DAT630
Clustering

Introduction to Data Mining, Chapter 8

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Supervised vs. Unsupervised Learning

- Supervised learning
  - Labeled examples (with target information) are available
- Unsupervised learning
  - Examples are not labeled

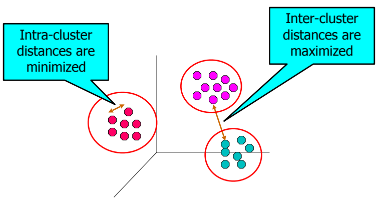
Outline

- Clustering
- Two algorithms:
  - K-means
  - Hierarchical (Agglomerative) Clustering

Clustering

Clustering

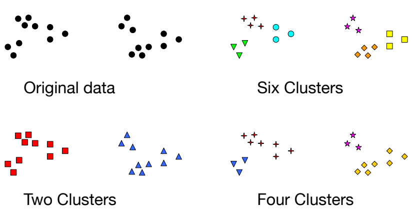
- Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups



Why?

- For **understanding**
  - E.g., biology (taxonomy of species)
  - Business (segmenting customers for additional analysis and marketing activities)
  - Web (clustering search results into subcategories)
- For **utility**
  - Some clustering techniques characterize each cluster in terms of a cluster prototype
  - These prototypes can be used as a basis for a number of data analysis and processing techniques

How many clusters?



- The notion of a cluster can be ambiguous

Types of Clustering

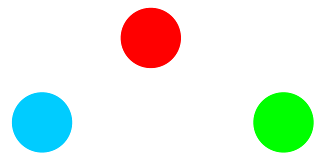
- Partitional vs. hierarchical
  - Partitional: non-overlapping clusters such that each data object is in exactly one cluster
  - Hierarchical: a set of nested clusters organized as a hierarchical tree
- Exclusive vs. non-exclusive
  - Whether points may belong to a single or multiple clusters

Types of Clustering (2)

- Partial versus complete
  - In some cases, we only want to cluster some of the data
- Fuzzy vs. non-fuzzy
  - In fuzzy clustering, a point belongs to every cluster with some weight between 0 and 1
  - Weights must sum to 1
  - Probabilistic clustering has similar characteristics

Different Types of Clusters

- Well-Separated Clusters
  - A cluster is a set of points such that any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster

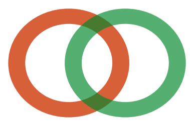


Different Types of Clusters

- Center-based (or prototype-based)
  - A cluster is a set of objects such that an object in a cluster is closer (more similar) to the "center" of a cluster, than to the center of any other cluster
  - The center of a cluster is often a centroid, the average of all the points in the cluster, or a medoid, the most "representative" point of a cluster

Different Types of Clusters

- Shared Property or Conceptual Clusters
  - Clusters that share some common property or represent a particular concept



Notation

- $\boldsymbol{x}$ an object (data point)
- m the number of points in the data set
- K the number of clusters
- C_i the ith cluster
- c_i the centroid of cluster C_i
- m_i the number of points in cluster C_i

K-means Clustering

K-means

- One of the oldest and most widely used clustering techniques
- Prototype-based clustering
  - Clusters are represented by their centroids
- Finds a user-specified number of clusters (K)

Basic K-means Algorithm

1. Select K points as initial centroids
2. **repeat**
   3. Form K clusters by assigning each point to its closest centroid
   4. Recompute the centroid of each cluster
5. **until** centroids do not change

Basic K-means Algorithm

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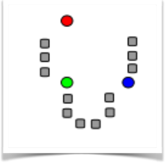

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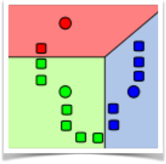

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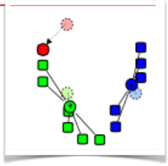

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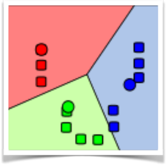

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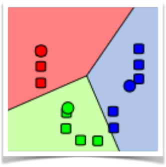
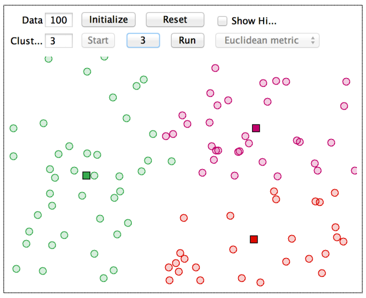


Interactive Demo



http://home.deib.polimi.it/matteucc/Clustering/tutorial_html/AppletKM.html

1. Choosing Initial Centroids

- Most commonly: select points (centroids) randomly
  - They may be poor
  - Possible solution: perform multiple runs, each with a different set of randomly chosen centroids

