Module 1: Introduction

TMA4268 Statistical Learning V2020

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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!

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 are the caveats.

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 an 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 an Rob Tibshirani -the inventors of statistical learning - all links here
2) All the lecture notes, **including any classnotes** made on the board (not necessarily 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/tma4268/2021v/start

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

The Statistical Learning Team 2021

The TAs:

- Emma Skarstein; PhD student
- Michail Spitieris; PhD student

The Lecturers

- Stefanie Muff; Associate Professor
- Thiago Guerrera Martins; NTNU/AIAscience (Modules 6, 7, 10)

Who is this course for?

Primary requirements

- Bachelor level: 3rd year student 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!
- Advangatge 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)
- **Module 12**: Summing up

Learning methods, activities and grading

- Lectures, exercises and works (projects).
- Portfolio assessment is the basis for the grade awarded in the course. This portfolio comprises
  - a written **final home examination (60%)**.
  - two projects / compulsory exercises ($2 \times 20\% = 40\%$).
- 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 12.15-14.00 online lectures and Fridays at 10.15-12.00 in S8 (if possible)

- 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_schedule2021.pdf for a tentative schedule.
- Some weeks the Tuesday lecture are supposed to be a bit more *interactive* or with some self-study / exercise component, where *active learning* is in focus. However, this will be a bit difficult if the lecture is online.
- **I suggest that you always have your laptop handy for the Tuesday lecture.** So you can run code or do an exercise in class.

The first week

- In the **first week of the course** you will have to work through parts 1-6 of the R course here: https://digit.ntnu.no/courses/course-v1:NTNU+IMF001+2020/course/

The weekly supervision sessions

Tuesdays 16.15-18:00 in room VE-E20

- For each module *recommended exercises* are uploaded. These are partly
    - theoretical exercises (from book or not)
    - computational tasks
    - data analysis
- These are supervised in the weekly exercise slots.
- Solutions will be provided to check yourself (no grading).
- We of course have to start with online supervision. How this works will be communicated.

The compulsory exercises

- 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**; handed in on Blackboard and be written in R Markdown (both .Rmd and .pdf handed in).
- The TAs grade the exercises.
- The compulsory exercises sum to 40% of the final evaluation in the course, the written exam the remaining 60%.

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

  Suggested submission deadline:

  Monday, 22. Februar 2021, 23:59h.

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

  Suggested submission deadline:

  Monday, 19. April 2021, 23:59h.

Tentative schedule

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

https://github.com/stefaniemuff/statlearning/blob/master/TMA4268_schedule2021.pdf

The lecture material

- All the material presented in class will be available on our course webpage (https://wiki.math.ntnu.no/tma4268/2021v/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.

Student active learning

Student's learning styles are different! Felder and Silverman (1988) suggested the following learning style axes:

1) **active - reflective**: How do you process information: actively (through physical activities and discussions), or reflexively (through introspection)?
2) **sensing-intuitive**: What kind of information do you tend to receive: sensitive (external agents like places, sounds, physical sensation) or intuitive (internal agents like possibilities, ideas, through hunches)?
3) **visual-verbal:** Through which sensorial channels do you tend to receive information more effectively: visual (images, diagrams, graphics), or verbal (spoken words, sound)? Many students have a visual learning style!
4) **sequential - global**: How do you make progress: sequentially (with continuous steps), or globally (through leaps and an integral approach)?

We try!

- ... to acknowledging these different learning style axes.
- ... to choose teaching styles that match the learning styles of as many students as possible.
- ... to provide learning environments, opportunities, interactions, and tasks that help to learn deeper.
- ... to provide guidance and support that challenges students based on their current ability.

We will now focus on *active* and *reflective* learning styles and learning methods.

Active vs. reflective learning styles

Reflective learning methods

- Plenary lectures
- Reading textbook
- Self study

Active learing methods

- Pause in plenary lecture to ask questions and let students think and/or discuss.
- In-class quizzes
- Projects - individual or in groups
- Group discussion
- Interactive lectures

Who are you - and what are your expectations?

In class - go to

https://docs.google.com/forms/d/e/1FAIpQLSccJumofq9vxWEJ5ZXQLbTOyzyflFGC-37ghllJkxOu58unWg/viewform?usp=sf_link

to answer these questions.

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)

Thanks to the three people that volunteered.

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

- 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/

You can log in with your Feide account.

