Cluster Analysis I

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Clustering is for?

For Understanding

For Utility

The big picture

- Clustering for Understanding

clustering and classification

  - Human beings are skilled at dividing objects into groups – clustering and assigning objects to existing groups (classification), way before we have statistics, let alone data science.
  - For data analysis: clusters are potential groups, cluster analysis is the study of techniques for automatically finding groups.
  - Broad applications in various fields as a (exploratory) learning approach:

1. Biology: (1) Taxonomy of all living things: Kingdom – phylum – class – order – family – genus – species; (2) Gene expression;

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2. Information retrieval: e.g. group results to your search query.
3. Medicine and Psychology: e.g. identify different types of depression
4. Business: e.g. segment customers for marketing

The big picture

- Clustering for Utility
  - Clustering techniques can characterize each cluster in terms of a cluster prototype – a data object representing of the other objects in the cluster
  1. Summarization – Use cluster prototypes instead entire data set to do analysis, with comparable results
  2. Compression – Tabulate data with "prototype index" – **Vector Quantization** – often applied to image/sound/video data
  3. Finding Nearest Neighbors much more efficiently – far away cluster prototypes tell that their cluster members are less likely (quite impossible) to be nearest neighbors

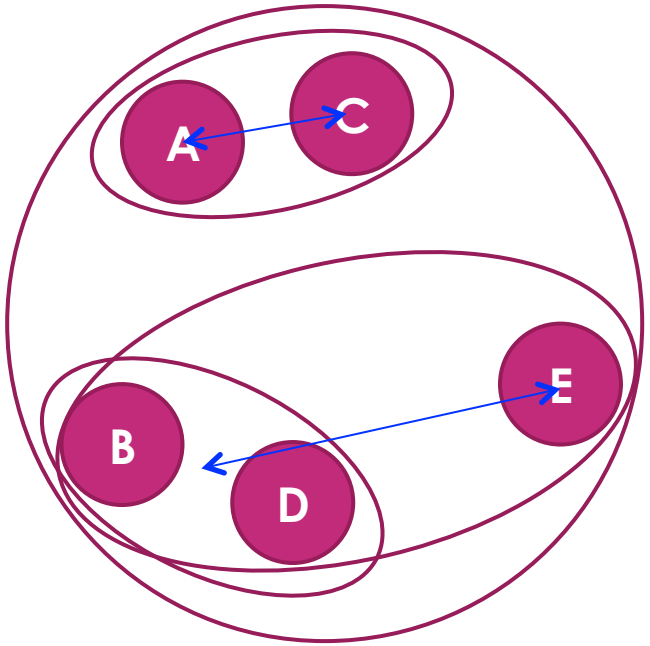
What is Cluster Analysis?

