TECHNISCHE UNIVERSITÄT DARMSTADT

Statistical Machine Learning

Lecture 01: Introduction

Kristian Kersting

TU Darmstadt

Summer Semester 2020

Today's Objectives

- Organizational issues
- Advertisement
- Introduction

Outline

1. Organizational Issues

2. Introduction

3. Wrap-Up

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Outline

1. Organizational Issues

2. Introduction

3. Wrap-Up

Instructors

- Kristian Kersting heads the AI and ML Lab at the Department of Computer Science at the TU Darmstadt. He has studied computer science and your can find him in the Alte Hauptgebäude, Room 074, Hochschulstrasse 1. You can also contact Kristian through kersting@cs.tu-darmstadt.de

- **Karl Stelzner** joined the AIML Lab as a Phd student in 2017. He is working on probabilistic (deep) learning, in particular for unsupervised image understanding. You can contact Karl via email stelzner@cs.tu-darmstadt.de.

PLEASE FEEL FREE TO EMAIL US WITH QUESTIONS!

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Website & Mailing list

- Moodle: `https://moodle.informatik.tu-darmstadt.de/course/view.php?id=928`

Course Language

...will be in **English**

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Why?

- Essentially *all* machine learning literature is in English.
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Questions and answers in emails/homework/exams may be answered in German (However, this is not encouraged...).

Feedback: Essential for both sides...

We appreciate
FEEDBACK!

Jeder Prof hat 'ne Meise. Meine dürfen Sie füttern!

Exam & Bonus Points from Homework

There will be a written exam.

- Approximate date: The weeks after the end of classes...

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- Will max out on bonus points!
- Please register in Moodle with groups of 2 students.

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Question: Favorite Homework-Frequency? 4 homeworks

Homework Assignments

- There will be **4** homework assignments!
- Each assignment will contain:
  - A few multiple choice questions
  - A few essay questions
  - Some programming exercises.

Background Reading

- We will add current papers & tutorials!
- Standard background reading:
  - **C.M. Bishop, Pattern Recognition and Machine Learning (2006), Springer**
  - **K.P. Murphy, Machine Learning: a Probabilistic Perspective (2012), MIT Press**
  - **S. Rogers, M. Girolami, A First Course in Machine Learning (2016), CRC Press**
- Mathematics for machine learning background:
  - **Marc Peter Deisenroth, A Aldo Faisal, and Cheng Soon Ong, Mathematics for Machine Learning, `https://mml-book.github.io/`**

Background Reading

- Other resources
  - D. Barber, Bayesian Reasoning and Machine Learning (2012), Cambridge University Press (http://web4.cs.ucl.ac.uk/staff/D.Barber/textbook/090310.pdf)
  - T. Hastie, R. Tibshirani, and J. Friedman (2015), The Elements of Statistical Learning, Springer Verlag (https://web.stanford.edu/~hastie/Papers/ESLII.pdf)
  - R.O. Duda, P.E. Hart, and D.G. Stork, Pattern Classification (2nd ed. 2001), Willey- Interscience
  - T.M. Mitchell, Machine Learning (1997), McGraw-Hill
  - R. Sutton, A. Barto. Reinforcement Learning - an Introduction, MIT Press (http://incompleteideas.net/book/RLbook2018.pdf)

How does it fit in your course plan? 1/3

VL *Statistical Machine Learning* is a good preparation for advanced lectures:

- **VL** *Lernende Robot* (aka *Robot Learning*)
- **VL** *Probababilistic Graphical Models*
- **VL** *Statistical Relational AI*
- **IP** *Robot Learning 1, 2*

How does it fit in your course plan? 2/3

Related Classes:

- Improve Foundations: *Data Mining and Machine Learning* (WiSe), *Robot Learning* (WiSe), *Deep Learning: Architectures and Methods* (WiSe)
- Useful Techniques: *Optimierung statischer und dynamischer Systeme*
- Applications of learning: *Computer Vision*

Theses: We always have B.Sc. or M.Sc. Theses on ML topics.

