Module 2, Part 2: Random vectors, covariance, multivariate Normal distribution TMA4268 Statistical Learning V2022

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Overview

- Random vectors
- The covariance and correlation matrix
- The multivariate normal distribution

$$X = \begin{pmatrix} x_{\rho} \\ \vdots \\ x_{\rho} \end{pmatrix}$$

Random vector



{0,15

- A random vector $X_{(p\times 1)}$ is a p-dimensional vector of random variables. For example
 - Weight of cork deposits in p = 4 directions (N, E, S, W).
 - Factors to predict body fat: bmi, age, weight, hip circumference,....
- Joint distribution function: (f(x))
- From joint distribution function to marginal (and conditional distributions).

$$\underbrace{f_1(x_1)} = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f(\underbrace{x_1, x_2, \dots, x_p}) \underbrace{dx_2 \cdots dx_p}$$

• Cumulative distribution (definite integrals!) used to calculate probabilites.

Moments

The moments are important properties of the distribution of X. We will look at:

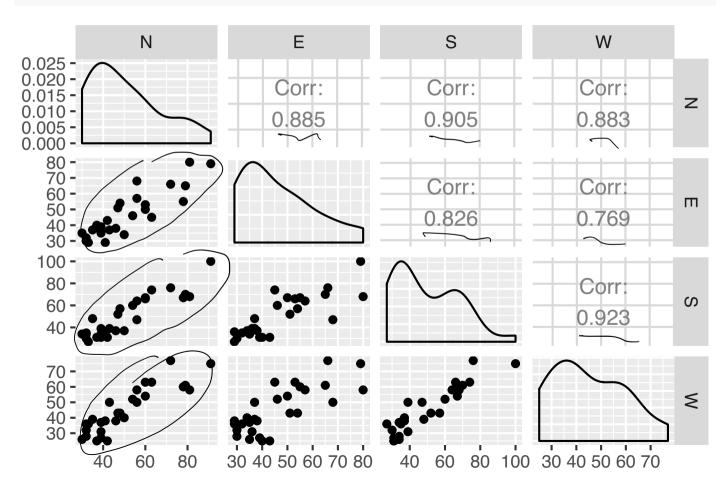
- E: Mean of random vector and random matrices.
- Cov: Covariance matrix.
- Corr: Correlation matrix.
- E and Cov of multiple linear combinations.

The Cork deposit data

- Classical multivariate data set from Rao (1948).
- Weigth of bark deposits of n = 28 cork trees in p = 4 directions (N, E, S, W).

Look at the data (always the first thing to do):

```
library(GGally)
corkds <- as.data.frame(corkds)
ggpairs(corkds)</pre>
```



- Here we have a random sample of n = 28 cork trees from the population and observe a p = 4 dimensional random vector for each tree.
- This leads us to the definition of random vectors and a random matrix for cork trees:

$$egin{aligned} m{X}_{(28 imes4)} &= egin{bmatrix} m{X}_{11} & m{X}_{12} & m{X}_{13} & m{X}_{14} \ m{X}_{21} & m{X}_{22} & m{X}_{23} & m{X}_{24} \ m{X}_{31} & m{X}_{32} & m{X}_{33} & m{X}_{34} \ dots & dots & \ddots & dots \ m{X}_{28,1} & m{X}_{28,2} & m{X}_{28,3} & m{X}_{28,4} \ \end{bmatrix} \ m{\chi} &= egin{bmatrix} m{\chi}_{1} & m{\chi}_{2} & m{\chi}_{3} & m{\chi}_{4} \ m{\chi}_{2} & m{\chi}_{3} & m{\chi}_{4} \ \end{bmatrix} m{\chi}_{1} \ m{\chi}_{2} & m{\chi}_{3} & m{\chi}_{4} \ \end{pmatrix}^{T}$$

Rules for means

• Random vector $\boldsymbol{X}_{(p\times 1)}$ with mean vector $\boldsymbol{\mu}_{(p\times 1)}$:

$$\boldsymbol{X}_{(p\times 1)} = \begin{bmatrix} \underbrace{X_1} \\ X_2 \\ \vdots \\ X_p \end{bmatrix}, \text{ and } \boldsymbol{\mu}_{(p\times 1)} = \mathrm{E}(\boldsymbol{X}) = \begin{bmatrix} \underline{\mathrm{E}}(X_1) \\ \underline{\mathrm{E}}(X_2) \\ \vdots \\ \underline{\mathrm{E}}(X_p) \end{bmatrix}.$$

- Same rule for random_matrices.
- Random matrix $X_{(n \times p)}$ and random matrix $Y_{(n \times p)}$:

(Rules of vector addition)
$$E(X + Y) = E(X) + E(Y).$$

$$E(X + Y) = E(X) + E(Y)$$

Observe that $E(X_j)$ is calculated from the marginal distribution of X_j and contains no information about dependencies between X_j and X_k , $k \neq j$.

