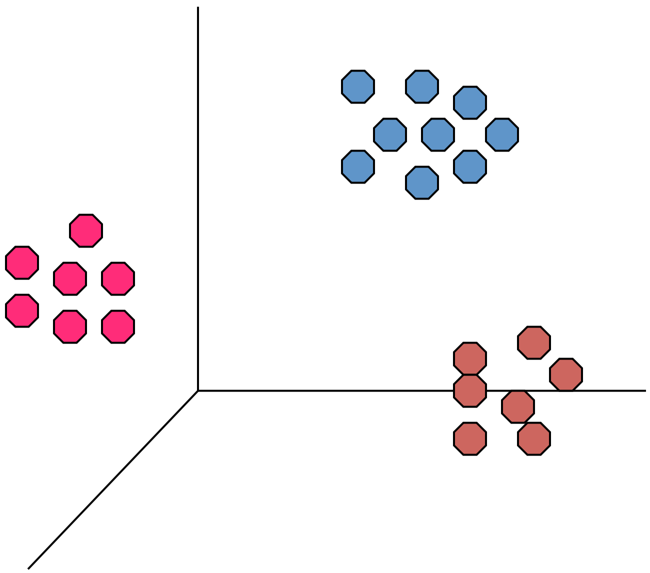
Clustering: Partition Clustering

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**



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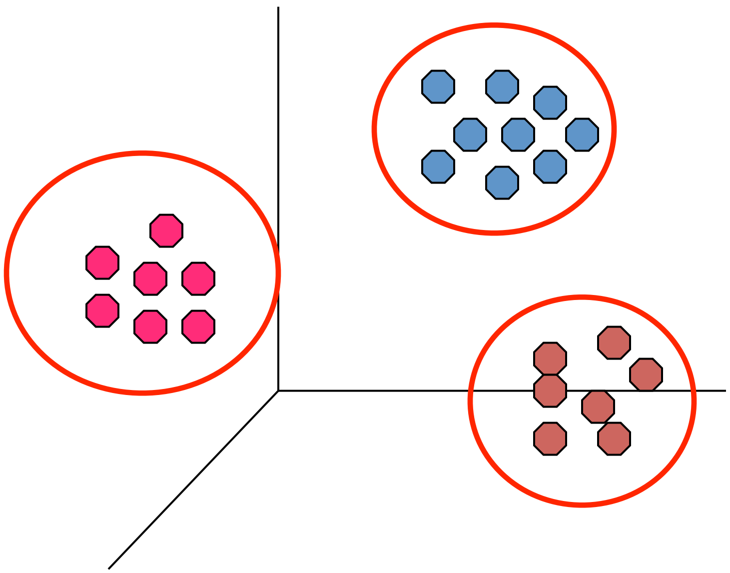

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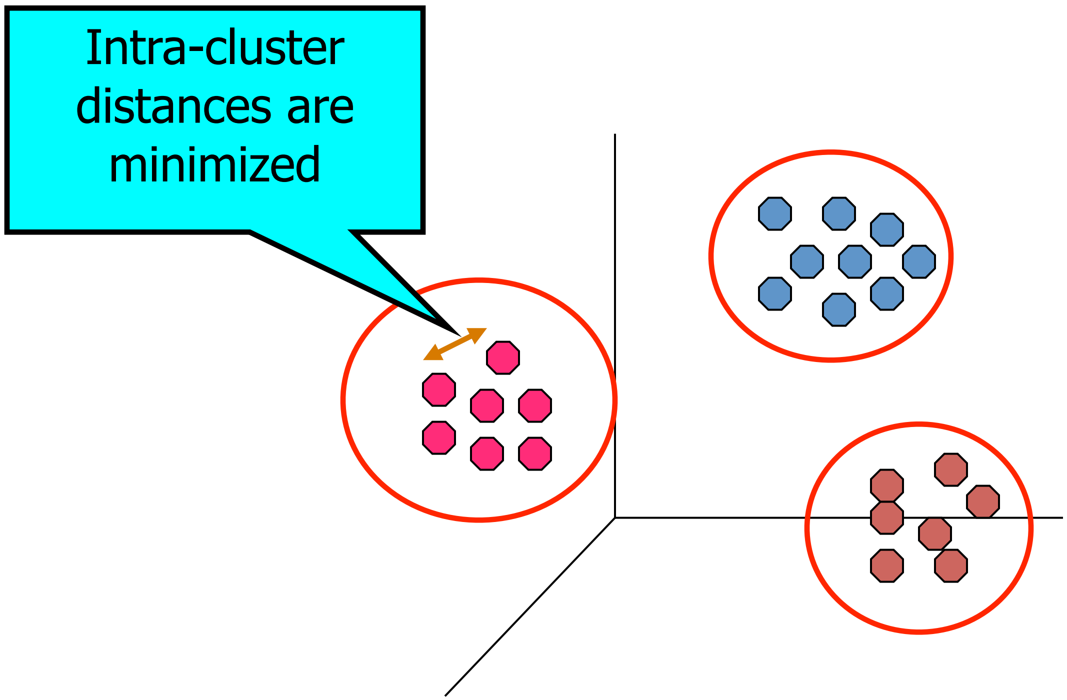

