}|.$$

• (HW3) If a partition matrix

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

then  $N(\mathbf{A}_{22}) \subset N(\mathbf{A}_{12})$  and  $C(\mathbf{A}_{21}) \subset C(\mathbf{A}_{22})$ .

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

$$0 \le \mathbf{x}' \mathbf{A} \mathbf{x} = \mathbf{x}_1' \mathbf{A}_{11} \mathbf{x}_1 + \alpha \mathbf{x}_2' \mathbf{A}_{21} \mathbf{x}_1 + \alpha \mathbf{x}_1' \mathbf{A}_{12} \mathbf{x}_2 + \alpha^2 \mathbf{x}_2' \mathbf{A}_{22} \mathbf{x}_2$$
$$= \mathbf{x}_1' \mathbf{A}_{11} \mathbf{x}_1 + 2\alpha \mathbf{x}_1' \mathbf{A}_{12} \mathbf{x}_2 \quad \text{since } \mathbf{A}_{21}' = \mathbf{A}_{12}, \ \mathbf{A}_{22} \mathbf{x}_2 = \mathbf{0}.$$

To satisfy that RHS  $\geq 0$  for  $\forall \alpha$  and  $\forall \mathbf{x}_1$ ,  $\mathbf{A}_{12}\mathbf{x}_2$  has to be zero, i.e.,  $\mathbf{x}_2 \in N(\mathbf{A}_{12})$ . Hence,  $N(\mathbf{A}_{22}) \subset N(\mathbf{A}_{12})$ . It follows from this relationship that

$$N(\mathbf{A}_{22}) \subset N(\mathbf{A}_{12}) \Leftrightarrow \mathbf{C}(\mathbf{A}_{22}')^{\perp} \subset \mathbf{C}(\mathbf{A}_{12}')^{\perp}$$
  
 $\Leftrightarrow C(\mathbf{A}_{22})^{\perp} \subset C(\mathbf{A}_{21})^{\perp} \text{ since } \mathbf{A}_{22}' = \mathbf{A}_{22}, \mathbf{A}_{12}' = \mathbf{A}_{21}$   
 $\Leftrightarrow C(\mathbf{A}_{21}) \subset C(\mathbf{A}_{22}).$ 

#### 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

$$(A + UBV)^{-1} = A^{-1} - A^{-1}UB(B + BVA^{-1}UB)^{-1}BVA^{-1}$$
$$= A^{-1} - A^{-1}U(B^{-1} + VA^{-1}U)^{-1}VA^{-1}.$$

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

If **A** is singular, suppose  $\mathbf{A} \in \mathbb{R}^{m \times n}$  with  $\operatorname{rank}(\mathbf{A}) = r$ . By the rank factorization, we obtain  $\mathbf{A} = \mathbf{CR}$ , 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  $\mathbf{ABA} = (\mathbf{CR})\mathbf{B}(\mathbf{CR}) = \mathbf{C}(\mathbf{RBC})\mathbf{R}$ , we want to find **B** s.t.  $\mathbf{RBC} = \mathbf{I}$  so that  $\mathbf{ABA} = \mathbf{A}$ . As mentioned before,  $\mathbf{C'C}$  and  $\mathbf{RR'}$  are non-singular even though **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  $\mathbf{RBC} = \mathbf{I}$ . Especially, if  $\mathbf{A}$  is full column rank,  $\mathbf{B} = (\mathbf{A}'\mathbf{A})^{-1}\mathbf{A}'$  is a g- inverse of  $\mathbf{A}$ . Similarly, if  $\mathbf{A}$  is full row rank,  $\mathbf{B} = \mathbf{A}'(\mathbf{A}\mathbf{A}')^{-1}$  is a g- inverse of  $\mathbf{A}$ .

- $A^-$  is not unique. There are several ways of getting it: If  $A^-$  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  $\mathbf{AGA} = \mathbf{A}(\mathbf{A}^- + (\mathbf{I} \mathbf{A}^- \mathbf{A}) \mathbf{W}) \mathbf{A} = \mathbf{A} \mathbf{A}^- \mathbf{A} + (\mathbf{A} \mathbf{A} \mathbf{A}^- \mathbf{A}) \mathbf{W} \mathbf{A} = \mathbf{A}$ , 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  $\mathbf{AGA} = \mathbf{AA}^- \mathbf{A}^- + (\mathbf{A}\mathbf{u})\mathbf{v}'\mathbf{A} = \mathbf{A}$ .
- 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 Ax = b is  $x = A^{-}b$ , which is not unique, as  $A(A^{-}b) = AA^{-}Ax = Ax = b$ .
- If  $A^-$  also satisfies three more conditions: (ii)  $A^-AA^- = A^-$ , (iii)  $(AA^-)' = AA^-$ , and (iv)  $(A^-A)' = A^-A$ , then  $A^-$  is denoted by  $A^+$ , which is called the **Moore-Penrose inverse**.
- $\bullet$  Moore-Penrose inverse  $A^+$  is unique. If  $B^+$  is another Moore-Penrose inverse, then

$$\mathbf{B}^{+} = \mathbf{B}^{+} \mathbf{A} \mathbf{B}^{+} = \mathbf{B}^{+} \mathbf{A} \mathbf{A}^{+} \mathbf{A} \mathbf{B}^{+} = \mathbf{A}' (\mathbf{B}^{+})' \mathbf{A}^{+} (\mathbf{B}^{+})' \mathbf{A}' = \mathbf{A}' (\mathbf{A}^{+})' \mathbf{A}' (\mathbf{B}^{+})' \mathbf{A}^{+} (\mathbf{B}^{+})' \mathbf{A}' (\mathbf{A}^{+})' \mathbf{A}'$$

$$= \mathbf{A}^{+} \mathbf{A} \mathbf{B}^{+} \mathbf{A} \mathbf{A}^{+} \mathbf{A} \mathbf{A}^{+} = \mathbf{A}^{+} \mathbf{A} \mathbf{A}^{+} \mathbf{A} \mathbf{A}^{+} = \mathbf{A}^{+} \mathbf{A} \mathbf{A}^{+} = \mathbf{A}^{+}.$$

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

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  $\mathbf{x} \in C(\mathbf{A}')$ , 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 PA'A = QA'A, then PA' = QA' for any comfortable matrices P and Q.

