Statistical Machine Learning

Lecture 1: Organization & Introduction

Simone Schaub-Meyer & Marcus Rohrbach
Department of Computer Science
TU Darmstadt

Summer Term 2025

Outline

1. Organizational Aspects

2. Introduction to ML

3. Wrap-Up

Instructors

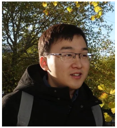
- **Simone Schaub-Meyer** is an assistant professor at TU Darmstadt leading the Image & Video Group and is affiliated with the Hessian Center for AI. Her research focuses on efficient, robust, and interpretable methods. She earned her Ph.D. from ETH Zurich in collaboration with Disney Research Zurich.

- **Marcus Rohrbach** is a professor at TU Darmstadt. He leads the Multimodal Reliable AI lab. His research focuses on computer vision, machine learning, and computational linguistics. Previously, he worked at Meta AI and UC Berkeley. He earned his Ph.D. from the Max Planck Institute for Informatics.

Teaching Assistants

- **Tobias Braun** is a PhD student in the Multimodal AI Lab at TU Darmstadt, working on multimodal reliable AI. You can contact Tobias at `tobias.braun@mai.tu-darmstadt.de`.

- **Jiayun Li** is a PhD student in the Interactive Robot Perception & Learning lab at TU Darmstadt, working on motion planning. You can contact Jiayun at `jiayun.li@tu-darmstadt.de`.



For Q&As, please use Moodle.
For personal matters, contact us directly at `smlstaff@visinf.tu-darmstadt.de`.

Website & Discussion Board

- Moodle:
  https://moodle.tu-darmstadt.de/course/view.php?id=42016
  - Lecture slides
  - Pointers to readings
  - Homework assignments + hand in
- Discussion board on Moodle
  - Please use it to ask questions of public interest.
  - You are encouraged to discuss with each other.
  - However: Please do not share solutions or give strong hints about the solutions to the homework problems.
  - Asking questions via the discussion boards on Moodle is the preferred form of communication with the course staff!

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Course Language

...will be in **English**

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Why?

- Essentially *all* machine learning literature is in English.
- Knowing the proper *terminology* is essential.
- Good to improve your English skills.

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Organization

- Lecture (13:25 – 15:05)
  - One lecture per week (exceptions announced on Moodle)
  - No lecture on the 4th of June (TU meet and move)
  - We will cover the foundational aspects of each topic
  - We might record and upload the lectures in the Moodle

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- Exercises, homework, etc.
  - Exercise session before the lecture (12:35–13:20)
  - We will cover some practical aspects, show general problem-solving and discuss the homework assignments
  - Time for Q&A
  - Mostly: Time to work on your homework assignments

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Exam & Bonus Points from Homework

There will be a written exam.

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- Date: Tuesday, 2nd of September (exact information, see TUCaN)

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Homework Exercises:

- Homework exercises are crucial for the exam!
- The points from the homework will count as bonus toward the final grade.
- Up to 1.0 higher grade (maxing out the departmental rules)
- Until next week: Register in Moodle with groups of 3 students.

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- Homework assignment 1 will be released on 30.04.2025
- 2 homework assignments will be checked in person
  - Groups randomly selected
  - Probably Tuesdays, more information in the exercise session

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Background Reading

- We will add current papers & tutorials.
- Standard background reading:
  - ***C.M. Bishop, Pattern Recognition and Machine Learning (2006), Springer,*** https://www.microsoft.com/en-us/research/uploads/prod/2006/01/Bishop-Pattern-Recognition-and-Machine-Learning-2006.pdf
  - ***K.P. Murphy, Probabilistic Machine Learning: An Introduction (2022), MIT Press,*** https://probml.github.io/pml-book/book1.html
  - ***S. Rogers, M. Girolami, A First Course in Machine Learning (2016), CRC Press***
- Mathematics background for machine learning:
  - ***M.P. Deisenroth, A. Aldo Faisal, and C.S. Ong, Mathematics for Machine Learning (2020), Cambridge University Press*** https://mml-book.github.io/

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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)

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How does it fit in your course plan?

VL *Statistical Machine Learning* prepares you for advanced courses:

- **VL** *Reinforcement Learning*
- **VL** *Lernende Roboter* (aka *Robot Learning*)
- **IP** *Robot Learning*
- **VL** *Intelligente Robotermanipulation*
- **VL** *Probababilistic Graphical Models*
- **VL** *Computer Vision I and II*
- **VL** *Multimodal Artificial Intelligence*
- **VL** *Deep Learning for NLP*

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

Questions about course organization

Time for your questions regarding the course organization!

