*** Applied Machine Learning Fundamentals *** Clustering

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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
   - What is Clustering?
   - Clustering Strategies Overview
2. k-Means
   - Introduction
   - k-Means Algorithm
   - Use Case: Image Compression
   - Problems and Issues
3. Hierarchical Clustering
   - Agglomerative Clustering Algorithm
   - Agglomerative Clustering: Example
   - Distance Metrics between Clusters
4. Spectral Clustering
   - Motivation
   - A Bit of Graph Theory
   - Spectral Clustering Algorithm
5. Wrap-Up
   - Summary
   - Self-Test Questions
   - Lecture Outlook
   - Recommended Literature and further Reading
   - Meme of the Day

Section:

Introduction

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Clustering Introduction

- Clustering belongs to the category of **unsupervised learning**
- A clustering algorithm tries to **find structure** in the data
- Once the clusters are found, they first have to be interpreted...
- ...and can then be used for prediction purposes

A cluster should be **internally homogeneous**, but simultaneously **externally heterogeneous**. (Elements of one cluster should be similar to each other, but should differ significantly from elements belonging to other clusters.)

Example Use Cases for Clustering

- **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, ...

Clustering Strategies

1. **EM-based clustering**, e. g.: k-Means
2. **Hierarchical clustering**, e. g.:
   - Agglomerative clustering
   - Divisive clustering
3. **Affinity-based clustering**, e. g.:
   - Spectral clustering
   - DBSCAN

Section:

k-Means

Important

k-Means: Procedure

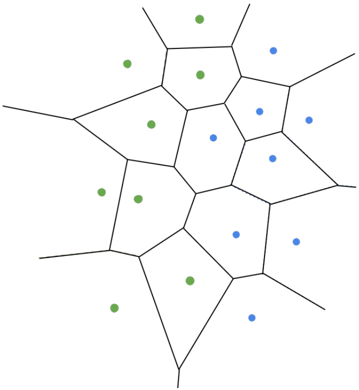
- The algorithm is an instance of vector quantization
  - It represents data points by a single vector (centroid) which is close to them
  - This is useful for **data compression**!
- **How to**: Create k partitions ($\hat{=}$ clusters) of the data set $\mathcal{D}$, such that the sum of squared deviations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

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

- Where $\mathcal{D}_j \equiv j$-th cluster, $\boldsymbol{\mu}_j \equiv$ 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: $\mathcal{D} = \{\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \ldots, \boldsymbol{x}^{(n)}\} \in \mathbb{R}^{n \times m}$, number of clusters k
- Algorithm:
  1. $t \longleftarrow 1$
  2. Randomly choose k means $\boldsymbol{\mu}_1^{\langle 1 \rangle}, \boldsymbol{\mu}_2^{\langle 1 \rangle}, \ldots, \boldsymbol{\mu}_k^{\langle 1 \rangle}$
  3. While not converged:

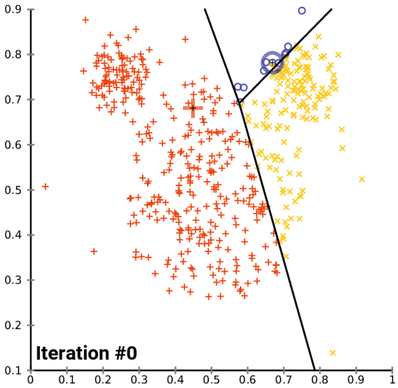
     3a Assign each $\boldsymbol{x}^{(i)} \in \mathcal{D}$ to the closest cluster:

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

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

$$\boldsymbol{\mu}_j^{\langle t+1 \rangle} = \frac{1}{|\mathcal{D}_j^{\langle t \rangle}|} \sum_{\boldsymbol{x}^{(i)} \in \mathcal{D}_j^{\langle t \rangle}} \boldsymbol{x}^{(i)} \qquad \text{then update } t\text{:} \quad t \longleftarrow t + 1$$

k-Means Algorithm (Ctd.)

