Introduction to Data Mining

Lecture #14: Clustering

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In This Lecture

- Learn the motivation, applications, and goal of clustering
- Understand the basic methods of clustering (bottom-up and top-down): representing clusters, nearness of clusters, etc.
- Learn the k-means algorithm, and how to set the parameter k

Outline

- ☐ **Overview**
- ☐ K-Means Clustering

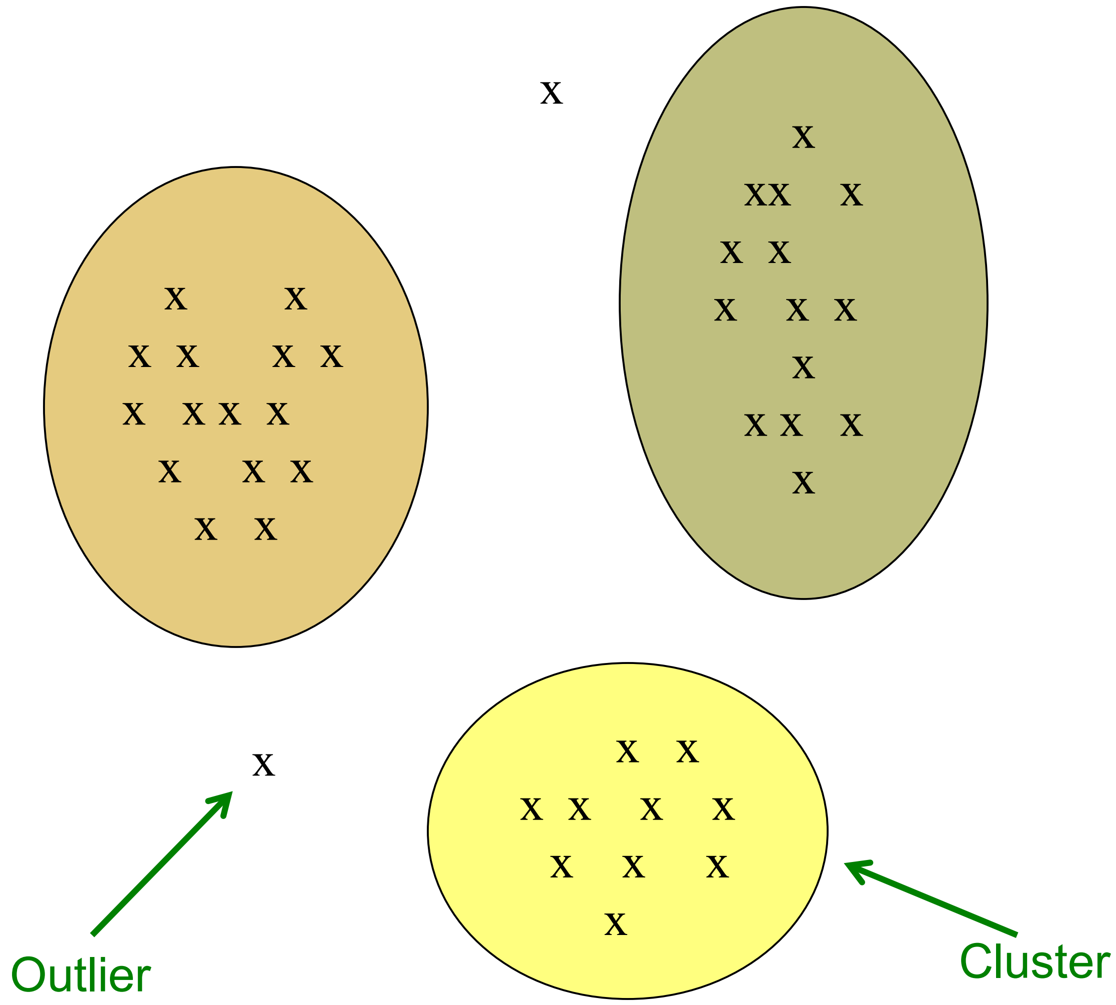
High Dimensional Data

- **Given a cloud of data points we want to understand its structure**

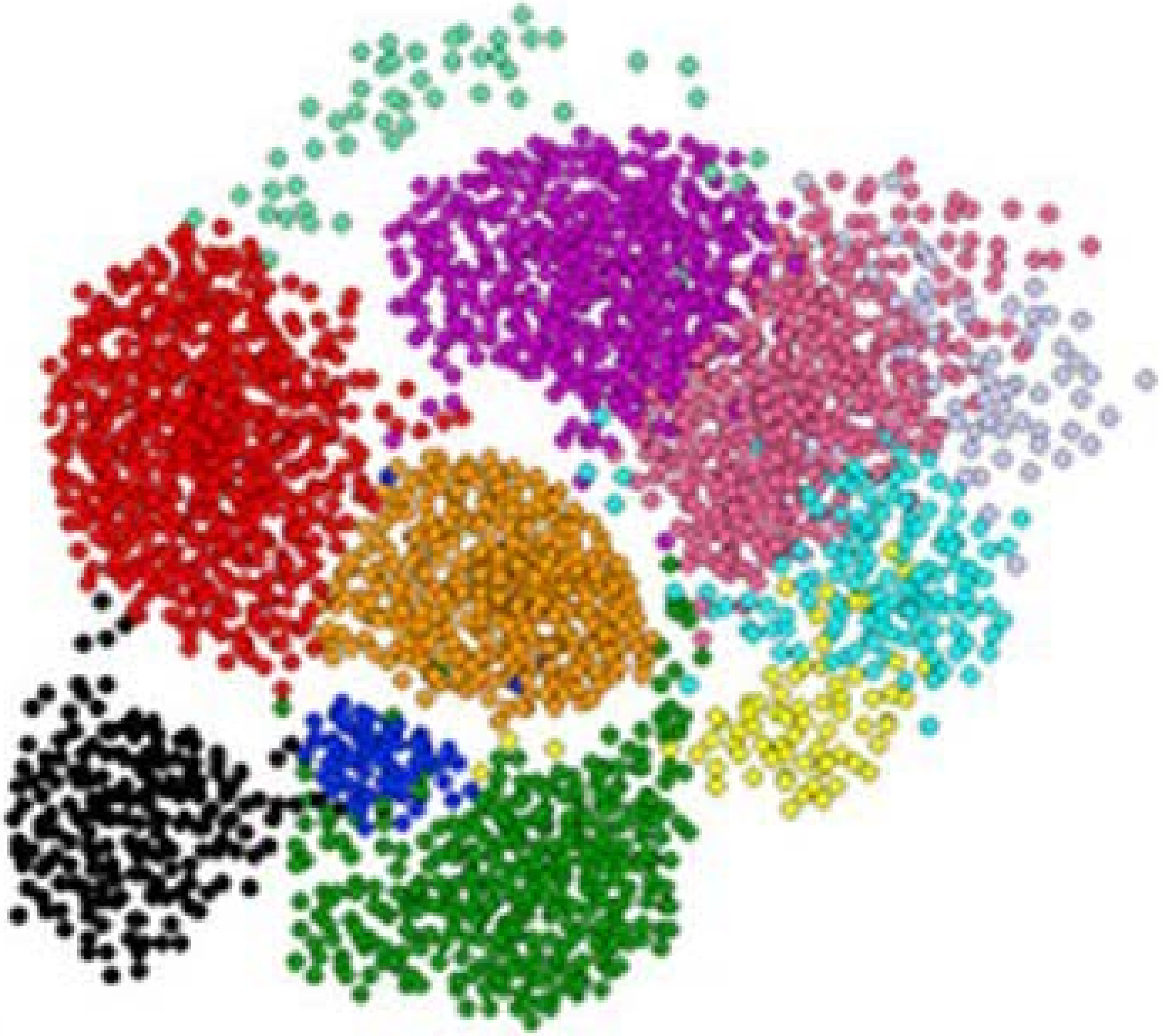
The Problem of Clustering

- Given a **set of points**, with a notion of **distance** between points, **group the points** into some number of ***clusters***, so that
  - Members of a cluster are close/similar to each other
  - Members of different clusters are dissimilar
- **Usually:**
  - Points are in a high-dimensional space
  - Similarity is defined using a distance measure
    - Euclidean, Cosine, Jaccard, edit distance, …

