

Module 1: Introduction

TMA4268 Statistical Learning V2022

Stefanie Muff, Department of Mathematical Sciences, NTNU

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Acknowledgements

- This course had been built up by Mette Langaas at NTNU in 2018 and 2019. I am using a some of her material, and material from her TAs, throughout the course.

I would like to thank Mette for her great work and for the permission to use her material!

- Thanks to Julia Debik for contributing to this module page.

Learning outcomes of TMA4268

1. **Knowledge.** The student has knowledge about the most popular statistical learning models and methods that are used for *prediction* and *inference* in science and technology. Emphasis is on regression- and classification-type statistical models.
2. **Skills.** The student can, based on an *existing data* set, choose a suitable statistical model, apply sound statistical methods, and perform the analyses using statistical software. The student can present, interpret and communicate the results from the statistical analyses, and knows which conclusions can be drawn from the analyses, and what the caveats are.

R
=

Learning material

- 1) **The main learning source** is the textbook by James, Witten, Hastie, Tibshirani (2013): “An Introduction to Statistical Learning”. The textbook can be downloaded here:
<https://www-bcf.usc.edu/~gareth/ISL/>
 - The ebook can also be downloaded from Springer:
<https://www.springer.com/gp/book/9781461471370> (NB, need to be on NTNU network or via vpn.)
 - There are 15 hours of youtube videos by two of the authors of the book, Trevor Hastie and Rob Tibshirani. Links will be added to the module subpages.
- 2) All the lecture notes, **including any classnotes** made on the iPad or black board (iPad notes will be made available online).
- 3) The R course here: <https://digit.ntnu.no/courses/course-v1:NTNU+IMF001+2020/course/>
- 4) **Additional reading material will be clearly indicated in the modules and on the course page.**

Course page

All the relevant information for the course can be found here:

<https://wiki.math.ntnu.no/tma4268/2022v/start>

On each module page, all the relevant learning material and exercises (incl. solutions) will be provided in due time.

The Statistical Learning Team 2022

The TAs:

- Emma Skarstein; PhD student
- Daesoo Lee; PhD student

The Lecturers

- Stefanie Muff; Associate Professor
- Thiago Guerrera Martins; NTNU/AIAscience (Modules 6, 7, 10)
- David Klindt; Postdoc/soon Meta (Module ~~12~~
11)

Who is this course for?

Primary requirements

- Bachelor level: 3rd year students from Science or Technology programs, and master/PhD level students with interest in performing statistical analyses.
- Statistics background: TMA4240/45 Statistics, ST1101+ST1201 (probability theory and statistical methods), or equivalent.
- No background in statistical software needed: but we will use the R statistical software extensively in the course. Knowing python will make this easier for you!
- Advantage with knowledge of computing - for example an introductory course in informatics, like TDT4105 or TDT4110.

Overlap

- **TDT4173 Machine learning** and case based reasoning: courses differ in philosophy (computer science vs. statistics).
- **TMA4267 Linear Statistical Models**: useful to know about multivariate random vectors, covariance matrices and the multivariate normal distribution. Overlap only for multiple linear regression (M3).

About the course

Focus: Statistical theory **and** doing analyses

- The course has focus on **statistical theory**, but we apply all models and theory using (mostly) available function in R and real data sets.
- It is important that the student in the end of the course **can analyse all types of data** (covered in the course) - not just understand the theory.
- And vice versa - the student must also **understand** the model, methods and algorithms used.

Teaching philosophy

- Divide the topics of the course into modular units with specific focus.
- This (hopefully) facilitates learning?
- Two weeks without lectures, time to work on the compulsory exercises.

Course content: The 12 Modules

- **Module 1:** Introduction & R course (this module)
- **Modules 2 - 11:**
 - 2) Statistical learning
 - 3) Multiple linear regression
 - 4) Classification
 - 5) Resampling methods
 - 6) Model selection/regularization
 - 7) Non-linearity
 - 8) Support vector machines
 - 9) Tree-based methods
 - 10) Unsupervised methods
 - 11) Neural networks (not in the course book) } not in course book
- **Module 12:** Summing up

course
book

Learning methods, activities and grading

- Lectures, exercises and works (projects). *compulsory exercises*
- Portfolio assessment is the basis for the grade awarded in the course. This portfolio comprises
 - a written **final (school!) examination (80%)**.
 - two projects / compulsory exercises ($2 \times \underline{10\%} = 20\%$).
- The results for the constituent parts are to be given in %-points, while the grade for the whole portfolio (course grade) is given by the letter grading system. Retake of examination may be given as an oral examination. The lectures are given in English.