3. Assigning Points to the Closest Centroid

- We need a proximity measure that quantifies the notion of "closest"
- Usually chosen to be simple
  - Has to be calculated repeatedly
- See distance functions from Lecture 1
  - E.g., Eucledian distance

4. Recomputing Centroids

- Objective function is selected
  - I.e., what is it that we want minimize/maximize
- Once the objective function and the proximity measure are defined, we can define mathematically the centroid we should choose
  - E.g., minimize the squared distance of each point to its closest centroid

Sum of Squared Error (SSE)

- Measures the quality of clustering in the Eucledian space
- Calculate the error of each data point (its Eucledian distance to the closest centroid), and then compute the total sum of the squared errors

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

- A clustering with lower SSE is better

Minimizing SSE

- It can be shown that the centroid that minimizes the SSE of the cluster is the mean
- The centroid of the *i*th cluster

$$\mathbf{c}_i = \frac{1}{m_i} \sum_{x \in C_i} \mathbf{x}$$

Example
Centroid computation

- What is the centroid of a cluster containing three 2-dimensional points: **(1,1), (2,3), (6,2)**?
- Centroid:
  ((1+2+6)/3, (1+3+2)/3) = **(3,2)**

5. Stopping Condition

- Most of the convergence occurs in the early steps
- "Centroids do not change" is often replaced with a weaker condition
  - E.g., repeat until only 1% of the points change

Exercise

Note

- There are other choices for proximity, centroids, and objective functions, e.g.,
- Proximity function: **Manhattan** (L1)
  Centroid: median
  Objective func: minimize sum of L1 distance of an object to its cluster centroid
- Proximity function: **cosine**
  Centroid: mean
  Objective func: maximize sum of cosine sim. of an object to ist cluster centroid

What is the complexity?

- *m* number of points, *n* number of attributes, *K* number of clusters
- Space requirements: *O(?)*
- Time requirements: *O(?)*

Complexity

- *m* number of points, *n* number of attributes, *K* number of clusters
- Space requirements: *O((m+K)*n)*
  - Modest, as only the data points and centroids are stored
- Time requirements: *O(I*K*m*n)*
  - *I* is the number of iterations required for convergence
  - Modest, linear in the number of data points

K-means Issues

- Depending on the initial (random) selection of centroids different clustering can be produced
- Steps 3 and 4 are only guaranteed to find a local optimum
- Empty clusters may be obtained

Bisecting K-means

- Straightforward extension of the basic K-means algorithm
- Idea:
  - Split the set of data points to two clusters
  - Select one of these clusters to split
  - Repeat until K clusters have been produced
- The resulting clusters are often used as the initial centroids for the basic K-means algorithm

Bisecting K-means Alg.

1. Initial cluster contains all data points
2. **repeat**
    3. Select a cluster to split
    4. **for** a number of trials
        5. Bisect the selected cluster using basic K-means
    6. end for
    7. Select the clusters from the bisection with the lowest total SSE
8. **until** we have *K* clusters

Selecting a Cluster to Split

- Number of possible ways
  - Largest cluster
  - Cluster with the largest SSE
  - Combine size and SSE
- Different choices result in different clusters

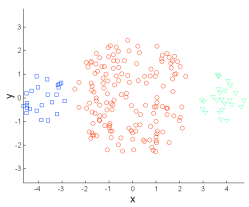
Hierarchical Clustering

- By recording the sequence of clusterings produced, bisecting K-means can also produce a hierarchical clustering

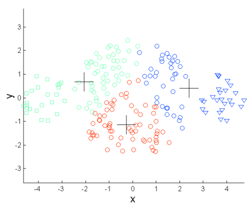
Limitations

- K-means has difficulties detecting clusters when they have
  - differing sizes
  - differing densities
  - non-spherical shapes
- K-means has problems when the data contains outliers

Example: differing sizes

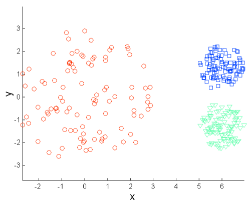


Original points



K-means (3 clusters)

Example: differing density



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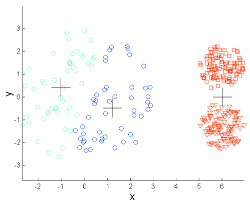
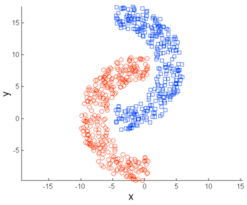


