Lecture 1: Overview
April 25, 2019

Machine Learning, Summer Term 2019

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University of Freiburg

Lecture Overview

1. Motivation: Why Study Machine Learning?
2. Organizational Issues
3. Introduction to Supervised Machine Learning
4. Other Types of Machine Learning
5. The Machine Learning Design Cycle
6. Wrapup: Summary, Other Courses, Resources, Preview

Lecture Overview

Where are you already using Machine Learning?

- You're probably using dozens of systems built on machine learning every day ...
- Let's hear some examples from you to get started! 

Machine Learning is Everywhere

- Spam classification

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- Computer game industry: self-configuration based on user actions

Machine Learning is Everywhere

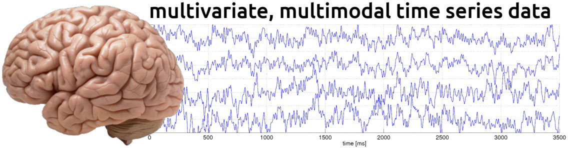
As of now, slightly less common examples:

- Autonomous cars
- Intelligent prostheses (BrainLinks-BrainTools)
- Autonomous helicopter flight
- Learning soccer robots (RoboCup)
- Learning to Design RNA

Success Story: Decoding of Brain Activity

A grand challenge! Brain signals ...

- are high-dimensional and noisy
- are subject specific
- have distributions that vary over time (fatigue, learning, strategies, ...)



Traditional way to do research:

- do the same experiment for many subjects
- average all the data
- do statistics and publish

Desired: single-trial decoding to run online applications!

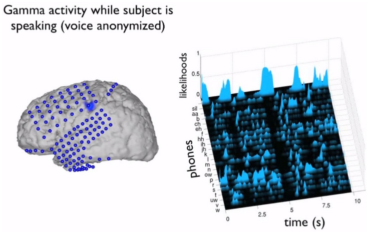
Estimate Movie Content from Brain Activity

Can you guess a movie's content from brain signals of the observer?

- Show subjects several hours of movies while recording brain signals (fMRI data).
- Train a movie-to-brain activity encoding model (regression).
- Show novel movies and record brain signals.
- Estimate the visual content with the trained model.

[Nishimoto et al., 2011, Current Biology, video from https://www.youtube.com/watch?v=nsjDnYxJ0bo]

Estimate Spoken Speech from Brain Activity



Reconstruct spoken speech from brain signals:

- Semi-invasive recordings
- Train a ECoG-to-phonemes decoder
- Use speech recognition technique + language models

[Herff et al., Front. Neurosci. 2015, http://dx.doi.org/10.3389/fnins.2015.00217]

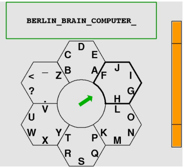
Example from our work: Estimate Mental Workload

Using BCI Technology to monitor brain processes in **real time**.
Driver's workload during:

- Driving task only (primary task)
- Driving + audio book listening
- Driving + mental calculation

Example from our work: Controlling a Brain-Computer Interface

Decode motor imagery classes (left hand, right hand, feet) from EEG signals to control a spelling application:



Today's BCI applications address:

- Communication for motor-impaired patients
- Device control
- Rehabilitation after stroke
- Mental state monitoring (workload, attention, ...)

- Many fields have big data to be mined
  - Medicine, biology, astronomy, finance, social network studies, ...

Machine Learning and Data Mining

- Many fields have big data to be mined
  - Medicine, biology, astronomy, finance, social network studies, ...
- We'd like to make inferences from the data
  - "We're drowning in data but starving for knowledge" (Futurist John Naisbitt)
  - Machine Learning lets us generalize (which is key to knowledge)

Machine Learning and Artificial Intelligence

- Machine learning is a subfield of AI

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  - Theorem proving
  - Classical planning

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- AI used to be focused on logics
  - Theorem proving
  - Classical planning
- Since the 1990s, AI focuses more on probabilistic reasoning
  - This is closer to machine learning
- One approach to solve AI is to build machine learning systems that resemble the human brain
  - Richard Feynman: "what we can't synthesize, we don't understand"
  - Deep neural networks are a (small) step in this direction

Machine Learning as A Different Way of Programming

- We don't understand how the human brain solves certain problems
  - Face recognition
  - Playing Atari games
  - Speech recognition
  - Picking the next move in the game of Go
- We can nevertheless learn these tasks from data/experience

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- If the task changes, we simply re-train
- We can construct computer systems that are too complex for us to understand anymore ourselves...
  - E.g., deep neural networks have millions of weights.
  - E.g., AlphaGo, the system that beat world champion Lee Sedol
    - David Silver, lead author of AlphaGo cannot explain its moves
    - Paraphrased: "You would have to ask a Go expert."

