

# Multivariate Statistical Analysis

## Lecture 03

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# Outline

- 1 Multivariate Normal Distribution
- 2 Linear Transformation
- 3 Marginal Distribution
- 4 Singular Normal Distributions

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- 1 Multivariate Normal Distribution
- 2 Linear Transformation
- 3 Marginal Distribution
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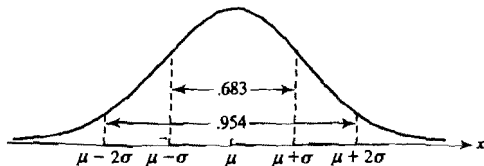
# Univariate Normal Distribution

A random variable  $x$  is normally distributed with mean  $\mu$  and standard deviation  $\sigma > 0$  can be written in the following notation

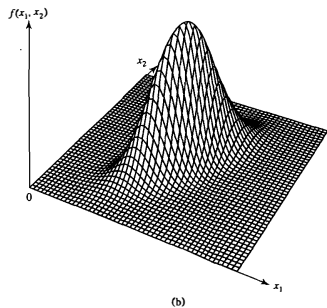
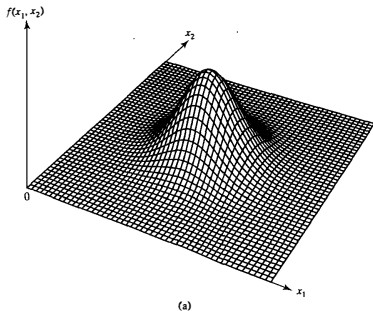
$$x \sim \mathcal{N}(\mu, \sigma^2).$$

The probability density function of univariate normal distribution is

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x - \mu)^2}{2\sigma^2}\right).$$



# Bivariate Normal Density



Two bivariate normal distributions:

- (a)  $\sigma_1 = \sigma_2$  and  $\rho_{12} = 0$
- (b)  $\sigma_1 = \sigma_2$  and  $\rho_{12} = 0.75$

# The Central Limit Theorem

Let  $x_1, \dots, x_n$  be independent and identically distributed random variables with the same arbitrary distribution, mean  $\mu$ , and variance  $\sigma^2$ .

Let  $\bar{x}_n = \frac{1}{n} \sum_{i=1}^n x_i$ , then the random variable

$$z = \lim_{n \rightarrow \infty} \sqrt{n} \left( \frac{\bar{x}_n - \mu}{\sigma} \right)$$

is a standard normal distribution.

The standard normal distribution is a normal distribution with a mean of 0 and standard deviation of 1.

What about multivariate case?

# The Central Limit Theorem

$$\lim_{n \rightarrow +\infty} \frac{1}{n} \sum_{i=1}^n$$



# Multivariate Normal Distribution

The multivariate normal distribution of a  $p$ -dimensional random vector  $\mathbf{x} = [x_1, \dots, x_p]^\top$  can be written in the following notation:

$$\mathbf{x} \sim \mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

or to make it explicitly known that  $\mathbf{x}$  is  $p$ -dimensional.

$$\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}),$$

with  $p$ -dimensional mean vector

$$\boldsymbol{\mu} = \mathbb{E}[\mathbf{x}] = \begin{bmatrix} \mathbb{E}[x_1] \\ \vdots \\ \mathbb{E}[x_p] \end{bmatrix} \in \mathbb{R}^p$$

and covariance matrix

$$\boldsymbol{\Sigma} = \mathbb{E} \left[ (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^\top \right] \in \mathbb{R}^{p \times p}.$$



# Multivariate Normal Distribution

The density function of univariate normal distribution is

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right),$$

where  $\mu$  is the mean and  $\sigma^2$  is the variance with  $\sigma > 0$ .

The density function of non-singular  $p$ -dimensional multivariate normal distribution is

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

where  $\boldsymbol{\mu} \in \mathbb{R}^p$  is the mean and  $\mathbf{\Sigma}$  is the  $p \times p$  (non-singular) covariance matrix.