Solution: If **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 **A** is singular and rank(**A**) = r, we have **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

$$PA'A = QA'A \Rightarrow (P-Q)A'A = O \Rightarrow (P-Q)R'C'CR = O.$$

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

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

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

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

Then  $\mathbf{A} = \mathbf{Q}\mathbf{R}$ , 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 **A** is a  $n \times n$  symmetric matrix, then  $\mathbf{A} = \mathbf{T} \Lambda \mathbf{T}' = \sum_{i} \lambda_{i} \mathbf{t}_{i}' \mathbf{t}_{i}'$ , or  $\mathbf{T}' \mathbf{A} \mathbf{T} = \Lambda$ , where  $\mathbf{\Lambda} = \operatorname{diag}(\lambda_{1}, \dots, \lambda_{n})$  and **T** is an orthogonal matrix (not symmetric in general) with eigenvectors. The columns of **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,

$$\underbrace{\mathbf{A}}_{n \times p} = \underbrace{\left(\mathbf{S}_r \mid \mathbf{S}_{p-r}\right)}_{n \times p} \begin{pmatrix} \mathbf{D}_r & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \end{pmatrix} \underbrace{\begin{pmatrix} \mathbf{T}'_r \\ \mathbf{T}'_{p-r} \end{pmatrix}}_{p \times p} \quad \text{(normal form)}$$

$$= \underbrace{\mathbf{S}_r}_{n \times r} \mathbf{D}_r \underbrace{\mathbf{T}'_r}_{r \times p} \quad \text{(reduced form)}$$

$$= \underbrace{\sum_{i=1}^r \sigma_i \mathbf{s}_i \mathbf{t}'_i}_{i} \quad \text{(outer product form)},$$

where  $\mathbf{D}_r = \operatorname{diag}(\sigma_1, \dots, \sigma_r)$  for  $\sigma_1 \ge \dots \ge \sigma_r > 0$ .  $\mathbf{S}_r' \mathbf{S}_r = \mathbf{T}_r' \mathbf{T}_r = \mathbf{I}_r$  (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 **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

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

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

Then,

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

Hence,

$$\mathbf{X} = \mathbf{S}_{r} \mathbf{D}_{r} \mathbf{T}_{r}' = \mathbf{s}_{1} \sigma_{1} \mathbf{t}_{1}' = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} (\sqrt{2}) \begin{pmatrix} 1 & 0 & 0 & 0 \end{pmatrix} \quad \text{(reduced form)}$$

$$= \mathbf{SDT}' = (\mathbf{s}_{1} \ \mathbf{s}_{2}) \begin{pmatrix} \sigma_{1} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{t}_{1}' \\ \mathbf{t}_{2}' \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \sqrt{2} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad \text{(normal form)}$$

In the normal form of SVD,  $s_2$  and  $t_2$  orthogonal to  $s_1$  and  $t_1$  were chosen, respectively.

• Cholesky's decomposition: If A is p.d., there exists a *unique* upper triangular matrix R with positive diagonal elements such that A = R'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 **Z** and comfortable matrices,  $E(\mathbf{AZB} + \mathbf{C}) = \mathbf{A}E(\mathbf{Z})\mathbf{B} + \mathbf{C}$ .
- $Cov(\mathbf{X}, \mathbf{Y}) = E[(\mathbf{X} E(\mathbf{X}))(\mathbf{Y} E(\mathbf{Y})'] \text{ and } Cov(\mathbf{X}, \mathbf{X}) = Var(\mathbf{X}).$
- $Cov(\mathbf{AX}, \mathbf{BY}) = \mathbf{A} Cov(\mathbf{X}, \mathbf{Y})\mathbf{B}'$ .
- $Var(a\mathbf{X} + b\mathbf{Y}) = a^2 Var(\mathbf{X}) + ab[Cov(\mathbf{X}, \mathbf{Y}) + Cov(\mathbf{Y}, \mathbf{X})] + b^2 Var(\mathbf{Y})$ . Note  $Cov(\mathbf{X}, \mathbf{Y}) \neq Cov(\mathbf{Y}, \mathbf{X})$ .
- Suppose  $\Sigma = \text{Var}(\mathbf{X})$ .  $E(\mathbf{x}'\mathbf{A}\mathbf{x}) = \text{tr}(\mathbf{A}\Sigma) + \mu'\mathbf{A}\mu$ .
  - $-E[(\mathbf{x}-\mathbf{b})'\mathbf{A}(\mathbf{x}-\mathbf{b})] = \operatorname{tr}(\mathbf{A}\boldsymbol{\Sigma}) + (\boldsymbol{\mu}-\mathbf{b})'\mathbf{A}(\boldsymbol{\mu}-\mathbf{b}) \text{ as } \operatorname{Var}(\mathbf{X}-\mathbf{b}) = \operatorname{Var}(\mathbf{X}).$
  - If  $\Sigma = \sigma^2 \mathbf{I}_n$ ,  $E(\mathbf{x}' \mathbf{A} \mathbf{x}) = \sigma^2 \operatorname{tr}(\mathbf{A}) + \mu' \mathbf{A} \mu = \sigma^2 (\text{sum of the coefficient of } X_i^2) + (\mathbf{x}' \mathbf{A} \mathbf{x})_{\mathbf{x} = \mu}$

#### 18 Multivariate normal distribution

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

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

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

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

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

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

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

- 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 **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  $\mathbf{a} \in \mathbf{R}^n \setminus \{\mathbf{0}\}$ ,  $\mathbf{a}' \mathbf{y} \sim N_1(\mathbf{a}' \boldsymbol{\mu}, \mathbf{a}' \boldsymbol{\Sigma} \mathbf{a})$ , i.e., a linear combination of  $y_i$ 's is univariate normal.
- Suppose  $\mathbb{E}(\mathbf{Y}) = \boldsymbol{\mu}$  and  $\operatorname{Var}(\mathbf{Y}) = \boldsymbol{\Sigma}$ .  $\mathbf{Y} \sim N_n(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \Leftrightarrow \mathbf{a}'\mathbf{Y}$  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 X are normal, X may not be normally distributed (See 250A HW).

• Consider the joint density of  $X \in \mathbb{R}^p$  and  $Y \in \mathbb{R}^q$ :

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

then  $X \perp \!\!\!\perp Y \Leftrightarrow \Sigma_{12} = \Sigma'_{21} = O_{p \times q}$  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.  $\psi_{X,Y}(t) = e^{t'\mu + t'\Sigma t} = e^{t'_1\mu_1 + t'_1\Sigma_{11}t_1 + t'_2\mu_2 + t'_2\Sigma_{22}t_2} = \psi_X(t_1)\psi_Y(t_2).$ 

• 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  $A_{22}$  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

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

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

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

• If  $A_{22}$  is not invertible, consider the transformation with g-inverse of  $A_{22}$ 

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

Then, covariance matrix

$$\begin{aligned} \operatorname{Var}\begin{pmatrix} \mathbf{Y} \\ \mathbf{X}_{2} \end{pmatrix} &= \begin{pmatrix} \mathbf{I}_{p} & -\mathbf{A}_{12}\mathbf{A}_{22}^{-} \\ \mathbf{O} & \mathbf{I}_{q} \end{pmatrix} \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{I}_{p} & \mathbf{O}' \\ -\mathbf{A}_{22}^{-}\mathbf{A}_{21} & \mathbf{I}_{q} \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-}\mathbf{A}_{21} & \mathbf{A}_{12} - \mathbf{A}_{12}\mathbf{A}_{22}^{-}\mathbf{A}_{22} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{I}_{p} & \mathbf{O}' \\ -\mathbf{A}_{22}^{-}\mathbf{A}_{21} & \mathbf{I}_{q} \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{A}_{11.2} - (\mathbf{A}_{12} - \mathbf{A}_{12}\mathbf{A}_{22}^{-}\mathbf{A}_{22})\mathbf{A}_{22}^{-}\mathbf{A}_{21} & \mathbf{A}_{12} - \mathbf{A}_{12}\mathbf{A}_{22}^{-}\mathbf{A}_{22} \\ \mathbf{A}_{21} - \mathbf{A}_{22}\mathbf{A}_{22}^{-}\mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix}. \end{aligned}$$

