Multivariate Statistics

Lecture 04

Fudan University

Outline

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Multivariate Normal Distribution (Conditional Distribution)

Let $\mathbf{x}$ be distributed according to $\mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ with $\boldsymbol{\Sigma} \succ \mathbf{0}$. Let us partition

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}^{(1)} \\ \mathbf{x}^{(2)} \end{bmatrix} \quad \text{with } \mathbf{x}^{(1)} \in \mathbb{R}^q \text{ and } \mathbf{x}^{(2)} \in \mathbb{R}^{p-q}.$$

The joint density of $\mathbf{y}^{(1)} = \mathbf{x}^{(1)} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\mathbf{x}^{(2)}$ and $\mathbf{y}^{(2)} = \mathbf{x}^{(2)}$ is

$$g(\mathbf{y}) = n(\mathbf{y}^{(1)} \mid \boldsymbol{\mu}^{(1)} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\mu}^{(2)}, \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{21})n(\mathbf{y}^{(2)} \mid \boldsymbol{\mu}^{(2)}, \boldsymbol{\Sigma}_{22}).$$

Consider that

$$\begin{bmatrix} \mathbf{y}^{(1)} \\ \mathbf{y}^{(2)} \end{bmatrix} = \begin{bmatrix} \mathbf{I} & -\boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{x}^{(1)} \\ \mathbf{x}^{(2)} \end{bmatrix} = \mathbf{u}(\mathbf{x})$$

and use

$$f(\mathbf{x}) = g(\mathbf{u}(\mathbf{x}))|\det(\mathbf{J}(\mathbf{x}))| = g(\mathbf{u}(\mathbf{x})).$$

Multivariate Normal Distribution (Conditional Distribution)

The resulting joint density of $\mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$ is

$$\begin{aligned}
& f(\mathbf{x}) = f(\mathbf{x}^{(1)}, \mathbf{x}^{(2)}) \\
=& n(\mathbf{y}^{(1)} \mid \boldsymbol{\mu}^{(1)} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\mu}^{(2)}, \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{21}) n(\mathbf{x}^{(2)} \mid \boldsymbol{\mu}^{(2)}, \boldsymbol{\Sigma}_{22}) \\
=& \frac{1}{\sqrt{(2\pi)^q \det(\boldsymbol{\Sigma}_{11.2})}} \exp\left(-\frac{1}{2}(\mathbf{x}_{11.2} - \boldsymbol{\mu}_{11.2})^\top \boldsymbol{\Sigma}_{11.2}^{-1}(\mathbf{x}_{11.2} - \boldsymbol{\mu}_{11.2})\right) \\
& \cdot \frac{1}{\sqrt{(2\pi)^{p-q} \det(\boldsymbol{\Sigma}_{22})}} \exp\left(-\frac{1}{2}\left(\mathbf{x}^{(2)} - \boldsymbol{\mu}^{(2)}\right)^\top \boldsymbol{\Sigma}_{22}^{-1}\left(\mathbf{x}^{(2)} - \boldsymbol{\mu}^{(2)}\right)\right)
\end{aligned}$$

where

$$\begin{aligned}
\mathbf{x}_{11.2} =& \mathbf{x}^{(1)} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\mathbf{x}^{(2)}, \\
\boldsymbol{\mu}_{11.2} =& \boldsymbol{\mu}^{(1)} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\mu}^{(2)}, \\
\boldsymbol{\Sigma}_{11.2} =& \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{21}.
\end{aligned}$$

Multivariate Normal Distribution (Conditional Distribution)

The marginal density of $\mathbf{x}^{(2)}$ is

$$
\begin{aligned}
& f(\mathbf{x}^{(2)}) = n(\mathbf{y}^{(2)} \mid \boldsymbol{\mu}^{(2)}, \boldsymbol{\Sigma}_{22}) \\
= & \frac{1}{\sqrt{(2\pi)^{p-q} \det(\boldsymbol{\Sigma}_{22})}} \exp\left(-\frac{1}{2}\left(\mathbf{x}^{(2)} - \boldsymbol{\mu}^{(2)}\right)^\top \boldsymbol{\Sigma}_{22}^{-1}\left(\mathbf{x}^{(2)} - \boldsymbol{\mu}^{(2)}\right)\right).
\end{aligned}
$$

