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 lot 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. **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/tma4268/2020v/start

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

The Statistical Learning Team 2020

The TAs:

- Martina Hall; PhD student
- Michail Spitieris; PhD student

The Lecturers

- Stefanie Muff; Associate Professor
- Thiago Guerrera Martins; NTNU/AIAscience (Modules 6 & 10)
- Andreas Strand; Postdoc (Module 7)

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, 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!
- Not a prerequisist but a good thing with knowledge of computing - preferably 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 it 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.

Course content

- Statistical learning
- Multiple linear regression
- Classification
- Resampling methods
- Model selection/regularization
- Non-linearity
- Support vector machines
- Tree-based methods
- Unsupervised methods
- Neural nets

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 examination (80%).
  - works (projects) ($2 \times 10\% = 20\%$).
- 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 may be given in English.

Exam from 2019

This is the digital exam held in Inspera.

- Problem set
- Tentative solutions
- Grading document

However, please note that this was the exam created by Mette Langaas and her team, and not by us. The recommended and compulsory exercises will give you hints abou the exam, so we highly recommend you will work on them.

Teaching philosophy

The modules

- Divide the topics of the course into modular units with specific focus.
- This (hopefully) facilitates learning?
- 12 modules (weeks of teaching) =
    - **Module 1**: introduction (this module)
    - **Modules 2 - 11**: the 10 topics listed previously
    - **Module 12**: summing up
- Two weeks without lectures (but supervision of exercises)

The lectures

Mondays at 10.15-12 in S1 and Fridays at 14.15-16.00 in S4

- We have $2 \cdot 2$ hours of lectures every week (except when working with the compulsory exercises).
- **Note**: The **first lecture of each module will be on Fridays**, the second lecture on **Mondays**, and the exercise that corresponds to this module on Thursdays.
- Some weeks the Monday lecture will be *interactive* or with some self-study / exercise component, where *active learning* is in focus.
- The other weeks (modules 3, 4, 6, 8, 10 and 11) the Monday lecture is a plenary lecture in S1.
- The first week of the course the second lecture is replaced by an R workshop!

The weekly supervision sessions

Thursdays 08.15-10 in Smia

- 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.

The compulsory exercises

- We will have **two compulsory exercises**, each with a maximal score of 100 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.
- This gives 20% of the final evaluation in the course, the written exam the remaining 80%.

The lecture material

- All the material presented in class will be available on our course webpage (https://wiki.math.ntnu.no/tma4268/2020v/start).
- There will be both a *.pdf and an .Rmd* version. This will allow you to check and use the code that I use to generate the slides.

Student active learning

Student's learning styles are different! Felder and Silverman (1988) suggested the following learning stlye 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 matche the learning styles of the students.
- … 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 (with the NTNU invention Kahoot!) - individual and team mode.
- Projects - individual or in groups.
- Group discussion
- Interactive lectures

Introduction

Aims of the first module

- What is statistical learning?
- Types of problems we will look at
- Course overview and learning outcome, activities and team
- Course modules, practical details (Blackboard)
- Getting to know you – who are you? Background?
- Key concepts from your first course in statistics – that you will need now, mixed with notation for this course
- 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 and 2.3.
- `Rbeginner` and `Rintermediate`
- Link to background on Matrix Algebra: Härdle and Simes (2015) - 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).
- Focuses on the whole chain:

model → method → algorithm → analysis → interpretation

- Both **prediction** and **understanding** (inference → drawing conclusions).
- Statistical learning is a statistical discipline.

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 the fields of statistical learning and machine learning.

Statistical Learning vs. “Data Science”

In data science the aim is to

- extract knowledge and understanding from data, and
- 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 (scraping 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:

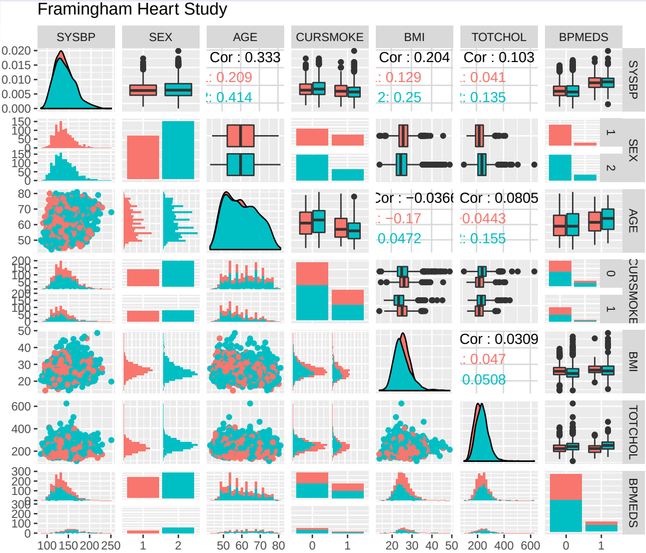
- Regression
- Classification
- Unsupervised methods

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.