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Why Machine Learning?

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- We generate much more data than we can analyze manually
  - "We are drowning in information and starving for knowledge."
    – John Naisbitt, author
  - 500 hours of video are uploaded to YouTube every minute (2022)
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!! ML is inherently data driven, data is at the core of ML. The goal of ML is to design general-purpose methodologies to extract valuable patterns from data, ideally without much domain-specific expertise.

Why Machine Learning?

Machine learning is a subfield of **artificial intelligence** that gives computers the ability to learn without explicitly being programmed. **Artificial intelligence systems** are used to perform complex tasks in a way that is similar to how humans solve problems.

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“Machine learning is changing, or will change, every industry, and leaders need to **understand** the basic principles, the potential, and the limitations”
–Aleksander Madry, director of the MIT Center for Deployable Machine Learning.

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Why Machine Learning?

- It's amazing what modern Machine Learning methods can do!
  - Image Generation (DALL-E, Midjourney, ...)
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In this class we will cover most of the topics you will need to get started in Machine Learning, like Projects, Thesis, Job Interviews

Machine Learning

What is ML? What is its goal?

Machine Learning

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According to T. Mitchell (1997):

- 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.
  in other words...

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  in other words…
- Develop a machine / an algorithm that learns to perform a task from experience.

Machine Learning

Why? What for?

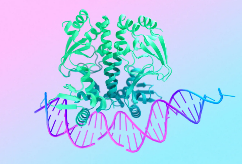
Machine Learning

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

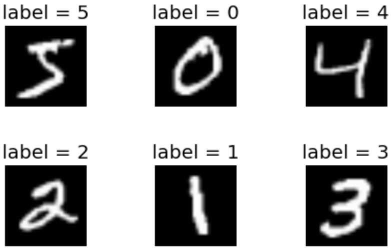
Machine Learning Impact & Successes

- **AlphaFold 3:** Predicts protein interactions with DNA/RNA — transforming biology and drug discovery.
- **Nobel Prize 2024:** Awarded to Hinton and Hopfield for their groundbreaking work in neural networks.
- **Autonomous Driving:** Tesla FSD V12.3 shows major real-world improvements.
- **ChatGPT / DeepSeek:** Powers human-like conversation, coding, tutoring, and creativity at scale.



Machine Learning Examples

Recognition of handwritten digits



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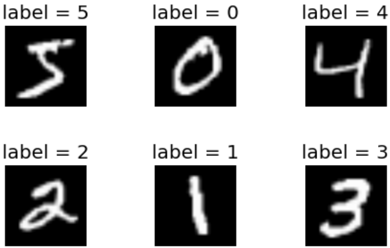

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Machine Learning Examples

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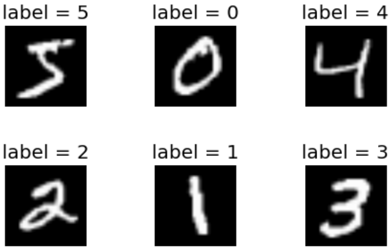
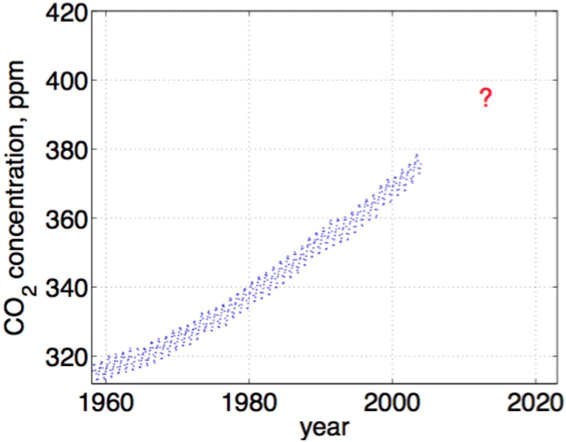


- These digits are given to us as small digital images
  - We have to build a "machine" to decide which digit it is
  - **Obvious challenge**: There are many different ways in which people handwrite

