Multivariate Statistical Analysis

Lecture 14

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Outline

1. Multivariate Analysis of Variance

2. Multivariate Linear Regression

3. Bayesian Multivariate Linear Regression

Outline

Multivariate Analysis of Variance

We consider testing the equality of means with common covariance.

Let $\mathbf{x}_\alpha^{(g)}$ be an observation from the g-th population $\mathcal{N}_p(\boldsymbol{\mu}^{(g)}, \boldsymbol{\Sigma})$ for $\alpha = 1, \ldots, N_g$ and $g = 1, \ldots, q$. We wish to test the hypothesis

$$H_0 : \boldsymbol{\mu}_1 = \cdots = \boldsymbol{\mu}_g.$$

Multivariate Analysis of Variance

The likelihood function is

$$L(\boldsymbol{\mu}^{(1)}, \ldots, \boldsymbol{\mu}^{(g)}, \boldsymbol{\Sigma})$$

$$= \prod_{g=1}^{q} \frac{1}{(2\pi)^{\frac{pN_g}{2}} (\det(\boldsymbol{\Sigma}))^{\frac{N_g}{2}}} \exp\left(-\frac{1}{2} \sum_{\alpha=1}^{N_g} \left(\mathbf{x}_{\alpha}^{(g)} - \boldsymbol{\mu}^{(g)}\right)^{\top} \boldsymbol{\Sigma}^{-1} \left(\mathbf{x}_{\alpha}^{(g)} - \boldsymbol{\mu}^{(g)}\right) \right).$$

1. We let $\boldsymbol{\theta} = \{\boldsymbol{\mu}^{(1)}, \ldots, \boldsymbol{\mu}^{(q)}, \boldsymbol{\Sigma}\}$ be the parameters.

2. The set Ω is the space in which $\boldsymbol{\Sigma}$ is positive definite and each $\boldsymbol{\mu}^{(g)}$ is any p-dimensional vector.

3. The set ω is the space in which $\boldsymbol{\mu}^{(1)} = \cdots = \boldsymbol{\mu}^{(g)}$ (p-dimensional vectors) and $\boldsymbol{\Sigma}$ is positive definite matrix.

Multivariate Analysis of Variance

The likelihood ratio criterion is

$$\lambda = \frac{\sup_{\boldsymbol{\theta} \in \omega} L(\boldsymbol{\theta})}{\sup_{\boldsymbol{\theta} \in \Omega} L(\boldsymbol{\theta})} = \frac{(\det(\hat{\boldsymbol{\Sigma}}_{\Omega}))^{\frac{N}{2}}}{(\det(\hat{\boldsymbol{\Sigma}}_{\omega}))^{\frac{N}{2}}},$$

where

$$\hat{\boldsymbol{\Sigma}}_{\Omega} = \frac{1}{N} \sum_{g=1}^{q} \sum_{\alpha=1}^{N_g} \big(\mathbf{x}_{\alpha}^{(g)} - \bar{\mathbf{x}}^{(g)}\big)\big(\mathbf{x}_{\alpha}^{(g)} - \bar{\mathbf{x}}^{(g)}\big)^{\top}$$

and

$$\hat{\boldsymbol{\Sigma}}_{\omega} = \frac{1}{N} \sum_{g=1}^{q} \sum_{\alpha=1}^{N_g} \big(\mathbf{x}_{\alpha}^{(g)} - \bar{\mathbf{x}}\big)\big(\mathbf{x}_{\alpha}^{(g)} - \bar{\mathbf{x}}\big)^{\top}.$$

Multivariate Analysis of Variance

We can write

$$N\hat{\boldsymbol{\Sigma}}_\omega = \mathbf{A} + \mathbf{B},$$

where

$$\mathbf{A} = N\hat{\boldsymbol{\Sigma}}_\Omega = \sum_{g=1}^{q} \sum_{\alpha=1}^{N_g} \left(\mathbf{x}_\alpha^{(g)} - \bar{\mathbf{x}}^{(g)}\right)\left(\mathbf{x}_\alpha^{(g)} - \bar{\mathbf{x}}^{(g)}\right)^\top \sim \mathcal{W}_p(\boldsymbol{\Sigma}, N - q)$$

and

$$\mathbf{B} = \sum_{g=1}^{q} N_g(\bar{\mathbf{x}}^{(g)} - \bar{\mathbf{x}})(\bar{\mathbf{x}}^{(g)} - \bar{\mathbf{x}})^\top \sim \mathcal{W}_p(\boldsymbol{\Sigma}, q - 1)$$

are independent.

