

Clustering

Agglomerative, K-Means, BFR

High Dimensional Data



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

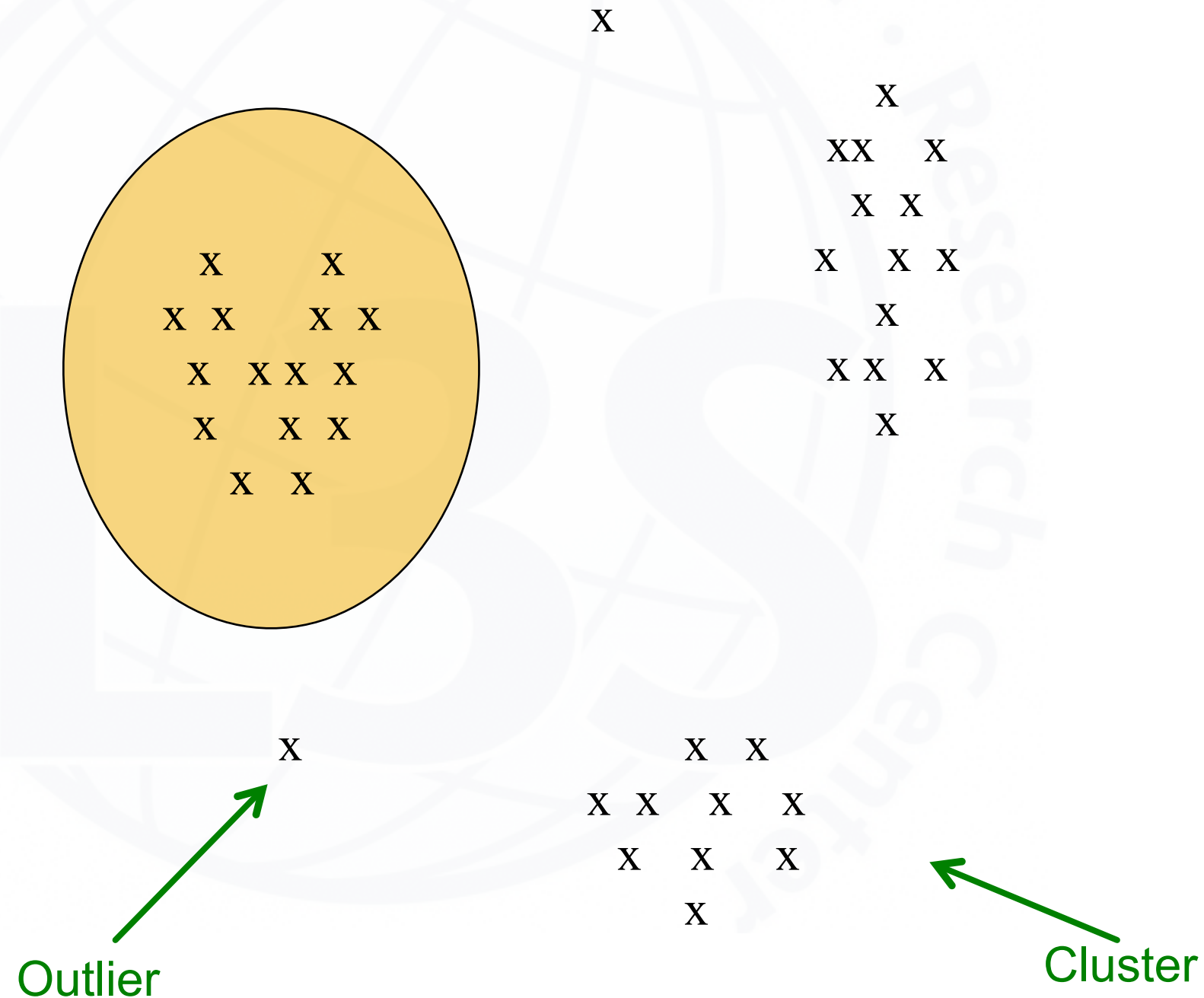
The Problem of Clustering

- 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, ...

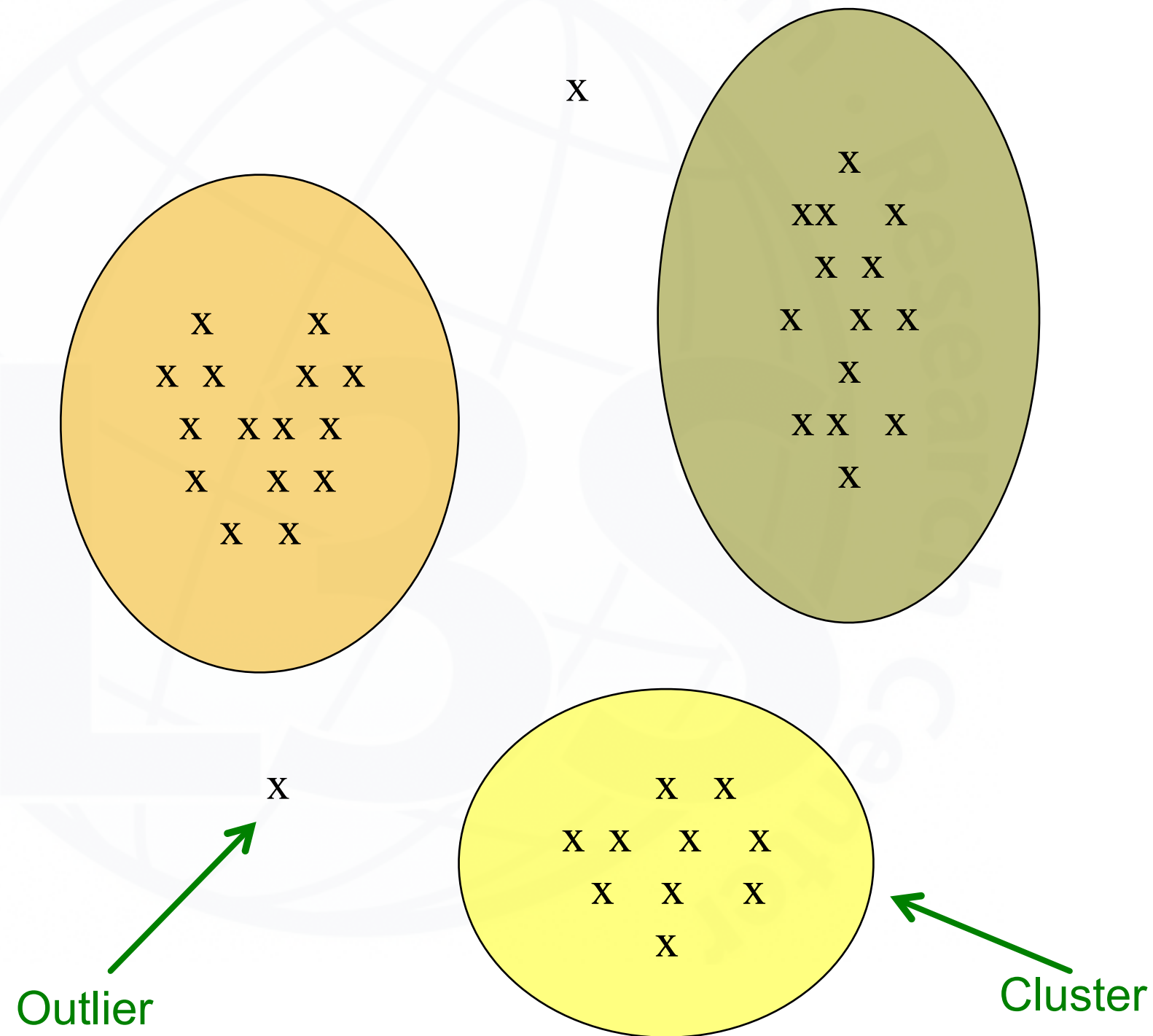
Example: Clusters & Outliers



Example: Clusters & Outliers



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

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
- 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

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, \dots, 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, \dots, x_k) , where $x_i = 1$ iff the i^{th} word (in some order) appears in the document
 - It actually doesn't matter if k is infinite; i.e., we don't limit the set of words
- **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**
 - **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):

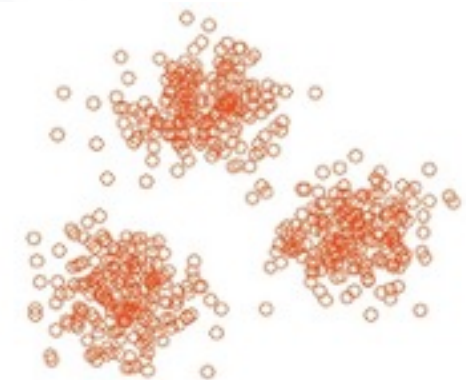
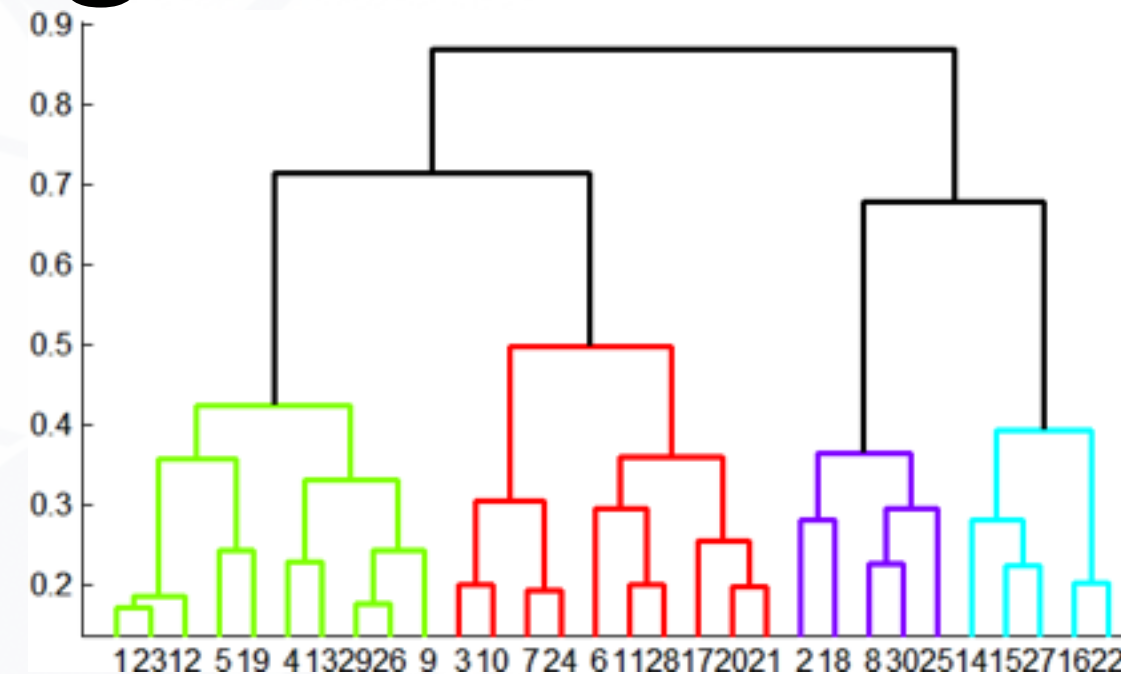
- Initially, each point is a cluster
 - Repeatedly combine the two “nearest” clusters into one

- **Divisive** (top down):

- Start with one cluster and recursively split it

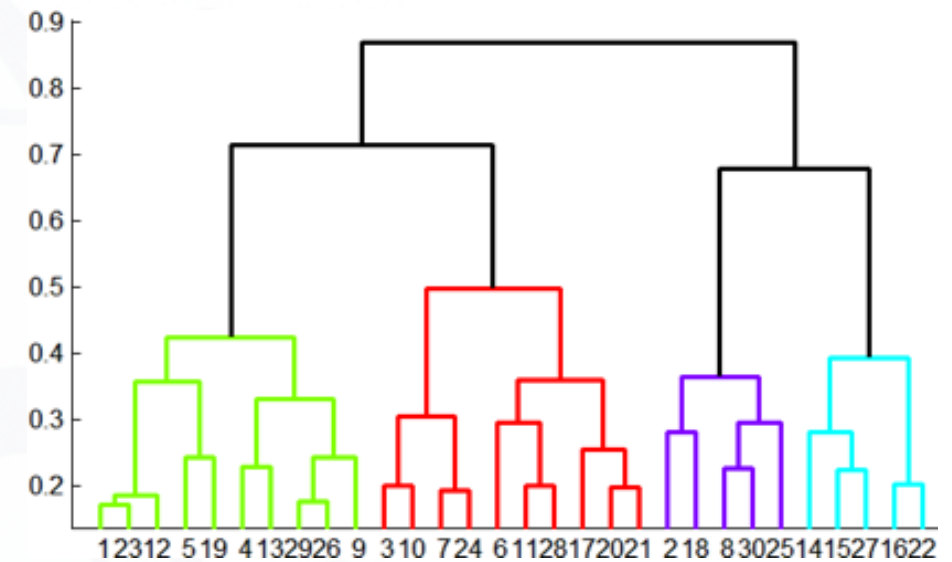
- **Point assignment:**

- Maintain a set of clusters
 - Points belong to “nearest” cluster



Hierarchical Clustering

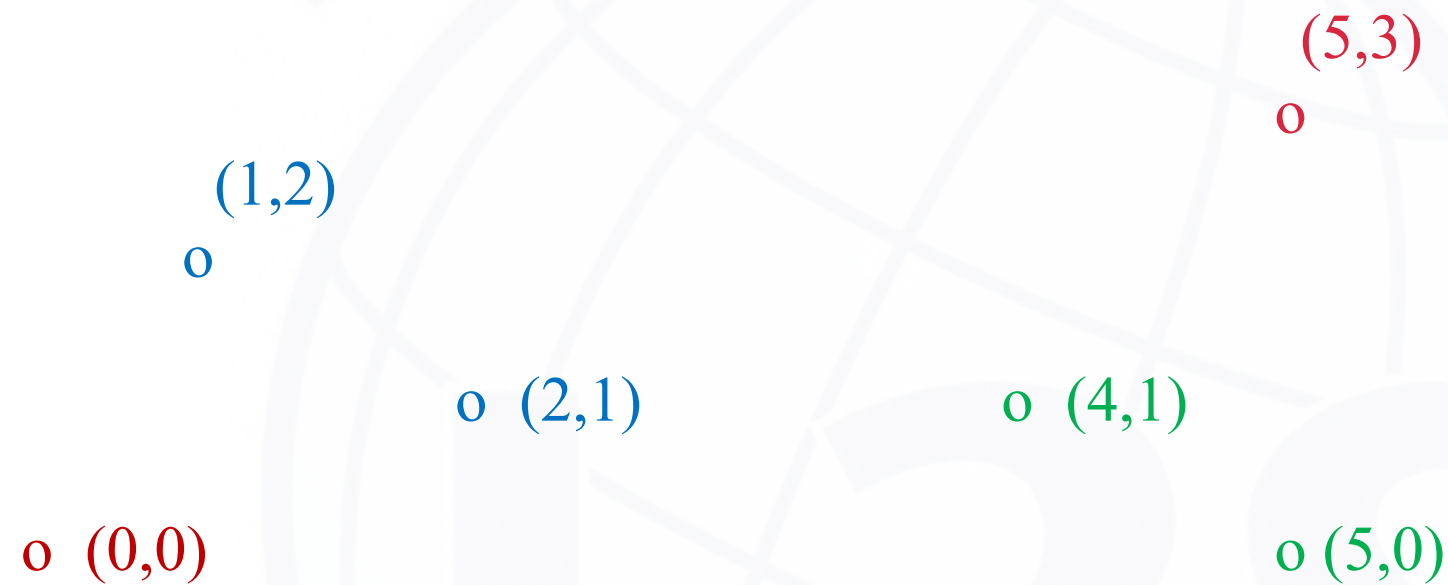
- **Key operation:**
Repeatedly combine two nearest clusters
- **Three important questions:**
 - 1) How do you represent a cluster of more than one point?
 - 2) How do you determine the “nearness” of clusters?
 - 3) When to stop combining clusters?



