ORGANISATIONAL MATTERS
LECTURE: UNSUPERVISED LEARNING AND EVOLUTIONARY COMPUTATION USING R

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26th Oct, 2024

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Research interests

- Heuristic Optimisation (in particular Evolutionary Algorithms)
- Theory of randomised search heuristics
- Combinatorial (Multi-Objective) Optimisation
- Evolutionary Diversity Optimisation (EDO) and Quality Diversity (QD)
- Automated Artificial Intelligence (AutoAI)

About me ii

Academic footprint

- 2005-2014: Studying Computer Science with minor Statistics at the TU-Dortmund University (degree: Diploma; M.Sc. equivalent)
- 09/2008-05/2013: Studying Statistics with minor Computer Science at the TU-Dortmund University (degree: B.Sc.)
- 02/2015-09/2019: Research Associate at the Department of Information Systems (Chair for Statistics and Optimization), University of Münster, Germany
- 11/2018: Doctoral degree in Information Systems (Dr. rer. pol.) at the University of Münster, Germany (supervisors: Prof. Dr. Heike Trautmann, Prof. Dr. Frank Neumann)
- 10/2019-08/2020: PostDoc Researcher at the School of Computer Science, The University of Adelaide, Australia in the Optimisation and Logistics group of Prof. Dr. Frank Neumann
- 09/2020-04/2022: PostDoc (Akademischer Rat auf Zeit) at the Department of Information Systems (Chair for Statistics and Optimization), University of Münster, Germany

About me iii

Academic footprint

- 04/2022-11/2023: Assistant Professor (Akademischer Rat auf Zeit) at the Department of Computer Science (Chair for AI Methodology), RWTH Aachen, Germany
- **Since 11/2023**: Assistant Professor (Akademischer Rat) at the Department of Computer Science (Machine Learning and Optimisation Group; short MALEO), Paderborn University, Germany

Dr. Urban Škvorc - Main Responsible for Tutorials

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Machine Learning and Optimisation group (MALEO)
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Research interests

- Benchmarking
- Exploratory Landscape Analysis (ELA)
- Black-box optimisation
- Automated Artificial Intelligence (AutoAI)

What is it all about?

The Epoch of Data

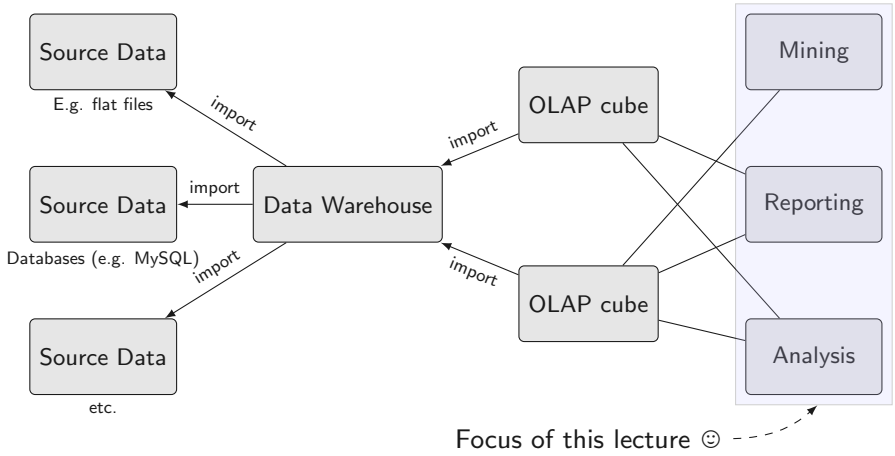
Undeniably we are living in the epoch of *(big) data*:

- Massive amounts of data is being collected ubiquitously: online transactions, online footprints, sensor data, any kind of measurements etc.
- According to IBM: by 2020, the overall amout of data is about 40 zetabytes.[1]
- Data is basically a set of oberservations (numbers, text etc.)
- Need for sophisticated methods to make sense of it!

[1] One zetabyte = 1 trillion gigabytes!

OLAP (Online Analytical Processing)

In a nutshell: the process of gathering, storing and analysing data.



