Multivariate Statistical Analysis

Lecture 16

Fudan University

luoluo@fudan.edu.cn

Outline

Outline

Factor Analysis

Let the observable vector $\mathbf{y} \in \mathbb{R}^p$ be written as

$$\mathbf{y} = \mathbf{W}\mathbf{x} + \boldsymbol{\mu} + \epsilon,$$

where

1. $\mathbf{W} \in \mathbb{R}^{p \times q}$ is the loading matrix (parameter),
2. $\mathbf{x} \in \mathbb{R}^q$ is the common factor (parameter/random vector),
3. $\boldsymbol{\mu} \in \mathbb{R}^p$ is the mean vector (parameter),
4. $\epsilon \in \mathbb{R}^p$ is the specific factor (random vector).

The model is similar to regression, but $\mathbf{x}$ is unobserved.

Factor Analysis

Example of sports games:

$$\mathbf{y} = \mathbf{W}\mathbf{x} + \boldsymbol{\mu} + \epsilon.$$

1. **y**: performance in real-world
2. **W**: system of the game
3. **x**: attributes in the game
4. $\boldsymbol{\mu}$: average attributes
5. ϵ: noise/exception

Outline

1 Factor Analysis

2 Probabilistic Principle Component Analysis

3 The Expectation-Maximization Algorithm

4 Course Summary

Probabilistic Principle Component Analysis

Let $\mathbf{y}_1, \ldots, \mathbf{y}_N \in \mathbb{R}^p$ be N independent observations and we have

$$\mathbf{y}_\alpha = \mathbf{W}\mathbf{x}_\alpha + \boldsymbol{\mu} + \epsilon_\alpha,$$

where

$$\mathbf{x}_\alpha \sim \mathcal{N}_q(\mathbf{0}, \mathbf{I}) \qquad \text{and} \qquad \epsilon_\alpha \sim \mathcal{N}_p(\mathbf{0}, \sigma^2\mathbf{I})$$

are independent for some $\sigma^2 > 0$ and $q < \min\{N, p\}$.

We target to estimate parameters

$$\mathbf{W} \in \mathbb{R}^{p \times q}, \quad \boldsymbol{\mu} \in \mathbb{R}^p \quad \text{and} \quad \sigma \in (0, +\infty)$$

by maximum likelihood estimation for given $\mathbf{y}_1, \ldots, \mathbf{y}_N$.

Probabilistic Principle Component Analysis

Consider that

$$\mathbf{y}_\alpha \sim \mathcal{N}_p(\boldsymbol{\mu}, \mathbf{W}\mathbf{W}^\top + \sigma^2 \mathbf{I}).$$

We construct the likelihood function

$$L(\boldsymbol{\mu}, \mathbf{W}, \sigma^2)$$
$$= \prod_{\alpha=1}^N \frac{1}{\sqrt{(2\pi)^p \det(\boldsymbol{\Sigma})}} \exp\left(-\frac{1}{2}(\mathbf{y}_\alpha - \boldsymbol{\mu})^\top (\mathbf{W}\mathbf{W}^\top + \sigma^2 \mathbf{I})^{-1}(\mathbf{y}_\alpha - \boldsymbol{\mu}) \right),$$

then we have

$$\ln L(\boldsymbol{\mu}, \mathbf{W}, \sigma^2)$$
$$\propto -\frac{N}{2} \ln \det(\mathbf{W}\mathbf{W}^\top + \sigma^2 \mathbf{I}) - \frac{1}{2}\sum_{\alpha=1}^N (\mathbf{y}_\alpha - \boldsymbol{\mu})^\top (\mathbf{W}\mathbf{W}^\top + \sigma^2 \mathbf{I})^{-1}(\mathbf{y}_\alpha - \boldsymbol{\mu}).$$

The Maximum Likelihood Estimators

The maximum likelihood estimators of $\boldsymbol{\mu}$, $\mathbf{W}$ and σ^2 are

$$\hat{\boldsymbol{\mu}} = \bar{\mathbf{y}} = \frac{1}{N}\sum_{\alpha=1}^{N}\mathbf{y}_\alpha, \quad \hat{\mathbf{W}} = \mathbf{U}_q(\boldsymbol{\Lambda}_q - \hat{\sigma}^2\mathbf{I})\mathbf{R} \quad \text{and} \quad \hat{\sigma}^2 = \frac{1}{p-q}\sum_{j=q+1}^{p}\lambda_j,$$

where

1. $\boldsymbol{\Lambda}_q \in \mathbb{R}^{q \times q}$ is diagonal with the largest q eigenvalues $\lambda_1, \ldots, \lambda_q$ of

$$\hat{\boldsymbol{\Sigma}} = \frac{1}{N}\sum_{\alpha=1}^{N}(\mathbf{y}_\alpha - \bar{\mathbf{y}})(\mathbf{y}_\alpha - \bar{\mathbf{y}})^\top;$$

2. $\mathbf{U}_q \in \mathbb{R}^{p \times q}$ is orthogonal column consisting of the eigenvectors associate with $\lambda_1, \ldots, \lambda_q$;

3. $\mathbf{R} \in \mathbb{R}^{q \times q}$ is any orthogonal matrix.

