Unsupervised Learning and Clustering

Muhammad Sarim

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    - Unsupervised methods can be used for feature extraction.
    - Exploratory data analysis can provide insight into the nature or structure of the data.

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- This description uses the assumption that the patterns form a cloud that can be modeled with a hyperellipsoidal shape.
- However, we must be careful about any assumptions we make about the structure of the data.

Data Description

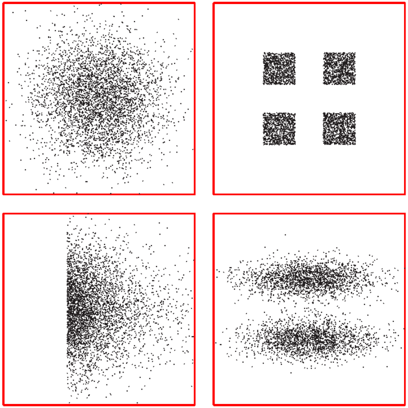

Figure: These four data sets have identical first-order and second-order statistics. We need to find other ways of modeling the structure. Clustering is an alternative way of describing the data in terms of groups of patterns.

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    - Clusters may be described as connected regions of a multi-dimensional space containing a relatively high density of points, separated from other such regions by a region containing a relatively low density of points.

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Clustering

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- Clustering is unsupervised. Category labels and other information about the source of data influence the interpretation of the clusters, not their formation.

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Figure: The number of clusters in the data often depend on the resolution (fine vs. coarse) with which we view the data. How many clusters do you see in this figure? 5, 8, 10, more?

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- Most of these algorithms are based on the following two popular techniques:
  - Iterative squared-error partitioning
  - Agglomerative hierarchical clustering
- One of the main challenges is to select an appropriate measure of similarity to define clusters that is often both data (cluster shape) and context dependent.

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Similarity Measures

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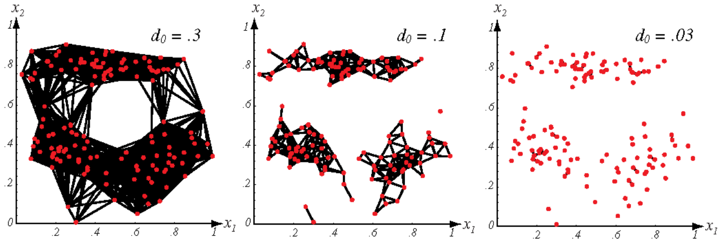

Figure: The distance threshold affects the number and size of clusters that are shown by lines drawn between points closer than the threshold.

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- The simplest and most widely used criterion function for clustering is the *sum-of-squared-error* criterion.

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- For a given cluster D_i, the mean vector m_i (centroid) is the best representative of the samples in D_i.

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- This algorithm, without step 5, is also known as the *k-means* algorithm.

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- The initial partition is often chosen by generating k random points uniformly distributed within the range of the data, or by randomly selecting k points from the data.

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- In model-based clustering, the value of k corresponds to the number of components in the mixture.

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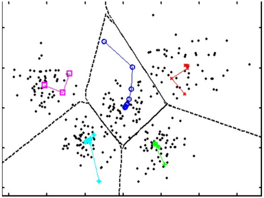
Examples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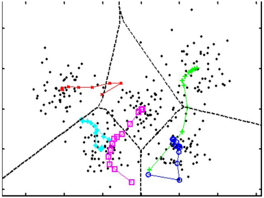
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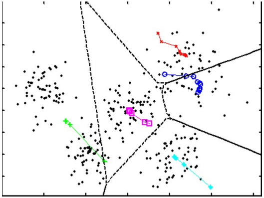
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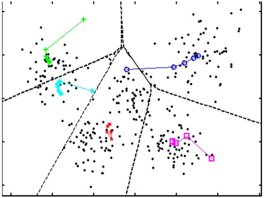
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Figure: Examples for k-means with different initializations of five clusters for the same data.