The lectures

Mondays at 14.15-16.00 in (S3) and Thursdays at 08.15-10.00 in (S2)

- We are starting with online classes due to the current restrictions around Covid.
- We have 2×2 hours of lectures every week (except when working with the compulsory exercises).
- See here https://github.com/stefaniemuff/statlearning/blob/master/TMA4268_schedule2022.pdf for a tentative schedule.
- **I suggest that you always have your laptop handy for the lecture.** So you can run code or do an exercise in class.

The first week: The R course

- In this **first week of the course** you will have to work through parts 1-6 of the R course on the openEdX page here:
<https://digit.ntnu.no/courses/course-v1:NTNU+IMF001+2020/course/>
- Log in with your Feide account (scroll a bit down).
- There is a discussion forum that you can use for the R course.

Recommended exercises

- For each module *recommended exercises* are uploaded. These are partly
 - theoretical exercises (from book or not)
 - computational tasks
 - data analysis Using R
- These are supervised in the weekly exercise slots.
- Solutions will be provided to check yourself (no grading).

Currently there are **three slots** in the schedule:

- Mon 8:15-10:00 (F2)
- Wed 12:15-14:00 (F6)
- Wed 14:15-16:00 (S4)

But **do we need all of those?**

Log into www.menti.com and use the code 9384 0003.

- We of course have to start with online supervision. How this works will be communicated (see also course website).

The compulsory exercises (projects / works)

- We will have **two compulsory exercises**, each with a maximal score of 50 points.
- These are supervised in the weekly exercise slots and there will be one week without lectures (only with supervision) for each compulsory exercise.
- Focus: theory, analysis in R, and interpretation.
- Work in **groups of maximum 3**; groups are formed in Blackboard (Bb). Also hand-in is via Bb in on Blackboard.
- Written in R Markdown (both .Rmd and .pdf handed in).
- The TAs grade the exercises.

- The **first compulsory exercise** will be held after Modules 1-5.

Suggested submission deadline:

Monday, 21. Februar 2022, 23:59h.

- The **second compulsory exercise** will be held after Modules 6-10.

Suggested submission deadline:

Monday, 4. April 2022, 23:59h.

Tentative schedule

A tentative schedule (i.e., with continuous updates) can be found under the following link (also available from our course page):

https://github.com/stefaniemuff/statlearning/blob/master/TMA4268_schedule2022.pdf

The lecture material

- All the material presented in class will be available on our course webpage (<https://wiki.math.ntnu.no/tma4268/2022v/start>).
- There will be .pdf, .html and .Rmd versions of the lecture notes and exercises. This will allow you to check and use the code that is used therein.

The discussion forum on Mattelab

- Use our discussion forum on Mattelab for all course-relevant questions: <https://mattelab2022v.math.ntnu.no/c/tma4268/9>
- Avoid writing emails to the course staff. By posting your question on Mattelab we get the chance to answer the questions to everyone.

Who are you - and what are your expectations?

We again use www.menti.com

Reference group

At least 3 members, ideally one from different programmes

- At least one from IndMat, year 3
- Any programme, year 4
- Not IndMat

Volunteers?

- (3 year Bachelor or MSMNFNA)
- (Industrial Mathematics) ✓ ✗
- (Other) ✓ ✗

August Arnstad

1 person in MLREAL
so far

Thanks to the three people that volunteer.

Simon Liabo

Module 1

Aims of the first module

- An introduction to statistical learning. What is it?
- Types of problems we will look at
- **Introduction to R and RStudio**

Learning material for this module

Required:

- Our textbook James et al (2013): An Introduction to Statistical Learning - with Applications in R (ISL).
 - Chapter 1 (Introduction)
 - 2.3 (Lab: Introduction to R)
- Go through parts 1 to 6 in the online R course:
<https://digit.ntnu.no/courses/course-v1:NTNU+IMF001+2020/course/>

Recommended:

- Watch the video lecture for Chapter 1 by Hastie and Tibshirani [here](#).
- Background on Matrix Algebra: Härdle and Simes (2015) - Chapter 2: A short excursion into Matrix Algebra (on the reading list for TMA4267 Linear statistical models).

What is statistical learning?

- Refers to *a vast set of tools to understanding data* (text book, p. 1).
- Main distinction: Supervised versus unsupervised learning. / M10
- Both prediction and inference (understanding → drawing conclusions).
- Statistical learning is **a statistical discipline**, but the borders are becoming more blurred.

Statistical Learning vs. “Machine Learning”

- Machine learning is more focused on the algorithmic part of learning, and is a *discipline in computer science*.
- But many methods/algorithms are common to both fields.

Statistical Learning vs. “Data Science”

Data science

- Aim: to extract knowledge and understanding from data.
- Requires a combination of statistics, mathematics, numerics, computer science and informatics.

