

# Multivariate Statistical Analysis

## Lecture 14

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- 1 Bayesian Multivariate Linear Regression
- 2 Principal Components Analysis
- 3 Principal Coordinate Analysis
- 4 Kernel Principal Component Analysis

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# 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

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

which leads to

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

# Bayesian Multivariate Linear Regression

We typically suppose

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

then the posterior likelihood function is

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

# 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

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

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

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- 1 Bayesian Multivariate Linear Regression
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# Population Principal Components Analysis

Let  $\mathbf{x}$  be a  $p$ -dimensional random vector with mean  $\mathbf{0}$  and covariance matrix  $\mathbf{\Sigma} \succ \mathbf{0}$ .

Let  $\mathbf{u}_1 \in \mathbb{R}^p$  with  $\|\mathbf{u}_1\|_2 = 1$  and maximizing the variance of  $\mathbf{u}_1^\top \mathbf{x}$ , then

$$(\mathbf{\Sigma} - \lambda_1 \mathbf{I})\mathbf{u}_1 = \mathbf{0},$$

where  $\lambda_1$  is the largest root of

$$\det(\mathbf{\Sigma} - \lambda \mathbf{I}) = 0.$$

- ① We call  $y_1 = \mathbf{u}_1^\top \mathbf{x}$  as the first principle component of  $\mathbf{x}$ .
- ② The pair  $\lambda_1 \in \mathbb{R}$  and  $\mathbf{u}_1 \in \mathbb{R}^p$  are the largest eigenvalue and corresponding eigenvector of  $\mathbf{\Sigma}$ .



# Population Principal Components Analysis

For the second principle components

$$y_2 = \mathbf{u}_2^\top \mathbf{x},$$

we determine  $\mathbf{u}_2 \in \mathbb{R}^p$  by maximizing the variance of  $y_2$  under the constraints  $\|\mathbf{u}_2\|_2 = 1$  and  $y_2$  be uncorrelated with  $y_1$ .

For the  $k$ -th principle component

$$y_k = \mathbf{u}_k^\top \mathbf{x},$$

we determine  $\mathbf{u}_k$  by maximizing the variance of  $y_k$  under the constraints  $\|\mathbf{u}_k\|_2 = 1$  and  $y_k$  be uncorrelated with  $y_1, \dots, y_{k-1}$ .

# Population Principal Components Analysis

Let vector  $\mathbf{u}_k \in \mathbb{R}^p$  the  $k$ -th principle component

$$y_k = \mathbf{u}_k^\top \mathbf{x}$$

holds that

$$(\mathbf{\Sigma} - \lambda_k \mathbf{I})\mathbf{u}_k = \mathbf{0},$$

where  $\lambda_k$  is the  $k$ -th largest root of

$$\det(\mathbf{\Sigma} - \lambda \mathbf{I}) = 0.$$

The pair  $\lambda_k \in \mathbb{R}$  and  $\mathbf{u}_k \in \mathbb{R}^p$  are the  $k$ -th largest eigenvalue and corresponding eigenvector of  $\mathbf{\Sigma}$ .

# Population Principal Components Analysis

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# PCA for dimensionality Reduction

We can write

$$\mathbf{U}_k = [\mathbf{u}_1 \quad \cdots \quad \mathbf{u}_k] \in \mathbb{R}^{p \times k} \quad \text{and} \quad \mathbf{\Lambda}_k = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_k \end{bmatrix} \in \mathbb{R}^{k \times k}$$

contains the top- $k$  eigenvectors and eigenvalues pairs of  $\mathbf{\Sigma}$ , that is

$$\mathbf{\Sigma} \mathbf{U}_k = \mathbf{U}_k \mathbf{\Lambda} \quad \text{with} \quad \mathbf{U}_k^\top \mathbf{U}_k = \mathbf{I}.$$

# PCA for dimensionality Reduction

We can keep  $\mathbf{U}_k \in \mathbb{R}^{p \times k}$  and transform  $\mathbf{x} \in \mathbb{R}^p$  to

$$\mathbf{U}_k^\top \mathbf{x} \in \mathbb{R}^k,$$

where  $k \ll p$ .