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*.
- Both **prediction** and **understanding** (inference $\rightarrow$ drawing conclusions).
- Statistical learning is **a statistical discipline**, but the boarders 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

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

This encompasses the whole process of data acquisition/scraping, going from unstructured to structured data, setting up a data model, performing data analysis, implementing tools and interpreting 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

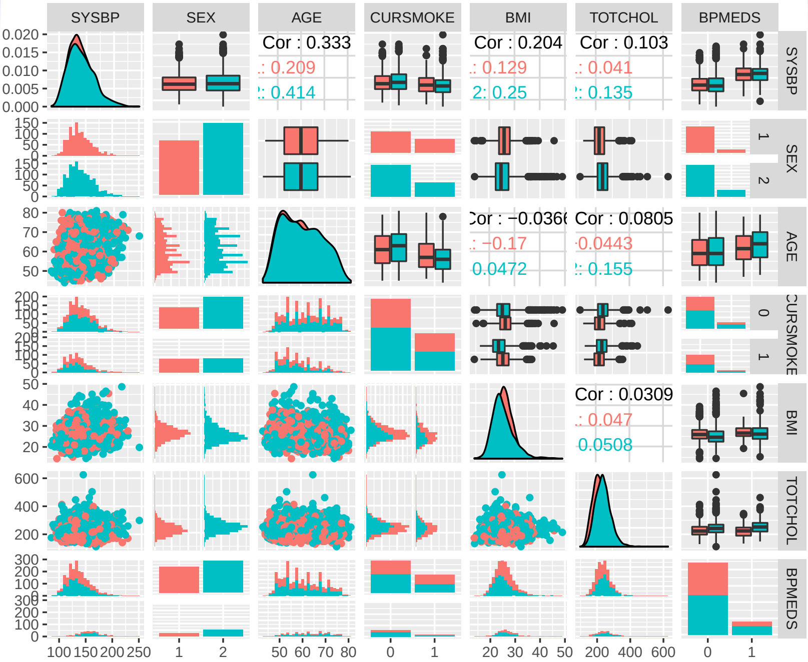
using data from science, technology, industry, economy/finance, ...

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.

- `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=currently using.

Framingham Heart Study



- 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?**

So we are interested in *inference* (explanation) and not predction!

- A *multiple normal linear regression model* was fit to the data set with
$$-\frac{1}{\sqrt{\texttt{SYSBP}}}$$
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.

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

summary(modelB)
```

```
##
## 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
```

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`.

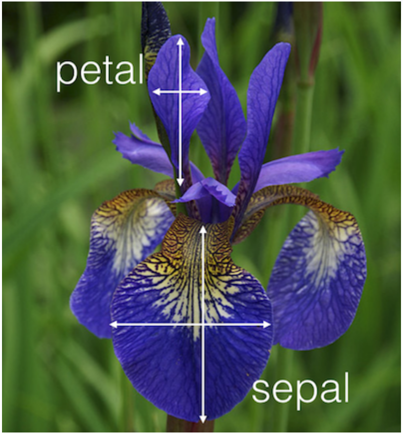


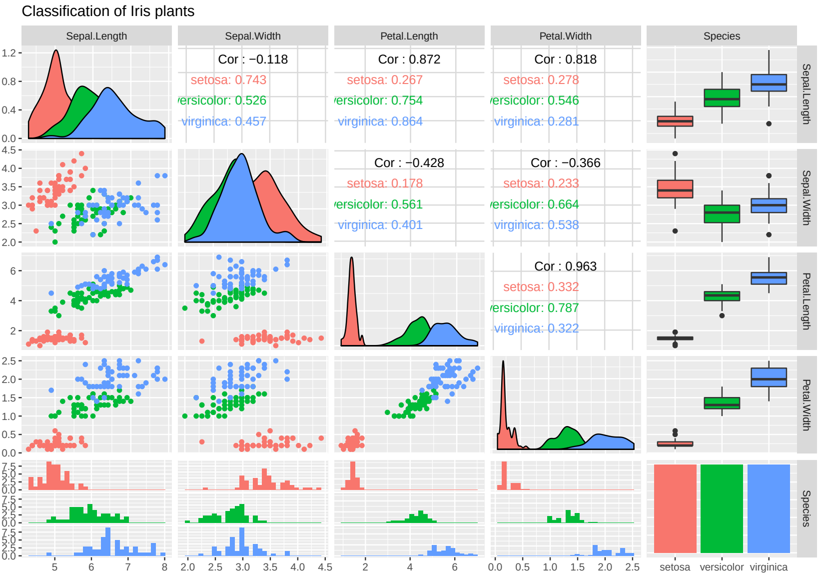
Figure 1: Iris plant with sepal and petal leaves

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

