CS 2750 Machine Learning
Lecture 18

Clustering

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Clustering

Groups together "similar" instances in the data sample

Basic clustering problem:

- distribute data into *k* different groups such that data points similar to each other are in the same group
- Similarity between data points is defined in terms of some distance metric (can be chosen)

Clustering is useful for:

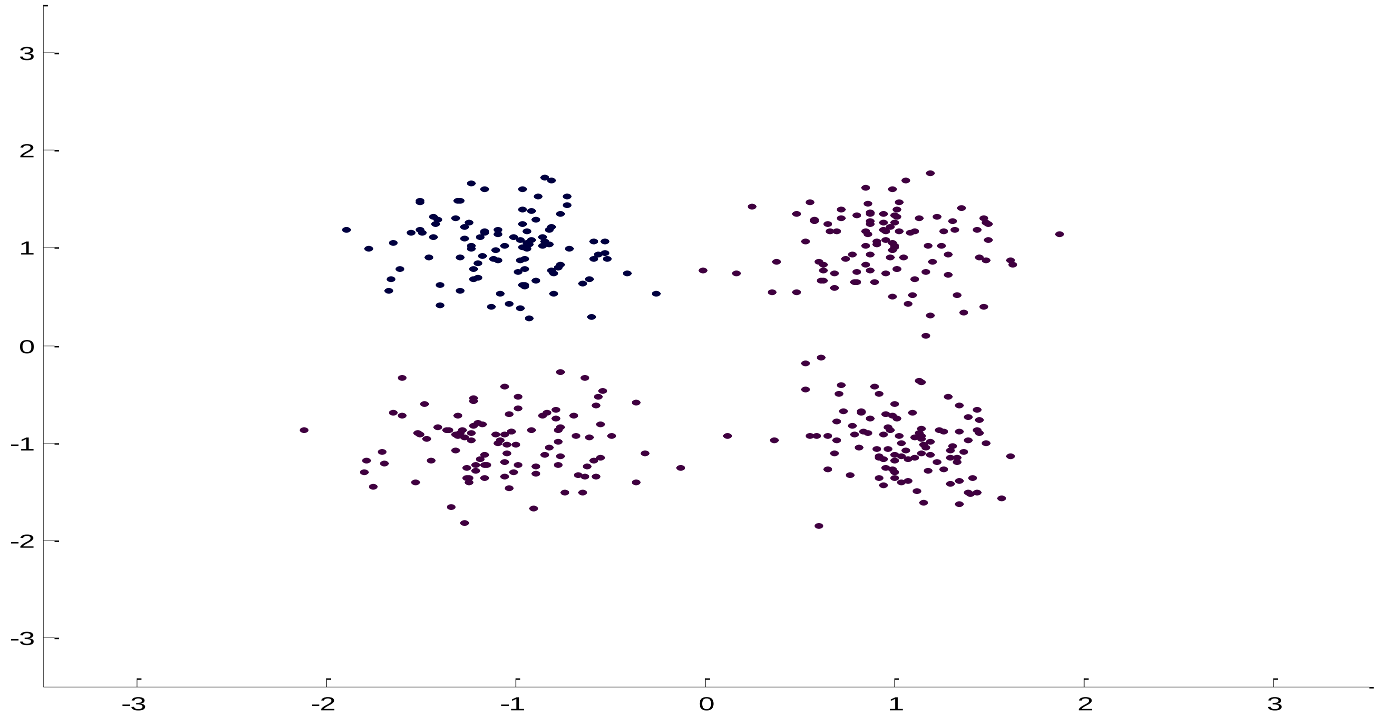
- **Similarity/Dissimilarity analysis**

  Analyze what data points in the sample are close to each other
- **Dimensionality reduction**

  High dimensional data replaced with a group (cluster) label

Clustering example

- We see data points and want to partition them into groups
- Which data points belong together?