Hence, the conditional density of $\mathbf{x}^{(1)}$ given that $\mathbf{x}^{(2)}$ is

$$
\begin{aligned}
& f(\mathbf{x}^{(1)} \mid \mathbf{x}^{(2)}) = \frac{f(\mathbf{x}^{(1)}, \mathbf{x}^{(2)})}{f(\mathbf{x}^{(2)})} \\
= & \frac{1}{\sqrt{(2\pi)^{q} \det(\boldsymbol{\Sigma}_{11.2})}} \exp\left(-\frac{1}{2}\left(\mathbf{x}_{11.2} - \boldsymbol{\mu}_{11.2}\right)^\top \boldsymbol{\Sigma}_{11.2}^{-1}\left(\mathbf{x}_{11.2} - \boldsymbol{\mu}_{11.2}\right)\right)
\end{aligned}
$$

Multivariate Normal Distribution (Conditional Distribution)

The conditional density of $\mathbf{x}^{(1)}$ given that $\mathbf{x}^{(2)}$ is

$$f(\mathbf{x}^{(1)} \mid \mathbf{x}^{(2)}) = \frac{f(\mathbf{x}^{(1)}, \mathbf{x}^{(2)})}{f(\mathbf{x}^{(2)})}$$
$$= \frac{1}{\sqrt{(2\pi)^q \det(\boldsymbol{\Sigma}_{11.2})}} \exp\left(-\frac{1}{2}(\mathbf{x}_{11.2} - \boldsymbol{\mu}_{11.2})^\top \boldsymbol{\Sigma}_{11.2}^{-1}(\mathbf{x}_{11.2} - \boldsymbol{\mu}_{11.2})\right)$$

Consider that $\mathbf{x}_{11.2} - \boldsymbol{\mu}_{11.2} = \mathbf{x}^{(1)} - \left(\boldsymbol{\mu}^{(1)} + \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{x}^{(2)} - \boldsymbol{\mu}^{(2)})\right)$.

The density $f(\mathbf{x}^{(1)} \mid \mathbf{x}^{(2)})$ is a q-variate normal density with mean

$$\mathbb{E}\left[\mathbf{x}^{(1)} \mid \mathbf{x}^{(2)}\right] = \boldsymbol{\mu}^{(1)} + \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{x}^{(2)} - \boldsymbol{\mu}^{(2)}) = \boldsymbol{\nu}(\mathbf{x}^{(2)})$$

and covariance matrix (not depend on $\mathbf{x}^{(2)}$)

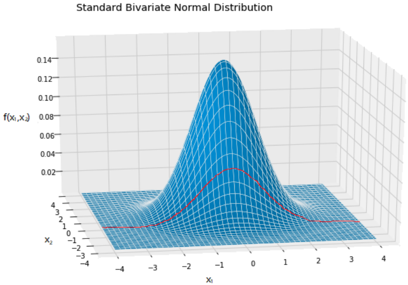
$$\mathrm{Cov}\left[\mathbf{x}^{(1)} \mid \mathbf{x}^{(2)}\right] = \mathbb{E}\left[(\mathbf{x}^{(1)} - \boldsymbol{\nu}(\mathbf{x}^{(2)}))(\mathbf{x}^{(1)} - \boldsymbol{\nu}(\mathbf{x}^{(2)}))^\top \mid \mathbf{x}^{(2)}\right]$$
$$= \boldsymbol{\Sigma}_{11.2} = \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{21} \preceq \boldsymbol{\Sigma}_{11}.$$

Multivariate Normal Distribution (Conditional Distribution)

The density $f(x_1, x_2)$ can be thought of as a surface $z = f(x_1, x_2)$ over the x_1, x_2-plane.