K-means (3 clusters)

Example: non-spherical shapes



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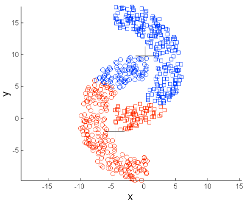
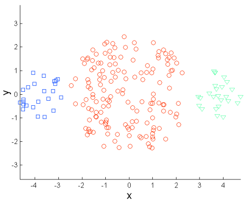


K-means (2 clusters)

Overcoming Limitations

- Use larger K values
- Natural clusters will be broken into a number of sub-clusters

Example: differing sizes



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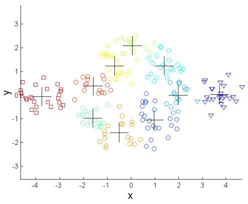
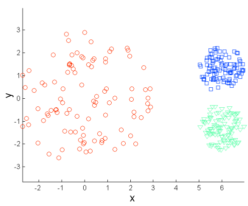


K-means clusters

Example: differing density



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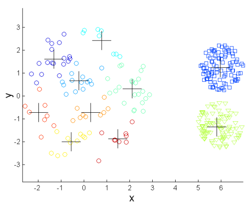
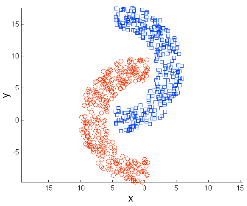


K-means clusters

Example: non-spherical shapes



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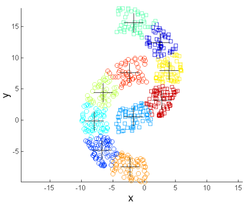


K-means clusters

Summary

- Efficient and simple
  - Provided that K is relatively small (K<<m)
- Bisecting variant is even more efficient and less susceptible to initialization problems
- Cannot handle certain types of clusters
  - Problems can be overcome by generating more (sub)clusters
- Has trouble with data that contains outliers
  - Outlier detection and removal can help

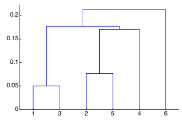
Hierarchical Clustering

Hierarchical Clustering

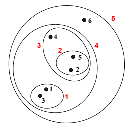
- Two general approaches
- Agglomerative
  - Start with the points as individual clusters
  - At each step, merge the closest pair of clusters
  - Requires a notion of *cluster proximity*
- Divisive
  - Start with a single, all-inclusive cluster
  - At each step, split a cluster, until only singleton clusters of individual points remain

Agglomerative Hierarchical Clustering

- Produces a set of nested clusters organized as a hierarchical tree
- Can be visualized
  - Dendrogram
  - Nested cluster diagram (only for 2D points)



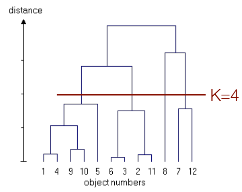
Dendogram

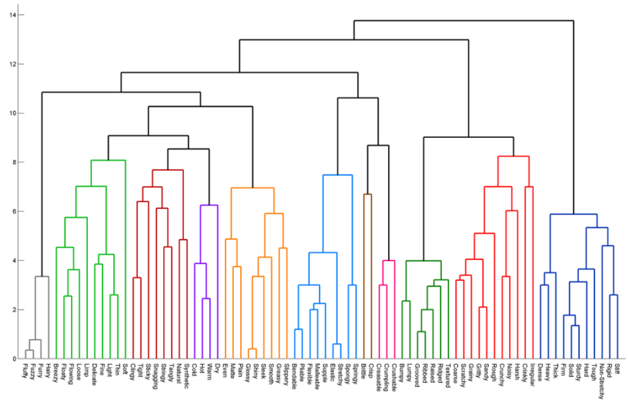


Nested cluster diagram

Strengths

- Do not have to assume any particular number of clusters
  - Any desired number of clusters can be obtained by cutting the dendogram at the proper level
- They may correspond to meaningful taxonomies
  - E.g., in biological sciences



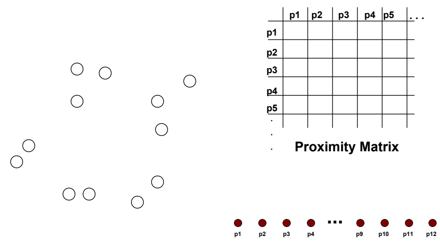


Basic Agglomerative Hierarchical Clustering Alg.