How does it fit in your course plan? 3/3

B.Sc. / M.Sc. Informatik:

- Human Computer Systems (see Modulhandbuch)
- If you are strongly interested in machine learning you should take:
  - Statistical Machine Learning for HCS credit
  - Data Mining and Machine Learning for DKE credit
  - Robot Learning for CE credit
  - Computer Vision for Visual Computing

M.Sc. in Autonome Systeme

M.Sc. in Visual Computing: Area “Computer Vision & ML”

Outline

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Why Machine Learning?

- “We are drowning in information and starving for knowledge.” - John Naisbitt

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- **Era of big data:**
  - In 2017 there are about 1.8 trillion webpages on the internet
  - 20 hours of video are uploaded to YouTube every minute
  - Walmart handles more than 1M transactions per hour and has databases containing more than 2.5 petabytes (2.5×10^{15}) of information.

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No human being can deal with the data avalanche!

Why Machine Learning?

"I keep saying the sexy job in the next ten years will be **statisticians** and **machine learners**. People think I'm joking, but who would've guessed that computer engineers would've been the sexy job of the 1990s? The ability to take data — to be able to understand it, to process it, to extract value from it, to visualize it, to communicate it — that's going to be a hugely important skill in the next decades."

Hal Varian, Chief Economist at Google, 2009

Job Perspective

"A significant constraint on realizing value from big data will be a shortage of talent, particularly of people with deep expertise in statistics and machine learning."

Big data: The next frontier for innovation, competition, and productivity, 2011, McKinsey Global Institute

Machine Learning

What is ML? What is its goal?

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- Develop a machine / an algorithm that learns to perform a task from past experience.

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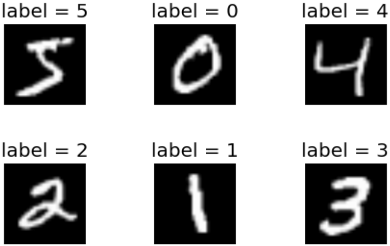
Why? What for?

- Fundamental component of every intelligent and / or autonomous system
- Discovering “rules” and patterns in data
- Automatic adaptation of systems
- Attempting to understand human / biological learning

Machine Learning in Action

Machine Learning Examples

Recognition of handwritten digits



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Machine Learning Examples

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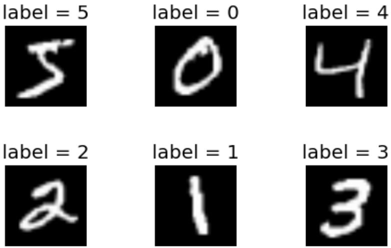

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Machine Learning Examples

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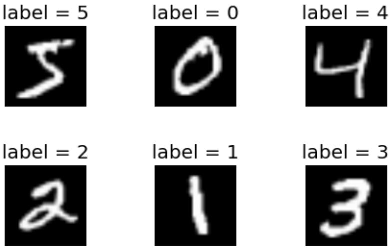
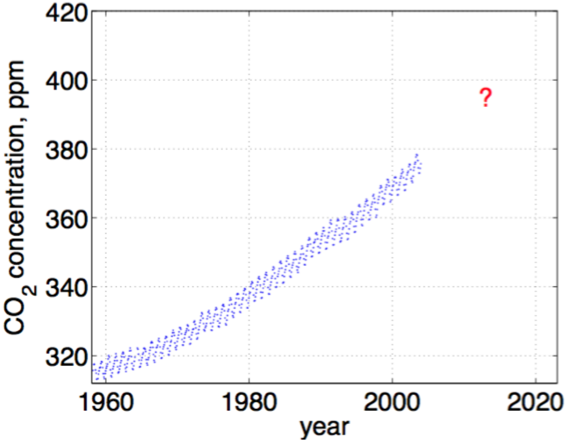


- These digits are given to us as small digital images
  - We have to build a “machine” to decide which digit it is
  - **Obvious challenge**: There are many different ways in which people handwrite