Example: Clusters & Outliers



Clustering is a hard problem!



Why is it hard?

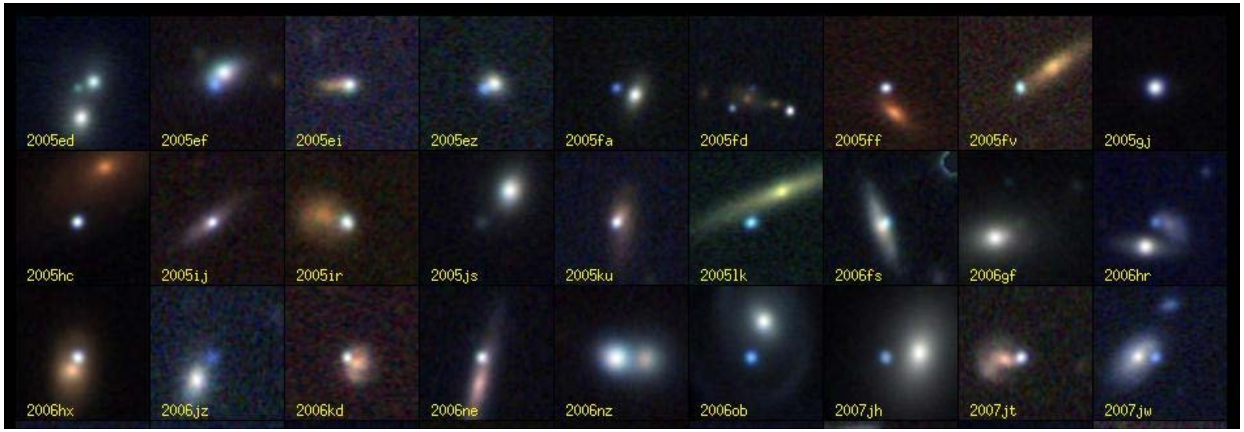
- Clustering in two dimensions looks easy
- Clustering small amounts of data looks easy
- And in most cases, looks are not deceiving

- But, many applications involve not 2, but 10 or 10,000 dimensions
- **High-dimensional spaces look different:** Almost all pairs of points are at about the same distance.
  - Distance between $(x_1..x_d)$ and $(y_1..y_d)$ = $\sqrt{\sum_{i=1}^{d}(x_i - y_i)^2}$

X_i ~ uniform distribution 0 to 1
E[(X_i - Y_i)^2] = mu
sample average converges to mu when number of sampling is large

Clustering Problem: Galaxies

- A catalog of 2 billion "sky objects" represents objects by their radiation in 7 dimensions (frequency bands)
- **Problem:** Cluster into similar objects, e.g., galaxies, nearby stars, quasars, etc.
- Sloan Digital Sky Survey



Clustering Problem: Music CDs

- **Intuitively: Music divides into categories, and customers prefer a few categories**
  - But what are categories really?

