38 Lecture 38: April 28

Last time

• Theoretical background of linear model

Today

- Course evaluation (7/17)
- Typo in HW3_keys
- \bullet Theoretical background of linear models cont.
 - Projections
 - Geometry of least squares solution
 - Multivariate normal distribution
 - Independence and Cochran's theorem

Additional reference

Course notes by Dr. Hua Zhou
"A Primer on Linear Models" by Dr. John F. Monahan

Projection

- A matrix $\mathbf{P} \in \mathbb{R}^{m \times n}$ is a projection onto a vector space \mathcal{V} if and only if
 - 1. P is idempotent
 - 2. $\mathbf{P}\mathbf{x} \in \mathcal{V}$ for any $\mathbf{x} \in \mathbb{R}^n$
 - 3. $\mathbf{Pz} = \mathbf{z}$ for any $\mathbf{z} \in \mathcal{V}$.
- Any idempotent matrix \mathbf{P} is a projection onto its own column space $\mathcal{C}(\mathbf{P})$. *Proof:*
- $\mathbf{A}\mathbf{A}^-$ is a projection onto the column space $\mathcal{C}(\mathbf{A})$. *Proof:*
- Start with $\mathbf{P}_{\mathbf{X}}\mathbf{X} = \mathbf{X}$, we have $\mathbf{X}(\mathbf{X}^T\mathbf{X})^-\mathbf{X}^T\mathbf{X} = \mathbf{X}$. Therefore, $(\mathbf{X}^T\mathbf{X})^-\mathbf{X}^T$ is a generalized inverse of \mathbf{X} which is sometimes called the <u>least-squares inverse</u>. And $\mathbf{P}_{\mathbf{X}}$ is a projection onto $\mathcal{C}(\mathbf{X})$.
- The projection matrix

$$\mathbf{P}_{\mathbf{X}} = \mathbf{X}_{n \times p} (\mathbf{X}^T \mathbf{X})^{-} \mathbf{X}^T$$

$$_{p \times p}$$

is unique.

Proof:

- Proposition: Let X, A, B be matrices, then $X^TXA = X^TXB$ if and only if XA = XB. *Proof:*
- $P_{X} \underset{n \times n}{\mathbf{X}} = X_{n \times p}$ Proof:
- Predicted values $\hat{\mathbf{Y}} = \mathbf{X}\hat{\mathbf{b}}_{ls}$ are invariant to choice of solution to the normal equation, where

$$\hat{\mathbf{b}}_{ls} = (\mathbf{X}^T \mathbf{X})^{-} \mathbf{X}^T \mathbf{Y}$$

is not necessarily unique. Proof:

Geometry of least squares

- $\mathbf{P}_{\mathbf{X}}^2 = \mathbf{P}_{\mathbf{X}}$ and $\hat{\mathbf{Y}} = \mathbf{P}_{\mathbf{X}}\mathbf{Y}$ is unique.
- Recall the column space of **X** is $C(\mathbf{X}) = \left\{ \mathbf{y} : \mathbf{y} = \mathbf{X} \mathbf{b} \text{ for some } \mathbf{b} \right\}$
- The vector in $C(\mathbf{X})$ that is closest in terms of squared norm $(L_2 \text{ norm: } ||\mathbf{a} \mathbf{b}||_2 = \sqrt{(\mathbf{a} \mathbf{b})^T(\mathbf{a} \mathbf{b})})$ to \mathbf{Y} is given by $\hat{\mathbf{Y}} = \mathbf{X}\hat{\mathbf{b}}_{ls} = \mathbf{P}_{\mathbf{X}}\mathbf{Y}$.

