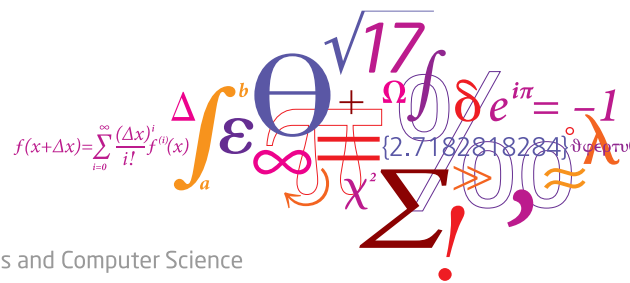
02450: Introduction to Machine Learning and Data Mining

Introduction

Georgios Arvanitidis

DTU Compute, Technical University of Denmark (DTU)

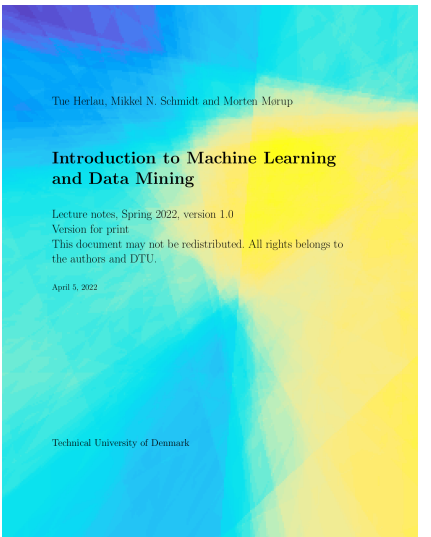


DTU Compute
Department of Applied Mathematics and Computer Science

Today

Reading material:

Chapter 1



Lecture Schedule

1. **Introduction**
   30 August: C1

   Data: Feature extraction, and visualization
2. Data, feature extraction and PCA
   6 September: C2, C3
3. Measures of similarity, summary statistics and probabilities
   13 September: C4, C5
4. Probability densities and data visualization
   20 September: C6, C7

   Supervised learning: Classification and regression
5. Decision trees and linear regression
   27 September: C8, C9
6. Overfitting, cross-validation and Nearest Neighbor
   4 October: C10, C12 **(Project 1 due before 13:00)**
7. Performance evaluation, Bayes, and Naive Bayes
   11 October: C11, C13
8. Artificial Neural Networks and Bias/Variance
   25 October: C14, C15
9. AUC and ensemble methods
   1 November: C16, C17

   Unsupervised learning: Clustering and density estimation
10. K-means and hierarchical clustering
    8 November: C18
11. Mixture models and density estimation
    15 November: C19, C20 **(Project 2 due before 13:00)**
12. Association mining
    22 November: C21

    Recap
13. Recap and discussion of the exam
    29 November: C1-C21

Online help: Piazza
Videos of lectures: `https://video.dtu.dk`
Streaming of lectures: Zoom (link on DTU Learn)

Public homepage

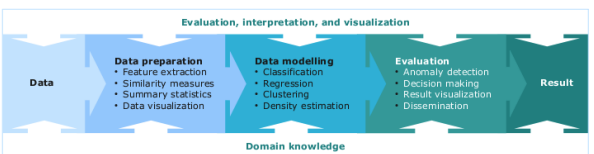
- Syllabus/homework also available on public homepage
  http://compute.dtu.dk/courses/02450
  and on DTU Learn (`02450syllabus_and_practicals.pdf`)

DTU Section for Cognitive Systems
DTU Compute

02450 Introduction to Machine Learning and Data Mining

Machine learning and data mining

The course is designed around a data modeling framework shown in the figure. Each lecture/assignment will focus on an aspect of the data modeling framework.



We emphasize the holistic view of modeling in order to motivate and stress the relevance of individual components and building blocks, disseminate the obtained competence (see the course learning obejctives), and make them applicable for a broad spectrum of engineering problems in e.g. biomedical engineering, chemistry, electrical engineering, and informatics.

Resources

DTU Learn


Georgios Arvanitidis


Bjørn Sand Jensen

Plan for today:

- What is machine learning?
- Why do we learn different methods?
- Impact of machine learning
- This course
- Pre-test
- Break
- Lecture 1, basic terminology
- Exercises in your favourite programming language (15:00–17:00)

Alan Turing (1946)

Alan Turing
(1912-1954)

- Universal computing
- Proposed machines should learn like children

We are not in a position to answer if a machine can think because the terms machine and think are undefined. Rather we should ask if a machine can imitate a human

(the imitation game)

Arthur Samuel (1959)

Arthur Samuel
(1901-1990)

- Samuels wrote a checkers playing program
  - Program played 10000 games against itself
  - Learned value of each board position by considering the resulting score

Machine learning: *(The) field of study that gives computers the ability to learn without being explicitly programmed*

Tom Michell (1999)

A well-posed learning problem: *A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at the tasks in T, as measured by P, improves with experience E*

- Checkers example
  - E: Playing 10'000 games
  - T: Playing checkers
  - P: Win or loose

Tom Michell

Quiz 01: Machine learning definition

Please answer this quiz on DTU Learn: https://learn.inside.dtu.dk/d2l/home/125816

Well posed learning problem: **"A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E."**

Tom Michell

Suppose a program watches as you label images of eyes as containing evidence of cataracts (clouding of the lens) or not, thereby learning to diagnose new examples. What is the experience E?