This encompasses the whole process of

1. data acquisition/scraping
2. going from unstructured to structured data
3. setting up a data model
4. implementing and performing data analysis
5. interpreting and communicating results

In statistical learning we will not work on the two first above (acquisition and unstructured to structured).

[R for Data Science](#) is an excellent read and relevant for this course!

Problems you will learn to solve

There are **three main types of problems** discussed in this course:

- Regression (supervised)
 - Classification (supervised)
 - Unsupervised methods
- } Modules 2-9, 11
} Module 10

using data from science, technology, industry, economy/finance, ...

Example 1: Regression (Etiology of CVD)

- The Framingham Heart Study investigates the underlying causes of cardiovascular disease (CVD) (see <https://www.framinghamheartstudy.org/>).
- Aim: modelling systolic blood pressure (SYSBP) using data from $n = 2600$ persons.
- For each person in the data set we have measurements of the following seven variables.

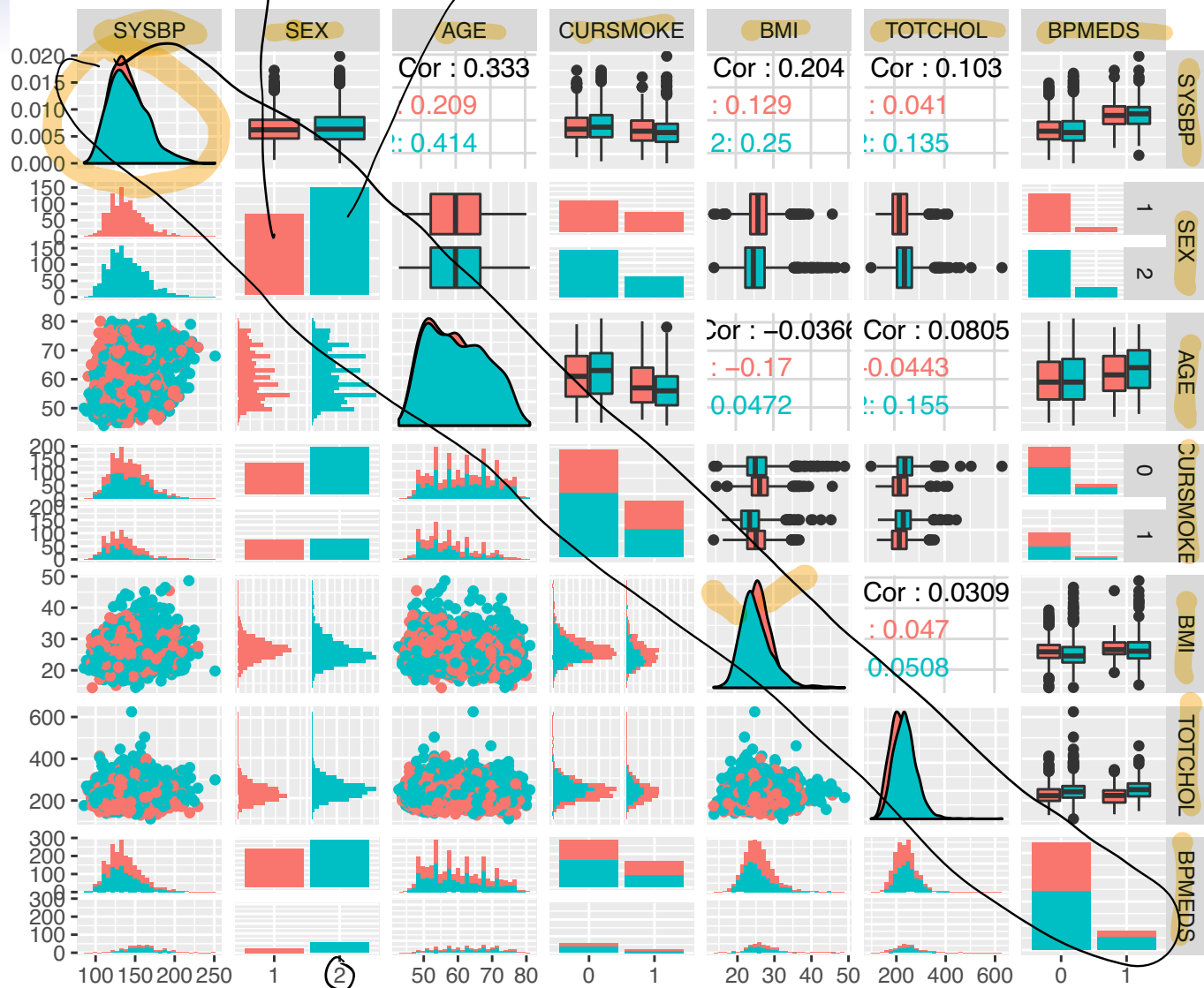
outcome (y)
covariates (x)

- SYSBP systolic blood pressure (mmHg),
- SEX 1=male, 2=female,
- AGE age (years),
- CURSMOKE current cigarette smoking at examination: 0=not current smoker, 1=current smoker,
- BMI body mass index,
- TOTCHOL serum total cholesterol (mg/dl),
- BPMEDS use of anti-hypertensive medication at examination: 0=not currently using, 1=current using.