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



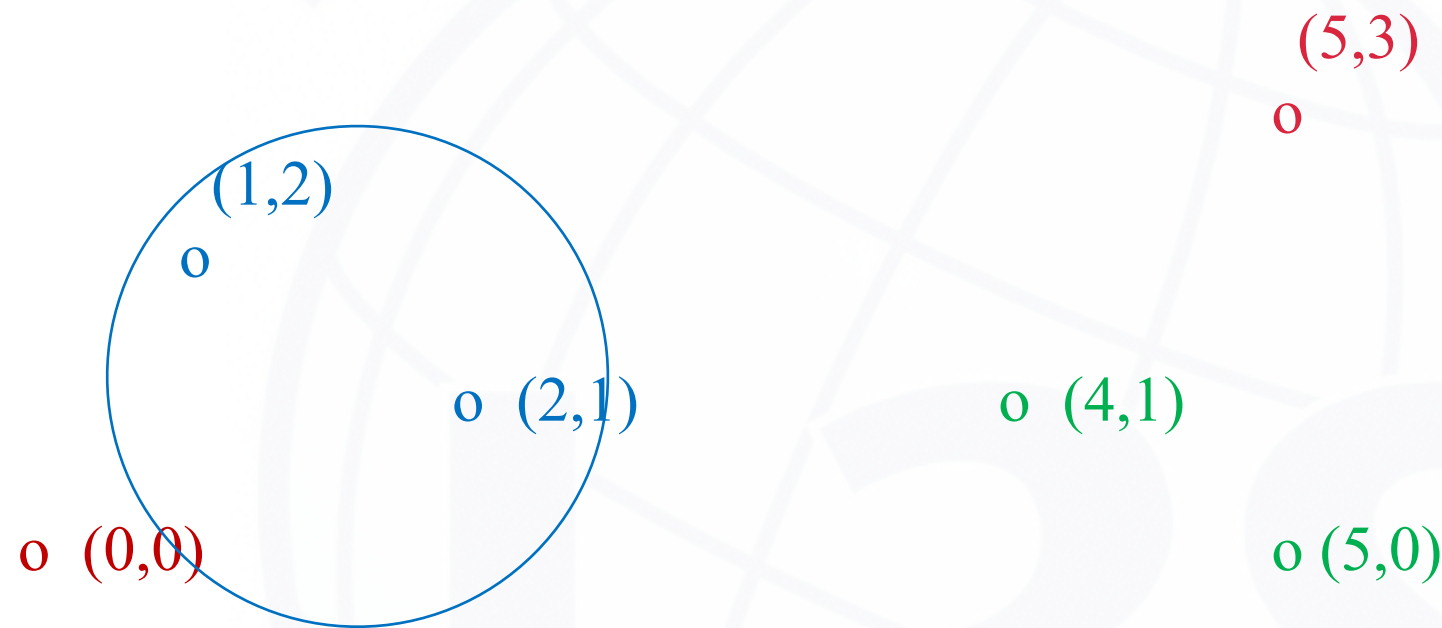
Data:

o ... data point

x ... centroid



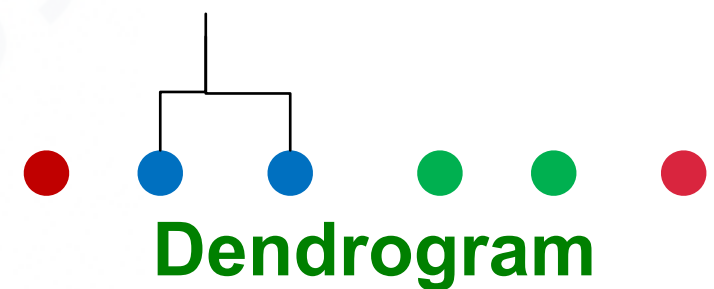
Example: Hierarchical clustering



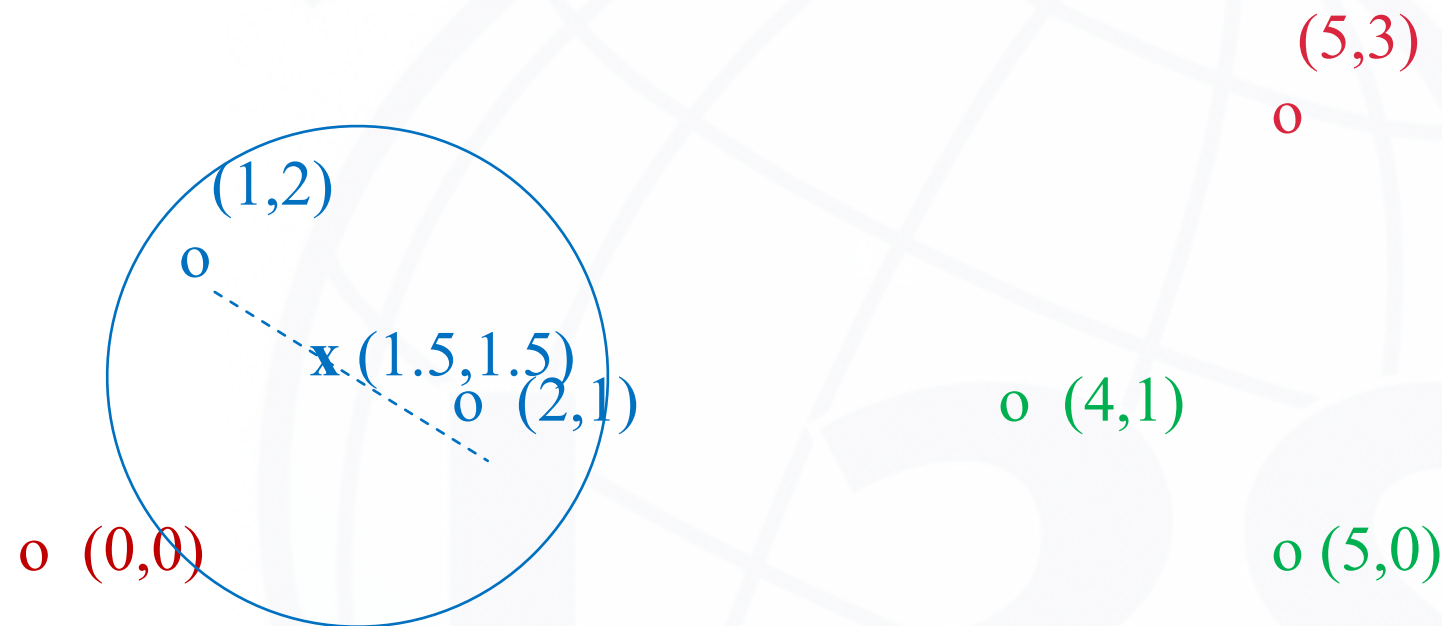
Data:

o ... data point

x ... centroid



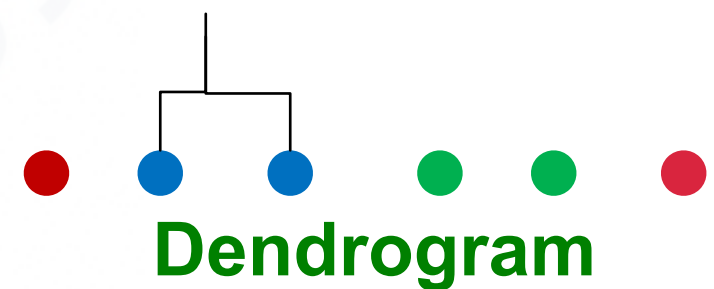
Example: Hierarchical clustering



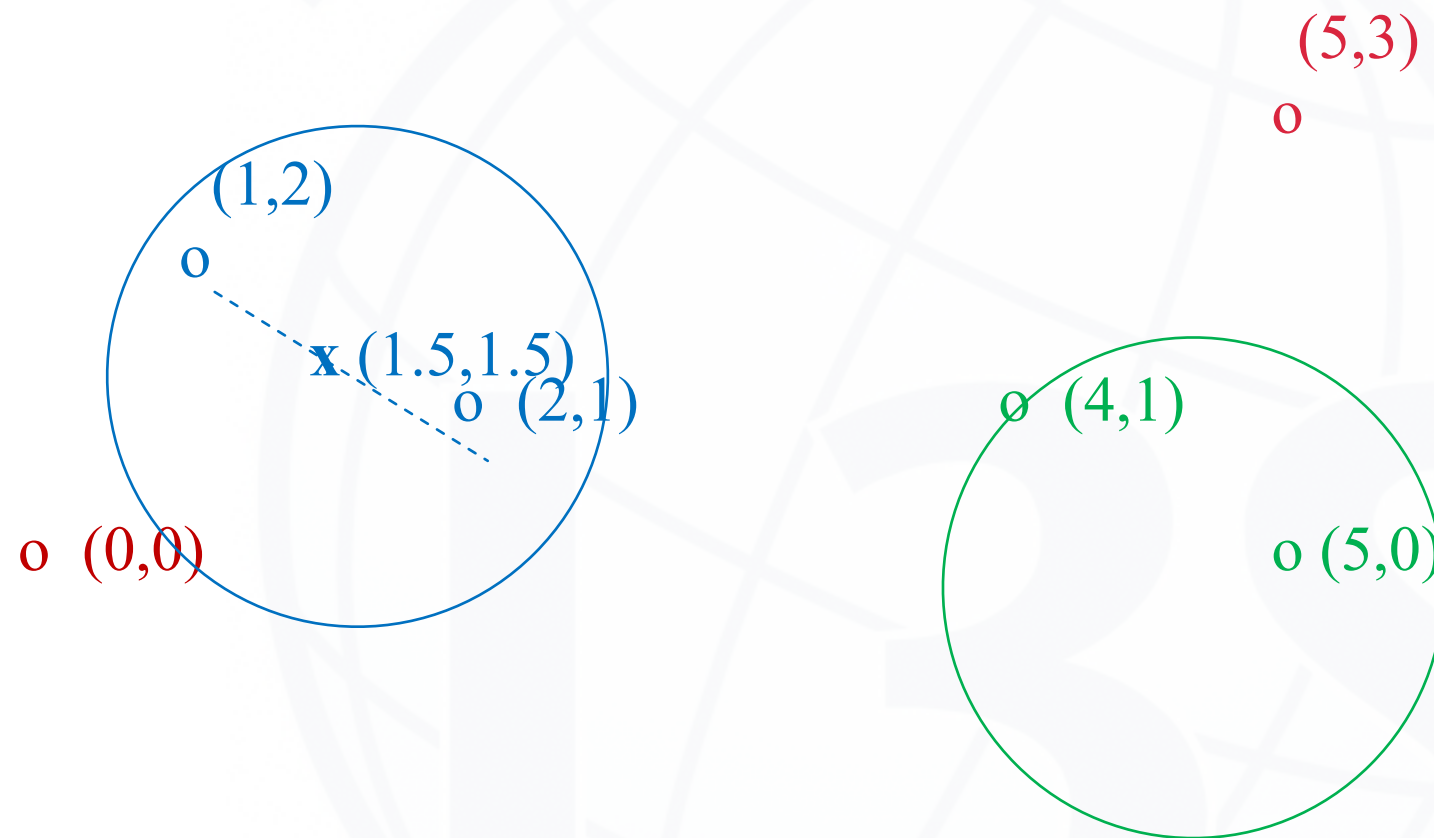
Data:

