DATA ANALYTICS

Unit 4: Brief Review of Unsupervised Learning Algorithms (k-means, Hierarchical agglomerative clustering)

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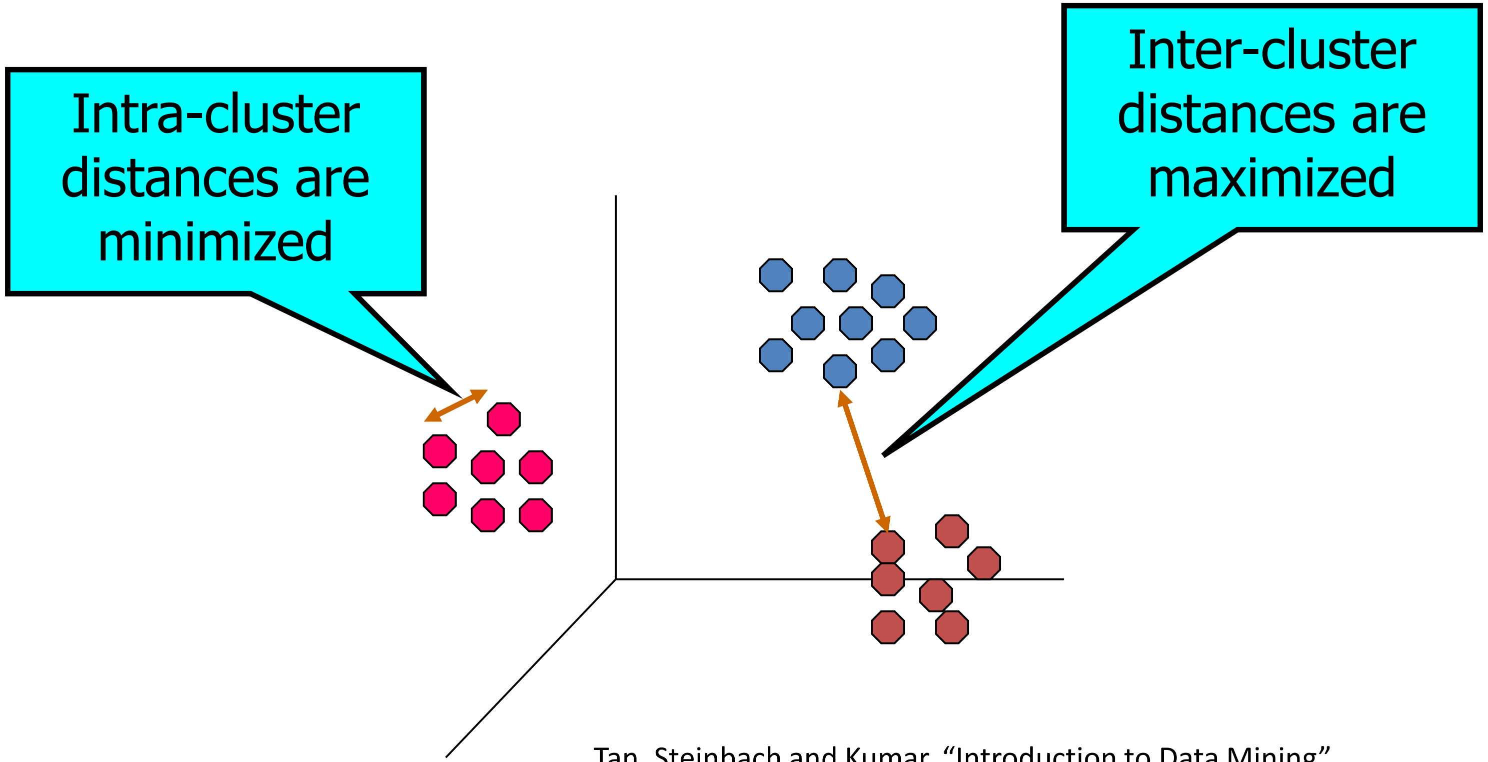
Introduction

- Mastering unsupervised learning opens up a broad range of avenues for a data scientist.
- Clustering has wide application across domains and industries
- Examples: Uber’s route optimization, Amazon’s recommendation system, Netflix’s customer segmentation, and so on…
- Why is it important?
  - Annotating data for supervised learning is time consuming, expensive and not always practical
  - We can use clustering to group similar data points for sampling
  - It provides a technique for describing the data and possibly getting insights (such as discovering subgroups within a known class, etc.)
- Basic clustering algorithms include K-Means clustering, hierarchical clustering, and the DBSCAN algorithm

What is clustering?

Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups



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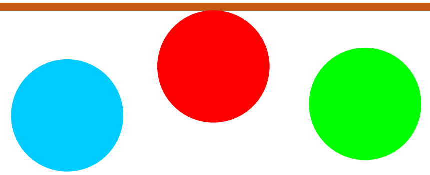
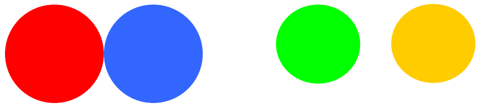
Types of clusters

- Well-separated clusters

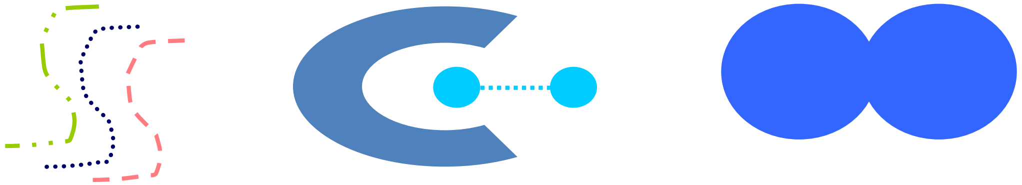


- Center-based clusters



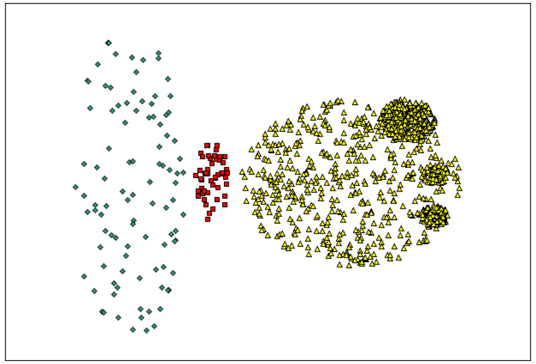
Mean or medioid is the ‘prototype’

- Contiguous clusters



NN or transitive

- Density-based clusters



- Property or Conceptual
- Described by an Objective Function

Minimize the edge weight between clusters
and maximize the edge weight within clusters

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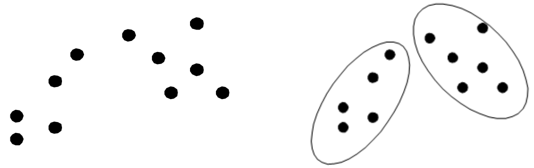
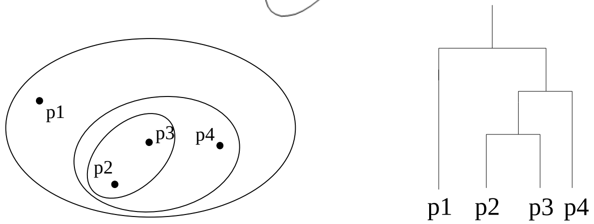
Types of clustering techniques

- Partitional



- Hierarchical



- Exclusive (vs nonexclusive) – points can belong to multiple clusters
- Fuzzy vs nonfuzzy – points belong to every cluster with a weight in (0,1)
- Property or Conceptual - we only want to cluster some of the data
- Described by an Objective Function – cluster of widely different sizes, shapes, and densities

k-means clustering

Partitional clustering approach

Each cluster is associated with a centroid (center point)

Each point is assigned to the cluster with the closest centroid

Number of clusters, K, must be specified

The basic algorithm is very simple

1: Select K points as the initial centroids.
2: **repeat**
3: Form K clusters by assigning all points to the closest centroid.
4: Recompute the centroid of each cluster.
5: **until** The centroids don't change

Tan, Steinbach and Kumar, "Introduction to Data Mining"

k-means parameters

- Initial centroids are often chosen randomly.
  - Clusters produced vary from one run to another.
- The centroid is (typically) the mean of the points in the cluster.
- 'Closeness' is measured by Euclidean distance, cosine similarity, correlation, etc.
- K-means will converge for common similarity measures mentioned above.
- Most of the convergence happens in the first few iterations.
  - Often the stopping condition is changed to 'Until relatively few points change clusters'
- Complexity is O(n * K * I * d)
  - n = number of points, K = number of clusters,
I = number of iterations, d = number of attributes

Evaluating k-means clusters

- Most common measure is Sum of Squared Error (SSE)
  - For each point, the error is the distance to the nearest cluster
  - To get SSE, we square these errors and sum them.

