# Introduction to Clustering

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# What is Clustering?

"Clustering" is a broad term for algorithms in statistics and machine learning that try to discover "natural groups" in data.

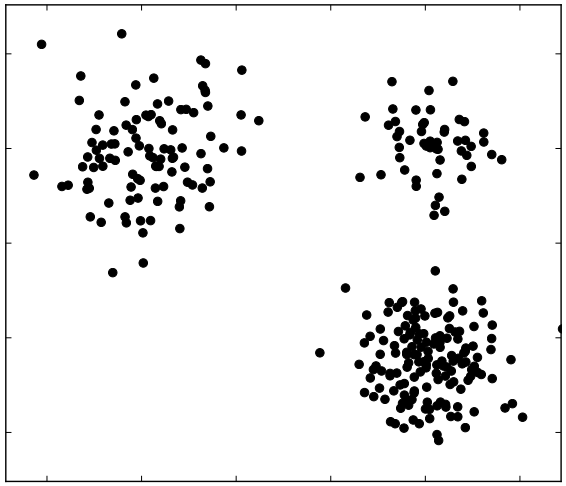
What's a "natural group"?

- Common sense definition: Groups of objects (or variables) where similarity between objects is higher within groups than between groups

# Natural Groups: Geometric Perspective

What's a "natural group"?

- Geometric definition: Patches of high density points surrounded by patches of lower density in the $p$-dimensional space defined by the variates.



# Similarity/Dissimilarity

## Intuition

Similarity is a measure of "likeness" between two entities of interest. Dissimilarity is the complement of similarity.

- Dissimilarities may be converted to similarities (and vise versa) by taking any monotonically decreasing function. For example:

$$s = 1 - d_{ij} \text{ (for } 0 \leq d_{ij} \leq 1)$$

- Dissimilarities are usually in range $0 \leq d_{ij} \leq C$ where $C$ is the maximum dissimilarity
- Distances are one measure of dissimilarity but distances are unbounded to the right

$$d_{ij} \in [0, \infty]$$

# Dissimilarity Measures for Quantitative Data

This simplest measure of dissimilarity is Euclidean distance.

$$d_{ij} = \left\{ \sum_{k=1}^{p} (x_{ik} - x_{jk})^2 \right\}^{1/2}$$

# Dissimilarity Measures for Quantitative Data, cont.

- Manhattan (taxi cab, city block) distance

$$d_{ij} = \sum_{k=1}^{p} |x_{ik} - x_{jk}|$$

- Chebychev distance

$$d_{ij} = max_k \left\{ |x_{ik} - x_{jk}| \right\}$$

- Minkowski Metric

$$d_{ij} = \left\{ \sum_{k=1}^{p} |x_{ik} - x_{jk}|^{\lambda} \right\}^{1/\lambda}$$

$\lambda = 1$ is Manhattan distance, $\lambda = 2$ is Euclidean distance, $\lambda = \infty$ is Chebychev distance.

# Dissimilarity Measures for Variables

Correlation provides a suitable measure of *similarity*. Common *dissimilarity* measures based on correlation include:

