## Multivariate Statistics

Lecture 05

Fudan University

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## The Maximum Likelihood Estimators

#### Theorem 1

If  $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$  constitute a sample from  $\mathcal{N}(\mu, \mathbf{\Sigma})$  with p < N, the maximum likelihood estimators of  $\mu$  and  $\mathbf{\Sigma}$  are

$$\hat{\boldsymbol{\mu}} = \bar{\mathbf{x}} = \frac{1}{N} \sum_{\alpha=1}^{N} \mathbf{x}_{\alpha} \quad \text{and} \quad \hat{\boldsymbol{\Sigma}} = \frac{1}{N} \sum_{\alpha=1}^{N} (\mathbf{x}_{\alpha} - \bar{\mathbf{x}}) (\mathbf{x}_{\alpha} - \bar{\mathbf{x}})^{\top}$$

respectively.

#### Lemma 1

If  $\mathbf{D} \in \mathbb{R}^{p \times p}$  is positive definite, the maximum of

$$f(\mathbf{G}) = -N \ln \det(\mathbf{G}) - \operatorname{tr}(\mathbf{G}^{-1}\mathbf{D})$$

with respect to positive definite matrices **G** exists, occurs at  $\mathbf{G} = \frac{1}{N}\mathbf{D}$ .

## The Maximum Likelihood Estimators

#### Theorem 1

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$$\hat{\boldsymbol{\mu}} = \bar{\mathbf{x}} = \frac{1}{N} \sum_{\alpha=1}^{N} \mathbf{x}_{\alpha} \quad \text{and} \quad \hat{\boldsymbol{\Sigma}} = \frac{1}{N} \sum_{\alpha=1}^{N} (\mathbf{x}_{\alpha} - \bar{\mathbf{x}}) (\mathbf{x}_{\alpha} - \bar{\mathbf{x}})^{\top}$$

respectively.

Can we guarantee  $\hat{\mathbf{\Sigma}} = \frac{1}{N} \sum_{\alpha=1}^{N} (\mathbf{x}_{\alpha} - \bar{\mathbf{x}}) (\mathbf{x}_{\alpha} - \bar{\mathbf{x}})^{\top}$  is positive definite?

In the univariate case, the mean of a sample is distributed normally and independently of the sample variance.

In the multivariate case, the sample mean  $\hat{\mu}$  is also distributed normally and independently of  $\hat{\Sigma}$ .

#### Lemma 1

Suppose  $\mathbf{x}_1, \dots, \mathbf{x}_N$  are independent, where  $\mathbf{x}_{\alpha} \sim \mathcal{N}_p(\boldsymbol{\mu}_{\alpha}, \boldsymbol{\Sigma})$ . Let  $\mathbf{C} \in \mathbb{R}^{N \times N}$  be an orthogonal matrix, then

$$\mathbf{y}_{lpha} = \sum_{eta=1}^{N} c_{lphaeta} \mathbf{x}_{eta} \sim \mathcal{N}_{m{p}}(m{
u}_{lpha}, m{\Sigma}),$$

where  $\nu = \sum_{\beta=1}^{N} c_{\alpha\beta} \mu_{\beta}$  for  $\alpha = 1, ..., N$  and  $y_1, ..., y_N$  are independent.

#### Lemma 2

If 
$$\mathbf{C} = \begin{bmatrix} c_{11} & c_{12} & \dots & c_{1N} \\ c_{21} & c_{22} & \dots & c_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ c_{N1} & c_{N2} & \dots & c_{NN} \end{bmatrix} = \begin{bmatrix} c_1^\top \\ c_2^\top \\ \vdots \\ c_N^\top \end{bmatrix} \in \mathbb{R}^{N \times N}$$
 is orthogonal, then 
$$\sum_{\alpha=1}^N \mathbf{x}_{\alpha} \mathbf{x}_{\alpha}^\top = \sum_{\alpha=1}^N \mathbf{y}_{\alpha} \mathbf{y}_{\alpha}^\top \text{ where } \mathbf{y}_{\alpha} = \sum_{\beta=1}^N c_{\alpha\beta} \mathbf{x}_{\beta} \text{ for } \alpha = 1, \dots, N.$$