Machine Learning is very Sought After

- AI is very popular
  - When university students in a wide range of fields were asked to list a field they would like to study other than their own, the most frequent answer was AI
  - Machine learning is one of the most exciting subfields of AI

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  - Machine learning is one of the most exciting subfields of AI
- Predictions by a 2011 McKinsey report (for the US):
  - Better data analysis could save the public sector 250 billion Euro/year
  - There will be a need for 140,000 to 190,000 machine learning experts
  - There will be a need for 1.5 million data-savvy managers

Lecture Overview

Organization: Instructors

Michael Tangermann
Research group leader
Brain State Decoding
Main Point of Contact

Frank Hutter
Professor
Machine Learning

Marius Lindauer
Junior Research Group Leader
Machine Learning

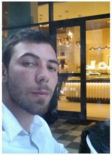
Organization: Assistants and Tutors

Sebastián Castaño

David Hübner

Jan Sosulski

Andreas Meinel



Arber Zela

Katharina Eggensperger

Simon Ging

Yi-Chun Lin

Baohe Zhang

Organization: Lectures

- Meeting times:
  Monday & Thursday 16:15-17:52 (S101, room 00 026)
  - Including a 7-minute break roughly in the middle
- Both Monday and Thursday slots might have lecture content and exercise discussion
  - We highly recommend that you attend both lectures & exercise sessions
- All lectures will be recorded & online soon after
  - Thanks to our Hiwis Simon, Yi-Chun & Bahoe

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- We strive for interaction!
  - Discuss with your neigbhor: ? (2 minutes)
  - Raise your hands to give answers:
  - Multiple-choice questions
    to be answered with colours on smartphone screens
    - E.g., "Color Screen" on iPhone, or go to:
    - https://ml.informatik.uni-freiburg.de/teaching/colors.html

Organization: Assignments

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- You can work in teams of up to 3 members

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- We'll try to optimize amount learned per time spent with assignments
  - Proposals for improvements are always welcome
- Keeping up with the assignments is the best preparation for the exam

Organization: Gitlab and ILIAS

- Gitlab Server
  - A private Git repository just for you (your team)
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  - Whatever is committed by the deadline is your submission
- ILIAS
  - All lecture materials will be posted in ILIAS (incl. assignments, code to get you started on assignments, etc)
  - There is a forum for questions of all kinds
    - Making a first post there is part of Assignment 1
    - Please answer a question if you know the answer
  - There is also a Wiki

Organization: Amount of Work / ECTS points

- This course yields 6 ECTS points $\rightarrow$ 180 working hours
- Lectures ($\approx$ 45 hours) + assignments + exam preparation
- Time management options
  - A 6-8 hours per assignment, little exam prep. RECOMMENDED
  - B 4-5 hours per assignment, much exam prep. MINIMUM
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- There is a written exam in the end
  - We'll make a mock exam available about two weeks before
  - We're trying to fix the exam date soon (likely mid August)
    - + Erasmus students: same exam as every one else
  - Doing all the exercise sheets and understanding everything behind them is the perfect preparation for the exam

Lecture Overview

Supervised Learning: The Basic Idea

- Use past experience to predict the future
  - Use labelled data points $\langle(\mathbf{x}_i, y_i)\rangle_{i=1}^{N}$ that we collected in the past
  - to automatically construct a model whose prediction $\hat{y}_{N+1}$ for a new data point $\mathbf{x}_{N+1}$ is close to the actual label y_{N+1}.

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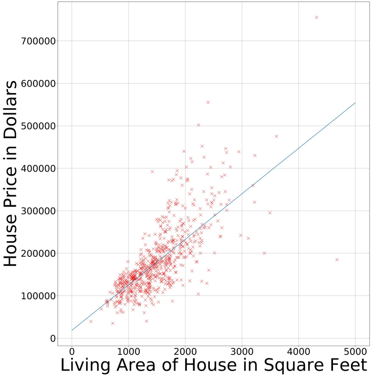
- First example: predicting house price based on size (in square feet)



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  - Data point $\mathbf{x}_i$, often a vector in $\mathbb{R}^D$
  - Label y_i
    - Regression: $y_i \in \mathbb{R}$
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- What is the dimensionality D in the house price example?

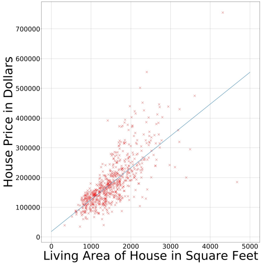
  ★ D=1 ★ D=2 ★ D=3 ★ D=4

Supervised Learning: A First Regression Example

Predicting housing prices

- For many houses in a training set, we know:
  - the square footage
  - the prize they sold for
- We'd like to predict the prize for houses based on their square footage
- One data point: square footage $\mathbf{x}_i$ and its prize y_i (in US$)
- This is a regression problem since $y_i \in \mathbb{R}$

Square footage x_i	Prize y_i
1.710	208.500
1.262	181.500
1.786	223.500
1.717	140.000
2.198	250.000
1.362	143.000
1.694	307.000
2.090	200.000
1.774	129.900
1.077	118.000
...	...