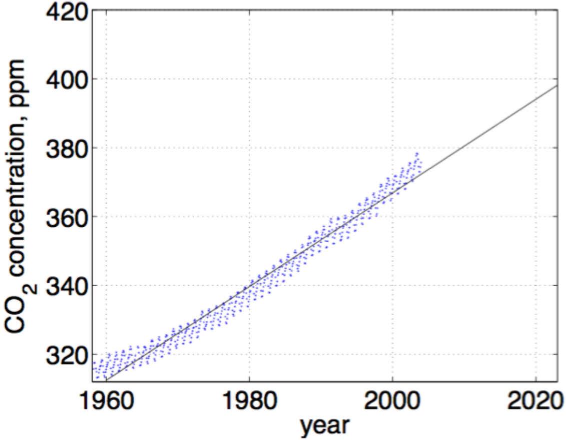
Machine Learning Examples

CO2 prediction



Machine Learning Examples

CO2 prediction



Machine Learning Examples

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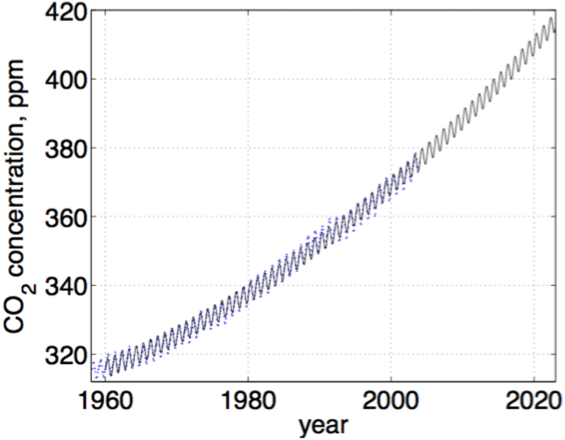

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Machine Learning Examples

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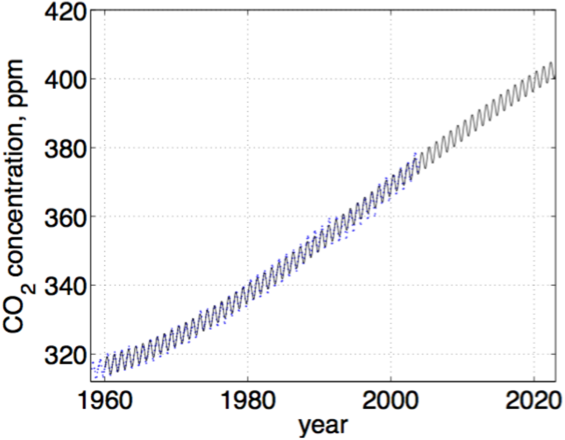

Machine Learning Examples

- **Email filtering**

x ε [a-z]+ → y ε [important, spam]

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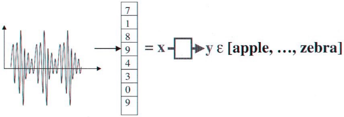
- **Speech recognition**



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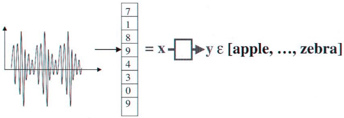
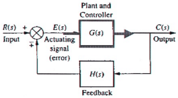


- **Vehicle control**



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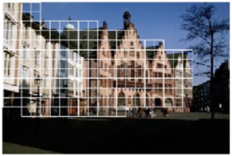
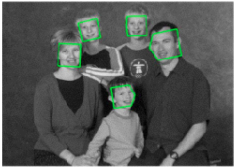
Machine Learning Impact & Successes

- Recognition of speech, letters, faces, ...
- Autonomous vehicle navigation
- Games
  - Backgammon world-champion
  - Chess: Deep-Blue vs. Kasparov
  - Go: AlphaGo, AlphaGo Zero
- Google
- Finding new astronomical structures
- Fraud detection (credit card applications)
- ...





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  - Input: $x \in I$ (images, text, sensor measurements, ...)
  - Output: $y \in O$
  - Parameters: $\theta \in \Theta$ (what needs to be "learned")

Classification vs Regression

Classification

- Learn a mapping into a discrete space, e.g.

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- Examples:

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- Examples:
  - Spam / not spam
  - Digit recognition
  - Part of Speech tagging

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  - $O = \mathbb{R}$
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- Examples

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Classification vs Regression

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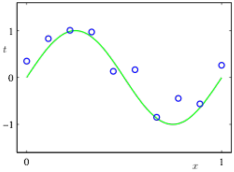
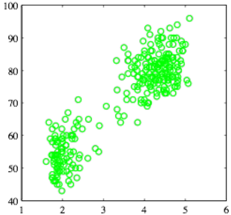
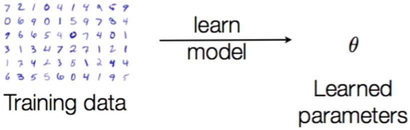
- Learn a mapping into a continuous space, e.g.
  - $O = \mathbb{R}$
  - $O = \mathbb{R}^3$
- Examples
  - Curve fitting, Financial Analysis, Housing prices, ...