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- In some applications, groups of patterns share some characteristics when looked at a particular level.
- Hierarchical clustering tries to capture these multi-level groupings using *hierarchical* representations rather than flat partitions.

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- Given any two samples, at some level they will be grouped together in the same cluster and remain together at all higher levels.

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- If there is an unusually large gap between the similarity values for two particular levels, one can argue that the level with fewer number of clusters represents a more natural grouping.

Hierarchical Clustering

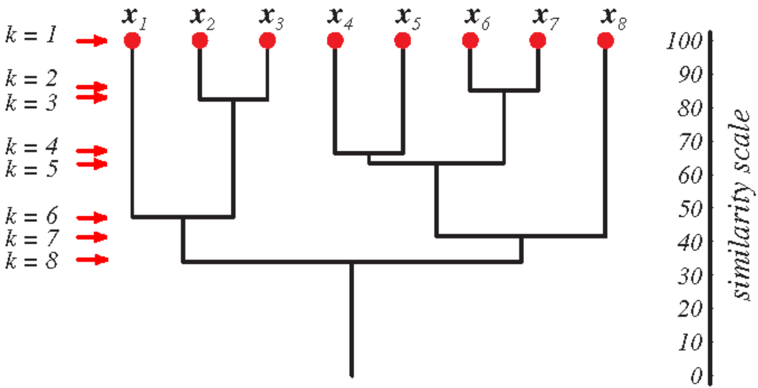

Figure: A dendrogram can represent the results of hierarchical clustering algorithms. The vertical axis shows a generalized measure of similarity among clusters.

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  4. Return the resulting clusters.

Hierarchical Clustering

- Popular distance measures (for two clusters D_i and D_j):

$$d_{\text{min}}(D_i, D_j) = \min_{\substack{x \in D_i \\ x' \in D_j}} \|x - x'\|$$

$$d_{\text{max}}(D_i, D_j) = \max_{\substack{x \in D_i \\ x' \in D_j}} \|x - x'\|$$

$$d_{\text{avg}}(D_i, D_j) = \frac{1}{\#D_i \, \#D_j} \sum_{x \in D_i} \sum_{x' \in D_j} \|x - x'\|$$

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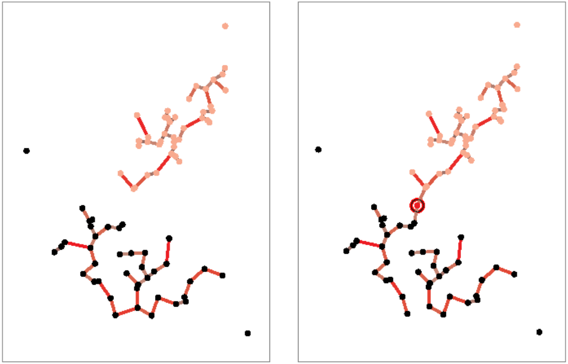

Figure: Examples for single linkage clustering.

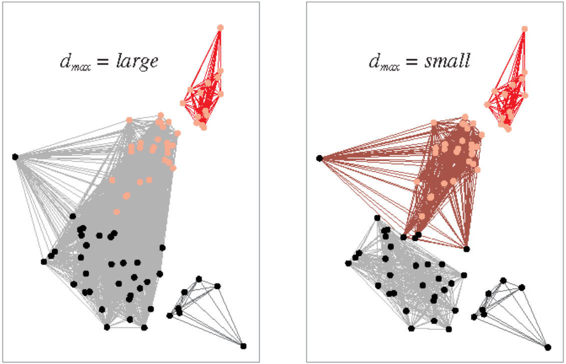

Figure: Examples for complete linkage clustering.

Contents

Hierarchical Clustering

- *Stepwise-Optimal Hierarchical Clustering:*

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- When the sum-of-squared-error criterion J_e is used, the pair of clusters whose merger increases J_e as little as possible is the pair for which the distance

$$d_e(D_i, D_j) = \frac{\#D_i \, \#D_j}{\#D_i + \#D_j} \|m_i - m_j\|^2$$

is minimum.