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  - That's why it is bold-faced
  - The dimensions of $\mathbf{x}_i$ are $D \times 1$
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$$\mathbf{X} = \begin{pmatrix} \mathbf{x}_1^\intercal \\ \dots \\ \mathbf{x}_N^\intercal \end{pmatrix} \qquad \mathbf{y} = \begin{pmatrix} y_1 \\ \dots \\ y_N \end{pmatrix}$$

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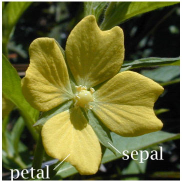
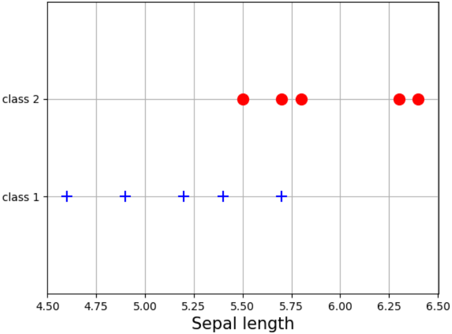
  - Thus, $\mathbf{X}$ is a $N \times D$ matrix; $\mathbf{y}$ is a $N \times 1$ matrix
    - $\mathbf{y}$ is bold-faced since it's a vector
    - $\mathbf{X}$ is capital and bold-faced since it's a matrix
  - $\mathbf{y}$ are the 'correct' labels; this is our supervisory signal (thus the name)

Supervised Learning: a Simple Classification Example

- A classical data set from Botany: classifying Iris flowers
  - feature 1: sepal length
  - feature 2: sepal width



$\mathbf{x}_{i,1}$	$\mathbf{x}_{i,2}$	y_i
6.40	2.90	2
5.50	2.50	2
5.20	3.50	1
4.60	3.60	1
5.70	3.80	1
6.30	2.50	2
5.80	2.60	2
4.90	3.10	1
5.70	2.80	2
5.40	3.90	1



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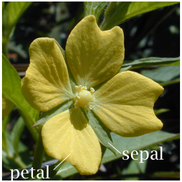

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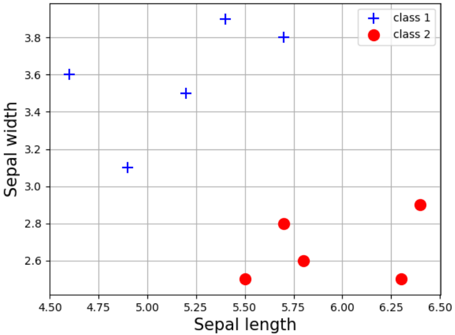

Mini-Quiz in Preparation for Assignment 1: Iris Data

- Classifying Iris flowers (the Iris data set)
  - You will learn a classifier based on 100 labelled Iris flowers
  - Iris flowers are described by 4 characteristics (sepal length/width, petal length/width)
  - There are 3 different classes of Iris flowers

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  - You learn a classifier based on $\mathbf{X}_{train}$ and $\mathbf{y}_{train}$
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- What is the correct dimensionality for the matrix $\mathbf{X}_{train}$?
  - ★ 100×3
  - ★ 3×4
  - ★ 100×4
  - ★ 4×100

Supervised Learning Example: Credit Risk

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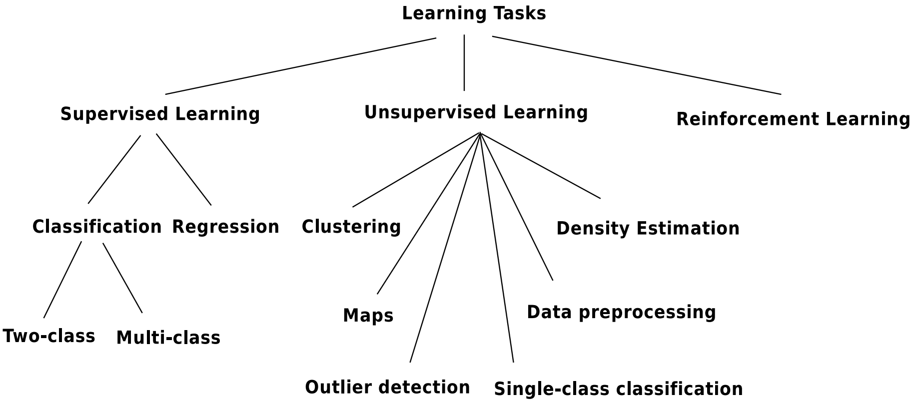
- Ways of casting this as a machine learning problem:
  - 1. Should the bank give the loan?
  - 2. How much interest should the bank charge to break even in expectation?
- Please raise the color of the correct statement:
  - ★ Both are regression tasks.
  - ★ Both are classification tasks.
  - ★ 1. is regression, 2. is classification.
  - ★ 1. is classification, 2. is regression.