• Random matrix $X_{(n \times p)}$ and conformable constant matrices A and B:

$$E(\underbrace{\overset{\ }{A}\overset{\ }{X}\overset{\ }{B}})=\underbrace{AE(X)B}$$

Proof: Board

Q:

• What are the univariate analogue to the formulas on the previous two slides (which you studied in your first introductory course in statistics)?

$$E(a \cdot X + b \cdot Y) = a E[X] + b E[Y]$$

$$E(a \times b) = a E[X) \cdot b$$

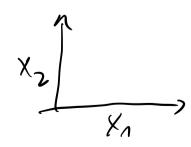
$$= ab \cdot E[X]$$

The covariance

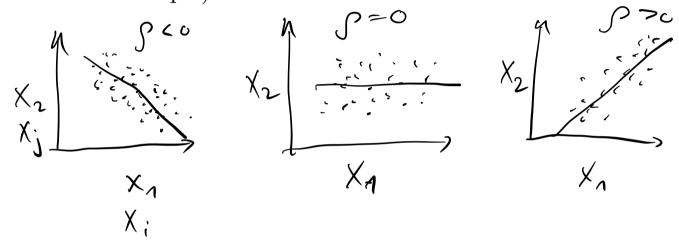
In the introductory statistics course we defined the covariance

$$\rho_{ij} = \operatorname{Cov}(X_i, X_j) = \operatorname{E}[(\underbrace{X_i - \mu_i})(\underbrace{X_j - \mu_j})]$$
$$= \operatorname{E}(X_i \cdot X_j) - \mu_i \mu_j.$$

- What is the covariance called when i = j? $\left\{ \left[\left(X_i \mu_i \right)^2 \right] = \right\}$ What does it mean when the covariance is
- What does it mean when the covariance is
 - negative
 - zero
 - positive?



Make a scatter plot for negative, zero and positive correlation (see also R example).



Variance-covariance matrix

• Consider random vector $X_{(p\times 1)}$ with mean vector $\mu_{(p\times 1)}$:

$$\boldsymbol{X}_{(p\times 1)} = \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_p \end{bmatrix}, \text{ and } \boldsymbol{\mu}_{(p\times 1)} = \mathrm{E}(\boldsymbol{X}) = \begin{bmatrix} \mathrm{E}(X_1) \\ \mathrm{E}(X_2) \\ \vdots \\ \mathrm{E}(X_p) \end{bmatrix}$$

• Variance-covariance matrix Σ (real and symmetric)

$$\Sigma = \underline{\text{Cov}(X)} = \underline{\text{E}[(X - \mu)(X - \mu)^T]}$$

$$= \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1p} \\ \sigma_{12} & \sigma_2^2 & \cdots & \sigma_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{1p} & \sigma_{2p} & \cdots & \sigma_p^2 \end{bmatrix} = \underline{\text{E}(XX^T)} - \mu\mu^T$$

- The diagonal elements in Σ , $\sigma_{ii} = \sigma_i^2$, are variances.
- The off-diagonal elements are covariances $\sigma_{ij} = E[(X_i \mu_i)(X_j \mu_j)] = \sigma_{ji}$.
- Σ is called variance, covariance and variance-covariance matrix and denoted both Var(X) and Cov(X).

Exercise: the variance-covariance matrix

Let $X_{4\times 1}$ have variance-covariance matrix

$$\Sigma = \begin{bmatrix} 2 & 1 & 0 & 0 \\ 1 & 2 & 0 & 1 \\ 0 & 0 & 2 & 1 \\ 0 & 1 & 1 & 2 \end{bmatrix}. \qquad \begin{matrix} \chi = \begin{pmatrix} \chi_{1} \\ \vdots \\ \chi_{q} \end{pmatrix}$$

Explain what this means.

where
$$3_1^2 = ... = 3_1^2 = 2$$

 $cov(X_1, X_2) = 1$
 $cov(X_2, X_4) = cov(X_3, X_4) = 1$
uncorrelated: $X_1 X_2 \times X_2 \times X_3 \times X_1 \times X_4$