- Represent a CD by a set of customers who bought it:

- Similar CDs have similar sets of customers, and vice-versa

Clustering Problem: Music CDs

Space of all CDs:

- Think of a space with one dim. for each customer
  - Values in a dimension may be 0 or 1 only
  - A CD is a point in this space $(x_1, x_2,\ldots, x_k)$, where $x_i = 1$ iff the i th customer bought the CD
- For Amazon, the dimension is tens of millions
- **Task:** Find clusters of similar CDs

Clustering Problem: Documents

Finding topics:

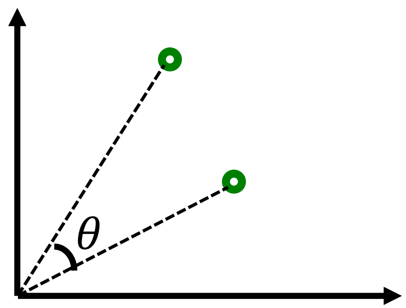
- Represent a document by a vector $(x_1, x_2,..., x_k)$, where $x_i = 1$ iff the i th word (e.g., in a dictionary order) appears in the document

- **Documents with similar sets of words may be about the same topic**

Cosine, Jaccard, and Euclidean

- **As with CDs we have a choice when we think of documents as sets of words or shingles:**
  - **Sets as vectors:** Measure similarity by the **cosine distance**

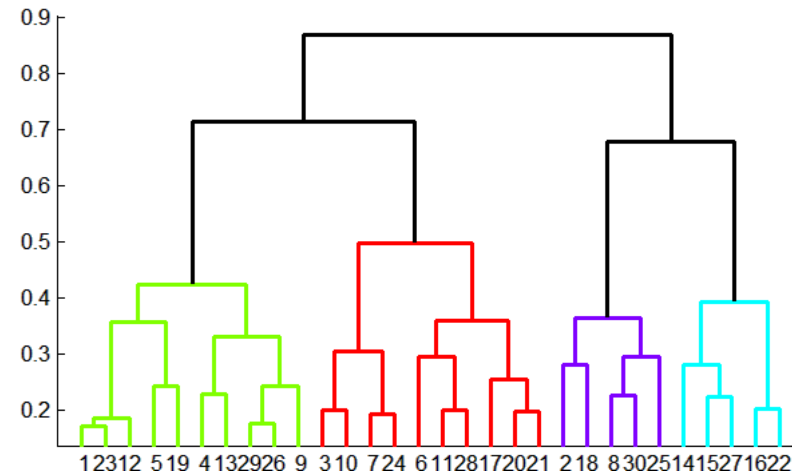
$$\cos\theta = \frac{x \cdot y}{|x||y|}$$



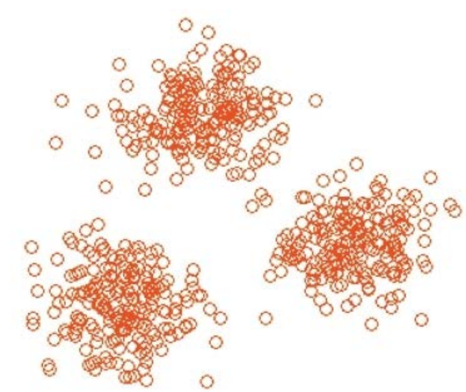
  - **Sets as sets:** Measure similarity by the **Jaccard distance**
  - **Sets as points:** Measure similarity by **Euclidean distance**

Overview: Methods of Clustering

- **Hierarchical:**
  - **Agglomerative** (bottom up):
    - Initially, each point is a cluster
    - Repeatedly combine the two "nearest" clusters into one
  - **Divisive** (top down):
    - Start with one cluster and recursively split it

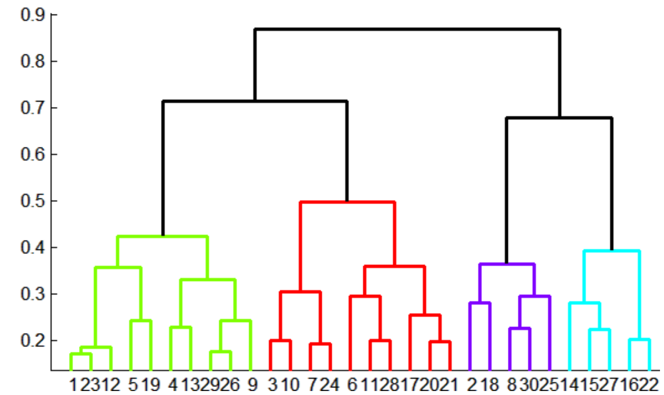


- **Point assignment:**
  - Maintain a set of clusters
  - Points belong to "nearest" cluster