Lecture Overview

Types of Learning Tasks



Types of learning tasks: Unsupervised Learning

- training data consists of a description of situations/ objects/ ...
- learn what is typical/ similar/ interesting/ strange within the data
- no teacher
- example: clustering of things that 'somehow belong together'
  - e.g. cluster customers into those with similar behavior
- example: novelty detection
  - detect objects, that are surprising / different from others
  - e.g. find suspicious outliers in radioactivity measurements

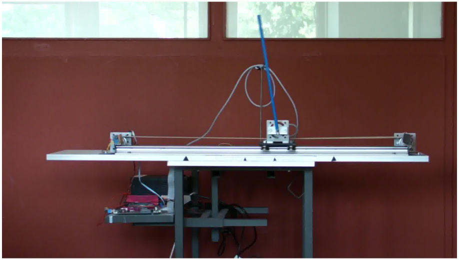
Types of learning tasks: Reinforcement learning

- training data consist of sequences of situations, actions and reward
- task is: learn a control strategy to maximize the reward
- no teacher
- (famous) example: learn to balance a pole

$\rightarrow$ treated in detail in lecture Reinforcement Learning

Example from our work: learning dynamics models for optimal control

- task is to swing up and balance a pole on a cart
- no knowledge of system dynamics
- use of regression technique to learn dynamics function from (random) interaction
- use model for planning locally optimal trajectories (model-based RL)



Example from our work: algorithm runtime prediction

- Task: predict how long an algorithm will run
  - on new inputs
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$\rightarrow$ regression problem

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- Task: will the algorithm terminate within 1 minute?

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$\rightarrow$ clustering problem

- Can we adapt the algorithm's parameters at runtime to make it better?

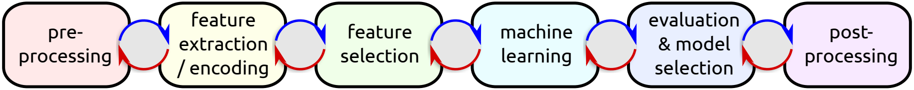
$\rightarrow$ reinforcement learning

Lecture Overview

Applying machine learning in practice

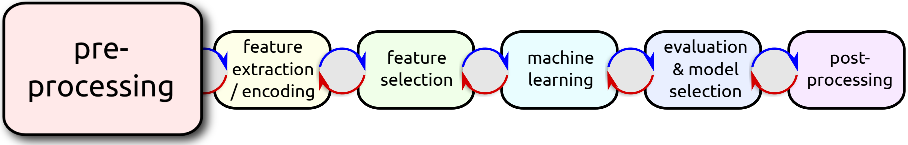
- Let's say we want to apply machine learning to a practical problem
- What do you think are some of the things we need to do?

The Machine Learning Design Cycle



- Real ML applications have many different steps, including:
  - Getting the data into the convenient (X,y) form
  - Casting your problem as an ML problem (supervised, unsupervised, RL)
  - Evaluating your solution & using it in practice

ML Design Cycle: Preprocessing



Get the data in the first place

- Design sensor systems, design questionaires
- Pay people for labels
- Get legal approval to use data, etc.

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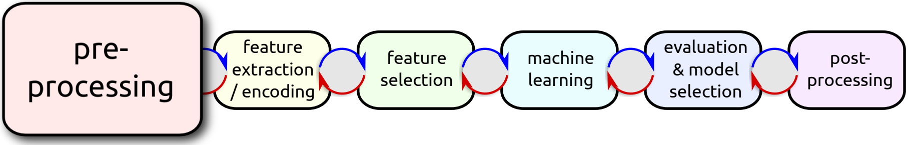

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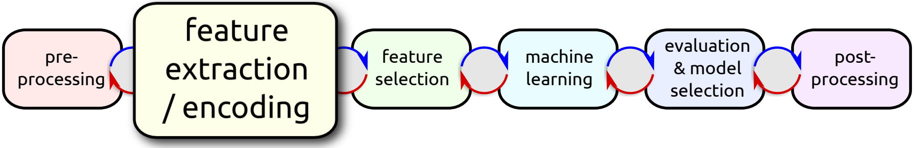
Clean the data

- Missing values may not be missing at random
- Outliers may be due to errors in data acquisition or carry meaning
- Imbalanced data → e.g., subsample majority class / create additional data from minority class, etc.