Clustering example

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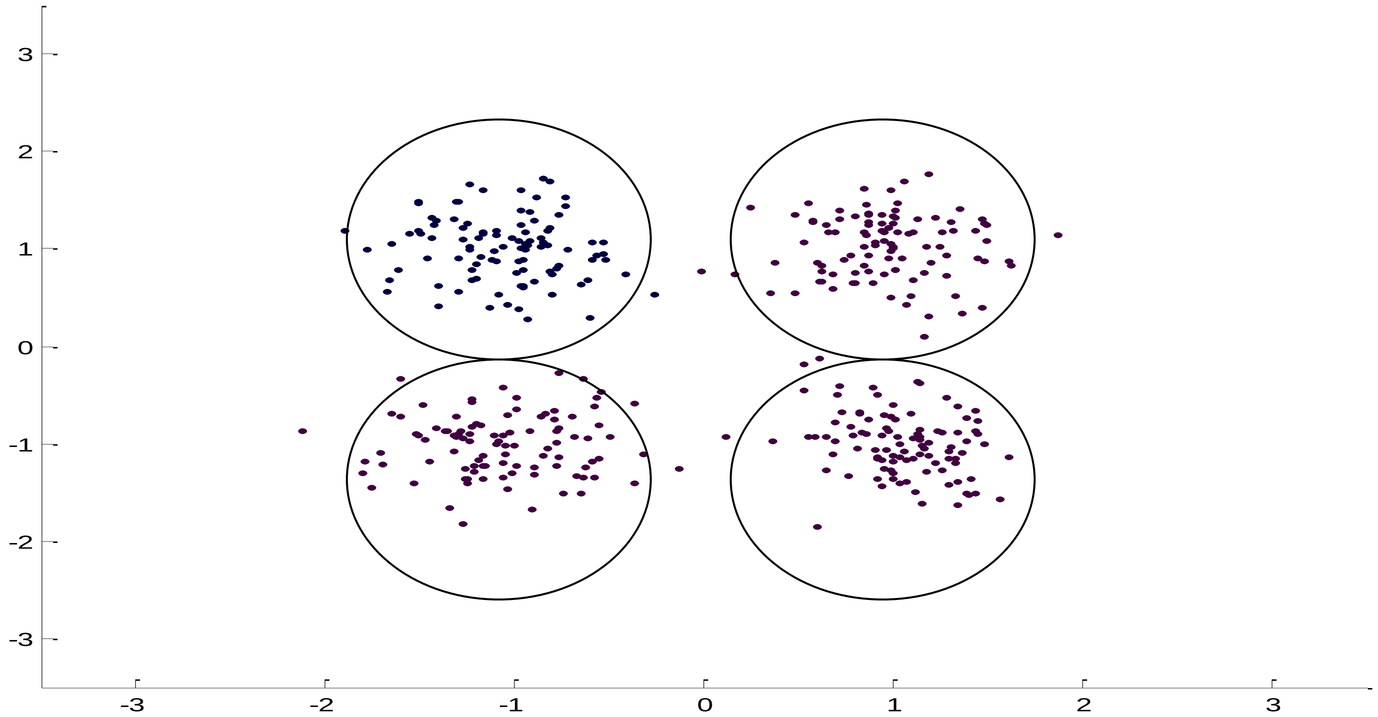
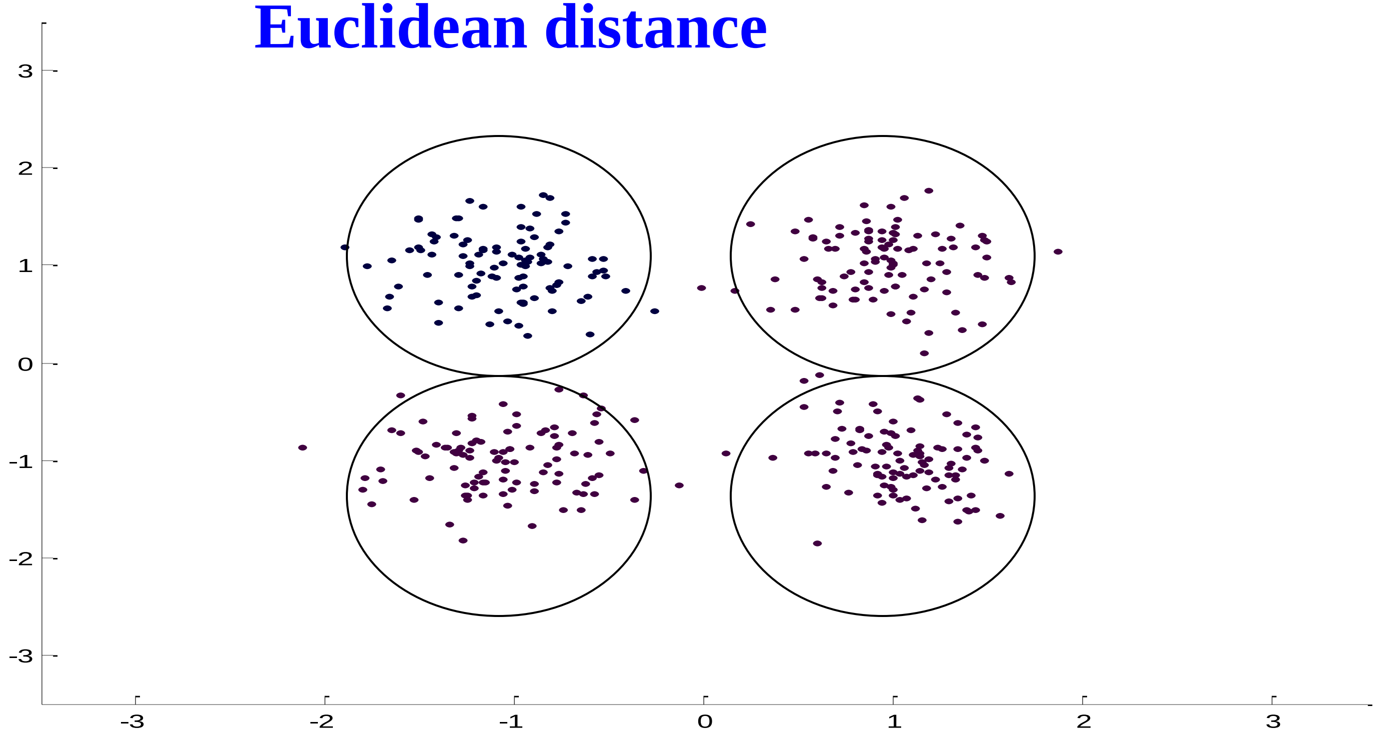


