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

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SAP SE

Winter term 2019/2020

Find all slides on GitHub

Lecture Overview

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

Agenda for this Unit

Section:

Introduction

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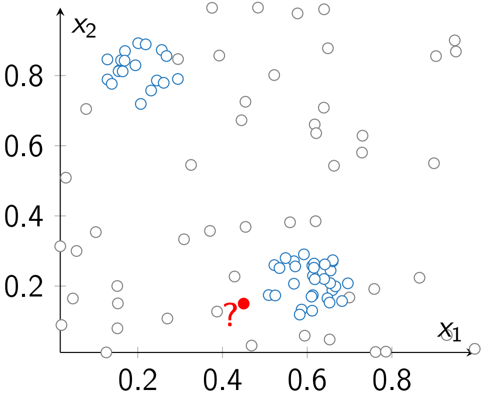
Introduction

- **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:

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

- Class priors:

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

Remember non-parametric density estimation?

Combine using Bayes' theorem:

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

Section:

Distance Metrics

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Distance Metrics

- How to measure the distance between two data points i and j?
  $\Rightarrow$ **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:

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

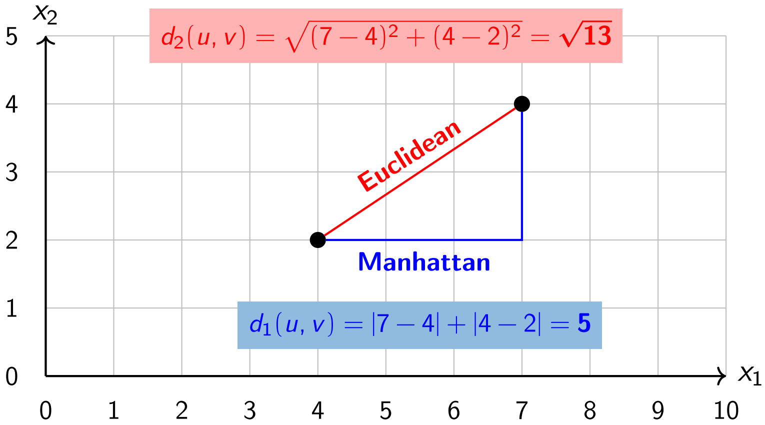
Manhattan distance: $(p = 1)$

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

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

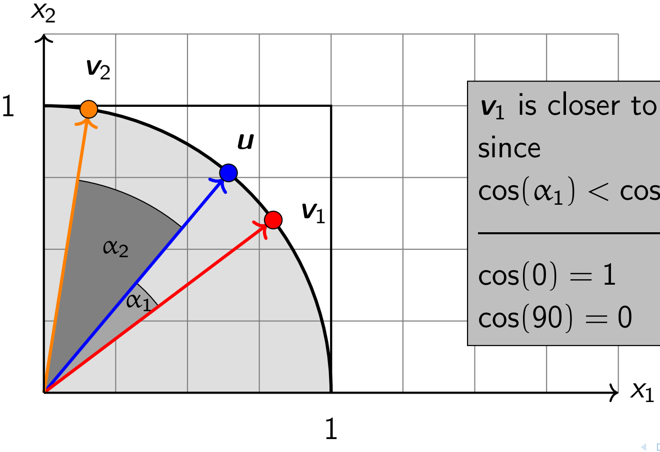
- Similarity metrics are an alternative to distance metrics
- **Example:** Cosine similarity
- The cosine similarity of two vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ is the cosine of the angle:

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

- The dot product is defined as:

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

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

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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**
   (if similarity metrics are used, sort in descending order)
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
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

- $\boldsymbol{x}^{(u)} = (0.45, 0.15)$
- 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 right)*
- Step ❸: Count the classes
  - **Class 0:** 3
  - **Class 1:** 7
- Step ❹: **Predict class 1!**

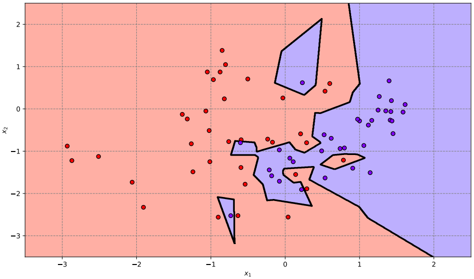
x_1	x_2	$\mathcal{C}$	$d_2(u, v)$
0.51	0.17	1	0.06
0.39	0.13	0	0.07
0.52	0.17	1	0.08
0.43	0.23	0	0.08
0.47	0.03	0	0.12
0.52	0.26	1	0.13
0.57	0.21	1	0.13
0.53	0.25	1	0.13
0.58	0.12	1	0.14
0.59	0.13	1	0.14
⋮	⋮	⋮	⋮

Section:

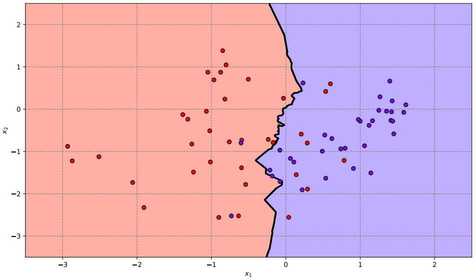
Choice of k

How to choose k?

The choice of k is important:



$k = 1$ (☠ overfitting ☠)



$k = 30$ (about right)

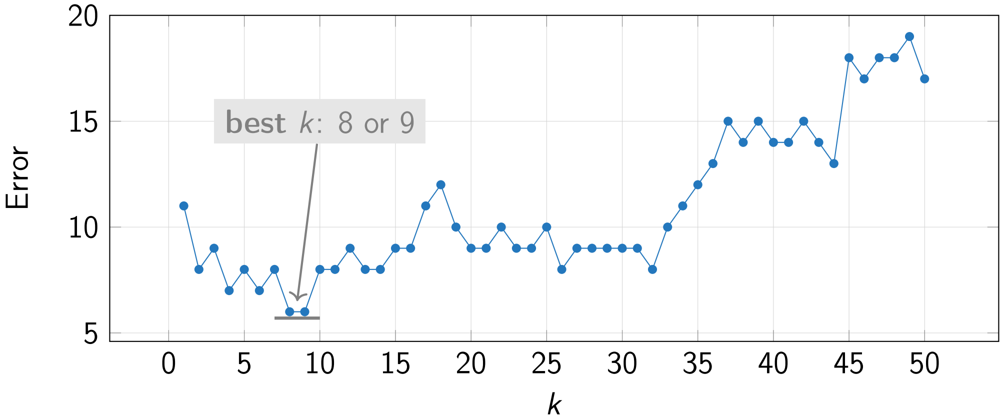
How to choose k? (Ctd.)

- 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

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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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Recommended Literature and further Reading

[1] Machine Learning

Tom Mitchell. McGraw-Hill Science. 1997.

→ Link, cf. chapter 8.2

Meme of the Day

Thank you very much for the attention!

Topic: *** Applied Machine Learning Fundamentals *** k-Nearest Neighbors
Term: Winter term 2019/2020

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Do you have any questions?