o ... data point

x ... centroid



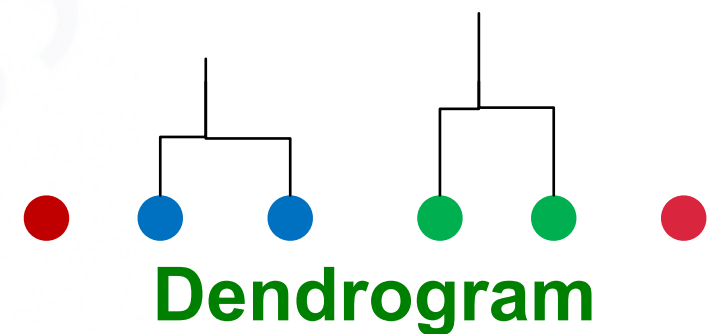
Example: Hierarchical clustering



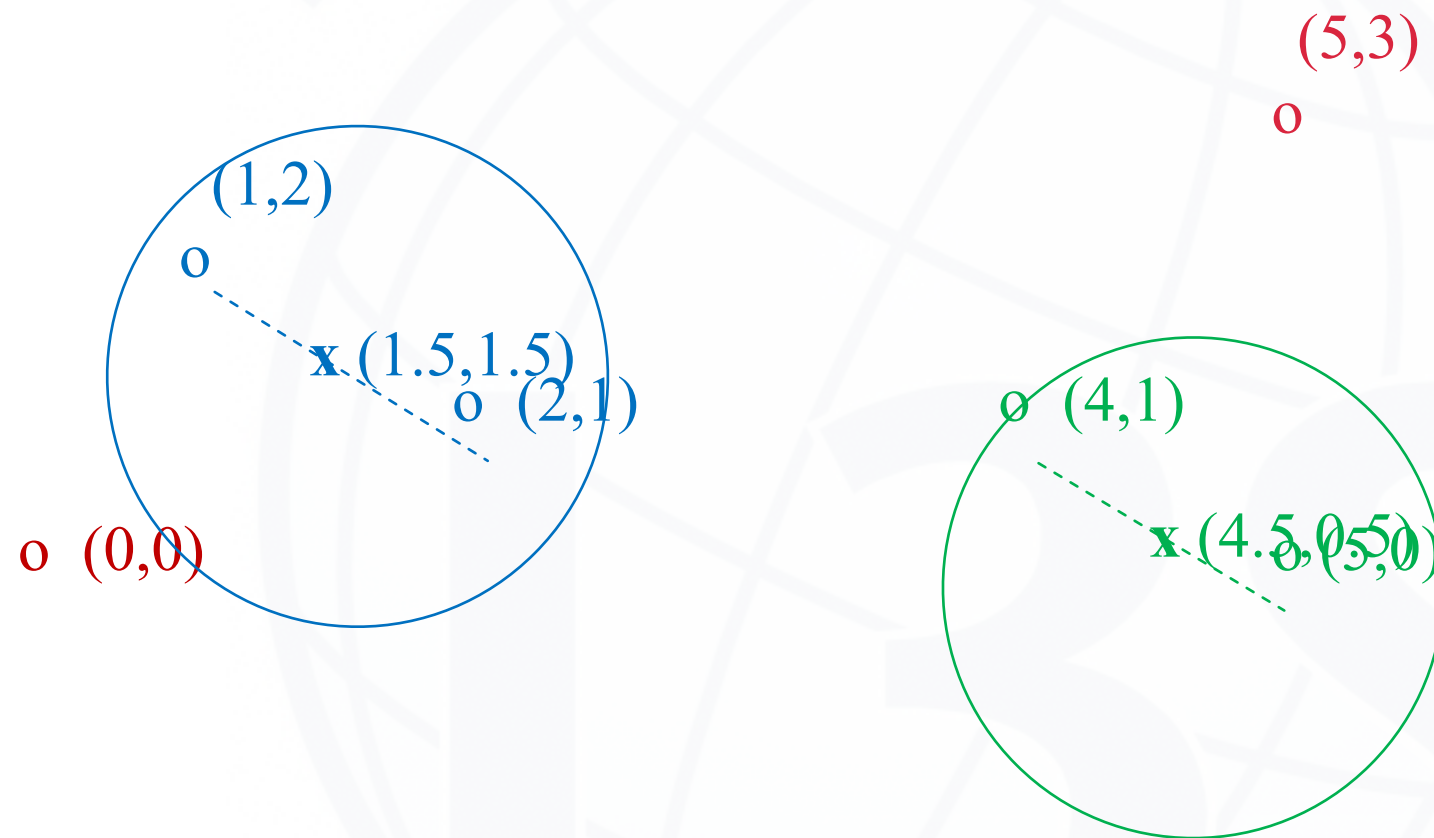
Data:

o ... data point

x ... centroid



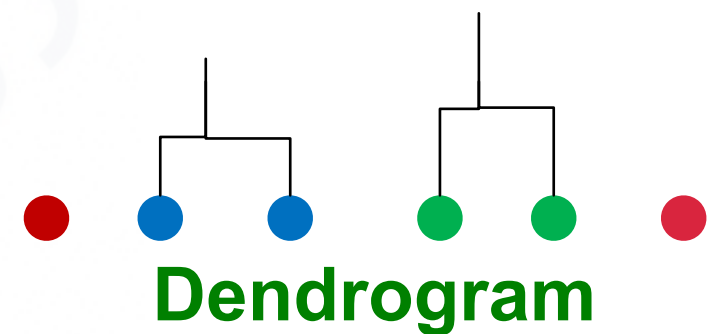
Example: Hierarchical clustering



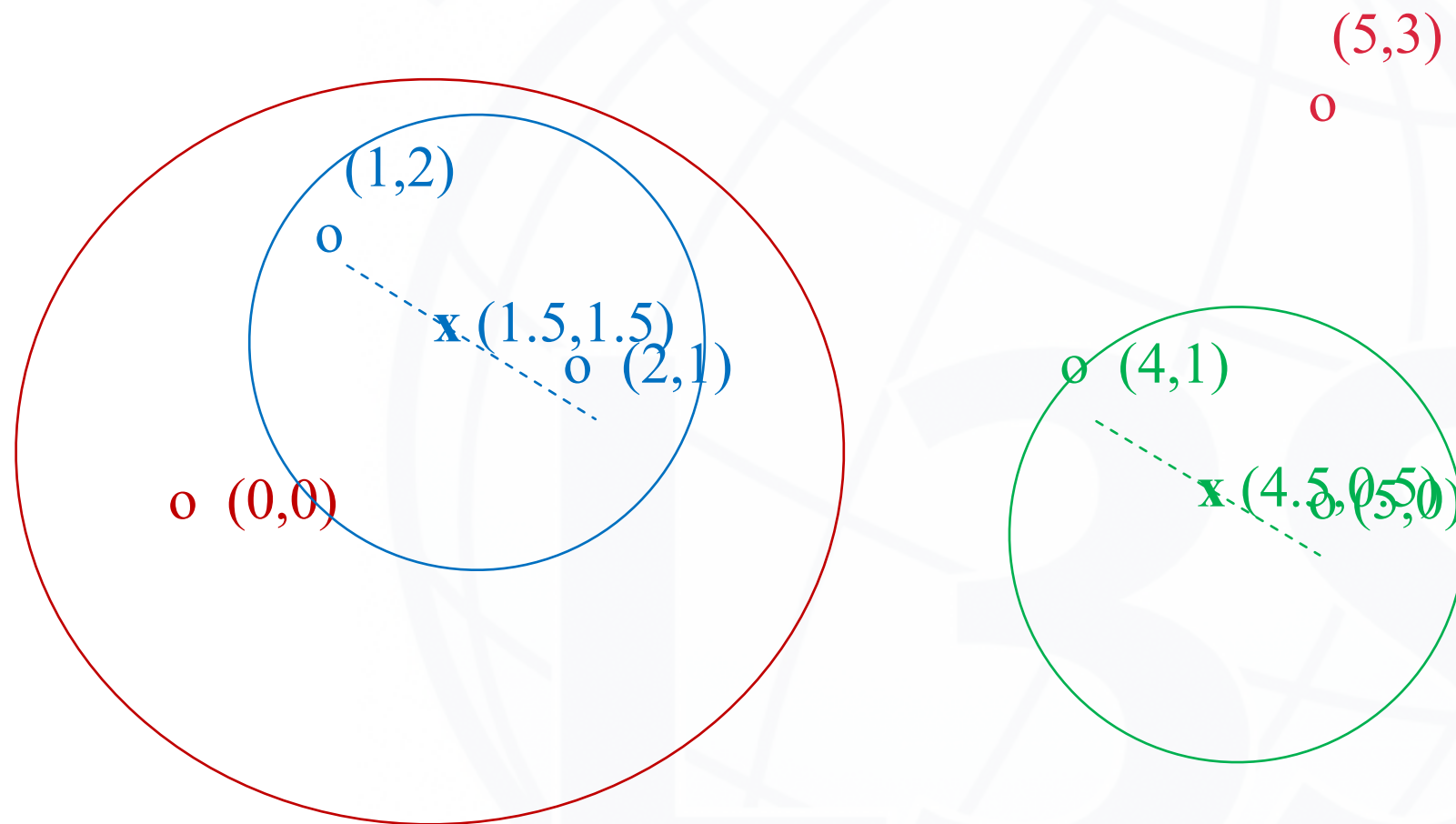
Data:

o ... data point

x ... centroid



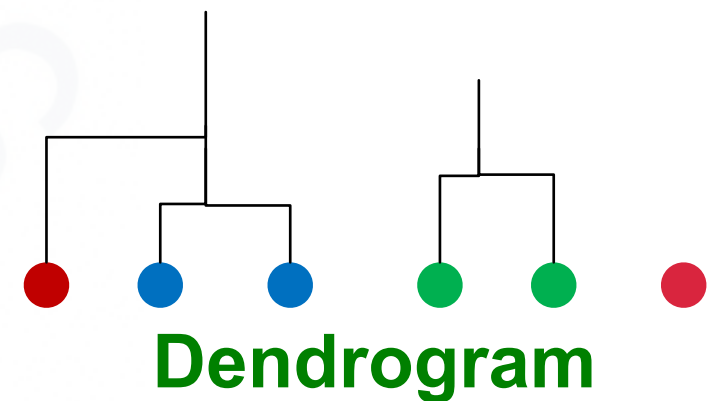
Example: Hierarchical clustering



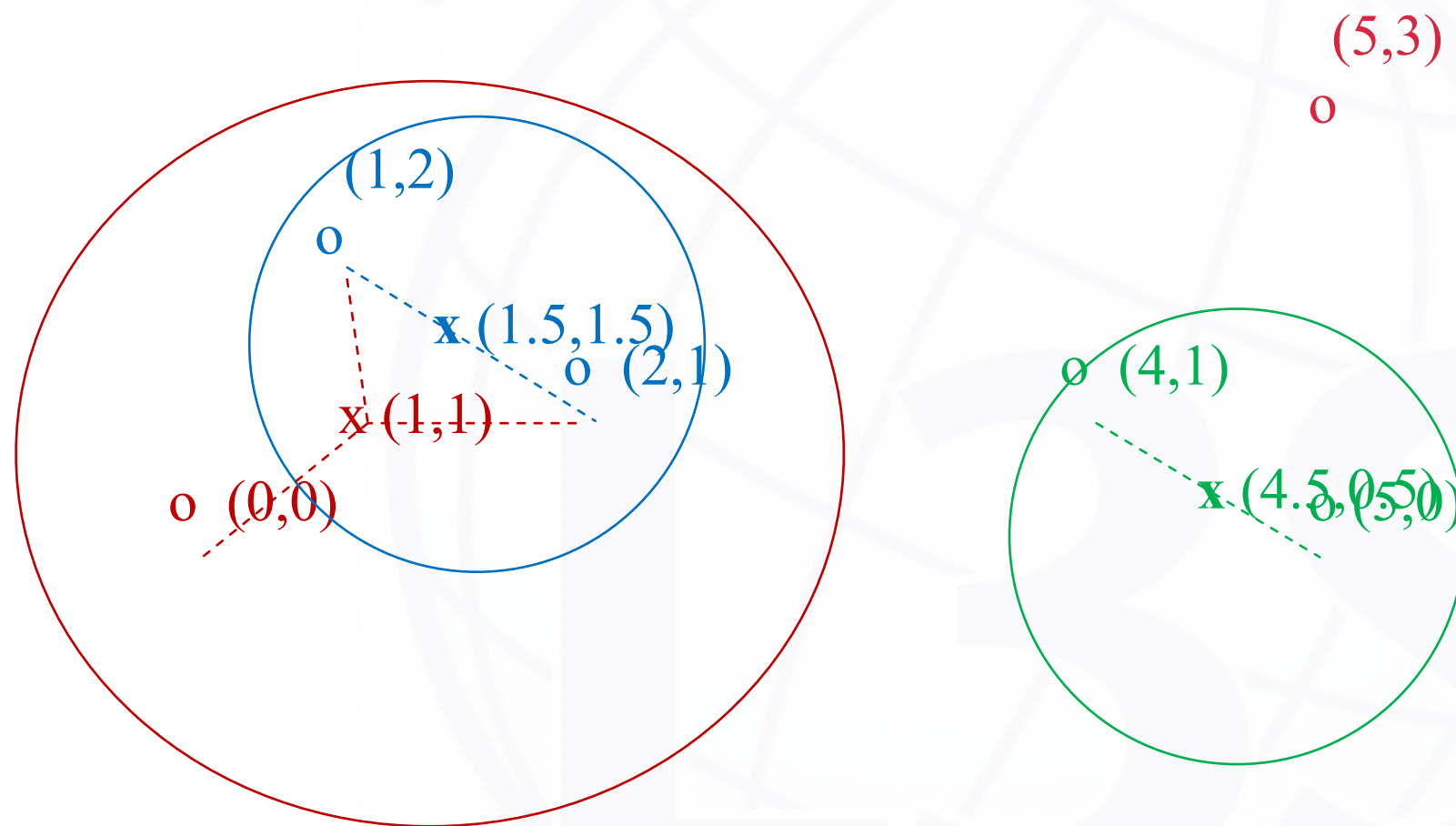
Data:

