Machine Learning, Artificial Intelligence, and Big Data Analytics (IL, 4th Semester)

Lecture 8

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Where we are (Supervised learning)

- Regression and Classification, generalization error, data splitting, Bootstrapping, Bagging/Boosting, model validation, …
- K-Nearest Neighbors
- Support Vector Machines
- Decision Trees
- Random Forest
- Adaboost
- XGBoost

Coming next (Unsupervised learning)

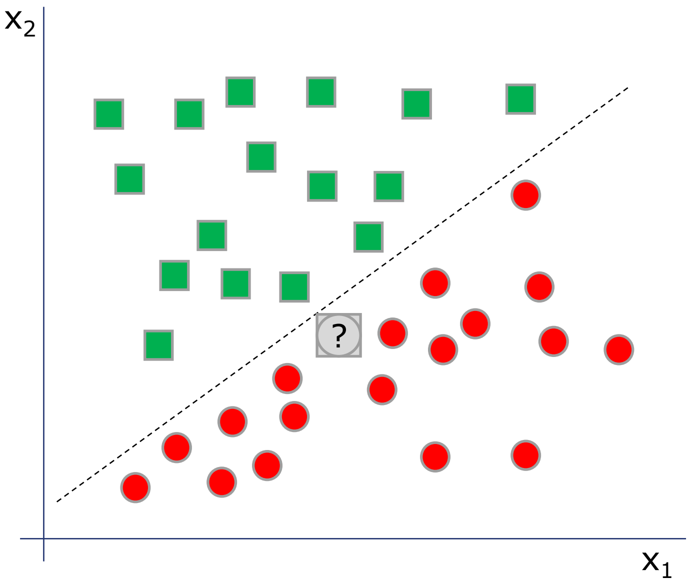
- Introduction to unsupervised learning
- **Clustering** objective
- Partitioning methods
  - K-means
  - Partitioning Around Medoids (PAM)
- Hierarchical methods
  - Agglomerative (AGNES)
  - Divisive (DIANA)
- Density-based methods
  - DBscan and OPTICS

Agenda

- Introduction to unsupervised learning
- Clustering
- Types of Clustering
- K-means algorithm
- K-means variants
- Validating clustering

Supervised learning

Training data is labeled (e.g., green square vs. red circle)

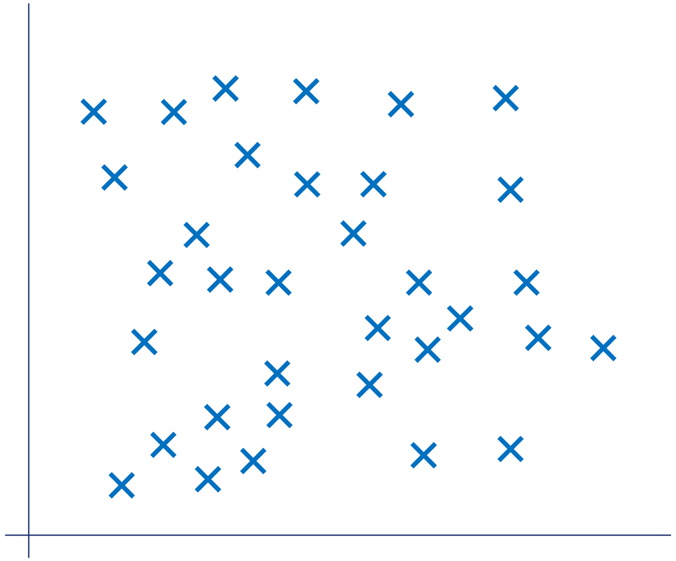


Training set: $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \cdots, (x^{(m)}, y^{(m)})\}$

