*** Applied Machine Learning Fundamentals *** Clustering

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SAP SE

Winter term 2019/2020

Find all slides on GitHub

Lecture Overview

Agenda for this Unit

Section:

Introduction

Duale Hochschule
Baden-Württemberg

k-Means: Introduction

- k-Means is a clustering algorithm and as such **unsupervised**
- A clustering algorithm tries to **find structure** in the data
- k defines the number of clusters to be found
- Once the clusters are found, they first have to be interpreted...
- ...and can then be used for prediction purposes

A cluster must be **internally homogeneous**, but simultaneously **externally heterogeneous**. (Elements of one cluster have to be very similar, but must differ significantly from elements in other clusters.)

k-Means: Example Use Cases

- **Behavioral segmentation**
  - Customer segmentation (e. g. **sinus milieus**)
  - Creating profiles based on activity monitoring
- **Sorting sensor measurements**
  - Image grouping
  - Detection of activity types in motion sensors
- **Inventory categorization**
  - Grouping inventory by sales activity
  - Grouping inventory by manufacturing metrics
- Many, many more, ...

k-Means: Procedure

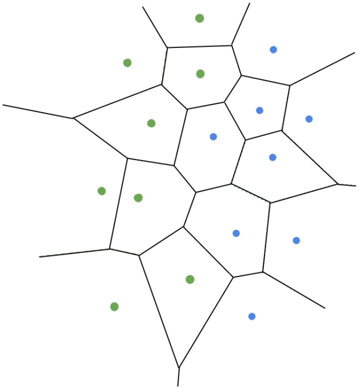
- **Vector quantization**
  - Represent data points by a single vector (here: called **centroid**) which is close to them
  - This is useful for **compression**!
- **How to**: Create k partitions ($\widehat{=}$ clusters) of the data set $\mathcal{D}$, such that the sum of squared deviations from the cluster centroids is **minimal**:

$$\min_{\boldsymbol{\mu}_j} \sum_{j=1}^{k} \sum_{\boldsymbol{x}^{(i)} \in \mathcal{D}_j} \left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}_j \right\|^2 \tag{1}$$

- With $\mathcal{D}_j \equiv j^{th}$ cluster, $\mu_j \equiv$ centroid of j^{th} cluster

Result: Voronoi Diagram

- The dots represent cluster centroids
- The lines visualize the **cluster boundaries**
- For a new point we can easily determine to which cluster it has to be assigned



k-Means Algorithm

- Input: $\mathcal{D} = \{\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \dots, \boldsymbol{x}^{(n)}\} \in \mathbb{R}^{n \times m}$, Number of clusters k
- Algorithm:
  1. $t \longleftarrow 1$
  2. Randomly choose k means $\boldsymbol{\mu}_1^{\langle 1 \rangle}, \boldsymbol{\mu}_2^{\langle 1 \rangle}, \dots, \boldsymbol{\mu}_k^{\langle 1 \rangle}$
  3. While not converged:

     3a Assign each $\boldsymbol{x}^{(i)} \in \mathcal{D}$ to the closest cluster:

     $$\mathcal{D}_j^{\langle t \rangle} = \left\{ \boldsymbol{x}^{(i)} : \|\boldsymbol{x}^{(i)} - \boldsymbol{\mu}_j^{\langle t \rangle}\|^2 \leqslant \|\boldsymbol{x}^{(i)} - \boldsymbol{\mu}_{j^*}^{\langle t \rangle}\|^2;\ \forall j^* = 1, 2, \dots, k; \boldsymbol{x}^{(i)} \in \mathcal{D} \right\}$$

     3b Update cluster centroids $\boldsymbol{\mu}_j$:

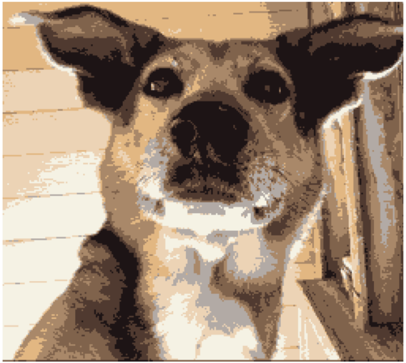
     $$\boldsymbol{\mu}_j^{\langle t+1 \rangle} = \frac{1}{|\mathcal{D}_i^{\langle t \rangle}|} \sum_{\boldsymbol{x}^{(i)} \in \mathcal{D}_j^{\langle t \rangle}} \boldsymbol{x}^{(i)}$$

     3c $t \longleftarrow t + 1$

Image Compression

Original image

Compressed image



Section:

Wrap-Up

Summary

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Self-Test Questions

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What's next...?

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**

Recommended Literature and further Reading

Thank you very much for the attention!

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Do you have any questions?