Clustering example

- We see data points and want to partition them into the groups
- Requires a distance measure to tell us what points are close to each other and are in the same group

Euclidean distance



Clustering example

- A set of patient cases
- We want to partition them into groups based on similarities

Patient #	Age	Sex	Heart Rate	Blood pressure …
Patient 1	55	M	85	125/80
Patient 2	62	M	87	130/85
Patient 3	67	F	80	126/86
Patient 4	65	F	90	130/90
Patient 5	70	M	84	135/85

Clustering example

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How to design the distance metric to quantify similarities?

Clustering example. Distance measures.

In general, one can choose an arbitrary distance measure.

Properties of distance metrics:

Assume 2 data entries *a*, *b*

Positiveness: $d(a,b) \geq 0$

Symmetry: $d(a,b) = d(b,a)$

Identity: $d(a,a) = 0$

Distance measures.

Assume pure real-valued data-points:

12	34.5	78.5	89.2	19.2
23.5	41.4	66.3	78.8	8.9
33.6	36.7	78.3	90.3	21.4
17.2	30.1	71.6	88.5	12.5

...

What distance metric to use?

Distance measures

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…

What distance metric to use?

Euclidian: works for an arbitrary k-dimensional space

$$d(a,b) = \sqrt{\sum_{i=1}^{k}(a_i - b_i)^2}$$

Distance measures

Assume pure real-valued data-points:

12	34.5	78.5	89.2	19.2
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What distance metric to use?

Squared Euclidian: works for an arbitrary k-dimensional space

$$d^2(a,b) = \sum_{i=1}^{k} (a_i - b_i)^2$$

Distance measures.

Assume pure real-valued data-points:

12	34.5	78.5	89.2	19.2
23.5	41.4	66.3	78.8	8.9
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Manhattan distance:

works for an arbitrary k-dimensional space

$$d(a,b) = \sum_{i=1}^{k} | a_i - b_i |$$

Etc. ..

Γ^{-1}

Distance measures

Generalized distance metric:

$$d^2(\mathbf{a},\mathbf{b}) = (\mathbf{a}-\mathbf{b})\boldsymbol{\Gamma}^{-1}(\mathbf{a}-\mathbf{b})^T$$

Γ semi-definite positive matrix

Γ^{-1} is a matrix that weights attributes proportionally to their importance. Different weights lead to a different distance metric.

If $\Gamma = I$ we get squared Euclidean

$\Gamma = \Sigma$ (covariance matrix) – we get the Mahalanobis distance that takes into account correlations among attributes

Distance measures.

