# Module 2, Part 2: Random vectors, covariance, multivariate Normal distribution TMA4268 Statistical Learning V2025

Stefanie Muff, Department of Mathematical Sciences, NTNU

January 17, 2025

# Overview

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

### Random vector

- 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).

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

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

#### Moments

The moments are important properties of the distribution of  $\boldsymbol{X}$ . 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).

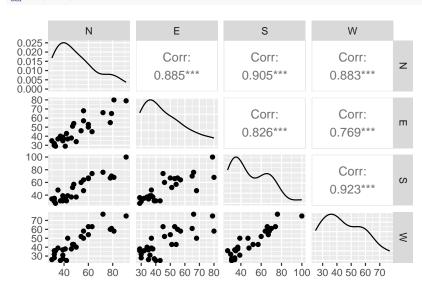
```
corkds=as.matrix(
  read.table("https://www.math.ntnu.no/emner/TMA4268/2019v/data/corkMKB.txt")
  )
  dimnames(corkds)[[2]]=c("N","E","S","W")
  head(corkds)

##    N    E    S    W
## [1,] 72 66 76 77
## [2,] 60 53 66 63
## [3,] 56 57 64 58
## [4,] 41 29 36 38
## [4,] 41 29 36 38
## [6,] 30 35 34 26
dim(corkds)

## [1] 28 4
```

# 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:

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

#### The mean vector

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

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

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

#### Rules for the mean I

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

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

(Rules of vector and matrix addition)

#### Rules for the mean II

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

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

Proof: Board

# $\mathbf{Q}$ :

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

#### 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 for negative, zero and positive correlation (see also R example).

#### Variance-covariance matrix

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

$$m{X}_{(p imes 1)} = \left[ egin{array}{c} X_1 \ X_2 \ dots \ X_p \end{array} 
ight], ext{ and } m{\mu}_{(p imes 1)} = \mathrm{E}(m{X}) = \left[ egin{array}{c} \mathrm{E}(X_1) \ \mathrm{E}(X_2) \ dots \ \mathrm{E}(X_p) \end{array} 
ight]$$

• Variance-covariance matrix  $\Sigma$  (real and symmetric)

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

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

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

#### Exercise: the variance-covariance matrix

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

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

Explain what this means.

#### Correlation matrix

Correlation matrix  $\rho$  (real and symmetric)

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

$$oldsymbol{
ho} = (oldsymbol{V}^{rac{1}{2}})^{-1} oldsymbol{\Sigma} (oldsymbol{V}^{rac{1}{2}})^{-1}, ext{ where } oldsymbol{V}^{rac{1}{2}} = \left[ egin{array}{cccc} \sqrt{\sigma_1^2} & 0 & \cdots & 0 \\ 0 & \sqrt{\sigma_2^2} & \cdots & 0 \\ dots & dots & \ddots & dots \\ 0 & 0 & \cdots & \sqrt{\sigma_p^2} \end{array} 
ight]$$

#### Exercise: the correlation matrix

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

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

Find the correlation matrix.

 $\mathbf{A}$ :

#### 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

$$oldsymbol{Z} = oldsymbol{C} oldsymbol{X} = oldsymbol{C} oldsymbol{C} = oldsymbol{C} oldsymbol{X} = oldsymbol{C} oldsymbol{C} = oldsymbol{C} = oldsymbol{C} oldsymbol{C} = o$$

have

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

**Exercise:** Follow the proof - 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  $\boldsymbol{Y}_{(3\times 1)} = \boldsymbol{C}_{(3\times 4)} \boldsymbol{X}_{(4\times 1)}$  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 given below.

Find C, such that  $Y_{(3\times 1)}=C_{(3\times 4)}X_{(4\times 1)}$  gives the three contrasts above:

$$\mathrm{Cov}(\boldsymbol{Y}) = \mathrm{Cov}(\boldsymbol{C}\boldsymbol{X}) = \dots$$

```
corkds <- as.matrix(read.table("https://www.math.ntnu.no/emner/TMA4268/2019v/data/corkMKB.txt"))
dimnames(corkds)[[2]] <- c("N", "E", "S", "W")
mu=apply(corkds,2,mean)
mıı
Sigma=var(corkds)
Sigma
##
## 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] [,3] [,4]
## [1,] 1 0 -1
## [2.] 0 1 0
## [3.] -1 1 -1 1
C %*% Sigma %*% t(C)
                       [,2]
                               [,3]
##
            [,1]
## [1,] 63.53439 -38.57672
                             21.02116
## [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

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

• 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  $\mathbf{b} \neq \mathbf{0}$ 

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

• 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 exercise

 ${\it Quizz\ on\ www.menti.com}$ 

# Question 1: Mean of sum

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

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

# Question 4: Mean of linear combinations

X is a p-dimensional random vector with mean  $\mu$  and covariance matrix  $\Sigma$ . 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  $\mu$  and covariance matrix  $\Sigma$ . 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  $X_{p\times 1}$  is multivariate normal  $N_p$  with mean  $\mu$  and (positive definite) covariate matrix  $\Sigma$ . 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?

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

- 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).

If you need a refresh, you might find that video useful: https://www.youtube.com/watch?v=eho8xH3E6mE 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  $\mu$  and have axes  $\pm \sqrt{b\lambda_i}e_i$ , where  $\Sigma e_i = \lambda_i e_i$  (eigenvector for  $\lambda_i$ ), 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.

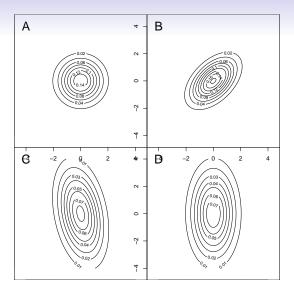
## Identify the mvNs from their contours

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

A second quizz on www.menti.com

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

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

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

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

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

## Acknowledgements

Thanks to Mette Langaas, who developed the first slide set in 2018 and 2019, and to Julia Debik for contributing to this module.