CS 1675 Introduction to Machine Learning
Lecture 18

Clustering

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Clustering

Groups together "similar" instances in the data sample

Basic clustering problem:

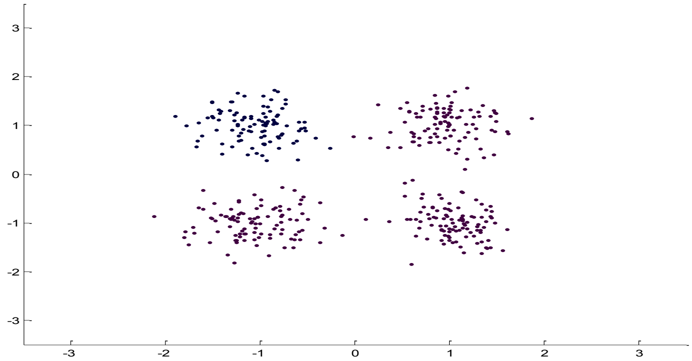
- distribute data into *k* different groups such that data points similar to each other are in the same group
- Similarity between data points is defined in terms of some distance metric (can be chosen)

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?



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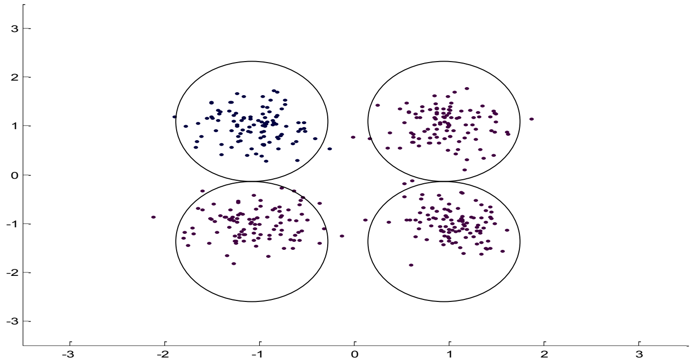
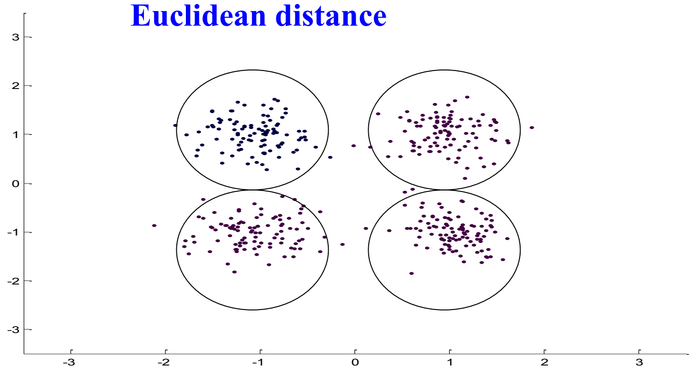


Clustering example

- We see data points and want to partition them into the groups
- Requires **a dissimilarity or a similarity measure** to tell us what points are close (similar) to each other and are in the

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

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How to design the dissimilarity/similarity measure to quantify similarities?

Similarity and dissimilarity measures

- **Dissimilarity measure**
  - Numerical measure of how different two data objects are
  - Often expressed in terms **of a distance metrics**
  - Euclidean:

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

- **Similarity measure**
  - Numerical measure of how alike two data objects are
  - Examples:
    - Gaussian kernel:

$$K(a,b) = \frac{1}{\left(2\pi h^2\right)^{d/2}} \exp\left[-\frac{\| a-b \|_2^2}{2h^2}\right]$$

    - Cosine similarity: $K(a,b) = a^T b$

Distance metrics

Dissimilarity is often measured with the help of a distance metrics.

Properties of distance metrics:

Assume 2 data entries *a, b*

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

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

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

Triangle inequality: $d(a,c) \leq d(a,b) + d(b,c)$

Distance metrics

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 metrics

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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 metrics

Assume pure real-valued data-points:

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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 metrics

Assume pure real-valued data-points:

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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

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:

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

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 categorical data where integers represent the different categories:

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?

Distance measures

Assume categorical data where integers represent the different categories:

0	1	1	0	0
1	0	3	0	1
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…

What distance metric to use?

