Clustering

Mining of Massive Datasets

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http://www.mmds.org

High Dimensional Data

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

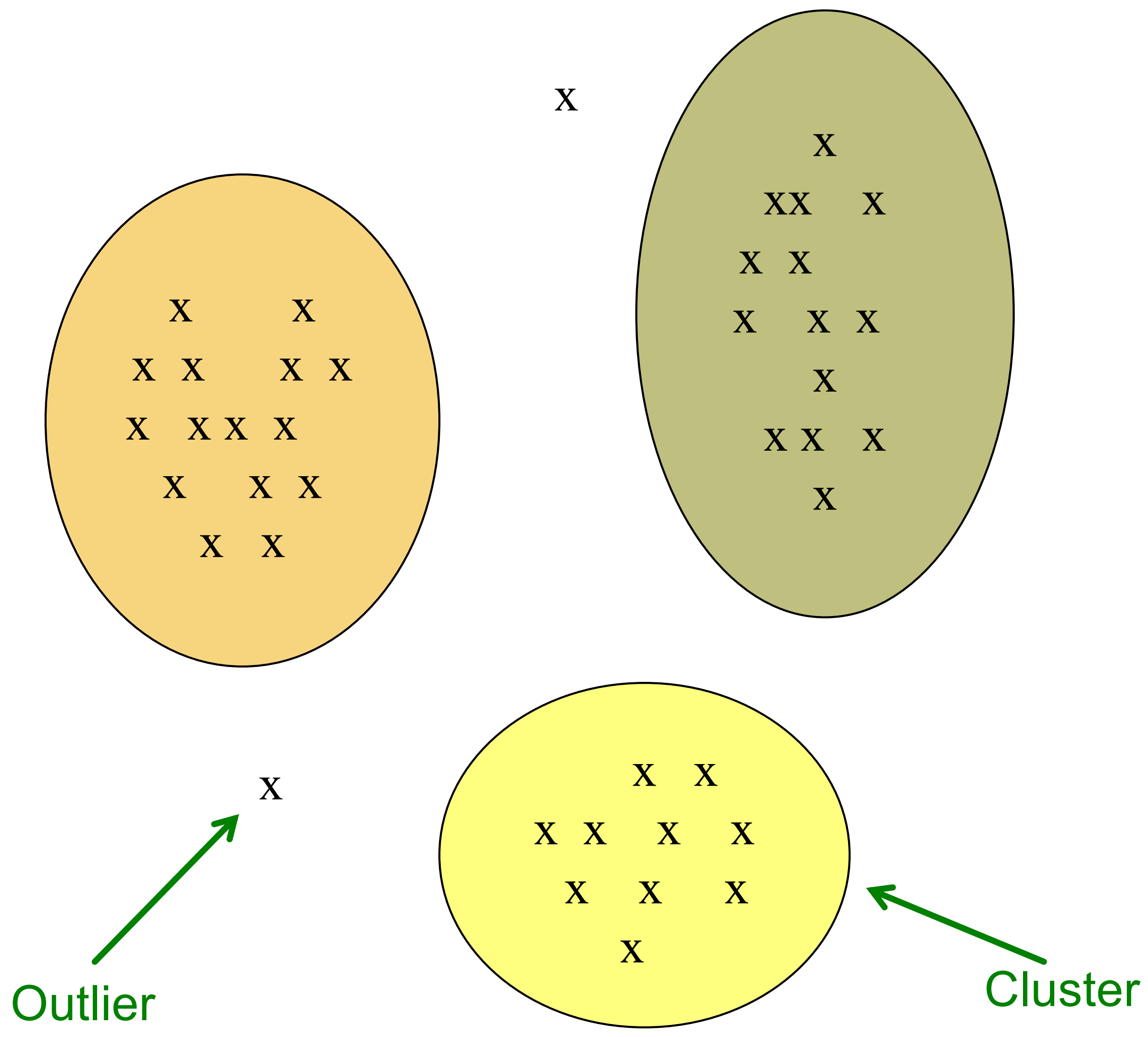
The Problem of Clustering

- 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

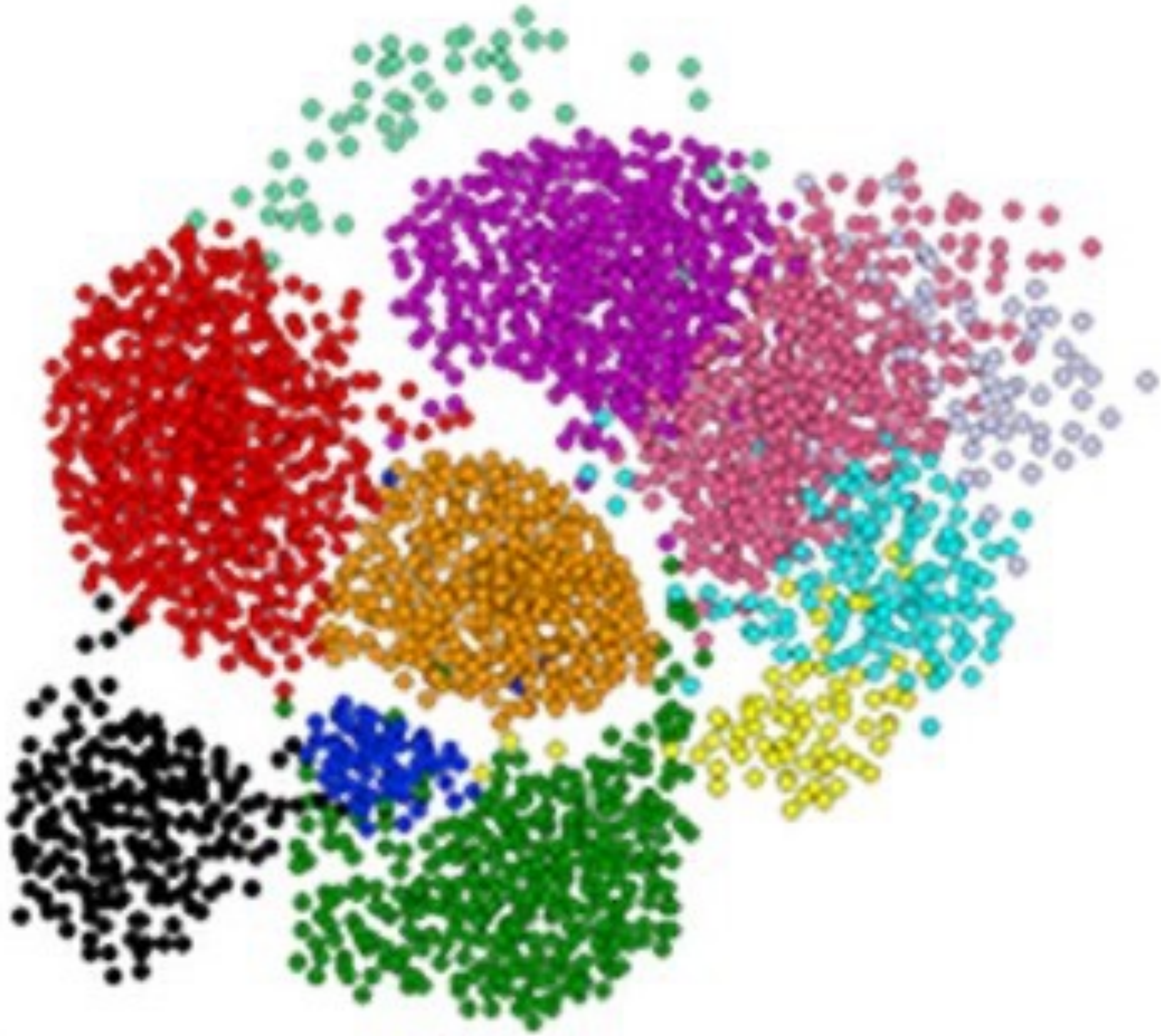
$$\mathbf{X} = \mathbf{USV}^\top$$

  - 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!



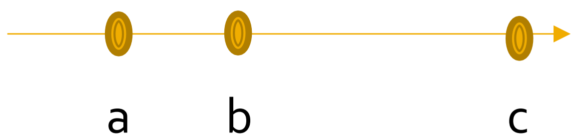
Why is it hard?

- Clustering in two dimensions looks easy