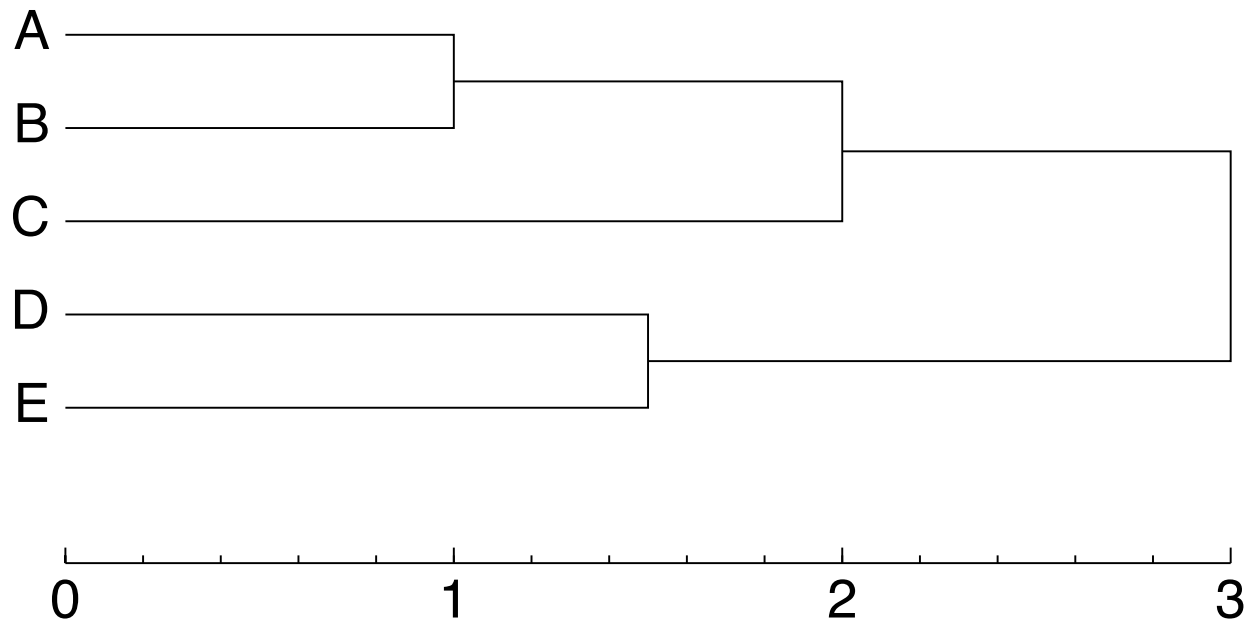
- $d_{kl} = 1 - r_{kl}$ if $r_{kl} = -1$ is taken to indicate maximum disagreement
- $d_{kl} = 1 - r_{kl}^2$ if $r_{kl} = 1$ and $r_{kl} = -1$ are treated equivalently (predictive power)
- Based on uncentered correlation:

$$d_{kl} = 1 - \frac{\sum_{i=1}^{n} x_{ik} x_{il}}{\sum_{i=1}^{n} x_{ik}^2 \sum_{i=1}^{n} x_{il}^2}$$

# Hierarchical Clustering

# Clustering Method: Hierarchical Clustering

For $n$ data points define a set of $n - 1$ "joins" that represent the groupings of objects at different levels of similarity. Represent the series of joins as a "tree" graph.



# Generic Algorithm for Hierarchical Clustering

1. Calculate a dissimilarity matrix for the $n$ items
2. Join the two nearest items, $i$ and $j$
3. Delete the $i$-th and $j$-th rows and columns of the dissimilarity matrix; and a new row/column that represents the dissimilarity of a new group $(i,j)$ to all other items
4. Repeat from step 2 until there is a single group

## Key Point

The different hierarchical clustering methods are determined by the function used to calculate the distance between groups in step 3.

# Single Linkage Clustering

## Group Distance Measure

Let $i$ and $j$ be groups, and $n_i$ and $n_j$ be the number of objects in the respective groups.

$D_{ij}$ is the *smallest* of the $n_i n_j$ dissimilarities between each element of $i$ and each element of $j$

Properties of Single Linkage Clustering

- Invariant under monotonic transformation of the $d_{ij}$
- Unaffected by ties
- Provably nice asymptotic properties
- Disadvantage: susceptible to chaining

# Hierarchical Clustering, Single Linkage Example

Step 1: Calculate Distance Matrix

Step 2: Find closest elements

| | A | B | C | D | E |
|---|---|---|---|---|---|
| A | 0 | | | | |
| B | 4 | 0 | | | |
| C | (1) | 4 | 0 | | |
| D | 4 | 2 | 4 | 0 | |
| E | 5 | 5 | 3 | 4 | 0 |

Step 3: Update distance matrix

| | (A,C) | B | D | E |
|---|---|---|---|---|
| (A,C) | 0 | | | |
| B | 4 | 0 | | |
| D | 4 | 2 | 0 | |
| E | 3 | 5 | 4 | 0 |