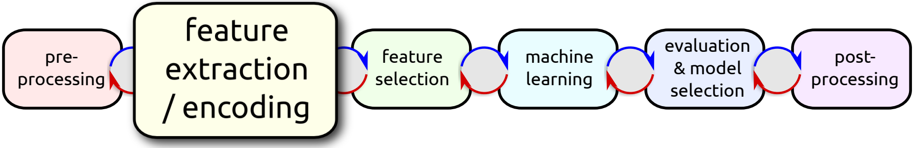
ML Design Cycle: Feature Extraction & Encoding (1/3)



Extract features: getting a nice X matrix

- Often unclear what the features should be.
  - E.g., what's a good feature representation of a human cell, a text, a sound, a brainwave, an image?
- Solution 1: use domain knowledge!
- Solution 2: representation learning (e.g., deep neural networks)

ML Design Cycle: Feature Extraction & Encoding (2/3)

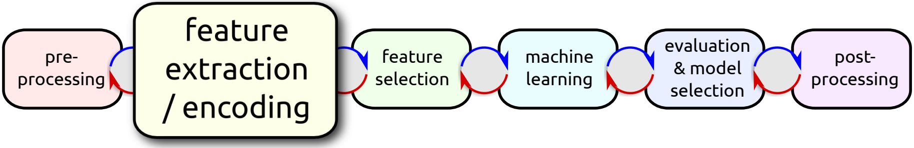


Combine features:

- We can use complex operations to combine features
- E.g., body mass index: $\text{BMI} = \text{weight}/\ (\text{height}^2)$

  (With weight in kg and height in cm)
- Combined features can be more expressive than their components

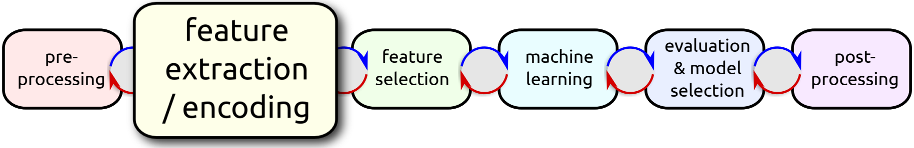
ML Design Cycle: Feature Extraction & Encoding (3/3)



Encode features: getting to a standard format

- Most prominent example: categorical features
  - Features with unordered, finite domain
  - E.g., {red, green, blue}
  - These could be coded as red=1, green=2, blue=3
  - But red is not closer to green than it is to blue ...

ML Design Cycle: Feature Extraction & Encoding (3/3)



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- Standard solution: one-hot-encoding (aka 1-in-k encoding)
  - k-ary feature is coded as k features in {0,1} with exactly one 1
  - E.g., red = [1,0,0]
  - E.g., green = [0,1,0]
  - E.g., blue = [0,0,1]

Mini-Quiz in Preparation for Assignment 1: Iris Data

- Classifying Iris Flowers
  - You will learn a classifier based on 100 labelled Iris flowers
  - Iris flowers are described by 4 characteristics (sepal length/width, petal length/width)
  - There are 3 different classes of Iris flowers
- Let's say we make an additional feature out of the class of flowers (and want to predict whether goats like the flower or not)
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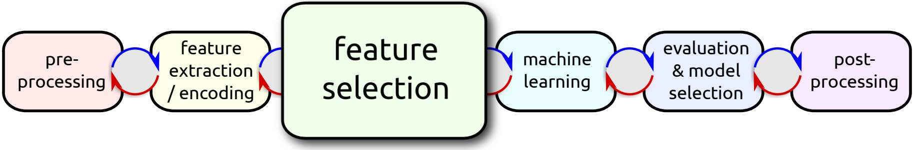
- What is the correct dimensionality for the matrix $\mathbf{X}_{train}$ now?
  - ★ Still 100×4
  - ★ 100×5
  - ★ 100×6
  - ★ 100×7

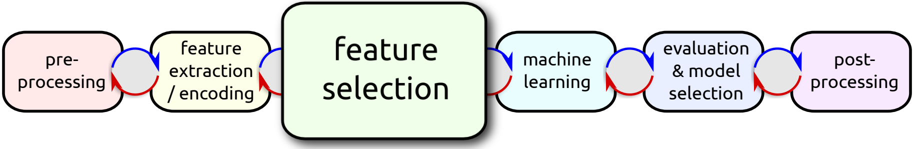
ML Design Cycle: Feature Selection



Select features: getting rid of distractions

- Sometimes, we have too many features (D features)
  - Source 1: original data (e.g., 20,000-25,000 human protein-coding genes)
  - Source 2: feature creation (e.g., trying lots of feature combinations)

