Module 2, Part 2: Random vectors, covariance, multivariate Normal distribution TMA4268 Statistical Learning V2020

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Overview

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

Warm up: Task

Find examples to explain the difference between supervised and unsupervised learning.

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- •
- •

Random vector

- A random vector $\boldsymbol{X}_{(p\times 1)}$ is a p-dimensional vector of random variables. For example
 - Weight of cork deposits in p = 4 directions (N, E, S, W).
 - Rent index in Munich: rent, area, year of construction, location, bath condition, kitchen condition, central heating, district.
- Joint distribution function: f(x).
- From joint distribution function to marginal (and conditional distributions).

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

- Cumulative distribution (definite integrals!) used to calculate probabilites.
- Independence: $f(x_1, x_2) = f_1(x_1) \cdot f(x_2)$ and $f(x_1 | x_2) = f_1(x_1)$.

Moments

The moments are important properties about 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

dimnames(corkds)[[2]] = c("N", "E", "S", "W")

[1] 28 4

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

corkds = as.matrix(read.table("https://www.math.ntnu.no/emner/TMA4268/2019v/data/corkMKB.txt"))

- 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:

$$\boldsymbol{X}_{(28\times4)} = \begin{bmatrix} X_{11} & X_{12} & X_{13} & X_{14} \\ X_{21} & X_{22} & X_{23} & X_{24} \\ X_{31} & X_{32} & X_{33} & X_{34} \\ \vdots & \vdots & \ddots & \vdots \\ X_{28,1} & X_{28,2} & X_{28,3} & X_{28,4} \end{bmatrix}$$

Rules for means

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

$$\boldsymbol{X}_{(p\times 1)} = \left[\begin{array}{c} X_1 \\ X_2 \\ \vdots \\ X_p \end{array} \right], \text{ and } \boldsymbol{\mu}_{(p\times 1)} = \mathrm{E}(\boldsymbol{X}) = \left[\begin{array}{c} \mathrm{E}(X_1) \\ \mathrm{E}(X_2) \\ \vdots \\ \mathrm{E}(X_p) \end{array} \right] \; .$$

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• Random matrix $X_{(n \times p)}$ and random matrix $Y_{(n \times p)}$:

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

(Rules of vector addition)

¹Observe 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:

$$\mathrm{E}(\boldsymbol{A}\boldsymbol{X}\boldsymbol{B}) = \boldsymbol{A}\mathrm{E}(\boldsymbol{X})\boldsymbol{B}$$

Proof: Look at element (i, j) of AXB

$$e_{ij} = \sum_{k=1}^{n} a_{ik} \sum_{l=1}^{p} X_{kl} b_{lj}$$

(where a_{ik} and b_{lj} are elements of \boldsymbol{A} and \boldsymbol{B} respectively), and see that $E(e_{ij})$ is the element (i,j) if $\boldsymbol{A}E(\boldsymbol{X})\boldsymbol{B}$.

\mathbf{Q} :

- What are the univariate analogue to the formulas on the previous two slides (which you studied in your first introductory course in statistics)?
- What do you think happens if we look at E(X) + d when X and d are of the same dimension?

The covariance

In the introductory statistics course we defined the covariance

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

= \text{E}(X_i \cdot X_j) - \mu_i \mu_j.

- What is the covariance called when i = j?
- What does it mean when the covariance is
 - negative
 - zero
 - positive?

Make a scatter plot to show this.

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)

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

$$= \begin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1p} \\ \sigma_{12} & \sigma_{22} & \cdots & \sigma_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{1p} & \sigma_{2p} & \cdots & \sigma_{pp} \end{bmatrix} = \operatorname{E}(\boldsymbol{X}\boldsymbol{X}^T) - \boldsymbol{\mu}\boldsymbol{\mu}^T$$

- The diagonal elements in Σ , $\sigma_{ii} = \sigma_i^2$, are variances.
- The off-diagonal elements are covariances

$$\sigma_{ij} = \mathrm{E}[(X_i - \mu_i)(X_j - \mu_j)] = \sigma_{ji}.$$
• Σ is called variance, covariance and variance-co

• 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

$$\Sigma = \left[\begin{array}{cccc} 2 & 1 & 0 & 0 \\ 1 & 2 & 0 & 1 \\ 0 & 0 & 2 & 1 \\ 0 & 1 & 1 & 2 \end{array} \right].$$

Explain what this means.