o ... data point

x ... centroid



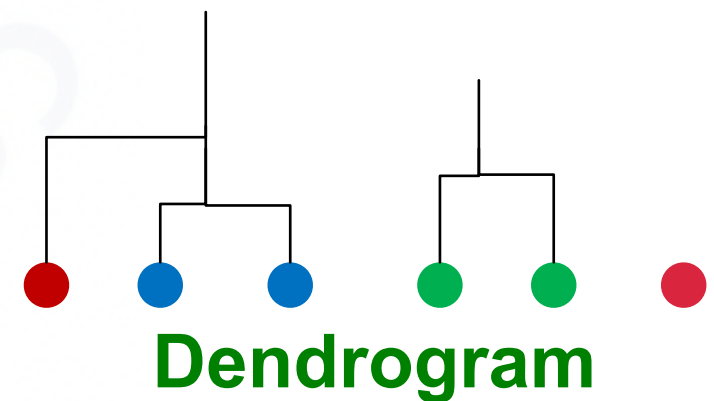
Example: Hierarchical clustering



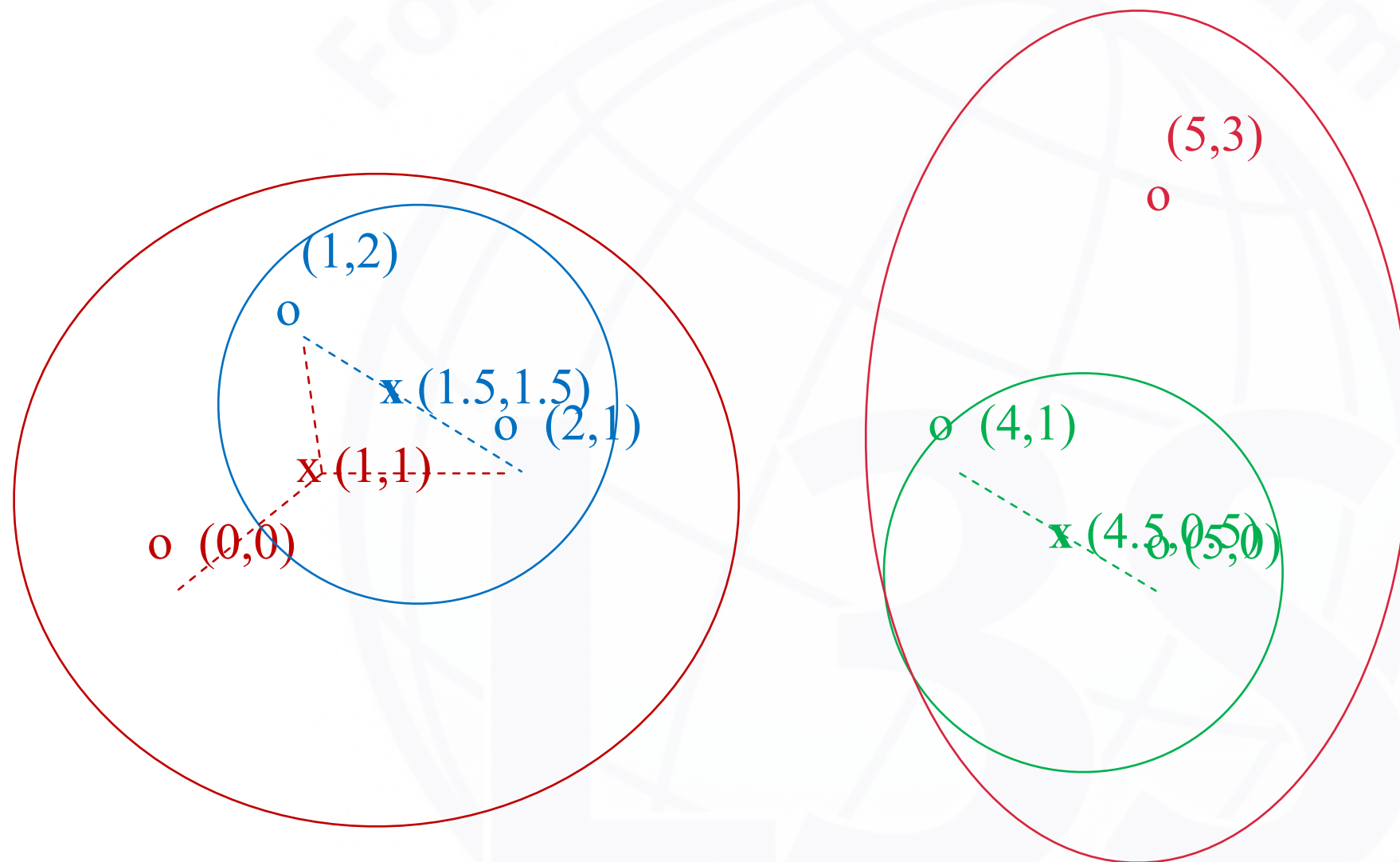
Data:

o ... data point

x ... centroid



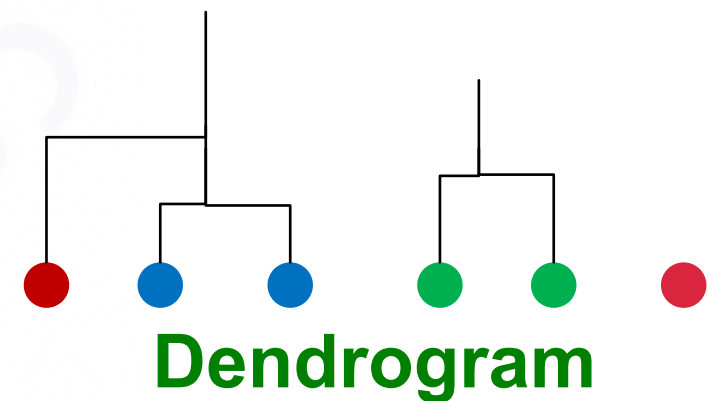
Example: Hierarchical clustering



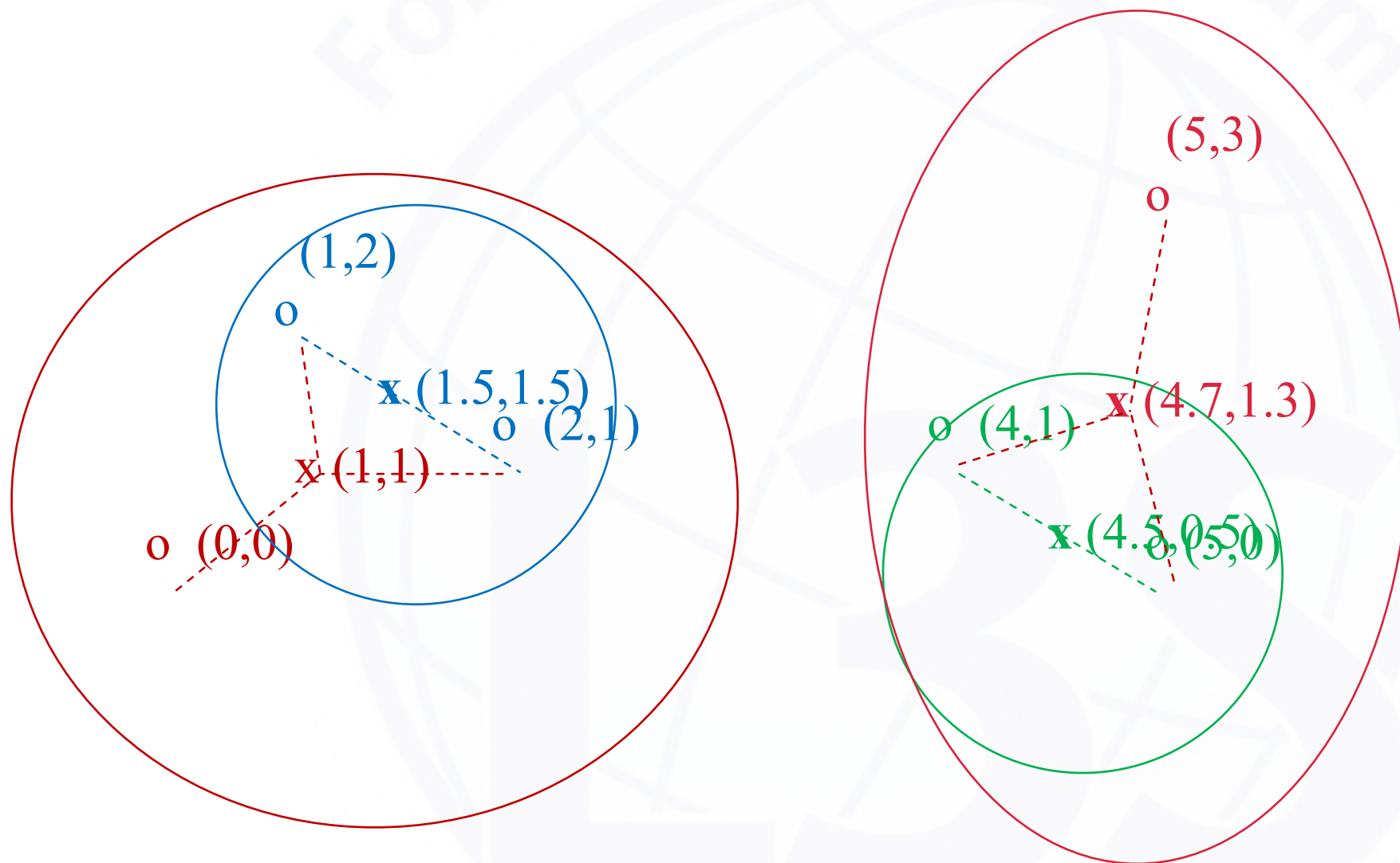
Data:

o ... data point

x ... centroid



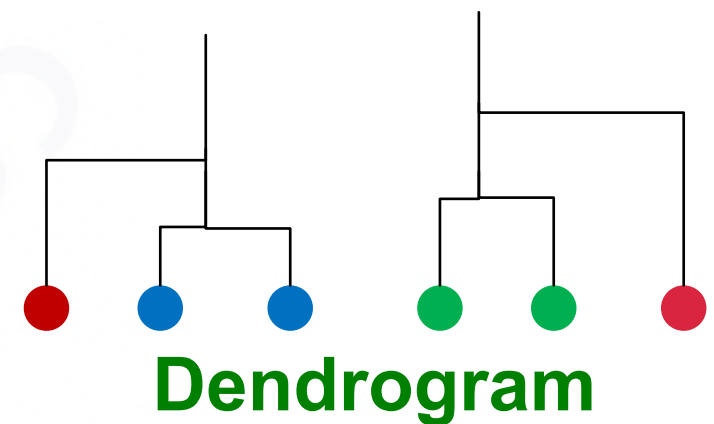
Example: Hierarchical clustering



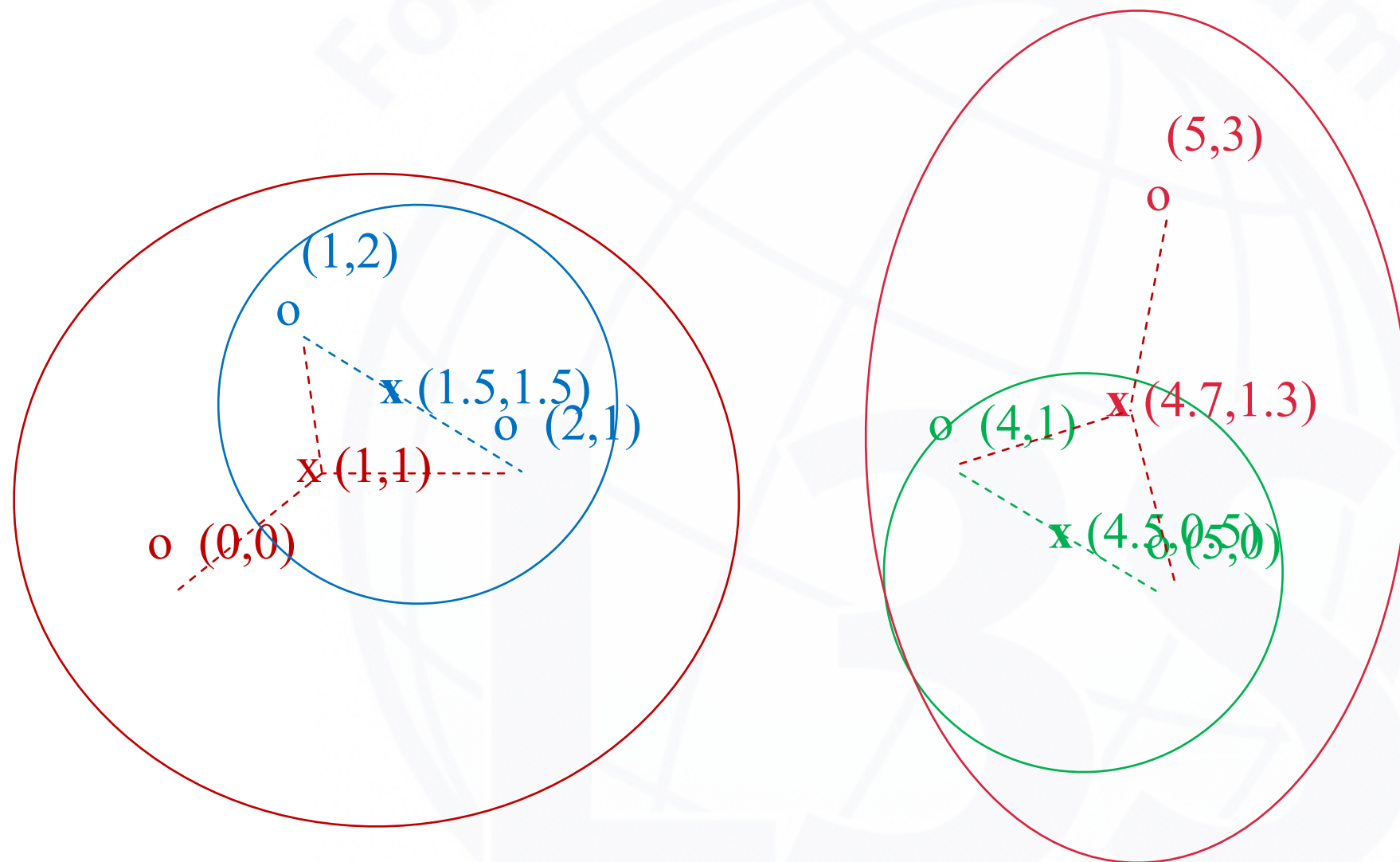
Data:

o ... data point

x ... centroid



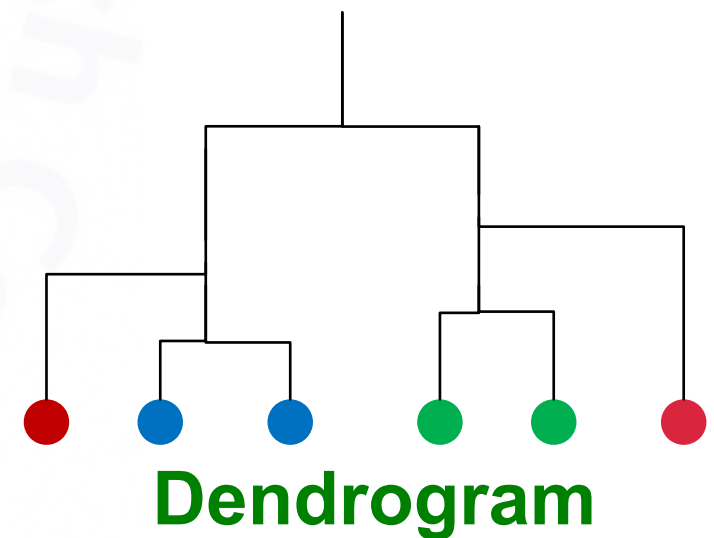
Example: Hierarchical clustering



Data:

o ... data point

x ... centroid



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?