Framingham Heart Study

males

females



- Diagonal: density plot (generalization of histogram), or barplot.
- Lower diagonals: scatterplot, histograms
- Upper diagonals: correlations, boxplots or barplots

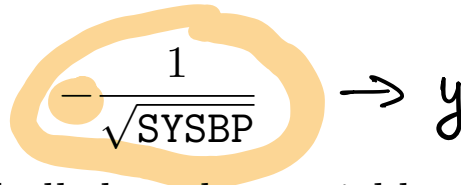
We use `sex` to color the graph.

Etiology of CVD

The question: **What are the factors that cause high SBP?**

→ we are interested in *inference* (*explanation*), not prediction!

- A *multiple normal linear regression model* was fit to the data set with

A diagram showing a regression coefficient. It consists of a horizontal line with a '1' above it, and a square root symbol containing 'SYSBP' below it. This entire fraction is enclosed in a hand-drawn orange oval. To the right of the oval is an arrow pointing to the letter 'y'.
$$-\frac{1}{\sqrt{\text{SYSBP}}} \rightarrow y$$

as response (output) and all the other variables as covariates (inputs).

- The results are used to formulate hypotheses about the etiology of CVD - to be studied in new trials.

linear model

```
modelB = lm(-1/sqrt(SYSBP) ~ SEX + AGE + CURSMOKE + BMI + TOTCHOL + BPMEDS, data = thisds)
summary(modelB)
```

y $x_1 + x_2 + \dots + x_6$ } 2 code

```
##
## Call:
## lm(formula = -1/sqrt(SYSBP) ~ SEX + AGE + CURSMOKE + BMI + TOTCHOL +
##     BPMEDS, data = thisds)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.0207366 -0.0039157 -0.0000304  0.0038293  0.0189747
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) -1.106e-01  1.342e-03 -82.413  < 2e-16 ***
## SEX2        -2.989e-04  2.390e-04  -1.251  0.211176
## AGE         2.378e-04  1.434e-05  16.586  < 2e-16 ***
## CURSMOKE1   -2.504e-04  2.527e-04  -0.991  0.321723
## BMI         3.087e-04  2.955e-05  10.447  < 2e-16 ***
## TOTCHOL     9.288e-06  2.602e-06   3.569  0.000365 ***
## BPMEDS1     5.469e-03  3.265e-04  16.748  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.005819 on 2593 degrees of freedom
## Multiple R-squared:  0.2494, Adjusted R-squared:  0.2476
## F-statistic: 143.6 on 6 and 2593 DF, p-value: < 2.2e-16
```

p-value

output

Example 2: Classification (iris plants)

The `iris` flower data set is a very famous multivariate data set introduced by the British statistician and biologist Ronald Fisher in 1936.

The data set contains

- **three plant species** {setosa, virginica, versicolor}
- **four features measured** for each corresponding sample:
 - **Sepal.Length**
 - Sepal.Width
 - **Petal.Length**
 - Petal.Width.