$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist^2(m_i, x)$$

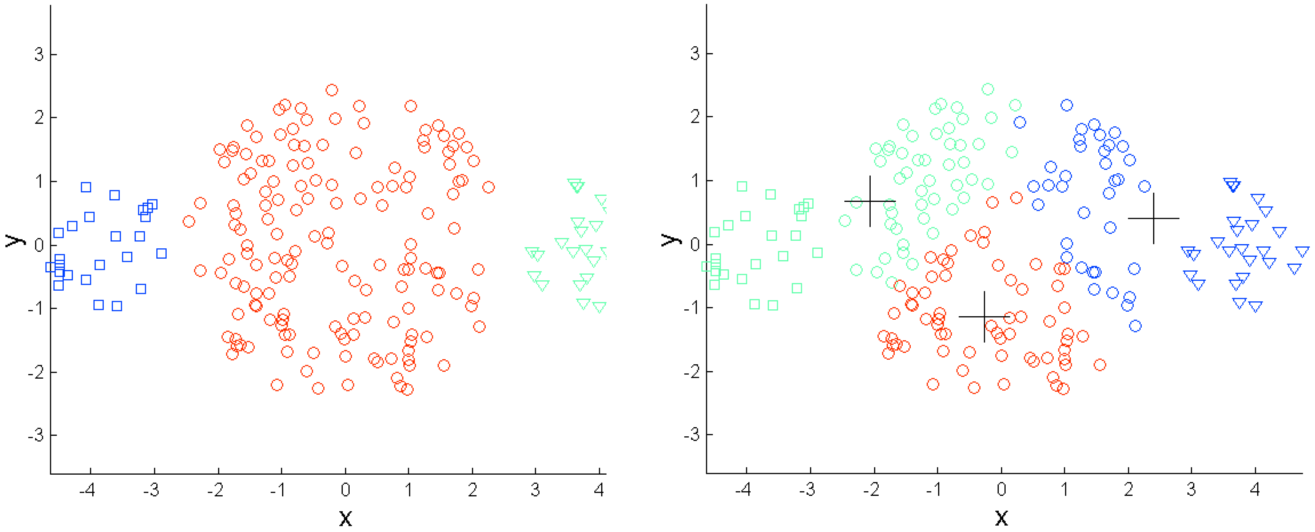
  - x is a data point in cluster C_i and m_i is the representative point for cluster C_i
    - can show that m_i corresponds to the center (mean) of the cluster
  - Given two clusters, we can choose the one with the smallest error
  - One easy way to reduce SSE is to increase K, the number of clusters
    - A good clustering with smaller K can have a lower SSE than a poor clustering with higher K