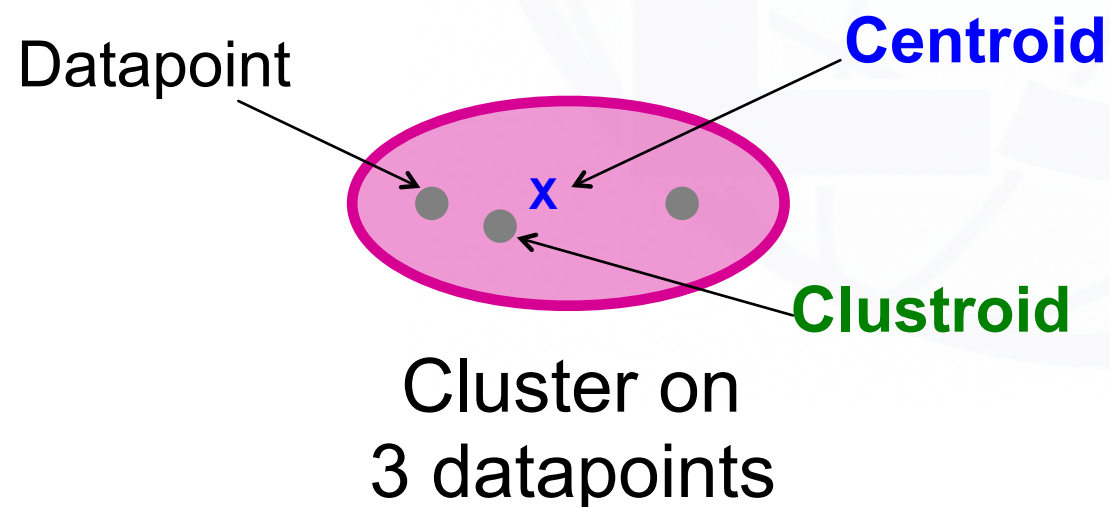
- (1) How to represent a cluster of many points?

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



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

Implementation

- **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 $O(N^2 \log N)$
 - **Still too expensive for really big datasets that do not fit in memory**

