

*** 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	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

① Introduction

- Overview of the Algorithm
- Derivation of the Algorithm

② Distance Metrics

- Properties of Distance Metrics
- Minkowski, Manhattan, Euclidean
- Cosine Similarity

③ k -nearest Neighbors Algorithm

- General Procedure
- Calculation of Distances

Prediction of the Class Label

④ Choice of k

- Danger of Overfitting
- Selection Strategies

⑤ Wrap-Up

- Summary
- Self-Test Questions
- Lecture Outlook
- Recommended Literature and further Reading
- Meme of the Day

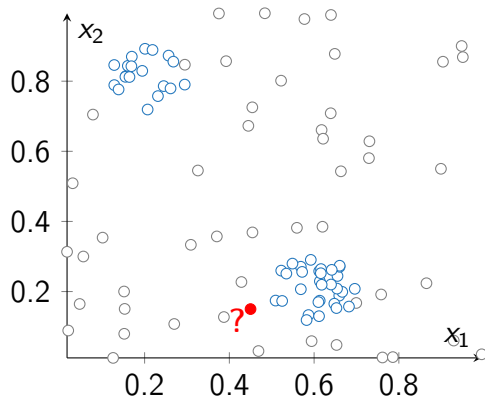
Section:
Introduction



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:

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

Remember non-parametric
density estimation?

Combine them using Bayes' theorem:

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

Section:
Distance Metrics



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 $d(u, k) \leq d(u, v) + d(v, k)$ (**triangle inequality**)

Distance Metrics (Ctd.)

Minkowski distance:

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

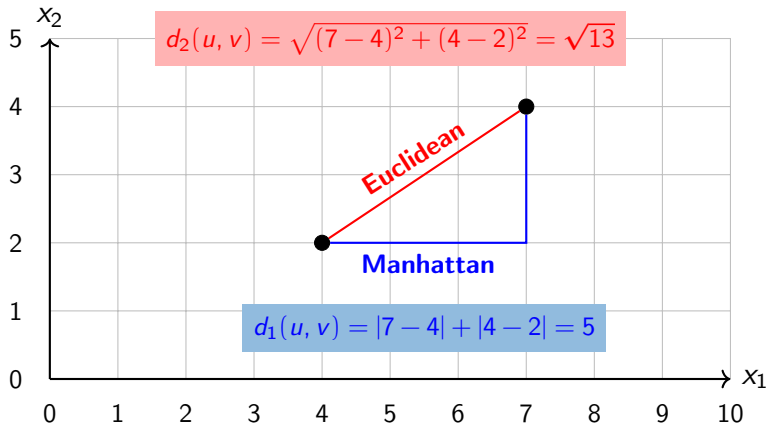
Manhattan distance: ($p = 1$)

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

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

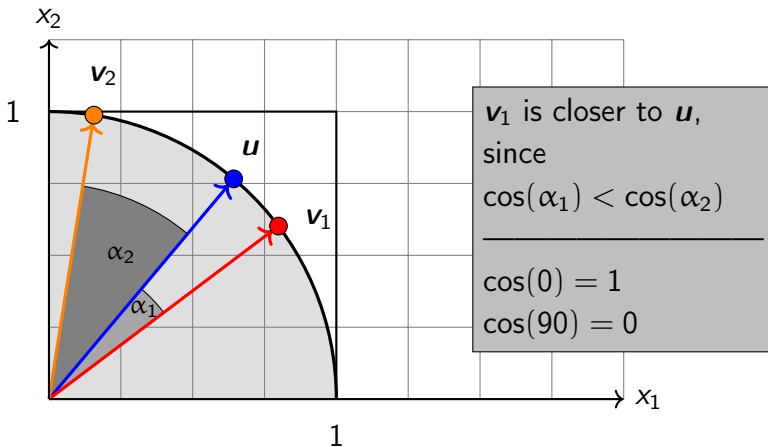
- **Similarity metrics** are an alternative to distance metrics
- **Example: Cosine similarity**
- The cosine similarity of two vectors \mathbf{a} and \mathbf{b} is the cosine of the angle:

$$\cos \angle(\mathbf{a}, \mathbf{b}) = \frac{\mathbf{a}^\top \mathbf{b}}{\|\mathbf{a}\| \cdot \|\mathbf{b}\|} = \frac{\sum_{j=1}^m a_j \cdot b_j}{\sqrt{\sum_{j=1}^m (a_j)^2} \cdot \sqrt{\sum_{j=1}^m (b_j)^2}} \quad (3)$$