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

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
…

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

How about squared Euclidean?

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

Distance measures.

Assume pure binary values data:

0 1 1 0 1
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One metric is the **Hamming distance:** The number of bits that need to be changed to make the entries the same

How about the squared Euclidean?

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

The same as Hamming distance.

Distance measures

Combination of real-valued and categorical attributes

Patient #	Age	Sex	Heart Rate	Blood pressure …
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What distance metric to use?

Distance measures.

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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

Distance metrics and similarity

- **Dissimilarity/distance measure**
  - Numerical measure of how different two data objects are
  - Expressed in terms of distance metrics
- **Similarity measure**
  - Numerical measure of how alike two data objects are
  - Example: Gaussian kernel:

$$K(a,b) = \frac{1}{\left(2\pi h^2\right)^{d/2}} \exp\left[-\frac{\| a-b \|_2^2}{2h^2}\right]$$

  - Cosine similarity:

$$K(a,b) = a^T b$$

  - Do not have to satisfy the properties like the ones for the distance metric

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 data-points with a point representing the group mean

Challenges:

- How to measure similarity (problem/data specific)?
- How to choose the 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) = soft clustering**
  - **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**

Clustering algorithms

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K-means clustering algorithm

- an iterative clustering algorithm
- works in the d-dimensional *R* space representing **x**

K-Means clusterting algorithm:

Initialize randomly *k* values of means (centers)

Repeat

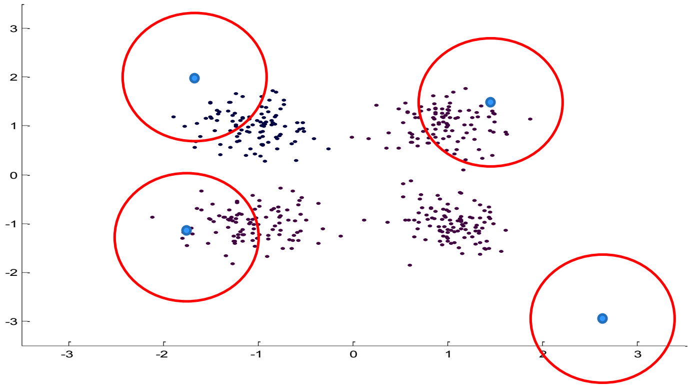
– Partition the data according to the current set of means (using the similarity measure)