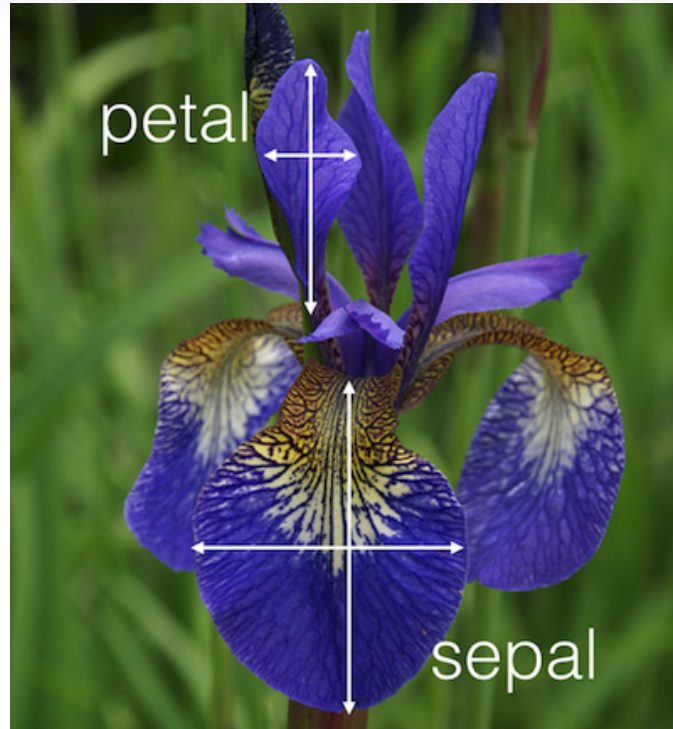


Figure 1: Iris plant with sepal and petal leaves

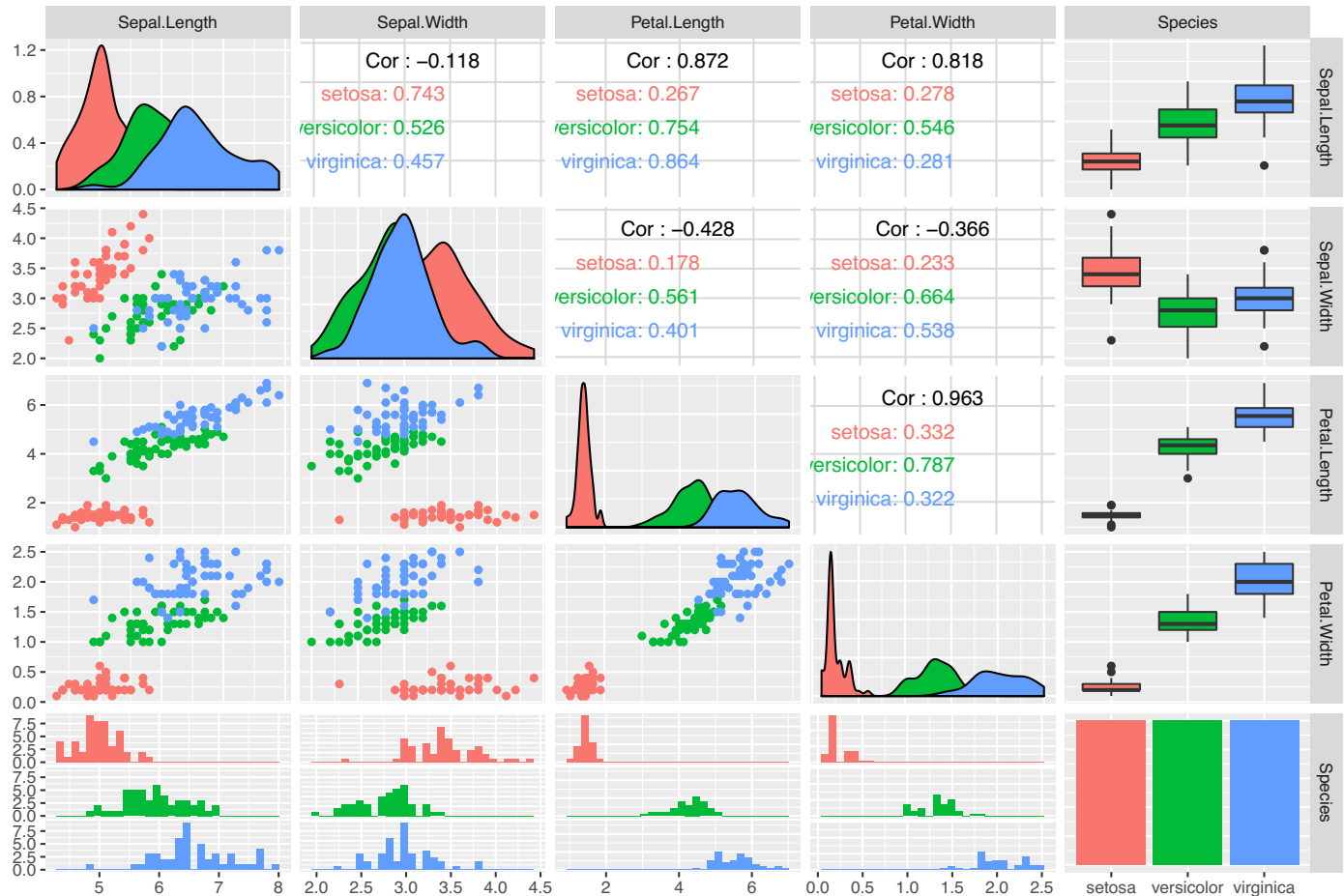
<http://blog.kaggle.com/2015/04/22/scikit-learn-video-3-machine-learning-first-steps-with-the-iris-dataset/>

```
head(iris)
```

##	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species	
## 1	5.1	3.5	1.4	0.2	setosa	→ plant 1
## 2	4.9	3.0	1.4	0.2	setosa	→ plant 2
## 3	4.7	3.2	1.3	0.2	setosa	.
## 4	4.6	3.1	1.5	0.2	setosa	:
## 5	5.0	3.6	1.4	0.2	setosa	:
## 6	5.4	3.9	1.7	0.4	setosa	}