- Clustering small amounts of data looks easy

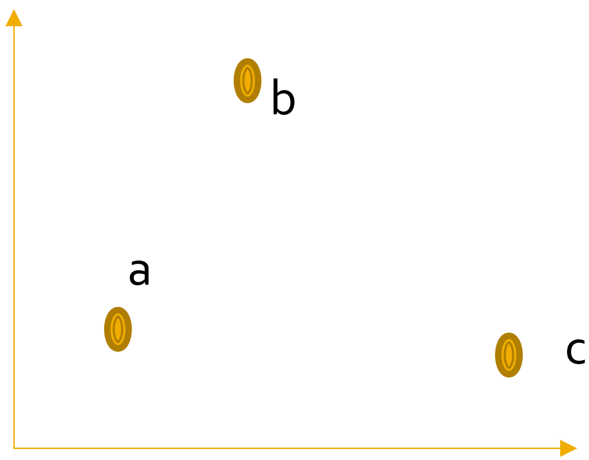
- Many applications involve not 2, but 10 or 10,000 dimensions
- **High-dimensional spaces look different:** Almost all pairs of points are at about the same distance

High Dimension: Euclidean

- Consider a set of data points on a line
  - dist(a, b) < dist(a, c)

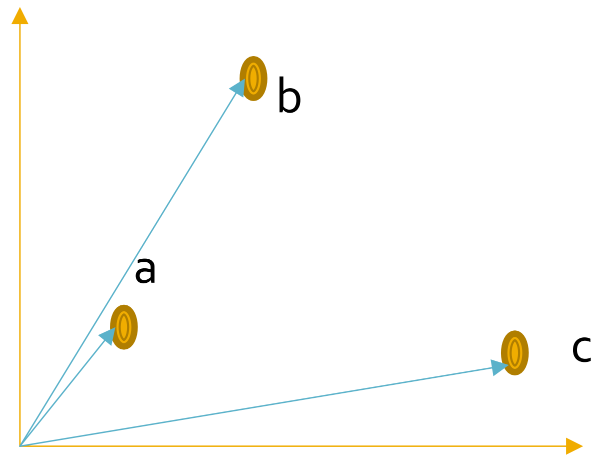


- Consider increasing the dimension by 1
  - dist(a, b) ~ dist(a, c)

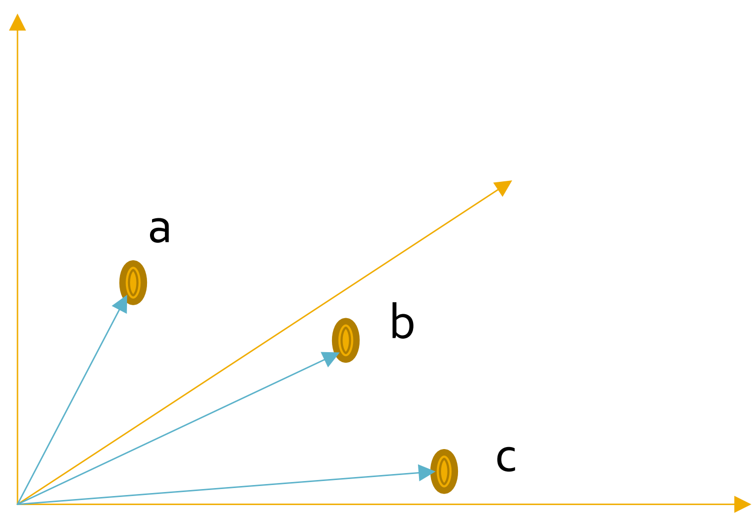


High Dimension: Cosine

- Cosine(a, b) > Cosine(a, c)