Correlation matrix

Correlation matrix ρ (real and symmetric)

$$\rho = \begin{bmatrix} \frac{\sigma_{11}}{\sqrt{\sigma_{11}\sigma_{11}}} & \frac{\sigma_{12}}{\sqrt{\sigma_{11}\sigma_{22}}} & \cdots & \frac{\sigma_{1p}}{\sqrt{\sigma_{11}\sigma_{pp}}} \\ \frac{\sigma_{12}}{\sqrt{\sigma_{11}\sigma_{22}}} & \frac{\sigma_{22}}{\sqrt{\sigma_{22}\sigma_{22}}} & \cdots & \frac{\sigma_{2p}}{\sqrt{\sigma_{22}\sigma_{pp}}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\sigma_{1p}}{\sqrt{\sigma_{11}\sigma_{pp}}} & \frac{\sigma_{2p}}{\sqrt{\sigma_{22}\sigma_{pp}}} & \cdots & \frac{\sigma_{pp}}{\sqrt{\sigma_{pp}\sigma_{pp}}} \end{bmatrix} = \begin{bmatrix} 1 & \rho_{12} & \cdots & \rho_{1p} \\ \rho_{12} & 1 & \cdots & \rho_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{1p} & \rho_{2p} & \cdots & 1 \end{bmatrix}$$

$$\boldsymbol{\rho} = (\boldsymbol{V}^{\frac{1}{2}})^{-1} \boldsymbol{\Sigma} (\boldsymbol{V}^{\frac{1}{2}})^{-1}, \text{ where } \boldsymbol{V}^{\frac{1}{2}} = \begin{bmatrix} \sqrt{\sigma_{11}} & 0 & \cdots & 0 \\ 0 & \sqrt{\sigma_{22}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{\sigma_{pp}} \end{bmatrix}$$

Exercise: the correlation matrix

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

$$\mathbf{\Sigma} = \left[\begin{array}{cccc} 2 & 1 & 0 & 0 \\ 1 & 2 & 0 & 1 \\ 0 & 0 & 2 & 1 \\ 0 & 1 & 1 & 2 \end{array} \right].$$

Find the correlation matrix.

 \mathbf{A} :

$$\rho = \left[\begin{array}{cccc} 1 & 0.5 & 0 & 0 \\ 0.5 & 1 & 0 & 0.5 \\ 0 & 0 & 1 & 0.5 \\ 0 & 0.5 & 0.5 & 1 \end{array} \right]$$

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

$$oldsymbol{Z} = oldsymbol{C} oldsymbol{X} = oldsymbol{C} oldsymbol{X} = oldsymbol{C} oldsymbol{X} = oldsymbol{C} oldsymbol{X} = oldsymbol{\sum}_{j=1}^p c_{2j} X_j \ dots \ \sum_{j=1}^p c_{kj} X_j \ \end{bmatrix}$$

have

$$\mathrm{E}(oldsymbol{Z}) = \mathrm{E}(oldsymbol{C}oldsymbol{X}) = oldsymbol{C}oldsymbol{\mu}$$
 $\mathrm{Cov}(oldsymbol{Z}) = \mathrm{Cov}(oldsymbol{C}oldsymbol{X}) = oldsymbol{C}oldsymbol{\Sigma}oldsymbol{C}^T$

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

Exercise: Linear combinations

$$\boldsymbol{X} = \begin{bmatrix} X_N \\ X_E \\ X_S \\ X_W \end{bmatrix}, \boldsymbol{\mu} = \begin{bmatrix} \mu_N \\ \mu_E \\ \mu_S \\ \mu_W \end{bmatrix}, \text{ and } \boldsymbol{\Sigma} = \begin{bmatrix} \sigma_{NN} & \sigma_{NE} & \sigma_{NS} & \sigma_{NW} \\ \sigma_{NE} & \sigma_{EE} & \sigma_{ES} & \sigma_{EW} \\ \sigma_{NS} & \sigma_{EE} & \sigma_{SS} & \sigma_{SW} \\ \sigma_{NW} & \sigma_{EW} & \sigma_{SW} & \sigma_{WW} \end{bmatrix}$$

