*** Applied Machine Learning Fundamentals ***
k-Nearest Neighbors

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SAP SE / DHBW Mannheim

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Find all slides on GitHub (DaWe1992/Applied_ML_Fundamentals)

Lecture Overview

Unit I	Machine Learning Introduction
Unit II	Mathematical Foundations
Unit III	Bayesian Decision Theory
Unit IV	Regression
Unit V	**Classification I**
Unit VI	Evaluation
Unit VII	Classification II
Unit VIII	Clustering
Unit IX	Dimensionality Reduction

Agenda for this Unit

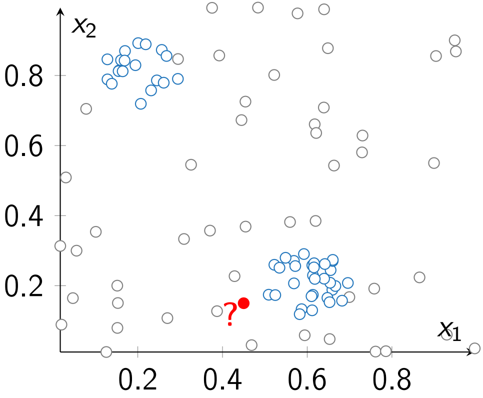
Section:

Introduction

Introduction

- **Basic idea:** Predict the class label based on nearby known examples
- Instance-based learning, a. k. a. lazy learning

We do not learn any model, the data speaks for itself!



Derivation of the Algorithm

- Unconditional density:

$$p(\mathbf{x}) = \frac{k}{n \cdot v}$$

- Class priors:

$$p(\mathcal{C}_j) = \frac{n_j}{n}$$

Combine them using Bayes' theorem:

$$p(\mathcal{C}_j|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_j) \cdot p(\mathcal{C}_j)}{p(\mathbf{x})} = \frac{\frac{k_j}{n_j \cdot v} \cdot \frac{n_j}{n}}{\frac{k}{n \cdot v}} = \frac{k_j}{k} \tag{1}$$

Section:

Distance Metrics

Properties of Distance Metrics
Minkowski, Manhattan, Euclidean
Cosine Similarity

Distance Metrics

- How to measure the distance between two data points u and v?
  $\Rightarrow$ **distance metrics**
- Let d be a function $d : (u, v) \mapsto \mathbb{R}^+$ (including 0)
- Function d has the following properties:

1. $d(u, v) = d(v, u)$ **(commutativity)**
2. $d(u, v) = 0 \Rightarrow u = v$
3. $d(u, k) \leqslant d(u, v) + d(v, k)$ **(triangle inequality)**

Distance Metrics (Ctd.)

Minkowski distance:

$$d_p(u, v) = \left(\sum_{j=1}^{m} |x_j^{(u)} - x_j^{(v)}|^p \right)^{1/p} \tag{2}$$

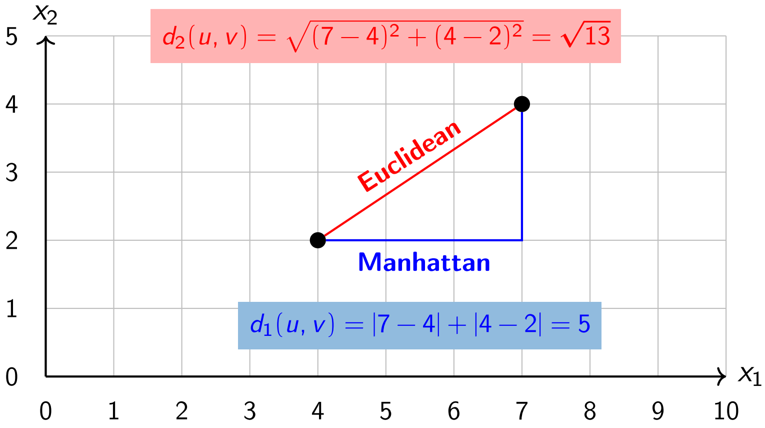
Manhattan distance: $(p = 1)$

$$d_1(u, v) = \sum_{j=1}^{m} |x_j^{(u)} - x_j^{(v)}|$$

Euclidean distance: $(p = 2)$

$$d_2(u, v) = \sqrt{\sum_{j=1}^{m} |x_j^{(u)} - x_j^{(v)}|^2}$$

Distance Metrics (Ctd.)



