Lecture 8: Unsupervised learning

Introduction to Machine Learning

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Definition: unsupervised learning

Question

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Unsupervised learning

Unsupervised learning* is a type of algorithm that **learns patterns from untagged data**: through likeliness, algorithms build a concise representation of the data to generate imaginative content.

Definition: unsupervised learning

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- **Clustering methods**
- Latent models
- Anomaly detection

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Several types of unsupervised learning exist in the literature:

- **Clustering methods**
- Latent models
- Anomaly detection

In this course, we'll focus on **clustering methods**.

Definition: clustering

Clustering

Clustering consists in **grouping a set of objects** so that objects in the same group (called a **cluster**) are more "similar" to each other than to those in other groups.
There is no class to be predicted but **the instances are to be divided into natural groups**.

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Given a set of j individuals described by their features $(x_{j,1}, \ldots, x_{j,n})$, assign each individual into a cluster i $(1 \leq i \leq m)$.

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Clustering consists in finding **groups** where:

- Individuals **within** the group are similar
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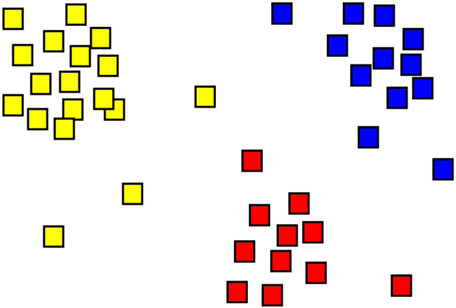
There are many different clustering algorithms, that have a different interpretetation of "similar" and "cluster". Similar to supervised learning, **there is no single best method for all datasets**.

Example: clustering

Height	Weight	Cluster
10	5	?
8	3	?
20	15	?
17	16	?



Example use-cases

Possible use-cases for clustering:

- Finding groups within the data: streaming behavior, shopping behavior (market segmentation . . .) . . .
- Finding outlier individuals in the dataset (individuals too far apart need to be investigated further)
- Semi-supervised learning: mapping samples to a set of class and using it for training.

Definition: clustering

Selecting the right number of clusters can be done:

- Natively by the selected algorithm
- Iteratively by testing different values, evaluating different number of clusters and selecting the best

Clustering is also sensitive to overfitting: the variance-bias trade-off also applies here.

Definition: clustering

Clustering can be:

- **Hard* clustering**: each individual belongs to **a single cluster**.
- **Soft* clustering** (*fuzzy*): an individual can belong to several clusters at the same time.

Clustering algorithms

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There are diverse algorithms:

- Centroid model based (k-means . . .)
- Connectivity models (hierarchical clustering . . .)
- Distribution-based clustering (latent models and gaussian mixtures . . .)
- Density based (DBSCAN . . .)

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As we have no **ground truth**, we cannot directly use supervised learning metrics.
We need some metrics specific to the **unsupervised learning task**.

Evaluation metrics

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What could be some good metrics to assess the performance of an algorithm for a clustering task ?

Different possible approaches:

- Internal evaluation (**find a score describing the performance of the algorithm**)

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What could be some good metrics to assess the performance of an algorithm for a clustering task ?

Different possible approaches:

- Internal evaluation (**find a score describing the performance of the algorithm**)
- Manual evaluation (**use a human expert to validate clusters meaning and see if they are consistent**)
- Empirical/indirect evaluation (**see if in practice the results of this clustering yields efficient information**)

Clustering scores

Clustering scores assign the best score to the algorithm that produces clusters with **high similarity within a cluster** and **low similarity between clusters**.

Possible scores include:

- Silhouette scores

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Possible scores include:

- Silhouette scores
- Davies-Boulin index

Silhouette scores

Silhouette

The silhouette score* measures **how similar an object is to its own cluster** compared to other clusters:
With a the mean intra-cluster distance and b the mean nearest-cluster distance, the silhouette score for an instance is:

$$\frac{b - a}{max(a, b)}$$

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It ranges from -1 to 1: a high value indicates that the objects is **well matched to its own cluster** and **poorly matched to neighboring clusters**.

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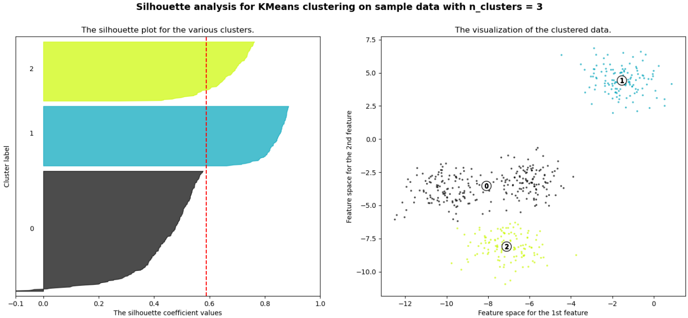
Silhouette scores

If most objects have a high value, then the clustering configuration is appropriate. If many points have a low or negative value (= individuals might have been clustered in the wrong cluster), then:

- Dataset may not be adequate for clustering
- Number of clusters may be poorly chosen (we will see for the different algorithms how to select the optimal number of clusters)

Silhouette scores

Silhouette scores are usually visually represented as a *silhouette* plot to visually see how well the algorithm behaves.



Silhouette scores: example

Question

Given the following clustering result, compute silhouette scores (Manhattan distance) and plot the graph.

ID	Height	Weight	Cluster
1	10	16	1
2	12	14	1
3	14	15	1
4	14	30	2
5	30	30	2

Davies-Bouldin index

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The **Davies-Boulin index*** measures the average similarity of each cluster with its most similar cluster, where similarity is **the ratio of within-cluster distances to between-cluster distances**.

Davies-Bouldin index

We define similarity between cluster i and j as:

$$R_{i,j} = \frac{s_i + s_j}{d_{i,j}}$$

with s_i the average distance between each point of cluster i and the centroid of that cluster and $d_{i,j}$ the distance between cluster centroids i and j.

$$DB = \frac{1}{k} \times \sum_{i=1}^{k} max_{i \neq j} R_{i,j}$$

Davies-Bouldin score: example

Question

Given the following clustering result, compute Davies-Bouldin index (Euclidean distance) and plot the graph.

ID	Height	Weight	Cluster
1	10	16	1
2	12	14	1
3	14	15	1
4	14	30	2
5	30	30	2

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Usually as hard as the clustering task itself !

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Possible interpretations of clusters can be done:

- By looking at the different scores to see how relevant clustering is
- By looking at estimator values of the different features within each cluster
- By plotting the different clusters against the features and understanding why they were clustered together.

Questions

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