What does this plot show?

Red: male; turquoise: female

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

Etiology of CVD - model

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

```
modelB = lm(-1/sqrt(SYSBP) ~ SEX + AGE + CURSMOKE + BMI + TOTCHOL + BPMEDS,
    data = thisds)
summary(modelB)$coeff
summary(modelB)$r.squared
summary(modelB)$adj.r.squared
```

```
##                  Estimate   Std. Error     t value     Pr(>|t|)
## (Intercept) -1.105693e-01 1.341653e-03 -82.4127584 0.000000e+00
## SEX2        -2.989392e-04 2.390278e-04  -1.2506465 2.111763e-01
## AGE          2.378224e-04 1.433876e-05  16.5859862 8.461545e-59
## CURSMOKE1   -2.504484e-04 2.526939e-04  -0.9911136 3.217226e-01
## BMI          3.087163e-04 2.954941e-05  10.4474583 4.696093e-25
## TOTCHOL      9.288023e-06 2.602433e-06   3.5689773 3.648807e-04
## BPMEDS1      5.469077e-03 3.265474e-04  16.7481874 7.297814e-60
## [1] 0.2493538
## [1] 0.2476169
```

```r
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} and **four features measured** for each corresponding sample: `Sepal.Length`, `Sepal.Width`, `Petal.Length` and `Petal.Width`.

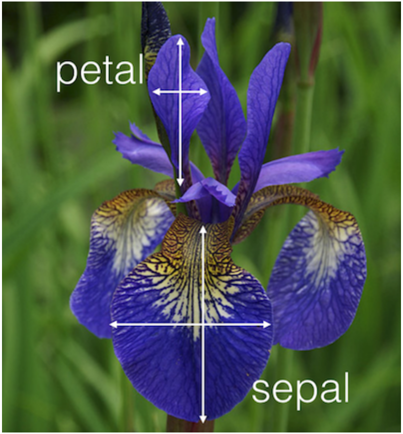


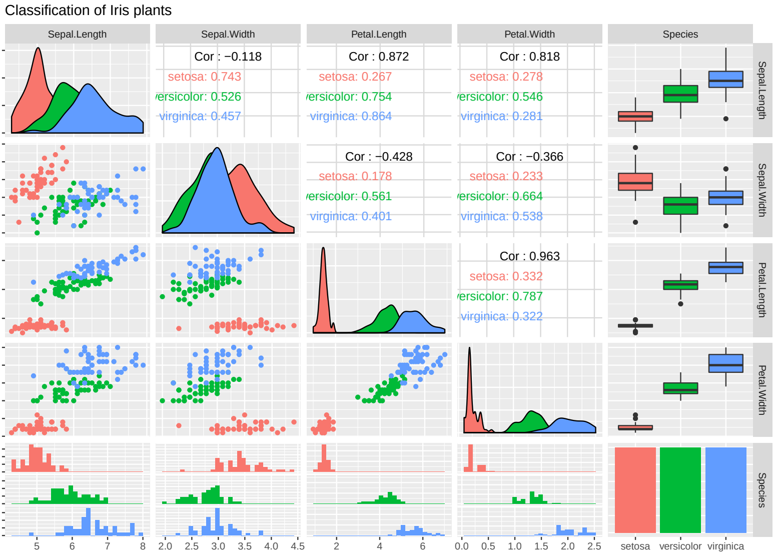
Figure 1: Iris plant with sepal and petal leaves

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

```r
head(iris)
```

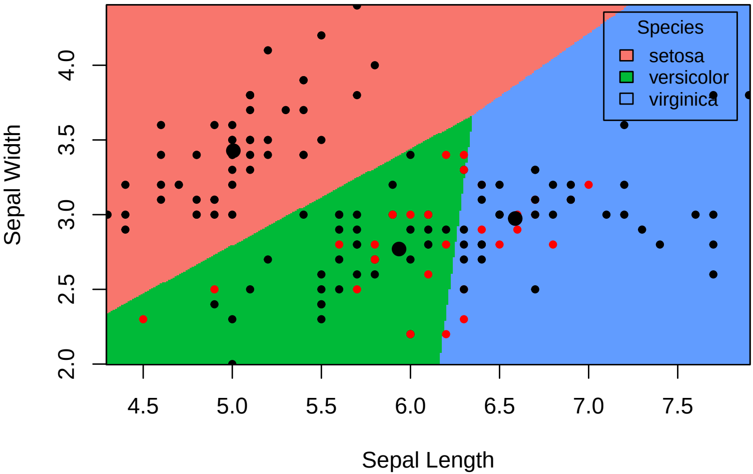
```
##   Sepal.Length Sepal.Width Petal.Length Petal.Width Species
## 1          5.1         3.5          1.4         0.2  setosa
## 2          4.9         3.0          1.4         0.2  setosa
## 3          4.7         3.2          1.3         0.2  setosa
## 4          4.6         3.1          1.5  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