 Proof:
- $\hat{\mathbf{Y}} \in \mathcal{C}(\mathbf{X})$
- $\hat{\mathbf{e}}_{n\times 1} = \mathbf{Y} \hat{\mathbf{Y}} = (\mathbf{I} \mathbf{P}_{\mathbf{X}})\mathbf{Y} \in \mathcal{N}(\mathbf{X}^T) \text{ where } \mathcal{N}(\mathbf{X}^T) = \left\{ \mathbf{v}_{n\times 1} : \mathbf{X}^T \mathbf{v} = \mathbf{0} \right\} \text{ is the } \frac{\text{null space of } \mathbf{X}^T.}{Proof:}$

Normal distribution in scaler case

• A random variable Z has a standard normal distribution, denoted $Z \sim \mathcal{N}(0,1)$, if

$$F_Z(t) = \Pr(Z \leqslant t) = \int_{-\infty}^{t} \frac{1}{\sqrt{2\pi}} e^{-z^2/2} dz,$$

or equivalently Z has density

$$f_Z(z) = \frac{1}{\sqrt{2\pi}} e^{-z^2/2}, \quad -\infty < z < \infty$$

or equivalently, Z has moment generating function (mgf)

$$m_Z(t) = \mathcal{E}(e^{tZ}) = e^{t^2/2}, \quad -\infty < z < \infty$$

• Non-standard normal random variable

– Definition 1: A random variable X has <u>normal distribution</u> with mean μ and variance σ^2 , denoted $X \sim \mathcal{N}(\mu, \sigma^2)$, if

$$X = \mu + \sigma Z$$

where $Z \sim \mathcal{N}(0,1)$

- Definition 2: $X \sim \mathcal{N}(\mu, \sigma^2)$ if

$$m_X(t) = E(e^{tX}) = e^{t\mu + \sigma^2 t^2/2}, \quad -\infty < t < \infty$$

- In both definitions, $\sigma^2 = 0$ is allowed. If $\sigma^2 > 0$, it has a density

$$f_X(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-(x-\mu)^2/2\sigma^2}, \quad -\infty < x < \infty$$

Multivariate normal distribution

- The <u>standard multivariate normal</u> is a vector of independent standard normals, denoted $\mathbf{Z} \sim \mathcal{N}(\mathbf{0}_p, \mathbf{I}_p)$. The joint density is

$$f_{\mathbf{Z}}(\mathbf{z}) = \frac{1}{(2\pi)^{p/2}} e^{-\sum_{i=1}^{p} z_i^2/2}.$$

The mgf is

$$m_{\mathbf{Z}}(\mathbf{t}) = \prod_{i=1}^{p} m_{Z_i}(t_1) = \prod_{i=1}^{p} e^{t_i^2/2} = e^{\mathbf{t}^T \mathbf{t}/2}.$$

– Consider the affine transformation $\mathbf{X} = \boldsymbol{\mu} + \mathbf{A}\mathbf{Z}$ where $\mathbf{Z} \sim \mathcal{N}(\mathbf{0}_p, \mathbf{I}_p)$. \mathbf{X} has mean and variance

$$E(\mathbf{X}) = \boldsymbol{\mu}, \quad Var(\mathbf{X}) = \mathbf{A}\mathbf{A}^T$$

and the moment generating function is

$$m_{\mathbf{X}}(\mathbf{t}) = \mathrm{E}(e^{\mathbf{t}^T(\boldsymbol{\mu} + \mathbf{A}\mathbf{Z})}) = e^{\mathbf{t}^T\boldsymbol{\mu}} \mathrm{E}(e^{\mathbf{t}^T\mathbf{A}\mathbf{Z}}) = e^{\mathbf{t}^T\boldsymbol{\mu} + \mathbf{t}^T\mathbf{A}\mathbf{A}^T\mathbf{t}/2}.$$

 $-\mathbf{X} \in \mathbb{R}^p$ has a <u>multivariate normal distribution</u> with mean $\boldsymbol{\mu} \in \mathbb{R}^p$ and covariance $\mathbf{V} \in \mathbb{R}^{p \times p}, \mathbf{V} \succeq_{p.s.d.} \mathbf{0}$, denoted $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{V})$, if its mgf takes the form

$$m_{\mathbf{X}}(\mathbf{t}) = e^{\mathbf{t}^T \boldsymbol{\mu} + \mathbf{t}^T \mathbf{V}^T \mathbf{t}/2}, \quad \mathbf{t} \in \mathbb{R}^p$$