If we intersect this surface with the plane $x_2 = c$, we obtain a curve $z = f(x_1, c)$ over the line $x_2 = c$ in the x_l, x_2-plane.

The ordinate of this curve is proportional to the conditional density of x_1 given $x_2 = c$; that is, it is proportional to the ordinate of the curve of a univariate normal distribution.



Correlation Coefficient

Recall that for random vector $\mathbf{x} = [x_1, x_2, \dots, x_p]^\top$, we define the covariance matrix as

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1p} \\ \sigma_{21} & \sigma_{22} & \cdots & \sigma_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{p1} & \sigma_{p2} & \cdots & \sigma_{pp} \end{bmatrix} \in \mathbb{R}^{p \times p}$$

and the correlation coefficient between x_i and x_j as (suppose $\boldsymbol{\Sigma} \succ \mathbf{0}$)

$$\rho_{ij} = \frac{\sigma_{ij}}{\sqrt{\sigma_{ii}}\sqrt{\sigma_{jj}}}.$$

Partial Correlation Coefficient

Now consider the partition

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}^{(1)} \\ \mathbf{x}^{(2)} \end{bmatrix} \quad \text{with} \quad \mathbf{x}^{(1)} \in \mathbb{R}^q \quad \text{and} \quad \mathbf{x}^{(2)} \in \mathbb{R}^{p-q}.$$

Let

$$\mathbf{\Sigma}_{11.2} = \begin{bmatrix} \sigma_{11\cdot q+1,\dots,p} & \sigma_{12\cdot q+1,\dots,p} & \cdots & \sigma_{1q\cdot q+1,\dots,p} \\ \sigma_{21\cdot q+1,\dots,p} & \sigma_{22\cdot q+1,\dots,p} & \cdots & \sigma_{2q\cdot q+1,\dots,p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{q1\cdot q+1,\dots,p} & \sigma_{q2\cdot q+1,\dots,p} & \cdots & \sigma_{qq\cdot q+1,\dots,p} \end{bmatrix} \in \mathbb{R}^{q\times q}.$$

We define

$$\rho_{ij\cdot q+1,\dots,p} = \frac{\sigma_{ij\cdot q+1,\dots,p}}{\sqrt{\sigma_{ii\cdot q+1,\dots,p}}\sqrt{\sigma_{jj\cdot q+1,\dots,p}}}$$

as the partial correlation between x_i and x_j holding $x_{q+1},\dots,x_p$ fixed.

Multiple Correlation Coefficient

We again consider $\mathbf{x} \sim \mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ such that

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}^{(1)} \\ \mathbf{x}^{(2)} \end{bmatrix}, \quad \boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}^{(1)} \\ \boldsymbol{\mu}^{(2)} \end{bmatrix} \quad \text{and} \quad \boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{bmatrix} \succ \mathbf{0}.$$

Then, we study some properties of $\mathbf{B}\mathbf{x}^{(2)}$, where

$$\mathbf{B} = \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}$$

is the matrix of regression coefficients of $\mathbf{x}^{(1)}$ on $\mathbf{x}^{(2)}$.

The vector $\mathbb{E}\big[\mathbf{x}^{(1)} \mid \mathbf{x}^{(2)}\big] = \boldsymbol{\mu}^{(1)} + \mathbf{B}(\mathbf{x}^{(2)} - \boldsymbol{\mu}^{(2)})$ is called the regression function.

The vector

$$\mathbf{x}^{(11.2)} = \mathbf{x}^{(1)} - (\boldsymbol{\mu}^{(1)} + \mathbf{B}(\mathbf{x}^{(2)} - \boldsymbol{\mu}^{(2)}))$$

is the vector of residuals of $\mathbf{x}^{(1)}$ from its regression on $\mathbf{x}^{(2)}$.