GOAL: learn $f(x) \rightarrow y$

Unsupervised learning

Training data is not labeled



Training set: $\{x^{(1)}, x^{(2)}, x^{(3)}, \cdots, x^{(m)}\}$

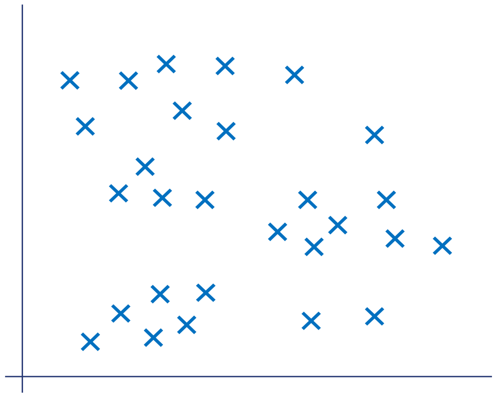
GOAL: find interesting things in data

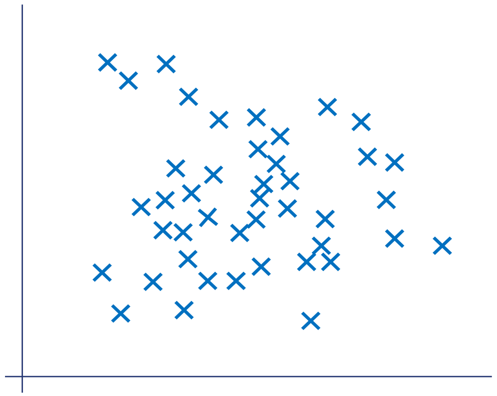
Examples of unsupervised learning techniques

- Clustering
- Dimensionality reduction
- Anomaly detection
- Association rules mining
- Pattern recognition

Clustering

- Cluster analysis: Given a set of data objects find the proper grouping such that
  - Points in the same groups are similar to each other
  - Points in one group differ from points in other groups
- In other words: Finding natural groupings among objects in a dataset





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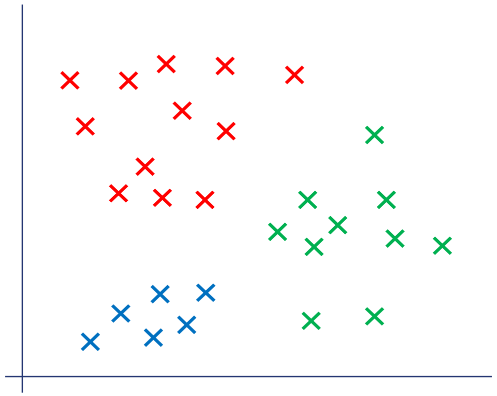
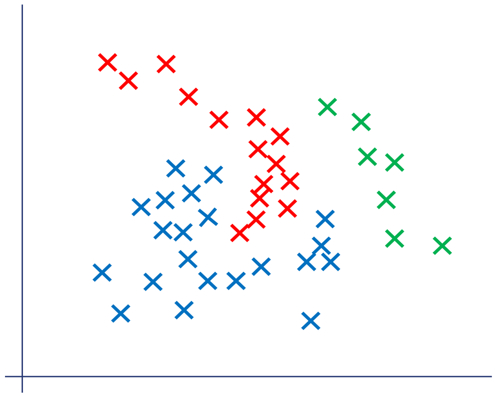
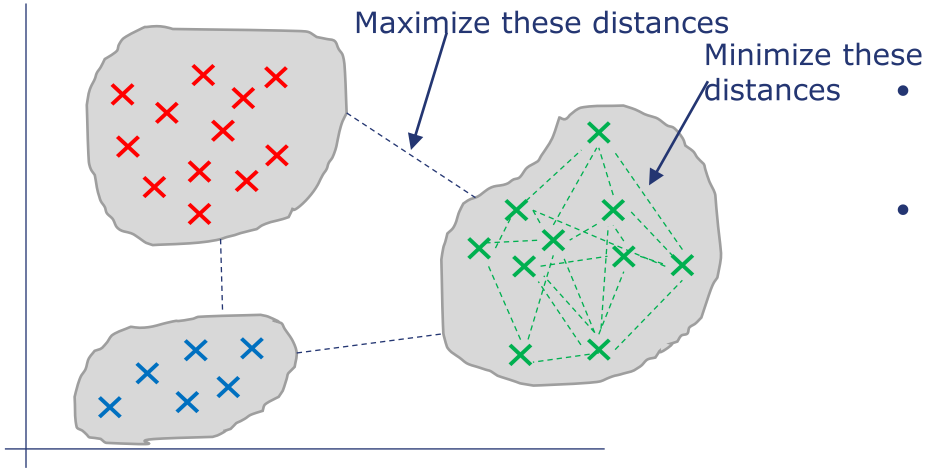




Clustering

- Optimal clusters should
  - Maximize similarity within clusters (intra-cluster): *cohesive* within clusters
  - Minimize similarity between clusters (inter-cluster): *distinctive* between cluster



- dissimilarity is expressed in terms of a distance function, typically metric: $d(i, j)$
- The definitions of distance functions are usually rather different for interval-scaled, boolean, categorical, ordinal ratio, and vector variables

Example of clustering

- Biology: Taxonomy of living things: kingdom, phylum, class, order, family, genus and species
- Behavioral: Understanding behavior of the masses
- Information retrieval: Document clustering
- Marketing: Discover distinct groups in their customer bases (customer segments), and use this knowledge to develop targeted marketing programs
- Climate: Understanding earth climate, find patterns
- Mobility: Understanding mobility patterns
- …