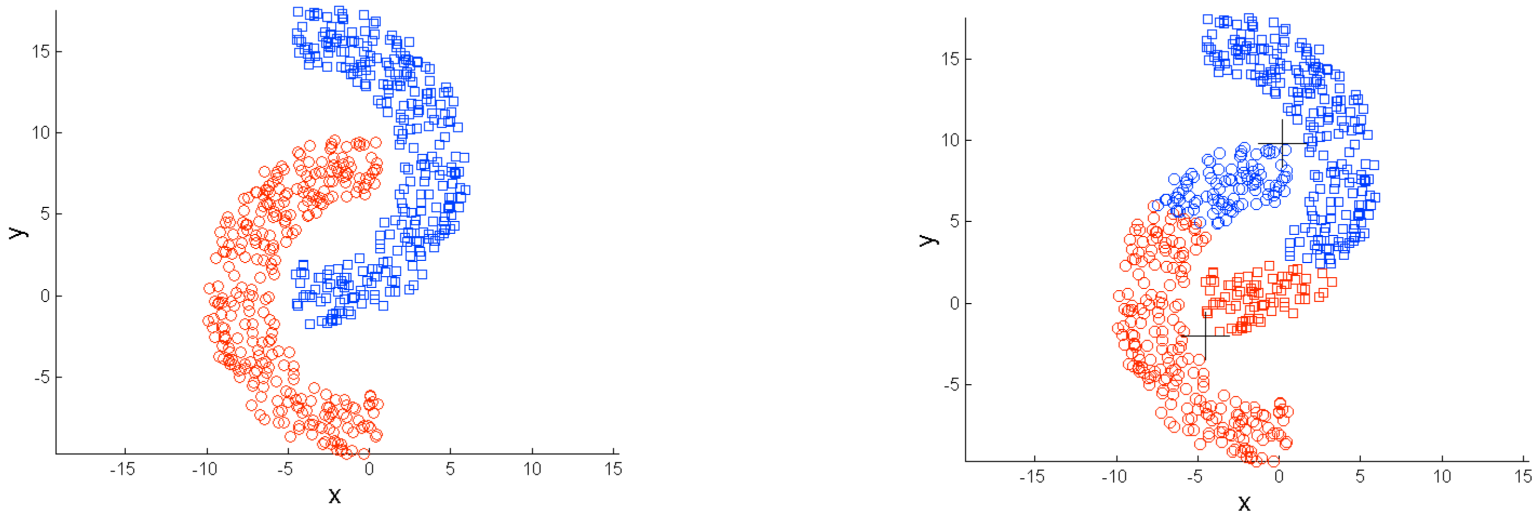
k-means clustering – some cons

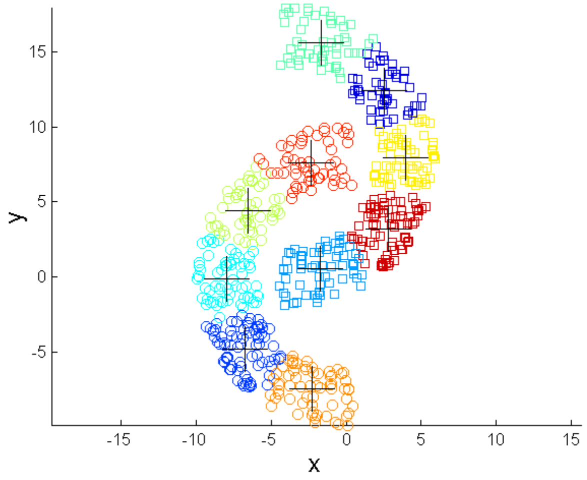
- Different configurations for each run due to random initialization
- Works well only for similarly shaped (or sized clusters)
- Does not work well for inherently nonglobular clusters

Try: (1) Choosing k>> no. of clusters

(2) Run kmeans multiple times; select the best configuration







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Quality and optimal number of clusters

- Number of clusters and recommended index (Calinski and Harabasz)

$$CH(k) = \frac{B(k)/k-1}{W(k)/(n-k)}$$

- Hartigan statistic

$$H(k) = \{(W(k)/W(k-1)) - 1\}/(n-k-1)$$

- Silhouette statistic

$$S(i) = (b(i)-a(i)/max\{a(i),b\{i\}))$$

Which can be also written as:

$$s(i) = \begin{cases} 1 - a(i)/b(i), & \text{if } a(i) < b(i) \\ 0, & \text{if } a(i) = b(i) \\ b(i)/a(i) - 1, & \text{if } a(i) > b(i) \end{cases}$$

From the above definition it is clear that

$$-1 \leq s(i) \leq 1$$

For data point $i \in C_i$ (data point i in the cluster C_i), let

$$a(i) = \frac{1}{|C_i| - 1} \sum_{j \in C_i, i \neq j} d(i,j) \qquad b(i) = \min_{k \neq i} \frac{1}{|C_k|} \sum_{j \in C_k} d(i,j)$$

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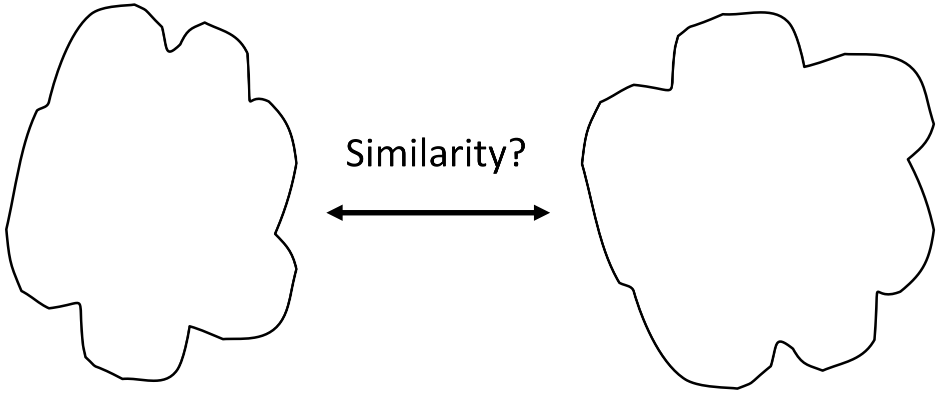
Agglomerative hierarchical clustering



	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
  – Ward's Method uses squared error

References

Text Book:

"Business Analytics, The Science of Data-Driven Making", U. Dinesh Kumar, Wiley 2017 (Chapter 14.1-14.2.6, 14.3-14.6)

"Recommender Systems, The text book, Charu C. Aggarwal, Springer 2016 Section 1.and Section 2.

Image Courtesy

https://www.analyticsvidhya.com/blog/2020/09/how-dbscan-clustering-works/

THANK YOU

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