MA8701 Advanced methods in statistical inference and learning

L1: Introduction and core concepts

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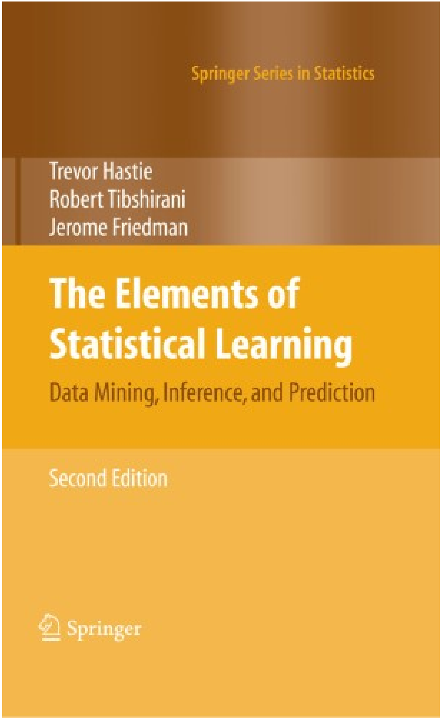
Course topics

The starting point is that we cover important parts of

The Elements of Statistical Learning: Data Mining, Inference, and Prediction, Second Edition (Springer Series in Statistics, 2009) by Trevor Hastie, Robert Tibshirani, and Jerome Friedman.

but, since the book is from 2009 (2nd edition, 12th corrected printing from 2017) this means that for many topic we need (to be up to date) additional selected material in the form of book chapters and research articles.

Download book at https://hastie.su.domains/ElemStatLearn/download.html (this is 12th corrected printing) or sign in at NTNU vpn at Springer (but I am not sure if this is an earlier print without the version 12 corrections).


Springer Series in Statistics
Trevor Hastie
Robert Tibshirani
Jerome Friedman
The Elements of Statistical Learning
Data Mining, Inference, and Prediction
Second Edition
Springer

Part 1: Core concepts [3 weeks]

Sort out assumed background knowledge, and learn something new

- Notation
- Repetition of core concepts (regression and classification)
- Statistical decision theoretic framework (partly new) ELS 2.4
- Model selection and model assessment - including bias-variance trade-off (mostly new) ELS 7
- Missing data ELS 9.6, Handbook of Missing data (chapters 11 and 12) and Flexible Imputation of Missing Data (parts of chapters 2 and 3)

Part 2: Shrinkage and regularization [3 weeks]

or "Regularized linear and generalized linear models", with focus on the ridge and lasso regression (in detail).

- ELS 3.2.3,3.4, 3.8, 4.4.4.
- Hastie, Tibshirani, Wainwright (HTW): "Statistical Learning with Sparsity: The Lasso and Generalizations". Selected sections from chapters 1,2,3,4,6.
- Selective inference (articles)

Part 3: Ensembles [4 weeks]

- trees, bagging and random forests
- xgboost
- general ensembles (including super learner)
- hyper-parameter tuning

Selected chapters in ELS (8.7, 8.8, 9.2, parts of 10, 15, 16) and several articles.

Part 4: XAI [2 weeks]

Lectured by Kjersti Aas https://www.nr.no/~kjersti/.
Articles on

- LIME,
- partial dependence plots,
- Shapley values,
- relative weights and
- counterfactuals.

Part 5: Closing [2 weeks]

“Required” previous knowledge

- TMA4267 Linear statistical methods
- TMA4268 Statistical learning
- TMA4295 Statistical inference
- TMA4300 Computer intensive statistical methods
- TMA4315 Generalized linear models
- Good understanding and experience with R, or with Python, for statistical data analysis.
- Knowledge of markdown for writing reports and presentations (Rmarkdown/Quarto, Jupyther).
- Skills in group work - possibly using git or other collaborative tools.

Some observations about the course

- Mainly a frequentist course, but some of the concepts and methods have a Bayesian version that might give insight into why and how the methods work. Then Bayesian methods will be used.
- Focus is on regression and classification, and unsupervised learning is not planned to be part of the course.
- The required previous knowledge is listed because this is a phd-course designed for statistics studenets. The background make the students go past an overview level of understanding of the course parts (move from algorithmic to deep understanding).

Learning

Learning outcome

1. Knowledge

- Understand and explain the central theoretical aspects in statistical inference and learning.
- Understand and explain how to use methods from statistical inference and learning to perform a sound data analysis.
- Be able to evaluate strengths and weaknesses for the methods and choose between different methods in a given data analysis situation.

2. Skills

Be able to analyse a dataset using methods from statistical inference and learning in practice (using R or Python), and give a good presentation and discussion of the choices done and the results found.