Wilks' Lambda distribution

For two independent random matrices $\mathbf{A} \sim \mathcal{W}_p(\boldsymbol{\Sigma}, n)$ and $\mathbf{B} \sim \mathcal{W}_p(\boldsymbol{\Sigma}, m)$ with $n \geq p$, the ratio

$$\frac{\det(\mathbf{A})}{\det(\mathbf{A} + \mathbf{B})}$$

has Wilks' Lambda distribution with degrees of freedom n and m, which is typically written as

$$\frac{\det(\mathbf{A})}{\det(\mathbf{A} + \mathbf{B})} \sim \Lambda_{p,n,m}.$$

Wilks' Lambda distribution

Theorem

Let $\mathbf{A} \sim \mathcal{W}_p(\mathbf{\Sigma}, n)$ and $\mathbf{B} \sim \mathcal{W}_p(\mathbf{\Sigma}, m)$ be two independent Wishart distributed variables, then we can write

$$\frac{\det(\mathbf{A})}{\det(\mathbf{A} + \mathbf{B})} = \prod_{i=1}^{p} u_i \sim \Lambda_{p,n,m},$$

where $u_1, \ldots, u_p$ are independent distributed as

$$u_i \sim \mathrm{Beta}\left(\frac{n+1-i}{2}, \frac{m}{2}\right).$$

Generalized Variance

Let $\mathbf{A} \sim \mathcal{W}_p(\mathbf{\Sigma}, n)$, we can follow above theorem to show

$$\det(\mathbf{A}) = \det(\mathbf{\Sigma}) \prod_{i=1}^{p} v_i$$

with some independent random variables $v_1, \ldots, v_p$?

Properties of Wishart Distribution

Let $\mathbf{A} \sim \mathcal{W}_p(\mathbf{\Sigma}, n)$ and partition $\mathbf{A}$ and $\mathbf{\Sigma}$ into q and $p - q$ rows and columns as

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix} \qquad \text{and} \qquad \mathbf{\Sigma} = \begin{bmatrix} \mathbf{\Sigma}_{11} & \mathbf{\Sigma}_{12} \\ \mathbf{\Sigma}_{21} & \mathbf{\Sigma}_{22} \end{bmatrix},$$

then we have

(a) $\mathbf{A}_{11} \sim \mathcal{W}_q(\mathbf{\Sigma}_{11}, n)$ and $\mathbf{A}_{22} \sim \mathcal{W}_{p-q}(\mathbf{\Sigma}_{22}, n)$;

(b) if $q = 1$, then

$$\mathbf{a}_{21} \,|\, \mathbf{A}_{22} \sim \mathcal{N}_{p-q}(\mathbf{A}_{22} \mathbf{\Sigma}_{22}^{-1} \boldsymbol{\sigma}_{21}, \sigma_{11.2}^2 \mathbf{A}_{22})$$

where $\sigma_{11.2}^2 = \sigma_{11} - \boldsymbol{\sigma}_{21}^\top \mathbf{\Sigma}_{22}^{-1} \boldsymbol{\sigma}_{21}$;

(c) if $n > p - q$, then

$$\mathbf{A}_{11.2} = \mathbf{A}_{11} - \mathbf{A}_{12} \mathbf{A}_{22}^{-1} \mathbf{A}_{21} \sim \mathcal{W}_q(\mathbf{\Sigma}_{11.2}, n - p + q)$$

is independent on $\mathbf{A}_{22}$ and $\mathbf{A}_{12}$, where $\mathbf{\Sigma}_{11.2} = \mathbf{\Sigma}_{11} - \mathbf{\Sigma}_{12} \mathbf{\Sigma}_{22}^{-1} \mathbf{\Sigma}_{21}$.

Outline

Multivariate Linear Regression

Given dataset $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^N$, where $\mathbf{x}_i \in \mathbb{R}^p$ and $\mathbf{y}_i \in \mathbb{R}^q$ are the feature and the corresponding output of the i-th data.