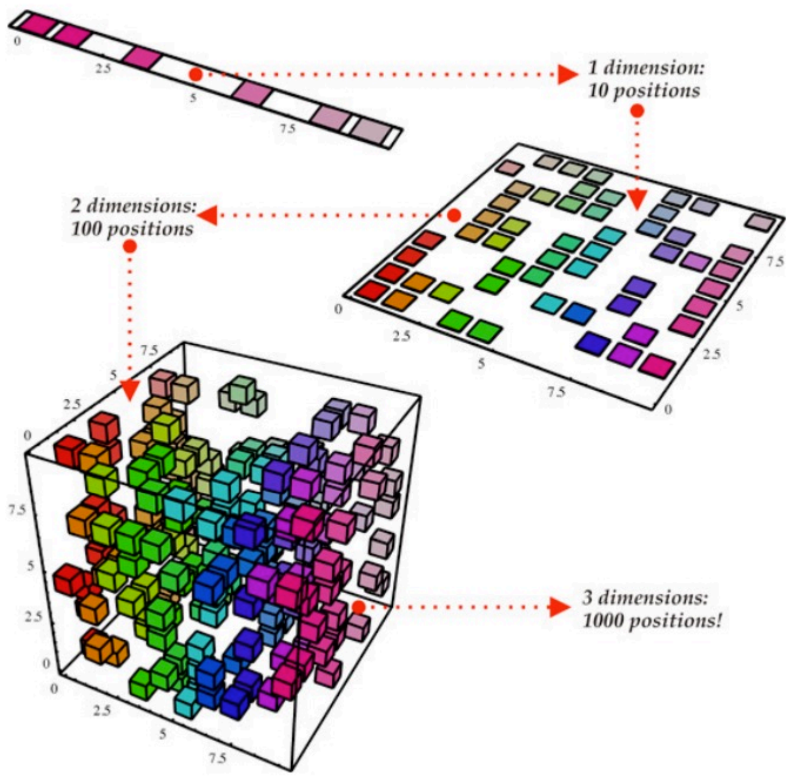
- Increase d to 3
  - Cosine(a, b) ~ Cosine(a, c)
- Higher d
  - Angle -> 90º
  - Cosine -> 0



Curse of Dimensionality

- Data points have similar distance btw each other
  - Euclidean distance breaks
  - almost all pairs of points are equally far away from one another

- Data vectors become orthogonal
  - Cosine function breaks
  - almost any two vectors are orthogonal



https://bigsnarf.wordpress.com/2013/06/14/curse-of-dimensionality/

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

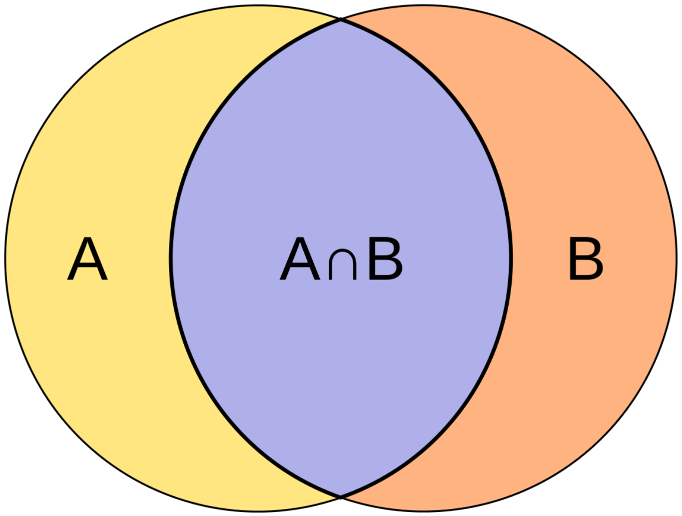
Space of all CDs:

- 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

Cosine, Jaccard, and Euclidean

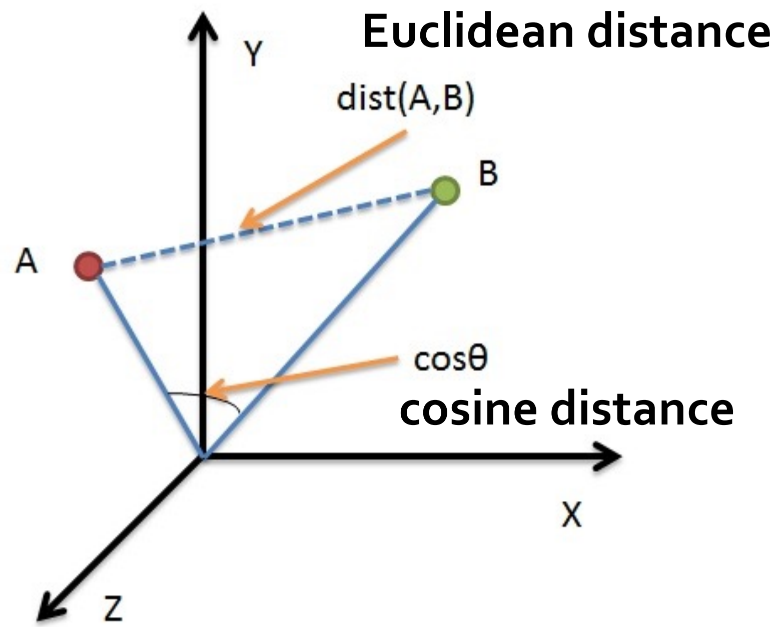
- **As with CDs we have a choice when we think of documents as sets of words or shingles:**
  - **as vectors:** Measure similarity by the **cosine distance**
  - **as sets:** Measure similarity by the **Jaccard distance**
  - **as points:** Measure similarity by **Euclidean distance**

