Maschinelles Lernen - Uebung 00

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Structure of this course

Goals

→ Learn the basics of Applied Machine Learning
→ Offer a place to discuss questions
→ Prepare you for the exam

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Structure

- There are no requirements to enter the exam (keine Studienleistung)
- There will be weekly exercises
- We will (probably) not publish sample solutions
- I will try to give a quick recap about the lecture each week
- We discuss what you deem necessary / interesting

Recap: Notation

Note The input space can be (nearly) everything
Make things easier focus on d–dimensional vectors $\vec{x} \in \mathcal{X} \subseteq \mathbb{R}^n$

$\mathcal{D}$	Feature 1	Feature 2	$\dots$	Feature d	Label
Example 1	x_{11}	x_{12}	$\dots$	x_{1d}	y_1
Example 2	x_{21}	x_{22}	$\dots$	x_{2d}	y_2
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
Example N	x_{N1}	x_{N1}	$\dots$	x_{Nd}	y_N

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Matrix $X \in \mathbb{R}^{d \times N}$

Vector $\vec{y} \in \mathcal{Y}^N$

then in short $\mathcal{D} = (X, \vec{y})$

Recap: Problems (1)

Supervised Learning

- **Given** Set of labeled training examples / data $\mathcal{D} = \{(\vec{x}_1, y_1), \ldots, (\vec{x}_N, y_N) \mid (\vec{x}_i, y_i) \in \mathcal{X} \times \mathcal{Y}\}$
- **Find** A model $f : \mathcal{X} \to \mathcal{Y}$ so that $f(\vec{x}_i) \approx y_i$

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Note 1 If $|\mathcal{Y}| = 2$ its called binary classification
Note 2 If $\mathcal{Y} = \mathbb{R}$ its called regression
Example Classify songs into pop music vs. rap music

Recap: Problems (2)

Unsupervised Learning

- **Given** Set of un-labeled training data $\mathcal{D} = \{\vec{x}_1, \ldots, \vec{x}_N\}$
- **Find** A plausible model M that explains the data well

Example Put songs into similar groups to find new songs

Recap: Problems (2)

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Example Put songs into similar groups to find new songs

Semi-Supervised Learning

- **Given** Set of partially-labeled training data $\mathcal{D} = \{\vec{x}_1, \ldots, \vec{x}_m, (\vec{x}_{m+1}, y_{m+1}), \ldots, (\vec{x}_n, y_n)\}$
- **Find** A plausible model M that explains the data well with $M(\vec{x}_i) \approx y_i$ for known y_i

Example Put songs into similar groups knowing that some belong together / should never be in the same group

Recap: Problems (3)

Active Learning

- **Given** Set of partially-labeled training data $\mathcal{D} = \{\vec{x}_1, \ldots, \vec{x}_m, (\vec{x}_{m+1}, y_{m+1}), \ldots, (\vec{x}_n, y_n)\}$
- **Find** $\vec{x}_i \in \mathcal{D}$, so that we acquire the true y_i

Example For which songs should I hire an expert to classify them?

Recap: Problems (3)

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Example For which songs should I hire an expert to classify them?

Reinforcement Learning

- **Given** A set of actions A and a reward function r
- **Goal** Find series of actions, so that reward is maximized

Example Maximize time the user listens to music by proposing new/similar songs

Recap: Principles of Machine Learning

Occam's Razor Favor simple models before complex ones

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Bias-Variance trade-off For squared error

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Bias-Variance trade-off For squared error
Assume: $t = f(x) + \varepsilon$ with $\varepsilon \in \mathcal{N}(0, \sigma^2)$, then

$$\begin{aligned} \mathbb{E}_{x,t,\mathcal{D}}[(t - f_{\mathcal{D}}(x))^2] &= (f(x) - \mathbb{E}_{\mathcal{D}|x}[f_{\mathcal{D}}(x)])^2 + \mathbb{V}_{\mathcal{D}|x}[f_D(x)] + \mathbb{V}_{t|x}[\varepsilon] \\ &= (bias)^2 + variance + noise \end{aligned}$$

Extra: Measure Model quality

Question So, what is model quality?

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1. how well explains the model training data?
2. can we give any guarantees for new predictions?
3. how well generalizes the model to new and unseen data?

Extra: Measure Model quality (2)

Fact In binary classification we have two choices: predict 0 or 1
$\longrightarrow$ 2 possible wrong predictions and 2 possible correct predictions

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Visualization Confusion matrix

	Predicted value	
True value	True positive (TP)	False negative (FN)
	False positive (FP)	True negative (TN)

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Visualization Confusion matrix

	Predicted value	
True value	True positive (TP)	False negative (FN)
	False positive (FP)	True negative (TN)

Accuracy $Acc = \frac{TP+TN}{N}$

Big Remark The accuracy only tells us something about the data $\mathcal{D}$ we know! There are no guarantees for new data

Extra: Measure Model quality (3)

Obviously The best model has $Acc = 1$, the worst has $Acc = 0$
Observation If we store all the data for look-up, then $Acc = 1$

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Question Is that what we want?
Clear This is just memorizing the training data, no real learning!
Question How well deals our model with new, yet unseen data?

