Lecture 9: The k-means algorithm

Introduction to Machine Learning

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L3 MIASHS — Semestre 2

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Reminder on previous session

Question

Can anyone remind me what is the definition of **unsupervised learning ?**

Principle

K-Means algorithm

The k-means algorithm* (*MacQueen, 1967*) is a clustering algorithm that partitions the space into k cluster by minimizing the *within-cluster variance*.

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K-Means algorithm

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Given a set of individuals described by their features $(X_1, \ldots, X_n)$ find k sets to partition the data into by minimzing *the within cluster variance*.

$$\sum_{i=1}^{k} \sum_{X \in S_i} = ||X - \mu_i||^2$$

with:

$$\mu_i = \frac{1}{|S_i|} \sum_{X \in S_i} X$$

(μ_i is the mean or centroid)

Medoids and centroids

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Medoids

A medoid* is a **member of the dataset** which sum of dissimilarities to all the objects in the cluster is minimal.

The k-means algorithm

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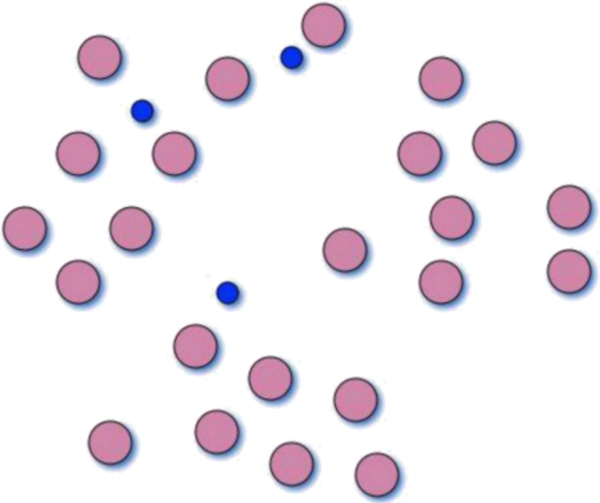
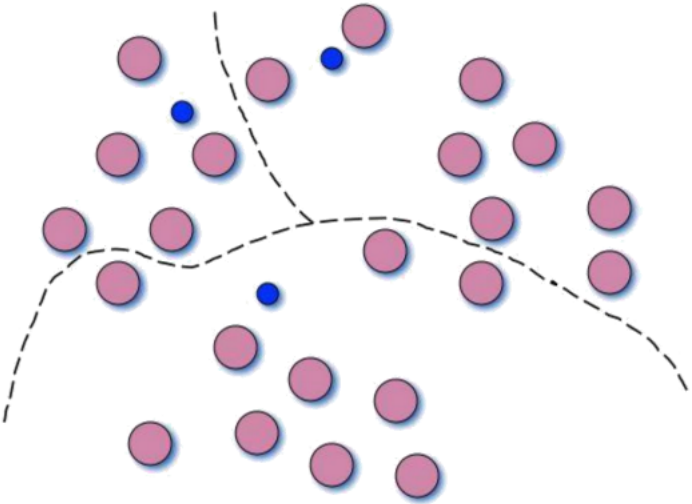
Run steps until assignment do not change.

There is no garantee to find the optimum (but efficient in practice).

