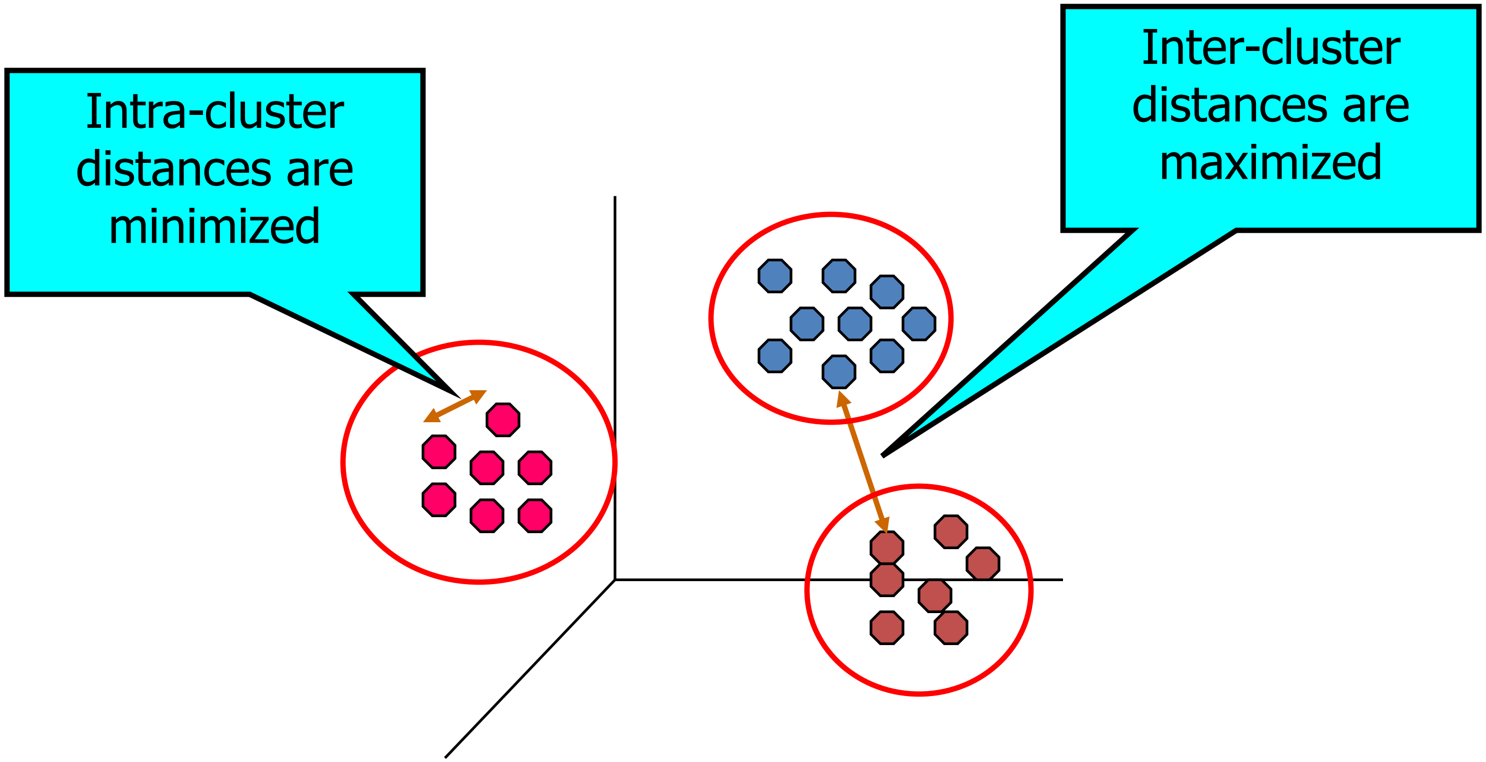
Clustering

Lecture outline

- Distance/Similarity between data objects
- Data objects as geometric data points
- Clustering problems and algorithms
  - K-means
  - K-median
  - K-center