Cosine Similarity

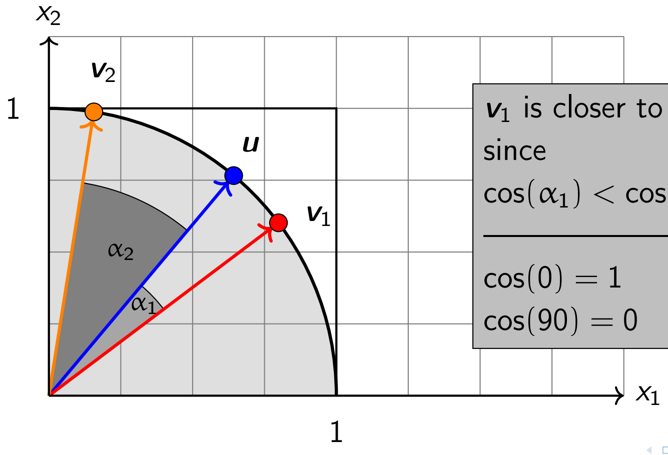
- **Similarity metrics** are an alternative to distance metrics
- **Example: Cosine similarity**
- The cosine similarity of two vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ is the cosine of the angle:

$$\cos \measuredangle(\boldsymbol{a}, \boldsymbol{b}) = \frac{\boldsymbol{a}^\intercal \boldsymbol{b}}{\|\boldsymbol{a}\| \cdot \|\boldsymbol{b}\|} = \frac{\sum_{j=1}^{m} a_j \cdot b_j}{\sqrt{\sum_{j=1}^{m} (a_j)^2} \cdot \sqrt{\sum_{j=1}^{m} (b_j)^2}} \tag{3}$$

- The dot product is defined as:

$$\boldsymbol{a}^\intercal \boldsymbol{b} = \|\boldsymbol{a}\| \cdot \|\boldsymbol{b}\| \cdot \cos \measuredangle(\boldsymbol{a}, \boldsymbol{b}) \tag{4}$$

Cosine Similarity (Ctd.)



$\boldsymbol{v}_1$ is closer to $\boldsymbol{u}$, since

$\cos(\alpha_1) < \cos(\alpha_2)$

$\cos(0) = 1$

$\cos(90) = 0$

Section:

k-nearest Neighbors Algorithm

Prediction with k-Nearest Neighbors (Ctd.)

k-nearest neighbors algorithm:

1. Calculate the distances between the new data point and **all data points in the data set**
2. Sort the data points by distances **in ascending order**
   (sort in descending order if similarity metrics are used)
3. Look at the first k examples and **count how often each class occurs**
4. Predict the class with **the maximum score**

❶ Calculation of Distances

v	x_1	x_2	$\mathcal{C}$	$d_2(u, v)$
1	0.66	0.24	1	0.23
2	0.25	0.79	1	0.67
3	0.16	0.81	1	0.73
4	0.57	0.21	1	0.13
5	0.21	0.72	1	0.62
6	0.66	0.27	1	0.24
7	0.27	0.11	0	0.19
8	0.39	0.13	0	0.07
9	0.39	0.86	0	0.71
10	0.44	0.67	0	0.52
11	0.31	0.33	0	0.23
12	0.03	0.51	0	0.55
⋮	⋮	⋮	⋮	⋮

- $\boldsymbol{x}^{(u)} = (0.45, 0.15)$
- Calculate the **Euclidean distance** between $\boldsymbol{x}^{(u)}$ and all other data points $\boldsymbol{x}^{(v)}$

Prediction is expensive!