# Worked Example, cont.

Repeat from Step 2

| | (A,C) | B | D | E |
|---|---|---|---|---|
| (A,C) | 0 | | | |
| B | 4 | 0 | | |
| D | 4 | (2) | 0 | |
| E | 3 | 5 | 4 | 0 |

| | (A,C) | (B,D) | E |
|---|---|---|---|
| (A,C) | 0 | | |
| (B,D) | 4 | 0 | |
| E | 3 | 4 | 0 |

Repeat from Step 2

| | (A,C) | (B,D) | E |
|---|---|---|---|
| (A,C) | 0 | | |
| (B,D) | 4 | 0 | |
| E | (3) | 4 | 0 |

| | ((A,C),E) | (B,D) |
|---|---|---|
| ((A,C),E) | 0 | |
| (B,D) | 4 | 0 |

# Worked Example, cont.

Repeat from Step 2

| | ((A,C),E) | (B,D) |
|---|---|---|
| ((A,C),E) | 0 | |
| (B,D) | (4) | 0 |

| Final Join |
|---|
| (((A,C),E),(B,D)) |

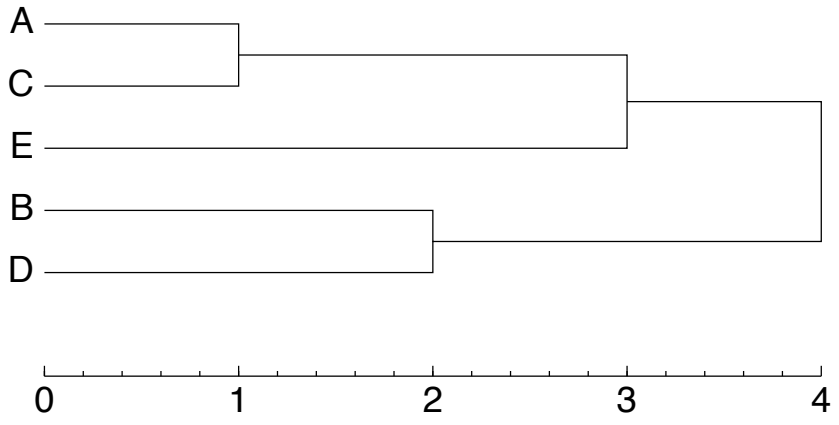



Figure: Final dendrogram for worked example

# More Hierarchical Clustering Functions

Complete Linkage – $D_{ij}$ is the maximum of the $n_i n_j$ dissimilarities between the two groups.

Group Average Methods – $D_{ij}$ is the average of the $n_i n_j$ dissimilarities between the two group (UPGMA, WPGMA)

Centroid Method – $D_{ij}$ is the squared Euclidean distance between the centroids of groups $i$ and $j$

# K-means Clustering

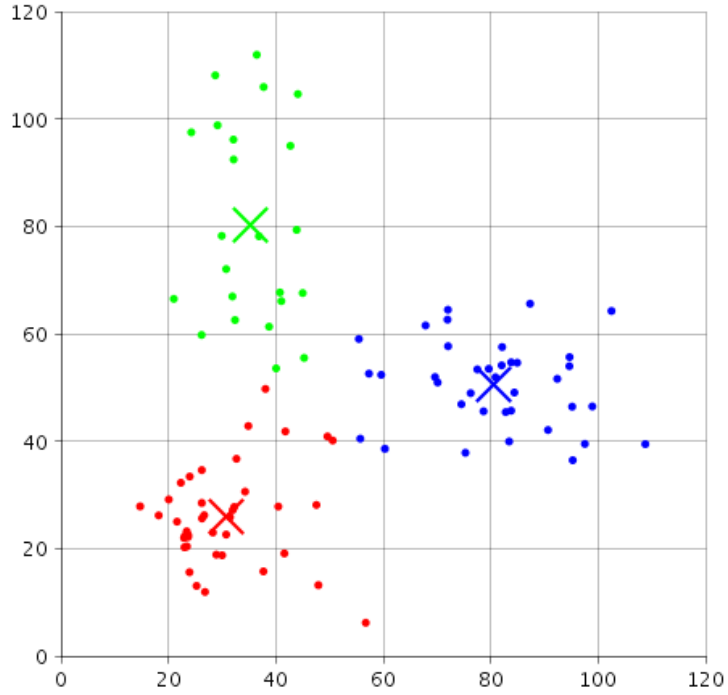
# K-mean Clustering

## General idea

Assign the $n$ data points (or $p$ variables) to one of $K$ clusters to as to optimize some criterion of interest.

- The most common criterion to minimize is the sum-of-squares from the group centroids.