$$\sum_{\alpha=1}^{N} \mathbf{x}_{\alpha} \mathbf{x}_{\alpha}^{\top} = \sum_{\alpha=1}^{N} \mathbf{y}_{\alpha} \mathbf{y}_{\alpha}^{\top} \text{ where } \mathbf{y}_{\alpha} = \sum_{\beta=1}^{N} c_{\alpha\beta} \mathbf{x}_{\beta} \text{ for } \alpha = 1, \dots, N.$$

$$\text{Let } \mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_M^\top \end{bmatrix} \text{ and } \mathbf{Y} = \begin{bmatrix} \mathbf{y}_1^\top \\ \mathbf{y}_2^\top \\ \vdots \\ \mathbf{y}_M^\top \end{bmatrix}, \text{ then } \mathbf{y}_\alpha = \mathbf{X}^\top \mathbf{c}_\alpha \text{ and } \mathbf{Y} = \mathbf{C}\mathbf{X}.$$

#### Theorem 2

Let  $\mathbf{x}_1, \dots, \mathbf{x}_N$  be independent, each distributed according to  $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ . Then the mean of the sample

$$\hat{\boldsymbol{\mu}} = \bar{\mathbf{x}} = rac{1}{N} \sum_{lpha=1}^{N} \mathbf{x}_{lpha}$$

is distributed according to  $\mathcal{N}(\pmb{\mu}, \frac{1}{N} \pmb{\Sigma})$  and independent of

$$\hat{oldsymbol{\Sigma}} = rac{1}{N} \sum_{lpha=1}^N (\mathbf{x}_lpha - ar{\mathbf{x}}) (\mathbf{x}_lpha - ar{\mathbf{x}})^ op.$$

Additionally, we have  $N\hat{\mathbf{\Sigma}} = \sum_{\alpha=1}^{N-1} \mathbf{z}_{\alpha} \mathbf{z}_{\alpha}^{\top}$ , where  $\mathbf{z}_{\alpha} \sim \mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$  for  $\alpha = 1, \dots, N-1$ , and  $\mathbf{z}_1, \dots, \mathbf{z}_{N-1}$  are independent.

#### Theorem 1

If  $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$  constitute a sample from  $\mathcal{N}(\mu, \mathbf{\Sigma})$  with p < N, the maximum likelihood estimators of  $\mu$  and  $\mathbf{\Sigma}$  are

$$\hat{\mu} = \bar{\mathbf{x}} = \frac{1}{N} \sum_{\alpha=1}^{N} \mathbf{x}_{\alpha}$$
 and  $\hat{\mathbf{\Sigma}} = \frac{1}{N} \sum_{\alpha=1}^{N} (\mathbf{x}_{\alpha} - \bar{\mathbf{x}}) (\mathbf{x}_{\alpha} - \bar{\mathbf{x}})^{\top}$ 

respectively.

#### Theorem 3

Using the notation of Theorem 1, if N>p, the probability is 1 of drawing a sample so that

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

is positive definite.

An estimator  ${f t}$  of a parameter vector  ${m heta}$  is unbiased if and only if

$$\mathbb{E}[\mathbf{t}] = \boldsymbol{\theta}.$$

For the estimators obtain from MLE for normal distribution, the vector  $\hat{\mu}$  is an unbiased estimator of  $\mu$  and  $\hat{\Sigma}$  is a biased estimator of  $\Sigma$ .

Consider the result of MLE for normal distribution:

We have

$$\mathbb{E}[\hat{oldsymbol{\mu}}] = \mathbb{E}[ar{f x}] = \mathbb{E}\left[\sum_{lpha=1}^N {f x}_lpha
ight] = oldsymbol{\mu}$$

and (not limited to normal distribution)

$$\mathbb{E}[\hat{\boldsymbol{\Sigma}}] = \mathbb{E}\left[\frac{1}{N}\sum_{\alpha=1}^{N-1} \mathbf{z}_{\alpha}\mathbf{z}_{\alpha}^{\top}\right] = \frac{N-1}{N}\boldsymbol{\Sigma}.$$

The sample covariance

$$\mathbf{S} = rac{1}{N-1} \sum_{lpha=1}^N (\mathbf{x}_lpha - ar{\mathbf{x}}) (\mathbf{x}_lpha - ar{\mathbf{x}})^ op$$

is an unbiased estimator of  $\Sigma$ .