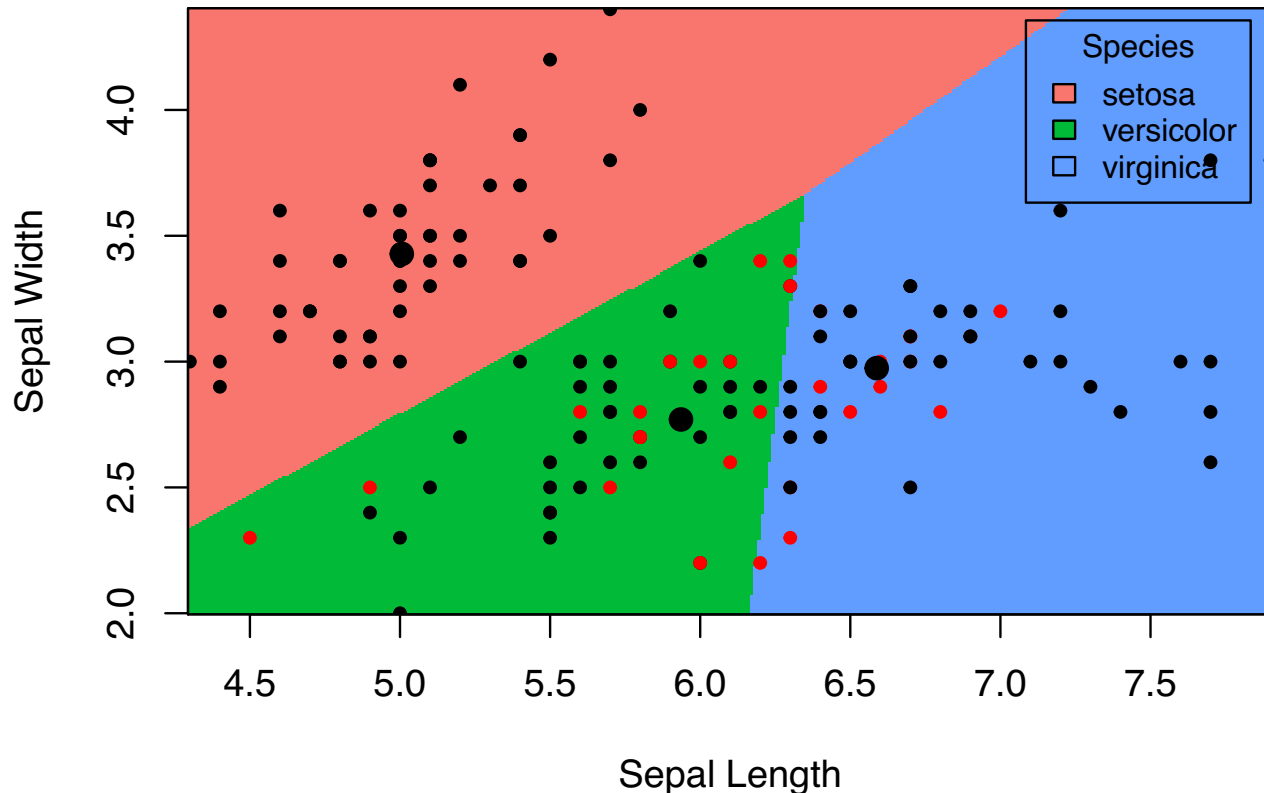
Aim: correctly classify the species of an iris plant from sepal length and sepal width.