Measure similarity

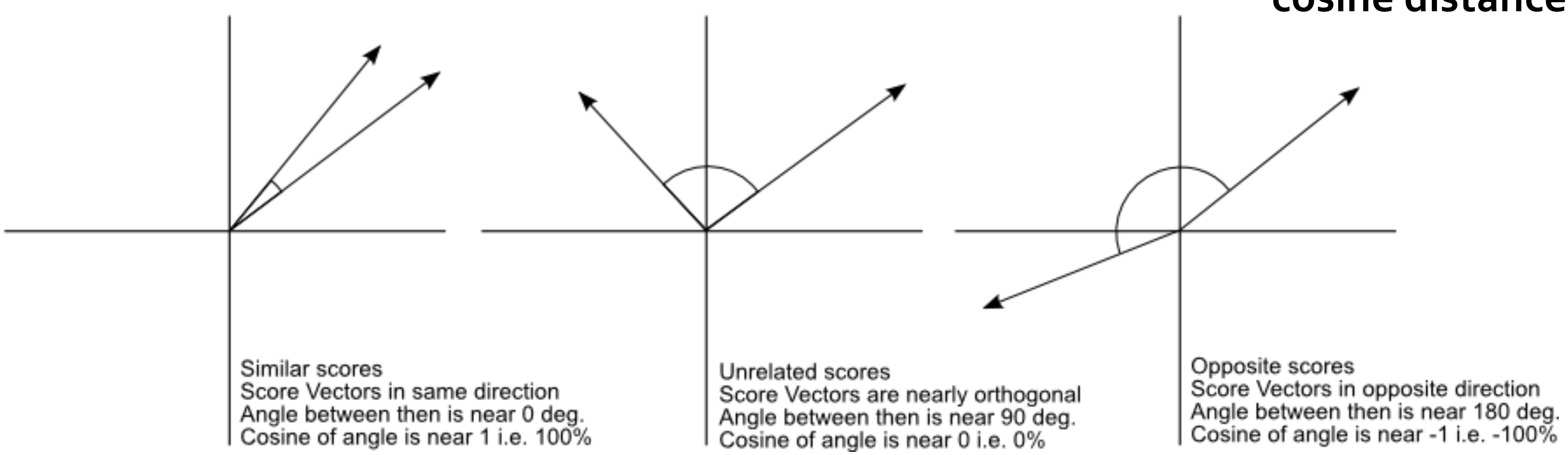


Jaccard distance

$$J(A,B) = \frac{|A \cap B|}{|A \cup B|}$$

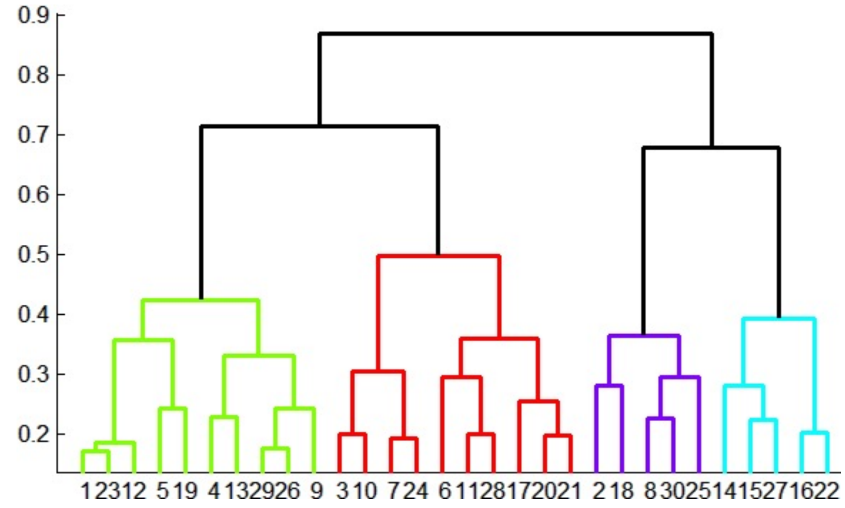


cosine distance

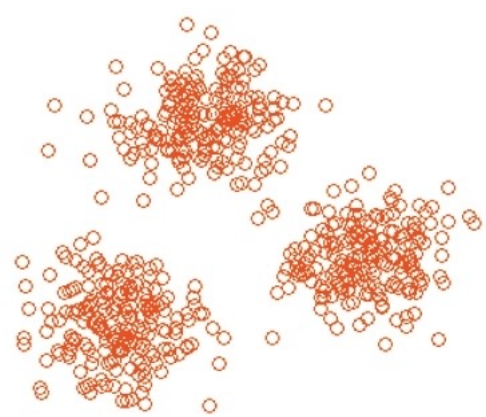


Overview: Methods of Clustering

- **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

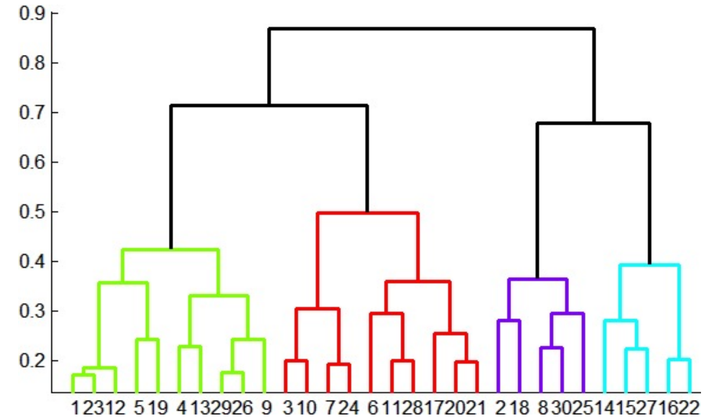


- **Point assignment:**
  - Maintain a set of clusters
  - Points belong to "nearest" cluster