Example (Data Analytics)

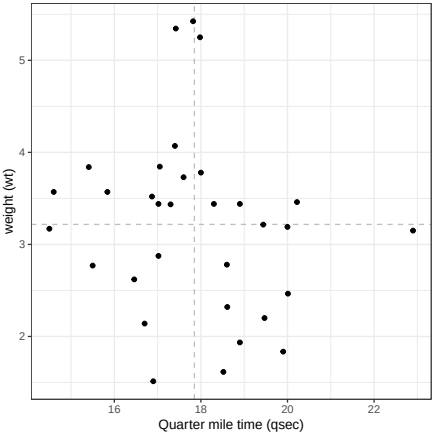
Starting point: *N observations* of *p features* or *variables*.

`mtcars` data: collected for 1974 Motor Trend US magazine, and comprises fuel consumption and 10 aspects of automobile design and performance for different automobiles.

	mpg	**cyl**	**disp**	**hp**	**drat**	**wt**	**qsec**	**vs**	**am**	**gear**	**carb**
Mazda RX4	21.0	6	160.0	110	3.90	2.620	16.46	0	1	4	4
Mazda RX4 Wag	21.0	6	160.0	110	3.90	2.875	17.02	0	1	4	4
Datsun 710	22.8	4	108.0	93	3.85	2.320	18.61	1	1	4	1
Hornet 4 Drive	21.4	6	258.0	110	3.08	3.215	19.44	1	0	3	1
Hornet Sportabout	18.7	8	360.0	175	3.15	3.440	17.02	0	0	3	2
Valiant	18.1	6	225.0	105	2.76	3.460	20.22	1	0	3	1
Duster 360	14.3	8	360.0	245	3.21	3.570	15.84	0	0	3	4
Merc 240D	24.4	4	146.7	62	3.69	3.190	20.00	1	0	4	2
Merc 230	22.8	4	140.8	95	3.92	3.150	22.90	1	0	4	2
Merc 280	19.2	6	167.6	123	3.92	3.440	18.30	1	0	4	4
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

Example (Data Analytics) II

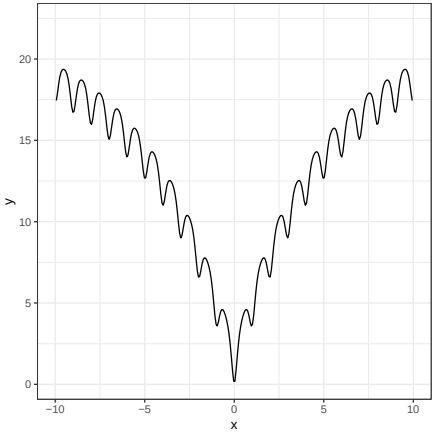
Goal: "Make sense" of the raw data! For example:



- Basic visualization
- Group identification
- Outlier detection
- Handling stream data
- Awareness that basically everything is problem-specific! ☺
- etc.

Example (Optimization)

Goal: Find optimal/"good" value(s) that optimize some given target(s).



- Optimization basics: classes of problems, hardness
- Single-objective problems
- Multi-objective problems
- Important class of algorithms: (bio-inspired) randomized search heuristics

Overview of Topics Covered in ULEOR

- Data preparation: collect, merge and transform data (make it "tidy").
- Exploratory data analysis (EDA): basic (multi-variate) visualizations and summary statistics.
- Data imputation: How to deal with missing data?
- Dimensionaly reduction: How to reduce high-dimensional data to a representative low-dimensional representation?
- Unsupervised learning: How do detect groups/clusters in data? I.e. similar observations.
- (Multi-objective) optimization: How to find optimal or at least good enough parameter values?
- Main tool: statistical programming language R.

Overview of Topics not Covered in ULEOR

- Further unsupervised learning: e.g. reinforcement learning
- Supervised learning: Regression and classification. How do make predictions for labelled data?
- Deep Learning: How do (deep) neural networks work?
- Parameter tuning/configuration: how to set the parameters of my machine learning algorithm to obtain the best possible performance?
- Feature selection: How to select a subset of my variables for learning to make my models simple yet high-performing?