Machine Learning Examples

CO2 prediction



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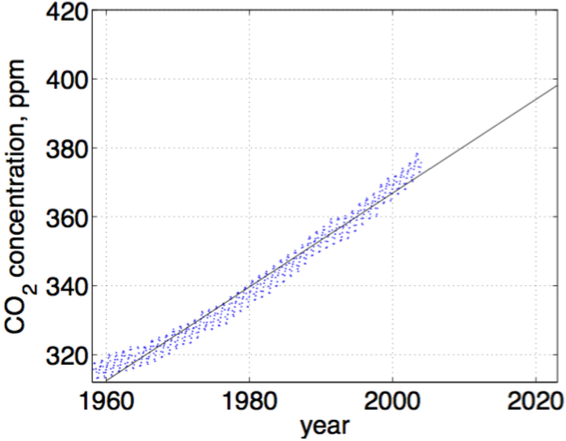
Machine Learning Examples

CO2 prediction



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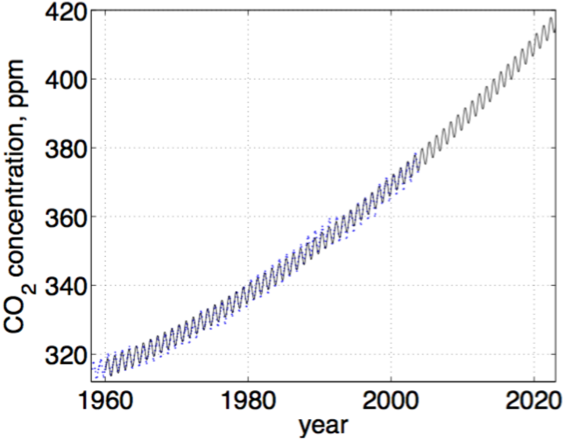

Machine Learning Examples

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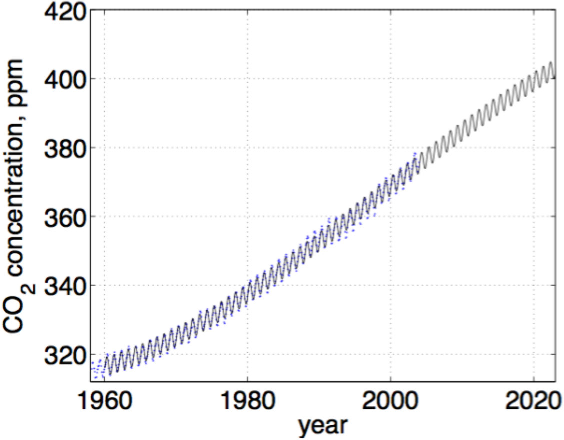

Machine Learning Examples

- **Email filtering**

$x \ \varepsilon\ [a\text{-}z]+ \longrightarrow \boxed{} \longrightarrow y \ \varepsilon\ [\text{important, spam}]$

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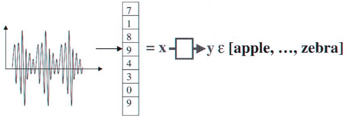
- **Speech recognition**



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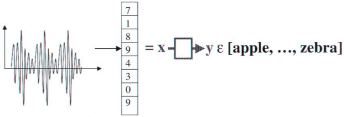
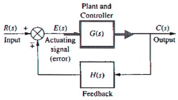


- **Vehicle control**



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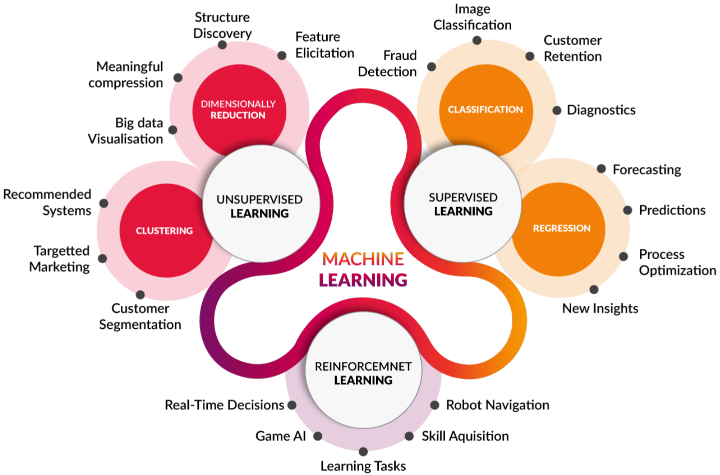
  - Input: $x \in I$ (images, text, sensor measurements, ...)
  - Output: $y \in O$
  - Parameters: $\theta \in \Theta$ (what needs to be “learned”)