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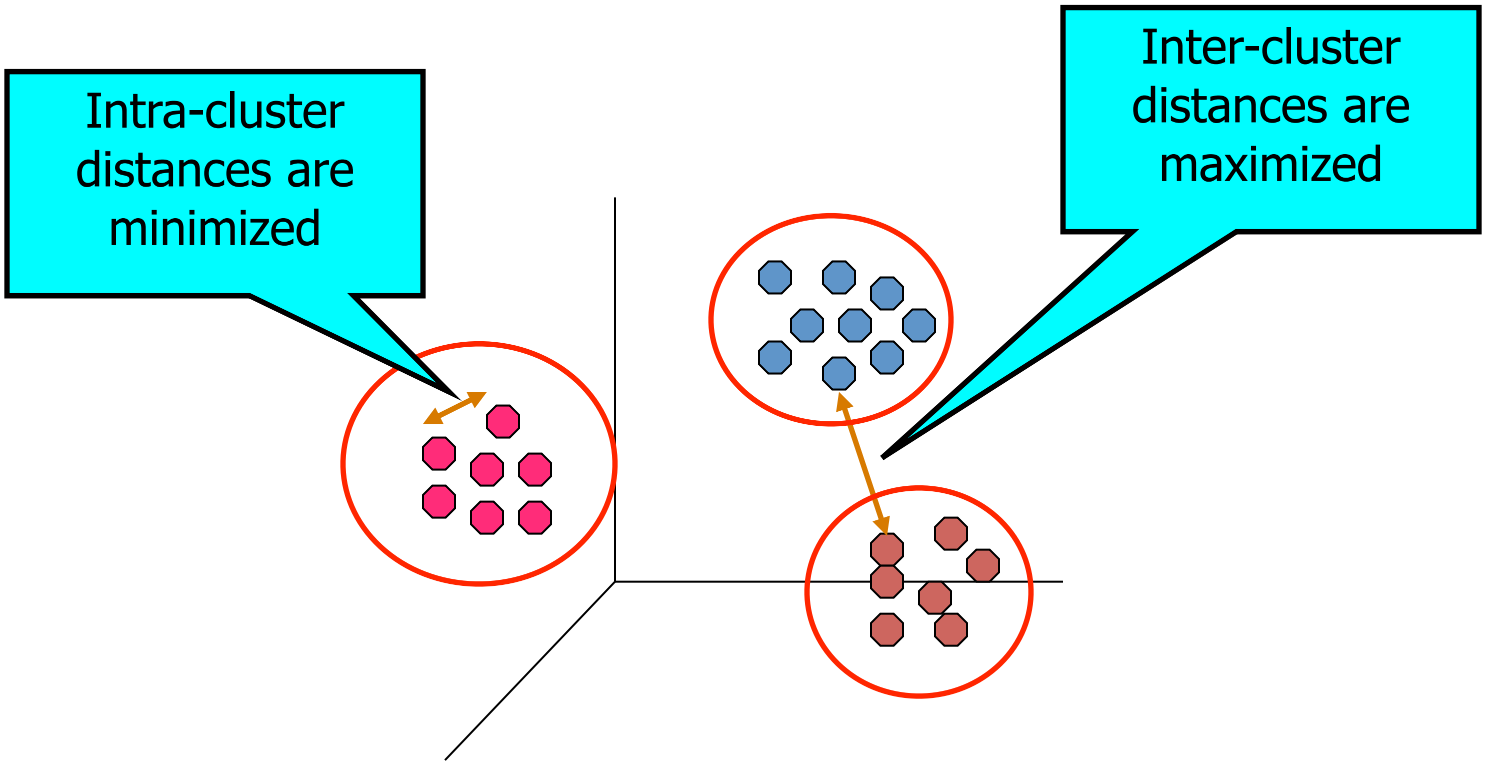
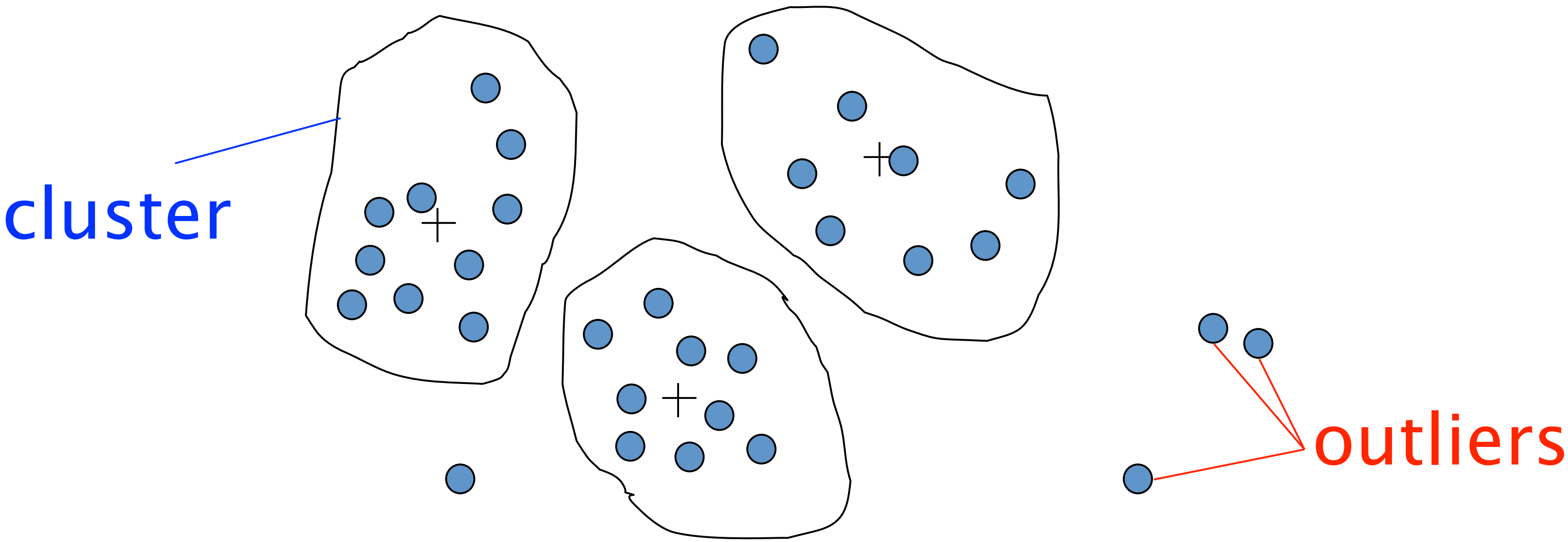