General Paradigm

Training



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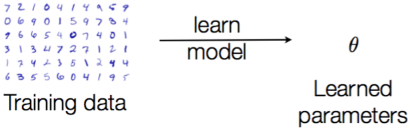

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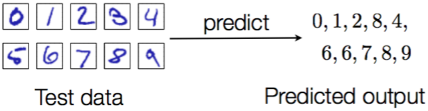

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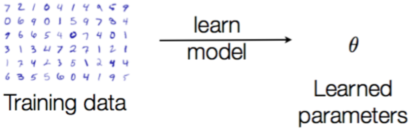

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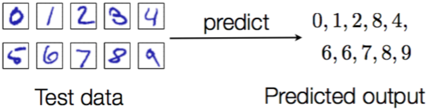

The test dataset needs to be different than the training dataset!

But ideally from the same underlying distribution.

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What data do we have for training?

- Data with labels (input / output pairs): supervised learning
  - Image with digit label
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  - Density Estimation
  - Dimensionality Reduction
- Data with and without labels: semi-supervised learning
- No examples: learn-by-doing
  - Reinforcement Learning

Some Key Challenges

- We need generalization!
  - We cannot simply memorize the training set.
- What if we see an input that we haven't seen before?
  - Different shape of the digit image (unknown writer)
  - "Dirt" on the picture, etc.
  - We need to learn what is important for carrying out our task.
- This is one of the most crucial points that we will return to many times.

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Generalization

How do we achieve generalization?

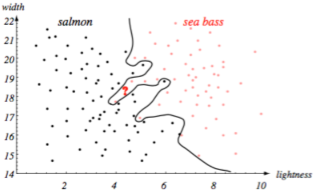

FIGURE 1.5. Overly complex models for the fish will lead to decision boundaries that are complicated. While such a decision may lead to perfect classification of our training samples, it would lead to poor performance on future patterns. The novel test point marked **?** is evidently most likely a salmon, whereas the complex decision boundary shown leads it to be classified as a sea bass. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

Generalization

How do we achieve generalization?

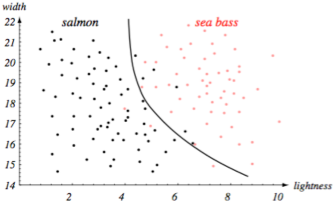

FIGURE 1.6. The decision boundary shown might represent the optimal tradeoff between performance on the training set and simplicity of classifier, thereby giving the highest accuracy on new patterns. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

Occam's Razor

Generalization

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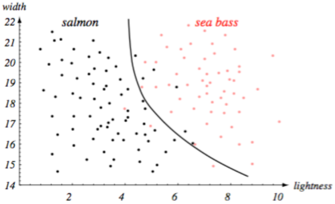

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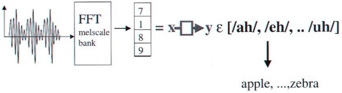
Occam's Razor

We should not make the model overly complex!

Prominent example of overfitting...


Some Key Challenges

- Input:



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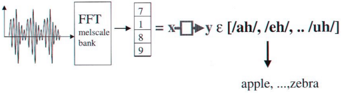
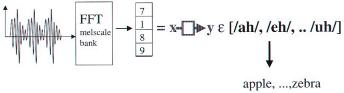


- Features

Some Key Challenges

- Input:



- Features
  - Choosing the “right” features is very important.
  - Coding and use of domain knowledge.
  - May allow for invariance (e.g., volume and pitch of voice).

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Some Key Challenges

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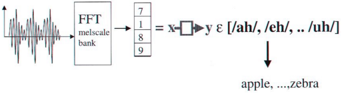

- Features
  - Choosing the "right" features is very important.
  - Coding and use of domain knowledge.
  - May allow for invariance (e.g., volume and pitch of voice).
- Curse of Dimensionality:
  - If the features are too high-dimensional, we will run into trouble
  - Dimensionality reduction.