Assume pure binary values data:

0	1	1	0	1
1	0	1	0	1
0	1	1	0	1
1	1	1	1	1
…				

What distance metric to use?

Distance measures.

Assume pure binary values data:

0	1	1	0	1
1	0	1	0	1
0	1	1	0	1
1	1	1	1	1
…				

What distance metric to use?

Hamming distance: The number of bits that need to be changed to make the entries the same

How about Euclidean distance?

Distance measures.

Assume pure categorical data:

0	1	1	0	0
1	0	3	0	1
2	1	1	0	2
1	1	1	1	2

…

What distance metric to use?

Hamming distance: The number of number of values that need to be changed to make them the same

Distance measures.

Combination of real-valued and categorical attributes

Patient #	**Age**	**Sex**	**Heart Rate**	**Blood pressure …**
Patient 1	55	M	85	125/80
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What distance metric to use?

Distance measures.

Combination of real-valued and categorical attributes

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What distance metric to use?

A weighted sum approach: e.g. a mix of Euclidian and Hamming distances for subsets of attributes

Clustering

Clustering is useful for:

- **Similarity/Dissimilarity analysis**

  Analyze what data points in the sample are close to each other
- **Dimensionality reduction**

  High dimensional data replaced with a group (cluster) label
- **Data reduction:** Replaces many datapoints with the point representing the group mean

Problems:

- Pick the correct similarity measure (problem specific)
- Choose the correct number of groups
  - Many clustering algorithms require us to provide the number of groups ahead of time

Clustering algorithms

- **K-means algorithm**
  - **suitable** only when data points have continuous values; groups are defined in terms of cluster centers (also called **means**). Refinement of the method to categorical values: **K-medoids**
- **Probabilistic methods (with EM)**
  - **Latent variable models**: class (cluster) is represented by a latent (hidden) variable value
  - Every point goes to the class with the highest posterior
  - **Examples:** mixture of Gaussians, Naïve Bayes with a hidden class
- **Hierarchical methods**
  - **Agglomerative**
  - **Divisive**

K-means

K-Means algorithm:

Initialize randomly k values of means (centers)

Repeat two steps until no change in the means:

– Partition the data according to the current set of means (using the similarity measure)

– Move the means to the center of the data in the current partition

Stop when no change in the means

Properties:

- Minimizes the sum of **squared center-point distances** for all clusters

$$\arg\min_{S} \sum_{i=1}^{k} \sum_{x_j \in S_i} \left\| x_j - u_i \right\|^2$$

- The algorithm always converges (to the local optima).

K-means algorithm

- **Properties:**
  - converges to centers minimizing the sum of squared center-point distances (still local optima)
  - The result is sensitive to the initial means' values
- **Advantages:**
  - Simplicity
  - Generality – can work for more than one distance measure
- **Drawbacks:**
  - Can perform poorly with overlapping regions
  - Lack of robustness to outliers
  - Good for attributes (features) with continuous values
    - Allows us to compute cluster means
    - k-medoid algorithm used for discrete data

Probabilistic (EM-based) algorithms

- **Latent variable models**

  Examples: Naïve Bayes with hidden class

  Mixture of Gaussians

- **Partitioning:**
  - the data point belongs to the class with the highest posterior
- **Advantages:**
  - Good performance on overlapping regions
  - Robustness to outliers
  - Data attributes can have different types of values
- **Drawbacks:**
  - EM is computationally expensive and can take time to converge
  - Density model should be given in advance

Hierarchical clustering.

Uses an arbitrary similarity/dissimilarity measure.

Typical similarity measures *d(a,b)* :

Pure real-valued data-points:

- Euclidean, Manhattan, Minkowski distances

Pure binary values data:

- Hamming distance - Number of matching values
- the same as Euclidean

Pure categorical data:

- Number of matching values

Combination of real-valued and categorical attributes

- Weighted, or Euclidean

Hierarchical clustering

Approach:

- **Compute dissimilarity matrix for all pairs of points**
  – uses standard or other distance measures
- **Construct clusters greedily:**
  – **Agglomerative approach**
    - Merge pair of clusters in a bottom-up fashion, starting from singleton clusters
  – **Divisive approach:**
    - Splits clusters in top-down fashion, starting from one complete cluster
- **Stop the greedy construction** when some criterion is satisfied
  – E.g. fixed number of clusters