Hierarchical Clustering

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

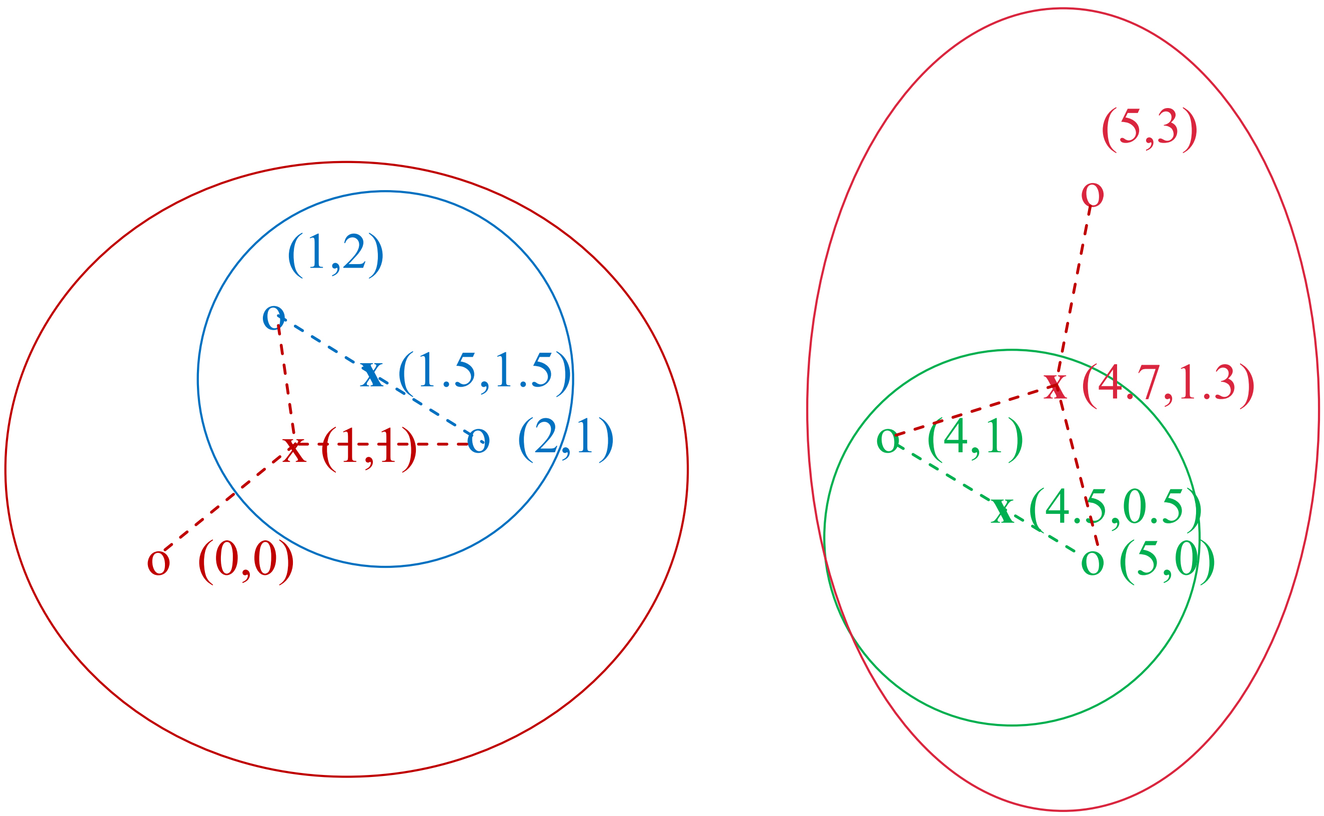


- **Three important questions:**
  - **1)** How do you represent a cluster of more than one point?
  - **2)** How do you determine the “nearness” of clusters?
  - **3)** When to stop combining clusters?

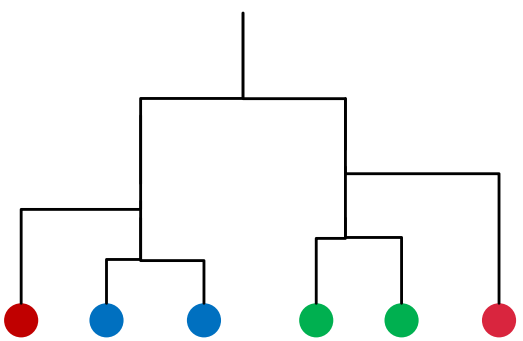
Hierarchical Clustering

- **Key operation:** **Repeatedly combine two nearest clusters**
- **(1) How to represent a cluster of many points?**
  - **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

And in the Non-Euclidean Case?

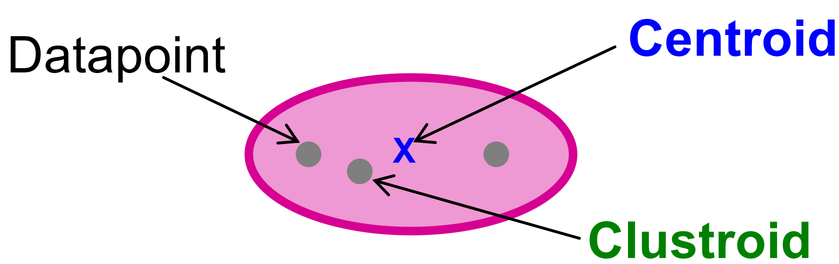
What about the Non-Euclidean case?

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

- **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: $\min_{c} \sum_{x \in C} d(x,c)^2$



Cluster on
3 datapoints

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 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
    - 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

Example

- Consider a cluster of 4 points:
  - abcd, aecdb, abecb, ecdab

- Their edit distances:

Insertion
Deletion
Substitution

	aecdb	abecb	ecdab
abcd	3	3	5
aecdb		2	2
abecb			4

Determine Clusteroid

- aecdb will be chosen as clusteroid
  - Located in “center” judged by all 3 measures

	aecdb	abecb	ecdab
abcd	3	3	5
aecdb		2	2
abecb			4

Point	Sum	Sum-sq	Max
abcd	11	43	5
aecdb	**7**	**17**	**3**
abecb	9	29	4
ecdab	11	45	5

Complexity of Hierarchical Clustering

- n data points
- At most n – 1 step of merging

- Naive implementation, e.g., storing pairwise cluster distances in a matrix

	C1	C2	C3	C4
C1	0	2	3	2
C2		0	4	5
C3			0	3
C4				0

Complexity of Naive Implementation

- Initially, $O(n^2)$ for creating matrix and finding pair with minimum distance

- Subsequent merge, assuming matrix: k x k
  - Delete columns for old clusters: $O(k)$
  - Add new column for new cluster C': $O(k)$
  - Compute dist. of C' with other clusters: $O(k)$
  - Find new pair of clusters with min. dist: $O(k^2)$