ML Design Cycle: Feature Selection



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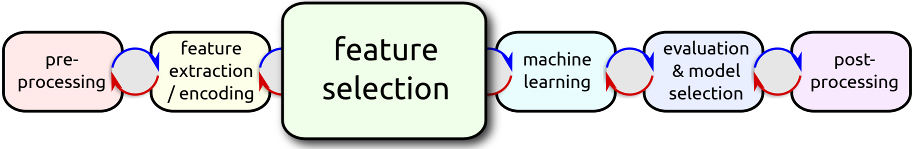
  - Strongly depends on the learning algorithm applied
  - Some algorithms do 'automatic' feature selection, scale to large D

ML Design Cycle: Feature Selection



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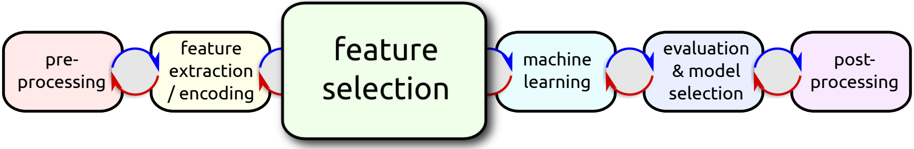

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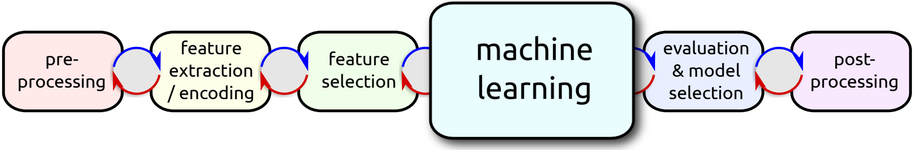
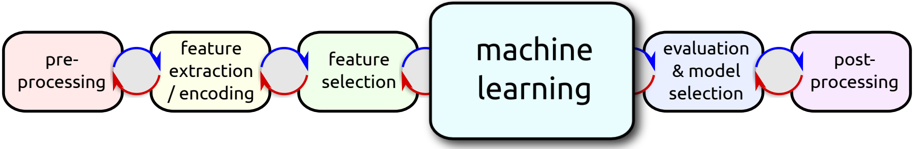
  - Some algorithms do ‘automatic’ feature selection, scale to large D
  - Some algorithms’ computational complexity scales poorly in D
    - They simply run out of memory when D is too large
  - Some algorithms’ predictive performance scales poorly in D
    - They won’t break but simply won’t do very well

ML Design Cycle: ‘Machine Learning’



- The ‘core’ of a machine learning system
- Different algorithms we could use to solve a problem
- This is where 90% of machine learning research happens
  - Computational efficiency
  - Statistical efficiency
  - Provable properties

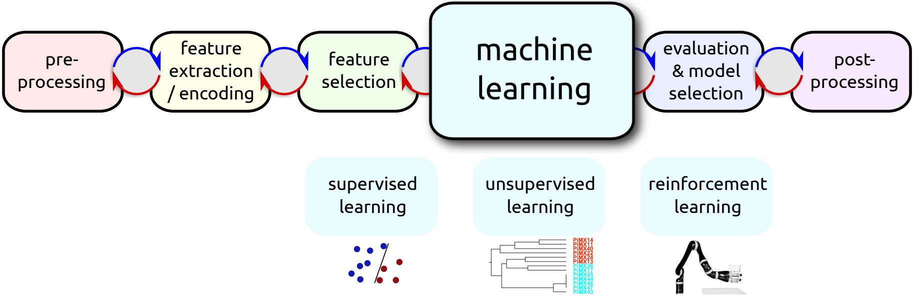
ML Design Cycle: ‘Machine Learning’



- The ‘core’ of a machine learning system
- Different algorithms we could use to solve a problem
- This is where 90% of machine learning research happens
  - Computational efficiency
  - Statistical efficiency
  - Provable properties

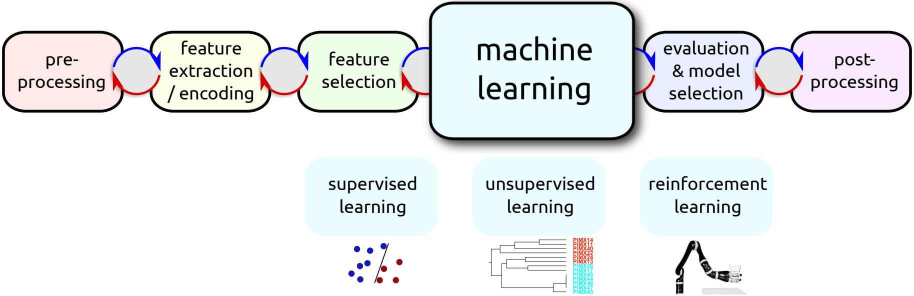
- In practice, this is not much more important than the other parts
- We’ll still focus on this part (since there is the most ‘meat’)
  - But we connect to the other parts whereever possible
  - In practice, the features are often more important than the algorithm