Correlation matrix

Correlation matrix ρ (real and symmetric)

$$\rho = \begin{bmatrix} \frac{\sigma_1^2}{\sqrt{\sigma_1^2 \sigma_1^2}} & \frac{\sigma_{12}}{\sqrt{\sigma_1^2 \sigma_2^2}} & \cdots & \frac{\sigma_{1p}}{\sqrt{\sigma_1^2 \sigma_p^2}} \\ \frac{\sigma_{12}}{\sqrt{\sigma_1^2 \sigma_2^2}} & \frac{\sigma_2^2}{\sqrt{\sigma_2^2 \sigma_2^2}} & \cdots & \frac{\sigma_{2p}}{\sqrt{\sigma_2^2 \sigma_p^2}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\sigma_{1p}}{\sqrt{\sigma_1^2 \sigma_2^2}} & \frac{\sigma_{2p}}{\sqrt{\sigma_2^2 \sigma_p^2}} & \cdots & \frac{\sigma_p^2}{\sqrt{\sigma_p^2 \sigma_p^2}} \end{bmatrix} = \begin{bmatrix} \mathbf{1} & \rho_{12} & \cdots & \rho_{1p} \\ \rho_{12} & \mathbf{1} & \cdots & \rho_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{1p} & \rho_{2p} & \cdots & \mathbf{1} \end{bmatrix}$$

Standardization of the con matrix:
$$\rho = \underbrace{(\boldsymbol{V}^{\frac{1}{2}})^{-1}\boldsymbol{\Sigma}(\boldsymbol{V}^{\frac{1}{2}})^{-1}}_{\text{there }\boldsymbol{V}^{\frac{1}{2}}}, \text{ where } \boldsymbol{V}^{\frac{1}{2}} = \begin{bmatrix} \sqrt{\sigma_1^2} & 0 & \cdots & 0 \\ 0 & \sqrt{\sigma_2^2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{\sigma_p^2} \end{bmatrix}$$

Exercise: the correlation matrix

Let $X_{4\times 1}$ have variance-covariance matrix

$$\Sigma = \begin{bmatrix} 2 & 1 & 0 & 0 \\ 1 & 2 & 0 & 1 \\ 0 & 0 & 2 & 1 \\ 0 & 1 & 1 & 2 \end{bmatrix}. \qquad \mathcal{P} = \begin{bmatrix} 1 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 1 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} & 1 \end{bmatrix}$$

Find the correlation matrix.

$$3i = 2$$
 => Stendardization with $\frac{1}{2 \cdot 2} = \frac{1}{2}$ for all entries!

A:

Linear combinations

Consider a random vector $\boldsymbol{X}_{(p\times 1)}$ with mean vector $\boldsymbol{\mu}=\mathrm{E}(\boldsymbol{X})$ and variance-covariance matrix $\boldsymbol{\Sigma}=\mathrm{Cov}(\boldsymbol{X}).$

The linear combinations

have

$$Z = CX = \begin{bmatrix} \sum_{j=1}^{p} c_{1j}X_j \\ \sum_{j=1}^{p} c_{2j}X_j \\ \vdots \\ \sum_{j=1}^{p} c_{kj}X_j \end{bmatrix}$$

$$E(Z) = E(CX) = C\mu$$

$$Cov(Z) = Cov(CX) = C\Sigma C^T$$

Exercise: Follow the proof (board) - what are the most important transitions?

Exercise: Linear combinations

$$\boldsymbol{X} = \begin{bmatrix} X_N \\ X_E \\ X_S \\ X_W \end{bmatrix}, \boldsymbol{\mu} = \begin{bmatrix} \mu_N \\ \mu_E \\ \mu_S \\ \mu_W \end{bmatrix}, \text{ and } \boldsymbol{\Sigma} = \begin{bmatrix} \sigma_N^2 & \sigma_{NE} & \sigma_{NS} & \sigma_{NW} \\ \sigma_{NE} & \sigma_E^2 & \sigma_{ES} & \sigma_{EW} \\ \sigma_{NS} & \sigma_{SE} & \sigma_S^2 & \sigma_{SW} \\ \sigma_{NW} & \sigma_{EW} & \sigma_{SW} & \sigma_W^2 \end{bmatrix}$$

Scientists would like to compare the following three *contrasts*: N-S, E+W and (E+W)-(N+S), and define a new random vector $\mathbf{Y}_{(3\times1)} = \mathbf{C}_{(3\times4)} \mathbf{X}_{(4\times1)}$ giving the three contrasts.