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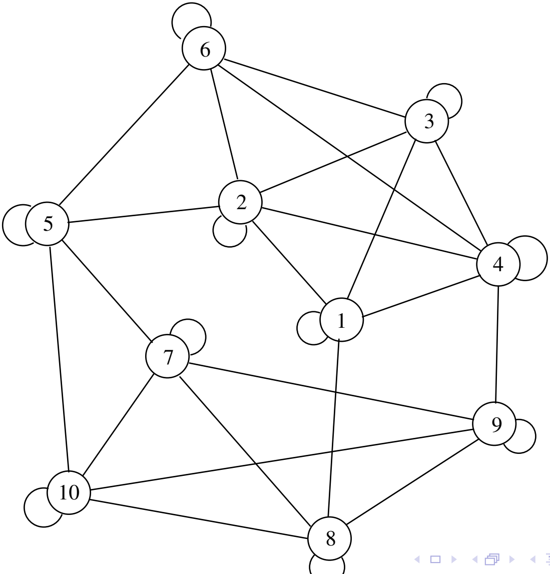
- **Clique**: Set of nodes that are all connected to each other, $\{P \subseteq S | P \times P \subseteq R\}$.
- **Goal**: Find clusters in a graph that are not as dense as cliques but are compact enough within user specified thresholds.

Graph-Theoretic Clustering



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- **Conditional density** $D(Y|X)$ is the number of nodes in the neighborhood of X which have Y as a neighbor,

$$\begin{aligned} D(Y|X) &= \#\{N \in S \mid (N, Y) \in R \text{ and } (X, N) \in R\} \\ &= D(X|Y) \\ &= \#\{\text{Neighborhood}(X) \cap \text{Neighborhood}(Y)\}. \end{aligned}$$

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- $Z(X) = Z(X, J)$ is a **dense region candidate** around X where

$$J = \max\{K \mid \#Z(X, K) \geq K\}$$

  because if M is a major clique of size L, then $X, Y \in M$ implies that $D(Y|X) \geq L$. Thus $M \subseteq Z(X, L)$ and $K \leq L \leq \#Z(X, K)$.

Graph-Theoretic Clustering

- **Association** of a node X to a subset B of S is

$$A(X|B) = \frac{\#\{\text{Neighborhood}(X) \cap B\}}{\#B}$$

where $0 \leq A(X|B) \leq 1$.

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- **Compactness** of a subset B of S is

$$C(B) = \frac{1}{\#B} \sum_{X \in B} A(X|B)$$

where $0 \leq C(B) \leq 1$.

Graph-Theoretic Clustering

- A **dense region** B of the graph (S, R) should satisfy
  1. $B = \{N \in Z(X) \mid A(N|Z(X)) \geq \tau_a\}$ for some $X \in S$,
  2. $C(B) \geq \tau_c$,
  3. $\#B \geq \tau_s$

  where τ_a, τ_c and τ_s are thresholds supplied by the user for minimum association, minimum compactness, and minimum size, respectively.

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$$F = \{(B_1, B_2) \mid B_1, B_2 \text{ are dense regions of } R, \\ \frac{\#B_1 \cap B_2}{\#B_1} \geq \tau_o \text{ or } \frac{\#B_1 \cap B_2}{\#B_2} \geq \tau_o\}$$

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  3. Iterate until no regions can be merged.

Graph-Theoretic Clustering

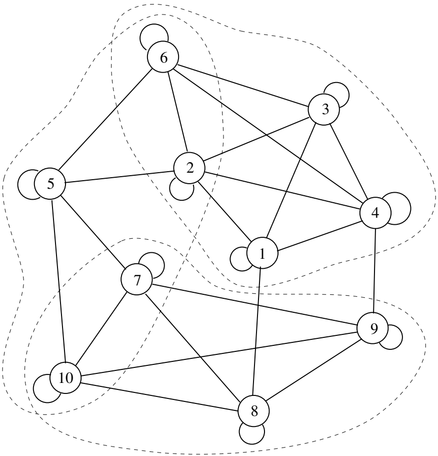

Figure: Clusters found in the example graph using the thresholds $\tau_a = 0.5, \tau_c = 0.6, \tau_s = 3, \tau_o = 0.9$: $\{1, 2, 3, 4, 6\}$ (compactness=0.92), $\{7, 8, 9, 10\}$ (compactness=1.00), $\{2, 5, 6, 7, 10\}$ (compactness=0.68).

