## CS 2750 Machine Learning
## Lecture 19

# Clustering

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## Clustering

Groups together "similar" instances in the data sample

**Basic clustering problem:**

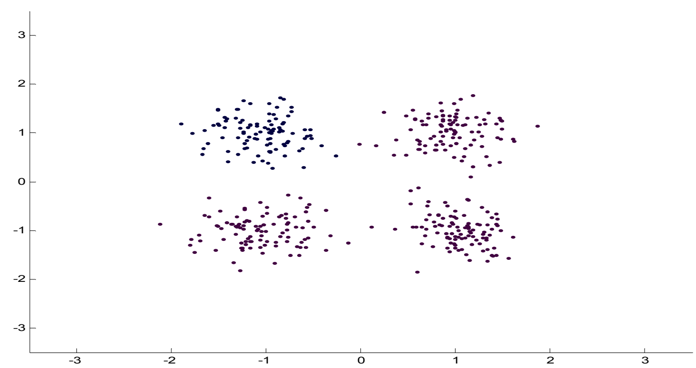
- distribute data into *k* different groups such that data points similar to each other are in the same group
- Similarity between data points is defined in terms of some distance metric (can be chosen)

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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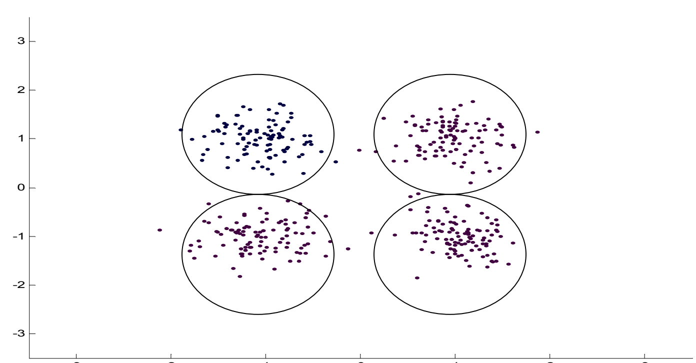
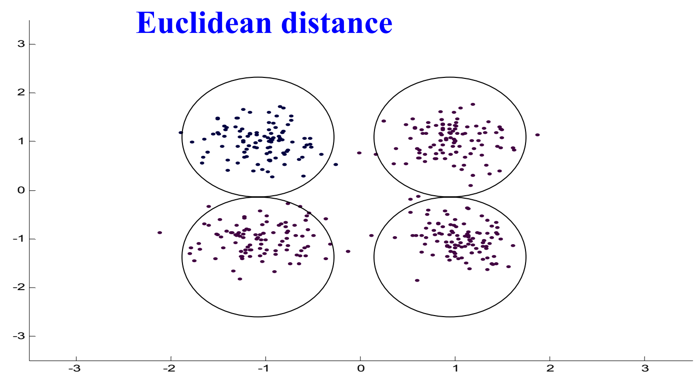


# Clustering example

- 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






# Clustering example

- A set of patient cases
- We want to partition them into the 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 distance metric to quantify similarities?**



## Clustering example. Distance measures.

**In general, one can choose an arbitrary distance measure.**

**Properties of the distance measures:**

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.

**Assume pure real-valued data-points:**

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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:**

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What distance metric to use?

**Manhattan:** works for an arbitrary k-dimensional space

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

Etc. ..



## 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?

**Edit distance:** The number of attributes that need to be changed to make the entries the same

**The same metric can be used for pure categorical values**



## 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.

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What distance metric to use?