The components of $\mathbf{x}^{(11.2)}$ are uncorrelated with the components of $\mathbf{x}^{(2)}$ since we have

$$\mathbf{x}^{(11.2)} = \mathbf{y}^{(1)} - \mathbb{E}[\mathbf{y}^{(1)}],$$

such that

$$\begin{bmatrix} \mathbf{y}^{(1)} \\ \mathbf{y}^{(2)} \end{bmatrix} = \begin{bmatrix} \mathbf{I} & -\boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{x}^{(1)} \\ \mathbf{x}^{(2)} \end{bmatrix} = \begin{bmatrix} \mathbf{x}^{(1)} - \mathbf{B}\mathbf{x}^{(2)} \\ \mathbf{x}^{(1)} \end{bmatrix}.$$

Multiple Correlation Coefficient

Theorem 1

For $\mathbf{x} \sim \mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ and every vector $\boldsymbol{\alpha} \in \mathbb{R}^{(p-q)}$, we have

$$\mathrm{Var}\left(x_i^{(11.2)}\right) \leq \mathrm{Var}\left(x_i - \boldsymbol{\alpha}^\top \mathbf{x}^{(2)}\right),$$

where $x_i^{(11.2)}$ and x_i are the i-th entry of $\mathbf{x}^{(11.2)}$ and the i-th entry of $\mathbf{x}$ respectively.

Observe that

$$\mathbb{E}[x_i] = \mu_i + \boldsymbol{\alpha}^\top \left(\mathbf{x}^{(2)} - \boldsymbol{\mu}^{(2)}\right),$$

which means

$$\mu_i + \boldsymbol{\beta}_{(i)}^\top (\mathbf{x}^{(2)} - \boldsymbol{\mu}^{(2)})$$

is the best linear predictor of x_i in all functions of the form $\boldsymbol{\alpha}^\top \mathbf{x}^{(2)} + c$, the mean squared error of the above is a minimum.

Multiple Correlation Coefficient

The correlation of two variables z_1 and z_2 is defined as

$$\mathrm{Corr}(z_1, z_2) = \frac{\mathrm{Cov}[z_1, z_2]}{\sqrt{\mathrm{Var}[z_1]\mathrm{Var}[z_2]}}.$$

The maximum correlation between x_i and the linear combination $\boldsymbol{\alpha}^\top \mathbf{x}^{(2)}$ is called the multiple correlation coefficient between x_i and $\boldsymbol{\alpha}^\top \mathbf{x}^{(2)}$.

Corollary 1

Under the setting of Theorem 1, prove that

$$\mathrm{Corr}\left[x_i, \boldsymbol{\beta}_{(i)}^\top \mathbf{x}^{(2)}\right] \geq \mathrm{Corr}\left[x_i, \boldsymbol{\alpha}^\top \mathbf{x}^{(2)}\right]$$

for every $\boldsymbol{\alpha} \in \mathbb{R}^{(p-q)}$.

Outline

1. Multivariate Normal Distribution (Conditional Distribution)
2. Characteristic Function
3. Maximum Likelihood Estimator of Mean and Covariance

Characteristic Function

The characteristic function of a p-dimensional random vector $\mathbf{x}$ is

$$\phi(\mathbf{t}) = \mathbb{E}\left[\exp(\mathrm{i}\,\mathbf{t}^\top \mathbf{x})\right]$$

defined for every real vector $\mathbf{t} \in \mathbb{R}^p$.

For the complex-valued function $g(z)$ be written as

$$g(z) = g_1(z) + \mathrm{i}\, g_2(z),$$

where $g_1(z)$ and $g_2(z)$ are real-valued, the expected value of $g(z)$ is

$$\mathbb{E}[g(z)] = \mathbb{E}[g_1(z)] + \mathrm{i}\,\mathbb{E}[g_2(z)].$$

Characteristic Function

Let $\mathbf{x} = \begin{bmatrix} \mathbf{x}^{(1)} \\ \mathbf{x}^{(2)} \end{bmatrix}$ be a p-dimensional random vector. If $\mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$ are independent and $g(\mathbf{x}) = g^{(1)}(\mathbf{x}^{(1)})g^{(2)}(\mathbf{x}^{(2)})$, then we have

$$\mathbb{E}\big[g(\mathbf{x})\big] = \mathbb{E}\big[g^{(1)}(\mathbf{x}^{(1)})\big]\mathbb{E}\big[g^{(2)}(\mathbf{x}^{(2)})\big].$$