Properties of the Maximum Likelihood Estimators

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## **Properties of Statistics**

Let

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

We shall show that  $\bar{\mathbf{x}}$  and  $\mathbf{S}$  are sufficient statistics and are complete.

# Sufficiency

A statistic  $\mathbf{t}(\mathbf{y})$  is sufficient for a family of distributions of random variable  $\mathbf{y}$  with parameter  $\boldsymbol{\theta}$ , if the conditional distribution of  $\mathbf{y}$  given  $\mathbf{t}(\mathbf{y}) = \mathbf{t}_0$  does not depend on  $\boldsymbol{\theta}$ .

The statistic  ${f t}$  gives as much information about  ${m heta}$  as the entire sample  ${f y}$ .

#### Theorem 4

A statistic  $\mathbf{t}(\mathbf{y})$  is sufficient for  $\theta$  if and only if the density  $f(\mathbf{y} \mid \theta)$  can be factored as

$$f(\mathbf{y} \mid \boldsymbol{\theta}) = g(\mathbf{t}(\mathbf{y}), \boldsymbol{\theta})h(\mathbf{y})$$

where  $g(\mathbf{t}(\mathbf{y}), \theta)$  and  $h(\mathbf{y})$  are nonnegative and  $h(\mathbf{y})$  does not depend on  $\theta$ .

For the MLE of normal distribution, we apply this theorem with

$$\boldsymbol{\theta} = \{\boldsymbol{\mu}, \boldsymbol{\Sigma}\}, \quad \boldsymbol{y} = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_{\mathcal{N}}\} \quad \text{and} \quad \boldsymbol{t}(\boldsymbol{y}) = \{\bar{\boldsymbol{x}}, \boldsymbol{S}\}.$$

# Sufficiency

#### Theorem 5

If  $x_1, ..., x_N$  are observations from  $\mathcal{N}(\mu, \Sigma)$ , then  $\bar{x}$  and S are sufficient for  $\mu$  and  $\Sigma$ .

If  $\Sigma$  is given,  $\bar{\mathbf{x}}$  is sufficient for  $\mu$ . However, if  $\mu$  is given,  $\mathbf{S}$  is not sufficient for  $\Sigma$ ;

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# Completeness

## Definition (Completeness)

A family of distributions of  $\mathbf{y}$  indexed by  $\boldsymbol{\theta}$  is **complete** if for every real-valued function  $g(\mathbf{y})$ , we have

$$\mathbb{E}[g(\mathbf{y})] \equiv 0$$

identically in  $\theta$  implies  $g(\mathbf{y}) = 0$  except for a set of  $\mathbf{y}$  of probability 0 for every  $\theta$ .

If the family of distributions of a sufficient set of statistics is complete, the set is called a complete sufficient set.

# Completeness

#### Theorem 6

The sufficient set of statistics  $\bar{\mathbf{x}}$ ,  $\mathbf{S}$  is complete for  $\boldsymbol{\mu}, \boldsymbol{\Sigma}$  when the sample is drawn from  $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ .

Sketch of the proof:

• We have  $N\hat{m{\Sigma}} = \sum_{lpha=1}^{N-1} {m{z}}_lpha {m{z}}_lpha^ op$ , where  ${m{z}}_lpha = \sum_{eta=1}^N b_{lphaeta} {m{x}}_eta$  and

$$\mathbf{B} = \begin{bmatrix} \times & \dots & \times \\ \vdots & \ddots & \vdots \\ \frac{1}{\sqrt{N}} & \dots & \frac{1}{\sqrt{N}} \end{bmatrix}$$

② The condition  $\mathbb{E}[g(\bar{\mathbf{x}}, n\mathbf{S})] \equiv 0$  implies the Laplace transform of  $g(\bar{\mathbf{x}}, \mathbf{B} - N\bar{\mathbf{x}}\bar{\mathbf{x}}^{\top}) h(\bar{\mathbf{x}}, \mathbf{B})$  is zero, where  $\mathbf{B} = \sum_{\alpha=1}^{N-1} \mathbf{z}_{\alpha} \mathbf{z}_{\alpha}^{\top} + N\bar{\mathbf{x}}\bar{\mathbf{x}}^{\top}$  and  $h(\bar{\mathbf{x}}, \mathbf{B})$  is the joint density of  $\bar{\mathbf{x}}$  and  $\bar{\mathbf{B}}$ .