We suppose

$$\mathbf{y}_i = \mathbf{B}^\top \mathbf{x}_i + \boldsymbol{\epsilon}_i \quad \text{with} \quad \mathbf{B} \in \mathbb{R}^{p \times q} \qquad \text{and} \qquad \boldsymbol{\epsilon}_i \stackrel{\text{i.i.d}}{\sim} \mathcal{N}_q(\mathbf{0}, \boldsymbol{\Sigma})$$

for $i = 1, \ldots, N$, $\boldsymbol{\Sigma} \succ 0$ and $N > p$.

We regard $\mathbf{B} \in \mathbb{R}^{p \times q}$ and $\boldsymbol{\Sigma} \in \mathbb{R}^{q \times q}$ as parameters, then

$$\boldsymbol{\epsilon}_i = \mathbf{y}_i - \mathbf{B}^\top \mathbf{x}_i \sim \mathcal{N}_q(\mathbf{0}, \boldsymbol{\Sigma}).$$

Multivariate Linear Regression

We denote

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \vdots \\ \mathbf{x}_N^\top \end{bmatrix} \in \mathbb{R}^{N \times p}, \quad \mathbf{Y} = \begin{bmatrix} \mathbf{y}_1^\top \\ \vdots \\ \mathbf{y}_N^\top \end{bmatrix} \in \mathbb{R}^{N \times q} \quad \text{and} \quad \mathbf{E} = \begin{bmatrix} \boldsymbol{\epsilon}_1^\top \\ \vdots \\ \boldsymbol{\epsilon}_N^\top \end{bmatrix} \in \mathbb{R}^{N \times q},$$

and suppose $\mathbf{X}$ is full rank.

MLE for Multivariate Linear Regression

We construct the likelihood function for $\epsilon_1, \ldots, \epsilon_N$ as follows

$$
\begin{aligned}
&L(\mathbf{B}, \mathbf{\Sigma}) \\
&= \prod_{\alpha=1}^{N} \frac{1}{\sqrt{(2\pi)^p \det(\mathbf{\Sigma})}} \exp\left(-\frac{1}{2}(\mathbf{B}^\top \mathbf{x}_\alpha - \mathbf{y}_\alpha)^\top \mathbf{\Sigma}^{-1}(\mathbf{B}^\top \mathbf{x}_\alpha - \mathbf{y}_\alpha)\right) \\
&= \frac{1}{(2\pi)^{Np/2}(\det(\mathbf{\Sigma}))^{N/2}} \exp\left(-\frac{1}{2}\operatorname{tr}\left((\mathbf{X}\mathbf{B} - \mathbf{Y})\mathbf{\Sigma}^{-1}(\mathbf{X}\mathbf{B} - \mathbf{Y})^\top\right)\right).
\end{aligned}
$$

The maximum likelihood estimators are

$$
\hat{\mathbf{B}} = \left(\mathbf{X}^\top \mathbf{X}\right)^{-1} \mathbf{X}^\top \mathbf{Y} \qquad \text{and} \qquad \hat{\mathbf{\Sigma}} = \frac{1}{N} \mathbf{Y}^\top (\mathbf{I} - \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top) \mathbf{Y}.
$$

MLE for Multivariate Linear Regression

We write

$$\mathbf{B} = \begin{bmatrix} \boldsymbol{\beta}_1 & \cdots & \boldsymbol{\beta}_q \end{bmatrix} \in \mathbb{R}^{q \times p} \quad \text{and} \quad \hat{\mathbf{B}} = \begin{bmatrix} \hat{\boldsymbol{\beta}}_1 & \cdots & \hat{\boldsymbol{\beta}}_q \end{bmatrix} \in \mathbb{R}^{q \times p}.$$

Then the joint distribution of $\hat{\boldsymbol{\beta}}_1, \ldots, \hat{\boldsymbol{\beta}}_N$ is normal and we have

1. $\mathbb{E}[\hat{\boldsymbol{\beta}}_i] = \boldsymbol{\beta}_i$;
2. $\mathrm{Cov}[\hat{\boldsymbol{\beta}}_i, \hat{\boldsymbol{\beta}}_j] = \sigma_{ij}(\mathbf{X}^\top \mathbf{X})^{-1}$;
3. $\hat{\boldsymbol{\Sigma}} \sim \mathcal{W}_q \left(\frac{1}{N} \boldsymbol{\Sigma}, N - p \right)$.