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The clustering process

1. Formulate the problem
   - Given a set of <…>, I want to find <…>, based on <…>
2. Select a distance/(dis)similarity measure
   - Euclidean, Manhattan, Cosine, Jaccard, …
3. Select a clustering technique
   - K-means, PAM, Diana, DBScan, …
4. Decide on the number of clusters
5. Interpret the clusters
6. Assess the clustering

- Using Silhouette, Elbow, Dendograms, …

Types of clustering techniques

Types of algorithms

- **Partitional algorithms:**
  - Construct various partitions and then evaluate them by some criterion.
  - Typical methods: k-means, k-medoids/PAM.
- **Hierarchical algorithms:**
  - Create a hierarchical decomposition of the set of objects using some criterion.
  - Typical methods: Diana, Agnes.
- **Density-based algorithms:**
  - Based on Connectivity and density functions
  - Typical methods: DBscan, OPTICS.
- …

Types of clustering techniques

Hard vs. Soft Clustering

- **Hard clustering**
  - Each sample belongs to exactly one cluster
  - For example: An *animal* belong to a *species*

- **Soft clustering**
  - A sample can belong to more than one cluster (probabilistic)
  - For example: *Glasses* belong to *medical aid* and to *fashion item*

Partitioning algorithms

- Partitioning method: Partitioning a database ***D*** of ***n*** objects into a set of ***k*** clusters, such that the sum of intra-cluster squared distances is minimized
- Given *k*, find a partition of *k clusters* that optimizes the chosen partitioning criterion
  - Global optimal: exhaustively enumerate all partitions
  - Heuristic methods: *k-means* and *k-medoids* algorithms
    - *k-means*: Each cluster is represented by the center of the cluster
    - *k-medoids* or PAM (Partition around medoids): Each cluster is represented by one of the objects in the cluster

K-Means algorithm

- Input:
  - K (number of clusters)
  - Training set $\{x^{(1)}, x^{(2)}, x^{(3)}, \cdots, x^{(m)}\}$
- Algorithm
  - Randomly initialize K cluster centroids $\mu_1, \mu_2, \cdots, \mu_K \in \mathbb{R}^n$
  - Repeat{

for $i = 1$ to m

$c^{(i)} :=$ index (from 1 to K) of cluster centroid closest to $x^{(i)}$

Cluster assignment step

for $k = 1$ to K

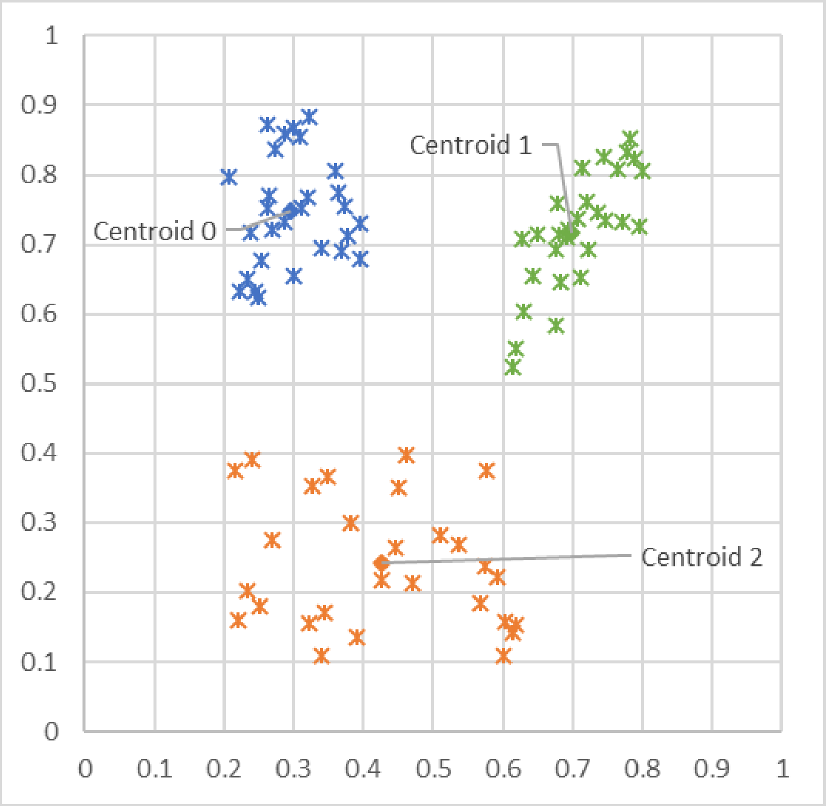
$\mu_k :=$ average (mean) of points assigned to cluster k

Centroid update step

}

K-Means visual example

- Unlabeled Data
- Initialize centroids to random data point locations
- Each point assigned to nearest centroid
- Update centroid locations to avg of assigned points



- Each point assigned to nearest centroid
- Update centroid locations to avg of assigned points
- Each point assigned to nearest centroid
- Converge!