A. The number of correctly diagnosed patients

B. A database containing images of eyes with their labels

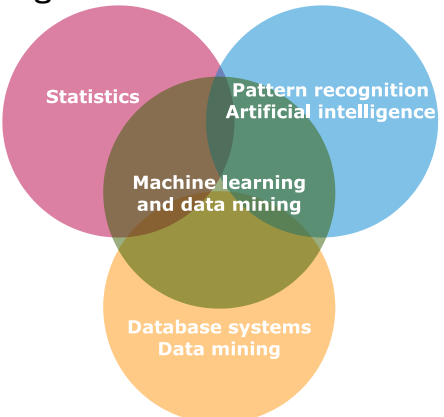
C. The errors the program commits when trying to label the images.

D. Physiological information about cataracts (genetic markers, disease progression, etc.)

E. Don't know.

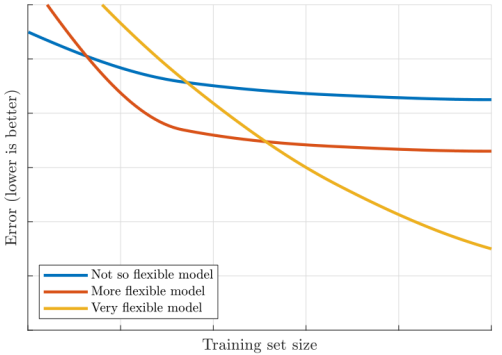
image obtained from https://www.pexels.com/photo/beautiful-blue-eyes-close-up-dhyamis-kleber-609549/

Machine-learning as a research area

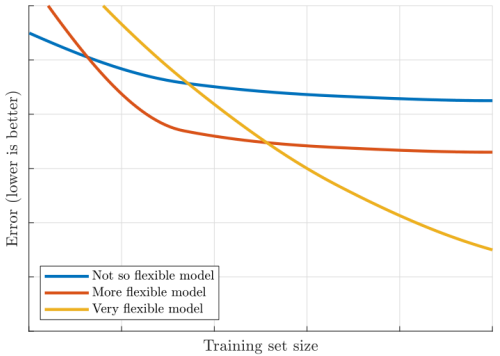


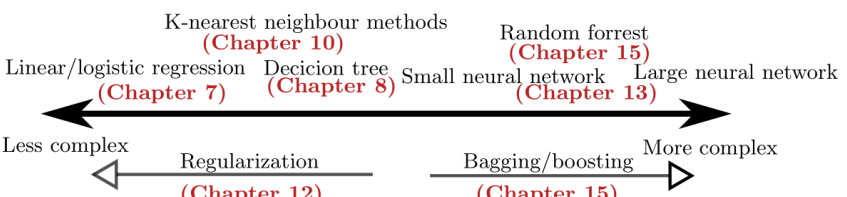
- Focus on a *learning algorithms* (rather than search, pathfinding, etc.)
- De-emphasize explicit knowledge representations, etc.
- Gradual improvements (training time, amount of data)
- *General* algorithms (or algorithmic ideas)

Machine-learning as a research area



Machine-learning as a research area





Man vs. Machine

2020, Breast cancer Outperforms radiologists in breast-cancer detection (Nature)

2019, Lung cancer Outperform six doctors with a 5% reduction in false negatives (Deepmind / Nature Medicine)

2019, Starcraft 1v1: OpenAI deep reinforcement learning exhibit high-level performance in SC2

2018, BERT: Superhuman performance on the SQuADv1.1 wikipedia question-answer task

2018, alphago: superhuman chess/go learned from scratch

2017, Dota2 1v1: OpenAI deep reinforcement learning bot beats top professionals in 1v1 DOTA

2017, Texas hold'em no limit: Libratus (Carnegie Mellon) beats top professional

2017, Go: Superhuman Go by reinforcement learning + imitation of expert games

2016, libreading : Superhuman libreading from Oxford and Google Deepmind

2016, conversational speech: Microsoft research demonstrate superhuman speech recognition

2016, Geoguessing Google PlaNet win 28 of 50 rounds; median localization error of 1132km vs. 2321km

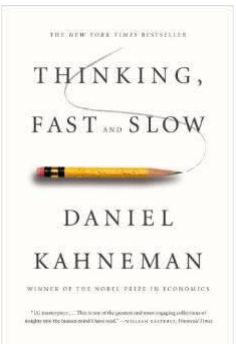
2015, closed-world image recognition Microsoft report error of 4.94% on ImageNet vs. 5.1% for top-human labeler

2015, Atari Google Deepmind obtain better-than-expert human performance on many Atari video games

List inspired by:
`https://finnaarupnielsen.wordpress.com/2015/03/15/status-on-human-vs-machines/`

Human abilities examined

The number of studies reporting comparisons of clinical and statistical predictions has increased to roughly two hundred (...) About 60% of the studies have shown significantly better accuracy for the algorithms. The other comparisons scored a draw in accuracy, but a tie is tantamount to a win for the statistical rules, which are normally much less expensive to use than expert judgement. No exception has been convincingly documented.