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

Until no change in the means

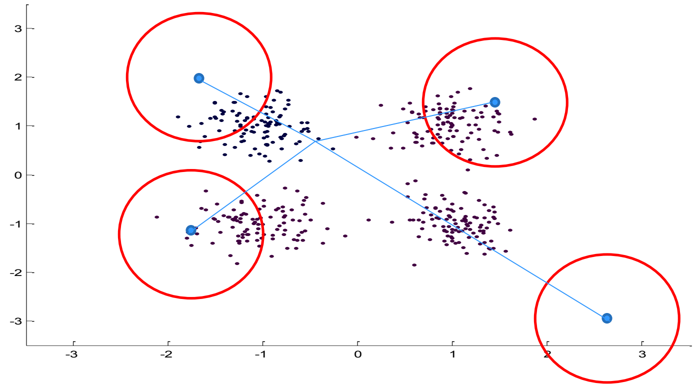
K-means: example

- **Initialize the cluster centers**



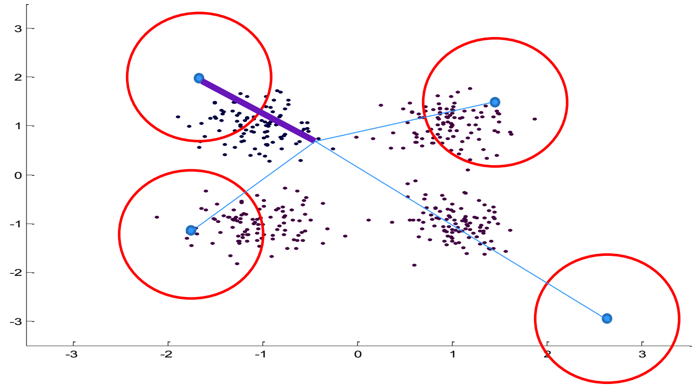
K-means: example

- Calculate the distances of each point to all centers



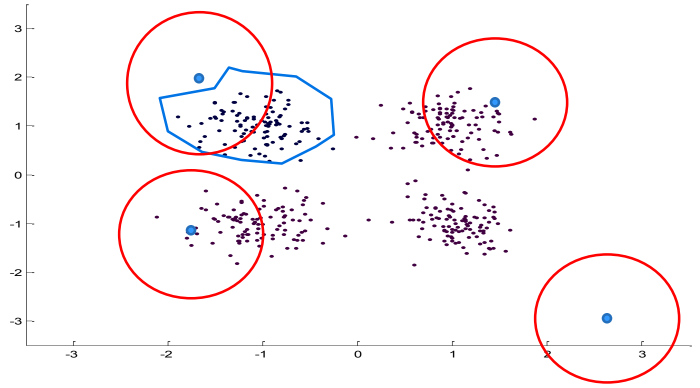
K-means: example

- For each example pick the best (closest) center



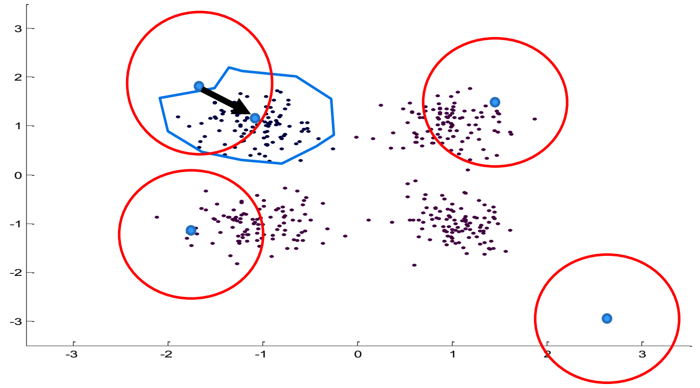
K-means: example

- Recalculate the new mean from all data examples assigned to the same cluster center



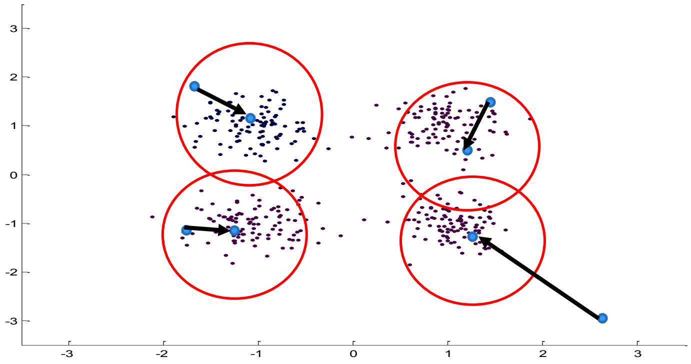
K-means: example

- Shift the cluster center to the new mean



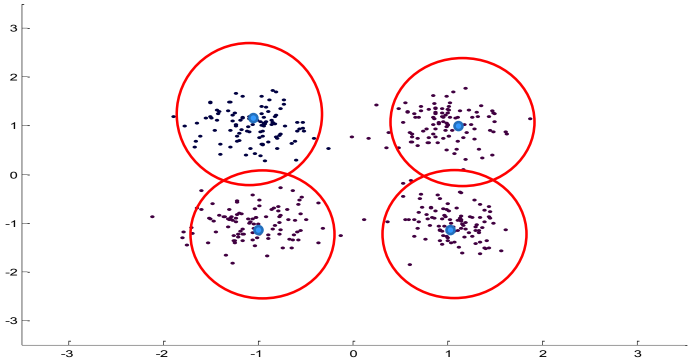
K-means: example

- Shift the cluster centers to the new calculated means



K-means: example

- And repeat the iteration …
- Till no change in the centers



K-means clustering algorithm

K-Means algorithm:

Initialize randomly *k* values of means (centers)

Repeat

– 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

Until no change in the means

Properties:

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

$$\min_{S} \sum_{i=1}^{k} \sum_{x_j \in S_i} || x_j - u_i ||^2 \qquad u_i = \text{center of cluster } S_i$$