K-Means - How to choose K

- Pick a K based on your understanding of the domain
- Run K-Means
- Examine samples from each cluster
- Adapt K based on what you find
  - If single clusters contain different entities, increase K
  - If entities spread across clusters, decrease K
- OR
- Try multiple values of K and pick the K that maximizes a specified metric

K-Means considerations

- The objective of k-means is to minimize the total sum of the squared distance of every point to its corresponding cluster centroid.
- Finding the global optimum is NP-hard.
- The k-means algorithm converges to a **<u>local</u>** optimum.
- Results can vary based on random seed selection.
- Some seeds can result in poor convergence rate, or convergence to sub-optimal clusterings.

K-Means weaknesses

- Sensitive to outliers
- Needs an initial guess on the number of clusters
- Results depend on the initial seeds
- Can be applied only to objects in a continuous n-dimensional space

Variants of K-means

- Many variants, usually differ by
  - Selection of the initial K
  - Initialization
  - Dissimilarity calculation
- Popular variants
  - K-medians:
    - Cluster center is the median
  - K-medoid:
    - Cluster center is an actual datapoint (not same as k-medians)
- Algorithms are similar to k-means

Evaluating the quality of clustering

- Two type of measures: intrinsic and extrinsic

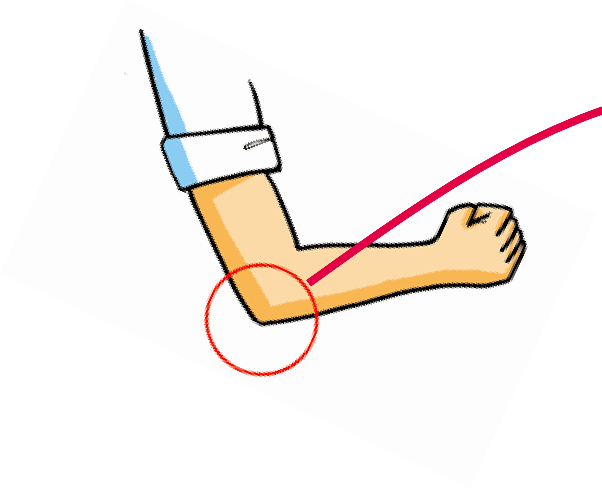
- Intrinsic: unsupervised, i.e., the ground truth is unavailable
    - Evaluate the goodness of a clustering by considering how well the clusters are separated, and how compact the clusters are (e.g., intracluster similarity, intercluster dissimilarity, the Silhouette coefficient)

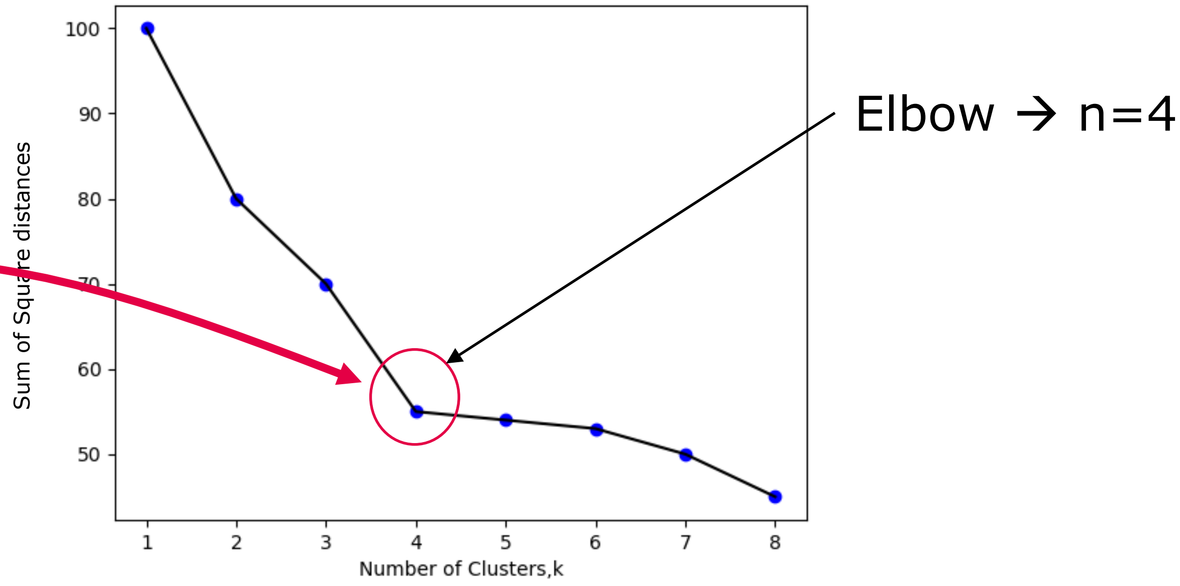
- Extrinsic: supervised, i.e., the ground truth is available for at least a subset of data
    - Compare a clustering against the ground truth using certain clustering quality measure