Hierarchical Clustering

- **Key operation:**
  Repeatedly combine two nearest clusters

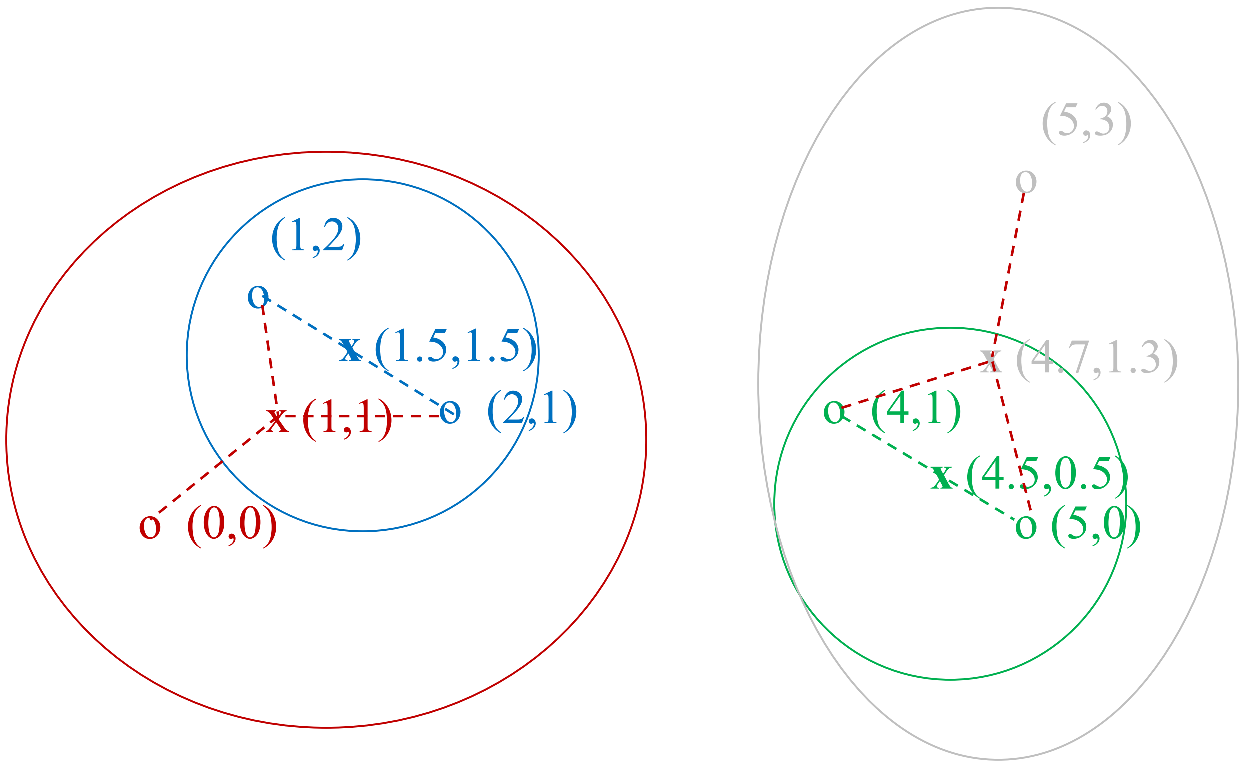


- **Three important questions:**
  - **1)** How do you represent a cluster of more than one point?
  - **2)** How do you determine the "nearness" of clusters?
  - **3)** When to stop combining clusters?

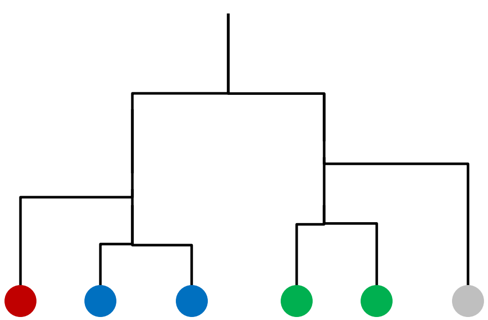
Hierarchical Clustering

- **Key operation: Repeatedly combine two nearest clusters**
- **(1) How to represent a cluster of many points?**
  - **Key problem:** As you merge clusters, how do you represent the "location" of each cluster, to tell which pair of clusters is closest?
- **Euclidean case:** each cluster has a ***centroid*** (= average of its (data)points)
- **(2) How to determine "nearness" of clusters?**
  - Measure cluster distances by distances of centroids

Example: Hierarchical clustering



Data:
o … data point
x … centroid



Dendrogram

When to Stop

- **(3) When to stop combining clusters?**
  - When we reach the predetermined number of clusters
  - When the quality of clusters (e.g. average distance to centroids) becomes very bad

And in the Non-Euclidean Case?

What about the Non-Euclidean case?

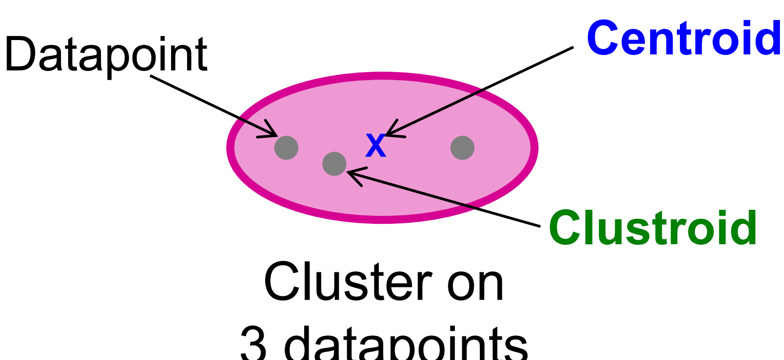
- The only "locations" we can talk about are the points themselves
  - E.g., there is no "average" of two sets

We cannot compute centroid and average. Clustroid

- **Approach 1:**
  - **(1) How to represent a cluster of many points?**
    clustroid (= (data)point "***closest***" to other points)
  - **(2) How do you determine the "nearness" of clusters?**
    Treat clustroid as if it were centroid, when computing inter-cluster distances

"Closest" Point?