1. Compute the proximity matrix
2. **repeat**
   3. Merge the closest two clusters
   4. Update the proximity matrix
5. **until** only one cluster remains

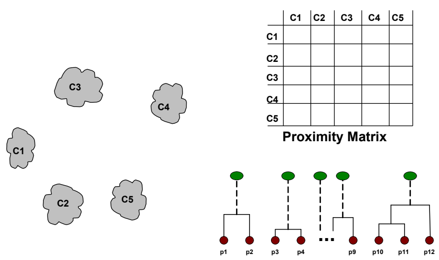
Example
Starting situation

- Start with clusters of individual points and a proximity matrix



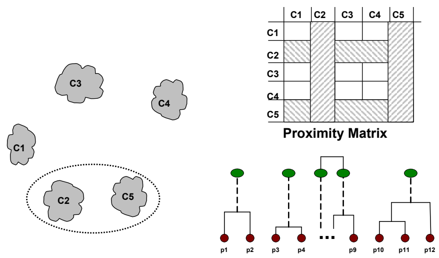
Example
Intermediate situation

- After some merging steps, we have some clusters



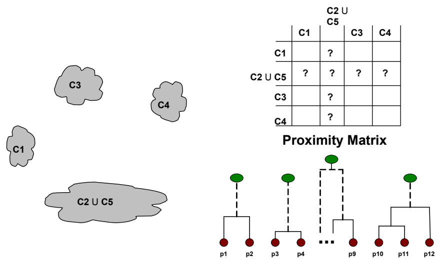
Example
Intermediate situation

- We want to merge the two closest clusters (C2 and C5) and update the proximity matrix



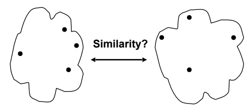
Example
After merging

- How do we update the proximity matrix?



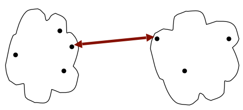
Defining the Proximity between Clusters

- MIN (single link)
- MAX (complete link)
- Group average
- Distance between centroids



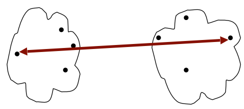
Single link (MIN)

- Similarity of two clusters is based on the two most similar (closest) points in the different clusters
  - Determined by one pair of points, i.e., by one link in the proximity graph



Complete link (MAX)

- Similarity of two clusters is based on the two least similar (most distant) points in the different clusters
  - Determined by all pairs of points in the two clusters

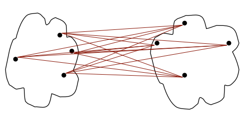


Group average

- Proximity of two clusters is the average of pairwise proximity between points in the two clusters

$$proximity(C_i, C_j) = \frac{\sum_{x \in C_i, y \in C_j} proximity(x, y)}{m_i \cdot m_j}$$

  - Need to use average connectivity for scalability since total proximity favors large clusters

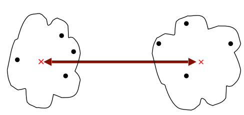


Strengths and Weaknesses

- Single link (MIN)
  - Strength: can handle non-elliptical shapes
  - Weakness: sensitive to noise and outliers
- Complete link (MAX)
  - Strength: less susceptible to noise and outliers
  - Weakness: tends to break large clusters
- Group average
  - Strength: less susceptible to noise and outliers
  - Weakness: biased towards globular clusters

Prototype-based methods

- Represent clusters by their centroids
  - Calculate the proximity based on the distance between the centroids of the clusters



- Ward's method
  - Similarity of two clusters is based on the increase in SSE when two clusters are merged
    - Very similar to group average if distance between points is distance squared

Exercise

Key Characteristics

- No global objective function that is directly optimized
- No problems with choosing initial points or running into local minima
- Merging decisions are final
  - Once a decision is made to combine two clusters, it cannot be undone

What is the complexity?

- *m* is the number of points
- Space complexity *O(?)*
- Time complexity *O(?)*

Complexity

- Space complexity $O(m^2)$
  - Proximity matrix requires the storage of $m^2/2$ proximities (it's symmetric)
  - Space to keep track of clusters is proportional to the number of clusters (*m-1*, exclusing singleton clusters)
- Time complexity $O(m^3)$
  - Computing the proximity matrix $O(m^2)$
  - *m-1* iterations (Steps 3 and 4)
  - It's possible to reduce the total cost to $O(m^2 \log m)$ by keeping data in a sorted list (or heap)

Summary

- Typically used when the underlying application requires a hierarchy
- Generally good clustering performance
- Expensive in terms of computation and storage