```r
head(iris)
```

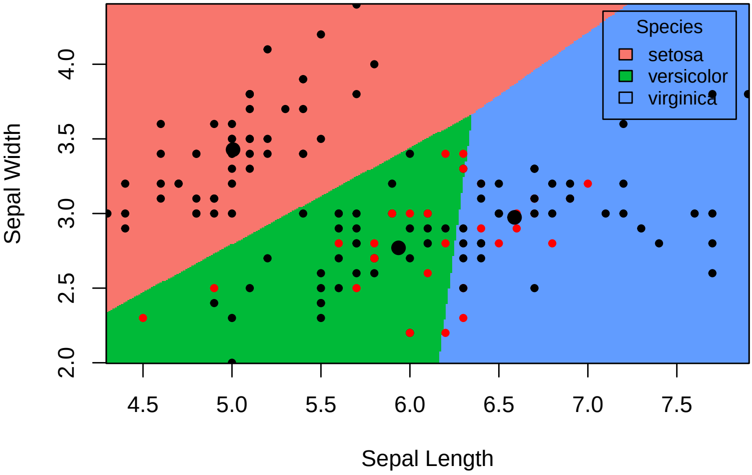
```
##   Sepal.Length Sepal.Width Petal.Length Petal.Width Species
## 1          5.1         3.5          1.4         0.2  setosa
## 2          4.9         3.0          1.4         0.2  setosa
## 3          4.7         3.2          1.3         0.2  setosa
## 4          4.6         3.1          1.5         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.



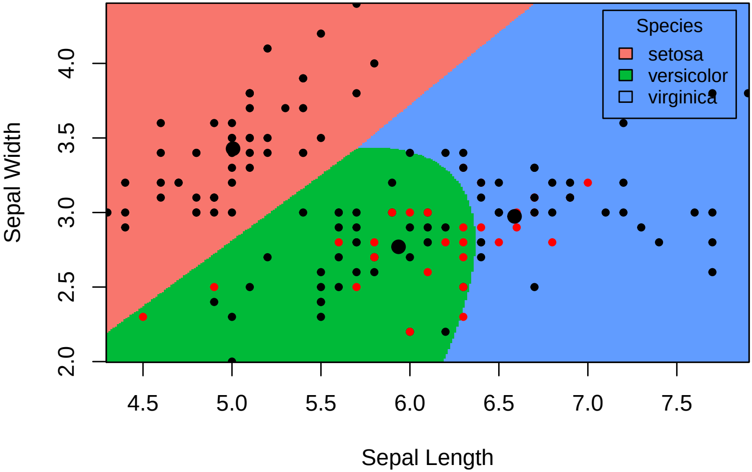
Linear boundaries

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 more suitable boundary is not linear.



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 seditary or trained.
- Transcripts significantly related to running capacity and training were identified.
- To further present the findings heat map of the most significant transcripts were presented (high expression are shown in red and transcripts with a low expression are shown in yellow).
- This is hierarchical cluster analysis with pearson correlation distance measure.

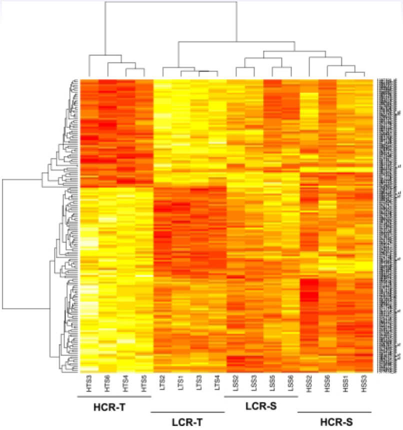


Figure 2: Heat map of the most significant transcripts. Transcripts with a high expression are shown in red and transcripts with a low expression are shown in yellow.

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

Example 4: Unsupervised methods (Network clustering)

Finding clusters in protein-protein-interaction networks.

MUFF, RAO, AND CAFLISCH PHYSICAL REVIEW E **72**, 056107 (2005)

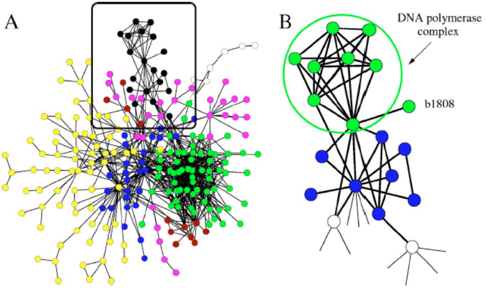


FIG. 4. (Color online) (a) Largest connected component of the PPI of *E. coli*. The colors represent the clusterization found by optimizing modularity. (b) *LQ* clusterization of the black *Q* cluster. The green circle contains proteins belonging to the DNA polymerase complex. The unknown protein b1808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

Plan for this week

- You can work through parts 1 - 6 in the R 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.

Acknowledgements

Thanks to Julia Debik for contributing to this module page.