- **(1) How to represent a cluster of many points?**
  clustroid = point "***closest***" to other points
- **Possible meanings of "closest":**
  - Smallest maximum distance to other points
  - Smallest average distance to other points
  - Smallest sum of squares of distances to other points
    - For distance metric ***d*** clustroid ***c*** of cluster ***C*** is: $\arg\min_{c} \sum_{x \in C} d(x, c)^2$



Centroid is the avg. of all (data)points in the cluster. This means centroid is an "artificial" point.
Clustroid is an **existing** (data)point that is "closest" to all other points in the cluster.

Defining "Nearness" of Clusters

- **(2) How do you determine the "nearness" of clusters?**
  - **(Approach 1: slide 17)** distance between clustroids
  - **Approach 2:**
    Intercluster distance = minimum of the distances between any two points, one from each cluster
  - **Approach 3:**
    Pick a notion of "**cohesion**" of clusters, *e.g.*, maximum distance from the clustroid of the new merged cluster
    - Merge clusters whose *union* is most cohesive

Cohesion

- **Approach 3.1:** Use the **diameter** of the merged cluster = maximum distance between points in the cluster
- **Approach 3.2:** Use the **average distance** between points in the cluster
- **Approach 3.3:** Use a **density-based approach**
  - Take the diameter or avg. distance, e.g., and divide by the number of points in the cluster

Implementation

- **Naïve implementation of hierarchical clustering:**
  - At each step, compute pairwise distances between all pairs of clusters, then merge
  - $N^2 + (N-1)^2 + (N-2)^2 + \ldots = O(N^3)$
- Careful implementation using priority queue (e.g. Heap) can reduce time to $O(N^2 \log N)$
  - **Still too expensive for really big datasets that do not fit in memory**

Outline

- ☑ Overview
- ☐ **K-Means Clustering**

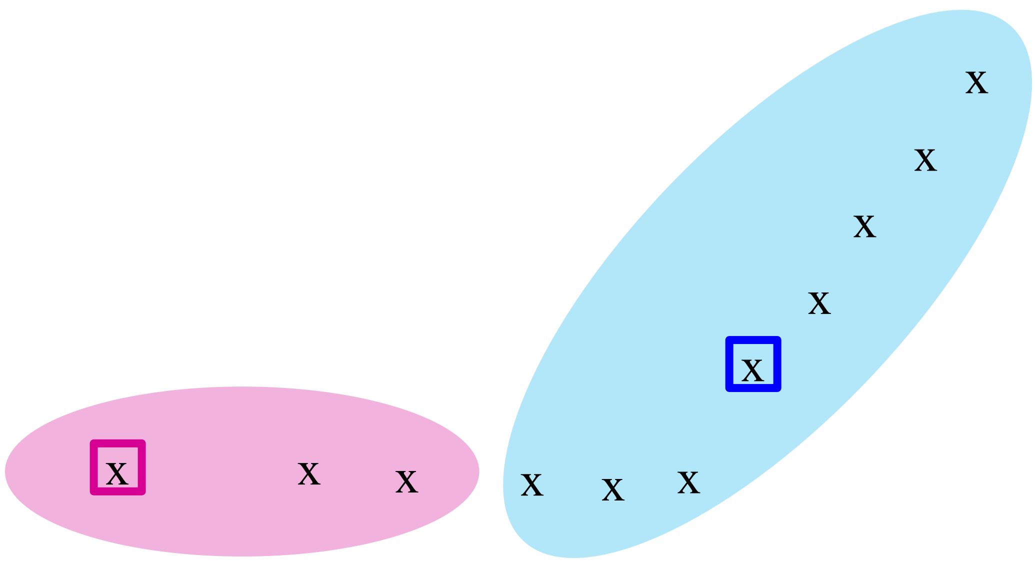
k–means Algorithm(s)

- Assumes Euclidean space/distance
- Start by picking ***k***, the number of clusters
  - We will see how to select the "right" k later
- Initialize clusters by picking one point per cluster
  - **Example:** Pick one point at random, then ***k*-1** other points, each as far away as possible from the previous points

Populating Clusters

- **Step 1)** For each point, place it in the cluster whose current centroid is nearest
- **Step 2)** After all points are assigned, update the locations of centroids of the ***k*** clusters
- **Step 3)** Reassign all points to their closest centroid
  - Sometimes moves points between clusters
- **Repeat steps 2 and 3 until convergence**
  - **Convergence:** Points don't move between clusters and centroids stabilize