=> Overall complexity: $O(n^3)$

Implementation Summary

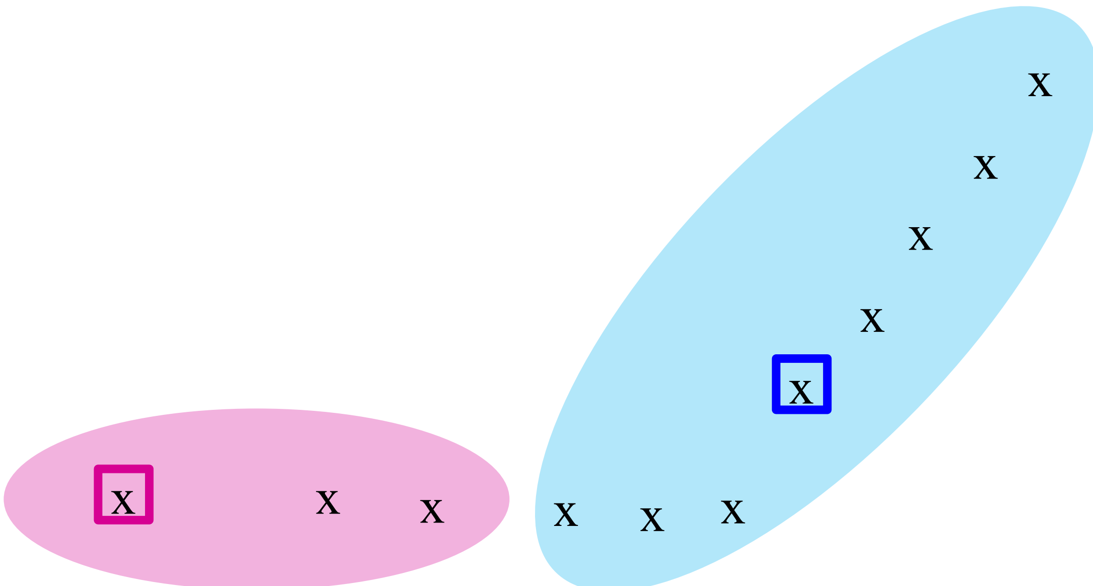
- **Naïve implementation of hierarchical clustering:**
  - At each step, compute pairwise distances between all pairs of clusters, then merge
  - O(N^3)
- Careful implementation using priority queue can reduce time to O($N^2 \log N$) (read textbook)
  - **Still too expensive for really big datasets that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

k-means clustering

k–means Algorithm(s)

- Assumes Euclidean space/distance
- Start by picking ***k***, the number of clusters
- 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