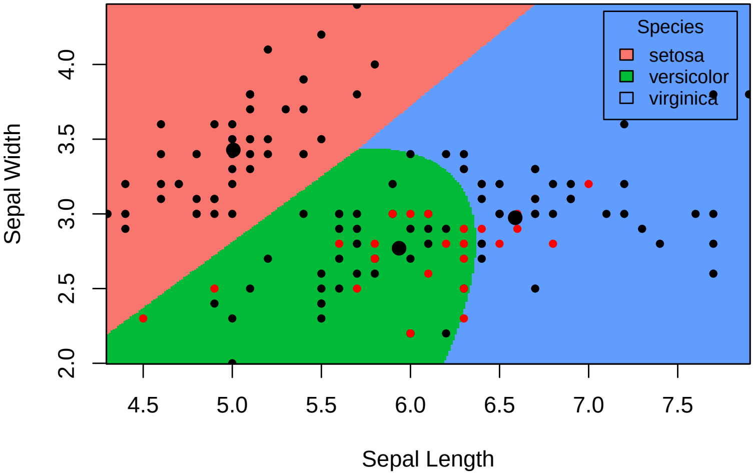
Linear boundaries

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)

- In a collaboration with researchers the Faculty of Medicine and Health 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.

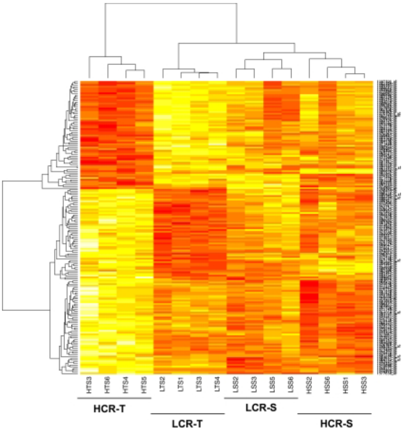


Figure 2: Heatmap with dendrograms

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

The course modules

(PL=plenary lecture in S4 (Mondays) or F6 (Thursdays),
IL=interactive lecture in Smia, E=exercise in Smia)

A detailed overview is found on Bb, and outside Bb in this table.

1. Introduction

[Ch 1, ML] 2019-w2 (PL: 07.01, R-workshop (IL/E): 10.01)

- About the course
- Key concepts in statistics.
- Intro to R and RStudio

2. Statistical Learning

[Ch 2, ML] 2019-w3 (PL: 14.01, IL: 17.01 and E: 17.01)

- Estimating f (regression, classification), prediction accuracy vs model interpretability.
- Supervised vs. unsupervised learning
- Bias-variance trade-off
- The Bayes classifier and the KNN - a flexible method for regression and classification

First hours of IL: bias-variance trade off. Second hour: we target students that doesn't plan to take TMA4267 Linear statistical models, and we work with random vectors, covariance matrices and the multivariate normal distribution (very useful before Modules 3 and 4).

3. Linear Regression

[Ch 3, ML] 2019-w4 (PL: 21.01, PL: 24.01 and E: 24.01)

- Simple and multiple linear regression: model assumptions and data sets
- Inference: Parameter estimation, CI, hypotheses, model fit
- Coding of qualitative predictors
- Problems and extensions
- Linear regression vs. KNN.

4. Classification

[Ch 4, ML] 2019-w5 (PL: 28.01, PL: 31.01 and E: 31.01)

- When to use classification (and not regression)?
- Logistic regression
- Linear discriminant analysis LDA and quadratic discriminant analysis QDA
- Comparison of classificators

5. Resampling methods

[Ch 5, ML] 2019-w7 (PL: 04.02, IL: 07.02, E: 07.02)

Two of the most commonly used resampling methods are cross-validation and the bootstrap. Cross-validation is often used to choose appropriate values for tuning parameters. Bootstrap is often used to provide a measure of accuracy of a parameter estimate.