For the top left,

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

$$\mathbf{Y} \mid \mathbf{X}_{2} = \mathbf{x}_{2} \sim N_{p}(\boldsymbol{\mu}_{1} - \mathbf{A}_{12}\mathbf{A}_{22}^{-}\boldsymbol{\mu}_{2}, \ \mathbf{A}_{11.2})$$
  
 $\Rightarrow \mathbf{X}_{1} \mid \mathbf{X}_{2} = \mathbf{x}_{2} \sim N_{p}(\boldsymbol{\mu}_{1} + \mathbf{A}_{12}\mathbf{A}_{22}^{-}(\mathbf{x}_{2} - \boldsymbol{\mu}_{2}), \ \mathbf{A}_{11.2})$ 

#### 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  $\mathbb{E}(Q) = \operatorname{tr}(A\Sigma) + \mu'A\mu$ . Proof:

$$\mathbb{E}(x'Ax) = \mathbb{E}[\operatorname{tr}(x'Ax)] = \mathbb{E}[\operatorname{tr}(Axx')] = \mathbb{E}[\operatorname{tr}(A(x-\mu)(x-\mu)' + A\mu\mu')]$$
$$= \operatorname{tr} A\mathbb{E}[((x-\mu)(x-\mu)'] + \operatorname{tr}(A\mu\mu').$$

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

$$(n-1)S^{2} = \sum_{i=1}^{n} (x_{i} - \overline{x})^{2} = x' \left( I_{n} - \frac{1_{n} 1'_{n}}{n} \right) x := x' A x,$$

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

• 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,

$$Q = y'T\Lambda T'y = z'\Lambda z = \sum_{i=1}^{r} z_i^2 \sim \chi_r^2(0) \quad \because z = T'y \sim N_n(0, \ T'T = I_n)$$
$$= y'T_1T'_1y = z'_rz_r = \sum_{i=1}^{r} z_i^2 \sim \chi_r^2(0) \quad \because z_r = T'_1y \sim N_r(0, \ T'_1T_1 = I_r)$$

 $(\Rightarrow)$  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,

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

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

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

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

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  $Q_i = y'A_iy \sim \chi_{r_i}^2$  for i = 1, 2. Then  $Q_1 \perp Q_2 \Leftrightarrow A_1A_2 = O$ . 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,  $(A_1 + A_2)^2 = A_1 + A_2 \quad \Rightarrow \quad A_1A_2 + A_2A_1 = O.$ 

Left and right multiplications by  $A_1$  yield  $A_1A_2 + A_1A_2A_1 = A_1A_2A_1 + A_2A_1 \Rightarrow A_1A_2 = A_2A_1 = O$ . ( $\Leftarrow$ ) Suppose  $A_1A_2 = 0$ . Find the Mgf of  $Q_1$  and  $Q_2$ :

$$\psi_{Q_1,Q_2}(t_1,t_2) = E(e^{t_1Q_1 + t_2Q_2}) = \int (2\pi)^{-p/2} \exp\left[-\frac{1}{2}y'(I - 2t_1A_1 - 2t_2A_2)y\right] dy$$

$$= \frac{1}{|I - 2t_1A_1 - 2t_2A_2|^{1/2}}$$

$$= \frac{1}{|I - 2t_1A_1|^{\frac{1}{2}}} \frac{1}{|I - 2t_2A_2|^{\frac{1}{2}}} \quad \because A_1A_2 = O$$

$$= \psi_{Q_1}(t_1)\psi_{Q_2}(t_2),$$

meaning that  $Q_1 \perp Q_2$ .

• If  $y \sim N_p(0, \Sigma)$ ,  $A_i$  is symmetric and  $Q_i = y'A_iy \sim \chi_{r_i}^2$  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  $A_1\Sigma A_2 = 0$ ,  $E(e^{t_1Q_1+t_2Q_2}) = |\Sigma|^{-\frac{1}{2}}|\Sigma^{-1} - 2tA_1 - 2tA_2|^{-\frac{1}{2}} = |I - 2tA_1\Sigma|^{-\frac{1}{2}}|I - 2tA_2\Sigma|^{-\frac{1}{2}}.$ Proof 2: Let  $x = \Sigma^{-\frac{1}{2}}y \sim N_p(0, \mathbf{I}_p)$ , then  $Q_i = x'\Sigma^{\frac{1}{2}}A_1\Sigma^{\frac{1}{2}}x$ . Hence, by the above theorem,

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

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

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

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

$$0 \le z'(A_1 - A_2)z = -z'A_2z \le 0 \quad :: A_2 \succeq O$$

so that  $z'A_2z = z'A_2^2z = ||A_2z||^2 = 0 \Rightarrow A_2z = 0 \Rightarrow z \in N(A_2)$ . 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

$$A_2(I_p - A_1)y = 0, \ \forall y \quad \Rightarrow \quad A_2 - A_2A_1 = O \quad \text{and} \quad A_2 - A_1A_2 = O \quad \therefore A_1' = A_1, A_2' = A_2.$$

Using the equation to get  $(A_1 - A_2)A_2 = A_1A_2 - A_2^2 = A_1A_2 - A_2 = O \Rightarrow Q_1 - Q_2 \perp \!\!\!\perp Q_2$  and

$$(A_1 - A_2)^2 = A_1 - A_1 A_2 - A_2 A_1 + A_2 = A_1 - A_2,$$
  

$$\operatorname{rank}(A_1 - A_2) = \operatorname{tr}(A_1 - A_2) = \operatorname{tr}(A_1) - \operatorname{tr}(A_2) = r_1 - r_2,$$

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

• 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 **T** is orthogonal, **T**<sub>1</sub> has k column eigenvectors corresponding to eigenvalues 1 ( $\mathbf{AT}_1 = \mathbf{T}_1$ ), and **T**<sub>2</sub> consists of p - k column eigenvectors corresponding to eigenvalues 0 ( $\mathbf{AT}_2 = \mathbf{O}$ ). 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

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

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

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

Hence, Q = y'Ay 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 rank $(A) = r \leq p$ , then

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

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  $\operatorname{rank}(A\Sigma) = r \leq p$ , then  $D = I_r$  so that

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

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  $X_i \stackrel{ind}{\sim} N(\mu_i, 1)$ ,  $i = 1, \ldots, n$  and  $\mu = (\mu_1, \ldots, \mu_n)'$ , 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:

$$A = \begin{pmatrix} a'_1 \\ a'_2 \\ \vdots \\ a'_n \end{pmatrix} \quad \text{s.t.} \quad A'A = AA' = I_n \ (a'_i a_j = \delta_{ij}).$$

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, ..., n, and  $Cov(W) = A Cov(X)A' = AA' = I_n$ . Hence,

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

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

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

$$var(Y) = var(W_1^2) + var\left(\sum_{i=2}^n W_i^2\right) = [E(W_1^4) - E(W_1^2)^2] + 2(n - 1)$$

$$= [(\delta^2 + 6\delta + 3) - (\delta + 1)^2] + 2n - 2 = 2n + 4\delta.$$

since  $E(X^2) = \mu^2 + \sigma^2$  and  $E(X^4) = \mu^4 + 6\mu^2\sigma^2 + 3\sigma^4$  if  $X \sim N(\mu, \sigma^2)$ .

• 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 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  $U'U \sim \chi_p^2(\alpha'\alpha)$ 

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

• 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

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

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

#### 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.
- $\bullet$  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  $S^2 = \sum_{i=1}^n (x_i - \overline{x})^2 / (n-1)$ . What is the dist. of  $\sqrt{n}(\overline{X} - a) / S$ ?