If the components of $\mathbf{x}$ are mutually independent, then

$$\mathbb{E}\big[\exp(\mathrm{i}\,\mathbf{t}^\top \mathbf{x})\big] = \mathbb{E}\left[\prod_{j=1}^{p} \exp(\mathrm{i}\, t_j x_j)\right].$$

Characteristic Function

Theorem 2

The characteristic function of $\mathbf{x}$ distributed according to $\mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ is

$$\phi(\mathbf{t}) = \exp\left(\mathrm{i}\,\mathbf{t}^\top\boldsymbol{\mu} - \frac{1}{2}\mathbf{t}^\top\boldsymbol{\Sigma}\mathbf{t}\right).$$

for every $\mathbf{t} \in \mathbb{R}^p$.

Sketch of the proof

1. The characteristic function of $\mathbf{y} \sim \mathcal{N}_p(\mathbf{0}, \mathbf{I})$ is $\phi_0(\mathbf{t}) = \exp\left(-\frac{1}{2}\mathbf{t}^\top\mathbf{t}\right)$.
2. For $\mathbf{x} \sim \mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, we have $\mathbf{x} = \mathbf{A}\mathbf{y} + \boldsymbol{\mu}$ such that $\boldsymbol{\Sigma} = \mathbf{A}\mathbf{A}^\top$.
3. Using $\phi_0(\mathbf{t})$ to present the characteristic function of $\mathbf{x} \sim \mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.

Characteristic Function

Theorem 2

The characteristic function of $\mathbf{x}$ distributed according to $\mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ is

$$\phi(\mathbf{t}) = \exp\left(\mathrm{i}\,\mathbf{t}^\top \boldsymbol{\mu} - \frac{1}{2}\mathbf{t}^\top \boldsymbol{\Sigma}\mathbf{t}\right).$$

for every $\mathbf{t} \in \mathbb{R}^p$.

We can use this theorem to prove $\mathbf{z} = \mathbf{D}\mathbf{x} \sim \mathcal{N}(\mathbf{D}\boldsymbol{\mu}, \mathbf{D}\boldsymbol{\Sigma}\mathbf{D}^\top)$ easily.

Characteristic Function

The following theorem can be viewed as another definition of multivariate normal distribution.

Theorem 3

If every linear combination of the components of a random vector **y** is normally distributed, then **y** is normally distributed.

In other words, if the *p*-dimensional random vector **y** leads to the univariate random variable

$$\mathbf{u}^\top \mathbf{y}$$

is normally distributed for any fixed $\mathbf{u} \in \mathbb{R}^p$, then **y** is normally distributed.

Problem in Exam

Let $\mathbf{x} \sim \mathcal{N}_p(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)$, $\mathbf{y} \sim \mathcal{N}_p(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)$ and $\mathbf{z} = \mathbf{x} + \mathbf{y}$. Suppose that $\mathbf{x}$ and $\mathbf{y}$ are independent. Prove $\mathbf{z} \sim \mathcal{N}_p(\boldsymbol{\mu}_1 + \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_1 + \boldsymbol{\Sigma}_2)$.

Use characteristic function to avoid using density.

Characteristic Function and Density

The characteristic function determines the density function uniquely (if the density exists).

Theorem 4

If the p-dimensional random vector $\mathbf{x}$ has the density $f(\mathbf{x})$ and the characteristic function $\phi(\mathbf{t})$, then

$$f(\mathbf{x}) = \frac{1}{(2\pi)^p} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \exp(-\mathrm{i}\,\mathbf{t}^\top \mathbf{x})\,\phi(\mathbf{t})\,\mathrm{d}t_1 \ldots \mathrm{d}t_p.$$

See the proof in Section 10.6 of "Cramer, H. (1946). Mathematical Methods of Statistics. Princeton University Press".