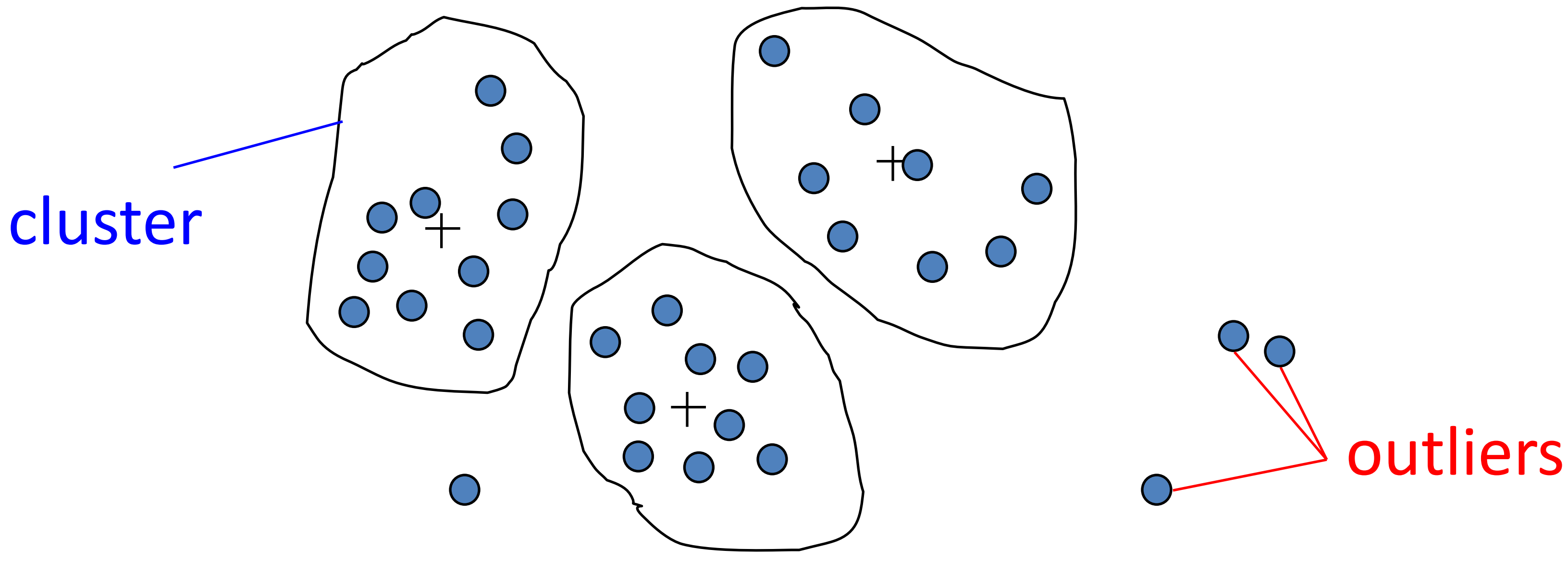
What is clustering?

- A **grouping** of data objects such that the objects **within a group are similar** (or related) to one another **and different from (or unrelated to) the objects in other groups**



Outliers

- **Outliers** are **objects that do not belong to any cluster** or form clusters of very small cardinality



- In some applications we are interested in discovering outliers, not clusters (outlier analysis)

Why do we cluster?

- Clustering : given a collection of data objects group them so that
  - Similar to one another within the same cluster
  - Dissimilar to the objects in other clusters

- Clustering results are used:
  - As a stand-alone tool to get insight into data distribution
    - Visualization of clusters may unveil important information
  - As a preprocessing step for other algorithms
    - Efficient indexing or compression often relies on clustering

Applications of clustering?

- Image Processing
  - cluster images based on their visual content
- Web
  - Cluster groups of users based on their access patterns on webpages
  - Cluster webpages based on their content
- Bioinformatics
  - Cluster similar proteins together (similarity wrt chemical structure and/or functionality etc)
- Many more…

The clustering task

- Group observations into groups so that the observations belonging in the same group are similar, whereas observations in different groups are different

- **Basic questions:**
  – What does “similar” mean
  – What is a good partition of the objects? I.e., how is the quality of a solution measured
  – How to find a good partition of the observations

Observations to cluster

- Real-value attributes/variables
  – e.g., salary, height
- Binary attributes
  – e.g., gender (M/F), has_cancer(T/F)
- Nominal (categorical) attributes
  – e.g., religion (Christian, Muslim, Buddhist, Hindu, etc.)
- Ordinal/Ranked attributes
  – e.g., military rank (soldier, sergeant, lutenant, captain, etc.)
- Variables of mixed types
  – multiple attributes with various types