Further Topics not Covered in ULEOR

- Data Warehousing (DWH) concepts
- Databases (relational algebra, SQL[2], modern architectures concepts)
- The Online Analytical Processing (OLAP) pipeline as a whole
- Business Intelligence (BI) tools like: Microsoft PowerBI, Oracle Business Intelligence Enterprise Edition etc.

[2] Structured Query Language

General Information

General Information I

Lecture

- In-person lectures/tutorials in F1.101.
- Lecture: Mondays, 1:15pm - 3:45pm
- Please (at least try to) arrive here in time!!!

General Information II

Participation

- Do not just "consume" my presentations: do not hesitate to ask questions.[3]
- Use the discussion forum in PANDA
  (ask and respond, search for learning groups etc.)
- Search for more information online
- Invest time on a weekly basis!
- Aim to understand the tools and methods. I.e., do not just memorize "recipes"

[3] I am sure many other students will have the same questions, but won't ask (for some reason).

General Information III

Get in touch

- Use the PANDA discussion forum to ask questions that might be of interest for all or aat least some other students
- Via mail for individual questions

General Information IV

Tutorials

- Exercise sheets will be uploaded weekly on Tuesday (first one October 22nd)
- Mixture of applied and "theoretical" exercises.
- Discussion of (hopefully *your*) results the week after
- Examplary solutions will be made available
- The good thing: working on exercise sheets is optional ☺
- But the bad thing is: you will fail to pass the exam with overwhelming probability if you skip working actively on the tutorials ☹

General Information V

Exam

- Written exam at the end of the lecture period (100% of the final grade)
- Duration: 90 minutes
- Content: Mix-up of applied exercices (e.g. apply algorithm A on some toy problem), reproducible (e.g. explain how clustering algorithm A works in your own words), multiple choice, maybe a R related exercise and maybe some theoretical stuff (show that something holds)
- All covered topics are relevant!
- Best way to prepare: learn actively, do the exercises etc.

General Information VI

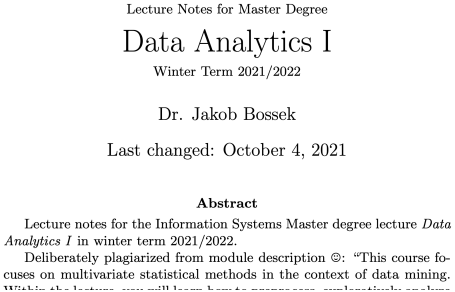
Do I need programming skills?

- This is an applied course: we will use R
- Short introduction[4] into R
- In the final exam: 1-2 R exercise(s) $\rightsquigarrow$ you can pass without knowledge of R
- However: you should teach yourself the basics! Why?
  - R gains increasing interest in industry (pimp your CV ☺)
  - R really shines when it comes to data analysis (very active community)
  - It is always good to learn a new programming language

[4] This is not a course on programming language basics.

How to prepare/postprocess the lectures/tutorials

Lecture Notes I



Lecture Notes for Master Degree

Data Analytics I

Winter Term 2021/2022

Dr. Jakob Bossek

Last changed: October 4, 2021

Abstract

Lecture notes for the Information Systems Master degree lecture *Data Analytics I* in winter term 2021/2022.

Deliberately plagiarized from module description ☺: "This course focuses on multivariate statistical methods in the context of data mining. Within the lectures, you will learn how to preprocess, exploratively analyze

- Kind of a lecture-specific book with additonal information and exercises.
- Not finished! Will evolve in the course of the winter term.
- Not perfect! Read with care. Please report any typos, unclear formulations, ideas for improvement etc.

Call for participation!

- Report typos
- Give constructive feedback on how to improve the manuscript
- Discuss stuff with others in the Learnweb
- There are many additional exercises with no sample solutions: send me your solutions
- **Benefit for you**: fame and honor, my gratitude, no price or whatever (sorry! ☺)

How to post-process?

Simple fact

You have no chance to pass the module without intense and active learning!