Evaluating the quality of clustering

The "Elbow method"

- SSE (or WSS): Sum of Squared Distances between data points and their assigned cluster's centroid





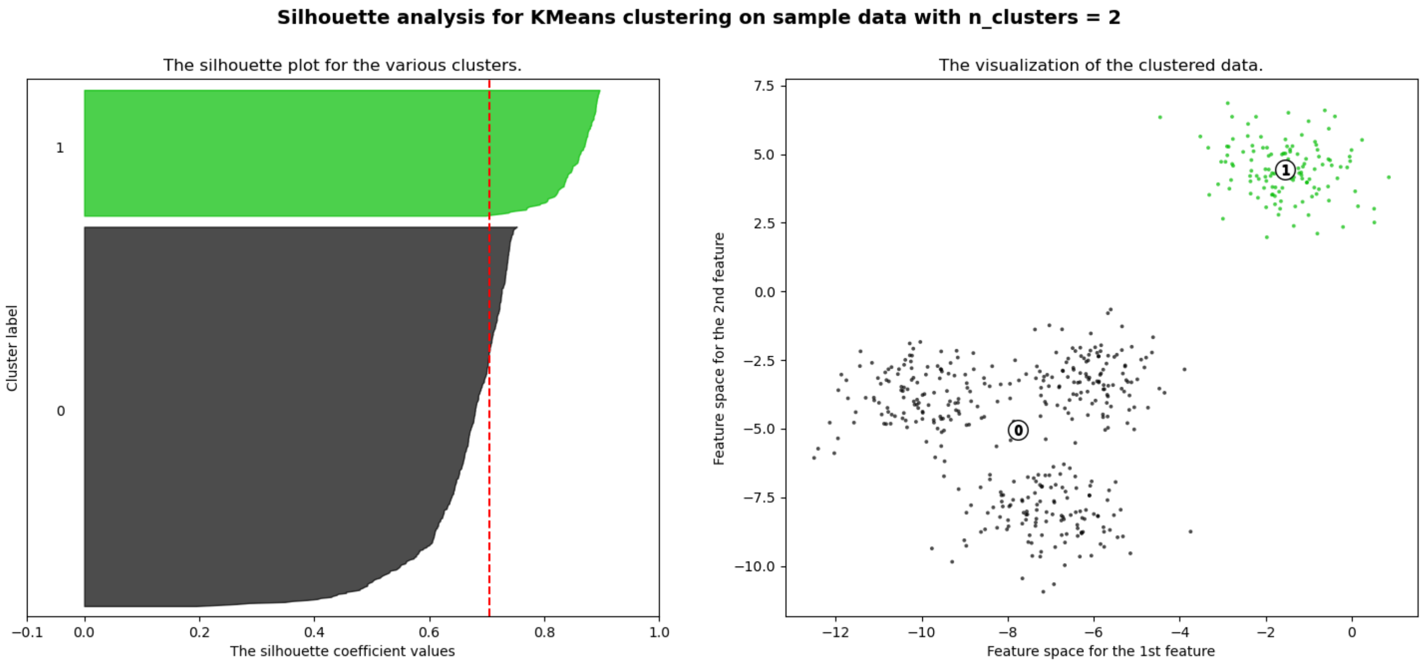
Evaluating the quality of clustering

The silhouette method

- Silhouette of one observation: $s(i) = \frac{b(i)-a(i)}{\max\{a(i),b(i)\}}$
- Where
  - *a(i) = average distance between i and all points in the same cluster*
  - *b(i) = average distance between i and all points in the closest different cluster*
- Interpretation:
  - *s(i) = 1* → observation fits well in its cluster and is far from other clusters
  - *s(i) = 0* → observation is as close to its cluster as to the neighbor cluster
  - *s(i) = -1* → observation is closer to the neighbor cluster than to its own
- Silhouette Score
  - SS=*mean{s(i)}* is a generic measure of cluster cohesiveness and distinction.