- Write down \boldsymbol{C} .
- Explain how to find $E(Y_1)$ and $Cov(Y_1, Y_3)$.
- Use R to find the mean vector, covariance matrix and correlations matrix of Y, when the mean vector and covariance matrix for X given below.

```
corkds <- as.matrix(read.table("https://www.math.ntnu.no/emner/TMA4268/2019v/data/corkMKB.txt"))</pre>
dimnames(corkds)[[2]] <- c("N", "E", "S", "W")</pre>
mu = apply(corkds, 2, mean)
mu
Sigma = var(corkds)
Sigma
##
          N
                   Ε
                             S
## 50.53571 46.17857 49.67857 45.17857
##
            N
                     Ε
                               S
## N 290.4061 223.7526 288.4378 226.2712
## E 223.7526 219.9299 229.0595 171.3743
## S 288.4378 229.0595 350.0040 259.5410
## W 226.2712 171.3743 259.5410 226.0040
(C \leftarrow matrix(c(1, 0, -1, 0, 0, 1, 0, 1, -1, 1, -1, 1), byrow = T, nrow = 3))
##
## [1,]
## [2,]
## <u>[</u>3,]
##
             [,1]
                         [,2]
## [1,] 63.53439
                   -38.57672
## [2,] -38.57672 788.68254 -149.94180
## [3,] (21.02116)-149.94180 128.71958
```

The covariance matrix - more requirements?

Random vector $\boldsymbol{X}_{(p\times 1)}$ with mean vector $\boldsymbol{\mu}_{(p\times 1)}$ and covariance matrix

$$\boldsymbol{\Sigma} = \text{Cov}(\boldsymbol{X}) = \text{E}[(\boldsymbol{X} - \boldsymbol{\mu})(\boldsymbol{X} - \boldsymbol{\mu})^T] = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1p} \\ \sigma_{12} & \sigma_2^2 & \cdots & \sigma_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{1p} & \sigma_{2p} & \cdots & \sigma_p^2 \end{bmatrix}$$

• The covariance matrix is by construction symmetric, and it is common to require that the covariance matrix is positive semidefinite. This means that, for every vector $\mathbf{b} \neq \mathbf{0}$

$$\begin{array}{c|c}
- \square \\
b^T \Sigma b \ge 0. & b^T = (b_1, \dots, b_p) \\
\hline
\text{Scalur}
\end{array}$$

• Why do you think that is?

Hint: Is it possible that the variance of the linear combination $\mathbf{Y} = \mathbf{b}^T \mathbf{X}$ is negative?

Random vectors - Single-choice exercise

Quizz on www.menti.com, code 3967 5773

Question 1: Mean of sum

X and Y are two bivariate random vectors with $E(X) = (1, 2)^T$ and $E(Y) = (2, 0)^T$. What is E(X + Y)?

- A: $(1.5,1)^T$
- B: $(3,2)^T$
- C: $(-1,2)^T$
- D: $(1,-2)^T$

Question 2: Mean of linear combination

X is a 2-dimensional random vector with $E(X) = (2,5)^T$, and $b = (0.5, 0.5)^T$ is a constant vector. What is $E(b^T X)$?

- A: 3.5
- B: 7
- C: 2
- D: 5

Question 3: Covariance

X is a p-dimensional random vector with mean μ . Which of the following defines the covariance matrix?

- A: $E[(\boldsymbol{X} \boldsymbol{\mu})^T (\boldsymbol{X} \boldsymbol{\mu})]$
- B: $E[(X \mu)(X \mu)^T]$
- C: $E[(X \mu)(X \mu)]$
- D: $E[(X \mu)^T (X \mu)^T]$

Question 4: Mean of linear combinations

X is a p-dimensional random vector with mean μ and covariance matrix Σ . C is a constant matrix. What is then the mean of the k-dimensional random vector Y = CX?

- \mathbb{A} : $C\mu$
- B: **CΣ**
- C: $C\mu C^T$
- D: $C\Sigma C^T$

Question 5: Covariance of linear combinations

X is a p-dimensional random vector with mean μ and covariance matrix Σ . C is a constant matrix. What is then the covariance of the k-dimensional random vector Y = CX?