How to avoid failing

- Ideally before and after a lecture: read the corresponding lecture notes chapter(s) / book chapters
- Try to solve the exercises! (this can take a while; do not give up quickly and google the solution $\rightsquigarrow$ you cheat yourself this way)
- Naturally, some things will be hard to understand:
  - Ask questions: lecturer, learnweb, stackoverflow etc.
  - Actively search for further sources online (e.g., on YouTube)
  - In R: make mistakes, google error messages etc.

Course achievement and exam

Exam Modalities

Course achievement

- Case study in R
- Mid december; to be submitted mid January
- Submission of running and documented R-code
- Submission of sumarising report in PDF format (using our LaTeX-template)
- **Has to be passed to be admitted to exam**

PAUL (de)registrations

Course achievement

- If you did not pass the course achievement, you will be de-registered from the exam automatically

Exam

- 1st-phase registration: 21 Oct until 21 Nov 2024
- 2nd-phase registration: 24 Feb untol 7 Mar 2025
- De-registration from exam is possible until two days before the examination date!

Literature Recommendations

Literature: Machine Learning

1. Gareth James, Daniela Witten, Trevor John Hastie & Robert Tibshirani (2021). An Introduction to Statistical Learning. 2nd Edition. Springer. (James et al. 2013)★
   ⇝ Focus on understanding, excellent introductory text to grasp the working principles.

2. Trevor John Hastie, Robert Tibshirani & Jerome Harold Friedman (2009). The Elements of Statistical Learning. 2nd Edition, Springer. (Hastie, Tibshirani, and Friedman 2009)
   ⇝ Advanced computer science perspective, focus on mathematics.

3. Ethem Alpaydin (2014). Introduction to Machine Learning. MIT press. (Alpaydin 2014)
   ⇝ Rather advanced.

Literature: Data Analysis with R

1. Hadley Wickham & Garrett Grolemund (2017). R for Data Science: Import, Tidy, Transform, Visualize, and Model Data. O'Reilly. (Wickham and Grolemund 2017)

2. Hadley Wickham (2016). `ggplot2`: Elegant Graphics for Data Analysis. Springer. (Wickham 2009)

3. Hadley Wickham (2014). Advanced R. Chapman & Hall/CRC The R Series. Taylor & Francis. (Wickham 2014)

4. Hadley Wickham (2015). R Packages. 1st Edition. O'Reilly Media. (Wickham 2015)

Wrap-Up

Wrap-Up

Todays content

Mainly organizational stuff ☺

Your task(s)

- Download and install both R[5] and R Studio[6].
- Optional: Check the introduced literature (recall that most of this stuff is free).
- Optional: Read the introduction of An Introduction to Statistical Learning (James et al. 2013).

[5] URL: `https://www.r-project.org`
[6] URL: `https://www.rstudio.com`

References I

James, Gareth et al. (2013). *An Introduction to Statistical Learning: with Applications in R*. Springer.

Hastie, Trevor, Robert Tibshirani, and Jerome H. Friedman (2009). *The Elements of Statistical Learning: Data Mining, Inference, and Prediction, 2nd Edition*. Springer Series in Statistics. Springer. ISBN: 9780387848570.

Alpaydin, Ethem (2014). *Introduction to Machine Learning*. 3rd ed. Adaptive Computation and Machine Learning. Cambridge, MA: MIT Press. ISBN: 978-0-262-02818-9.

Wickham, Hadley and Garrett Grolemund (Jan. 2017). *R for Data Science: Import, Tidy, Transform, Visualize, and Model Data*. 1st ed. O'Reilly Media. ISBN: 1491910399.

Wickham, Hadley (2009). *ggplot2: elegant graphics for data analysis*. Springer New York. ISBN: 978-0-387-98140-6.

— (2014). *Advanced R*. Chapman & Hall/CRC The R Series. Taylor & Francis. ISBN: 9781466586963. URL: `https://books.google.de/books?id=PFHFNAEACAAJ`.

— (2015). *R Packages*. 1st. O'Reilly Media, Inc. ISBN: 1491910593.