The Maximum Likelihood Estimators

The maximum likelihood estimators also minimize the error with respect to Frobenius norm

$$\left(\hat{\mathbf{W}}, \ \hat{\sigma}^2\right) = \underset{\mathbf{W} \in \mathbb{R}^{p \times q}, \sigma^2 \in \mathbb{R}^+}{\arg \min} \left\| \hat{\mathbf{\Sigma}} - \left(\mathbf{W}\mathbf{W}^\top + \sigma^2 \mathbf{I}\right) \right\|_F.$$

Outline

The Expectation-Maximization Algorithm

For the model

$$\mathbf{y} = \mathbf{W}\mathbf{x} + \boldsymbol{\mu} + \epsilon,$$

where $\mathbf{x} \sim \mathcal{N}_q(\mathbf{0}, \mathbf{I})$ and $\epsilon \sim \mathcal{N}_p(\mathbf{0}, \sigma^2\mathbf{I})$ are independent.

We regard $\{\mathbf{x}_\alpha\}_{\alpha=1}^N$ as missing data and $\{\mathbf{x}_\alpha, \mathbf{y}_\alpha\}_{\alpha=1}^N$ as the complete data, then we can achieve

$$\mathbf{y}_\alpha \,|\, \mathbf{x}_\alpha \sim \mathcal{N}_p(\mathbf{W}\mathbf{x}_\alpha + \boldsymbol{\mu}, \sigma^2\mathbf{I})$$

and

$$\mathbf{x}_\alpha \,|\, \mathbf{y}_\alpha \sim \mathcal{N}_q(\mathbf{M}^{-1}\mathbf{W}^\top(\mathbf{y}_\alpha - \boldsymbol{\mu}), \sigma^2\mathbf{M}^{-1}),$$

where $\mathbf{M} = \mathbf{W}^\top\mathbf{W} + \sigma^2\mathbf{I}$.

The Expectation-Maximization Algorithm

The update of the EM algorithm

1. In E-step, we take the expectation

$$l_C = \mathbb{E}\left[\ln\left(\prod_{\alpha=1}^{N} f(\mathbf{x}_\alpha \mid \mathbf{y}_\alpha)\right)\right].$$

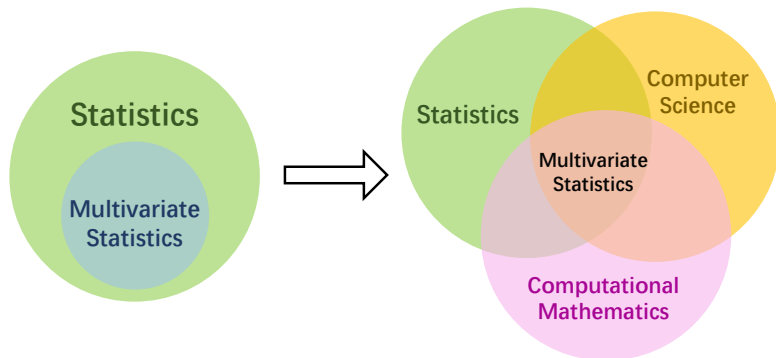2. In the M-step, we maximized l_C with respect to $\mathbf{W}$ and σ^2:

$$\mathbf{W}_+ = \hat{\boldsymbol{\Sigma}}\mathbf{W}(\sigma^2\mathbf{I} + \mathbf{M}^{-1}\mathbf{W}^\top\hat{\boldsymbol{\Sigma}}\mathbf{W})^{-1},$$
$$\sigma_+^2 = \frac{1}{p}\mathrm{tr}\left(\hat{\boldsymbol{\Sigma}} - \hat{\boldsymbol{\Sigma}}\mathbf{W}\mathbf{M}^{-1}\mathbf{W}_+^\top\right).$$

Note that the computational complexity of EM is $\mathcal{O}(Npq)$, while the spectral decomposition in MLE requires $\mathcal{O}(Np^2 + p^3)$.

Outline

Multivariate Statistics

Final Exam

**Multivariate Statistical Analysis
(DATA 13004)**

Machine Learning

Matrix Calculus

Statistics

Linear Algebra

Optimization