Evaluating the quality of clustering

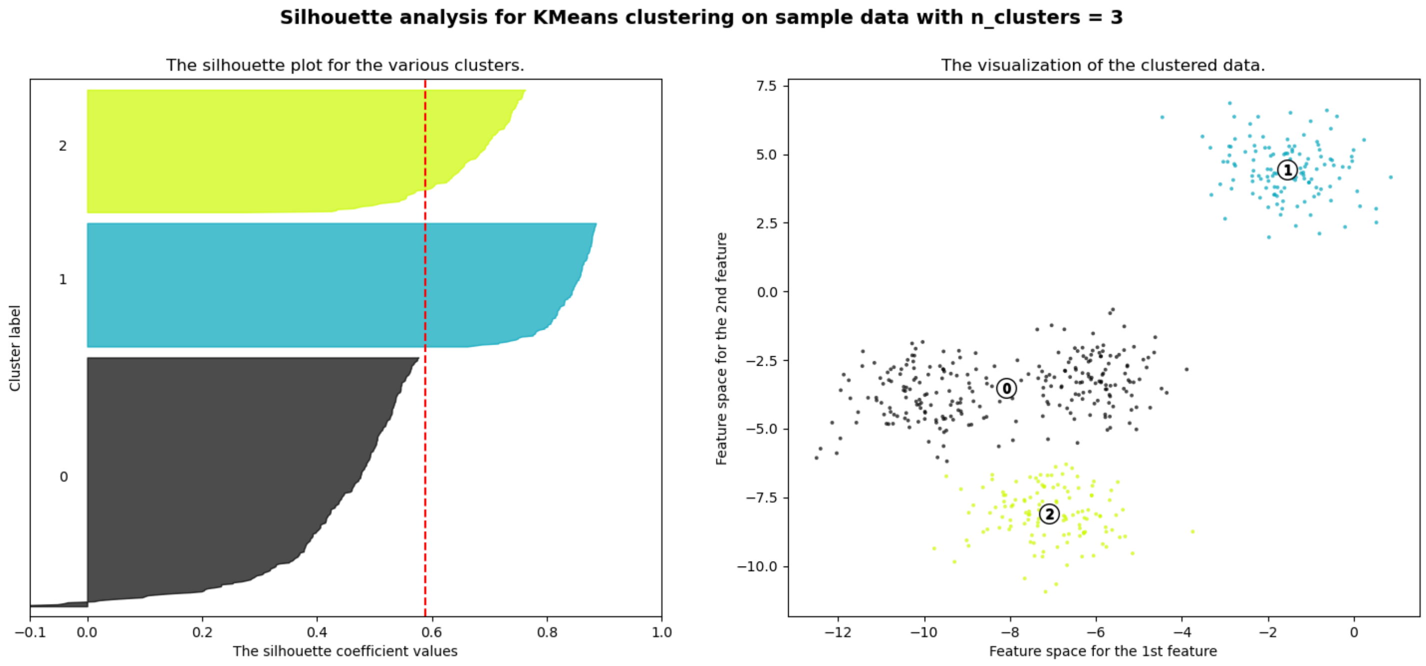
The silhouette method (example)



From: https://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_silhouette_analysis.html

Evaluating the quality of clustering

The silhouette method (example)



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Evaluating the quality of clustering