The range of predicted outcomes has expanded to cover medical variables such as longevity of cancer patients, the length of hospital stayes, the diagnosis of cardiac disease, and the susceptibility of babies to sudden infant death syndrome; economic measures such as the prospect of success for new businesses, the evaluation of credit risks by banks, and the future career satisfaction of workers; questions of interest to government agencies, including assessment of the suitability of foster parents, the odds of recidivism among juvenile offenders, and the likelihood of other forms of violent behaviour; and the miscallaneous outcomes such as the evaluation of scientific presentations, the winners of football games, and the future prices of Bordeaux wine. Each of these domains entails a significant degree of uncertainty and unpredictability. We describe them as “low-validity environments.”. **In every case, the accuracy of experts was matched or exceeded by a simple algorithm.** (Kahneman 2011)

Why now?

Scientific Advances in algorithmic ideas

Empirical Increased availability of large/good datasets

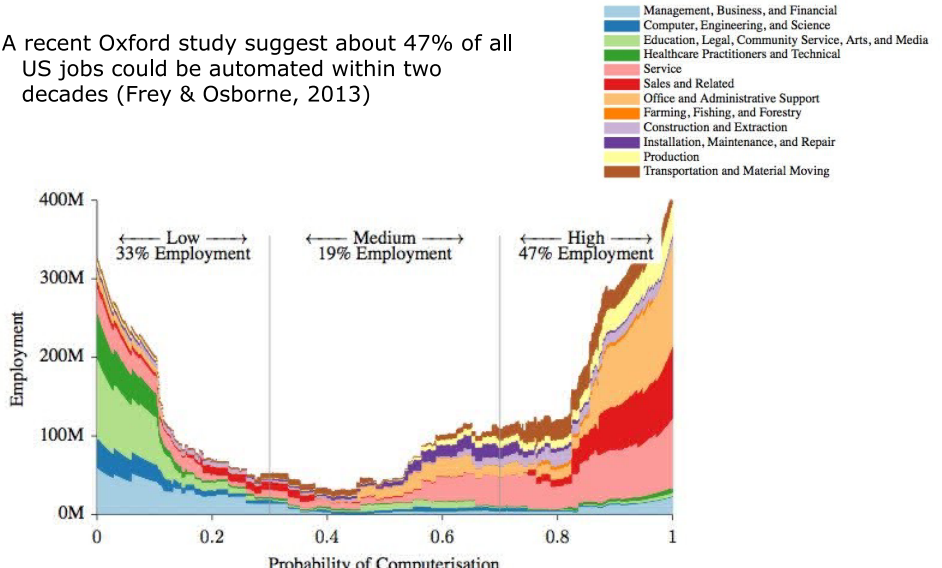
Technological Faster computers

Social Libraries which automate routine tasks; increased sharing of code, etc.

Economical Greatly increased resource allocation

Machine learning as a disruptive technology

- A recent Oxford study suggest about 47% of all US jobs could be automated within two decades (Frey & Osborne, 2013)



Economical impact I

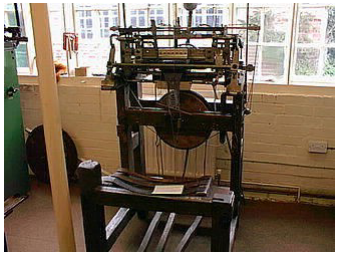
- Basic economics: When things become cheap, we will use it in more places
- Example: Microprocessors perform computations
- Microprocessors did not change the world because people did a lot of computations in 1950, but because nearly everything can at least partially be turned into a computation problem (bookkeeping, telephony, photography, entertainment, navigation, design, education, economics, science, etc.)
- We should not ask what situations are as of now a machine-learning problem, but which can be turned into one

Economical impact II

Many jobs match this description

1. Recognize what situation you are in
2. Collect relevant data
3. Given data about situation make a prediction such as: (i) outcome of performing a given action in the situation or (ii) which action is appropriate
4. Perform action
5. Repeat ...

Machine learning can, in principle, learn 3



https://en.wikipedia.org/wiki/William_Lee_(inventor)
William Lee (1563–1614) was an English clergyman and inventor who devised the first stocking frame knitting machine in 1589

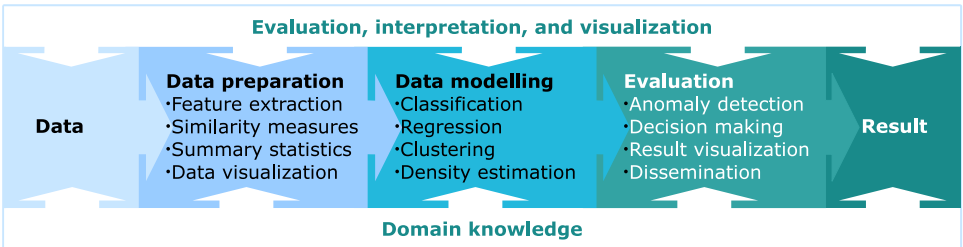
Elizabeth I: ”Thou aimest high, Master Lee. Consider thou what the invention could do to my poor subjects. It would assuredly bring to them ruin by depriving them of employment, thus making them beggars."