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

It follows that

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

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

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

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

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

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

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

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

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

• Let  $(X_i, Y_i)$ , i = 1, ..., 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

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

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

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

where  $\nu^2 = \nu_1^2 - 2r\nu_1\nu_2 + \nu_2^2$ . It follows that

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

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

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

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  $V \perp \!\!\! \perp W$ , 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.
- $\bullet$  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

$$Var(F) = \left(\frac{m}{n}\right)^{2} Var\left(\frac{X}{Y}\right) = \left(\frac{m}{n}\right)^{2} \left[E(X^{2})E(Y^{-2}) - E(X)^{2}E(Y^{-1})^{2}\right]$$

$$= \left(\frac{m}{n}\right)^{2} \left[\frac{2n + 4\theta + (n + \theta)^{2}}{(m - 2)(m - 4)} - \frac{(n + \theta)^{2}}{(m - 2)^{2}}\right]$$

$$= 2\frac{(n + 2\theta)(m - 2) + (n + \theta)^{2}}{(m - 2)^{2}(m - 4)} \left(\frac{m}{n}\right)^{2}, \quad m > 4.$$

• (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  $\widehat{Y}$  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  $\|\widehat{Y}\| = Y'PY \sim \chi_2^2(\theta'P\theta)$  and  $\|Y - \widehat{Y}\|^2 = Y'QY \sim \chi_3^2(\theta'Q\theta)$ . 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 Cov(u, v) = AB' = O, then  $u \perp \!\!\! \perp v$  and  $u'u \perp \!\!\! \perp v'v$ .
- 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

$$C'x = (A'_1 \mid B'_1) {x_{l_1} \choose x_{l_1}} = 0 \quad \Rightarrow \quad A'_1 x_{k_1} = B'_1 x_{l_1} = 0 \quad \Rightarrow \quad x = 0.$$

• 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  $Q_i \perp Q_j \Leftrightarrow A_i A_j = O$ .
- Loynes' lemma. If  $M^2 = M = M'$ ,  $P = P' \succeq O$ , and  $I M P \succeq O$ , then MP = PM = O.

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

$$0 < \mathbf{y}'(\mathbf{I} - \mathbf{M} - \mathbf{P})\mathbf{y} = -\mathbf{y}'\mathbf{P}\mathbf{y} < 0 \quad \because \mathbf{P} \succ O.$$

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

- Marsaglia-Garaybill's Lemma. If  $\mathbf{D}_1, \mathbf{D}_2, \dots, \mathbf{D}_q$  are symmetric  $n \times n$  matrices, then any of two of the following statements imply the third:
  - (i)  $\mathbf{D}_1, \mathbf{D}_2, \dots, \mathbf{D}_q$  are idempotent;
  - (ii)  $\mathbf{D}_i \mathbf{D}_j = \mathbf{O}, \ \forall i \neq j.$
  - (iii)  $\mathbf{D} = \mathbf{D}_1 + \mathbf{D}_2 + \cdots + \mathbf{D}_q$  is idempotent;

Proof:

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

- (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),

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

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 rank $(\mathbf{A}_i) = r_i$ ,  $i = 1, \ldots, k$ . 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  $Q_i \sim \chi^2_{r_i}(0)$ .

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

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

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

- (iii)  $\rightarrow$  (i): Let  $\alpha_1, \ldots, \alpha_{r_i}$  be eigenvalues of  $\mathbf{A}_i$  and  $\mathbf{T}$  be an orthogonal matrix such that  $\mathbf{T}'\mathbf{A}_i\mathbf{T} = \operatorname{diag}(\alpha_1, \ldots, \alpha_{r_i}, 0, \ldots 0)$  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  $\mathbf{T}' \mathbf{A}_{(-i)} \mathbf{T} = \operatorname{diag}(\beta_1, \dots, \beta_p)$ . Then

$$\mathbf{I} = \operatorname{diag}(\alpha_1 + \beta_1, \dots, \alpha_{r_i} + \beta_{r_1}, \beta_{r_i+1}, \dots, \beta_p)$$

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

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

leading to rank( $\mathbf{T'A}_{(-i)}\mathbf{T}$ ) =  $p - r_i \Rightarrow \beta_1 = \cdots = \beta_{r_i} = 0 \Rightarrow \alpha_1 = \cdots = \alpha_{r_i} = 1 \Rightarrow \mathbf{A}_i$  is (symmetric and) idempotent for  $i = 1, \ldots, k$ . 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  $\mathbf{MG}$  lemma and hence  $Q_i \perp \!\!\!\perp Q_j$  by Craig's theorem if  $\mathbf{\Sigma} = \mathbf{I}$ .

# 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  $\{x_1, \ldots, x_r\}$  be an **orthogonal basis** for  $\Omega$ . Expand this to an **orthogonal basis** for V by adding  $\{x_{r+1}, \ldots, x_k\}$ . 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  $\{x_1, \ldots, x_r, x_{r+1}, \ldots, x_k\}$  be an orthogonal basis for  $V = \mathbb{R}^n$ . WLOG, assume that  $\{x_1, \ldots, x_r\}$  is an orthogonal basis for  $\Omega$ . Then, if  $y \in V$ , we can write

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

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

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

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,  $P = U\Lambda U' = U_1U_1'$ , 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:  $AA^{-}A = A$ ,

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

- 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  $Cov(\boldsymbol{\epsilon}) = \sigma^2 \mathbf{I}_n$ . 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, i.e.,  $(\mathbf{X}'\mathbf{X})^{-}$  and  $\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{y}$  (biased) are *not* unique.

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

#### 27 Gauss Markov's Theorem

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

*Proof*: Suppose  $\underline{a'y}$  is a linear unbiased estimator of  $\underline{c'\theta}$ , i.e.,  $\mathbb{E}(a'y) = c'\theta$ . Since  $\mathbb{E}(y) = \theta$ ,  $\underline{a'\theta} = \underline{c'\theta}$ ,  $\forall \theta \Rightarrow a = c$ . Then, the difference in variance between a'y and  $c'\widehat{\theta} = c'X\widehat{\beta} = c'X(X'X)^{-1}X$  is

$$\operatorname{Var}(a'y) - \operatorname{Var}(c'\widehat{\theta}) = \sigma^2[a'a - c'X(X'X)^{-1}X] = \sigma^2a'(I_n - P_X)a \succeq O,$$

so that  $Var(a'y) \succeq Var(c'\hat{\theta})$ , which is minimum variance.

• Similarly,  $c'\widehat{\beta}$  is BLUE for  $c'\beta$ : Suppose a'y is a linear unbiased estimator of  $c'\beta$ , then  $a'X\beta = c'\beta$ ,  $\forall \beta \Rightarrow a'X = c'$ . Then  $\operatorname{Var}(a'y) - \operatorname{Var}(c'\widehat{\beta}) = \sigma^2 a'a - \sigma^2 c'(X'X)^{-1}c = \sigma^2 a'(I_n - P_X)a \succeq O$ .