Outline

Bayesian Multivariate Linear Regression

We can additionally suppose each b_{ij} independently follows

$$b_{ij} \sim \mathcal{N}(0, \tau^2),$$

then the posterior likelihood function is

$$
\begin{aligned}
&L(\mathbf{B}, \boldsymbol{\Sigma}) \\
=&\prod_{i=1}^{N} \frac{1}{\sqrt{(2\pi)^p \det(\boldsymbol{\Sigma})}} \exp\left(-\frac{1}{2}(\mathbf{B}^\top \mathbf{x}_i - \mathbf{y}_i)^\top \boldsymbol{\Sigma}^{-1}(\mathbf{B}^\top \mathbf{x}_i - \mathbf{y}_i)\right) \\
&\cdot \prod_{i=1}^{p}\prod_{j=1}^{q} \frac{1}{\sqrt{2\pi\tau^2}} \exp\left(-\frac{b_{ij}^2}{2\tau^2}\right) \\
\propto& \frac{1}{(\det(\boldsymbol{\Sigma}))^{N/2}} \exp\left(-\frac{1}{2}\mathrm{tr}\left((\mathbf{X}\mathbf{B} - \mathbf{Y})\boldsymbol{\Sigma}^{-1}(\mathbf{X}\mathbf{B} - \mathbf{Y})^\top\right) - \frac{1}{2\tau^2}\|\mathbf{B}\|_F^2\right),
\end{aligned}
$$

which leads to

$$\mathrm{vec}(\hat{\mathbf{B}}) = (\mathbf{I}_q \otimes \tau^2 \mathbf{X}^\top \mathbf{X} + \boldsymbol{\Sigma} \otimes \mathbf{I}_p)^{-1}\mathrm{vec}(\tau^2 \mathbf{X}^\top \mathbf{Y}).$$

Bayesian Multivariate Linear Regression

We typically suppose

$$\boldsymbol{\beta}_{(i)} \overset{\text{i.i.d}}{\sim} \mathcal{N}_q(\mathbf{0}, \tau^2 \boldsymbol{\Sigma}), \qquad \text{where} \qquad \mathbf{B} = \begin{bmatrix} \boldsymbol{\beta}_{(1)}^\top \\ \vdots \\ \boldsymbol{\beta}_{(p)}^\top \end{bmatrix} \in \mathbb{R}^{p \times q},$$

then the posterior likelihood function is

$$
\begin{aligned}
&L(\mathbf{B}, \boldsymbol{\Sigma}) \\
=& \prod_{i=1}^{N} \frac{1}{\sqrt{(2\pi)^p \det(\boldsymbol{\Sigma})}} \exp\left(-\frac{1}{2} (\mathbf{B}^\top \mathbf{x}_i - \mathbf{y}_i)^\top \boldsymbol{\Sigma}^{-1} (\mathbf{B}^\top \mathbf{x}_i - \mathbf{y}_i) \right) \\
&\cdot \prod_{j=1}^{p} \frac{1}{\sqrt{(2\pi)^q \det(\boldsymbol{\Sigma})}} \exp\left(-\frac{1}{2\tau^2} \boldsymbol{\beta}_{(j)}^\top \boldsymbol{\Sigma}^{-1} \boldsymbol{\beta}_{(j)} \right) \\
\propto& \frac{1}{(\det(\boldsymbol{\Sigma}))^{N/2}} \exp\left(-\frac{1}{2} \text{tr}\left((\mathbf{X}\mathbf{B} - \mathbf{Y}) \boldsymbol{\Sigma}^{-1} (\mathbf{X}\mathbf{B} - \mathbf{Y})^\top \right) - \frac{1}{2\tau^2} \mathbf{B} \boldsymbol{\Sigma}^{-1} \mathbf{B}^\top \right).
\end{aligned}
$$

Bayesian Multivariate Linear Regression

We have

$$\hat{\mathbf{B}}_\lambda = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{Y},$$

and

$$\hat{\mathbf{\Sigma}}_\lambda = \frac{1}{N} \mathbf{Y}^\top (\mathbf{I} - \mathbf{X}(\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top) \mathbf{Y},$$

where $\lambda = 1/\tau^2$.