Characteristic Function and Probability

If $\mathbf{x}$ does not have a density, the characteristic function uniquely defines the probability of any continuity interval.

Theorem 5

Let $\{F_j(\mathbf{x})\}$ be a sequence of cdfs, and let $\{\phi_j(\mathbf{t})\}$ be the sequence of corresponding characteristic functions. A necessary and sufficient condition for $F_j(\mathbf{x})$ to converge to a cdf $F(\mathbf{x})$ is that, for every $\mathbf{t}$, $\phi_j(\mathbf{t})$ converges to a limit $\phi(\mathbf{t})$ that is continuous at $\mathbf{t} = 0$. When this condition is satisfied, the limit $\phi(\mathbf{t})$ is identical with the characteristic function of the limiting distribution $F(\mathbf{x})$.

See the proof in Section 10.7 of "Cramer, H. (1946). Mathematical Methods of Statistics. Princeton University Press"

Characteristic Function and Moments

If the n-th moment of random variable x, denoted by $\mathbb{E}[x^n]$, exists and is finite, then its characteristic function is n times continuously differentiable and

$$\mathbb{E}[x^n] = \frac{1}{\mathrm{i}^n} \frac{\mathrm{d}^n \phi(t)}{\mathrm{d} t^n}\bigg|_{t=0},$$

which is because of

$$\begin{aligned}
\frac{\mathrm{d}^n \phi(t)}{\mathrm{d} t^n} &= \frac{\mathrm{d}^n}{\mathrm{d} t^n} \mathbb{E}\left[\exp(\mathrm{i}\, tx)\right] \\
&= \mathbb{E}\left[\frac{\mathrm{d}^n}{\mathrm{d} t^n} \exp(\mathrm{i}\, tx)\right] \\
&= \mathbb{E}\left[(\mathrm{i}\, x)^n \exp(\mathrm{i}\, tx)\right] \\
&= \mathrm{i}^n \, \mathbb{E}\left[x^n \exp(\mathrm{i}\, tx)\right].
\end{aligned}$$

Characteristic Function and Moments

For normal distributed random vector $\mathbf{x} \sim \mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ and its characteristic function $\phi(\mathbf{t}) = \exp\left(\mathrm{i}\, \mathbf{t}^\top \boldsymbol{\mu} - \frac{1}{2}\mathbf{t}^\top \boldsymbol{\Sigma}\mathbf{t}\right)$, we have

$$\mathbb{E}[x_h] = \frac{1}{\mathrm{i}} \frac{\mathrm{d}\phi(\mathbf{t})}{\mathrm{d}t_h}\bigg|_{\mathbf{t}=\mathbf{0}} = \frac{1}{\mathrm{i}} \left(\mathrm{i}\, \mu_h - \sum_{j=1}^{p} \sigma_{hj} t_j\right) \phi(\mathbf{t})\bigg|_{\mathbf{t}=\mathbf{0}} = \mu_h$$

and

$$\begin{aligned}
\mathbb{E}[x_h x_j] &= \frac{1}{\mathrm{i}^2} \frac{\partial^2 \phi(t)}{\partial t_h\, \partial t_j}\bigg|_{\mathbf{t}=\mathbf{0}} \\
&= \frac{1}{\mathrm{i}^2} \left(\left(-\sum_{k=1}^{p} \sigma_{hk} t_k + \mathrm{i}\, \mu_h\right) - \sigma_{hj}\right)\left(\left(-\sum_{k=1}^{p} \sigma_{kj} t_k + \mathrm{i}\, \mu_j\right) - \sigma_{hj}\right) \phi(\mathbf{t})\bigg|_{\mathbf{t}=\mathbf{0}} \\
&= \sigma_{hj} + \mu_h \mu_j.
\end{aligned}$$