Cluster merging

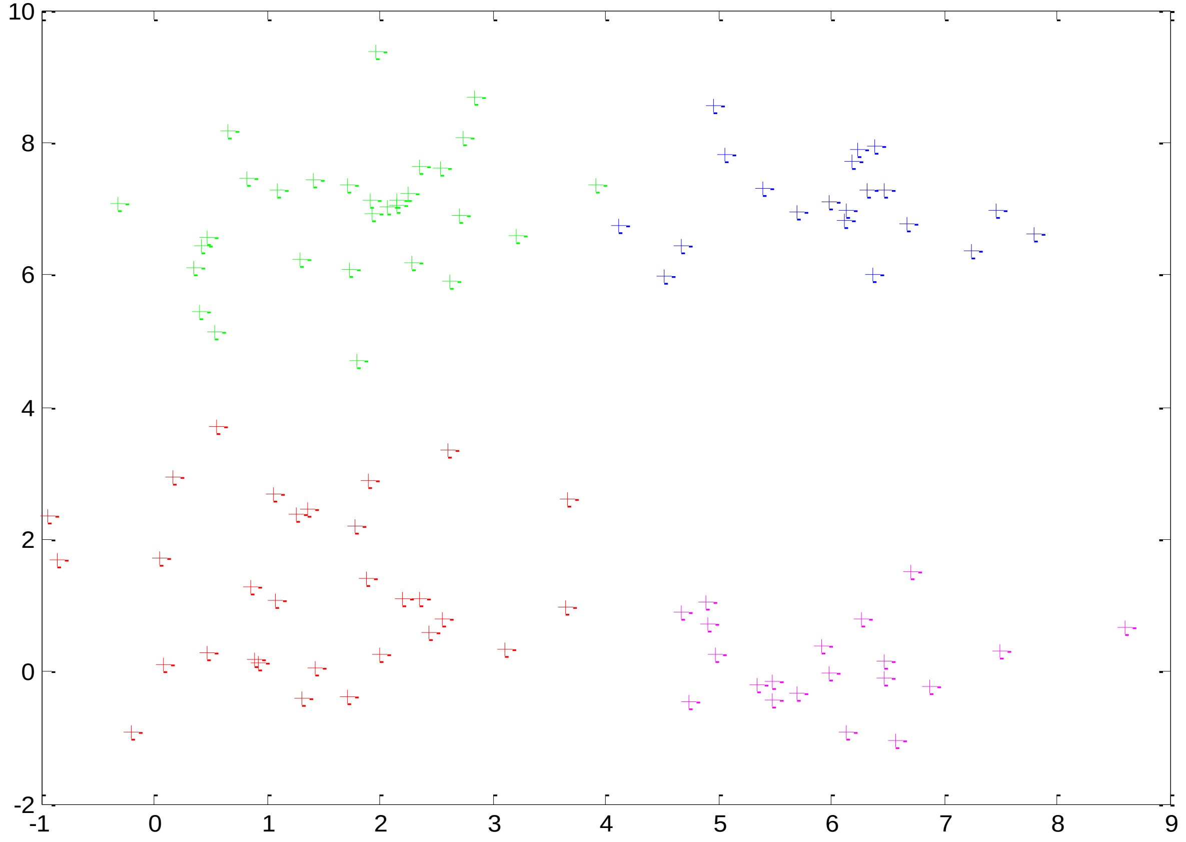
- **Construction of clusters through greedy agglomerative approach**
  - Merge pair of clusters in a bottom-up fashion, starting from singleton clusters
  - Merge clusters based on **cluster (or linkage) distances**. Defined in terms of point distances. **Examples:**