Classification of Iris plants



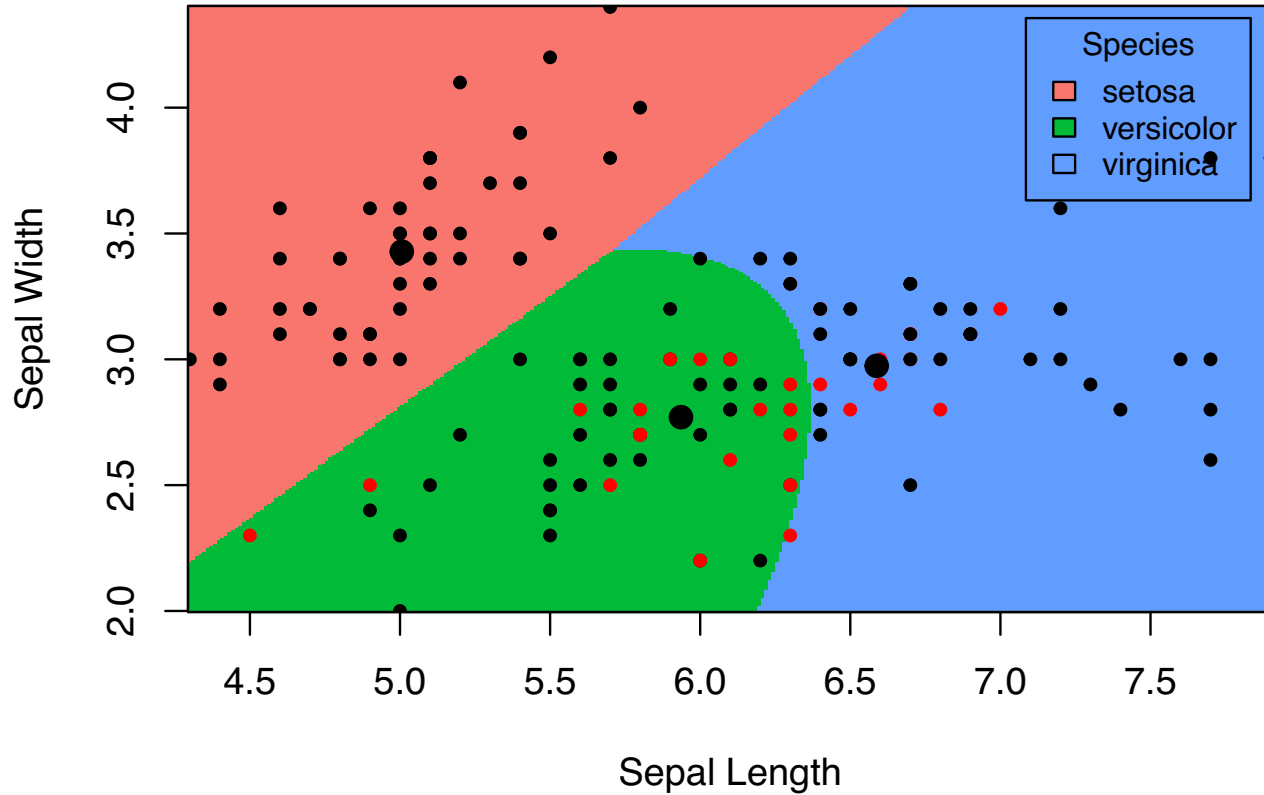
Linear boundaries

In this plot the small black dots represent correctly classified iris plants, while the red dots represent misclassifications. The big black dots represent the class means.



Non-linear boundaries

Sometimes a non-linear boundary is more suitable.



Example 3: Unsupervised methods (Gene expression)

- The relationship between inborn maximal oxygen uptake and skeletal muscle gene expression was studied.
- Rats were artificially selected for high- and low running capacity (HCR and LCR, respectively).
- Rats were either kept sedentary or trained.
- Transcripts significantly related to running capacity and training were identified.
- Heat maps showing the expression level for the most significant transcripts were presented graphically.
- This is *hierarchical cluster analysis* with pearson correlation distance measure (module 10).