> *”our discovery of means of economising the use of labour can outrun the pace at which we can find new uses for labour, as Keynes (1933) pointed out.* ***The reason why human labour has prevailed relates to its ability to adopt and acquire new skills by means of education (Goldin and Katz, 2009). Yet as computerisation enters more cognitive domains this will become increasingly challenging*** *(Brynjolfsson and McAfee, 2011).”*
> (Taken from Frey & Osborne, 2013)

Economical impact III

- We don't know what will happen
- Plausibly, many tasks will become so cheap humans will no longer perform them
  - Essential, non-automated tasks will both become more valuable, inhibit progress
  - Humans will do fewer jobs, play a relatively smaller role in the economy (the share of capital will increase relative to labor)
  - The most destructive forms of automation is when tasks are only slightly better done by machines

Machine learning and data mining pipeline of this course



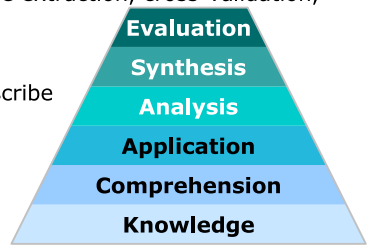
Learning objectives

1.Describe the major steps involved in data modeling from preparing the data, modeling the data to evaluating and disseminating the results.
(Knowledge)

2.Discuss key machine learning concepts such as feature extraction, cross-validation, generalization and over-fitting, prediction and curse of dimensionality.
(Comprehension)

3.Sketch how the data modeling methods work and describe their assumptions and limitations.
(Knowledge and Comprehension)

4.Match practical problems to standard data modeling problems such as regression, classification, density estimation, clustering and association mining.
(Comprehension and Application)



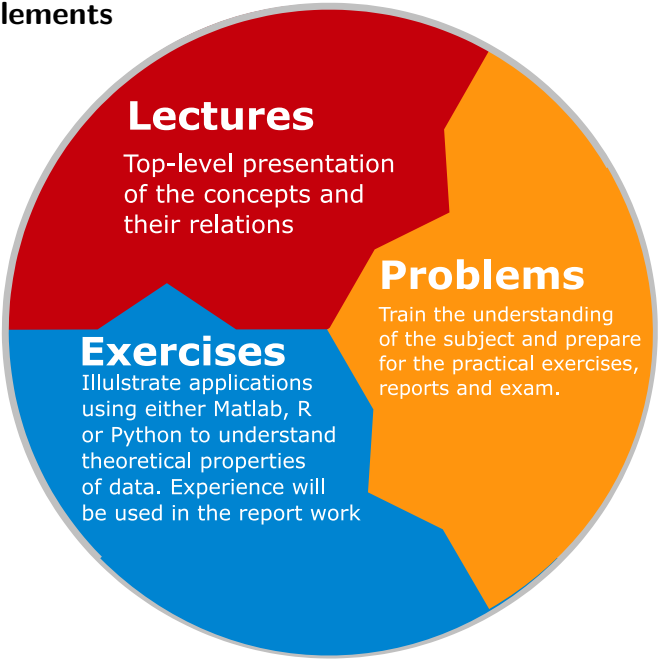
5.Apply the data modeling framework to a broad range of application domains in medical engineering, bio-informatics, chemistry, electrical engineering and computer science.
(Application)

6.Compute the results of the data modeling framework by use of Matlab, R or Python.
(Application)

7.Use visualization techniques and statistics to evaluate model performance, identify patterns and data issues.
(Analysis)

8.Combine and modify data modeling tools in order to analyze a data set of their own and disseminate the results of the analysis.
(Application, Analysis, Synthesis and Evaluation)

Course Elements



Group Learning

- You should form groups of 2-3 students (max 3 students for the reports).
  - **During class** You are encouraged to work together and discuss the online Quiz questions.
  - **During exercises** Each exercise consist of computer exercises relevant for the report work as well as a conceptual multiple-choice question from a previous exam. Please only spend about 15 minutes on the multiple-choice question.
- You have to register your group at DTU Learn > My Course > Groups. Inform your TA about your: 1) Group number, 2) student IDs of the members, and 3) full names of the members.

Online help

- https://piazza.com/dtu.dk/fall2022/02450 (Sign up!)
- Use forum for 24/7 help
- Ensure everyone have access to the same information
  - **Bad: very general questions, i.e. can you explain GMM?**
    Good: Here is what I understand, but I don't get equation ...
  - **Bad: error without context, i.e. I tried to do a PCA but I get an error the matrix has the wrong size?**
    Good: What language are you using and what is the error; code which produced the mistake; what did you try to accomplish?
  - **Bad: Can you explain the PCA question in the Fall 2009 exam?**
    Good: Insert screenshot of fall 2009 exam, explain what part of the solution is unclear

Examination

Exam has two components

- 4 hours written multiple choice exam (homework problems are from previous exams)
- 2 project reports

  Report 1 October 4, *Data: Feature extraction, and visualization*
  Report 2 November 15, *Supervised learning: Classification and regression*

- Final grade based on overall assessment of reports and written exam. The written exam is weighted more than the reports ($\approx 75\%$ vs $\approx 25\%$)

Reminder: Structure of the course and activities

- **Workload**: DTU's **nominal** workload for a 5 ECTS course is **9 hours per week** during the 13-week period and 140 hours in total.
- **Structure and study-activities** :
  - Lecture session [2 hours per week]:
    - **High-level lectures** including quizzes and in-class discussions (formative, i.e. not assessed)
  - Supervised **exercises** (formative) [2 hours per week]
    - Focus on the central aspects of the exercises, not the project work.
    - Do not underestimate the importance of attempting the exam questions; anecdotal evidence would suggest that students who attempt exam questions do better on the exam.
    - TAs have be instructed to prioritise questions on the central aspects of the exercises (including the suggested exam questions).
  - Self-study, preparation & project work [5 hours per week]
    - We assign **readings, homeworks, quizzes** and provide **old exams** to help you study more effectively (not assessed).
    - **Project work** (**assessed**), you apply the taught theory to your own data.
    - Online help/assistance on any aspect of the course via Piazza.
  - **Exam** (**assessed**) [4h + preparation (19h)]

Course format

Lecture session [2 hours per week]

- Physically - main auditorium 116-81. [275 seats]
- Physically - secondary auditorium 116-83 where we live broadcast. [100 seats]
- Online - live stream via Zoom (link on DTU Learn).