Example: Assigning Clusters

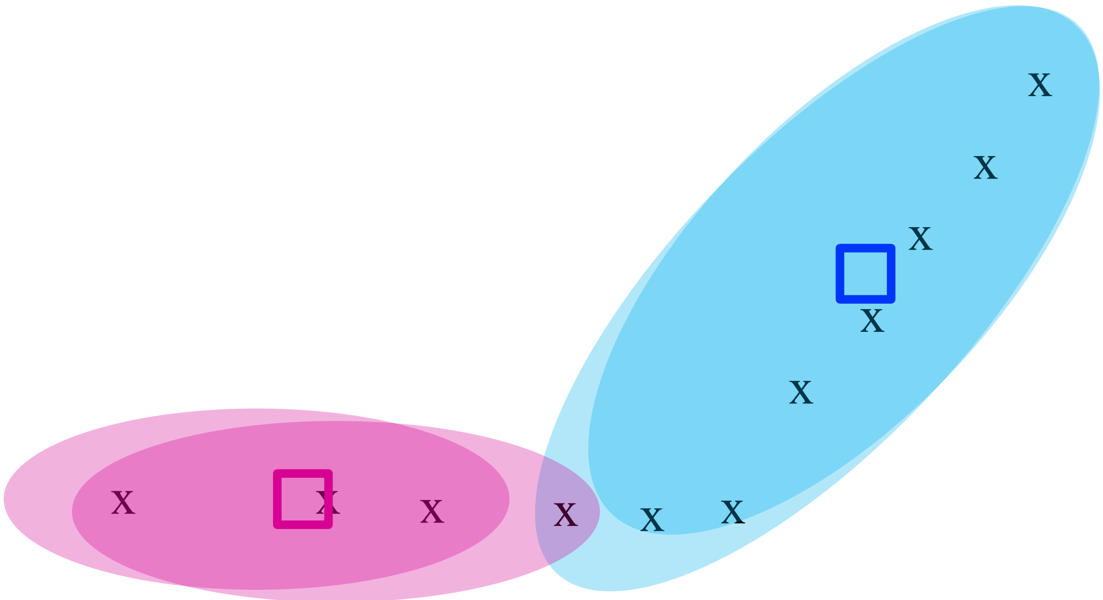


x … data point

… centroid

Clusters after round 1

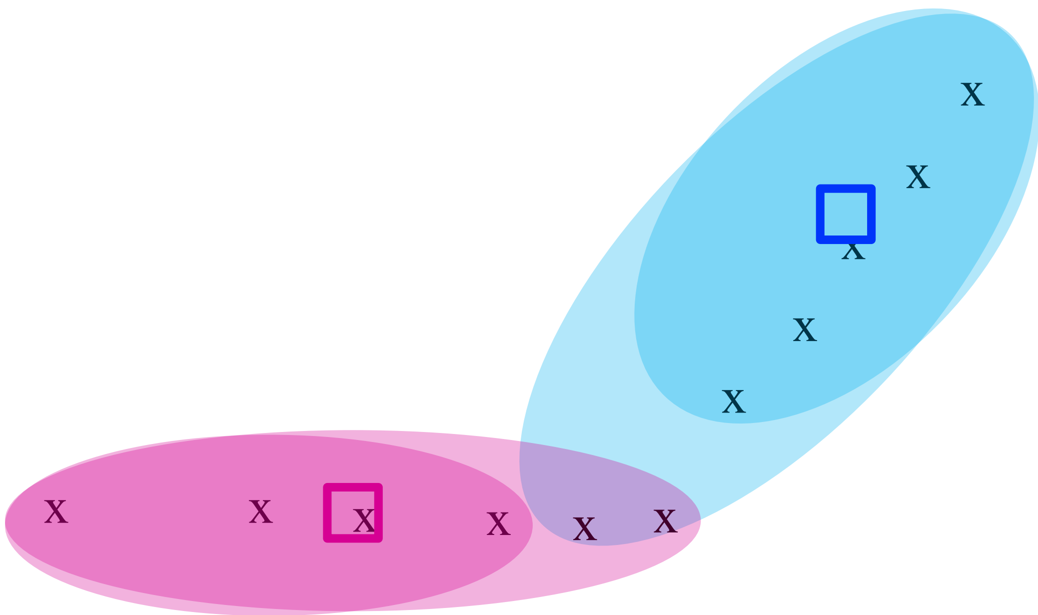
Example: Assigning Clusters



x … data point
… centroid

Clusters after round 2

Example: Assigning Clusters



x … data point
□ … centroid

Clusters at the end

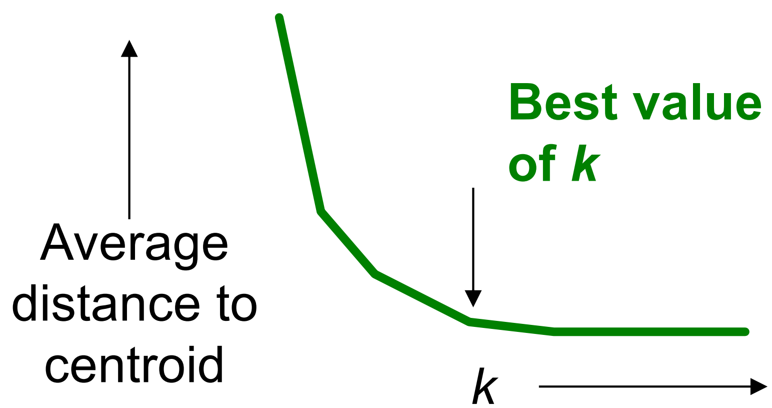
Populating Clusters

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

Getting the *k* right

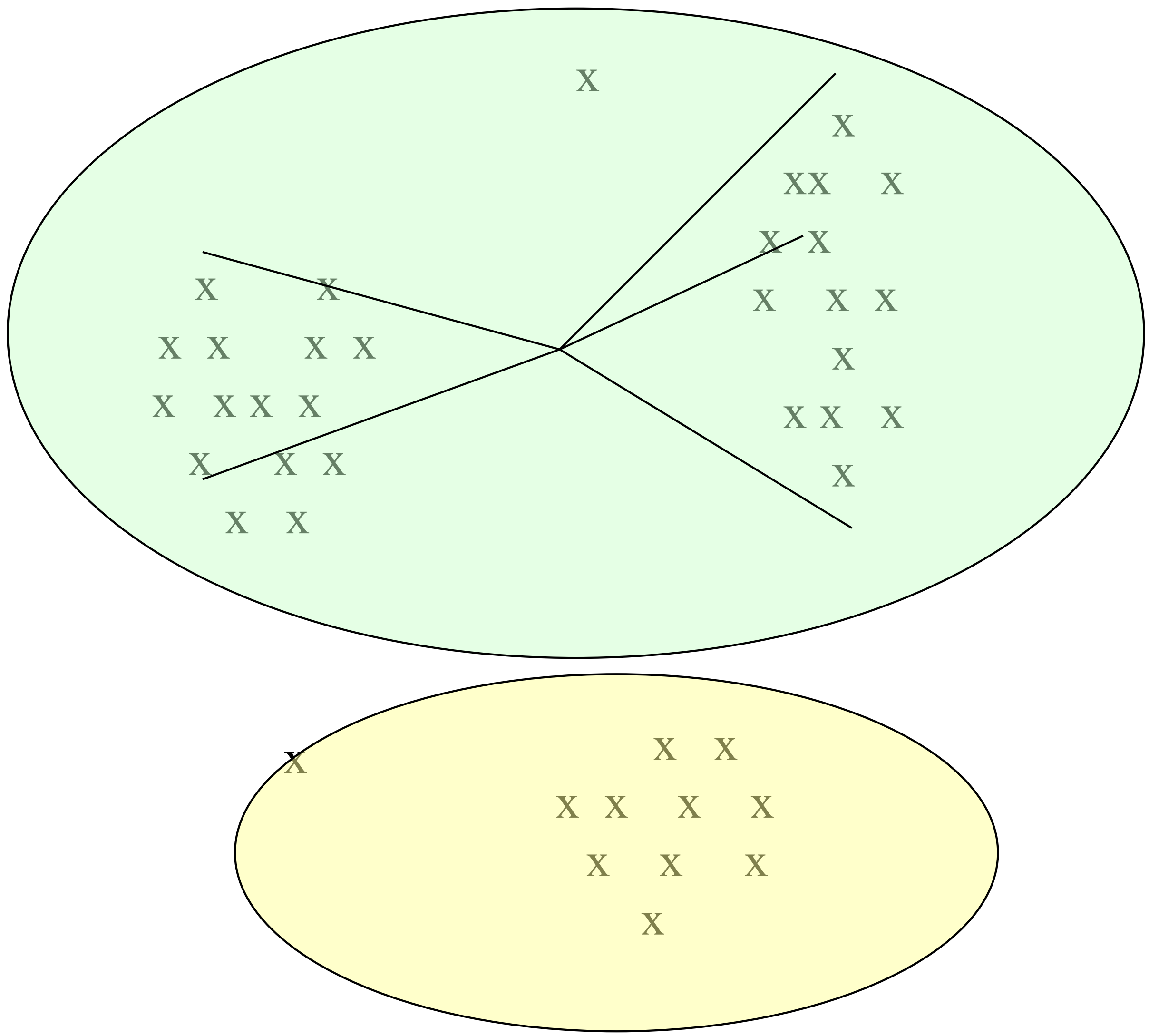
How to select *k*?