3. Competence

- The students will be able to participate in scientific discussions, read research presented in statistical journals.
- They will be able to participate in applied projects, and analyse data using methods from statistical inference and learning.

Learning methods and activities

Herbert A. Simon (Cognitive science, Nobel Laureate): *Learning results from what the student does and thinks and only from what the student does and thinks. The teacher can advance learning only by influencing what the student does to learn.*

Course elements

Course wiki at https://wiki.math.ntnu.no/ma8701/2023v/start

- Lectures
- Office hours (poll?)
- Problem sets to work on between lectures.
- Study techniques (share)
- Ethical considerations
- Compulsory work
- Final individual oral exam in May

The learning material is also available at https://github.com/mettelang/MA8701V2023.

Questions?

Class activity

Aim: get to know each other - to improve on subsequent group work!

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while (at least one student not presented)
   lecturer give two alternatives, you choose one.
   lecturer choose a few students to present their view
   together with giving their name and study programme
   (and say if they are looking for group members)
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- Dog person or cat person?
- When performing logistic regression - do you then say you do statistical learning or machine learning?
- I will show you the result of a descriptive analysis: summary or graphical display?
- Learning something new: read a book or watch a video?
- Analysing data: R or python?
- Analysing data: report p-values and or confidence intervals
- In class: taking notes or not?
- Use camel case or snake case for programming?

camel: writing compound words such that each word in the middle of the phrase begins with a capital letter, with no intervening spaces or punctuation. "camelCase" or "CamelCase".

snake: writing compound words where the elements are separated with one underscore character (_) and no spaces, with each element's initial letter usually lower cased within the compound and the first letter either upper- or lower case as in "foo_bar"

Plan for part 1

L1:

- Notation
- Remind about assumed background knowledge (already known),
  - Regression (ELS ch 3, except 3.2.3, 3.2.4, 3.4, 3.7, 3.8)
- Statistical decision theoretic framework (partly new: ELS 2.4)

L2: continue with the same framework but for classification

- Classification (ELS ch 4.1-4.5, except 4.4.4)

W2: L3-4: Then, cover new aspects for

- Model selection and assessment (ELS Ch 7.1-7.6, 7.10-7.12), including statistical learning and the bias-variance trade-off (ELS ch 2)

W3: L5-6

- How to handle missing data in data analyses (ELS 9.6), and chapters from the Van Buuren (2018): Flexible Imputation of Missing Data.

Core concepts

Notation

(mainly from ELS)

We will only consider supervised methods.

- Response Y (or G): dependent variable, outcome, usually univariate (but may be multivariate)
  - quantitative Y: for regression
  - qualitative, categorical G: for classification, some times dummy variable coding used (named one-hot coding in machine learning)
- Covariates $X_1, X_2, \ldots, X_p$: "independent variables", predictors, features
  - continuous, discrete: used directly
  - categorical, discrete: often dummy variable coding used

We aim to construct a rule, function, learner: $f(X)$, to predict Y (or G).

Random variables and (column) vectors are written as uppercase letters X, and Y, while observed values are written with lowercase (x, y). (Dimensions specified if needed.)

Matrices are presented with bold face: $\mathbf{X}$, often $N \times (p + 1)$.

ELS uses boldface also for $\mathbf{x}_j$ being a vector of all N observations of variable j, but the vector of observed variables for observation i is just x_i.

Both the response *and covariates* will be considered to be random, and drawn from some joint distribution $P(X_1, X_2, \ldots, X_p, Y) = P(X, Y)$ or $P(X, G)$.

Joint to conditional and marginal distribution:
$P(X, Y) = P(Y \mid X)P(X)$ or $P(Y \mid X = x)P(X = x)$ or
$P(Y = y, X = x) = P(Y = y \mid X = x)P(X = x)$

and we may then calculate the expected value in a sequential (iterated) manner:

$$\mathsf{E}[L(Y, f(X))] = \mathsf{E}_{X,Y}[L(Y, f(X))] = \mathsf{E}_X \mathsf{E}_{Y|X}[L(Y, f(X))]$$

where L is a loss function (to be defined next) and $f(X)$ some function to predict Y (or G). (No, $f(X)$ is not the density pdf.)

Random variables and random vectors

Maybe brush up on this?

Resources

- From TMA4268: Module 2 - Random vectors
- From TMA4267: Part 1: Multivariate random variables and the multivariate normal distribution

Training set

(ELS 2.1)

A set of size N of independent pairs (x_i, y_i) is called the *training set* and often denoted T.

The training data is used to estimate the unknown function f.

Test data

Test data is in general thought of as future data, and plays an important role in both

- model selection (finding the best model among a candidate set) and also for
- model assessment (assess the performance of the fitted model on future data).