Observations to cluster

- Usually data objects consist of a set of attributes (also known as **dimensions**)

- J. Smith, 20, 200K

- If all **d** dimensions are ***real-valued*** then we can ***visualize*** each data point as points in a ***d-dimensional space***

- If all **d** dimensions are ***binary*** then we can think of each data point as a ***binary vector***

Distance functions

- The distance **d(x, y)** between two objects **x**and **y** is a metric if

  - **$d(i, j) \geq 0$** (non-negativity)
  - **$d(i, i)=0$** (isolation)
  - **$d(i, j)= d(j, i)$** (symmetry)
  - **$d(i, j) \leq d(i, h)+d(h, j)$** (triangular inequality) [**Why do we need it?**]

- The definitions of distance functions are usually different for real, boolean, categorical, and ordinal variables.

- Weights may be associated with different variables based on applications and data semantics.

Data Structures

- *data* matrix

$$\text{tuples/objects}\left\{\overbrace{\begin{bmatrix} x_{11} & \cdots & x_{1\ell} & \cdots & x_{1d} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{i1} & \cdots & x_{i\ell} & \cdots & x_{id} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{n1} & \cdots & x_{n\ell} & \cdots & x_{nd} \end{bmatrix}}^{\text{attributes/dimensions}}\right.$$

- *Distance* matrix

$$\text{objects}\left\{\overbrace{\begin{bmatrix} 0 & & & & \\ d(2,1) & 0 & & & \\ d(3,1) & d(3,2) & 0 & & \\ : & : & : & & \\ d(n,1) & d(n,2) & \ldots & \ldots & 0 \end{bmatrix}}^{\text{objects}}\right.$$

Distance functions for binary vectors

- **Jaccard similarity** between binary vectors **X** and **Y**

$$JSim(X,Y) = \frac{X \cap Y}{X \cup Y}$$

- **Jaccard distance** between binary vectors **X** and **Y**

  Jdist(X,Y) = 1- JSim(X,Y)

- Example:
  - JSim = 1/6
  - Jdist = 5/6

	Q1	Q2	Q3	Q4	Q5	Q6
X	1	0	0	1	1	1
Y	0	1	1	0	1	0

Distance functions for real-valued vectors

- **L_p** norms or *Minkowski distance*:

$$L_p(x,y)=\left(|x_1-y_1|^p+|x_2-y_2|^p+\ldots+|x_d-x_d|^p\right)^{1/p}=\left(\sum_{i=1}^{d}(x_i-y_i)\right)^{1/p}$$

where ***p*** is a positive integer

- If **p = 1, L_1** is the *Manhattan (or city block)* distance:

$$L_1(x,y)=|x_1-y_1|+|x_2-y_2|+\ldots+|x_d-y_d|=\sum_{i=1}^{d}\left|x_i-y_i\right|$$

Distance functions for real-valued vectors

- If **p = 2, L_2** is the **Euclidean distance**:

$$d(x,y)=\sqrt{(|x_1-y_1|^2+|x_2-y_2|^2+...+|x_d-y_d|^2)}$$

- Also one can use **weighted distance**:

$$d(x,y)=\sqrt{(w_1|x_1-x_1|^2+w_2|x_2-x_2|^2+...+w_d|x_d-y_d|^2)}$$

$$d(x,y)=w_1\left|x_1-y_1\right|+w_2\left|x_2-y_2\right|+...+w_d\left|x_d-y_d\right|$$

- Very often **L_p^p** is used instead of L_p (why?)

Partitioning algorithms: basic concept

- Construct a partition of a set of ***n*** objects into a set of ***k*** clusters
  - Each object belongs to **exactly one** cluster
  - The number of clusters **k** is given in advance

The k-means problem

- Given a set **X** of **n** points in a **d**-dimensional space and an integer **k**

- **Task:** choose a set of **k** points $\{c_1, c_2,\ldots,c_k\}$ in the **d**-dimensional space to form clusters $\{C_1, C_2,\ldots,C_k\}$ such that

$$Cost(C) = \sum_{i=1}^{k} \sum_{x \in C_i} L_2^{\,2}\left(x - c_i\right)$$

  is minimized
- Some special cases: k = 1, k = n

Algorithmic properties of the k-means problem

- NP-hard if the dimensionality of the data is at least 2 (**d>=2**)
- Finding the best solution in polynomial time is infeasible
- For **d=1** the problem is solvable in polynomial time (how?)
- A simple iterative algorithm works quite well in practice