K-means clustering 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

Clustering algorithms

- K-means algorithm
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  - **Examples:** mixture of Gaussians, Naïve Bayes with a hidden class
- Hierarchical methods
  - Agglomerative
  - Divisive

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

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Hierarchical clustering

Can use many different dissimilarity measures

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

Pure real-valued data-points:

– Euclidean, Manhattan, Minkowski distances

Pure categorical data:

– Hamming distance, Number of matching values

Combination of real-valued and categorical attributes

– Weighted, or Euclidean

Hierarchical clustering

Two versions of the hierarchical clustering

- **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

Hierarchical (agglomerative) 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
- **Stop the greedy construction** when some criterion is satisfied
  - E.g. fixed number of clusters

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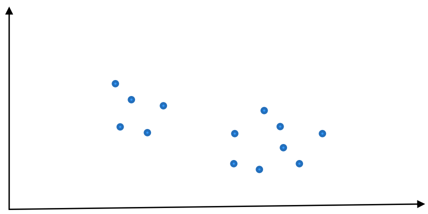

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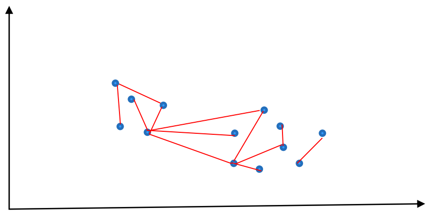

N datapoints, $O(N^2)$ pairs, $O(N^2)$ distances

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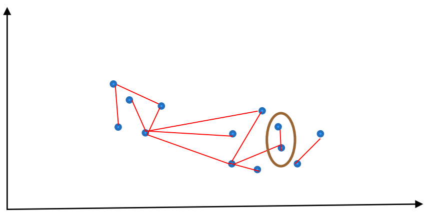

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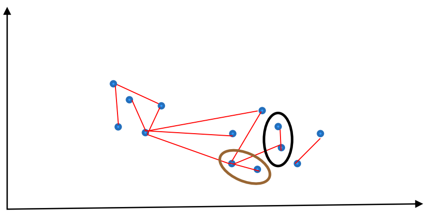

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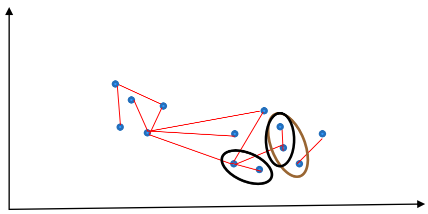

Hierarchical (agglomerative) clustering

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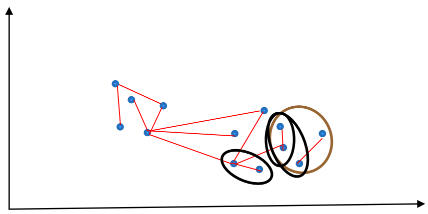
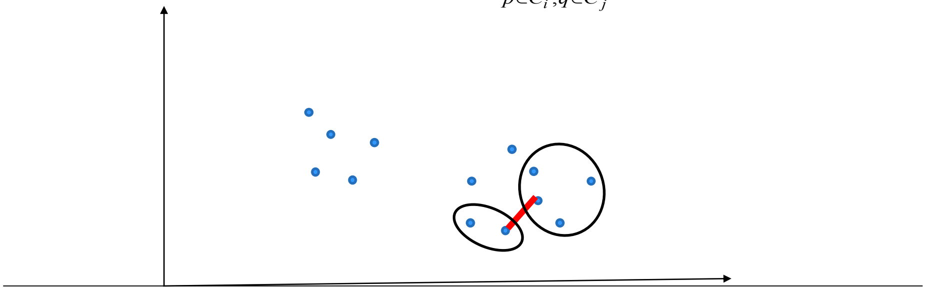