ML Design Cycle: ‘Machine Learning’



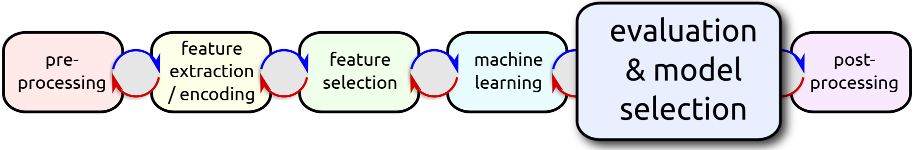
- Sometimes, you can phrase your learning problem in various ways
- Or you can combine various machine learning paradigms
- E.g., AlphaGo:
  - classification to predict expert moves
  - regression to evaluate board positions
  - reinforcement learning by self-play

ML Design Cycle: ‘Machine Learning’



- E.g., learning in infants
  - Lots of unsupervised data
    - + Continuous perception of the environment
    - + Can suffice to learn a representation
  - Very few data points with a supervision signal y
    - + E.g., ‘Look, that’s called a dog!’
    - → Infants can learn the class ‘dog’ from a handful of examples

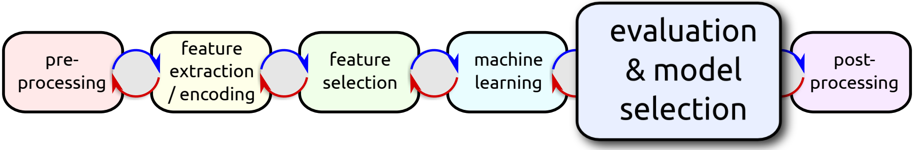
ML Design Cycle: Evaluation and Model Selection 1/3



Evaluation:

- We want our models to generalize
  - I.e., perform well on previously unseen data points
- What does it mean to perform well?
  - Precision, recall, false positives, false negatives
  - Speed at training time, speed at test time, memory, accuracy

ML Design Cycle: Evaluation and Model Selection 2/3



Model Selection: Which Algorithm to Use?

- Computational efficiency, accuracy
- Estimates of generalization performance
- Simplest approach: split dataset into training and validation set
  - Choose algorithm that does best on the validation set
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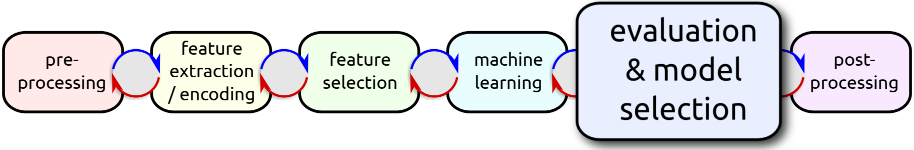
ML Design Cycle: Evaluation and Model Selection 2/3



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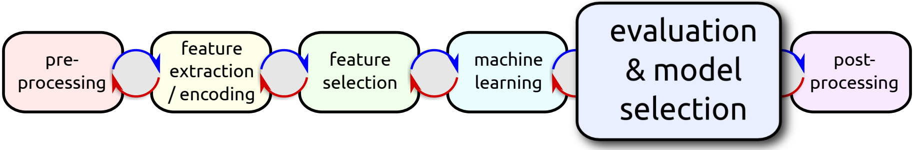
- Simplest approach: split dataset into training and validation set
  - Choose algorithm that does best on the validation set
  - Only that algorithm gets deployed and applied to new test data
  - To evaluate on a fixed dataset
    + Split dataset into training/validation/test
    + Lock away test set for final test
    + Train on training part, choose best w.r.t. validation part

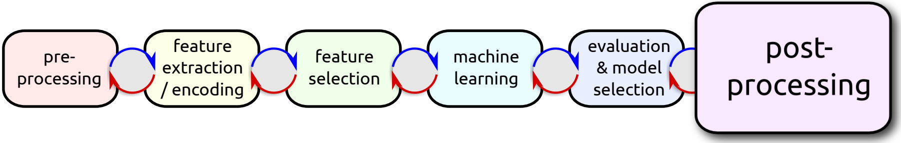
ML Design Cycle: Evaluation and Model Selection 3/3



Model Selection: How to set free parameters of the algorithm?