Example: Assigning Clusters

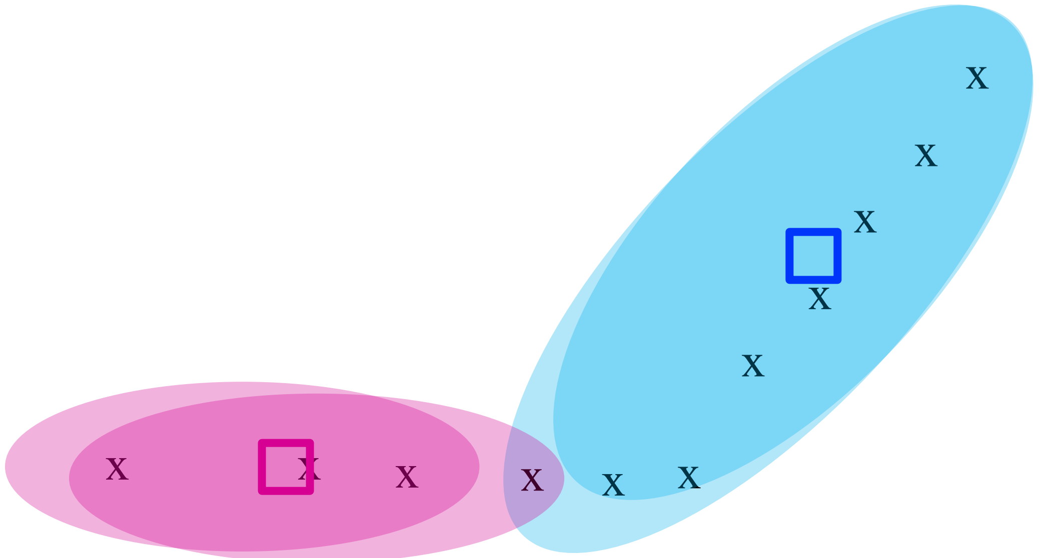


x … data point

… centroid

Clusters after round 1

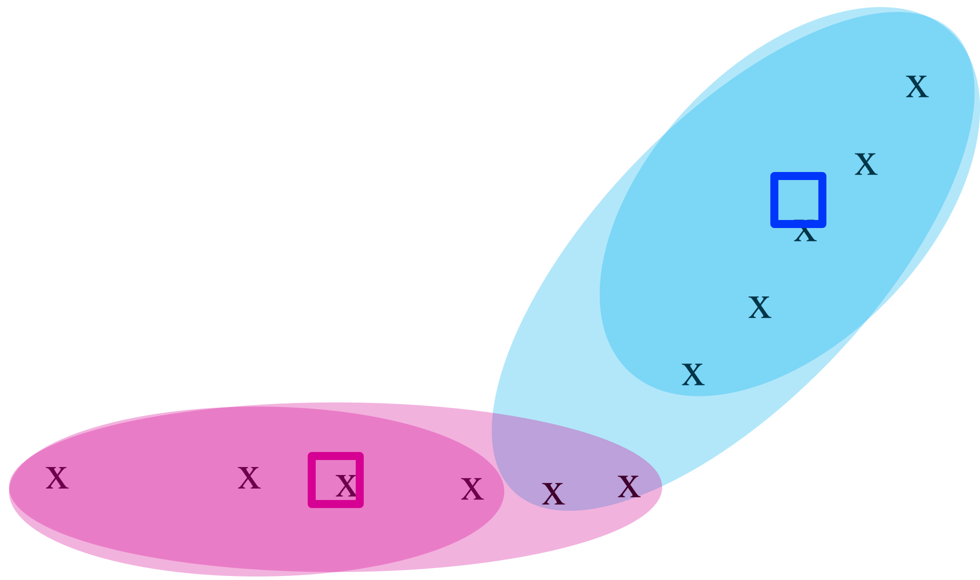
Example: Assigning Clusters



x … data point
□ … centroid

Clusters after round 2

Example: Assigning Clusters



x … data point

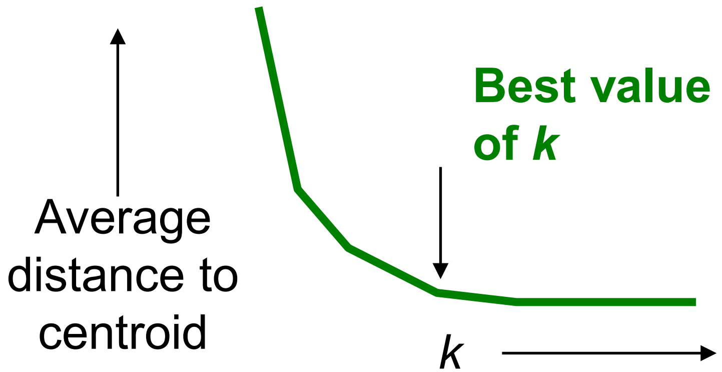
… centroid

Clusters at the end

Getting the *k* right