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

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

Example: Assigning Clusters

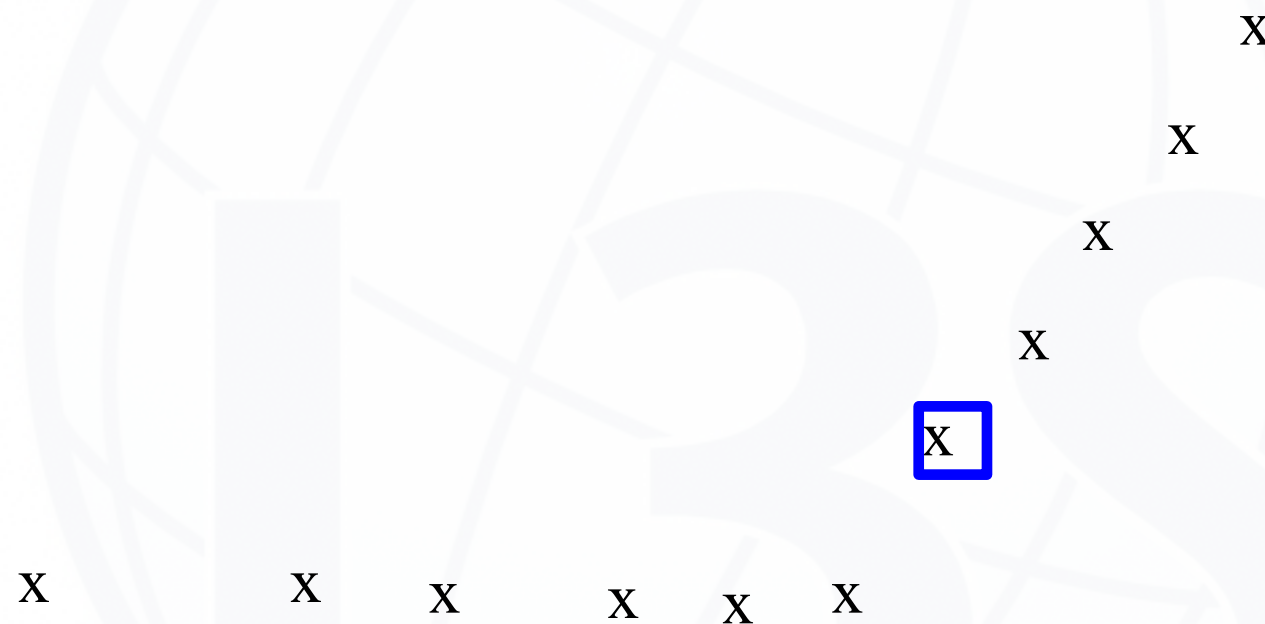


x ... data point

□ ... centroid

Clusters after round 1

Example: Assigning Clusters

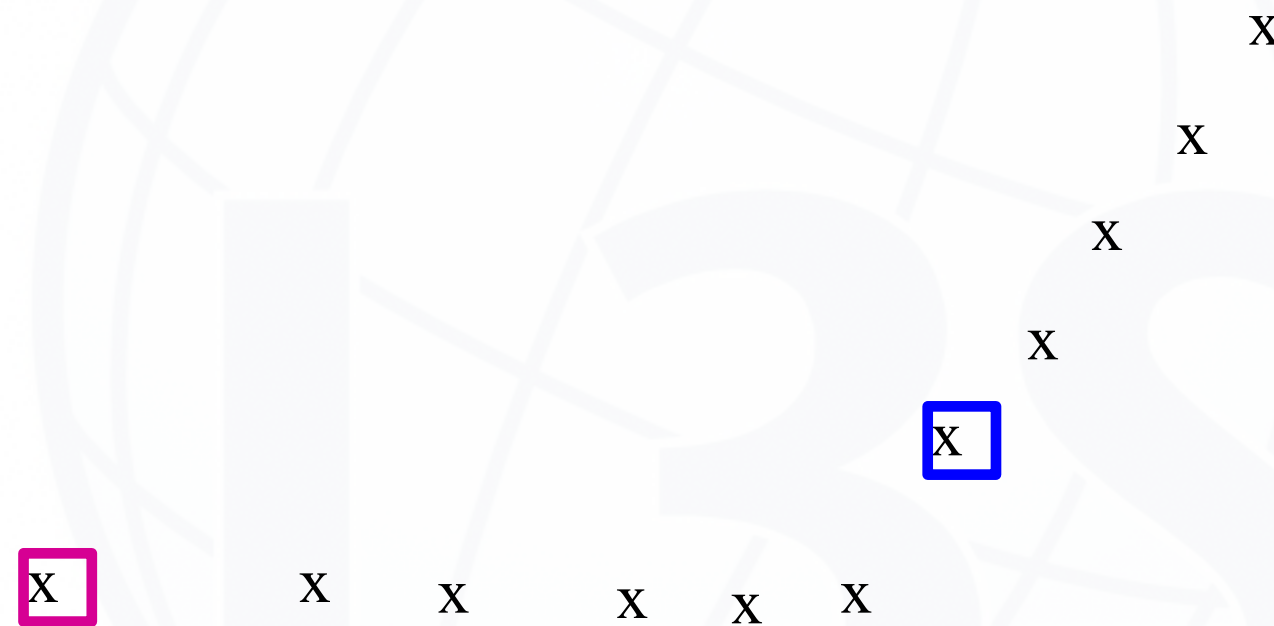


x ... data point

□ ... centroid

Clusters after round 1

Example: Assigning Clusters



x ... data point

□ ... centroid

Clusters after round 1

Example: Assigning Clusters

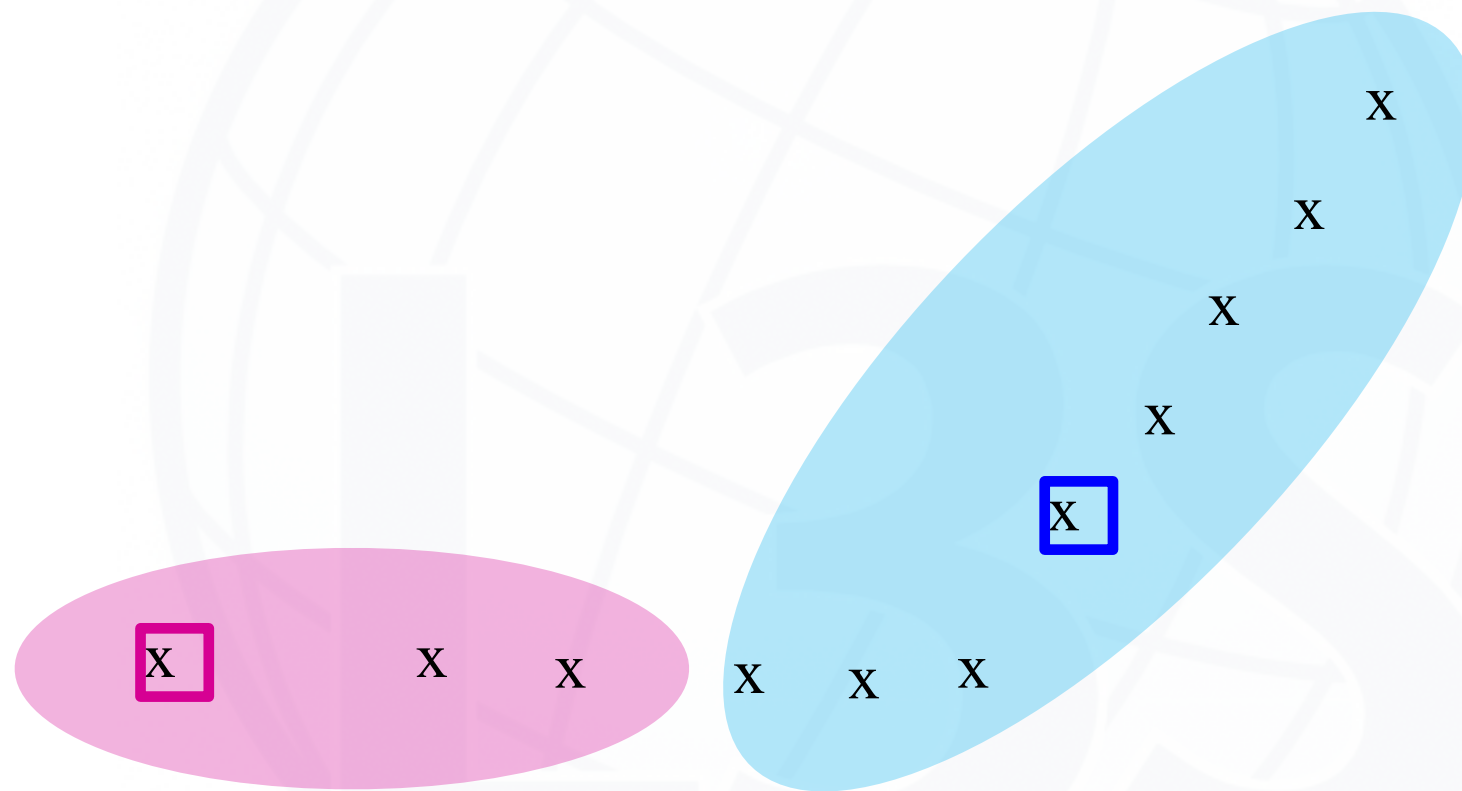


x ... data point

□ ... centroid

Clusters after round 1

Example: Assigning Clusters

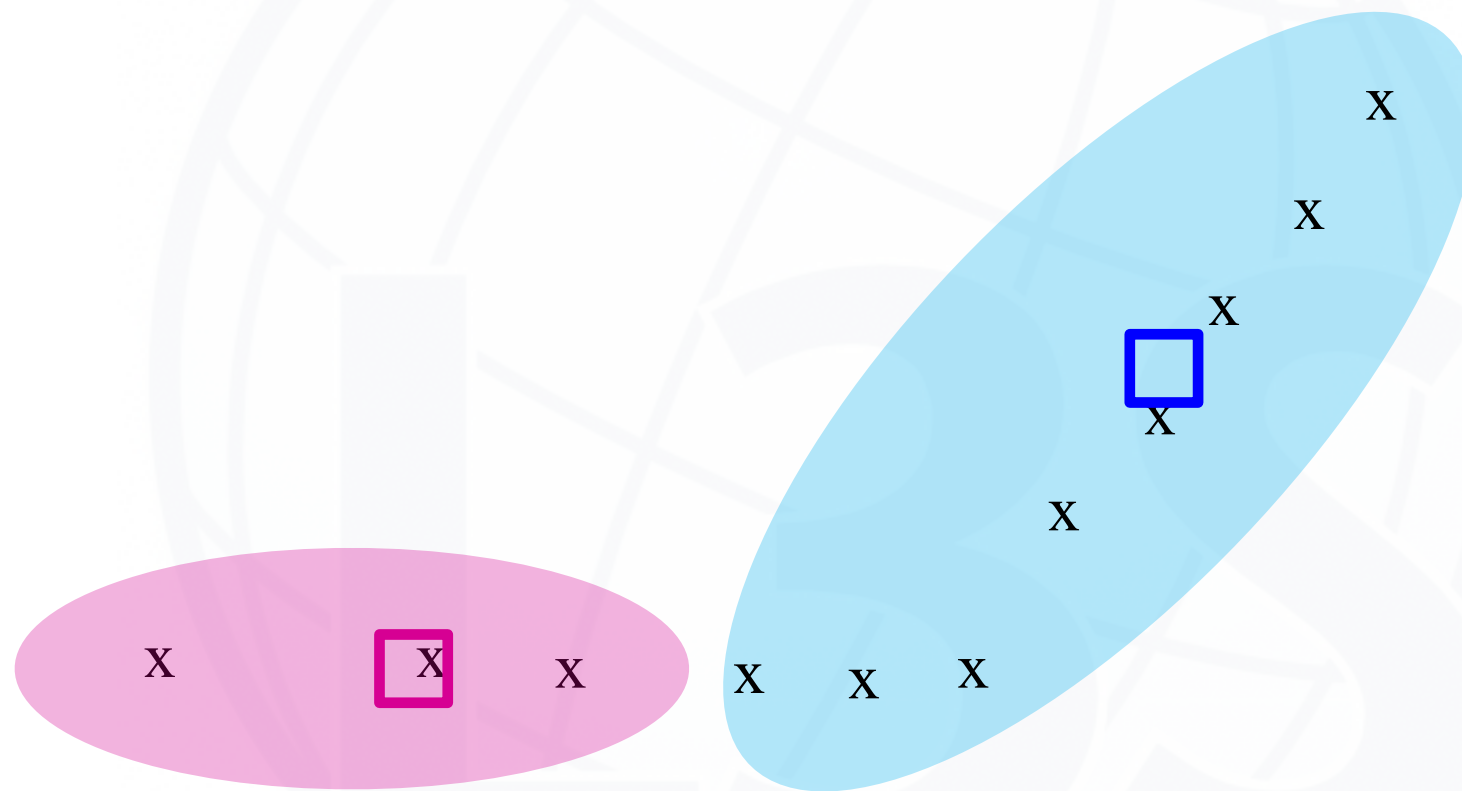


x ... data point

□ ... centroid

Clusters after round 1

Example: Assigning Clusters

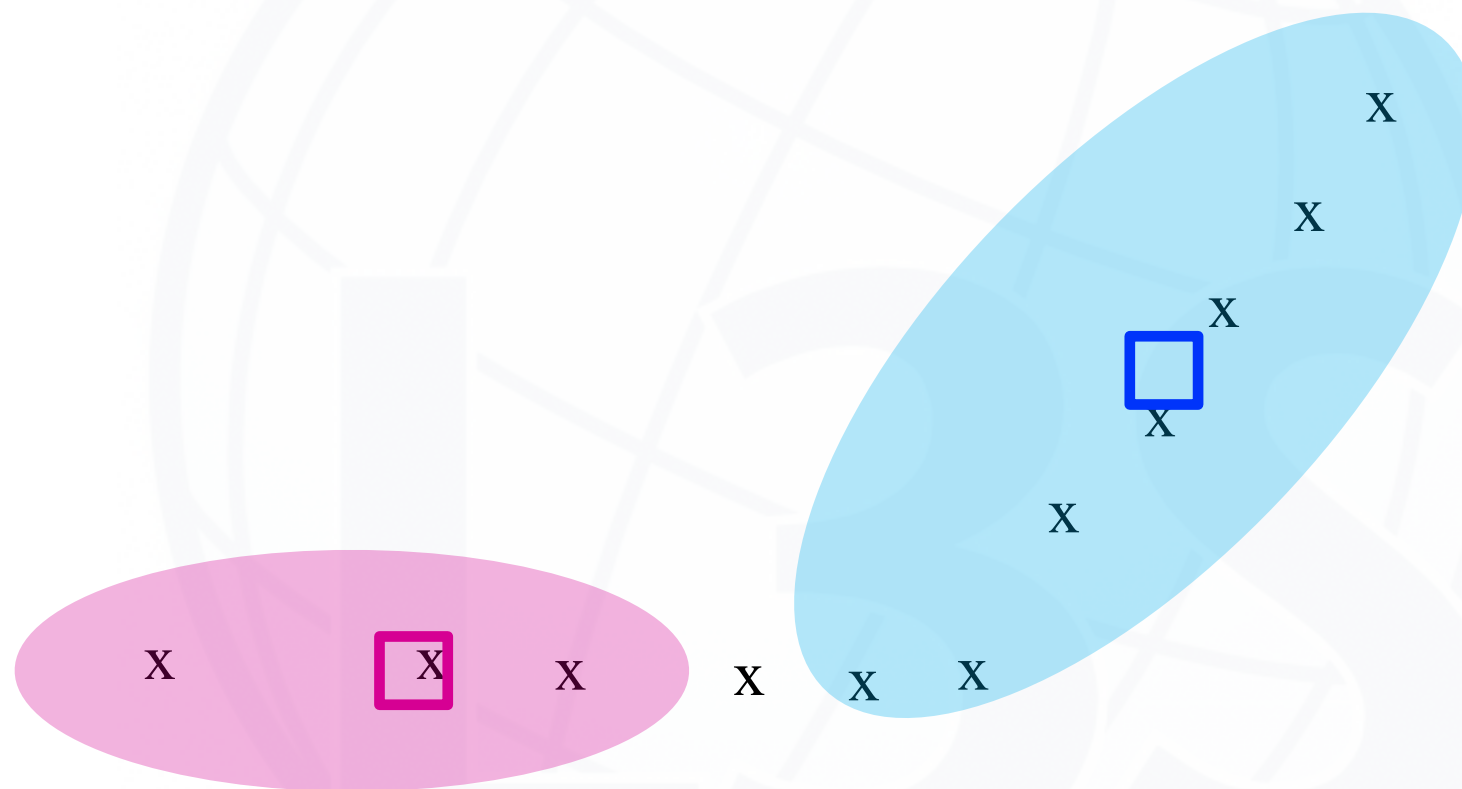


x ... data point

□ ... centroid

Clusters after round 2

Example: Assigning Clusters