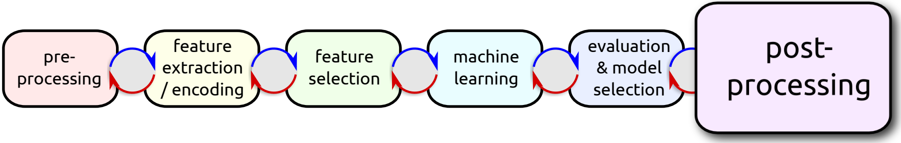
- In machine learning, free tuning parameters are called hyperparameters
  - in contrast to internal model parameters
- Find the hyperparameter setting with best validation performance
- Exponential number of possible settings

The Machine Learning Design Cycle



- Ensure fairness / avoid algorithmic bias
  - E.g., model should not discriminate based on race, gender, religion, sexual orientation, ...

The Machine Learning Design Cycle



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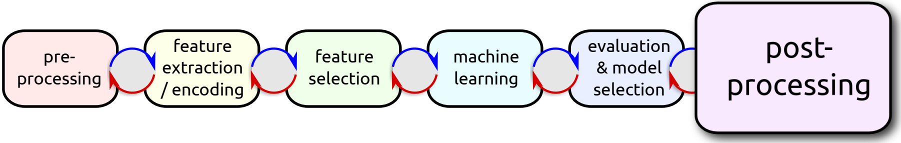

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  - E.g., prediction of side effects
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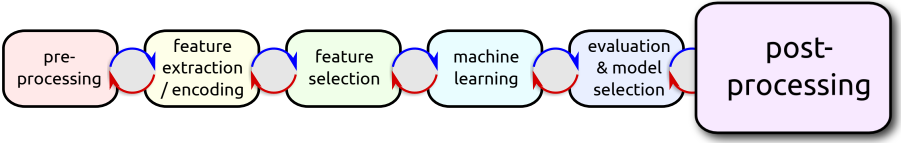

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  - E.g., prediction whether a treatment would help a patient
  - E.g., prediction of side effects
  - E.g., prediction whether the ward has a free bed . . .
- Deploy the model we found to achieve something
  - Don't just predict, but act based on the model

Lecture Overview

Summary by learning goals

Having heard this lecture, you can now . . .

- explain why so many people are interested in machine learning
- give examples for successful machine learning applications
- describe supervised machine learning
- distinguish between classification and regression problems
- distinguish supervised machine learning from other machine learning problems
- describe the parts of the machine learning pipeline

Most related courses at Uni Freiburg

- Statistical pattern recognition
  - By Thomas Brox, this term
  - A probabilistic machine learning course
  - Our course is designed to be complementary
  - If your main interest is machine learning,
    we strongly encourage you to take this course as well

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- Lab Course Deep Learning
  - By groups Boedecker, Brox, Burgard, Hutter, SS
  - More advanced course that builds on the Deep Learning course

Other related courses at Uni Freiburg

- Artificial Intelligence
  - By groups Burgard, Nebel, Boedecker, Hutter
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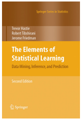
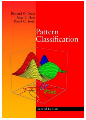
- Information Retrieval
  - By Hannah Bast, WS
- Automated Machine Learning (AutoML)
  - By Marius Lindauer & Frank Hutter, SS
  - More advanced course that builds on this current course & Deep Learning

We'll use material from several books, including these

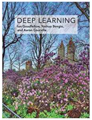
- The Elements of Statistical Learning
  by Hastie, Tibshirani and Friedman
  - Available online for free: `https://web.stanford.edu/~hastie/ElemStatLearn/`



- Pattern Classification by Duda, Hart and Stork



- Deep Learning
  by Goodfellow, Bengio and Courville
  - HTML version available online for free: `http://www.deeplearningbook.org/`



Python tutorials

- General:
  - Official tutorial: https://docs.python.org/3/tutorial/index.html
  - For beginners: www.learnpython.org/
  - For programmers: http://stephensugden.com/crash_into_python/
  - Many more: http://docs.python-guide.org/en/latest/intro/learning/
- Libraries:
  - Numpy: http://wiki.scipy.org/Tentative_NumPy_Tutorial
  - SciPy: http://docs.scipy.org/doc/scipy/reference/tutorial/
  - Matplotlib: http://matplotlib.org/users/beginner.html
- Feel free to discuss about these and additional ones on ILIAS . . .

Other resources for the course

We'll also refer to other sources for background throughout. Here is one to start with:

- Khan Academy: `https://www.khanacademy.org/`
  - Useful to review linear algebra, etc
- Again, please post resources you find useful on ILIAS

Preview of Assignment 1

- Set up infrastructure for the remainder of the course
- Explore a simple classification dataset
- Classify with some manually-derived rules

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- On Monday:
  - Bring your (charged!) laptops with the VM image on it!
  - We'll set up the teams
  - Space-permitting, we'll arrange seating so we can walk through & help