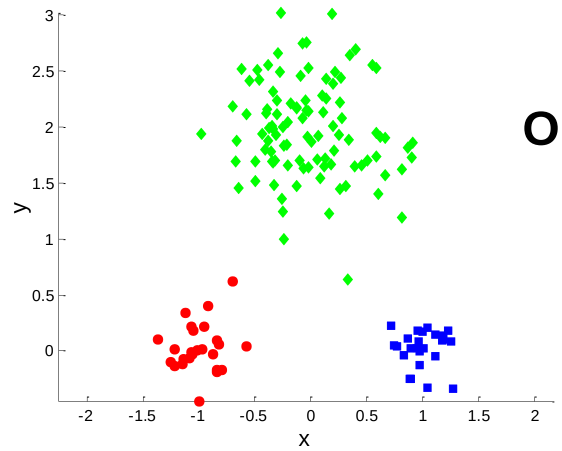
The k-means algorithm

- One way of solving the **k**-means problem
- Randomly pick **k** cluster centers $\{c_1,\ldots,c_k\}$
- For each **i**, set the cluster C_i to be the set of points in **X** that are closer to c_i than they are to c_j for all $i \neq j$
- For each **i** let c_i be the center of cluster C_i (mean of the vectors in C_i)
- Repeat until convergence

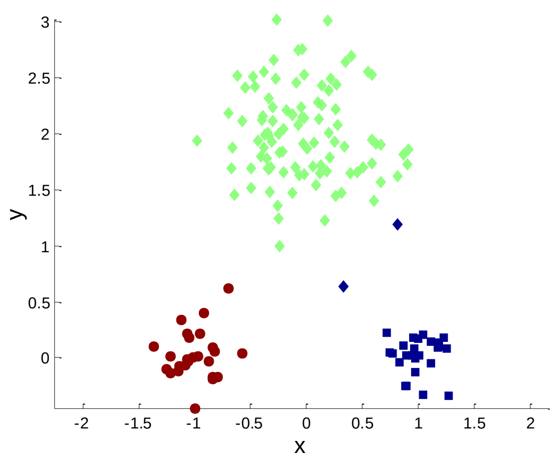
Properties of the k-means algorithm

- Finds a local optimum
- Converges often quickly (but not always)
- The choice of initial points can have large influence in the result

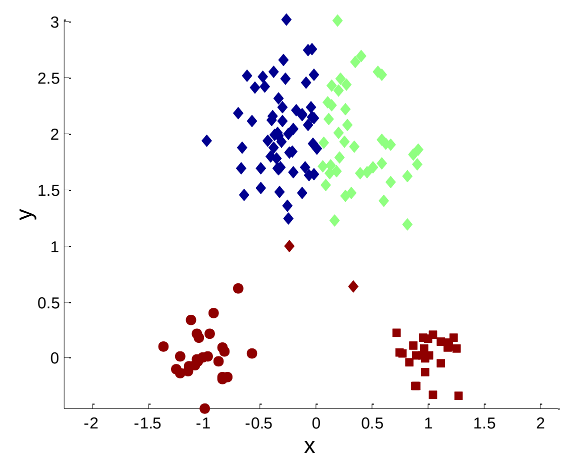
Two different K-means Clusterings



Original Points



Optimal Clustering



Sub-optimal Clustering

Discussion k-means algorithm

- Finds a local optimum
- Converges often quickly (but not always)
- The choice of initial points can have large influence
  - Clusters of different densities
  - Clusters of different sizes

- Outliers can also cause a problem (Example?)