- if $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{V})$ and \mathbf{V} is non-singular, then
 - * $\mathbf{V} = \mathbf{A}\mathbf{A}^T$ for some non-singular \mathbf{A}
 - * $\mathbf{A}^{-1}(\mathbf{X} \boldsymbol{\mu}) \sim \mathcal{N}(\mathbf{0}_p, \mathbf{I}_p)$
 - * The density of X is

$$f_{\mathbf{X}}(\mathbf{x}) = \frac{1}{(2\pi)^{p/2} |\mathbf{V}|^{1/2}} e^{-(\mathbf{x} - \boldsymbol{\mu})^T \mathbf{V}^{-1} (\mathbf{x} - \boldsymbol{\mu})/2}.$$

- (Any affine transform of normal is normal) If $\mathbf{X} \in \mathbb{R}^p$, $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{V})$ and $\mathbf{Y} = \mathbf{a} + \mathbf{B}\mathbf{X}$, where $\mathbf{a} \in \mathbb{R}^q$ and $\mathbf{B} \in \mathbb{R}^{q \times p}$, then $\mathbf{Y} \sim \mathcal{N}(\mathbf{a} + \mathbf{B}\boldsymbol{\mu}, \mathbf{B}\mathbf{V}\mathbf{B}^T)$.
- (Marginal of normal is normal) If $\mathbf{X} \in \mathbb{R}^p$, $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{V})$, then any subvector of \mathbf{X} is normal too.
- A convenient fact about normal random variables/vectors is that zero correlation/covariance implies independence.

If $X \sim \mathcal{N}(\mu, V)$ and is partitioned as

$$\mathbf{X} = \left[egin{array}{c} \mathbf{X}_1 \ dots \ \mathbf{X}_m \end{array}
ight], \quad oldsymbol{\mu} = \left[egin{array}{c} oldsymbol{\mu}_1 \ dots \ oldsymbol{\mu}_m \end{array}
ight], \quad \mathbf{V} = \left[egin{array}{c} \mathbf{V}_{11} & \dots & \mathbf{V}_{1m} \ dots & & dots \ \mathbf{V}_{m1} & \dots & \mathbf{V}_{mm} \end{array}
ight]$$

then $\mathbf{X}_1, \dots, \mathbf{X}_m$ are jointly independent if and only if $\mathbf{V}_{ij} = \mathbf{0}$ for all $i \neq j$. *Proof:*

Independence and Cochran's theorem

- (Independence between two linear forms of a multivariate normal) Let $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{V})$, $\mathbf{Y}_1 = \mathbf{a}_1 + \mathbf{B}_1 \mathbf{X}$ and $\mathbf{Y}_2 = \mathbf{a}_2 + \mathbf{B}_2 \mathbf{X}$. Then \mathbf{Y}_1 and \mathbf{Y}_2 are independent if and only if $\mathbf{B}_1 \mathbf{V} \mathbf{B}_2^T = 0$. *Proof:*
- Consider the normal linear model $\mathbf{y} \sim \mathcal{N}(\mathbf{X}\mathbf{b}, \sigma^2\mathbf{I}_n)$
 - Using $\mathbf{A} = (1/\sigma^2)(\mathbf{I} \mathbf{P_X})$, we have

$$SSE/\sigma^2 = ||\hat{\boldsymbol{\epsilon}}||_2^2/\sigma^2 = \mathbf{y}^T \mathbf{A} \mathbf{y} \sim \chi_{n-r}^2,$$

where $r = \text{rank} \mathbf{X}$. Note the noncentrality parameter is

$$\phi = \frac{1}{2} (\mathbf{X}\mathbf{b})^T (1/\sigma^2) (\mathbf{I} - \mathbf{P}_{\mathbf{X}}) (\mathbf{X}\mathbf{b}) = 0$$
 for all \mathbf{b} .