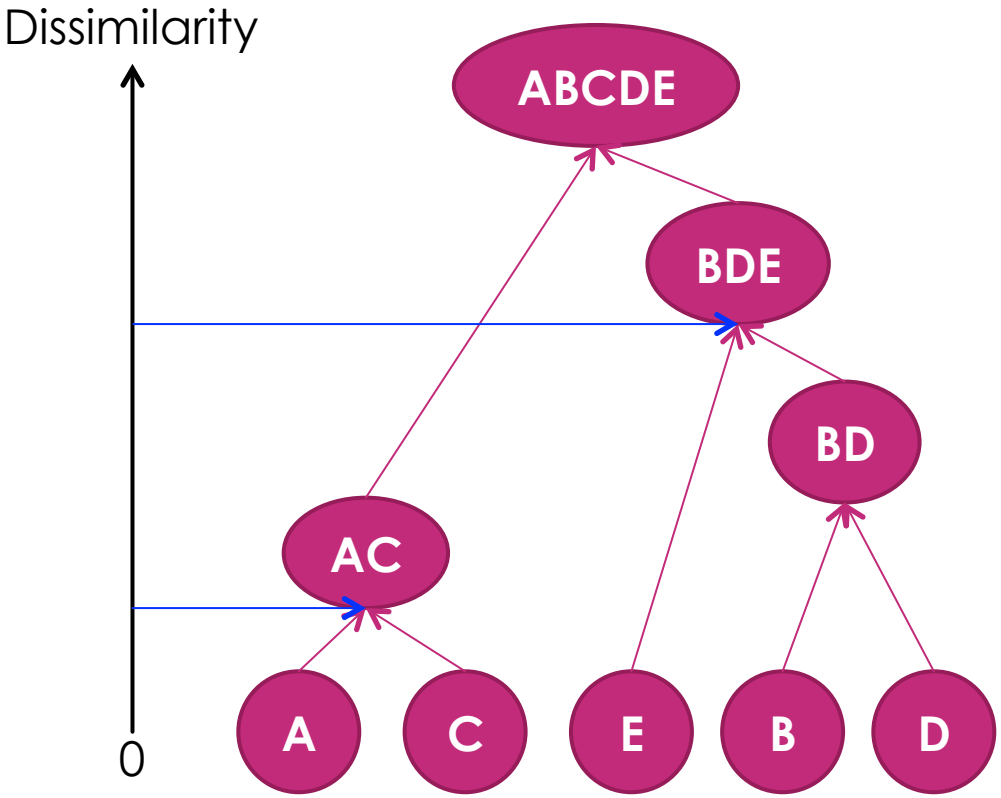
- Definition: To group data objects based on ONLY information found in the data, which tells what are the objects and what are their relationships.
- Goal: Objects in a group are similar to one another, AND different from the objects in other groups [two levels!]
  - The greater the within-group similarity + the greater the between-group difference → the better the clustering
- Cluster analysis vs. Classification – Unsupervised vs. Supervised

Types of Clustering of our focus

1. Hierarchical techniques
   - Agglomerative – build up clusters from individual observations – solve clustering for all possible numbers of cluster at once – choose desired number of cluster afterward
   - Vs. Divisive – start with one group for all and then split off clusters – computational burden
2. K-means clustering
3. Model-based clustering

Agglomerative Hierarchical Clustering





- **Join observations that are closest until only one cluster is left**

Measure dissimilarity between **observations**

- Any dissimilarity we have learnt before can be used
- **Euclidean**
- Manhattan
- Simple matching coefficient

距离度量

$$SMC = \frac{\text{Number of Matching Attributes}}{\text{Number of Attributes}} = \frac{M_{00} + M_{11}}{M_{00} + M_{01} + M_{10} + M_{11}}$$

- Jaccard dissimilarity: Jaccard similarity coefficient is defined as $J(\mathbf{x}, \mathbf{y}) = \frac{\sum_i \min(x_i, y_i)}{\sum_i \max(x_i, y_i)}$, and Jaccard distance is $d_J(\mathbf{x}, \mathbf{y}) = 1 - J(\mathbf{x}, \mathbf{y})$.
- Gower's dissimilarity
- More…

Measure dissimilarity between **groups**

- Inter-individual distance: $d_{ij} = \sqrt{\sum_{k=1}^{q}(x_{ik} - x_{jk})^2}$

三种常见的度量

- Two simple inter-group measures by the IAMA author:

1 $d_{AB} = \min_{\substack{i \in A \\ i \in B}}(d_{ij})$ *Single Linkage Clustering*

2 $d_{AB} = \max_{\substack{i \in A \\ i \in B}}(d_{ij})$ *Complete Linkage Clustering*

Invariant under monotone transformation of the original inter-individual distance

3 $d_{AB} = \frac{1}{n_A n_B}\sum\sum_{i \in A i \in B} d_{ij}$ *Average Linkage Clustering*

Measure dissimilarity between **groups** (cont'd)

- None is perfect, normally choose complete linkage to get started

1. *Single Linkage:* suitable for finding elongated cluster