- A: $C\mu$
- B: **CΣ**
- C: $C\mu C^T$
- D: $C\Sigma C^T$

Question 6: Correlation

X is a 2-dimensional random vector with covariance matrix

$$\mathbf{\Sigma} = \left[egin{array}{cc} 4 & 0.8 \\ 0.8 & 1 \end{array}
ight]$$

Then the correlation between the two elements of X are:

- A: 0.10
- B: 0.25
- C: 0.40
- D: 0.80

$$y_{1}^{2}=1$$

$$= 2 \cos((X_1, X_2)) = \frac{0.8}{2}$$

$$= 2 \cos((X_1, X_2)) = \frac{0.8}{2}$$

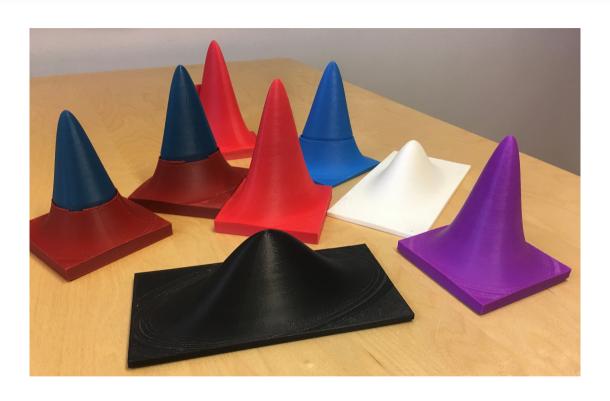
$$= 0.4$$

$$\frac{1}{4\cdot 1} = \frac{1}{2} = 0.$$

The multivariate normal distribution

Why is the mvN so popular?

- Many natural phenomena may be modelled using this distribution (just as in the univariate case).
- Multivariate version of the central limit theorem- the sample mean will be approximately multivariate normal for large samples.
- Good interpretability of the covariance.
- Mathematically tractable.
- Building block in many models and methods.



3D multivariate Normal distributions

The multivariate normal (mvN) pdf

The random vector $X_{p\times 1}$ is multivariate normal N_p with mean μ and (positive definite) covariate matrix Σ . The pdf is:

$$f(\boldsymbol{x}) = \frac{1}{(2\pi)^{\frac{p}{2}} \Sigma^{\frac{1}{2}}} \exp\{-\frac{1}{2} (\boldsymbol{x} - \boldsymbol{\mu})^{T} \Sigma^{-1} (\boldsymbol{x} - \boldsymbol{\mu})\}$$

Questions:

• How does this compare to the univariate version?

$$\begin{cases} f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\{-\frac{1}{2\sigma^2}(x) - \mu^2\} \end{cases}$$

- Why do we need the constant in front of the exp?
- What is the dimension of the part in exp?
- What happens if the determinant $|\Sigma| = 0$ (degenerate case)?

Four useful properties of the mvN

Let $X_{(p\times 1)}$ be a random vector from $N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.

- 1. The grapical contours of the mvN are ellipsoids (can be shown using spectral decomposition).
- 2. Linear combinations of components of X are (multivariate) normal.
- 3. All subsets of the components of X are (multivariate) normal (special case of the above).
- 4. Zero covariance implies that the corresponding components are independently distributed (in contrast to general distributions).

 Entry n is tero => X; X;

If you need a refresh, you might find that video useful: https://www.youtube.com/watch?v=eho8xH3E6mE

$$(COL(X_i, X_i) = O \subset X_i, X_i) = O \subset X_i, X_i$$
 indep.

are independent!

All of these are proven in TMA4267 Linear Statistical Models.

The result 4 is rather useful! If you have a bivariate normal and observed covariance 0, then your variables are independent.

Contours of multivariate normal distribution

• Contours of constant density for the p-dimensional normal distribution are ellipsoids defined by x such that

$$(\boldsymbol{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu}) = b$$

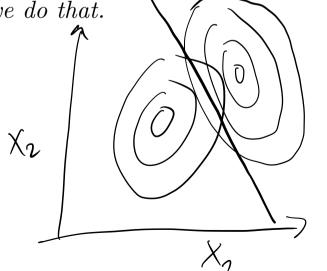
where b > 0 is a constant.

- These ellipsoids are centered at μ and have axes $\pm \sqrt{b\lambda_i} e_i$, where $\Sigma e_i = \lambda_i e_i$ (eigenvector for λ_i), for i = 1, ..., p.
- To see this the spectral decomposition of the covariance matrix is useful.

Note:

In M4: Classification the mvN is very important and we will often draw contours of the mvN as ellipses (in 2D space). This is the reason why we do that.