❷/❸/❹ Prediction of the Class Label

- Let k be set to 10
- Step ❷: Sort data set by distances *(cf. table on the right)*
- Step ❸: Count class occurrences
  - **Class 0:** 3
  - **Class 1:** 7
- Step ❹: **Predict class 1!**

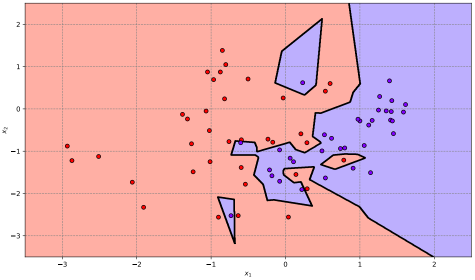
x_1	x_2	$\mathcal{C}$	$d_2(u, v)$
0.51	0.17	1	0.06
0.39	0.13	0	0.07
0.52	0.17	1	0.08
0.43	0.23	0	0.08
0.47	0.03	0	0.12
0.52	0.26	1	0.13
0.57	0.21	1	0.13
0.53	0.25	1	0.13
0.58	0.12	1	0.14
0.59	0.13	1	0.14
$\vdots$	$\vdots$	$\vdots$	$\vdots$

Section:
Choice of k

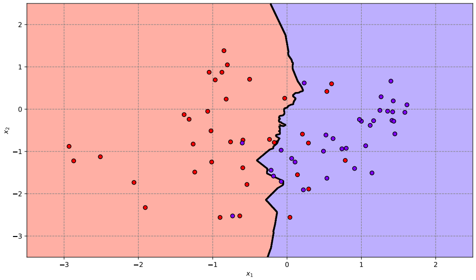
Danger of Overfitting
Selection Strategies

How to choose k?

The choice of k is important:



$k = 1$ (☠ overfitting ☠)



$k = 30$ (about right)

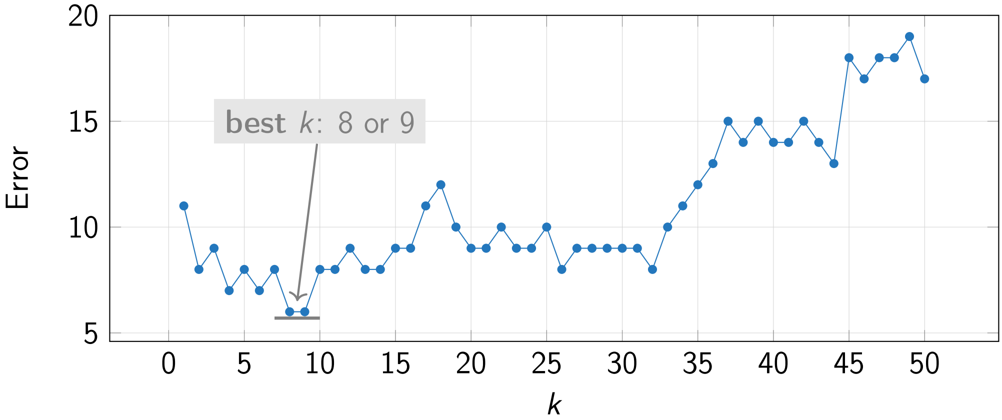
How to choose k? (Ctd.)

- First of all, it is recommended to use **odd values** for k *(no tie-breaking necessary)*
- Compute k depending on the size of the data set $\mathcal{D}$:

$$k = \sqrt{\frac{n}{2}} \qquad \text{or} \qquad k = \sqrt{n} \tag{5}$$

- **Other strategy:** Evaluate different k on a `dev` set and choose the best one

How to choose k? (Ctd.)



Section:

Wrap-Up

Summary
Self-Test Questions
Lecture Outlook

Summary

- The basic idea is to classify unknown instances **based on nearby examples**
- The algorithm is an example for **instance-based learning**
- **Distance metrics** allow to calculate the distance between data points:
  - Manhattan distance
  - Euclidean distance
  - Cosine similarity
- Choose the value of k wisely:
  - Too small: **Overfitting**
  - Too large: **Underfitting**

Self-Test Questions

1. Outline the k-nearest neighbors algorithm.
2. What is instance-based learning (in contrast to model-based learning)?
3. How can you compute distances? What properties do distance metrics have?
4. What is the intuition behind the triangle inequality?
5. How can you choose k?
6. Suppose you have a data set comprising $n = 50$ examples.
   If you set $k = n$, what class does the algorithm predict?
7. What are advantages and disadvantages of the algorithm?

What's next...?

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Thank you very much for the attention!

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Do you have any questions?