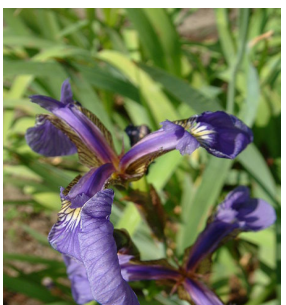
Exercise session [2 hours per week]

- Physically - find rooms & information on DTU Learn (recommended).
- Online - questions via Microsoft Teams channels.

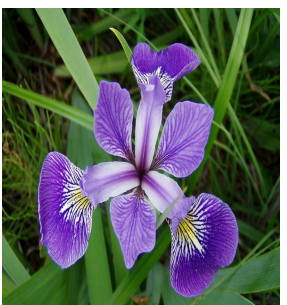
Project information

Dataset selection At least 60 observations (check for missing or erroneous values), at least 5 features with ideally at least 3 of the features to be continuous (interval or ratio).
Example Iris flower dataset, 50 observations, 3 classes: setosa, versicolor, virginica, and 4 features: length and width of sepals and petals.

- **Regression**: Predict the petal width using the rest of the features.
- **Classification**: Find the class using the 4 features.



(a) Iris setosa



(b) Iris versicolor

(c) Iris virginica

Subsequent ML courses

This course (02450) is recommended prerequisite for:

- 02456 Deep learning
- 02471 Machine learning for signal processing
- 02477 Bayesian machine learning
- 02460 Advanced Machine Learning (also recommended prerequisites 02456 / 02471 / 02477)

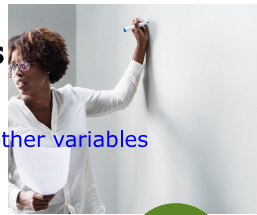
More courses will probably be added soon.

Pretest

- The purpose is to assess your background in order to adjust the presentation and measure your learning.
- Some of the questions will be hard and may seem unfair. Do not Google it. We want to know, if you know.
- **Not part of your assessment. We never look at individual results.**

Go to: DTU Learn > 02450 > Course Content > Quizzes > Pretest

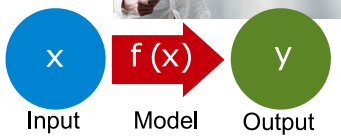
Data Mining and Machine Learning Tasks



Predictive tasks (Supervised learning)

– Use some variables to predict unknown or future values of other variables

- **Classification**
  - Discrete output
  (Determine which class a new data object belongs to)
- **Regression**
  - Continuous output
  (Determine the output value from the input variables)



Descriptive tasks (Unsupervised learning)

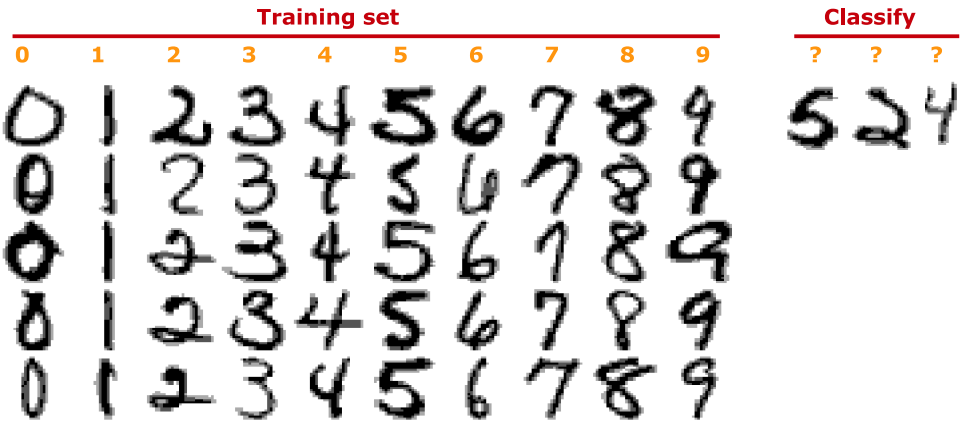
– Find human-interpretable patterns that describe the data

- **Clustering**
  – Discover group structure in data
- **Association rule discovery**
  – Discover how data objects relate to each other
- **Anomaly detection**
  – Find data objects that are abnormal

Classification: Definition

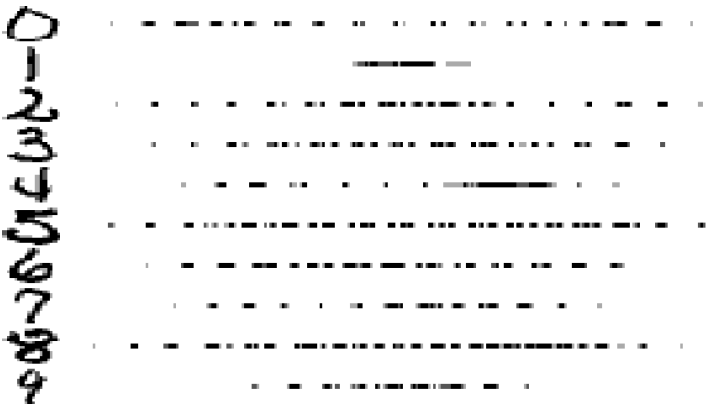
- Given a collection of data objects (**training set**)
  - Each object has associated a number of features
  - Each object belongs to a certain class
- Define a **model** for the class given the other features
- Goal: Assign a class label to a **previously unseen object**