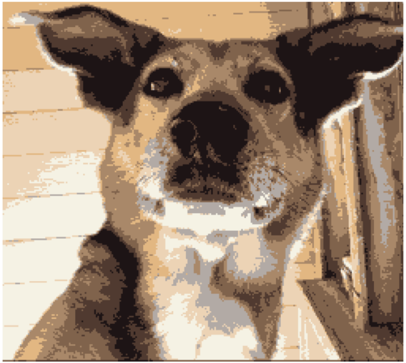


- The algorithm might need some iterations until the result is satisfactory
- **Caveat:** The algorithm might get stuck in local optima
  $\Rightarrow$ several restarts

Image Compression

Original image

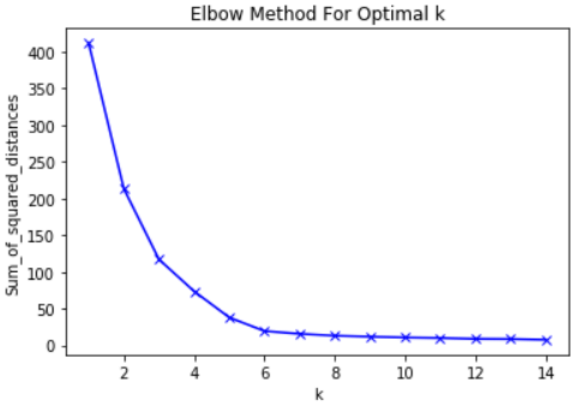
Compressed image



k-Means Issues

- The algorithm assumes that all clusters are **spherical** ($\neq$ affinity-based clustering)
- It does not have a notion of **outliers** (unlike DBSCAN)
- What is the correct value for k? $\Rightarrow$ Elbow-method:
  - Measure sum of squared distances from data points to cluster centers (inertia)
  - Record results for different values for k and plot them
  - Search for the 'elbow point'

Elbow Method



Section:

Hierarchical Clustering

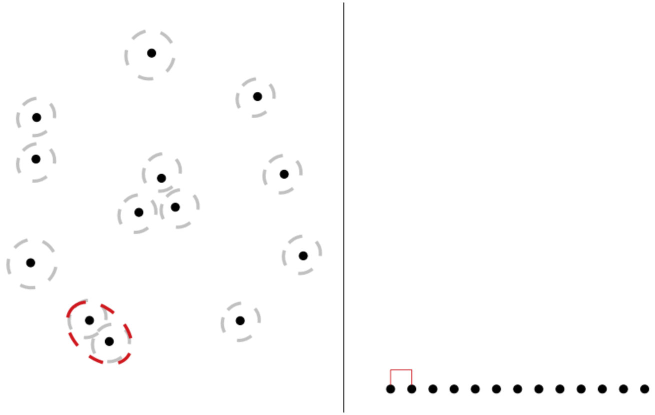
Agglomerative Clustering Algorithm

1. Start with one cluster for each instance: $C = \{\{\boldsymbol{x}^{(i)}\} : \boldsymbol{x}^{(i)} \in \mathcal{D}\}$
2. Compute distance $d(C_i, C_j)$ between all pairs of clusters C_i, C_j
3. Join clusters C_i and C_j with minimum distance into a new cluster C_p:

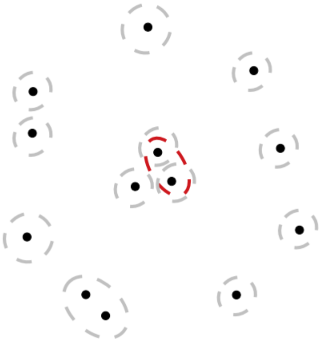
$$\begin{aligned} C_p &= \{C_i, C_j\} \\ C &= (C \setminus \{C_i, C_j\}) \cup \{C_p\} \end{aligned}$$

4. Compute distances between C_p and all other clusters in C
5. If $|C| > 1$, goto 3

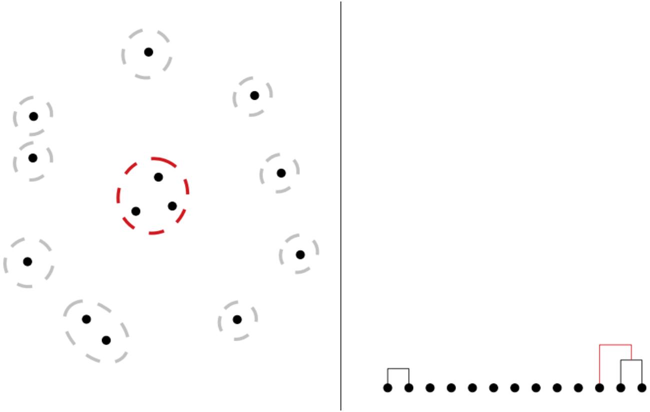
Agglomerative Clustering: Example



Agglomerative Clustering: Example (Ctd.)



Agglomerative Clustering: Example (Ctd.)