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Idea Split data into training $\mathcal{D}_{Train}$ and test data $\mathcal{D}_{Test}$
Then $\mathcal{D}_{Test}$ is new to the model f
Question How to split $\mathcal{D}$?

Extra: Measure Model quality (4)

1) Test/Train Split Split $\mathcal{D}$ by size, e.g. 80% training and 20% test data
$\rightarrow$ Fast and easy to compute, but sensitive for “bad” splits.
$\rightarrow$ Model quality might be over- or under-estimated

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$\rightarrow$ N models are computed, but insensitive for “bad” splits.
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3) K-fold cross validation Split data into k buckets. Use every bucket once for testing / train model on the rest. Average results.
$\rightarrow$ Insensitive for "bad" splits and practical. Usually $k \in \{5, 10\}$.

Extra: K nearest neighbor (K-NN) method

Goal Solve supervised problem

Thus We want a prediction method $\widehat{f}(\vec{x})$
Observation Examples $\vec{x}_i$ and $\vec{x}_j$ which are similar probably have the same label $y_i = y_j$

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Idea Given new and unseen observation $\vec{x}$

- use distance function $dist \colon \mathcal{X} \times \mathcal{X} \to \mathbb{R}$
- calculate $d(\vec{x}, \vec{x}_i)$ for all $i = 1, \ldots, N$
- find k nearest neighbors of $\vec{x}$ $S = \{(\vec{x}_1, y_1), \ldots, (\vec{x}_k, y_k)\}$
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Note If S has equal number of positive and negative examples, take a random class

Extra: K-NN (Some Notes)

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$$dist(\vec{x}_i, \vec{x}_j) = \sqrt{(\vec{x}_i - \vec{x}_j)^T \cdot (\vec{x}_i - \vec{x}_j)}$$
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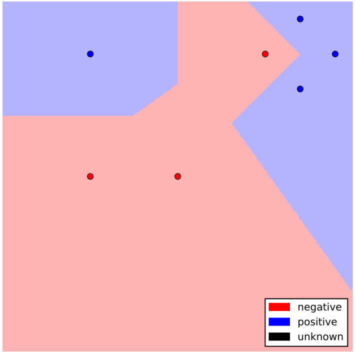
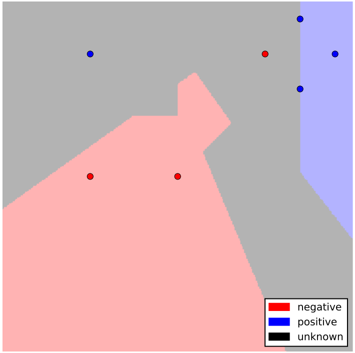
Note 2 K-NN can be used for regression as well. Just average the labels in S :

$$\widehat{f}(\vec{x}) = \frac{1}{k} \sum_{y \in S} y$$

Extra: K-NN Examples

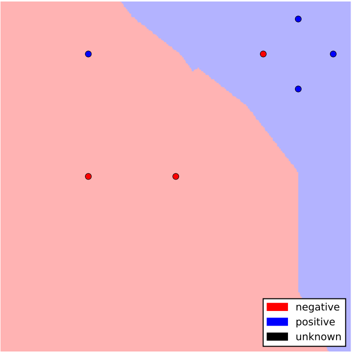


$k = 1$

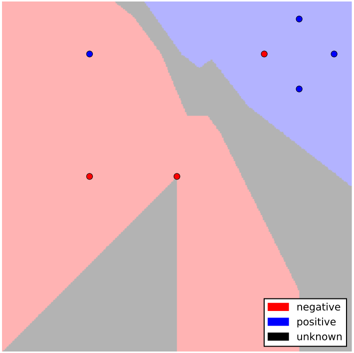


$k = 2$

Extra: K-NN More examples



$k = 3$



$k = 4$

Practical Data Science: Python

Data Scientist use `Python`

- Dynamically scripting language
- Usually interpreted
- Only syntax is checked before execution (fails late)
- Indentation is a part of syntax (e.g. tabs instead of '{')

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Why Python?

- **Fast** Important algorithm have fast C/GPU backends
- **Flexible** Easy to test and try new things
- **Extensible** There are a lot of packages

Practical Data Science: Packages

Important Packages

- `numpy` Contains linear algebra functions
- `scipy` Contains common functions for scientific computing
- `matplotlib` Produces nice plots
- `pandas` Reads and handles files efficiently

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Important tools

- `Python` I recommend version ≥ 3.5
- `pip/anaconda` Install/Manage new packages
- `IPython` (Enhanced) Interactive python shell
- `Jupyter` Browser notebook for 'story' driven programming
- `plotly` Interactive plots on the web

BUT Your editor and raw python is your best tool