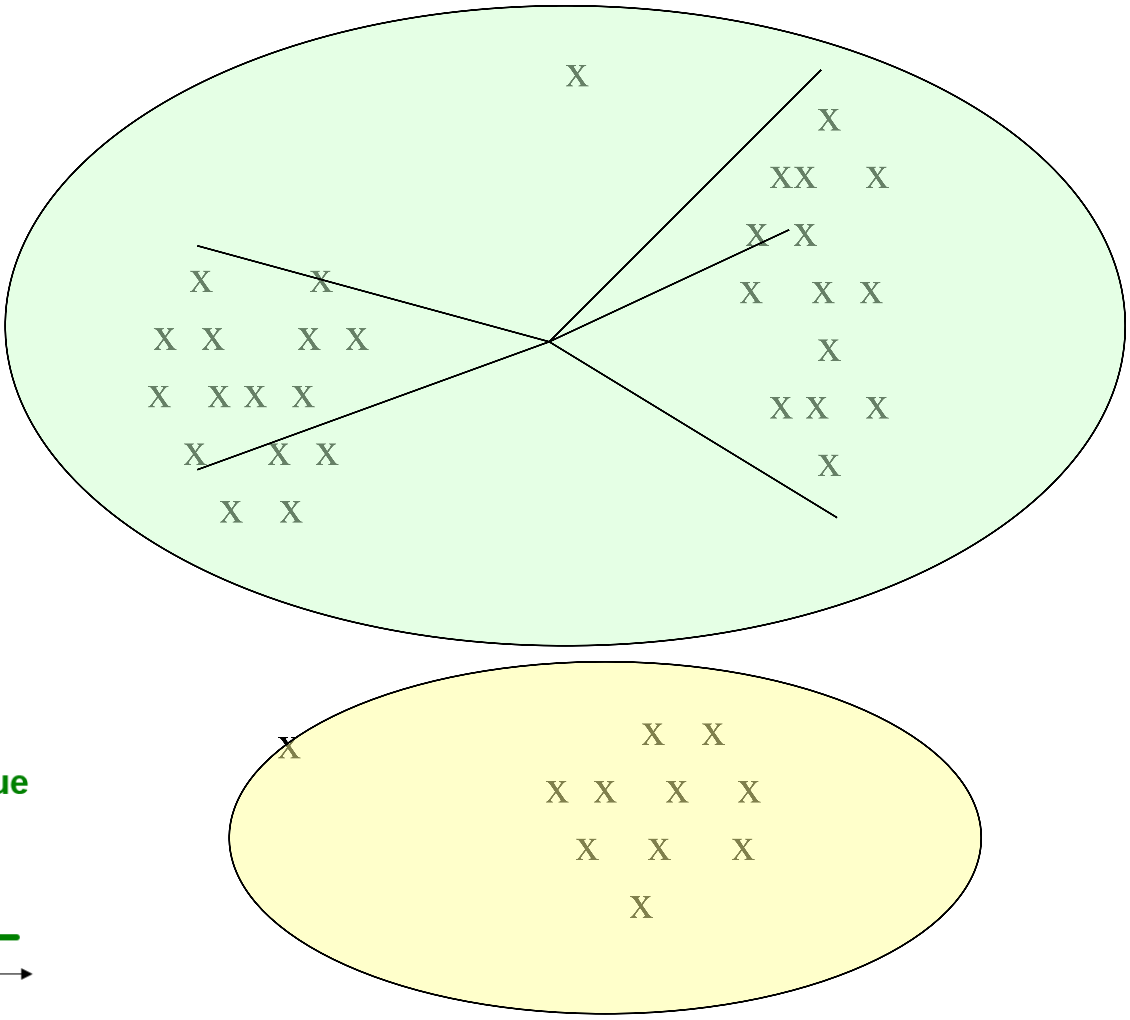
How to select *k*? "Finding the Knee" Method

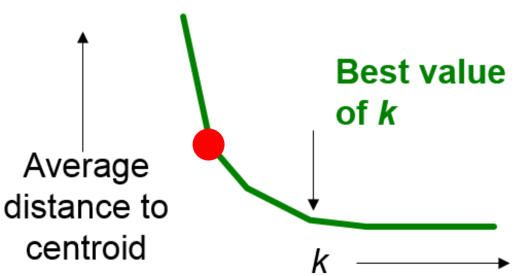
- Try different **k**, looking at the change in the average distance to centroid as **k** increases
- Average falls rapidly until right **k**, then changes little



Example: Picking *k*

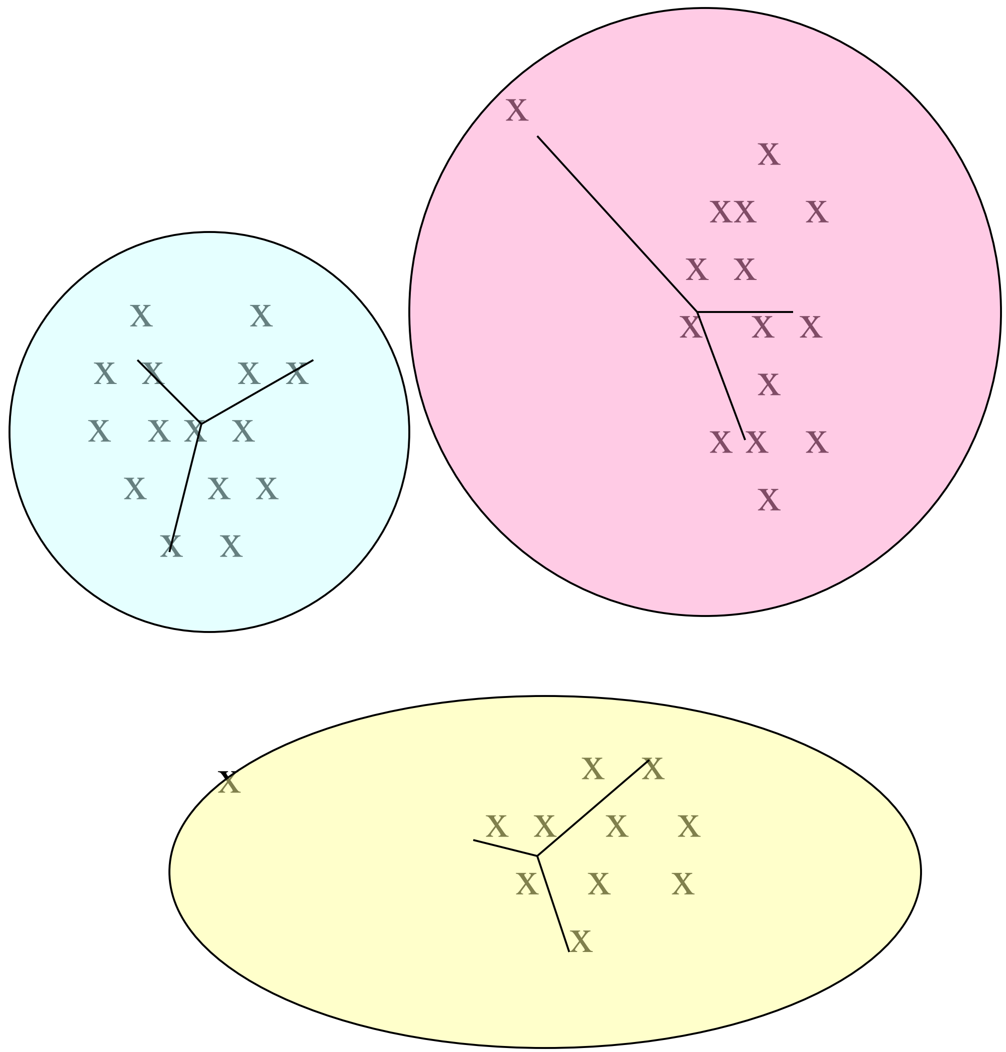
Too few;
many long distances to centroid.