# Density Function of Multivariate Normal Distribution

## Theorem

Suppose the  $p$ -dimensional random vector  $\mathbf{x}$  has the density function

$$f(\mathbf{x}) = K \exp \left( -\frac{1}{2} (\mathbf{x} - \mathbf{b})^\top \mathbf{A} (\mathbf{x} - \mathbf{b}) \right),$$

where  $K \in \mathbb{R}$ ,  $\mathbf{b} \in \mathbb{R}^p$  and  $\mathbf{A} \in \mathbb{R}^{p \times p}$  is symmetric positive definite. Then

$$K = \frac{1}{\sqrt{(2\pi)^p \det(\mathbf{\Sigma})}}, \quad \mathbf{b} = \boldsymbol{\mu} \quad \text{and} \quad \mathbf{A} = \mathbf{\Sigma}^{-1}.$$

The main idea of this section:



# Multivariate Normal Distribution

If the density of a  $p$ -dimensional random vector  $\mathbf{x}$  is

$$K \exp \left( -\frac{1}{2} (\mathbf{x} - \mathbf{b})^\top \mathbf{A} (\mathbf{x} - \mathbf{b}) \right),$$

where  $\mathbf{A} \in \mathbb{R}^{p \times p}$  is symmetric positive definite, then  $\mathbb{E}[\mathbf{x}] = \mathbf{b}$  and  $\text{Cov}[\mathbf{x}] = \mathbf{A}^{-1}$ .

Conversely, given a vector  $\boldsymbol{\mu} \in \mathbb{R}^p$  and a positive definite matrix  $\boldsymbol{\Sigma} \in \mathbb{R}^{p \times p}$ , there is a multivariate normal density

$$n(\mathbf{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^p \det(\boldsymbol{\Sigma})}} \exp \left( -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right).$$

# Bivariate Normal Distribution

We consider the (non-singular) bivariate normal distribution  $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ , where

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \quad \boldsymbol{\mu} = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \quad \text{and} \quad \boldsymbol{\Sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{bmatrix}.$$

We have

$$\boldsymbol{\Sigma}^{-1} = \frac{1}{\sigma_{11}\sigma_{22} - \sigma_{12}^2} \begin{bmatrix} \sigma_{22} & -\sigma_{12} \\ -\sigma_{12} & \sigma_{11} \end{bmatrix}.$$

Let  $\rho = \sigma_{12}/\sqrt{\sigma_{11}\sigma_{22}}$ , then we have  $\det(\boldsymbol{\Sigma}) = \sigma_{11}\sigma_{22}(1 - \rho^2)$  and

$$\begin{aligned} & (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \\ &= \frac{1}{1 - \rho^2} \left( \left( \frac{x_1 - \mu_1}{\sqrt{\sigma_{11}}} \right)^2 + \left( \frac{x_2 - \mu_2}{\sqrt{\sigma_{22}}} \right)^2 - 2\rho \left( \frac{x_1 - \mu_1}{\sqrt{\sigma_{11}}} \right) \left( \frac{x_2 - \mu_2}{\sqrt{\sigma_{22}}} \right) \right). \end{aligned}$$

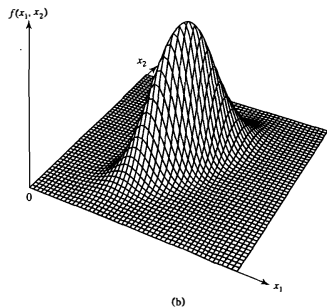
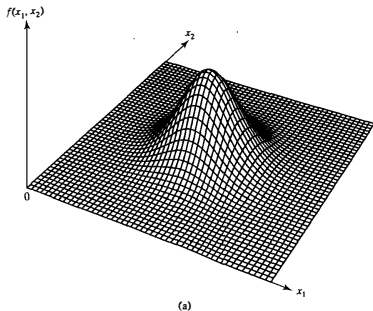
# Bivariate Normal Density

The density function is

$$\begin{aligned} & f(x_1, x_2) \\ &= \frac{1}{2\pi\sqrt{\sigma_{11}\sigma_{22}(1-\rho^2)}} \\ & \times \exp\left(-\frac{1}{2(1-\rho^2)}\left(\frac{(x_1-\mu_1)^2}{\sigma_{11}} + \frac{(x_2-\mu_2)^2}{\sigma_{22}} - \frac{2\rho(x_1-\mu_1)(x_2-\mu_2)}{\sqrt{\sigma_{11}\sigma_{22}}}\right)\right). \end{aligned}$$

If  $\rho = 0$ , then the variables  $x_1$  and  $x_2$  are independent.