Min distance $$d_{\min}(C_i, C_j) = \min_{p \in C_i, q \in C_j} d(p,q)$$

Max distance $$d_{\max}(C_i, C_j) = \max_{p \in C_i, q \in C_j} d(p,q)$$

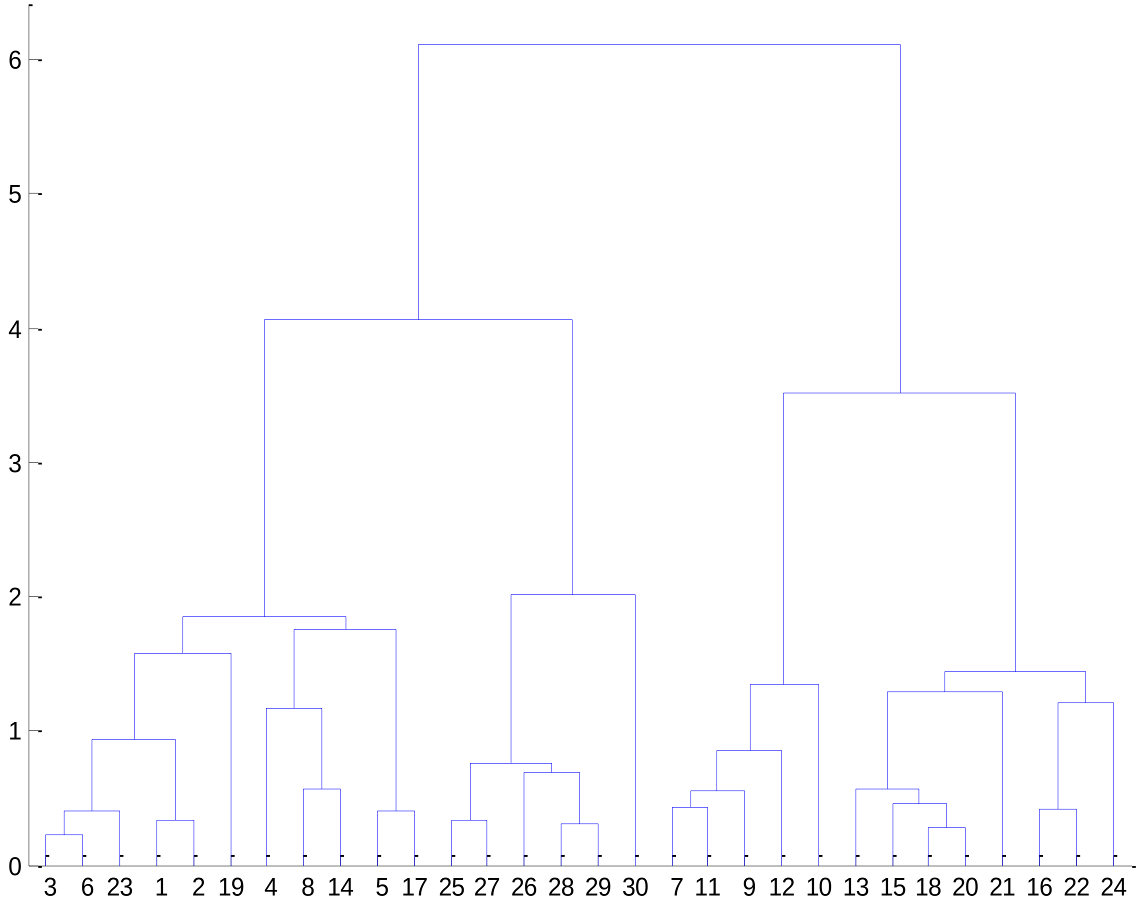
Mean distance $$d_{mean}(C_i, C_j) = \left| d\left(\frac{1}{|C_i|} \sum_i p_i ; \frac{1}{|C_j|} \sum_j q_j \right) \right|$$

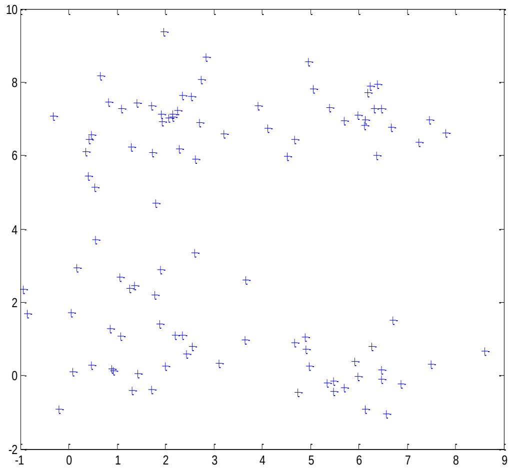
Hierarchical clustering example



Hierarchical clustering example

- **dendogram**





Hierarchical clustering

- **Advantage:**
  – Smaller computational cost; avoids scanning all possible clusterings
- **Disadvantage:**
  – Greedy choice fixes the order in which clusters are merged; cannot be repaired
- **Partial solution:**
    - combine hierarchical clustering with iterative algorithms like k-means

Other clustering methods

- **Spectral clustering**
  - Uses similarity matrix

- **Multidimensional scaling**
  - techniques often used in data visualization for exploring similarities or dissimilarities in data.