**A weighted sum approach: e.g. a mix of Euclidian and Edit 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

**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

**Partitioning 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.
  - **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:

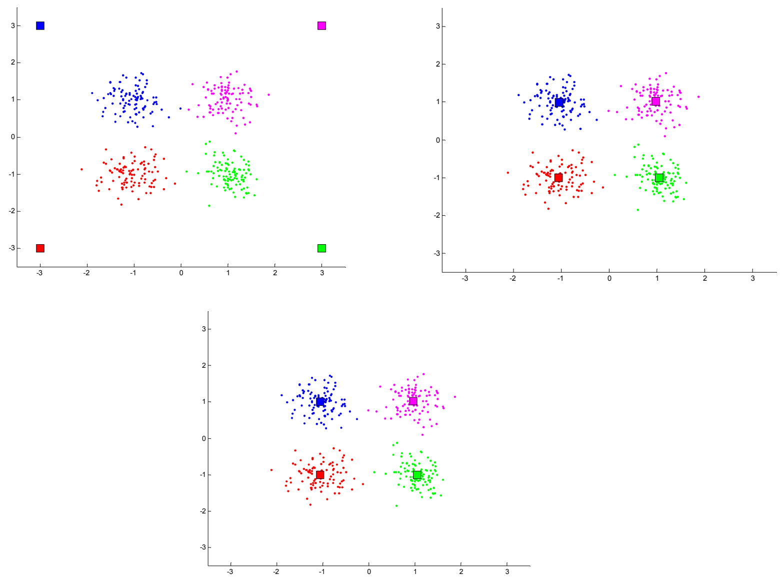
- Partition the data according to the current set of means (using the similarity measure)
- Move the means to the center of the data in the current partition

Stop when no change in the means

**Properties:**

- Minimizes the sum of squared center-point distances for all clusters
- The algorithm always converges (local optima).

# K-Means example





# 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

## 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:**
– Number of matching values

**Pure categorical data:**
– Number of matching values

**Combination of real-valued and categorical attributes**
– A weighted sum approach

## 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

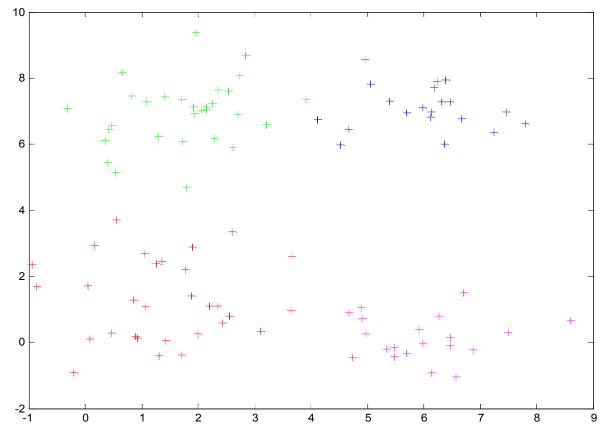
- **Construction of clusters through greedy agglomerative approach**
  - Merge pair of clusters in a bottom-up fashion, starting from singleton clusters
  - Merge clusters based on cluster (or linkage) distances. Defined in terms of point distances. **Examples:**

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

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

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

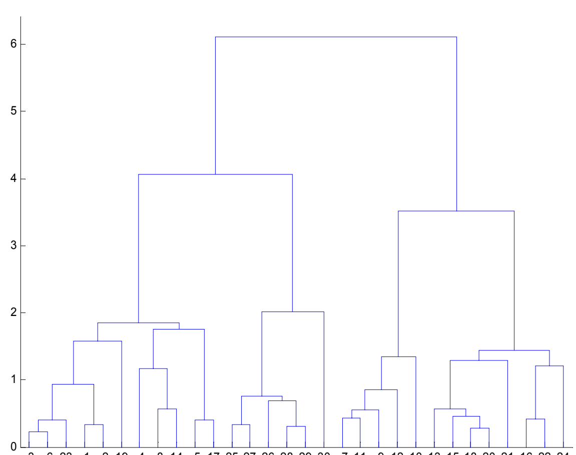
# Hierarchical clustering example

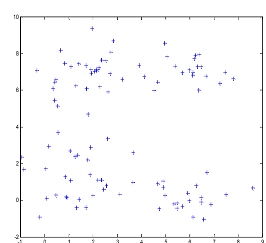





# Hierarchical clustering example

- **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