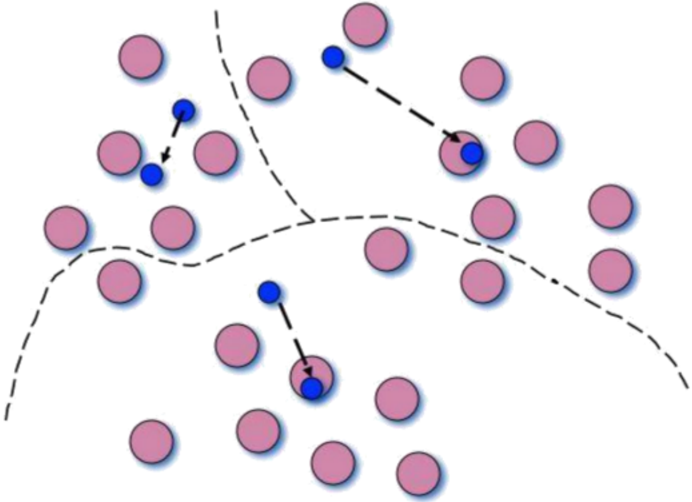
Initialization



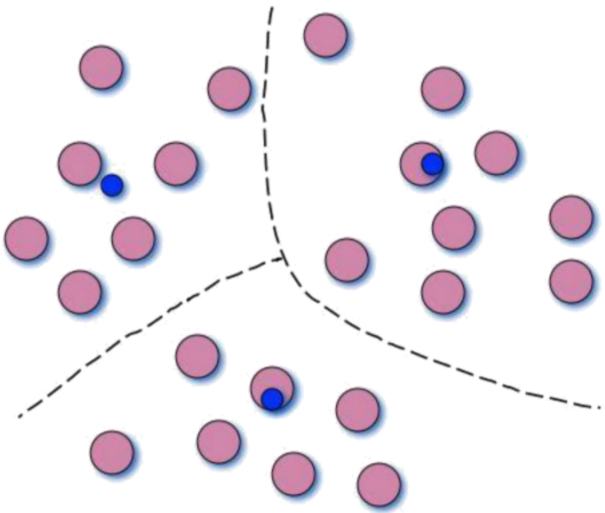
Assign each individual to a cluster



Compute new medoids



Repeat until stable



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- **Fully random approach**: randomly choose k vectors in the feature space.

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- **Fully random approach**: randomly choose k vectors in the feature space.
- **Forgy partition**: Randomly choose k observations from the dataset.
- **Random partition**: Randomly assign a cluster to each observation.

Example: k-means algorithm

Questions

1. Perform the k-means algorithm on the following dataset for k=2
2. Assign each individual to a cluster
3. Give coordinates of each centroid

ID	Sepal length	Sepal width
1	5	2
2	5	3
3	4	3
4	7	4
5	6	5

Hyperparameters

Question

What are the hyperparameters of the algorithm ?

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k !

Selecting the number of clusters using the elbow method

Elbow method

An elbow plot* is a visual method by plotting the *within cluster variance* against the number of clusters and selecting the number of clusters before the curve flattens.

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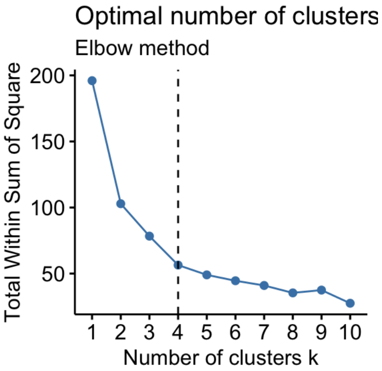

Selecting the number of clusters using silhouette score

The silhouette score (see previous lecture) reaches its global maximum for the optimum number of k.

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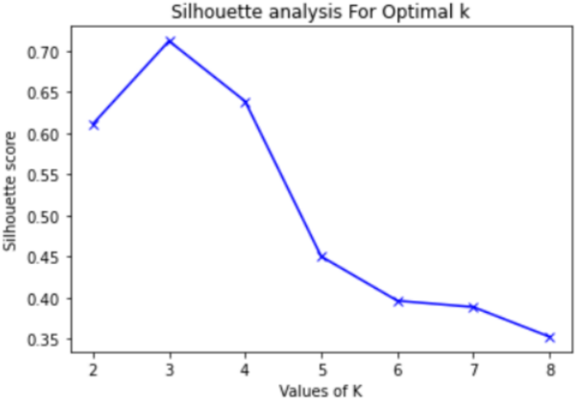

Line plot between K and Silhouette score

Advantages and drawbacks

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- Fast to compute
- Easy to understand
- Work very well when clusters have a spherical shape

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Limits

- Random algorithm
- No garantee to not be in a local optimum
- k must be chosen beforehand
- Class representative does not exist making it harder to interprete

Similar algorithm: PAM

Partitioning Around Medoids

Partitioning Around Medoids* (PAM) (*Leonard Kaufman and Peter J. Rousseeuw*) is a clustering algorithm that attempts to minimize the distance between points labeled to be in a cluster and a point designated as the center of that cluster.

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Partitioning Around Medoids* (PAM) (*Leonard Kaufman and Peter J. Rousseeuw*) is a clustering algorithm that attempts to minimize the distance between points labeled to be in a cluster and a point designated as the center of that cluster.

Fixes one of the problem of k-means: the *medoid* (instead of centroid) exists in the dataset.

PAM algorithm

The PAM algorithm is iterative:
Given k and a cost function $\sum_{i=1}^{k} \sum_{X \in S_i} = d(X, x^{(i)})$ with $x^{(i)}$ the medoid of cluster i and d a dissimilarity,

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Initialize: greedily select k of the n data points as the medoids to minimize the cost.

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Until the cost function does not decrease anymore:

1. Associate each non-medoid data point to the closest medoid
2. For each medoid m, and for each non-medoid data point o
   1. Swap m and o
   2. Compute the cost change
   3. If the cost decreases, the store the value for the cost decrease
3. Perform the swap of o and m that decreases the most the cost function

Example: PAM algorithm

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Limits:

- We need to decide a value for k
- Algorithm initialization is random

Questions

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