Outliers

- **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

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, …,c_k}** in the **d**-dimensional space to form clusters **{C_1, C_2,…,C_k}** such that

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

  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 $\{c_1,\dots,c_k\}$
- 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

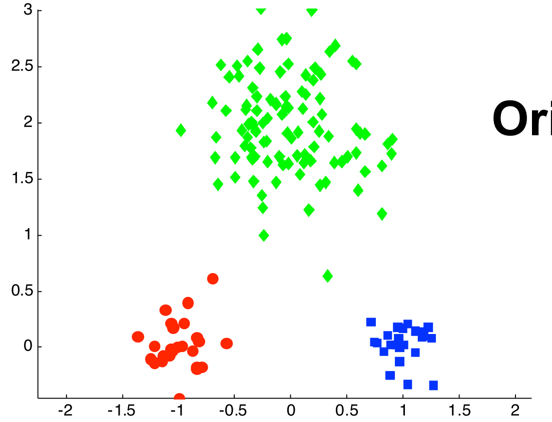
Properties of the k-means algorithm

- Finds a local optimum

- Converges often quickly (but not always)

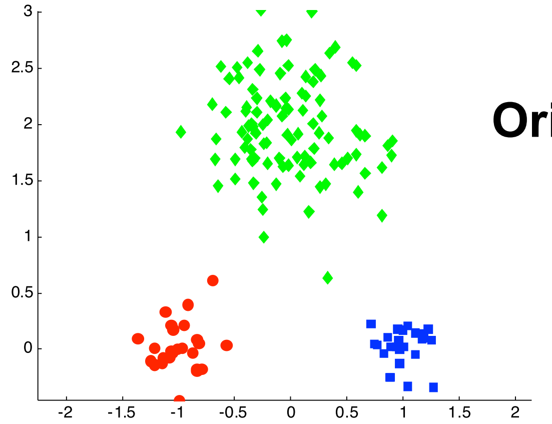
- The choice of initial points can have large influence in the result