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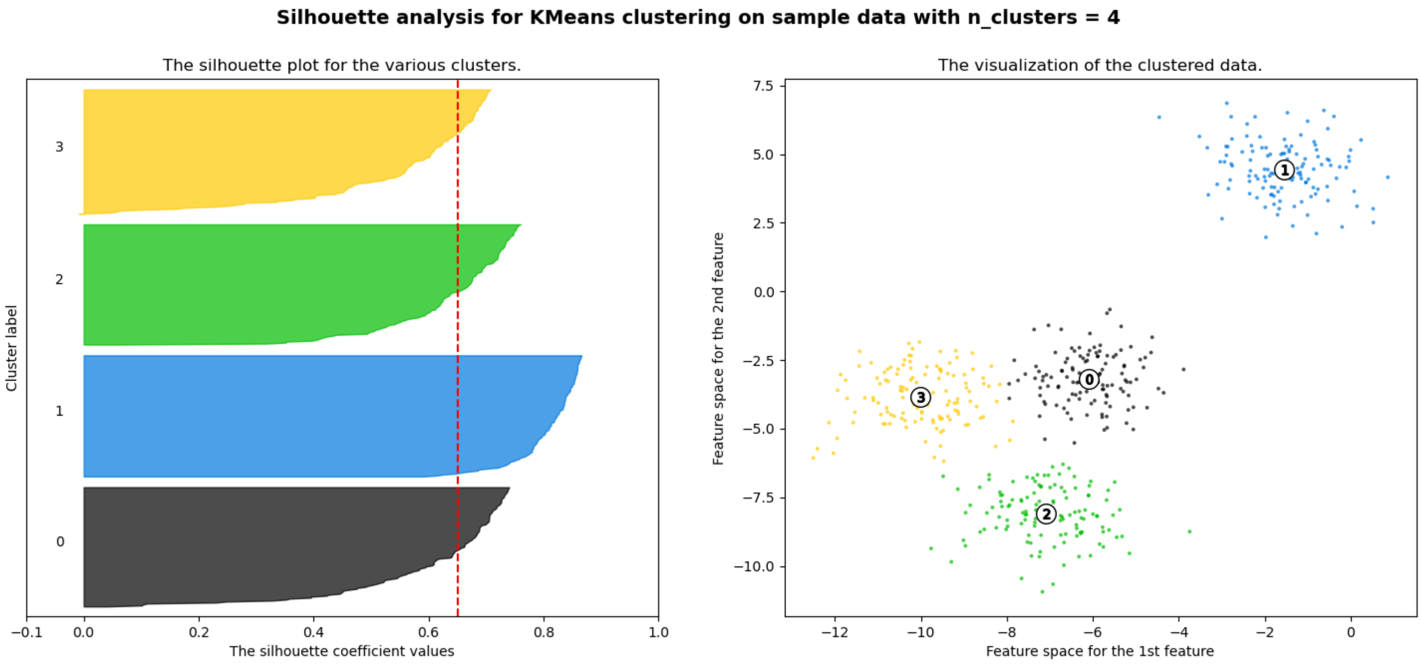

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Evaluating the quality of clustering

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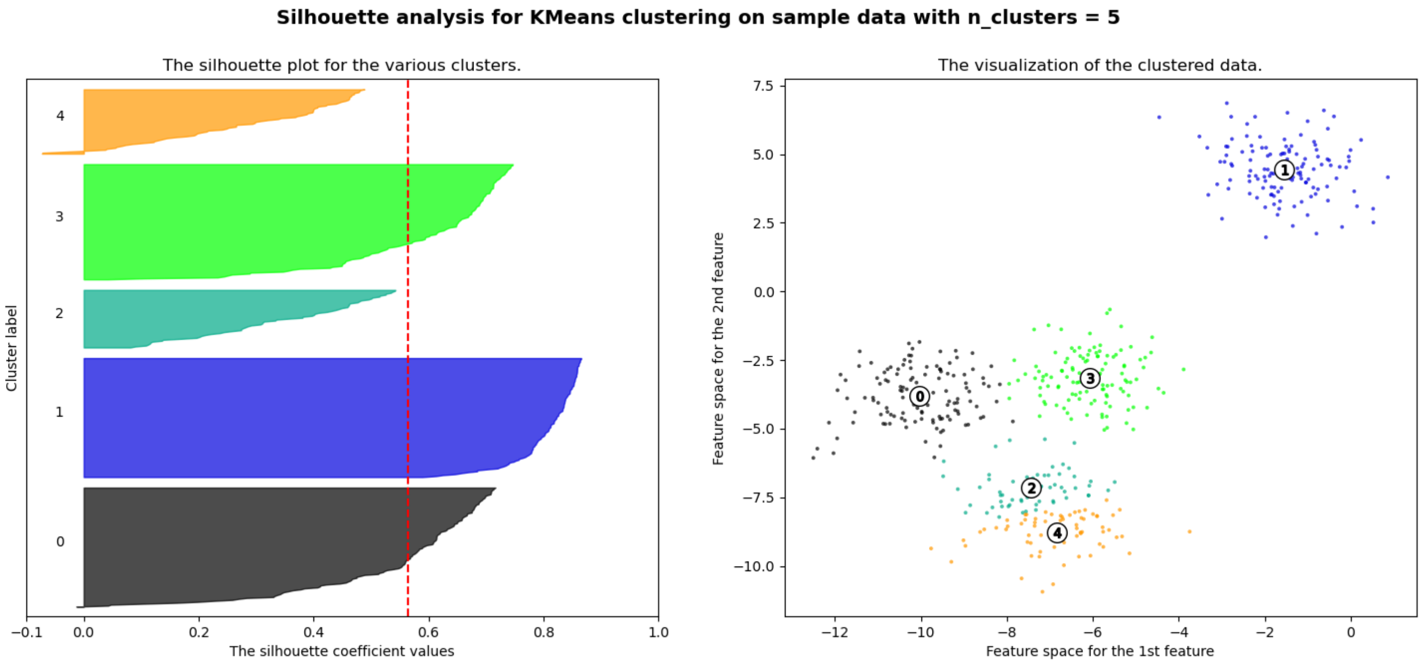