- Training, validation and test sets
- Cross-validation
- The bootstrap

Part 1: Modules 2-5

is finished with compulsory exercise 1. In week 7 we have supervision in Smia 11.02 (8.15-10.00), 14.02 (14.15-18.00).

To be decided: deadline for handing in Compulsory Ex 1. Suggestion: Friday 22.02 at 16?

6. Linear Model Selection and Regularization

[Ch 6, TGM] 2019-w8 (PL: 18.02, PL: 21.02, E: 21.02)

- Subset selection
- Shrinkage methods (ridge and lasso)
- Dimension reduction with principal components
- Issues when working in high dimensions

7. Moving Beyond Linearity

[Ch 7, AS/ML] 2019-w9 (PL: 25.02, IL: 28.02, E: 28.02)

- Polynomial regression
- Step functions
- Basis functions
- Regression and smoothing splines
- Local regression
- Generalized additive models

8. Tree-Based Methods

[Ch 8, ML/TR] 2019-w10 (PL: 04.03, PL: 07.03, E: 07.03)

- Classification and regression trees
- Trees vs linear models
- Bagging, boosting and random forests

9. Support Vector Machines

[Ch9, ML] 2019-w11 (PL: 11.03, IL: 14.03, E: 14.03)

- Maximal margin classifiers
- Support vector classifiers
- Support vector machines
- Two vs. many classes
- SVM vs. logistic regression

10. Unsupervised learning

[Ch 10, TGM] 2019-w12 (PL: 18.03, PL: 21.03, E:21.03)

- Principal component analysis
- Clustering methods

11. Neural Networks

[ML] (PL: 25.03, PL: 28.03, E: 28.03)

- Network design and connections to previous methods
- Fitting neural networks
- Issues in training neural networks

Part 2: Modules 6-11

is finished with compulsory exercise 2. In week 14 we have supervision in Smia 01.04 (8.15-10.00), 04.04 (14.15-18.00).
To be decided: deadline for handing in Compulsory Ex 2. Suggestion: Friday 12.04 at 16?

12. Summing up and exam preparation

[ML] 2019-w15 (PL: 08.04, E:11.04)

- Overview - common connections
- Exam and exam preparation.

Who are you - the students?

Todo: Find out about kahoot!!

In class - go to kahoot.it to answer these questions. Answers in class added, with 51 respondents.

Study programme

- MTFYMA FysMat ( )
- BMAT ( )
- MSMNFNA Master in Mathematical Sciences ( )
- Other ( )

Study year

- 1 or 2 ( )
- 3 ( )
- 4 ( )
- 5, >5 or PhD ( )

Have you/will you take TMA4267 Linear Statistical Models?

- Yes, previously= in 2019 or earlier ( )
- Yes, now= in 2020 ( )
- Yes, planned for 2021 or later ( )
- Not planned ( )

Do you know R?

- No ( )
- No, and I do not want to learn R ( )
- Yes, but only the basics ( )
- Yes, in depth ( )

Plenary lectures on Monday mornings at 8.15-10 - do you plan to attend?

- Yes ( )
- No, this is too early ( )
- No, since I rarely attend lectures. ( )
- No, for some other reason ( )

What do you think will be most fun in TMA4268?

- Learning new statistical theory ( )
- Trying out statistical theory in R ( )
- Analysing data ( )
- Learn new hot topics ( )

Practical details

- go to Blackboard

Guest access

Course information-Course modules-R resources-Compulsory exercises-Reading list and resources-Exam

Reference group

At least 3 members, one from ideall different programmes

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

Volunteers?

Key concepts (stats) and notation

Todo – compare to hand-written notes by Mette (M1L1notes.pdf);
Perhaps delete this slide then

Plan for this week: Workshop for R and RStudio

Thursday January 10 at 14.15-18.00 in Smia

Say here what the plan is

Please do this before the next lecture

- 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.

R, Rstudio, CRAN and GitHub - and R Markdown

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/
5. 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
We will use R Markdown for writing the Compulsory exercise reports in our course.

6. What is `knitr`? https://yihui.name/knitr/

A first look at R and R studio

- Rbeginner.html
- Rbeginner.pdf
- Rbeginner.Rmd

A second look at R and probability distributions

- Rintermediate.html
- Rintermediate.pdf
- Rintermediate.Rmd

To see solutions added to the files, add -sol to filename to get

- Rintermediate-sol.html

And resources about plots

- Rplots.html
- Rplots.pdf
- Rplots.Rmd

To see solutions added to the files, add -sol to filename to get

- Rplots-sol.html

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.