Two different K-means Clusterings



Original Points

Two different K-means Clusterings



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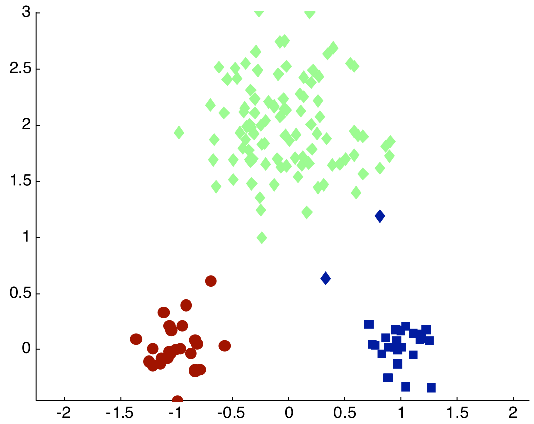
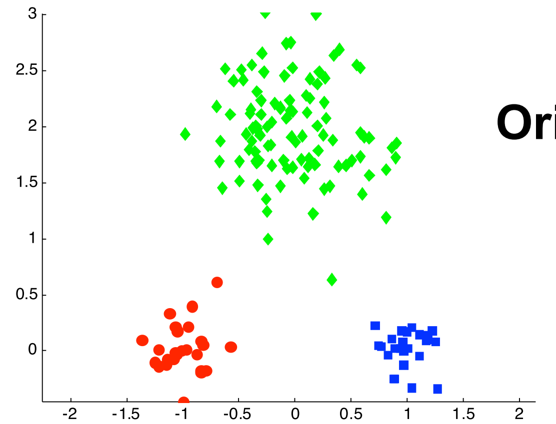


Optimal Clustering

Two different K-means Clusterings



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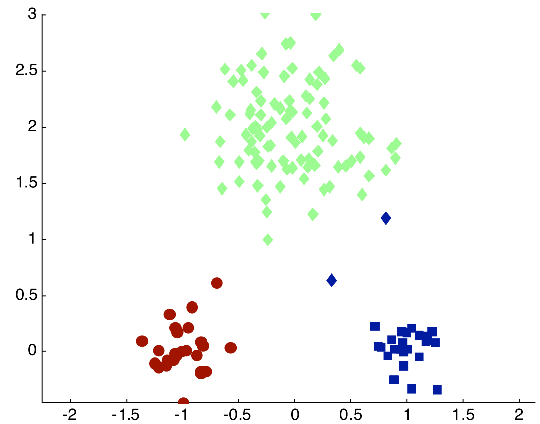
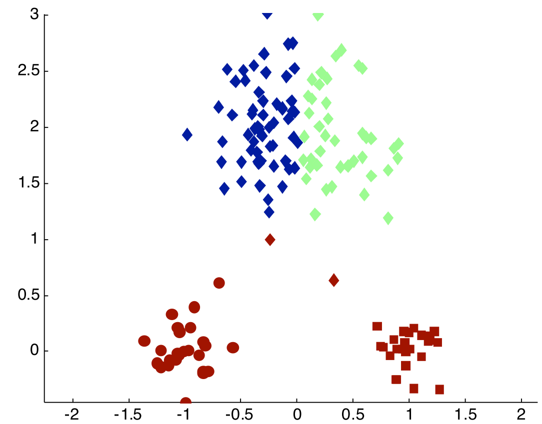


Optimal Clustering



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 $\{c_1,c_2,\ldots,c_k\}$ from X and form clusters $\{C_1,C_2,\ldots,C_k\}$ 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
- Strength: deals with larger data sets than PAM

- Weakness:
  - 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:** Partition the points in **X** in **k** clusters $\{C_1, C_2, \ldots, C_k\}$ such that

$$R(C) = \max_{i} \max_{x,x' \in C_i} d(x, x')$$

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 furthest-first traversal algorithm

- Pick any data point and label it as point **1**
- For **$i=2,3,\ldots,k$**
  - 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
  - **$\pi(i) = \text{argmin}_{j<i} d(i,j)$**
  - **$R_i = d(i,\pi(i))$**
- Assign the remaining unlabelled points to their closest labelled point

The furthest-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 furthest-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 furthest-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 $R(C) \leq 2xR(C^*)$
- **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**