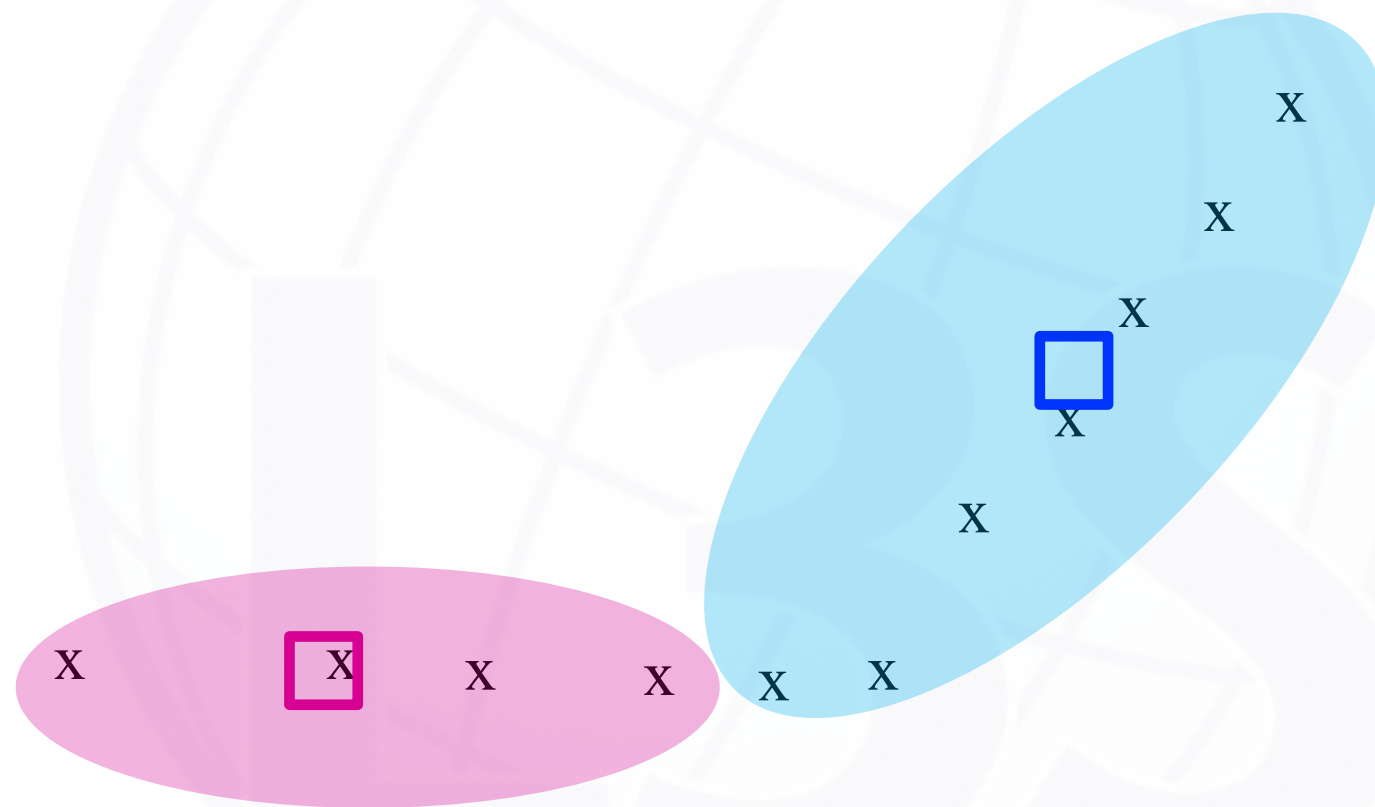


x ... data point

□ ... centroid

Clusters after round 2

Example: Assigning Clusters

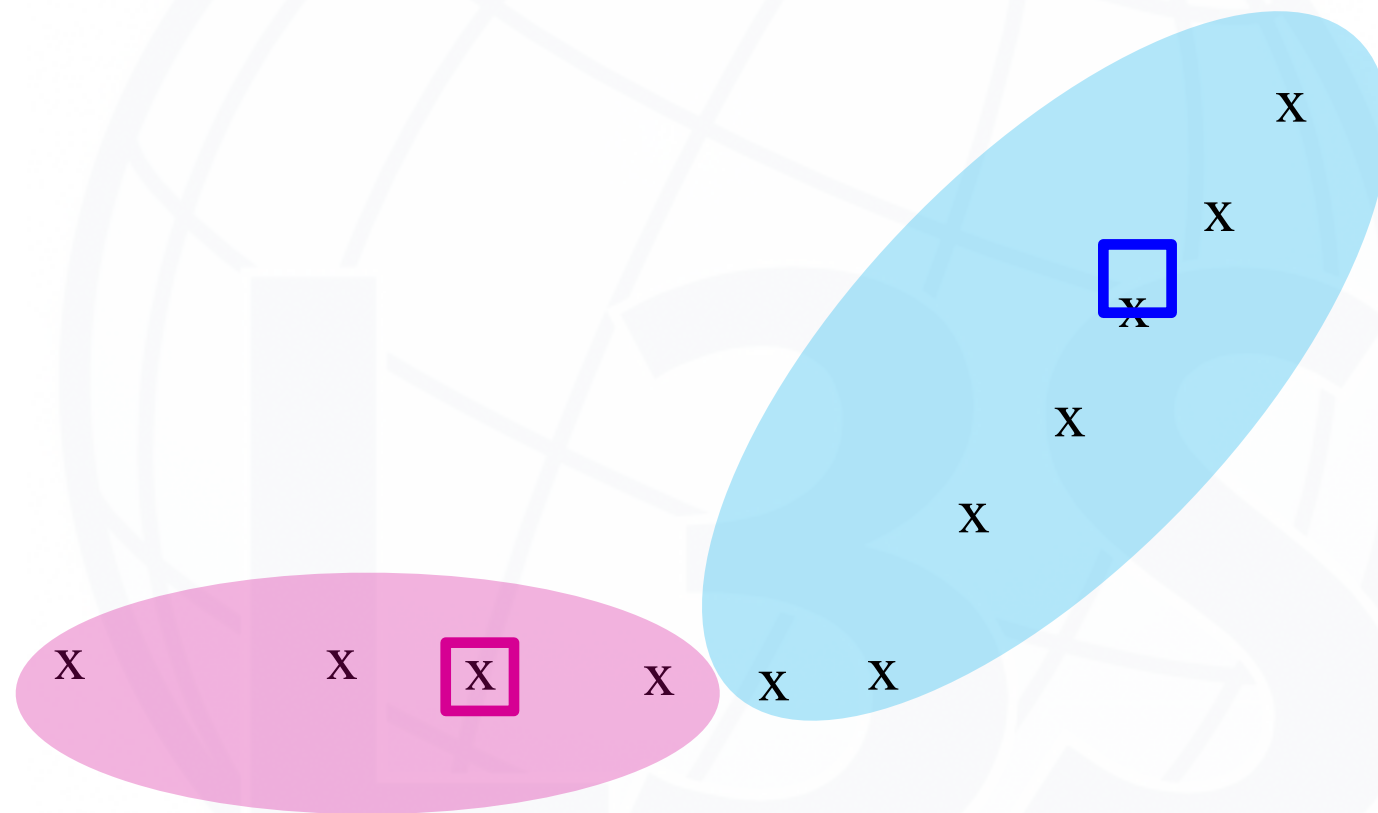


x ... data point

□ ... centroid

Clusters after round 2

Example: Assigning Clusters

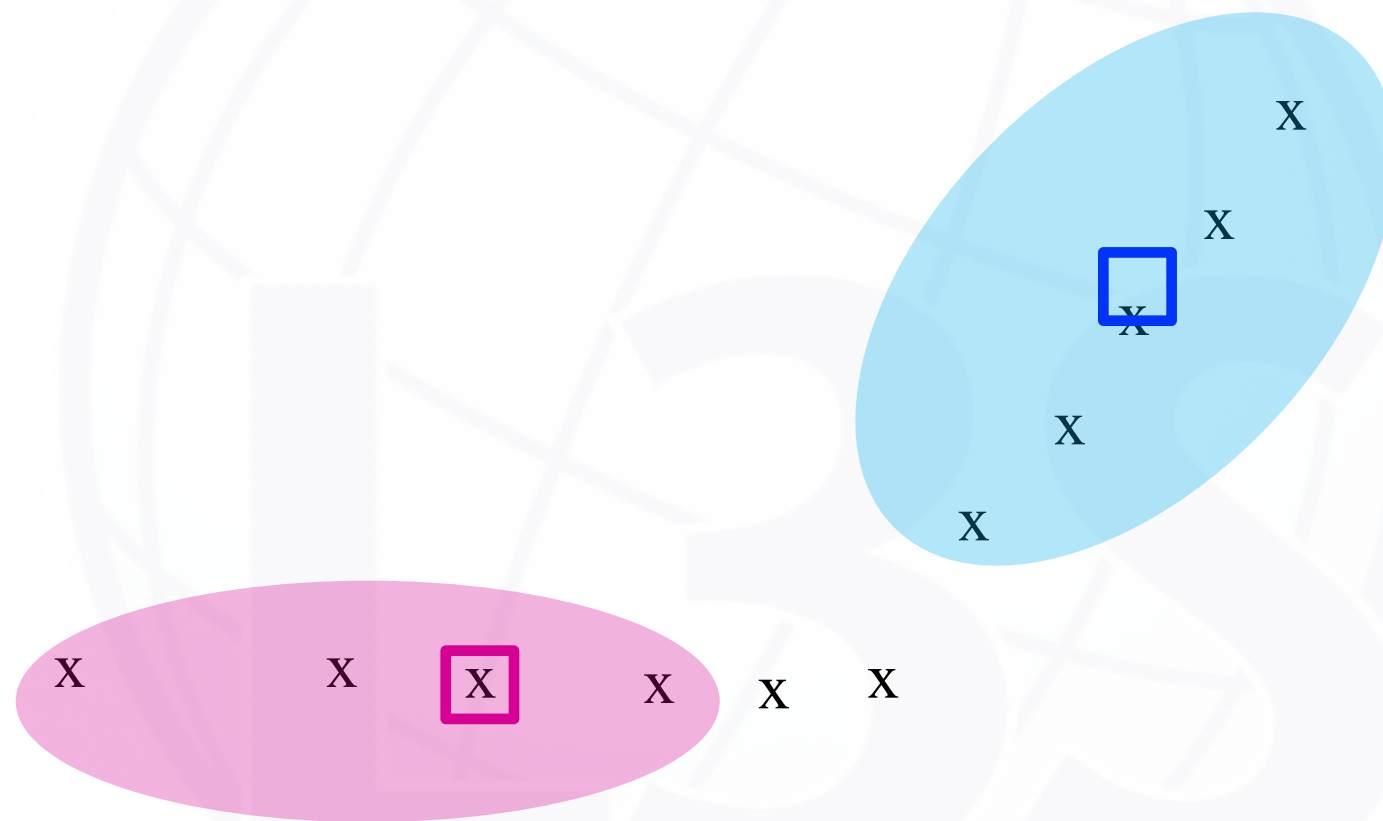


x ... data point

□ ... centroid

Clusters at the end

Example: Assigning Clusters

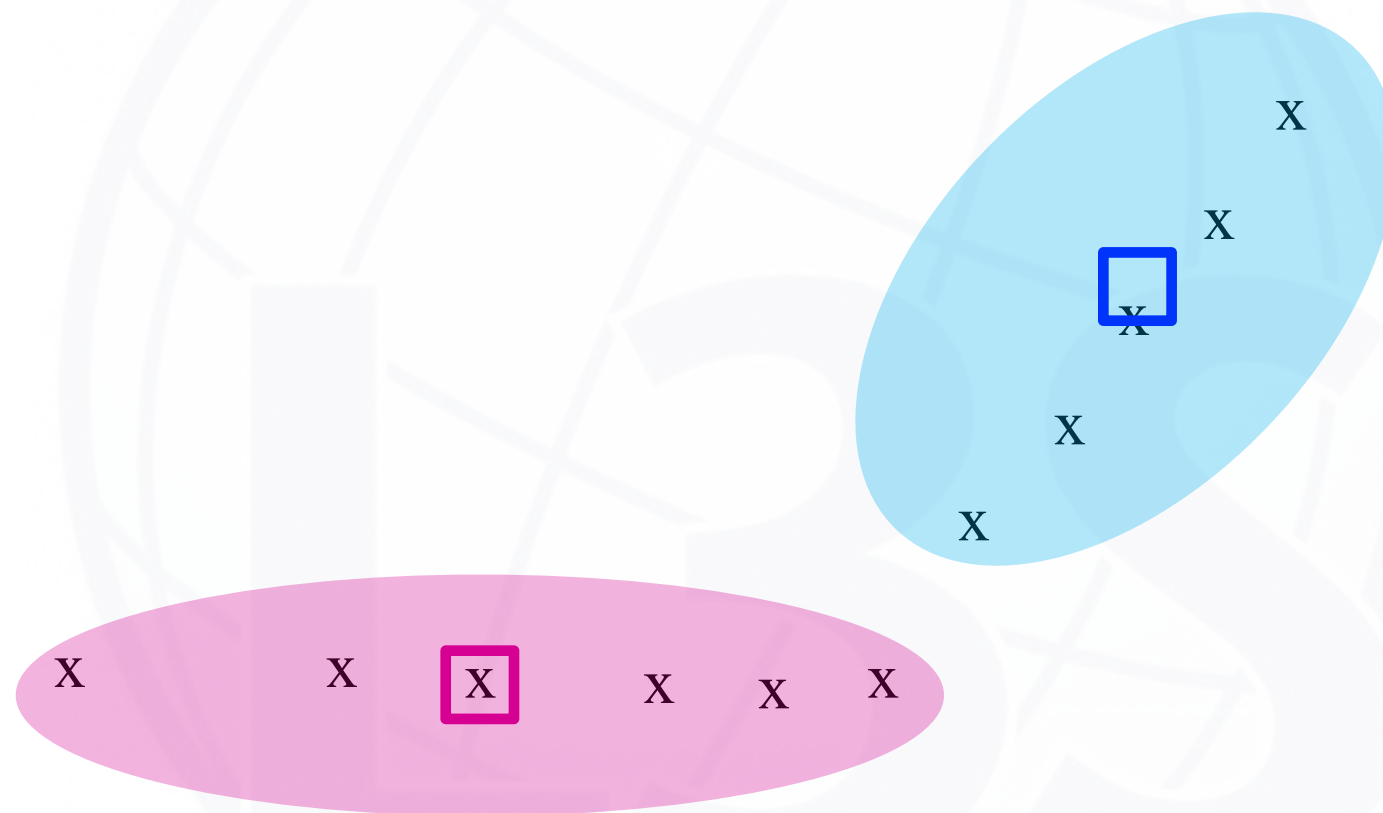


x ... data point

□ ... centroid

Clusters at the end

Example: Assigning Clusters



x ... data point

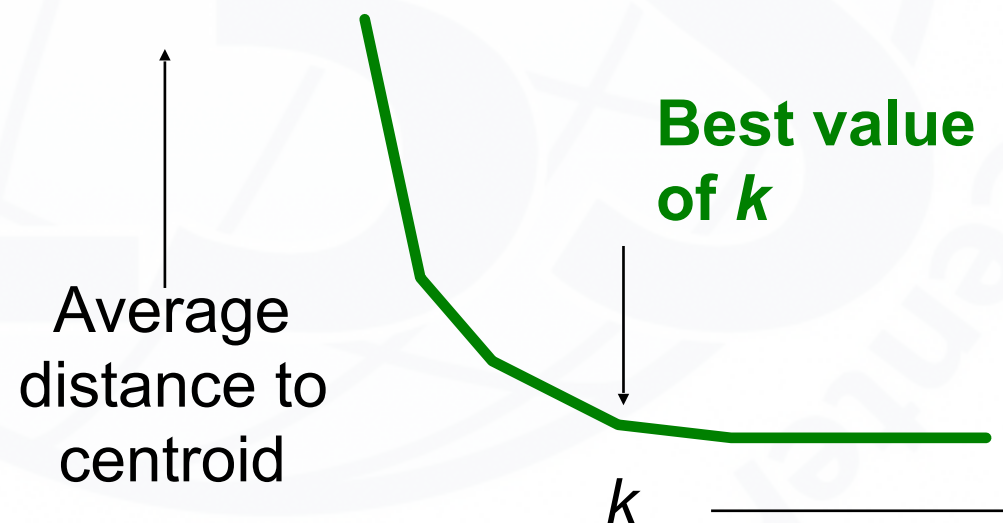
□ ... centroid

Clusters at the end

Getting the k right

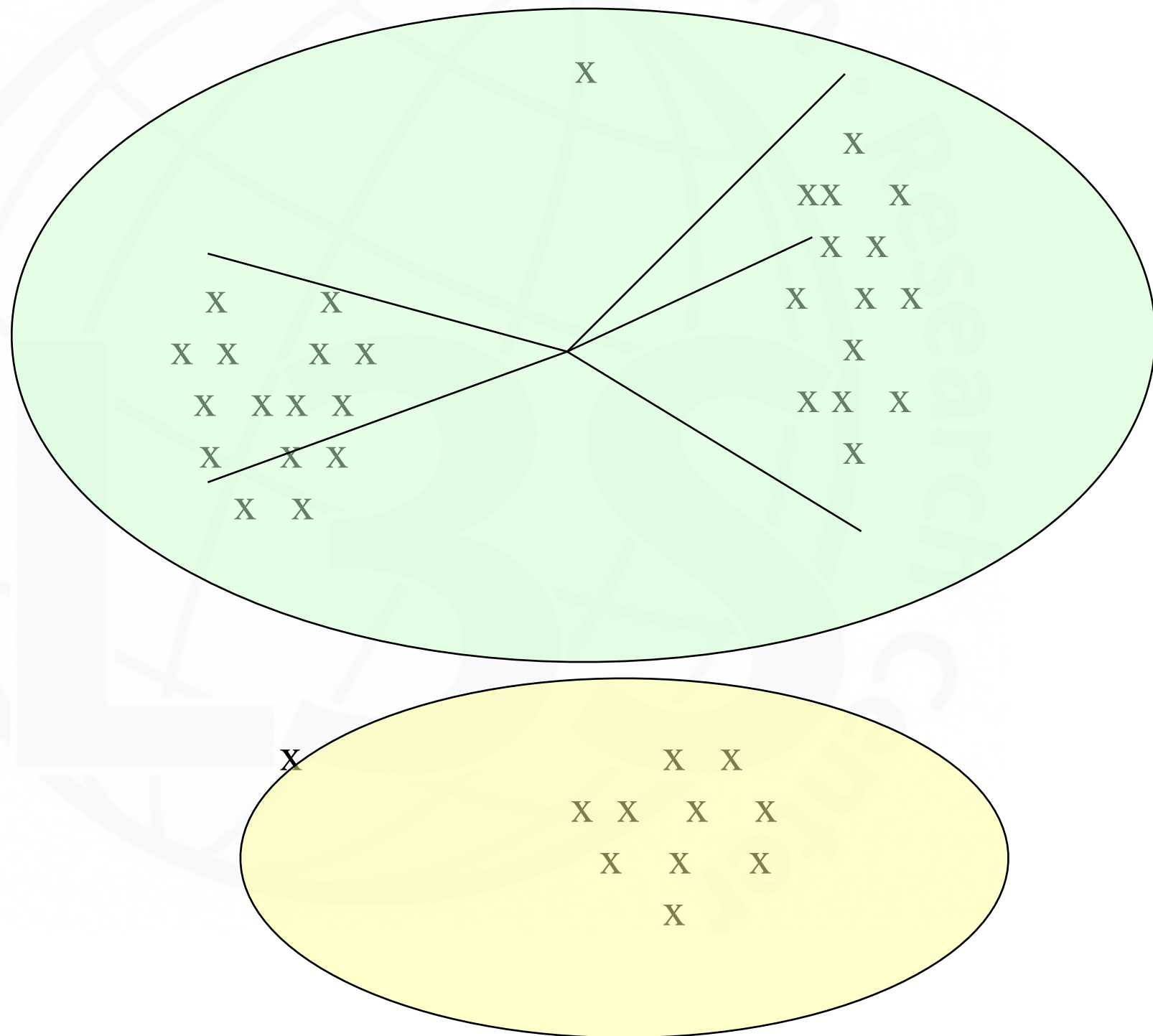
How to select k ?

- 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



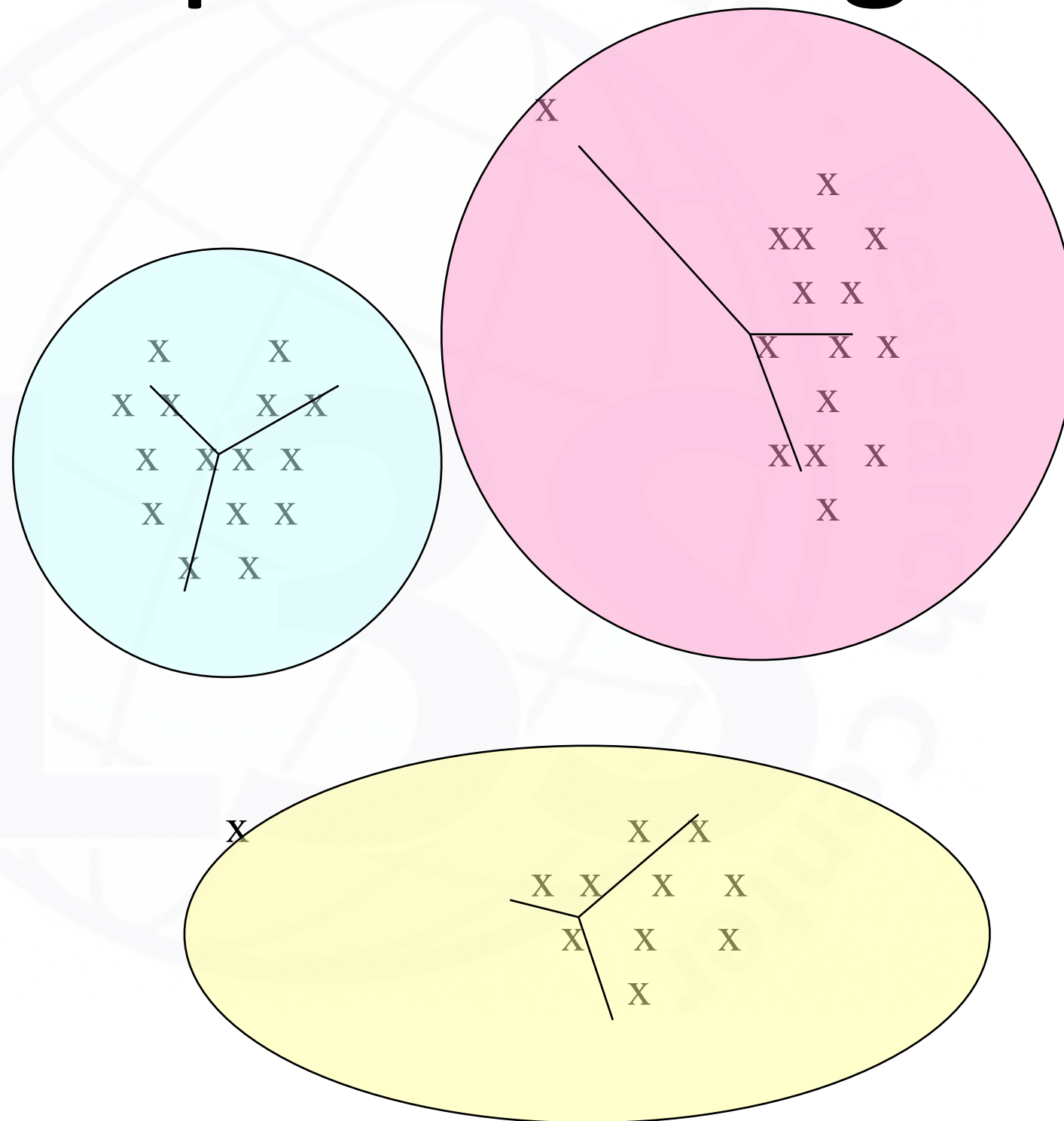
Example: Picking k

Too few;
many long
distances
to centroid.