Cluster merging

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



Cluster merging

- **Agglomerative approach**
  - Merge pair of clusters in a bottom-up fashion, starting from singleton clusters
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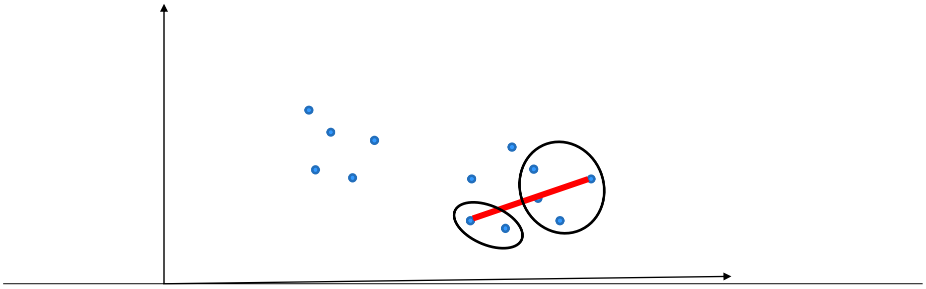
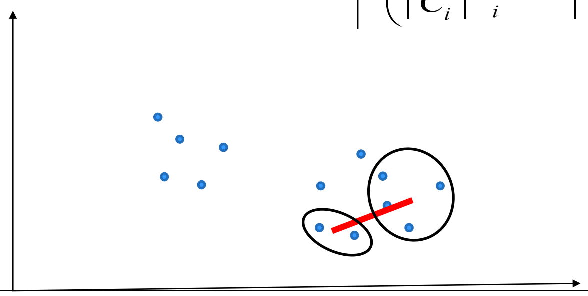
Max distance $$d_{\max}(C_i, C_j) = \max_{p \in C_i, q \in C_j} d(p,q)$$



Cluster merging

- **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:**

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 (agglomerative) clustering

Approach:

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- **Construct clusters greedily:**
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    - Merge pair of clusters in a bottom-up fashion, starting from singleton clusters
- **Stop the greedy construction** when some criterion is satisfied
  - E.g. fixed number of clusters

Hierarchical (divisive) clustering

Approach:

- **Compute dissimilarity matrix for all pairs of points**
  - uses standard distance or other dissimilarity 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
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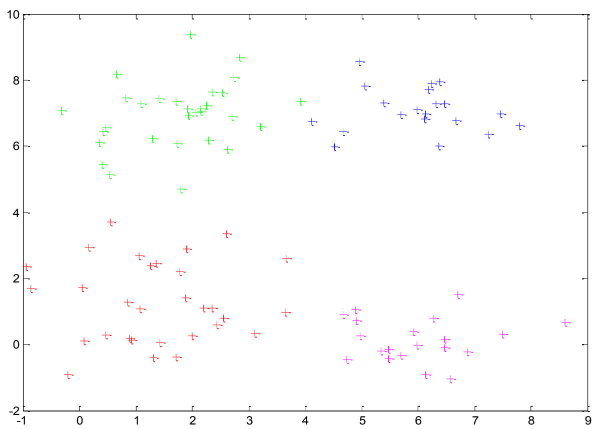
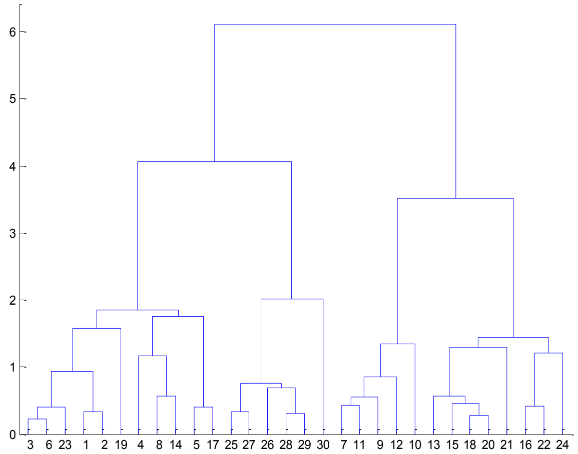
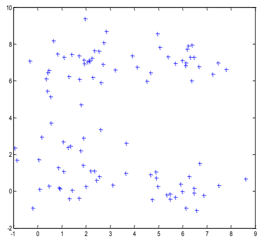
Hierarchical clustering example



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 algorithm

Other clustering methods

- **Spectral clustering**
  - Uses similarity matrix and its spectral decomposition (eigenvalues and eigenvectors)

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