Classification: Example



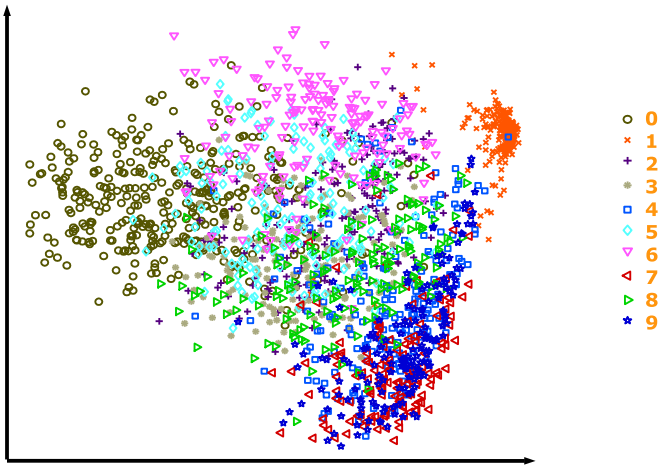
Classification: Example

Data representation

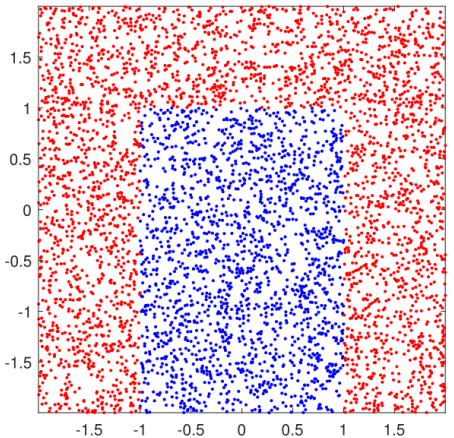


Classification: Example

Visualization



Quiz 02 (DTU Learn): Decision rules



The figures shows an example classification problem consisting of a large number of observations (x, y) along with their class (red and blue).

A *decision rule* is just a function which takes an (x, y) coordinate and outputs either the red or the blue class. Suppose we define:

$$z_1 = \max\{0, x - 1\} + \max\{0, -1 - x\}$$
$$z_2 = \max\{0, -1 + y\}$$

Which of the following *decision rules* solve the problem?

A. If $z_1 = z_2 = 0$ classify as blue and otherwise as red

B. If $z_1 = z_2 = 1$ classify as blue and otherwise as red

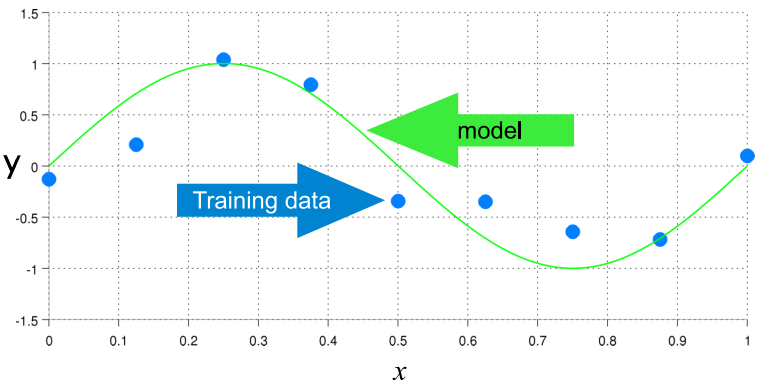
C. If $z_1 = 1$ and $z_2 = 0$ classify as blue and otherwise as red

D. If $z_1 = 0$ and $z_2 = 1$ classify as blue and otherwise as red

E. Don't know

Regression: Definition

- Given a collection of data objects
  - Each object has associated a number of features
  - Each object has associated a **continuous valued variable**
- Define a **model** for the variable given the features
- Goal: Predict the value of the variable for a **previously unseen object**



Regression: Example

- Predict **sales amounts** of new product based on
  - advertising expenditure
- Predict **wind velocity** as a function of
  - temperature, humidity, and air pressure
- Predict the value of a **stock market index** based on
  - previous index time series and market indicators

Regression: Example

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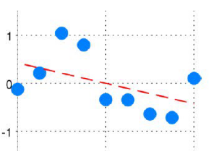
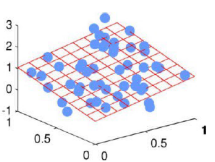
1-dimensional inputs

$$f(x) = w_0 + w_1 x$$

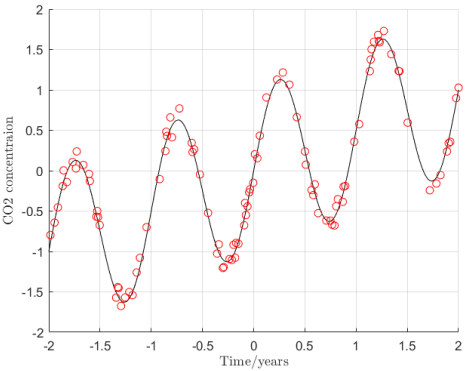


2-dimensional inputs

$$f(\boldsymbol{x}) = w_0 + w_1 x_1 + w_2 x_2$$



Quiz 03 (DTU Learn): Regression



The figures shows an example regression problem where the CO2 concentration is measured as a function of the time of year.