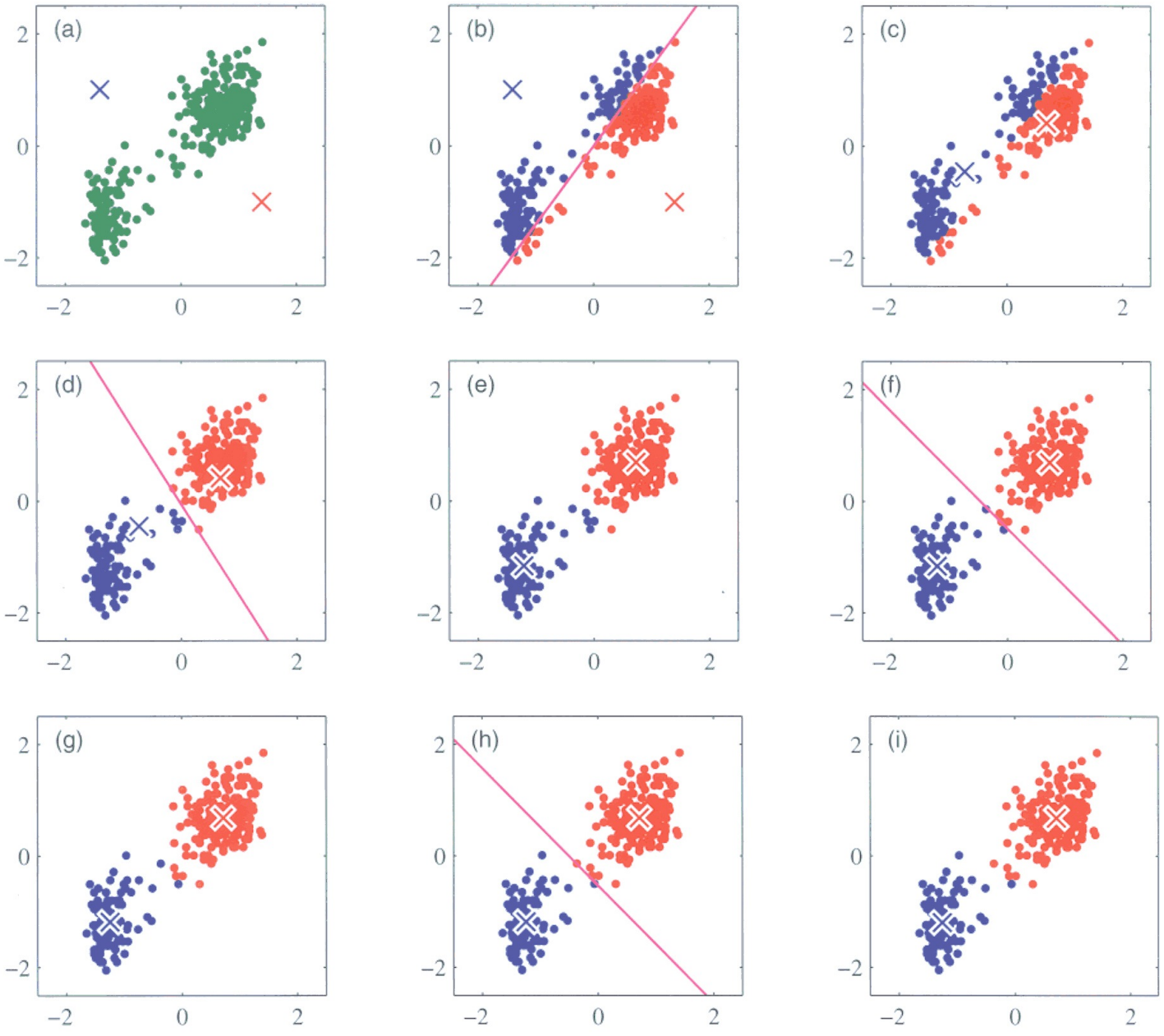
$$V = \sum_{i=1}^{k} \sum_{j \in g_i} |x_j - \mu_i|^2$$



# Simple algorithm for K-means clustering

1. Decide on $k$, the number of groups
2. Randomly pick $k$ of the objects to act as the initial centers
3. Assign each object to the group whose center it is closest to
4. Recalculate the $k$ centers as the centroids of the objects assigned to them
5. Repeat from step 3 until centroids no longer move (convergence)

# Illustration of K-means algorithm



# Things to note re: K-means clustering

- The algorithm described above does not necessarily find the global optimum
- The algorithm is sensitive to choice of initial cluster center; k-means is often run multiple-time with different initial centers to insure inferred clusters are robust.