Discriminant analysis



Identify the mvNs from their contours

Let
$$\Sigma = \begin{bmatrix} \widehat{\sigma_x^2} & \widehat{\rho} \widehat{\sigma_x} \widehat{\sigma_y} \\ \widehat{\rho} \widehat{\sigma_x} \widehat{\sigma_y} & \widehat{\sigma_y^2} \end{bmatrix}$$
.

The following four figure contours have been generated:

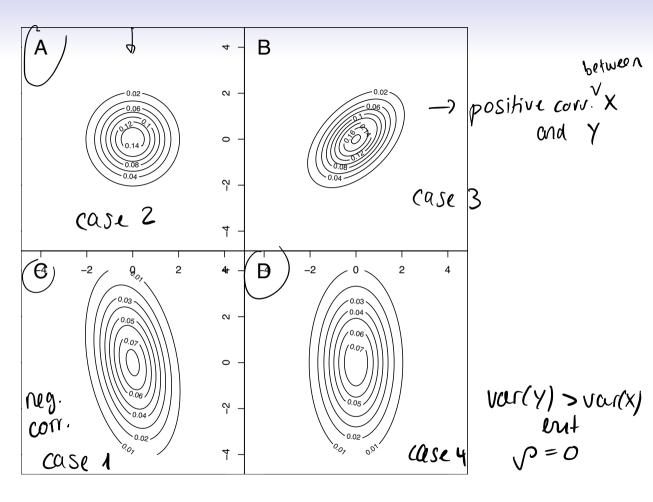
• 1:
$$\sigma_x = 1$$
, $\sigma_y = 2$, $\rho = -0.3$

• 2:
$$\sigma_x = 1$$
, $\sigma_y = 1$, $\rho = 0$ —

• 3:
$$\sigma_x = 1$$
, $\sigma_y = 1$, $\rho = 0.5$

• 4:
$$\sigma_x = 1$$
, $\sigma_y = 2$, $\rho = 0$

Match the distributions to the figures on the next slide.



Take a look at the contour plots - when are the contours circles, when ellipses?

Multiple choice - multivariate normal

A second quizz on www.menti.com, code 3967 5773 Choose the correct answer. Let's go!

Question 1: Multivariate normal pdf

The probability density function is $(\frac{1}{2\pi})^{\frac{p}{2}} \det(\Sigma)^{-\frac{1}{2}} \exp\{-\frac{1}{2}Q\}$ where Q is

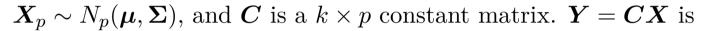
- A: $(x-\mu)^{T} \Sigma^{-1}(x-\mu) \rightarrow scalar$.
- B: $(\boldsymbol{x} \boldsymbol{\mu})\boldsymbol{\Sigma}(\boldsymbol{x} \boldsymbol{\mu})^T$
- C: $\Sigma \mu$

Question 2: Trivariate normal pdf

What graphical form has the solution to $f(\mathbf{x}) = \text{constant}$?

- A: Circle
- B: Parabola
- C: Ellipsoid
- D: Bell shape

Question 3: Multivariate normal distribution



- A: Chi-squared with k degrees of freedom
- B: Multivariate normal with mean $k\mu$
- C: Chi-squared with p degrees of freedom
- D: Multivariate normal with mean $C\mu$

Question 4: Independence

Let $X \sim N_3(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, with

$$\mathbf{\Sigma} = \left[egin{array}{ccc} 1 & 1 & 0 \\ 1 & 3 & 2 \\ 0 & 2 & 5 \end{array}
ight].$$

Which two variables are independent?

- A: X_1 and X_2
- B: X_1 and X_3
- C: X_2 and X_3
- D: None but two are uncorrelated.

mont == independent in muN case!

Question 5: Constructing independent variables?

Let $X \sim N_p(\mu, \Sigma)$. How can I construct a vector of independent standard normal variables from X?

- A: $\Sigma(X \mu)$
- B: $\Sigma^{-1}(X + \mu)$
- ullet C: $\Sigma^{-rac{1}{2}}(X-oldsymbol{\mu})$
- D: $\Sigma^{\frac{1}{2}}(X + \mu)$

$$cov\left(\sum_{i=1}^{n-2}X\right) = \sum_{i=1}^{n-2} cov(X) \left(\sum_{i=1}^{n-2}X\right)^{T}$$

$$= \sum_{i=1}^{n-2} \sum_{i=1}^{n} \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_$$

Aim:
$$Y \sim N_{\rho}(\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}) = I$$

Further reading/resources

• Videoes on YouTube by the authors of ISL, Chapter 2

Acknowledgements

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