Graph-Theoretic Clustering

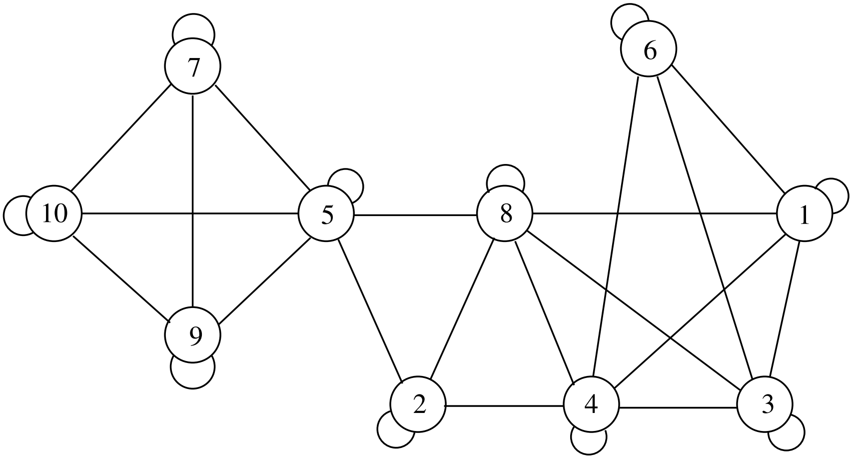

Figure: Another example graph.

Graph-Theoretic Clustering

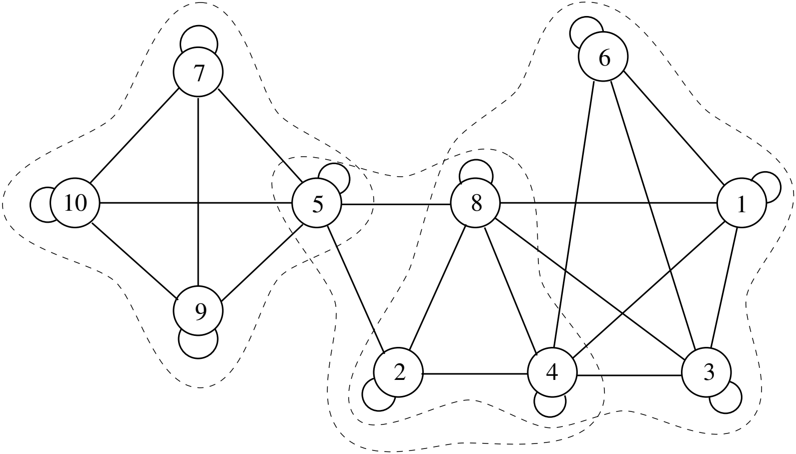

Figure: Clusters found in the second example graph using the thresholds $\tau_a = 0.5, \tau_c = 0.8, \tau_s = 3, \tau_o = 0.75$: $\{1, 2, 3, 4, 6, 8\}$ (compactness=0.78), $\{2, 4, 5, 8\}$ (compactness=0.88), $\{5, 7, 9, 10\}$

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- These may be reasonable assumptions for some applications but are usually unjustified if we are exploring a data set whose properties and structure are unknown.
- Furthermore, most of the iterative algorithms that we use may find a local extremum and may not give the best result.

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  - Evaluating the goodness-of-fit using measures such as the chi-squared or Kolmogorov-Smirnov statistics.
  - Formulating hypothesis tests that check whether multiple clusters found have been formed by chance, and whether the observed change in the error criterion has any significance.