- The dot product is defined as:

$$\mathbf{a}^\top \mathbf{b} = \|\mathbf{a}\| \cdot \|\mathbf{b}\| \cdot \cos \angle(\mathbf{a}, \mathbf{b}) \quad (4)$$

Cosine Similarity (Ctd.)



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**

① 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

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

Prediction is expensive!

②/③/④ Prediction of the Class Label

- Let k be set to 10
- Step ②: Sort data set by distances
(cf. table on the right)
- Step ③: Count class occurrences
 - Class 0: 3
 - Class 1: 7
- Step ④: Predict class 1!

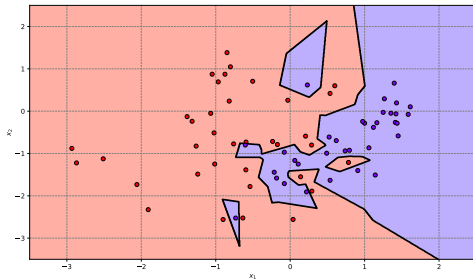
x_1	x_2	\mathcal{C}	$d_2(u, v)$
0.51	0.17	1	0.06
0.39	0.13	0	0.07
0.52	0.17	1	0.08
0.43	0.23	0	0.08
0.47	0.03	0	0.12
0.52	0.26	1	0.13
0.57	0.21	1	0.13
0.53	0.25	1	0.13
0.58	0.12	1	0.14
0.59	0.13	1	0.14
\vdots	\vdots	\vdots	\vdots

Section:
Choice of k

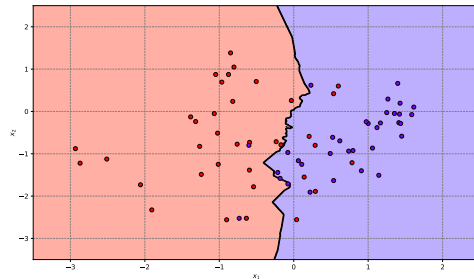


How to choose k ?

The choice of k is important:



$k = 1$ (💀 overfitting 💀)



$k = 30$ (about right)

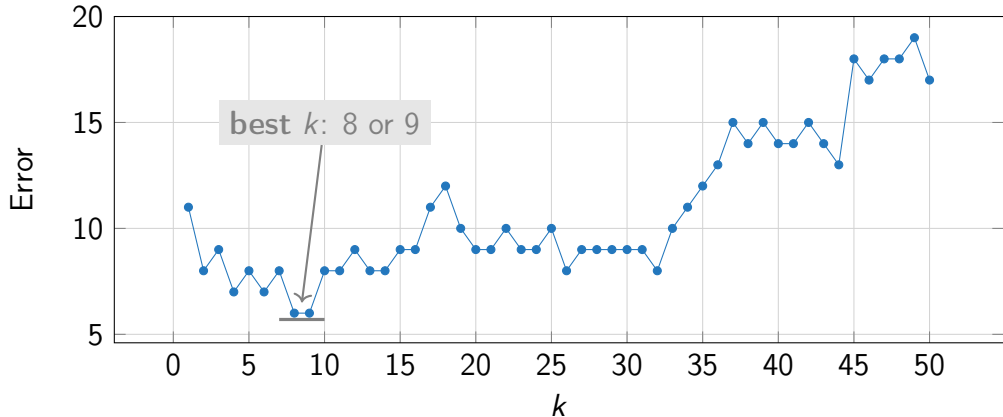
How to choose k ? (Ctd.)

- 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} :

$$k = \sqrt{\frac{n}{2}} \quad \text{or} \quad k = \sqrt{n} \quad (5)$$

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

How to choose k ? (Ctd.)



Section:
Wrap-Up



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 I



[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 2022/2023

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Do you have any questions?