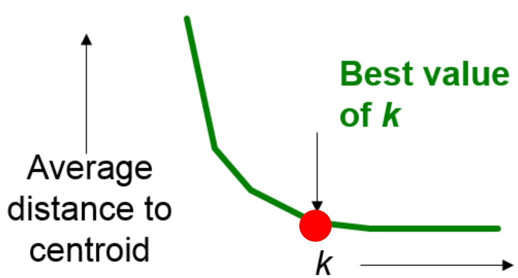




Example: Picking *k*

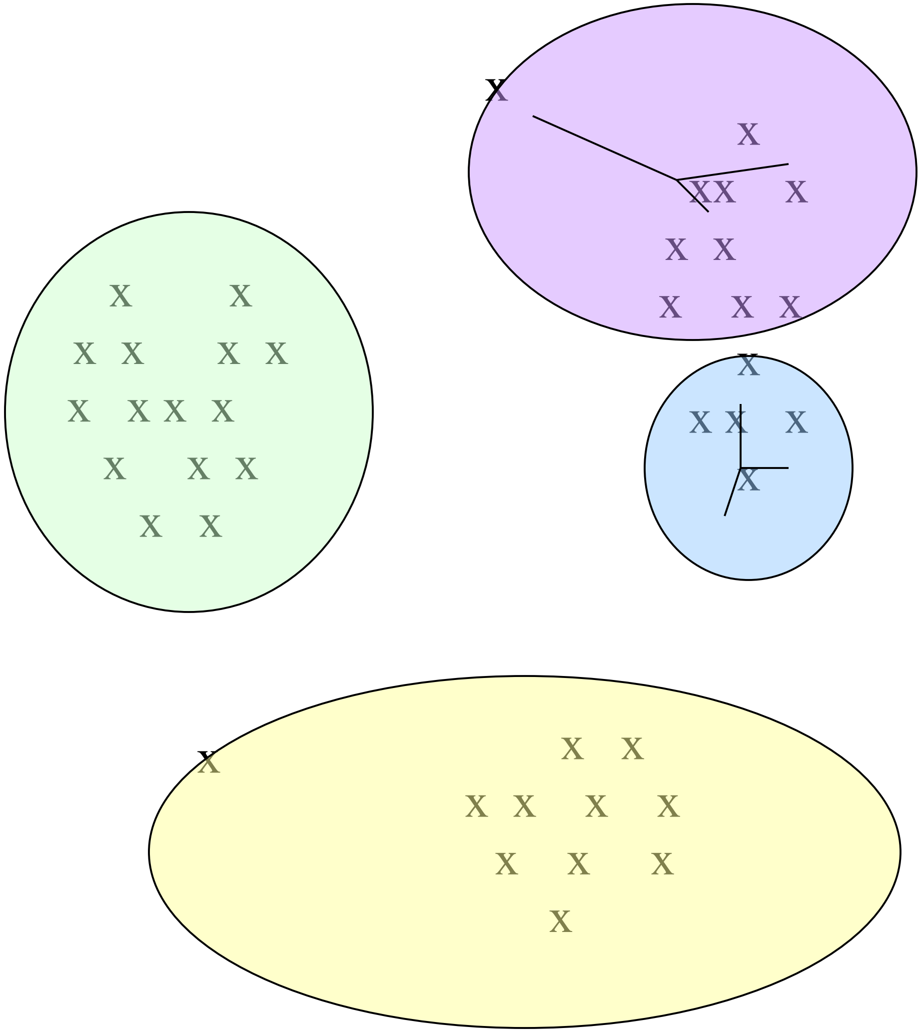
Just right;
distances
rather short.

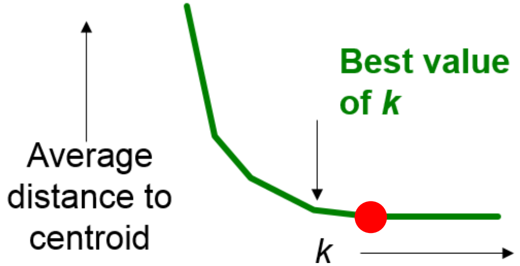




Example: Picking *k*

Too many;
little improvement in average distance.





Checklist

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- Understand the basic methods of clustering (bottom-up and top-down): representing clusters, nearness of clusters, etc.
- Learn the k-means algorithm, and how to set the parameter k

Questions?