# Bivariate Normal Density



Two bivariate normal distributions:

- (a)  $\sigma_1 = \sigma_2$  and  $\rho_{12} = 0$
- (b)  $\sigma_1 = \sigma_2$  and  $\rho_{12} = 0.75$

# Probability Density Contour

The density of a  $p$ -dimensional normal variable

$$n(\mathbf{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^p \det(\boldsymbol{\Sigma})}} \exp \left( -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right).$$

implies the multivariate normal density is constant on surfaces where the square of the distance  $(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})$  is a constant.

These paths are called contours:

$$\begin{aligned} \text{constant probability density contour} &= \{ \mathbf{x} : (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) = c^2 \} \\ &= \text{surface of an hyperellipsoid centered at } \boldsymbol{\mu}, \end{aligned}$$

where  $c > 0$  is a fixed constant.

# Probability Density Contour

Consider the hyperellipsoid with surface defined by  $\mathbf{x} \in \mathbb{R}^p$  such that

$$(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}) = c^2.$$

Denote the eigenvalue-eigenvector pairs of  $\boldsymbol{\Sigma}$  by

$$(\lambda_1, \mathbf{u}_1), (\lambda_2, \mathbf{u}_2), \dots, (\lambda_p, \mathbf{u}_p),$$

then the hyperellipsoid is centered at  $\boldsymbol{\mu}$  and have axes (vertices)

$$\pm c\sqrt{\lambda_1}\mathbf{u}_1, \pm c\sqrt{\lambda_2}\mathbf{u}_2, \dots, \pm c\sqrt{\lambda_p}\mathbf{u}_p.$$

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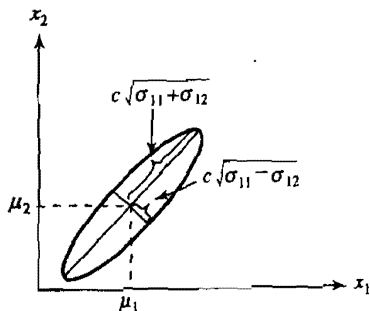


# Probability Density Contour

For bivariate normal distribution with  $\sigma_{11} = \sigma_{22}$ , we have

$$\lambda_1 = \sigma_{11} + \sigma_{12}, \quad \mathbf{u}_1 = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}, \quad \lambda_2 = \sigma_{11} - \sigma_{12} \quad \text{and} \quad \mathbf{u}_2 = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix}.$$

If we additionally suppose  $\sigma_{12} > 0$ , it leads to the following figure:



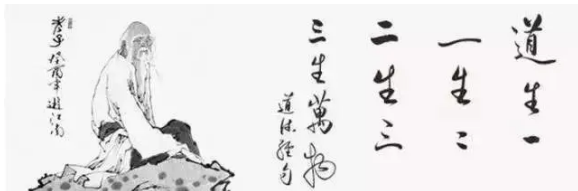
# Probability Density Contour

For the hyperellipsoid with surface defined by  $\mathbf{x} \in \mathbb{R}^p$  such that

$$(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}) = c^2,$$

how the connect the eigenvalue-eigenvector pairs of  $\boldsymbol{\Sigma}$  to the vertices of the hyperellipsoid?

The main idea:



# Normally Distributed Variables

Some properties of normally distributed variables:

- ① The linear transform of multivariate normal variates are normally distributed.
- ② The marginal distributions derived from multivariate normal distributions are also normal distributions.
- ③ The conditional distributions derived from multivariate normal distributions are also normal distributions.