The information of  $\mathbf{x}$  can be estimated by

$$\hat{\mathbf{x}} = \mathbf{U}_k (\mathbf{U}_k^\top \mathbf{x}) \in \mathbb{R}^p.$$

We have

$$\text{Cov}[\hat{\mathbf{x}}] = \mathbf{U}_k \mathbf{\Lambda}_k \mathbf{U}_k^\top,$$

which is the best rank- $k$  approximation of  $\mathbf{\Sigma}$ .

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# Sample Principal Components Analysis

Given observation  $\mathbf{x}_1, \dots, \mathbf{x}_N \in \mathbb{R}^p$ , we construct sample covariance

$$\mathbf{S} = \frac{1}{N-1} \sum_{\alpha=1}^N (\mathbf{x} - \bar{\mathbf{x}})(\mathbf{x} - \bar{\mathbf{x}})^\top, \quad \text{where } \bar{\mathbf{x}} = \frac{1}{N} \sum_{\alpha=1}^N \mathbf{x}_\alpha.$$

Let spectral decomposition of  $\mathbf{S}$  be  $\mathbf{S} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}$ , where  $\mathbf{U} \in \mathbb{R}^{p \times p}$  is orthogonal and  $\mathbf{\Lambda} \in \mathbb{R}^{p \times p}$  is diagonal.

We write

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \vdots \\ \mathbf{x}_N^\top \end{bmatrix} \in \mathbb{R}^{N \times p},$$

which results the sample principle components

$$\mathbf{Y} = \begin{bmatrix} (\mathbf{x}_1 - \bar{\mathbf{x}})^\top \mathbf{U}_k \\ \vdots \\ (\mathbf{x}_N - \bar{\mathbf{x}})^\top \mathbf{U}_k \end{bmatrix} = \mathbf{H}\mathbf{X}\mathbf{U}_k \in \mathbb{R}^{N \times k}, \quad \text{where } \mathbf{H} = \mathbf{I} - \frac{1}{N} \mathbf{1}_N \mathbf{1}_N^\top \in \mathbb{R}^{N \times N}.$$

# Principal Coordinate Analysis

We consider the case of  $p \geq N$  and define

$$\mathbf{T} = \frac{1}{N-1} \mathbf{H} \mathbf{X} \mathbf{X}^{\top} \mathbf{H} \in \mathbb{R}^{N \times N}$$

with spectral decomposition

$$\mathbf{T} = \mathbf{V} \mathbf{\Gamma} \mathbf{V}^{\top},$$

where  $\mathbf{V} \in \mathbb{R}^{N \times N}$  is orthogonal and  $\mathbf{\Gamma} \in \mathbb{R}^{N \times N}$  is diagonal.

The matrix  $\mathbf{Y} \in \mathbb{R}^{N \times k}$  can be written as

$$\mathbf{Y} = \mathbf{V}_k \mathbf{\Gamma}_k^{1/2} \in \mathbb{R}^{N \times k}.$$



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# Kernel Principal Component Analysis

We consider the case of  $p \geq N$  and define

$$\mathbf{T} = \frac{1}{N-1} \mathbf{H} \mathbf{X} \mathbf{X}^T \mathbf{H} \in \mathbb{R}^{N \times N}$$

with spectral decomposition

$$\mathbf{T} = \mathbf{V} \mathbf{\Gamma} \mathbf{V}^T,$$

where  $\mathbf{V} \in \mathbb{R}^{N \times N}$  is orthogonal and  $\mathbf{\Gamma} \in \mathbb{R}^{N \times N}$  is diagonal.

The matrix  $\mathbf{Y} \in \mathbb{R}^{N \times k}$  can be written as

$$\mathbf{Y} = \mathbf{V}_k \mathbf{\Gamma}_k^{1/2} \in \mathbb{R}^{N \times k}.$$