We wish to come up with a prediction rule $y = f(x)$ where y is the relative CO2 concentration and x is the time of year. Which of the following functions would be a good candidate?

A. $y = 0.5x + \cos(x)$

B. $y = -0.5x + \cos(x)$

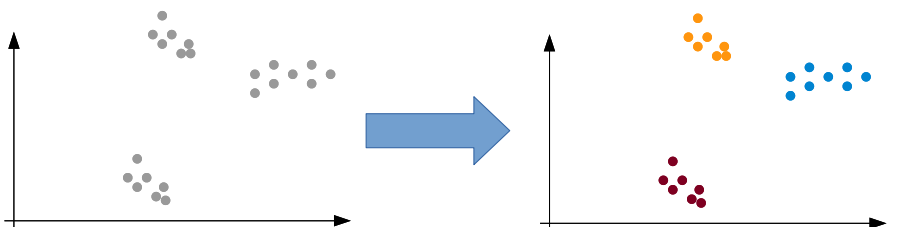
C. $y = 0.5x + \sin(2\pi x)$

D. $y = -0.5x + \sin(2\pi x)$

E. Don't know

Clustering: Definition

- Given a collection of data objects
  - Each object has associated a number of features
  - A measure of **similarity** between objects is defined
- Goal: **Group the objects** into clusters such that
  - Objects within each cluster are similar
  - Objects in separate clusters are less similar



Clustering: Example

Document clustering

- **Goal**
  - Find groups of similar documents based on the words appearing in them
- **Approach**
  - Identify frequently occurring words in each document
  - Define a similarity measure based on the word frequencies
  - Perform clustering to find groups of documents
- **Motivation**
  - Use the clusters to relate a new document to existing documents
  - Better search algorithms: Return documents that are similar but do not have the exact search keywords

Association rule discovery: Definition

- Given a set of **records**
  - Each containing a number of **items from a set**
- Goal: Produce dependency rules
  - Predict the occurence of an item based on occurences of other items

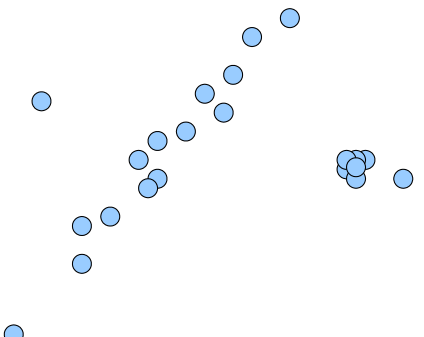
Association rule discovery: Example

Market basket analysis

Training set	Rules discovered
1.{Bread, Coke, Milk}	{Milk} ►{Coke}
2.{Beer, Bread}	{Diaper, Milk} ►{Beer}
3.{Beer, Coke, Diaper, Milk}	
4.{Beer, Bread, Diaper, Milk}	
5.{Coke, Milk}	

Anomaly detection: Definition

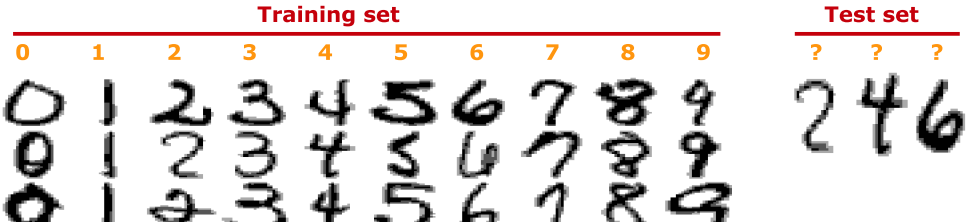
- Given a collection of data objects
  - Each object has associated a number of features
- Detect which objects **deviate from normal** behaviour



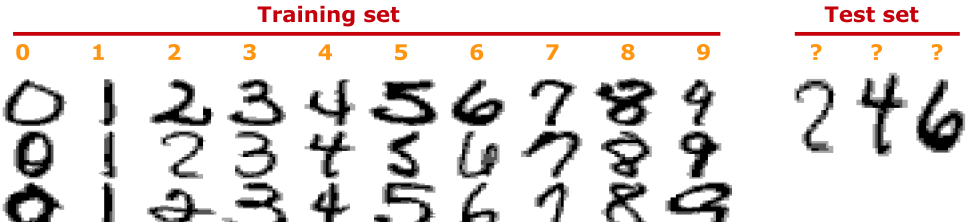
Anomaly detection: Example

- Credit card **fraud detection**
  - Recognize dubious credit card transactions based on the transaction history of the card holder
- Detection of **outliers** in data measurements
  - Remove erroneous measurements due to misreading from an instrument
- **Fault detection** in system health monitoring
  - Detect when a wind turbine performs poorly due to ice coating on blades