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Evaluating the quality of clustering

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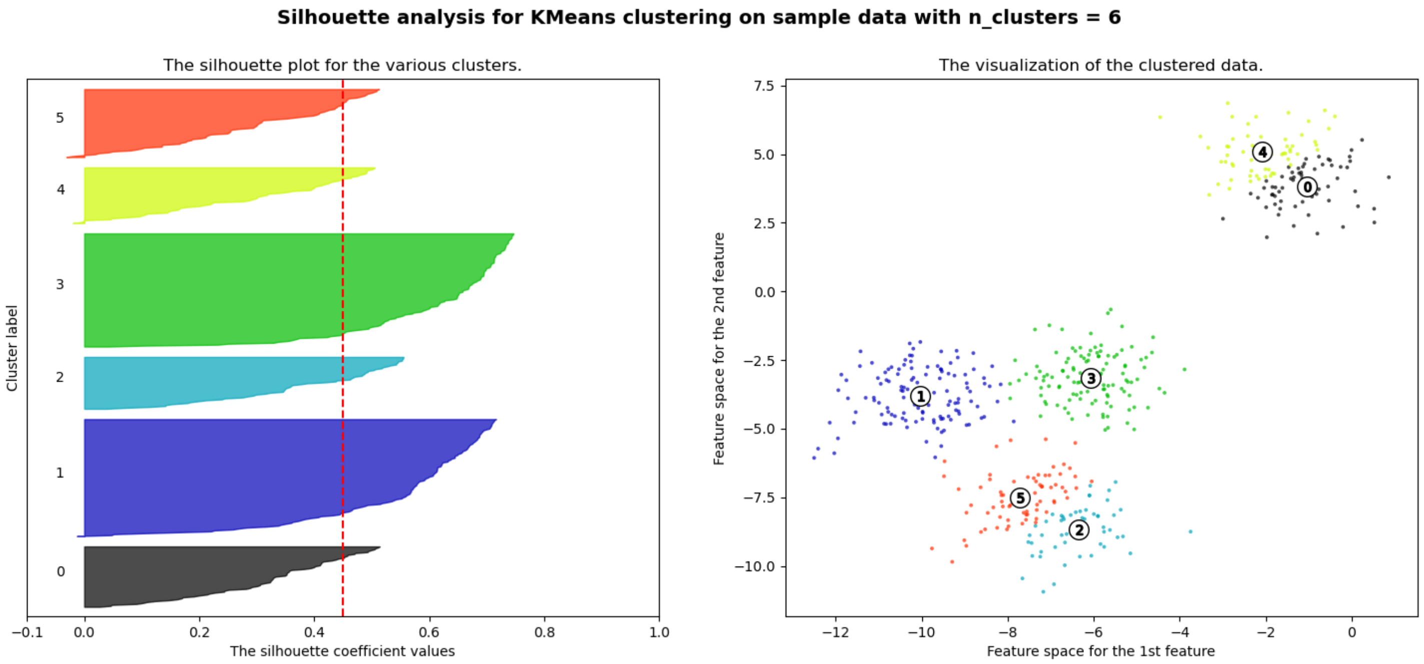

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Homework 3

DEADLINE: **May 8th, 09.00** (NO LATE SUBMISSIONS)
(MEGABONUS: **+5**) Do the assignment both in R and Python

- Create a report (**Rmarkdown and/or Jupyter notebook**) addressing the following assignments. The report must contain both code (cells) and results (no need to re-run)!

3.1 Mobile phone picture

- Take a picture with your smartphone. The picture must contain a piece of paper with your name on it and some type of background (walls, floor, window, etc.).
- Resize it to a manageable size (e.g., 256x256) either with R or Py
- The goal is to reduce the number of RGB colors by using k-means as in the lecture.
- Pick the k suggested by the elbow mechanism. Try also other k values.
- The report must contain the original pic, the WSS plot (elbow), & the final pictures

example

3.2 Drilling machine

- *drilling.csv* contains 400 operational measurements from a drilling machine.
- The machine can operate in different unknown states.

- Identify the number of states by using the known clustering techniques
  - K-means (iterate over k → elbow → final clustering)
  - Hierarchical clustering (iterate over linkages → AC/dendrograms → final clustering)
  - Dbscan (kNNdistplot → Eps → final clustering)
  - Optics
- The report must contain all plots and a final comparison of the different clustering outcomes

- Coding session