Types of Machine Learning



Source: `https://www.cognub.com/index.php/cognitive-platform/`

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Classification vs Regression

Classification

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

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  - $O = \{0, 1\}$
  - $O = \{0, 1, 2, 3, \ldots\}$
  - $O = \{\text{verb}, \text{noun}, \text{adjective}, \ldots\}$
- Examples:

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

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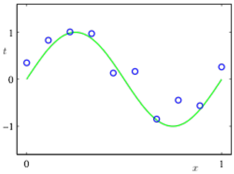
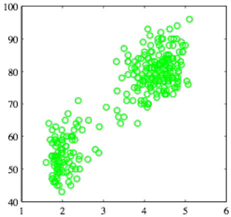
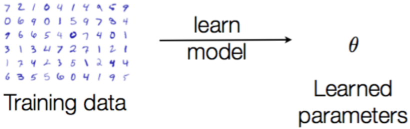
- Examples
  - Curve fitting, Financial Analysis, Housing prices, ...





General Paradigm

Training



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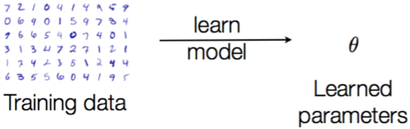

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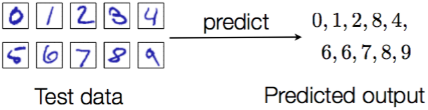

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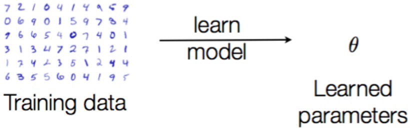

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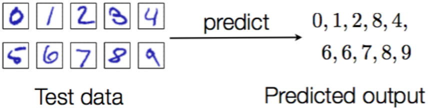

The test dataset needs to be different than the training dataset!

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
    - Sensory data for car with intended steering control

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- Data with and without labels: semi-supervised learning
- No examples: learning-by-doing
  - Reinforcement learning

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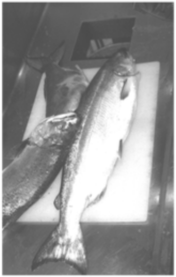
Some Key Challenges

- 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.

Generalization

How do we achieve generalization?



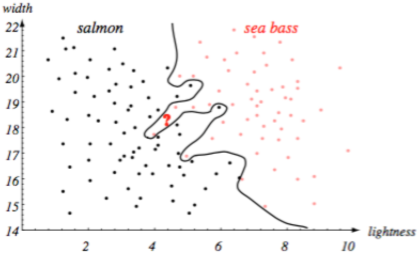


FIGURE 1.5. Overly complex models for the fish will lead to decision boundaries that are complicated. While such a decision may lead to perfect classification of our training samples, it would lead to poor performance on future patterns. The novel test point marked **?** is evidently most likely a salmon, 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.

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Generalization

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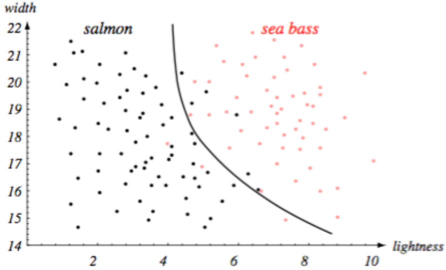

FIGURE 1.6. The decision boundary shown might represent the optimal tradeoff between performance on the training set and simplicity of classifier, thereby giving the highest accuracy on new patterns. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001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

Occam's Razor

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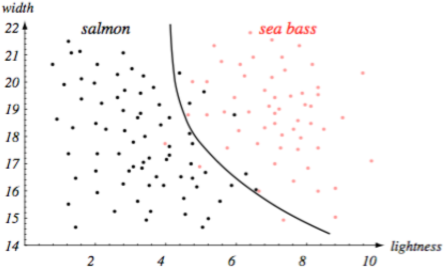

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Occam's Razor

We should not make the model overly complex!

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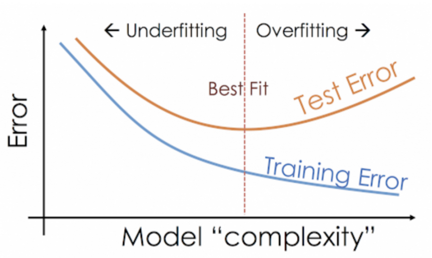
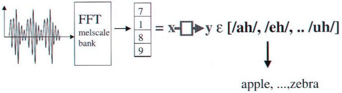
Example of overfitting...