Thus, we have

$$\begin{aligned}
\mathrm{Var}(x_h) &= \mathbb{E}[x_h - \mu_h]^2 = \mathbb{E}[x_h^2] - \mu_h^2 = \sigma_{hh}, \\
\mathrm{Cov}(x_h, x_j) &= \mathbb{E}[(x_h - \mu_h)(x_j - \mu_j)] = \mathbb{E}[x_h x_j] - \mu_h \mu_j = \sigma_{hj}.
\end{aligned}$$

Characteristic Function and Moments

If all the moments of a distribution exist, then the cumulants are the coefficients κ in

$$\log \phi(\mathbf{t}) = \sum_{s_1=0}^{\infty} \cdots \sum_{s_p=0}^{\infty} \kappa_{s_1 \dots s_p} \frac{(\mathrm{i}t_1)^{s_1} \dots (\mathrm{i}t_p)^{s_p}}{s_1! \dots s_p!}.$$

In the case of the multivariate normal distribution, we have

$$\kappa_{100\dots 0} = \mu_1, \quad \kappa_{010\dots 0} = \mu_2, \quad \dots \quad \kappa_{000\dots 1} = \mu_p,$$

and

$$\kappa_{200\dots 0} = \sigma_{11}, \quad \kappa_{110\dots 0} = \sigma_{12}, \quad \dots \quad \kappa_{000\dots 2} = \sigma_{pp}.$$

The cumulants for which $\sum s_i > 2$ are 0.

Outline

The Maximum Likelihood Estimators

Given a sample of (vector) observations from a p-variate (non-singular) normal distribution, we ask for estimators of the mean vector $\boldsymbol{\mu}$ and the covariance matrix $\boldsymbol{\Sigma}$ of the distribution.

Suppose our sample of N observations on the $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$, which are distributed according to $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, where $N > p$. The likelihood function is

$$
\begin{aligned}
L &= \prod_{\alpha=1}^{N} n(\mathbf{x}_\alpha \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) \\
&= \frac{1}{(2\pi)^{\frac{pN}{2}} (\det(\boldsymbol{\Sigma}))^{\frac{N}{2}}} \exp\left[-\frac{1}{2} \sum_{\alpha=1}^{N} (\mathbf{x}_\alpha - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x}_\alpha - \boldsymbol{\mu}) \right].
\end{aligned}
$$

The Maximum Likelihood Estimators

The likelihood function is

$$L = \frac{1}{(2\pi)^{\frac{pN}{2}} (\det(\boldsymbol{\Sigma}))^{\frac{N}{2}}} \exp\left[-\frac{1}{2} \sum_{\alpha=1}^{N} (\mathbf{x}_\alpha - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x}_\alpha - \boldsymbol{\mu}) \right].$$

The vectors $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ are fixed at the sample values and L is a function of $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$.

The logarithm of the likelihood function is

$$\ln L = -\frac{PN}{2} \ln 2\pi - \frac{N}{2} \ln\left(\det(\boldsymbol{\Sigma})\right) - \frac{1}{2} \sum_{\alpha=1}^{N} (\mathbf{x}_\alpha - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x}_\alpha - \boldsymbol{\mu}).$$

Since $\ln L$ is an increasing function of L, the maximum likelihood estimators of $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ are the vector and the positive definite matrix that maximize $\ln L$.

The Maximum Likelihood Estimators

Let the mean vector be

$$\bar{\mathbf{x}} = \frac{1}{N}\sum_{\alpha=1}^{N}\mathbf{x}_\alpha = \begin{bmatrix} \frac{1}{N}\sum_{\alpha=1}^{N} x_{1\alpha} \\ \vdots \\ \frac{1}{N}\sum_{\alpha=1}^{N} x_{p\alpha} \end{bmatrix} = \begin{bmatrix} \bar{x}_1 \\ \vdots \\ \bar{x}_p \end{bmatrix}$$

where

$$\mathbf{x}_\alpha = \begin{bmatrix} x_{1\alpha} \\ \vdots \\ x_{p\alpha} \end{bmatrix} \quad \text{and} \quad \bar{x}_i = \frac{1}{N}\sum_{\alpha=1}^{N} x_{i\alpha}.$$

Let the matrix of sums of squares and cross products of deviations about the mean be

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

The Maximum Likelihood Estimators

Theorem 6

If $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ constitute a sample from $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ with $p < N$, the maximum likelihood estimators of $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ 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 $\mathbf{G}$ exists, occurs at $\mathbf{G} = \frac{1}{N}\mathbf{D}$.