#### 28 Estimability

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

*Proof*: If there is a linear unbiased estimator for  $\beta$ , we have  $\mathbb{E}(a_i'y) = \beta_i$ , i = 1, ..., p. Setting  $A' = (a_1, ..., a_p)$  leads to  $E(Ay) = \beta \Rightarrow AX\beta = \beta$ ,  $\forall \beta \Rightarrow AX = I_p$ . However,  $p = \operatorname{rank}(I_p) = \operatorname{rank}(AX) \leq \operatorname{rank}(X) = r$ , which contradicts with r < p.

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

- By the above,  $Var[a'\beta] = a' Var[(X'X)^{-}X'y]a = \sigma^{2}a'[(X'X)^{-}X'X(X'X)^{-}]a = \sigma^{2}a'(X'X)^{-}a$ .
- If  $a'\beta$  is estimable,  $a'\widehat{\beta}$  is unique. Proof  $a' = b'X \Rightarrow a'\beta = b'X\beta = b'\theta$ . Similarly,  $a'\widehat{\beta} = b'X\widehat{\beta} = b'\widehat{\theta}$ , which is unique. By theorem for BLUE,  $b'\widehat{\theta}$  is the BLUE of  $b'\theta$ , so that  $a'\widehat{\beta}$  is the BLUE of  $a'\beta$ .
  - Since the GLS estimate is simply the OLS for a transformed model,  $a'\widehat{\beta}_W$  is the BLUE of  $a'\beta$ . This implies that the OLS estimate  $a'\widehat{\beta}$  is not BLUE in a less-than-full-rank model, although this is still unbiased. That is  $E(a'\widehat{\beta}) = E(a'\widehat{\beta}_w) = a'\beta$ , but  $\text{var}[b'Y] \ge \text{var}[a'\widehat{\beta}] \ge \text{var}[a'\widehat{\beta}_W]$ .
- $a'\mathbb{E}(\widehat{\beta})$  is an estimable function of  $\beta$ .  $Proof: a'\mathbb{E}(\widehat{\beta}) = a'\mathbb{E}[(X'X)^-X'Y] = a'(X'X)^-X'X\beta = c'\beta$ , 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  $Var(Y) = \sigma^2 I_n$ . a'Y is the linear unbiased estimate of E(a'Y) with minimum variance iff 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  $E(c'Y) = c'X\beta = a'X\beta = E(a'Y)$  for  $\forall b$  s.t. E(b'Y) = 0.  $\operatorname{var}(c'Y) = \operatorname{var}(a'Y) + \operatorname{var}(b'Y) + \operatorname{cov}(a'Y, b'Y) \ge \operatorname{var}(a'Y) + \operatorname{var}(b'Y)$  with equality iff  $\operatorname{cov}(a'Y, b'Y) = 0$ .

• Example: Consider a one-way ANOVA,  $y_{ij} = \mu + \tau_i + \epsilon_{ij}$ , i = 1, ..., a (No. of group),  $j = 1, ..., n_i$ 

(No. of obs in the *i*th group). Let  $n = \sum_{i=1}^{a} n_i$ . Then the model can be written as

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

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

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

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

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

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

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

# 29 Distribution Theory

- Consider  $y = X\beta + \epsilon \sim N_n(X\beta, \sigma^2 I_n)$ , where  $X : n \times p$ , rank(X) = p, and  $\beta : p \times 1$ .  $Q_X = I_n P_X$ .
- $\widehat{\beta} \sim N_p(\beta, \sigma^2(X'X)^{-1})$ .
- $(\widehat{\beta} \beta)' X' X (\widehat{\beta} \beta) / \sigma^2 \sim \chi_p^2(0)$  by above.
- $\widehat{\beta} \perp \!\!\!\perp y \widehat{y}$  since  $\operatorname{Cov}(\widehat{\beta}, y \widehat{y}) = \operatorname{Cov}((X'X)^{-1}X'y, Q_Xy) = (X'X)^{-1}X'(\sigma^2I_n)Q'_X = 0$ .
- $\widehat{\beta} \perp \!\!\! \perp S^2 = (y \widehat{y})'(y \widehat{y})/(n p) = y'Q_Xy/(n p)$  by above.
- $SSE/\sigma^2 = (n-p)S^2/\sigma^2 = y'Q_Xy/\sigma^2 \sim \chi_r^2(0)$ , where  $r = rank(Q_X) = n-p$ .

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

- $-E(SSE/\sigma^2) = n p \Rightarrow E(SSE/(n-p)) = \sigma^2$
- Another solution:  $E(y'Qy) = \operatorname{tr}(Q\sigma^2 I_n) + \mu Q\mu = \sigma^2(n-p)$
- MLE of  $\beta$  coincides with the least square estimate for  $\beta$ :  $\widehat{\beta} = (X'X)^{-1}X'y$ .
- MLE of  $\sigma^2$  is  $\widehat{\sigma}_{\text{MLE}}^2 = \text{SSE}/n = \|y X\widehat{\beta}\|^2/n$ , which is biased, while  $\widehat{\sigma}^2 = \text{SSE}/(n-p)$  is unbiased.

• The information matrix is given by

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

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

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

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

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

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

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

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

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

where  $\lambda_1 = n$  and  $\lambda_j$   $(j \geq 2)$  are eigenvalues of C.  $\operatorname{tr}(C) = c(p-1) = \sum_j \lambda_j$  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  $y_1, \ldots, y_n$  be a random sample from  $N_p(\mu, V)$ .
- Let  $A = \sum_{i=1}^{n} (y_i \overline{y})(y_i \overline{y})' \succ O$ , then log-likelihood is

$$\ell(\mu, V) = C - \frac{n}{2} \log |V| - \frac{1}{2} \sum_{i=1}^{n} (y_i - \mu)' V^{-1} (y_i - \mu)$$

$$= C - \frac{n}{2} \log |V| - \frac{1}{2} \sum_{i=1}^{n} (y_i - \overline{y})' V^{-1} (y_i - \overline{y}) - \frac{1}{2} \sum_{i=1}^{n} (\overline{y} - \mu)' V^{-1} (\overline{y} - \mu)$$

$$\leq C - \frac{n}{2} \log |V| - \frac{1}{2} \operatorname{tr}(V^{-1} A)$$

with equality (maximum) when  $\mu = \widehat{\mu} = \overline{y}$ .

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

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

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

#### 31 Generalized Least Square Estimate

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

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

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

$$SSE = (\widetilde{Y} - \widetilde{X}\widehat{\beta}_W)'(\widetilde{Y} - \widetilde{X}\widehat{\beta}_W) = (Y - X\widehat{\beta}_W)'V^{-1}(Y - X\widehat{\beta}_W)$$

• Let  $P_{\widetilde{X}}$  be the orthogonal projection such that  $P_{\widetilde{X}}y = \widetilde{X}\widehat{\beta}_W$ , then

$$SSE = (\widetilde{Y} - \widetilde{X}\widehat{\beta}_{W})'(\widetilde{Y} - \widetilde{X}\widehat{\beta}_{W}) = \widetilde{Y}'(I - P_{\widetilde{X}})\widetilde{Y} = (\widetilde{Y} - \widetilde{X}\beta)'(I - P_{\widetilde{X}})(\widetilde{Y} - \widetilde{X}\beta) = \widetilde{\epsilon}(I - P_{\widetilde{X}})\widetilde{\epsilon}$$

$$\Rightarrow \frac{SSE}{\sigma^{2}} = \frac{(Y - X\widehat{\beta}_{W})'V^{-1}(Y - X\widehat{\beta}_{W})}{\sigma^{2}} = \frac{\widetilde{\epsilon}(I - P_{\widetilde{X}})\widetilde{\epsilon}}{\sigma^{2}} \sim \chi_{n-p}^{2}(0)$$