We will consider theoretical results for future test data, and also look at different ways to split or resample available data.

Group discussion

Two core regression methods are multiple linear regression (MLR) and k-nearest neighbour (kNN).

For the two methods

- Set up the formal definition for f, and model assumptions made
- What top results do you remember? Write them down.
- What are challenges?
- If time: What changes need to be done to each of the two methods for classification?

Regression and MLR

Resources

(mostly what we learned in TMA4267, or ELS ch 3, except 3.2.3, 3.2.4, 3.4, 3.7, 3.8)

- From TMA4268: Overview and in particular Module 3: Linear regression
- From TMA4315: Overview and in particular Module 2: MLR

For kNN see also Problem 1 of the TMA4268 2018 exam with solutions

Statistical decision theoretic framework

(ELS ch 2.4)

is a mathematical framework for developing models f - and assessing optimality.

First, regression:

- $X \in \Re^p$
- $Y \in \Re$
- $P(X, Y)$ joint distribution of covariates and respons

Aim: find a function $f(X)$ for predicting Y from some inputs X.

Ingredients: Loss function $L(Y, f(X))$ - for *penalizing errors in the prediction*.

Criterion for choosing f: Expected prediction error (EPE)

$$\mathsf{EPE}(f) = \mathsf{E}_{X,Y}[L(Y, f(X))] = \int_{x,y} L(y, f(x))p(x,y)dxdy$$

Choose f to minimize the $\mathsf{EPE}(f)$.

What is the most popular loss function for regression?

Squared error loss

$$\mathsf{EPE}(f) = \mathsf{E}_{X,Y}[L(Y, f(X))] = \mathsf{E}_X \mathsf{E}_{Y|X}[(Y - f(X))^2 \mid X]$$

We want to minimize EPE, and see that it is sufficient to minimize $\mathsf{E}_{Y|X}[(Y - f(X))^2 \mid X]$ for each $X = x$ (pointwise):

$$f(x) = \mathsf{argmin}_c \mathsf{E}_{Y|X}[(Y - c)^2 \mid X = x]$$

This gives as result the conditional expectation - the best prediction at any point $X = x$:

$$f(x) = \mathsf{E}[Y \mid X = x]$$

Proof: by differentiating and setting equal 0.
In practice: need to estimate f.

Linear regression

Conditionally (known from before): if we assume that $(X, Y) \sim N_{p+1}(\mu, \Sigma)$ then we have seen (TMA4267) that $\mathrm{E}(Y \mid X)$ is linear in X and $\mathrm{Cov}(Y \mid X)$ is independent of X. Then we know we get $\hat{\beta} = (X^T X)^{-1} X^T Y$ (with matrices) using OLS or MLE.

But, also if we assume an approximate linear model: $f(x) \approx x^T\beta$

Marginally: $\text{argmin}_\beta \mathsf{E}[(Y - X^T\beta)^2]$ gives $\beta = \mathsf{E}[XX^T]^{-1}\mathsf{E}[XY]$ (now random vectors).

We may replace expectations with averages in training data to estimate β.

This is not conditional on X, but we have assumed a linear relationship.

Absolute loss

Regression with absolute (L1) loss: $L(Y, f(X)) = |Y - f(X)|$ gives $\hat{f}(x) = \text{median}(Y \mid X = x)$.
Proof: for example pages 8-11 of
https://getd.libs.uga.edu/pdfs/ma_james_c_201412_ms.pdf

Exercises

Getting started

Give a derivation of the law of total expectation:

$$\mathsf{E}[X] = \mathsf{E}[\mathsf{E}(X \mid Y)]$$

and the law of total variance:

$$\mathsf{Var}[X] = \mathsf{E}_Y \mathsf{Var}_{X|Y}[X] + \mathsf{Var}_Y \mathsf{E}_{X|Y}[X]$$

This will be useful to remember in this course. There is also a law of total covariance.

Quadratic loss and decision theoretic framework

Prove that $f(x) = \mathsf{E}[Y \mid X = x]$ for the quadratic loss.

Curse of dimensionality

Read pages 22-23 and then answer Exercise 2.3 - which is to "Derive equation (2.24)."

Important take home messages:

- All sample points are close to an edge of the sample.

Solutions to exercises

Please try yourself first, or take a small peek - and try some more - before fully reading the solutions. Report errors or improvements to Mette.Langaas@ntnu.no. (The solutions given here are very similar to the UiO STK-IN4300 solutions, see link under References.)

- Quadratic loss: Page 8 of https://getd.libs.uga.edu/pdfs/ma_james_c_201412_ms.pdf
- 2.3
- 2.9

References

- ELS official errata: and choose “Errata” in the left menu
- ELS solutions to exercises
- ELS solutions from UiO
- Camel_case
- Snake_case