The Maximum Likelihood Estimators

The maximum likelihood estimators of functions of the parameters are those functions of the maximum likelihood estimators of the parameters.

Theorem 7

Let $f(\boldsymbol{\theta})$ be a real-valued function defined on a set $\mathcal{S}$ and let ϕ be a single-valued function, with a single-valued inverse, on $\mathcal{S}$ to a set $\mathcal{S}^*$. Let

$$g(\boldsymbol{\theta}^*) = f\left(\phi^{-1}(\boldsymbol{\theta}^*)\right).$$

Then if $f(\boldsymbol{\theta})$ attains a maximum at $\boldsymbol{\theta} = \boldsymbol{\theta}_0$, then $g(\boldsymbol{\theta}^*)$ attains a maximum at $\boldsymbol{\theta}^* = \boldsymbol{\theta}_0^* = \phi(\boldsymbol{\theta}_0)$. If the maximum of $f(\boldsymbol{\theta})$ at $\boldsymbol{\theta}_0$ is unique, so is the maximum of $g(\boldsymbol{\theta}^*)$ at $\boldsymbol{\theta}_0^*$.

The Maximum Likelihood Estimators

Corollary 2

If on the basis of a given sample $\hat{\theta}_1, \ldots, \hat{\theta}_m$ are maximum likelihood estimators of the parameters $\theta_1, \ldots, \theta_m$ of a distribution, then $\phi_1(\hat{\theta}_1, \ldots, \hat{\theta}_m), \ldots, \phi_m(\hat{\theta}_1, \ldots, \hat{\theta}_m)$ are maximum likelihood estimator of $\phi_1(\theta_1, \ldots, \theta_m), \ldots, \phi_m(\theta_1, \ldots, \theta_m)$ if the transformation from $\theta_1, \ldots, \theta_m$ to $\phi_1, \ldots, \phi_m$ is one-to-one. If the estimators of $\theta_1, \ldots, \theta_m$ are unique, then the estimators of $\phi_1, \ldots, \phi_m$ are unique.

Corollary 3

If $\mathbf{x}_1, \ldots, \mathbf{x}_N$ constitutes a sample from $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, let $\rho_{ij} = \sigma_{ij}/(\sigma_i \sigma_j)$. Then the maximum likelihood estimator of ρ_{ij} is

$$\hat{\rho}_{ij} = \frac{\sum_{\alpha=1}^{N}(x_{i\alpha} - \bar{x}_i)(x_{j\alpha} - \bar{x}_j)}{\sqrt{\sum_{\alpha=1}^{N}(x_{i\alpha} - \bar{x}_i)^2}\sqrt{\sum_{\alpha=1}^{N}(x_{j\alpha} - \bar{x}_j)^2}}$$

The Maximum Likelihood Estimators

If $\phi : \mathcal{S} \to \mathcal{S}^*$ is not one-to-one, we let

$$\phi^{-1}(\boldsymbol{\theta}^*) = \{\boldsymbol{\theta} : \boldsymbol{\theta}^* = \phi(\boldsymbol{\theta})\}.$$

and define (the induced likelihood function)

$$g(\boldsymbol{\theta}^*) = \sup\{f(\boldsymbol{\theta}) : \boldsymbol{\theta}^* = \phi(\boldsymbol{\theta})\}.$$

If $\boldsymbol{\theta} = \hat{\boldsymbol{\theta}}$ maximize $f(\boldsymbol{\theta})$, then $\boldsymbol{\theta}^* = \phi(\hat{\boldsymbol{\theta}})$ also maximize $g(\boldsymbol{\theta}^*)$.