Some Key Challenges

- Input:



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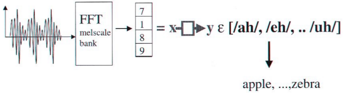

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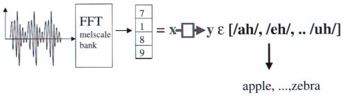

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  - Coding and use of domain knowledge.
  - May allow for invariance (e.g., volume and pitch of voice).

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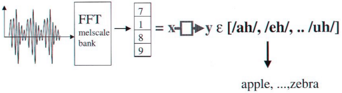

- Features
  - Choosing the “right” features is very important.
  - Coding and use of domain knowledge.
  - May allow for invariance (e.g., volume and pitch of voice).
- Curse of Dimensionality:
  - If the features are too high-dimensional, we will run into trouble
  - Dimensionality reduction.

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Some Key Challenges

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- Training vs. testing accuracy!

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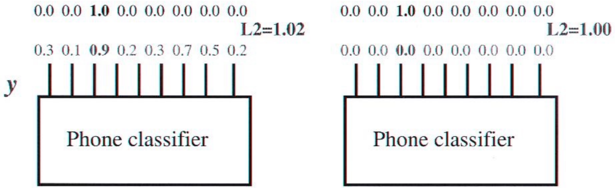
Some Key Challenges

- We also need to define the right error metric:



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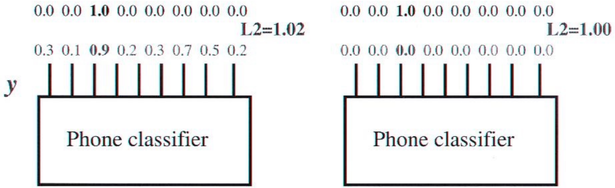


- Which is better?
- Euclidean distance (L2 norm) might be useless.

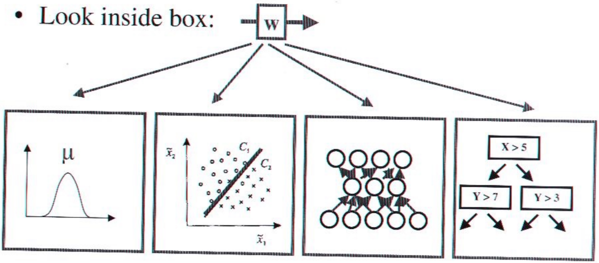
Some Key Challenges

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
- Often we have to deal with thousands, millions, billions, ..., of training examples
- Given a model, compute the prediction efficiently

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- Machine learning is a challenging problem that is far from being solved.
  - Our learning systems are primitive compared to us humans.
  - Think about what and how quickly a child can learn!
- 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
  - Natural language processing
  - Search (think Google)
  - Digital “assistants”
  - Computer systems
  - Robotics
  - ...

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- Because it is fun!

Preliminary Syllabus

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- Refresher of Linear Algebra & Statistics (next week)

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  - Bayes decision theory, Decision Boundary, Risk Minimization
  - Probability density estimation
  - Mixture models, expectation maximization

Preliminary Syllabus

- Linear Methods (~ 3 weeks)
  - Classification, Fisher linear discriminant
  - Linear regression
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Preliminary Syllabus

- Linear Methods (~ 3 weeks)
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- Fundamentals Part II (~ 1 week)
  - Clustering
  - Performance evaluation

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- Neural Networks (~ 2 week)
  - Neural Networks: From Inspiration to Application
  - Deep Learning: What is really different?

Credits

- These slides have been originally developed by Prof. Bernt Schiele and later modified by Profs. Jan Peters, Kristian Kersting, Stefan Schaal, Stefan Roth and myself for previous iterations of this course or similar classes.
- Many figures are directly taken out of the books by Chris Bishop and Duda, Hart & Stork and Kevin Murphy.

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Outline

3. Wrap-Up

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- The different types of learning problems.
- What classification and regression are.
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- What is generalization? What is overfitting?

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- Next week: Refresher Linear Algebra & Statistics

Before You Go

Please remember:

Register for an exercise group on Moodle
by next week, in teams of 3 students.

This is important for participating in the homework exercises.