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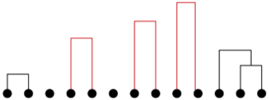

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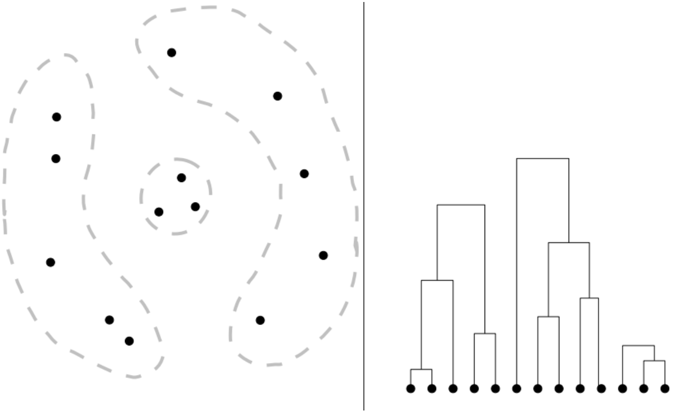

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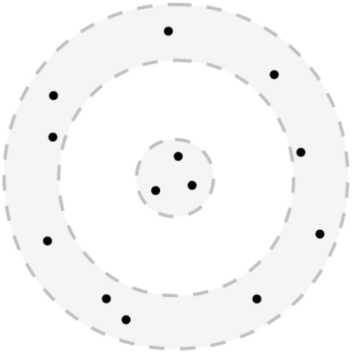
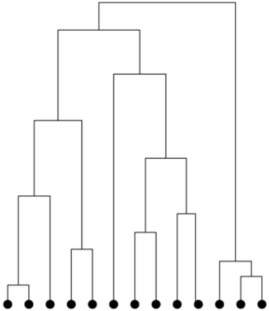


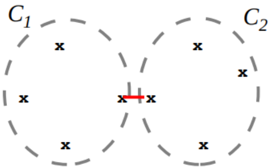


This is a **dendrogram**

Single Linkage

- How to compute the distance between two clusters C_1 and C_2?
- **Single linkage**:

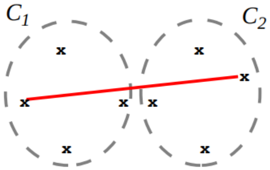
$$d(C_1, C_2) = \min\{d(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) : \mathbf{x}^{(i)} \in C_1, \mathbf{x}^{(j)} \in C_2\}$$



Complete Linkage

- How to compute the distance between two clusters C_1 and C_2?
- **Complete linkage**:

$$d(C_1, C_2) = \max\{d(\boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)}) : \boldsymbol{x}^{(i)} \in C_1, \boldsymbol{x}^{(j)} \in C_2\}$$



Section:

Spectral Clustering

Spectral Clustering

- Remember the disadvantage of k-Means? (spherical clusters)
- How can we cluster data without this assumption?

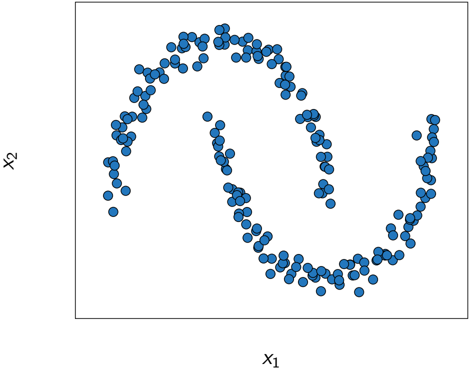
$\Rightarrow$ **Affinity-based clustering**

> **Affinity-based clustering** assumes **no shape** of the resulting clusters. It is based on the **connectedness of the data points**.

- Spectral clustering is affinity-based
- Whenever you hear *'spectral'*: It has something to do with eigen-vectors

Example Data Set

What would be the result of k-Means?



A short Introduction to Graphs

- A graph $\mathcal{G}$ is a tuple $\mathcal{G} = (\mathcal{V}, \mathcal{E})$
- $\mathcal{V} = \{v_1, v_2, \dots, v_n\}$ is the set of n vertices (nodes)
- $\mathcal{E} \in \mathcal{V} \times \mathcal{V}$ the set of edges (connections between nodes)
- **Adjacency matrix $\boldsymbol{A}$**
  - $A_{ij} = 1$, iff $(v_i, v_j) \in \mathcal{E}$ (v_i is a neighbor of v_j)
  - $\boldsymbol{A}$ is symmetric for undirected graphs, i. e. $A_{ij} = A_{ji}$
- The **degree matrix** $\boldsymbol{D} = diag(d_1, d_2, \dots, d_n)$ is a matrix of node degrees

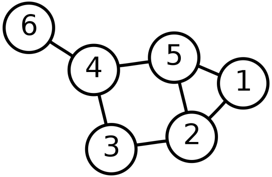
$$d_i = \sum_{j=1}^{n} A_{ij}$$

A short Introduction to Graphs (Ctd.)