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

- If  $\epsilon \sim N_n(0, \sigma^2 V)$ , then  $\widehat{\beta}_W \sim N_p(\beta, \sigma^2 (X'V^{-1}X)^{-1})$
- Suppose  $V = \operatorname{diag}(\omega_1, \dots, \omega_n)$ , where  $\omega_i = \operatorname{Var}(y_i)$ . If  $\omega_i$  depends only on the values of X, then errors are heteroscedastic.
- (Important) Let  $\widehat{\beta}$  be OLS estimate.  $\widehat{\beta}_W = \widehat{\beta} \Leftrightarrow C(V^{-1}X) = C(X) \Leftrightarrow C(VX) = C(X)$ . 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,  $C(X)^{\perp} \subseteq C(V^{-1}X)^{\perp} \Leftrightarrow C(X) \supseteq C(V^{-1}X)$ . However, by  $\operatorname{rank}(V^{-1}X) = \operatorname{rank}(X)$  and the **rank-nullity theorem**,  $C(V^{-1}X) = C(X)$ . Finally,

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

where W is a nonsingular matrix.

#### 32 Add Regressions to a Model

- Assume that  $\mathbb{E}(y) = X\beta$ , where  $\operatorname{Var}(\epsilon) = \sigma^2 I$  and then  $\widehat{\beta} = (X'X)^{-1}X'y$ .
- 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

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

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

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

• 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

$$\mathbb{E}(y) = X\beta + P_X Z\gamma + Q_X Z\gamma$$

$$= X[\beta + (X'X)^{-1} X'Z\gamma] + Q_X Z\gamma$$

$$= X\alpha + Q_X Z\gamma.$$

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

$$\widehat{\alpha} = (X'X)^{-1}X'y = \widehat{\beta}_G + (X'X)^{-1}X'Z\widehat{\gamma}_G = \widehat{\beta}_G + L\widehat{\gamma}_G,$$

$$\widehat{\gamma}_G = (Z'Q'_XQ_XZ)^{-1}Z'Q_Xy = (Z'Q_XZ)^{-1}Z'Q_Xy = MZ'Q_Xy,$$

$$\widehat{\beta}_G = (X'X)^{-1}X'(y - Z\widehat{\gamma}_G) = \widehat{\beta} - L\widehat{\gamma}_G,$$

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

Check that  $Z'Q_XZ$  is nonsingular: Suppose  $Z'Q_XZa=0$ . Then

$$a'Z'Q_XZa = ||Q_XZa|| = 0 \Rightarrow Q_XZa = 0 \Rightarrow Za = P_XZa = X(X'X)^{-1}X'Za \in C(X).$$

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

• Variance-covariance matrix is a bit complicated.

$$\operatorname{Var}(\widehat{\gamma}_{G}) = \sigma^{2} M Z' Q_{X} Z M = \sigma^{2} M$$

$$\operatorname{Cov}(\widehat{\beta}, \widehat{\gamma}_{G}) = \operatorname{Cov}((X'X)^{-1} X' y, M Z' Q_{X} y) = \sigma^{2} (X'X)^{-1} X' Q_{X} Z M = O$$

$$\operatorname{Var}(\widehat{\beta}_{G}) = \operatorname{Var}(\widehat{\beta} - L \widehat{\gamma}_{G}) = \operatorname{Var}(\widehat{\beta}) + L \operatorname{Var}(\widehat{\gamma}_{G}) L' = \sigma^{2} [(X'X)^{-1} + L M L'],$$

$$\operatorname{Cov}(\widehat{\beta}_{G}, \widehat{\gamma}_{G}) = \operatorname{Cov}(\widehat{\beta} - L \widehat{\gamma}_{G}, \widehat{\gamma}_{G}) = O - L \operatorname{Var}(\widehat{\gamma}_{G}) = -\sigma^{2} L M.$$

To summarize,

$$\operatorname{Cov}\begin{pmatrix} \widehat{\beta}_G \\ \widehat{\gamma}_G \end{pmatrix} = \sigma^2 \begin{pmatrix} (X'X)^{-1} + LML' & -LM \\ -ML' & M \end{pmatrix}.$$

We also see that  $\operatorname{Var}(\widehat{\beta}_G) = \sigma^2[(X'X)^{-1} + LML'] \succeq \sigma^2(X'X)^{-1} = \operatorname{Var}(\widehat{\beta})$  because  $a'LML'a = \|M^{1/2}L'a\|^2 > 0 \implies LML' \succeq O$ ,

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).

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

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

• Using this, SSE in G model is given by

$$SSE_G = y'(I - P_W)y = y'(I - P_X - Q_X Z(Z'Q_X Z)^{-1}Z'Q_X)y$$
$$= SSE - y'Q_X ZMZ'Q_X y \le SSE$$

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

#### 33 Estimate under Linear Constraints

- Consider  $y = X\beta + \epsilon$ , where  $\mathbb{E}(\epsilon) = 0$  and  $Cov(\epsilon) = \sigma^2 I_n$ . Assume  $X : n \times p$  and  $\beta : p \times 1$ .
- First, suppose 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

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

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

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

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

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

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

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

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

• 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

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

• Lemma 2:  $\omega^{\perp} \cap \Omega = C(P_{\Omega}A'_1)$ . Proof: Show  $\omega^{\perp} \cap \Omega \subseteq C(P_{\Omega}A'_1)$  and  $C(P_{\Omega}A'_1) \subseteq \omega^{\perp} \cap \Omega$  (See earlier).

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

$$\begin{split} \widehat{\theta}_{H} &= P_{\omega} \widetilde{y} = (P_{\Omega} - P_{\omega^{\perp} \cap \Omega}) \widetilde{y} \quad \text{by lemma 1} \\ &= (P_{\Omega} - P_{C(P_{\Omega} A_{1}')}) \widetilde{y} \quad \text{by lemma 2} \\ &= (P_{\Omega} - P_{\Omega} A_{1}' (A_{1} P_{\Omega} A_{1}')^{-1} A_{1} P_{\Omega}) (y - X \beta_{0}) \\ &= P_{\Omega} (y - X \beta_{0}) - P_{\Omega} A_{1}' (A_{1} P_{\Omega} A_{1}')^{-1} A_{1} P_{\Omega} (y - X \beta_{0}) \\ &= X (\widehat{\beta} - \beta_{0}) - P_{\Omega} A_{1}' (A_{1} P_{\Omega} A_{1}')^{-1} A_{1} X (\widehat{\beta} - \beta_{0}) \\ &= X (\widehat{\beta} - \beta_{0}) - X (X'X)^{-1} A' (A(X'X)^{-1} A)^{-1} A (\widehat{\beta} - \beta_{0}) \quad \because P_{\Omega} A_{1}' = X (X'X)^{-1} A' \\ &= X (\widehat{\beta} - \beta_{0}) - X (X'X)^{-1} A' (A(X'X)^{-1} A)^{-1} (A\widehat{\beta} - c). \end{split}$$

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

$$X\widehat{\beta}_{H} = X\widehat{\beta} - X(X'X)^{-1}A'(A(X'X)^{-1}A)^{-1}(A\widehat{\beta} - c)$$

$$\Rightarrow \widehat{\beta}_{H} = \widehat{\beta} - (X'X)^{-1}A'[A(X'X)^{-1}A']^{-1}(A\widehat{\beta} - c) \quad \therefore \text{ premultiply by } (X'X)^{-1}X'$$

Indeed,  $A\widehat{\beta}_H = A\widehat{\beta} - (A\widehat{\beta} - c) = c$ . We can use  $(X'X)^-$ , which is more complicated as shown later.