Some Key Challenges

- How do we measure performance?
  - 99% correct classification in speech recognition: What does that really mean?
  - We understand the meaning of the sentence? We understand every word? For all speakers?

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  - % of correctly classified letters
  - average distance driven (until accident...)
  - % of games won
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  - % correctly recognized words, sentences, etc.
- Training vs. testing performance!

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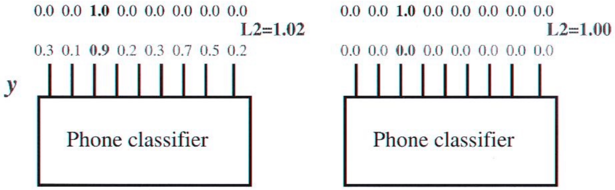
Some Key Challenges

- We also need to define the right error metric:



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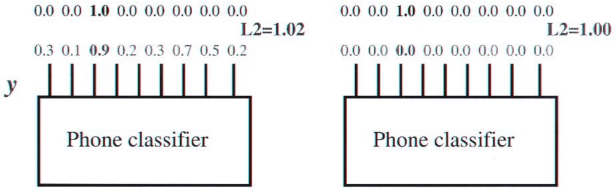

- Which is better?
- Euclidean distance (L2 norm) might be useless.

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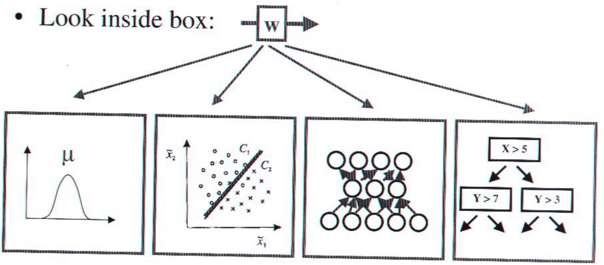
Some Key Challenges

Which is the right model?

Some Key Challenges

Which is the right model?

- The learned parameters (**w**) can mean a lot of different things:
  - May characterize the family of functions or the model space
  - May index the hypothesis space
  - **w** can be a vector, adjacency matrix, graph, ...



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Even if we have solved the other problems, computation is usually quite hard:

- Learning often involves some kind of optimization
- Find (search) best model parameters

Some Key Challenges

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- Given a model, compute the prediction efficiently

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- It combines insights and tools from many fields and disciplines:
  - Traditional artificial intelligence (logic, semantic networks, ...)
  - Statistics
  - Complexity theory
  - Artificial neural networks
  - Psychology
  - Adaptive control
  - ...

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- Allows you to apply theoretical skills that you may otherwise only use rarely.
- Has lots of applications:
  - Computer vision
  - Computer linguistics
  - Search (think Google)
  - Digital “assistants”
  - Computer systems
  - Robotics
  - ...

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- It is a growing field:
  - Many major companies are hiring people with machine learning knowledge.
  - Learning machine learning is probably the most promising route to such a 80-160.000 Euro Job...
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- Linear Methods (~ 3-4 weeks)
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  - PCA, robust PCA
  - Fisher linear discriminant
  - Generalized linear models

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  - Deep Learning: What is really different?
- Miscellaneous (~ 3 weeks)
  - Model averaging (bagging & boosting)
  - Graphical models (basic introduction)

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Credits

- These slides are essentially the slides of Jan Peters.
- Some parts of Jan's lecture material have been developed by Profs. Bernt Schiele, Stefan Roth and Stefan Schaal for the previous iterations of this course or similar classes.
- Many figures that I will use are directly taken out of the books by Chris Bishop and Duda, Hart & Stork and Kevin Murphy.

Outline

3. Wrap-Up

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You know now:

- What Machine Learning is and what it is not.
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- The different types of learning problems.
- What classification and regression are.
- The challenges in solving a problem with Machine Learning.

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- What is generalization? What is overfitting?

Homework

- Select some Machine Learning applications and check:
  - What type of learning is it?
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- Reading assignment
  - Jordan Book, Linear Algebra chapter (online)
  - Pedro Domingos, *A few useful things to know about Machine Learning* (`https://homes.cs.washington.edu/~pedrod/papers/cacm12.pdf`)
  - Bishop ch. 1