Some alternatives to random initialization of the central points

- Multiple runs
  - Helps, but probability is not on your side

- Select original set of points by methods other than random . E.g., pick the most distant (from each other) points as cluster centers (kmeans++ algorithm)

The k-median problem

- Given a set **X** of **n** points in a **d**-dimensional space and an integer **k**

- **Task:** choose a set of **k** points $\{c_1,c_2,\dots,c_k\}$ from **X** and form clusters $\{C_1,C_2,\dots,C_k\}$ such that

$$Cost(C)=\sum_{i=1}^{k}\sum_{x\in C_i} L_1(x,c_i)$$

  is minimized

The *k-medoids* algorithm

- *Or … PAM* (Partitioning Around Medoids, 1987)
  - Choose randomly **k** medoids from the original dataset **X**
  - Assign each of the **n-k** remaining points in **X** to their closest medoid
  - iteratively replace one of the medoids by one of the non-medoids if it improves the total clustering cost

Discussion of PAM algorithm

- The algorithm is very similar to the k-means algorithm
- It has the same advantages and disadvantages
- How about efficiency?

CLARA (Clustering Large Applications)

- It draws ***multiple samples*** of the data set, applies *PAM* on each sample, and gives the best clustering as the output
- <u>Strength</u>: deals with larger data sets than *PAM*

- <u>Weakness:</u>
  - Efficiency depends on the sample size
  - A good clustering based on samples will not necessarily represent a good clustering of the whole data set if the sample is biased

The k-center problem

- Given a set **X** of **n** points in a **d**-dimensional space and an integer **k**

- **Task:** choose a set of **k** points from **X** as cluster centers $\{c_1,c_2,\ldots,c_k\}$ such that for clusters $\{C_1,C_2,\ldots,C_k\}$

$$R(C) = \max_j \max_{x \in C_j} d(x, c_j)$$

is minimized

Algorithmic properties of the k-centers problem

- NP-hard if the dimensionality of the data is at least 2 (d>=2)
- Finding the best solution in polynomial time is infeasible
- For d=1 the problem is solvable in polynomial time (how?)
- A simple combinatorial algorithm works well in practice

The farthest-first traversal algorithm

- Pick any data point and label it as point **1**
- For **$i=2,3,\ldots,n$**
  - Find the unlabelled point furthest from **$\{1,2,\ldots,i-1\}$** and label it as **i**.

    //Use **$d(x,S) = \min_{y \in S} d(x,y)$** to identify the distance
    //of a point from a set
  - **$\pi(i) = \mathrm{argmin}_{j<i} d(i,j)$**
  - **$R_i=d(i,\pi(i))$**

The farthest-first traversal is a 2-approximation algorithm

- **Claim1**: $R_1 \geq R_2 \geq \ldots \geq R_n$

- **Proof:**
  - $R_j = d(j, \pi(j)) = d(j, \{1,2,\ldots,j-1\})$

    $\leq d(j, \{1,2,\ldots,i-1\})$ //$j > i$

    $\leq d(i, \{1,2,\ldots,i-1\}) = R_i$

The farthest-first traversal is a 2-approximation algorithm

- **Claim 2:** If **C** is the clustering reported by the farthest algorithm, then $R(C)=R_{k+1}$

- **Proof:**
  - For all $i > k$ we have that

    $d(i, \{1,2,\ldots,k\}) \leq d(k+1,\{1,2,\ldots,k\}) = R_{k+1}$

The farthest-first traversal is a 2-approximation algorithm

- **Theorem:** If **C** is the clustering reported by the farthest algorithm, and C^* is the optimal clustering, then then $R(C) \leq 2xR(C^*)$
- **Proof:**
  - Let $C^*_1, C^*_2, \ldots, C^*_k$ be the clusters of the optimal k-clustering.
  - If these clusters contain points $\{1,\ldots,k\}$ then $R(C) \leq 2R(C^*)$ (triangle inequality)
  - Otherwise suppose that one of these clusters contains two or more of the points in $\{1,\ldots,k\}$. These points are at distance at least R_k from each other. Thus clusters must have radius
    $½ R_k \geq ½ R_{k+1} = ½ R(C)$

What is the right number of clusters?

- …or who sets the value of **k**?
- For n points to be clustered consider the case where **k=n**. What is the value of the error function
- What happens when **k = 1**?
- Since we want to minimize the error why don’t we select always **k = n**?

Occam's razor and the minimum description length principle

- Clustering provides a description of the data
- For a description to be good it has to be:
  - Not too general
  - Not too specific

- Penalize for every extra parameter that one has to pay

- Penalize the number of bits you need to describe the extra parameter

- So for a clustering **C**, extend the cost function as follows:
- **NewCost(C) = Cost(C) + |C| x logn**