- Using $\mathbf{A} = (1/\sigma^2)\mathbf{P_X}$, we have

$$SSR/\sigma^2 = ||\hat{\mathbf{y}}||_2^2/\sigma^2 = \mathbf{y}^T \mathbf{A} \mathbf{y} \sim \chi_r^2(\phi),$$

with the noncentrality parameter

$$\phi = \frac{1}{2} (\mathbf{X}\mathbf{b})^T (1/\sigma^2) \mathbf{P}_{\mathbf{X}} (\mathbf{X}\mathbf{b}) = \frac{1}{2\sigma^2} ||\mathbf{X}\mathbf{b}||_2^2.$$

– The joint distribution of $\hat{\mathbf{y}}$ and $\hat{\boldsymbol{\epsilon}}$ is

$$\left[\begin{array}{c} \hat{\mathbf{y}} \\ \hat{\boldsymbol{\epsilon}} \end{array}\right] = \left[\begin{array}{c} \mathbf{P_X} \\ \mathbf{I}_n - \mathbf{P_X} \end{array}\right] \mathbf{y} \sim \mathcal{N} \left(\left[\begin{array}{c} \mathbf{X} \mathbf{b} \\ \mathbf{0}_n \end{array}\right], \left[\begin{array}{cc} \sigma^2 \mathbf{P_X} & \mathbf{0} \\ \mathbf{0} & \sigma^2 (\mathbf{I} - \mathbf{P_X}) \end{array}\right]\right).$$

So $\hat{\mathbf{y}}$ is independent of ϵ . Thus $||\hat{\mathbf{y}}||_2^2/\sigma^2$ is independent of $||\hat{\boldsymbol{\epsilon}}||_2^2/\sigma^2$ and

$$F = \frac{||\hat{\mathbf{y}}||_2^2/\sigma^2/r}{||\hat{\boldsymbol{\epsilon}}||_2^2/\sigma^2/(n-r)} \sim F_{r,n-r}(\frac{1}{2\sigma^2}||\mathbf{Xb}||_2^2).$$

- (Independence between linear and quadratic forms of a multivariate normal) Let $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{V})$. Then \mathbf{A} is symmetric with rank s. If $\mathbf{B}\mathbf{V}\mathbf{A} = \mathbf{0}$, then $\mathbf{B}\mathbf{X}$ and $\mathbf{X}^T\mathbf{A}\mathbf{X}$ are independent. *Proof:*
- (Independence between two quadratic forms of a multivariate normal) Let $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{V})$, \mathbf{A} be symmetric with rank r, and \mathbf{B} be symmetric with rank s. If $\mathbf{B}\mathbf{V}\mathbf{A} = \mathbf{0}$, then $\mathbf{X}^T\mathbf{A}\mathbf{X}$ and $\mathbf{X}^T\mathbf{B}\mathbf{X}$ are independent. *Proof:*
- (Cochran's theorem) Let $\mathbf{y} \sim \mathcal{N}(\boldsymbol{\mu}, \sigma^2 \mathbf{I}_n)$ and \mathbf{A}_i , i = 1, ..., k be symmetric idempotent matrix with rank s_i . If $\sum_{i=1}^k \mathbf{A}_i = \mathbf{I}_n$, then $(1/\sigma^2)\mathbf{y}^T\mathbf{A}_i\mathbf{y}$ are independent $\chi^2_{s_i}(\phi_i)$, with $\phi_i = \frac{1}{2\sigma^2}\boldsymbol{\mu}^T\mathbf{A}_i\boldsymbol{\mu}$ and $\sum_{i=1}^k s_i = n$. *Proof:*
- Application to the one-way ANOVA: $y_{ij} = \mu + \alpha_i + \epsilon_{ij}$. We have the classical ANOVA table

Source	df	Projection	SS	Noncentrality
Mean	1	$\mathbf{P_1}$	$SSM = n\bar{y}^2$	$\frac{1}{2\sigma^2}n(\mu+\bar{\alpha})^2$
Group	a-1	$\mathbf{P_X} - \mathbf{P_1}$	$SSA = \sum_{i=1}^{a} n_i \bar{y}_i^2 - n\bar{y}^2$	$\frac{1}{2\sigma^2} \sum_{i=1}^a n_i (\alpha_i - \bar{\alpha})^2$
Error	n-a	$\mathbf{I} - \mathbf{P_X}$	$SSE = \sum_{i=1}^{a} \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2$	0
Total	\overline{n}	I	$SST = \sum_{i} \sum_{j} y_{ij}^{2}$	$\frac{1}{\sigma^2} \sum_{i=1}^a n_i (\mu + \alpha_i)^2$