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

- Write down 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 is given below.

```
dimnames(corkds)[[2]] <- c("N", "E", "S", "W")
mu = apply(corkds, 2, mean)
mu
Sigma = var(corkds)
Sigma
## N E S
## 50.53571 46.17857 49.67857 45.17857
##
          N
                  E
## 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), bvrow = T, nrow = 3))
## [,1] [,2] [,3] [,4]
## [1.] 1 0 -1
## [2,] 0 1 0 1
## [3.] -1 1 -1 1
C %*% Sigma %*% t(C)
           [,1] [,2] [,3]
##
```

[1,] 63.53439 -38.57672 21.02116 ## [2,] -38.57672 788.68254 -149.94180 ## [3,] 21.02116 -149.94180 128.71958

corkds <- as.matrix(read.table("https://www.math.ntnu.no/emner/TMA4268/2019v/data/corkMKB.txt"))

The covariance matrix - more requirements?

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

$$\boldsymbol{\Sigma} = \operatorname{Cov}(\boldsymbol{X}) = \operatorname{E}[(\boldsymbol{X} - \boldsymbol{\mu})(\boldsymbol{X} - \boldsymbol{\mu})^T] = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1p} \\ \sigma_{12} & \sigma_{22} & \cdots & \sigma_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{1p} & \sigma_{2p} & \cdots & \sigma_{pp} \end{bmatrix}$$

• 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 $\mathbf{b} \neq \mathbf{0}$

$$\boldsymbol{b}^T \boldsymbol{\Sigma} \boldsymbol{b} \geq 0$$
.

• Why do you think that is?

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

Random vectors - Single-choice klicker exercise

In class - go to https://app.klicker.uzh.ch/join/bkx to answer the questions on the following slides

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

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

- 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: $E[(\boldsymbol{X} \boldsymbol{\mu})(\boldsymbol{X} \boldsymbol{\mu})^T]$
- 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?

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

Question 6: Correlation

 \boldsymbol{X} is a 2-dimensional random vector with covariance matrix

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

Then the correlation between the two elements of X are:

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



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 $\boldsymbol{X}_{p\times 1}$ is multivariate normal N_p with mean $\boldsymbol{\mu}$ and (positive definite) covariate matrix $\boldsymbol{\Sigma}$. The pdf is:

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

Questions:

• How does this compare to the univariate version?

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

- 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)?

Six 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).

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 $\Sigma e_i = \lambda_i e_i$, for i = 1, ..., p.
- To see this the spectral decomposition of the covariance matrix is useful.
- $(\boldsymbol{x} \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} \boldsymbol{\mu})$ is distributed as χ_p^2 .

Note:

In M4: Classification the mvN is very important and we will often draw contours of the mvN as ellipses- and this is the reason why we do that.

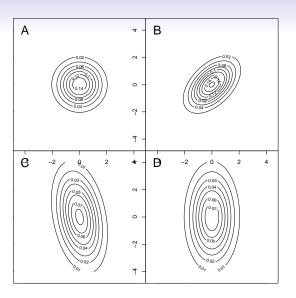
Identify the mvNs from their contours

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

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

Choose the correct answer - time limit was 30 seconds for each question! 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: $(\boldsymbol{x} \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} \boldsymbol{\mu})$
- 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(x) = constant?

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

Question 3: Multivariate normal distribution

 $\boldsymbol{X}_p \sim N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma}),$ and \boldsymbol{C} is a $k \times p$ constant matrix. $\boldsymbol{Y} = \boldsymbol{C}\boldsymbol{X}$ is

- 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

$$\Sigma = \left[\begin{array}{ccc} 1 & 1 & 0 \\ 1 & 3 & 2 \\ 0 & 2 & 5 \end{array} \right].$$

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.

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: $\Sigma^{-1}(X + \mu)$
- C: $\Sigma^{-\frac{1}{2}}(X \mu)$
- D: $\Sigma^{\frac{1}{2}}(X + \mu)$



Further reading/resources

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

Excursion: R Markdown and knitr

We will use R Markdown for writing the Compulsory exercise reports in our course.

1. What is R Markdown?

1-minute introduction video: https://rmarkdown.rstudio.com/lesson-1.html

Then, if more is needed also a chapter from the Data Science book: http://r4ds.had.co.nz/r-markdown.html

2. What is knitr? https://yihui.name/knitr/

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