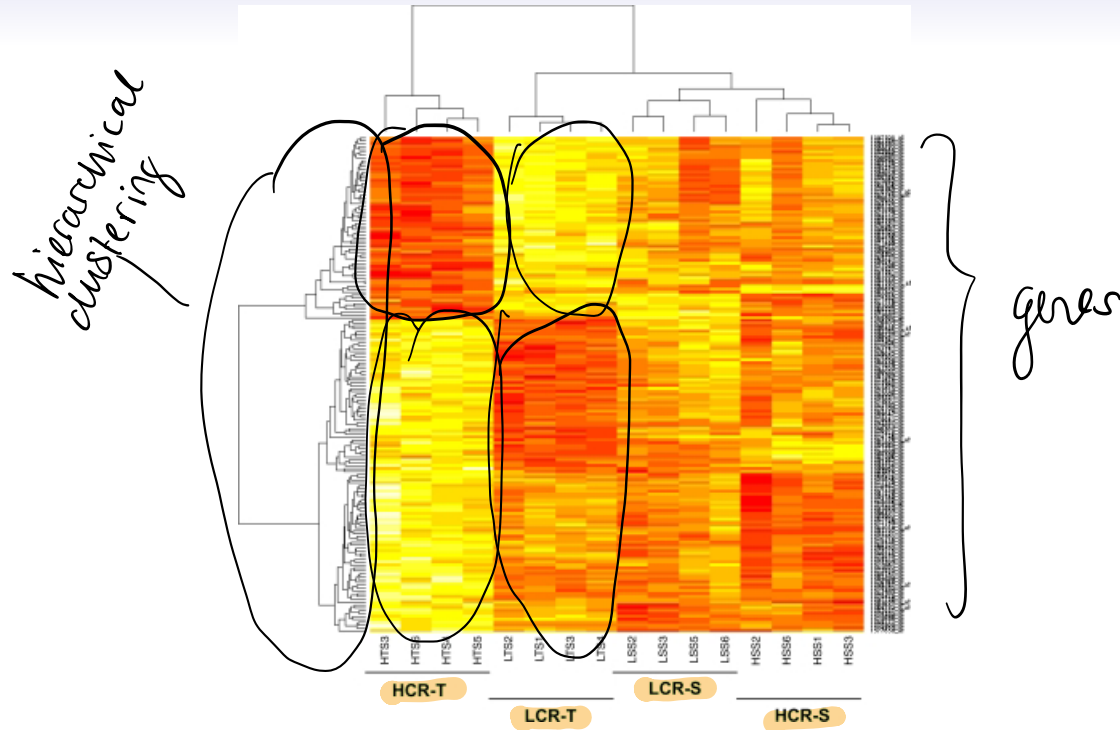


Figure 2: Heat map of the most significant transcripts. Transcripts with a high expression are shown in red and transcripts with a low expression are shown in yellow.

More: <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2585023/>

Example 4: Unsupervised methods (Network clustering)

Idea: Find structure in messy data

Finding clusters in protein-protein-interaction networks.

MUFF, RAO, AND CAFLISCH

PHYSICAL REVIEW E 72, 056107 (2005)

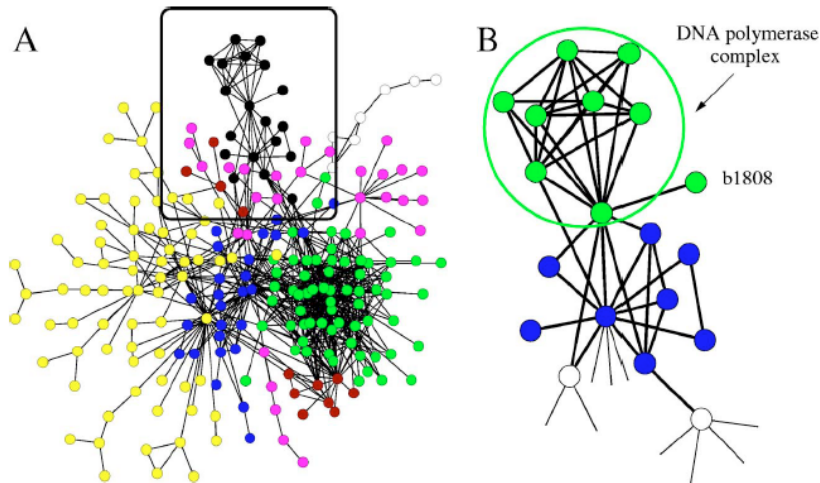


FIG. 4. (Color online) (a) Largest connected component of the PPI of *E. coli*. The colors represent the clusterization found by optimizing modularity. (b) LQ clusterization of the black Q cluster. The green circle contains proteins belonging to the DNA polymerase complex. The unknown protein b1808 is assigned to this complex according to LQ while the complete Q cluster is heterogeneous.

Plan for rest of the week

- You can work through parts 1 - 6 in the R course
[https://digit.ntnu.no/courses/course-v1:
NTNU+IMF001+2020/course/](https://digit.ntnu.no/courses/course-v1:NTNU+IMF001+2020/course/)
- Ideally use your Feide account to log in.
- There is a discussion forum (click on the “Discussion” tab).

Getting started with R

- Install R (use the Norwegian CRAN mirror):
<https://www.r-project.org>
- Install Rstudio <https://www.rstudio.com/products/rstudio/>

If you need help on installing R and RStudio on you laptop computer, contact orakel@ntnu.no.

Some additional links

- 1) What is R? <https://www.r-project.org/about.html>
- 2) What is RStudio? <https://www.rstudio.com/products/rstudio/>
- 3) What is CRAN? <https://cran.uib.no/>
- 4) What is GitHub and Bitbucket? Do we need GitHub or Bitbucket in our course?
<https://www.youtube.com/watch?v=w3jLJU7DT5E> and <https://techcrunch.com/2012/07/14/what-exactly-is-github-anyway/>

Additional nice R resources

- P. Dalgaard: Introductory statistics with R, 2nd edition, Springer, which is also available freely to NTNU students as an ebook: [Introductory Statistics with R](#).
- Grolemund and Hadwick (2017): “R for Data Science”, <http://r4ds.had.co.nz>
- Hadwick (2009): “ggplot2: Elegant graphics for data analysis” textbook: <https://ggplot2-book.org/>
- [Overview of cheat sheets from RStudio](#)
- Questions on R: ask the course staff, colleagues, and [stackoverflow](#).