- For graph analysis it is often useful to compute the **graph Laplacian** matrix:

$$\boldsymbol{L} = \boldsymbol{D} - \boldsymbol{A}$$

- Example:



Example: Computation of $\boldsymbol{A}$, $\boldsymbol{D}$ and $\boldsymbol{L}$

$$\boldsymbol{A} = \begin{bmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix} \qquad \boldsymbol{D} = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \qquad \boldsymbol{L} = \begin{bmatrix} 2 & -1 & 0 & 0 & -1 & 0 \\ -1 & 3 & -1 & 0 & -1 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ -1 & -1 & 0 & -1 & 3 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{bmatrix}$$

How to get the Graph for the Data Set?

- There are at least two possibilities:
  1. **ε-neighborhood graph**
     - Connect all instances whose pairwise distances are smaller than ε
     - **Problem:** How to choose ε?
  2. **k-nearest neighbor graph**
     - Connect instance $\boldsymbol{x}^{(i)}$ with instance $\boldsymbol{x}^{(j)}$, if $\boldsymbol{x}^{(j)}$ is among the k nearest neighbors of $\boldsymbol{x}^{(i)}$
     - Attention: This definition leads to a directed graph **(Why?)**
       $\Rightarrow$ Can be ignored
     - **Problem:** How to choose k?
- Both approaches are used in practice

Spectral Clustering Algorithm

- Input: $\mathcal{D} = \{\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \ldots, \boldsymbol{x}^{(n)}\} \in \mathbb{R}^{n \times m}$, number of clusters k
- Algorithm:
  1. Construct a similarity graph (adjacency matrix $\boldsymbol{A}$ and degree matrix $\boldsymbol{D}$)
  2. Compute the graph Laplacian matrix $\boldsymbol{L} = \boldsymbol{D} - \boldsymbol{A}$
  3. Perform **eigen-decomposition** on $\boldsymbol{L}$ (to obtain the eigen-vectors $\boldsymbol{Q}$)

$$\boldsymbol{L} = \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^{-1}$$

  4. Apply k-Means to the rows of matrix $\boldsymbol{Q}$ to obtain the clusters $\{C_1, C_2, \ldots, C_k\}$

Section:

Wrap-Up

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Summary

- Clustering belongs to the category of **unsupervised learning**
- With clustering we try to find **structure in the data**
- Different algorithms make **different assumptions** about the resulting clusters
- **Clustering Strategies:**
  - EM-based clustering (e. g. k-Means)
  - Hierarchical clustering
  - Affinity-based clustering (e. g. spectral clustering, DBSCAN)

Self-Test Questions

1. What is clustering?
2. What is the definition of a cluster. Which properties should it have?
3. Describe the general procedure of k-Means. What are disadvantages?
4. What is a dendrogram?
5. How do we obtain the graphs for spectral clustering?
6. What is affinity-based clustering? How does it differ from k-Means?
7. How to calculate the graph Laplacian matrix?

What's next...?

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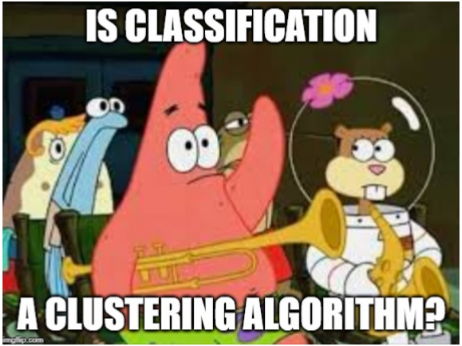
Unit IX	Clustering
Unit X	**Dimensionality Reduction**

Recommended Literature and further Reading I

- **[1] Pattern Recognition and Machine Learning**
  Christopher Bishop. Springer. 2006.
  → Link, cf. chapter 9

- **[2] Machine Learning: A Probabilistic Perspective**
  Kevin Murphy. MIT Press. 2012.
  → Link, cf. chapter 25

Meme of the Day



Thank you very much for the attention!

Topic: *** Applied Machine Learning Fundamentals *** Clustering
Term: Winter term 2021/2022

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Do you have any questions?