Models in machine learning

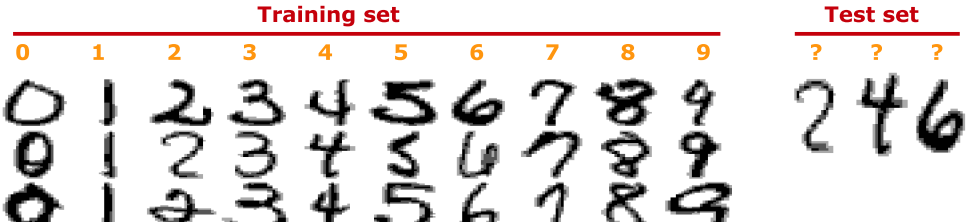


Models in machine learning

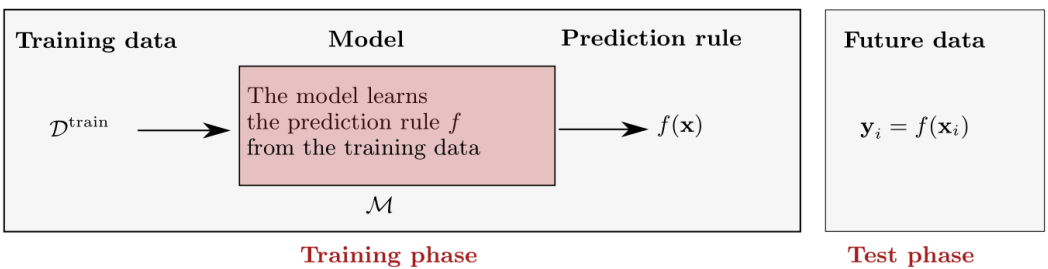


Classifying digits is a mapping $f : \mathbb{R}^M \rightarrow \{0, 1, \ldots, 9\}$

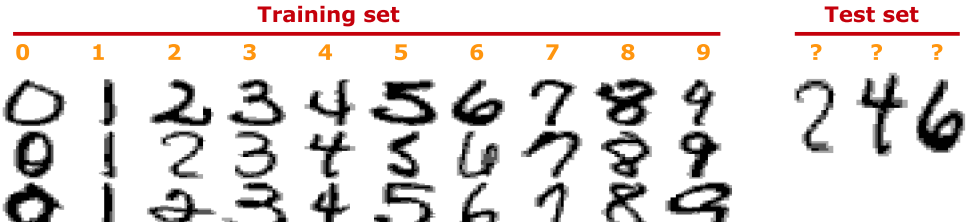
Models in machine learning



Classifying digits is a mapping $f : \mathbb{R}^M \rightarrow \{0, 1, \ldots, 9\}$



Models in machine learning



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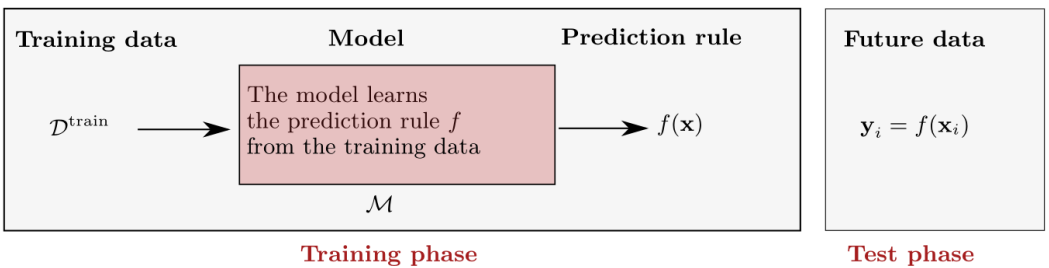

How often the learned function f makes errors in the future is the **generalization error**

Exercises

We support **Matlab**, **Python**, and **R**

- Exercise 0 guided your through installing your chosen environment
- If you have no experience with either, we recommend **Python**

Rooms for exercises:

- Building 116, auditorium A081, (Python, Matlab, R), [capacity: 137]
- Building 116, auditorium A083, (Matlab, Python, R), [capacity: 50]
- Building 116, room H010, (Python), [capacity: 54]
- Building 116, room H012, (Python), [capacity: 54]
- Building 116, room H016, (Python, Matlab), [capacity: 50]
- Building 116, room H015, (Python), [capacity: 30]
- Building 116, room H011, (Python), [capacity: 30]
- Building 116, room H040, (Python), [capacity: 48]
- Building 116, room H042, (Python), [capacity: 36]
- Building 116, room H049, (Python), [capacity: 36]

Exercises Today

- Follow exercise instructions available on DTU learn (Exercise 1)
- Form groups (max 3 students) and select a dataset for the reports
- Instruction for finding a dataset on DTU Learn > 02450 > Shared files > Project descriptions > `02450finding_a_dataset_for_reports`
- Please have your dataset approved and your group registered (talk to your TA)

Resources

https://www.mckinsey.com Impact assessment of automation by McKinsey (https://www.mckinsey.com/featured-insights/artificial-intelligence/notes-from-the-ai-frontier-modeling-the-impact-of-ai-on-the-world-economy)

https://towardsdatascience.com Another introduction to machine learning basics (https://towardsdatascience.com/introduction-to-machine-learning-db7c668822c4)

https://www.economicsofai.com conference on modelling economical impact of AI (https://www.economicsofai.com/nber-conference-toronto-2017/)

https://deepmind.com Obviously google-focused, but otherwise a great resource for what is hot right now (https://deepmind.com/)