- 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



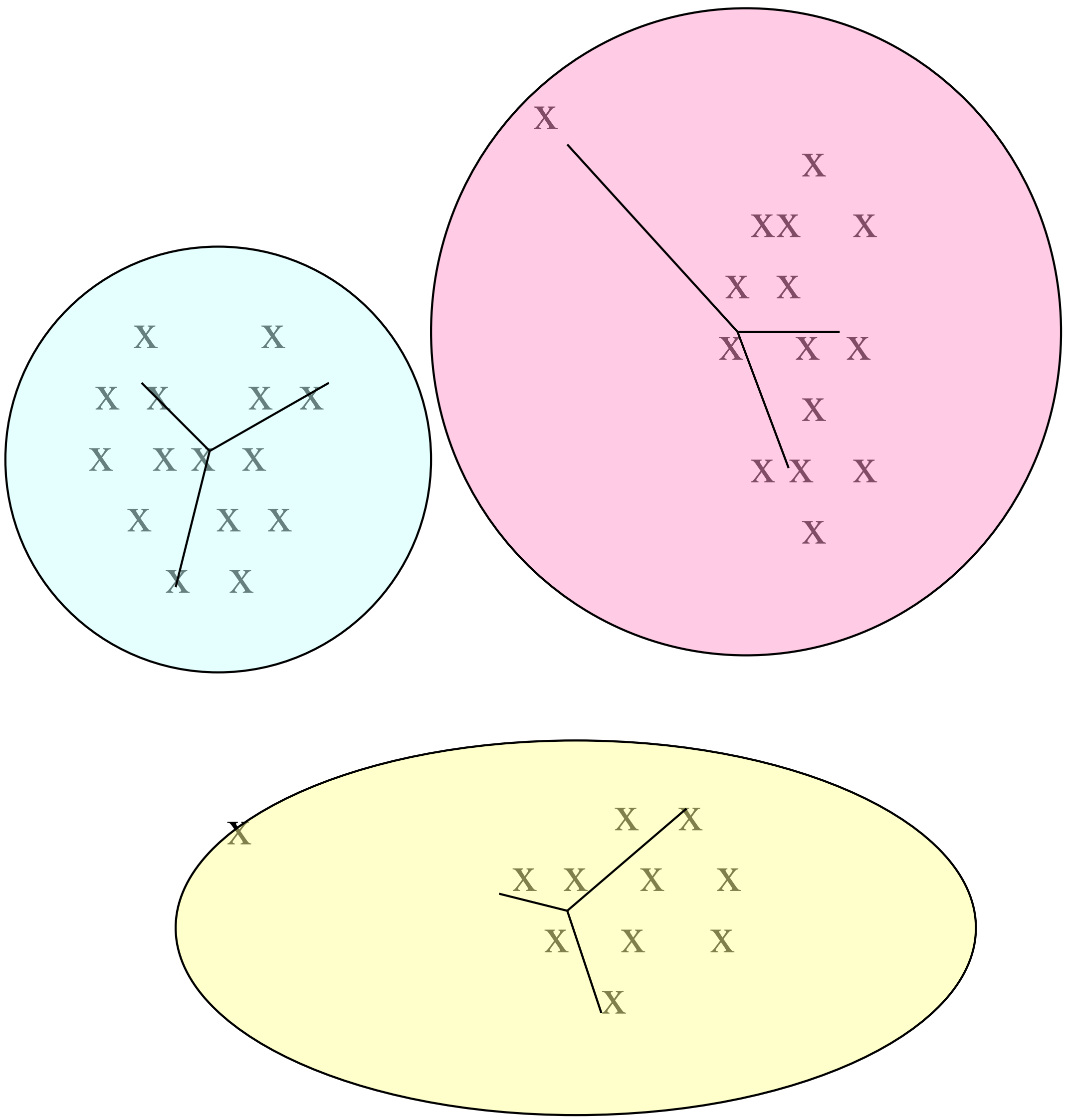
Example: Picking *k*

Too few;
many long
distances
to centroid.



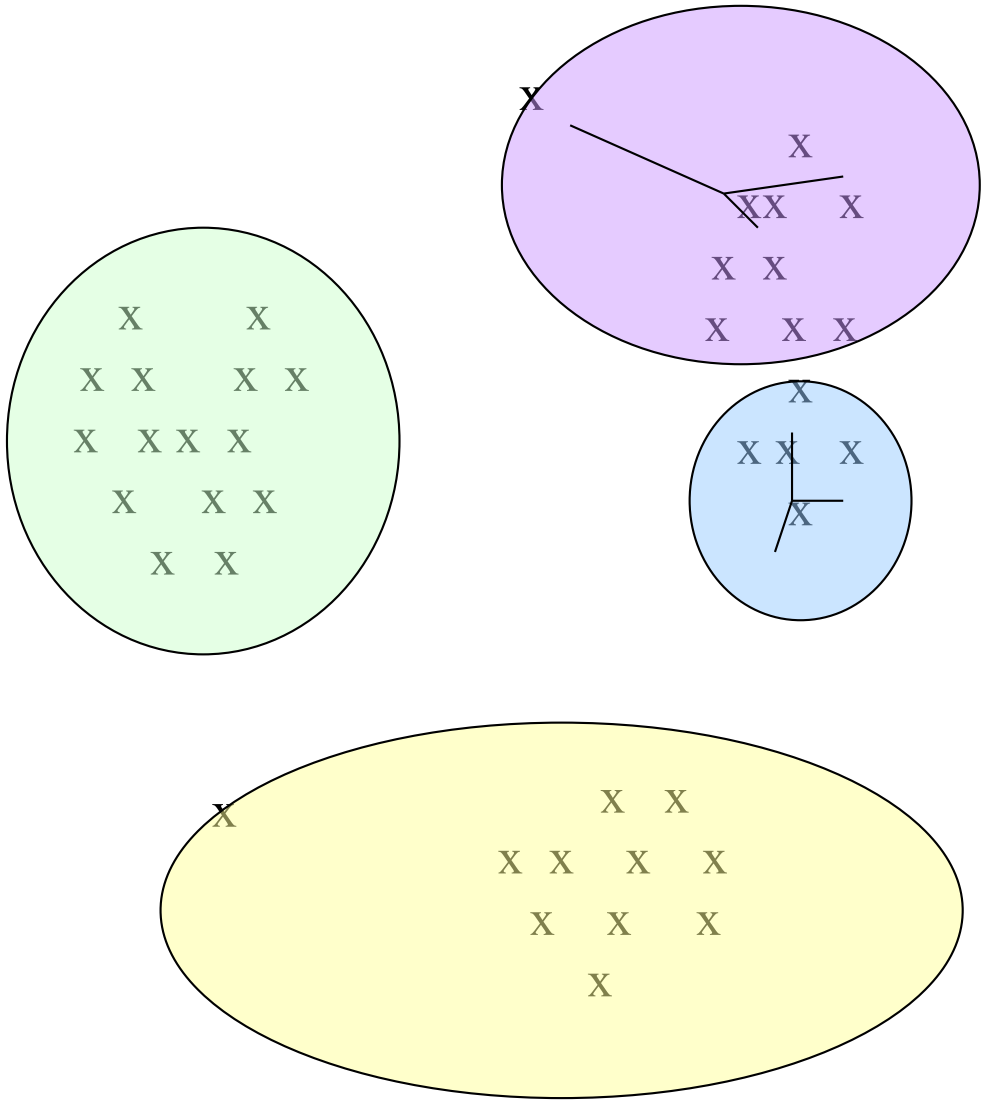
Example: Picking *k*

Just right;
distances
rather short.



Example: Picking *k*

Too many;
little improvement
in average
distance.



Summary

- **Clustering:** Given a **set of points**, with a notion of **distance** between points, **group the points** into some number of ***clusters***
- **Algorithms:**
  - Agglomerative **hierarchical clustering**:
    - Centroid and clustroid
  - ***k*-means:**
    - Initialization, picking *k*