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## Theorem 1

Let  $\mathbf{x} \sim \mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ , with  $\boldsymbol{\Sigma} \succ \mathbf{0}$ . Then

$$\mathbf{y} = \mathbf{C}\mathbf{x}$$

is distributed according to  $\mathcal{N}_p(\mathbf{C}\boldsymbol{\mu}, \mathbf{C}\boldsymbol{\Sigma}\mathbf{C}^\top)$  for non-singular  $\mathbf{C} \in \mathbb{R}^{p \times p}$ .

Sketch of the proof:

- 1 Let  $f(\mathbf{x})$  be the density function of  $\mathbf{x}$ .
- 2 Let  $g(\mathbf{y})$  be the density function of  $\mathbf{y}$ .
- 3 The relation  $\mathbf{x} = \mathbf{C}^{-1}\mathbf{y}$  implies

$$g(\mathbf{y}) = f(\mathbf{u}^{-1}(\mathbf{y})) |\det(\mathbf{J}^{-1}(\mathbf{y}))|$$

with  $\mathbf{u}(\mathbf{x}) = \mathbf{C}\mathbf{x}$ ,  $\mathbf{u}^{-1}(\mathbf{y}) = \mathbf{C}^{-1}\mathbf{y}$  and  $\mathbf{J}^{-1}(\mathbf{y}) = \mathbf{C}^{-1}$ .

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## Theorem

If  $\mathbf{x} = [x_1, \dots, x_p]^\top \sim \mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$  with  $\boldsymbol{\Sigma} \succ \mathbf{0}$ . Let

$$\mathbf{x}^{(1)} = [x_1, \dots, x_q]^\top \quad \text{and} \quad \mathbf{x}^{(2)} = [x_{q+1}, \dots, x_p]^\top$$

for  $q < p$ . A necessary and sufficient condition for  $\mathbf{x}^{(1)}$  and  $\mathbf{x}^{(2)}$  to be independent is that each covariance of a variable from  $\mathbf{x}^{(1)}$  and a variable from  $\mathbf{x}^{(2)}$  is 0.

- 1 The random vectors  $\mathbf{x}^{(1)}$  and  $\mathbf{x}^{(2)}$  can be replaced by any subset of  $\mathbf{x}$  the subset consisting of the remaining variables respectively.
- 2 The necessity does not depend on the assumption of normality.

If two random variables are normally distributed, can we say they are independent?



## Corollary

We use the notation in above theorem such that

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}^{(1)} \\ \mathbf{x}^{(2)} \end{bmatrix} \sim \mathcal{N} \left( \begin{bmatrix} \boldsymbol{\mu}^{(1)} \\ \boldsymbol{\mu}^{(2)} \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{bmatrix} \right)$$

It shows that *if  $\mathbf{x}^{(1)}$  is uncorrelated with  $\mathbf{x}^{(2)}$* , the marginal distribution of  $\mathbf{x}^{(1)}$  is  $\mathcal{N}(\boldsymbol{\mu}^{(1)}, \boldsymbol{\Sigma}_{11})$  and the marginal distribution of  $\mathbf{x}^{(2)}$  is  $\mathcal{N}(\boldsymbol{\mu}^{(2)}, \boldsymbol{\Sigma}_{22})$ .

In fact, this result holds even if the two sets are NOT uncorrelated.

## Theorem

*If  $\mathbf{x} \sim \mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$  with  $\boldsymbol{\Sigma} \succ \mathbf{0}$ , the marginal distribution of any set of components of*

$$\mathbf{x} = [x_1, x_2, \dots, x_p]^\top$$

*is multivariate normal with means, variances, and covariances obtained by taking the corresponding components of  $\boldsymbol{\mu}$  and  $\boldsymbol{\Sigma}$ , respectively.*

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# Singular Normal Distributions

In previous section, we focus on non-singular normal normally distributed variate  $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$  with  $\boldsymbol{\Sigma} \succ \mathbf{0}$  whose density function is

$$n(\mathbf{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^p \det(\boldsymbol{\Sigma})}} \exp \left( -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}) \right).$$

What about the case of singular  $\boldsymbol{\Sigma}$ ?