•  $\operatorname{var}(\widehat{\beta}_{Hj}) \leq \operatorname{var}(\widehat{\beta}_j)$  as

$$\operatorname{Var}(\widehat{\beta}_{H}) = \operatorname{Var}[(I - (X'X)^{-1}A'[A(X'X)^{-1}A']^{-1}A)\widehat{\beta}]$$

$$= \sigma^{2}[(X'X)^{-1} - (X'X)^{-1}A'[A(X'X)^{-1}A']^{-1}A(X'X)^{-1}]$$

$$\leq \sigma^{2}(X'X)^{-1} = \operatorname{Var}(\widehat{\beta}).$$

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

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

# 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 (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  $\sum_j \gamma_j = 0$ :

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

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

- Suppose  $\operatorname{rank}(X) = r < p$  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  $i = 1, \ldots, q$ , then  $\forall m_i$ , such that  $\mathbb{E}(m_i'y) = a_i'\beta \Rightarrow m_i'X = a_i'$ . Hence, we have A = MX, where  $M = (m_1, \ldots, m_q)' \in \mathbb{R}^{q \times n}$  with rank q as  $q = \operatorname{rank}(A) = \operatorname{rank}(MX) \leq \operatorname{rank}(M) \leq q$ .
- Recall that we consider  $\mathbb{E}(\widetilde{y}) = X\gamma = \theta \in \Omega = C(X)$ . Then  $M\theta = MX\gamma = A(\beta \beta_0) = 0$ , so that  $\theta \in N(M) \cap \Omega := \omega \subseteq \Omega$ . Using this, we form  $X\widehat{\gamma}_H = \widehat{\theta}_H = P_{\omega}\widetilde{y} = (P_{\Omega} P_{C(P_{\Omega}M')})\widetilde{y}$ . 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:

$$X(\widehat{\beta}_{H} - \beta_{0}) = (P_{\Omega} - P_{C(P_{\Omega}M')})\widetilde{y}$$

$$= (P_{\Omega} - P_{\Omega}M'(MP_{\Omega}M')^{-}MP_{\Omega})(y - X\beta_{0})$$

$$= (I_{n} - P_{\Omega}M'(MP_{\Omega}M')^{-}M)(P_{\Omega}y - P_{\Omega}X\beta_{0})$$

$$= (I_{n} - P_{\Omega}M'(MP_{\Omega}M')^{-}M)X(\widehat{\beta} - \beta_{0})$$

$$= X(\widehat{\beta} - \beta_{0}) - P_{\Omega}M'(MP_{\Omega}M')^{-}MX(\widehat{\beta} - \beta_{0})$$

$$= X(\widehat{\beta} - \beta_{0}) - X(X'X)^{-}A'(A(X'X)^{-}A')^{-}A(\widehat{\beta} - \beta_{0})$$

and similarly to full rank X,

$$X\widehat{\beta}_{H} = X\widehat{\beta} - X(X'X)^{-}A'(A(X'X)^{-}A')^{-}A(\widehat{\beta} - \beta_{0})$$

$$\Rightarrow X'X\widehat{\beta}_{H} = X'X\widehat{\beta} - X'X(X'X)^{-}A'(A(X'X)^{-}A')^{-}A(\widehat{\beta} - \beta_{0})$$

$$\Rightarrow X'X\widehat{\beta}_{H} = X'X\widehat{\beta} - A'(A(X'X)^{-}A')^{-}A(\widehat{\beta} - \beta_{0})$$

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

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

$$\widehat{\beta}_{H} = (X'X)^{-} X' X \widehat{\beta} - (X'X)^{-} A' (A(X'X)^{-} A')^{-} A(\widehat{\beta} - \beta_{0})$$

$$= (X'X)^{-} X' y - (X'X)^{-} A' (A(X'X)^{-} A')^{-} A(\widehat{\beta} - \beta_{0})$$

$$= \widehat{\beta} - (X'X)^{-} A' (A(X'X)^{-} A')^{-} (A\widehat{\beta} - c).$$

- 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 (rank $(P_{\Omega}M') = q$ ). Lemma 3:  $P_{\Omega}M'$  has full column rank  $\Leftrightarrow \Omega^{\perp} \cap C(M') = \{0\}$ . Proof:
  - ( $\Rightarrow$ ) Suppose 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: rank $(P_{\Omega}M') < q \Rightarrow \Omega^{\perp} \cap C(M') \neq \{0\}$ . Suppose rank $(P_{\Omega}M') < q$ . For  $\exists \alpha \in \mathbb{R}^q \setminus \{\mathbf{0}\}$  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,  $\operatorname{rank}(P_{\Omega}M') = q$  (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

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

- 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

$$SSE_{H} = \|y - X\widehat{\beta}_{H}\|^{2} = \|y - X\widehat{\beta} + X\widehat{\beta} - X\widehat{\beta}_{H}\|^{2} = SSE + (\widehat{\beta}_{H} - \widehat{\beta})'X'X(\widehat{\beta}_{H} - \widehat{\beta})$$

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

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

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

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

• 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  $B = A(X'X)^{-1}A$ ,

$$\mathbb{E}[SSE_H - SSE] = \mathbb{E}[Z'B^{-1}Z)] = \operatorname{tr}(B^{-1}(\sigma^2 B)) + (A\beta - c)'B^{-1}(A\beta - c)$$
$$= \sigma^2 q + (A\beta - c)'[A(X'X)^{-1}A]^{-1}(A\beta - c)$$
$$= \sigma^2 q + (SSE_H - SSE)_{\widehat{\beta} = \beta}.$$

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

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

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

This is not enough! Need to show  $SSE_H - SSE \perp \!\!\! \perp SSE$ 

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

$$X'y \perp \!\!\!\perp Q_X y \Rightarrow (X'X)^{-1}X'y \perp \!\!\!\perp y'Q_X y \Rightarrow \widehat{\beta} \perp \!\!\!\perp SSE \Rightarrow SSE_H - SSE \perp \!\!\!\perp SSE$$

as  $SSE_H - SSE$  is a function of  $\widehat{\beta}$ .

• Let  $S_H^2 = (\mathrm{SSE}_H - \mathrm{SSE})/q$  and  $S^2 = \mathrm{SSE}/(n-p)$ . 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  $SSE_H - SSE = \|\widehat{Y} - \widehat{Y}_H\|^2 = \epsilon'(P - P_H)\epsilon$ . We have

$$SSE_{H} - SSE = (A\widehat{\beta} - c)'[A(X'X)^{-1}A']^{-1}(A\widehat{\beta} - c)$$

$$= (\widehat{\beta} - \beta)'A'[A(X'X)^{-1}A']^{-1}A(\widehat{\beta} - \beta)$$

$$= (Y - X\beta)'X(X'X)^{-1}A'B^{-1}A(X'X)^{-1}X'(Y - X\beta)$$

$$= \epsilon'(P - P_{H})\epsilon.$$

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

$$X'X = \begin{pmatrix} n & 1'x \\ 1'x & x'x \end{pmatrix} = \begin{pmatrix} n & n\overline{x} \\ n\overline{x} & \sum_{i} x_{i}^{2} \end{pmatrix}$$

$$\Rightarrow (X'X)^{-1} = \frac{1}{n \sum_{i} (x_{i} - \overline{x})^{2}} \begin{pmatrix} \sum_{i} x_{i}^{2} & -n\overline{x} \\ -n\overline{x} & n \end{pmatrix} = \frac{1}{\sum_{i} (x_{i} - \overline{x})^{2}} \begin{pmatrix} \frac{1}{n} \sum_{i} x_{i}^{2} & -\overline{x} \\ -\overline{x} & 1 \end{pmatrix}$$

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

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

F statistics for testing

 $- H : \beta_1 = c \text{ is}$ 

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

 $- H : \beta_0 = c \text{ is}$ 

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

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

$$SSE = \sum_{i} (Y_{i} - \widehat{Y}_{i})^{2} = \sum_{i} \left[ Y_{i} - \overline{Y} - \widehat{\beta}_{1}(x_{i} - \overline{x}) \right]$$

$$= \sum_{i} (Y_{i} - \overline{Y})^{2} - 2\widehat{\beta}_{1} \sum_{i} (Y_{i} - \overline{Y})(x_{i} - \overline{x}) + \widehat{\beta}_{1}^{2} \sum_{i} (x_{i} - \overline{x})^{2}$$

$$= \sum_{i} (Y_{i} - \overline{Y})^{2} - \widehat{\beta}_{1}^{2} \sum_{i} (x_{i} - \overline{x})^{2}$$

$$= \sum_{i} (Y_{i} - \overline{Y})^{2} - \sum_{i} (\widehat{Y}_{i} - \overline{Y})^{2}.$$

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

$$r^{2} = \frac{\text{SSReg}}{\text{SSTO}} = \frac{\sum_{i} (\widehat{Y}_{i} - \overline{Y})^{2}}{\sum_{i} (Y_{i} - \overline{Y})^{2}} = \frac{\widehat{\beta}_{1}^{2} \sum_{i} (x_{i} - \overline{x})^{2}}{\sum_{i} (Y_{i} - \overline{Y})^{2}} = \frac{\left[\sum_{i} (Y_{i} - \overline{Y})(x_{i} - \overline{x})^{2}\right]^{2}}{\sum_{i} (Y_{i} - \overline{Y})^{2} \sum_{i} (x_{i} - \overline{x})^{2}},$$

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

$$(1 - r^2) \sum_{i} (Y_i - \overline{Y})^2 = \sum_{i} (Y_i - \hat{Y}_i)^2 = SSE.$$

Using SSE and r, the F statistic for testing

 $- H : \beta_1 = 0$  is

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

 $- H: \beta_0 = 0$  is

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

## 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,

$$\widehat{\beta}_{H} = \widehat{\beta} - (X'X)^{-1}A'[A(X'X)^{-1}A']^{-1}(A\widehat{\beta} - c)$$

$$= \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} - \frac{4}{3} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \frac{1}{3} \begin{pmatrix} -1 \\ 2 \\ 5 \end{pmatrix}.$$

• (b) Determine  $Cov(\widehat{\beta}_H)$ .

$$Cov(\widehat{\beta}_H) = Cov[(I_3 - (X'X)^{-1}A'[A(X'X)^{-1}A']^{-1}A)\widehat{\beta}]$$
  
=  $Cov[(I_3 - 3^{-1}1'_31_3)\widehat{\beta}]$   
=  $\sigma^2(I_3 - 3^{-1}1'_31_3)^2 \preceq \sigma^2I_3 = Cov(\widehat{\beta}),$ 

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

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

For the numerator,

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

Therefore,

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

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  $I'_4\theta = 0$ , 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

$$\widehat{Y}_i = \widehat{\theta}_i = Y_i - \overline{Y} \quad \Leftrightarrow \quad \widehat{Y} = \widehat{\theta} = (I_4 - 11'/4)Y$$

so that the denominator of the F-statistic is

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

• 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

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

Then the numerator of the F is

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

• 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  $\widehat{\theta}_0$  and  $\widehat{\theta}$  be MLEs of  $\theta$  for each space. Then LRT statistic and its asymptotic distribution are

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

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

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

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

so that

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

leading to

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

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

• Instead, using this notation, we have

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

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  $Var(X) = E(X^2) E(X)^2 \ge 0 \Rightarrow E(X^2) \ge E(X)^2$ . So if  $f(x) = x^2$ , then  $E(f(X)) \ge f(E(X))$ . This implies that

$$f(x)$$
 is a convex function  $(f''(x) > 0) \Rightarrow E(f(X)) \ge f(E(X))$ 

$$f(x)$$
 is a concave function  $(f''(x) < 0) \implies E(f(X)) \le f(E(X))$ .

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

#### 40 Iterative Algorithms

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

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

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

• Newton method:

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

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

$$\mathbf{u}(\widehat{\boldsymbol{ heta}}) = \frac{\partial \ell(\widehat{\boldsymbol{ heta}}, \mathbf{y})}{\partial \boldsymbol{ heta}} = \mathbf{0}.$$

Taylor expansion of  $\mathbf{u}(\widehat{\boldsymbol{\theta}})$  around an initial value  $\boldsymbol{\theta}_0$  up to the first order gives

$$\mathbf{u}(\widehat{oldsymbol{ heta}}) pprox \mathbf{u}(oldsymbol{ heta}_0) + rac{\partial \mathbf{u}(oldsymbol{ heta}_0)}{\partial oldsymbol{ heta}}(\widehat{oldsymbol{ heta}} - oldsymbol{ heta}_0) = \mathbf{u}(oldsymbol{ heta}_0) + \mathbf{H}(oldsymbol{ heta}_0)(\widehat{oldsymbol{ heta}} - oldsymbol{ heta}_0) = \mathbf{0} \ \Rightarrow \ \widehat{oldsymbol{ heta}} = oldsymbol{ heta}_0 - \mathbf{H}^{-1}(oldsymbol{ heta}_0)\mathbf{u}(oldsymbol{ heta}_0).$$

#### 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  $a'T'Q_STa = 0$ . Since  $a'T'Q_STa = \|Q_S^{1/2}Ta\|^2$ ,

$$a'T'Q_STa = 0 \Leftrightarrow \|Q_S^{1/2}Ta\|^2 = 0 \Leftrightarrow Q_STa = \mathbf{0} \Leftrightarrow Ta = S(S'S)^{-1}S'Ta \Leftrightarrow a = \mathbf{0}$$
 as  $S \perp \!\!\! \perp T$  implies  $C(S) \cap C(T) = \{\mathbf{0}\}.$ 

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

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

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

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

• (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  $||x||e_1 = ||y||e_1 \Rightarrow H_1x = H_2y \Rightarrow H_2H_1x = y$ , where  $T = H_2H_1$  is orthogonal.

• (HW4) Let  $X_1, \ldots, X_{n_1}$  and  $Y_1, \ldots, Y_{n_2}$  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

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

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

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

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  $X_i \perp \!\!\! \perp S_2^2$  that is a function of  $Y_i$ ,

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

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