# General Linear Transformation

- ① Let  $\mathbf{x} \sim \mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ , with  $\boldsymbol{\Sigma} \succ \mathbf{0}$ . Then

$$\mathbf{y} = \mathbf{C}\mathbf{x}$$

is distributed according to  $\mathcal{N}_p(\mathbf{C}\boldsymbol{\mu}, \mathbf{C}\boldsymbol{\Sigma}\mathbf{C}^\top)$  for non-singular  $\mathbf{C} \in \mathbb{R}^{p \times p}$ .

- ② Let  $\mathbf{x} \sim \mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ , with  $\boldsymbol{\Sigma} \succ \mathbf{0}$ . Then

$$\mathbf{z} = \mathbf{C}\mathbf{x}$$

is distributed according to  $\mathcal{N}_q(\mathbf{C}\boldsymbol{\mu}, \mathbf{C}\boldsymbol{\Sigma}\mathbf{C}^\top)$  for  $\mathbf{C} \in \mathbb{R}^{q \times p}$  of rank  $q \leq p$ .

- ③ Let  $\mathbf{x} \sim \mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ . Then

$$\mathbf{z} = \mathbf{C}\mathbf{x}$$

is distributed according to  $\mathcal{N}_q(\mathbf{C}\boldsymbol{\mu}, \mathbf{C}\boldsymbol{\Sigma}\mathbf{C}^\top)$  for any  $\mathbf{C} \in \mathbb{R}^{q \times p}$ .

# Transformation



$5.3 \times 10^5$

$$c \neq 0$$

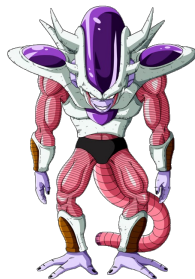
$$\sigma^2 > 0$$



$> 1.0 \times 10^6$

$$\mathbf{C} \in \mathbb{R}^{p \times p} \text{ is non-singular}$$

$$\Sigma \succ 0$$



$2.0 \times 10^6 \sim 3.0 \times 10^6$

$$\mathbf{C} \in \mathbb{R}^{q \times p} \text{ of rank } q \leq p$$

$$\Sigma \succ 0$$



$> 3.0 \times 10^7$

$$\mathbf{C} \in \mathbb{R}^{p \times p}$$

$$\Sigma \preceq 0$$

# General Linear Transformation

## Theorem

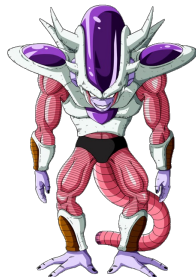
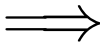
Let  $\mathbf{x} \sim \mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ , with  $\boldsymbol{\Sigma} \succ \mathbf{0}$ . Then

$$\mathbf{z} = \mathbf{D}\mathbf{x}$$

is distributed according to  $\mathcal{N}_q(\mathbf{D}\boldsymbol{\mu}, \mathbf{D}\boldsymbol{\Sigma}\mathbf{D}^\top)$  for  $\mathbf{D} \in \mathbb{R}^{q \times p}$  of rank  $q \leq p$ .



non-singular



full-rank

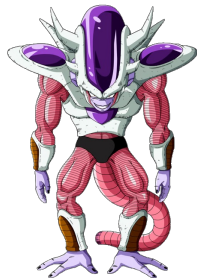
# General Linear Transformation

## Theorem

Let  $\mathbf{x} \sim \mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ . Then

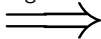
$$\mathbf{z} = \mathbf{D}\mathbf{x}$$

is distributed according to  $\mathcal{N}_q(\mathbf{D}\boldsymbol{\mu}, \mathbf{D}\boldsymbol{\Sigma}\mathbf{D}^\top)$  for any  $\mathbf{D} \in \mathbb{R}^{q \times p}$ .



full-rank

understand the singular normal distribution



no limitation