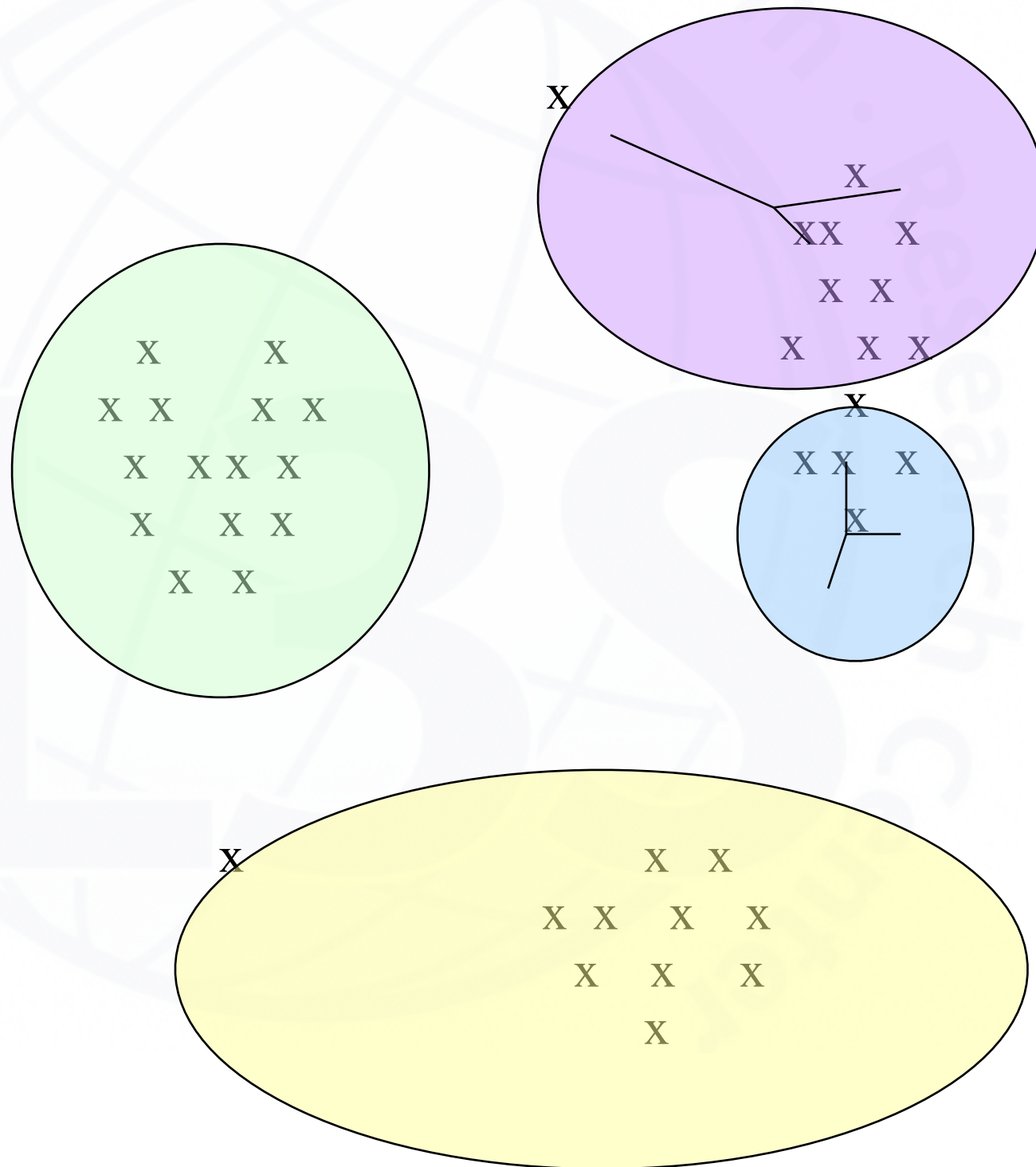
Example: Picking k

Just right;
distances
rather short.

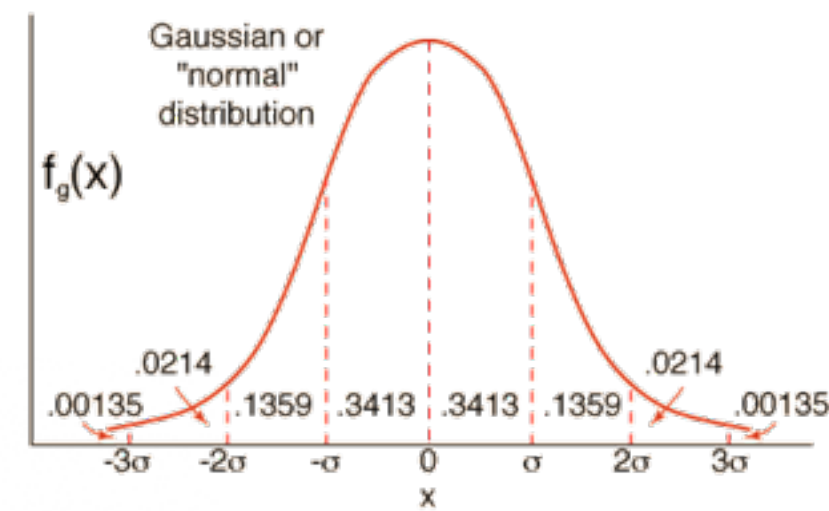


Example: Picking k

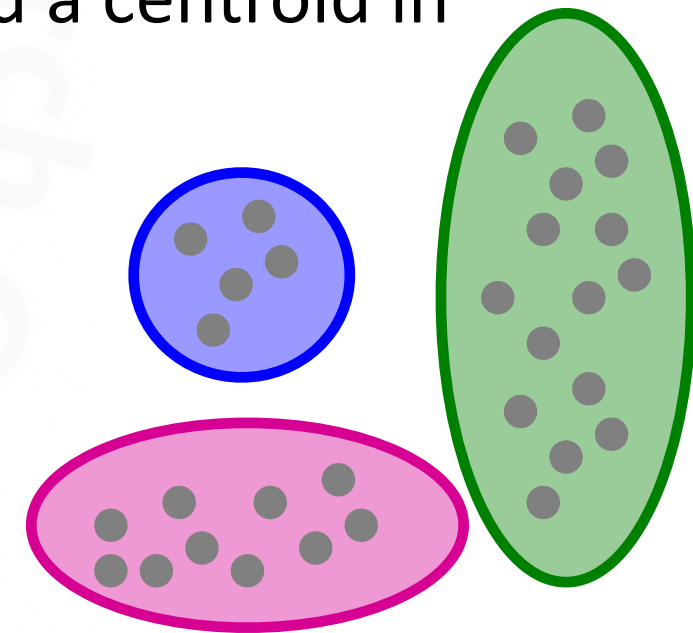
Too many;
little improvement
in average
distance.



BFR Algorithm



- **BFR** [Bradley-Fayyad-Reina] is a variant of k -means designed to handle **very large** (disk-resident) data sets
- **Assumes** that clusters are normally distributed around a centroid in a Euclidean space
 - Standard deviations in different dimensions may vary
 - Clusters are axis-aligned ellipses
- **Efficient way to summarize clusters**
(want memory required $O(\text{clusters})$ and not $O(\text{data})$)



BFR Algorithm

- Points are read from disk one main-memory-full at a time
- Most points from previous memory loads are summarized by **simple statistics**
- To begin, from the initial load we select the initial k centroids by some sensible approach:
 - Take k random points
 - Take a small random sample and cluster optimally
 - Take a sample; pick a random point, and then $k-1$ more points, each as far from the previously selected points as possible

Three Classes of Points

3 sets of points which we keep track of:

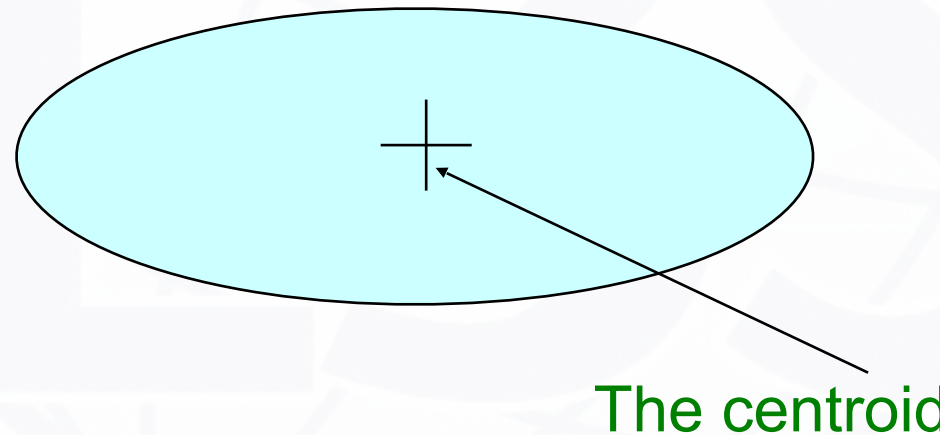
- **Discard set (DS):**
 - Points close enough to a centroid to be summarized
- **Compression set (CS):**
 - Groups of points that are close together but not close to any existing centroid
 - These points are summarized, but not assigned to a cluster
- **Retained set (RS):**
 - Isolated points waiting to be assigned to a compression set

BFR: “Galaxies” Picture



Discard set (DS): Close enough to a centroid to be summarized
Compression set (CS): Summarized, but not assigned to a cluster
Retained set (RS): Isolated points

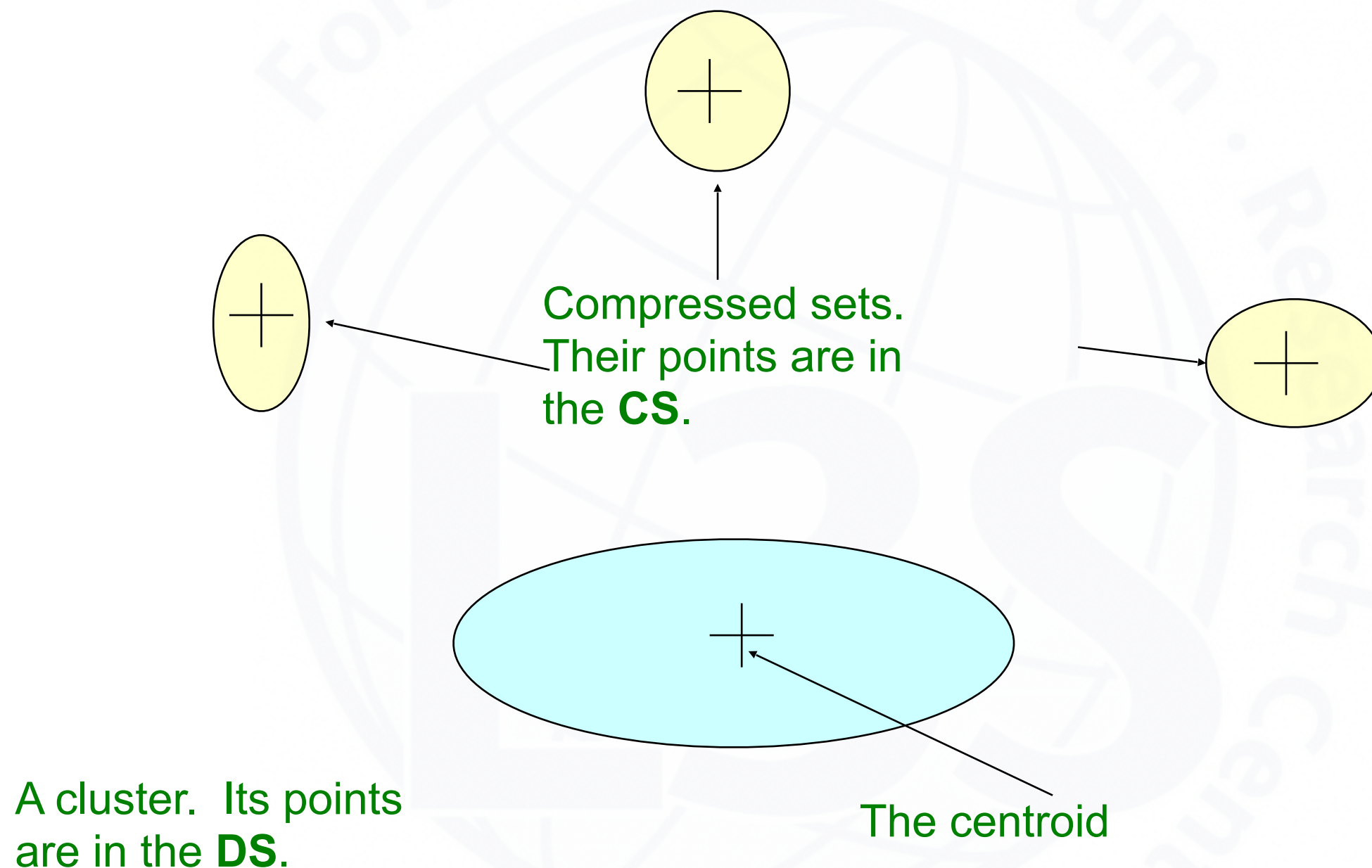
BFR: “Galaxies” Picture



A cluster. Its points are in the **DS**.

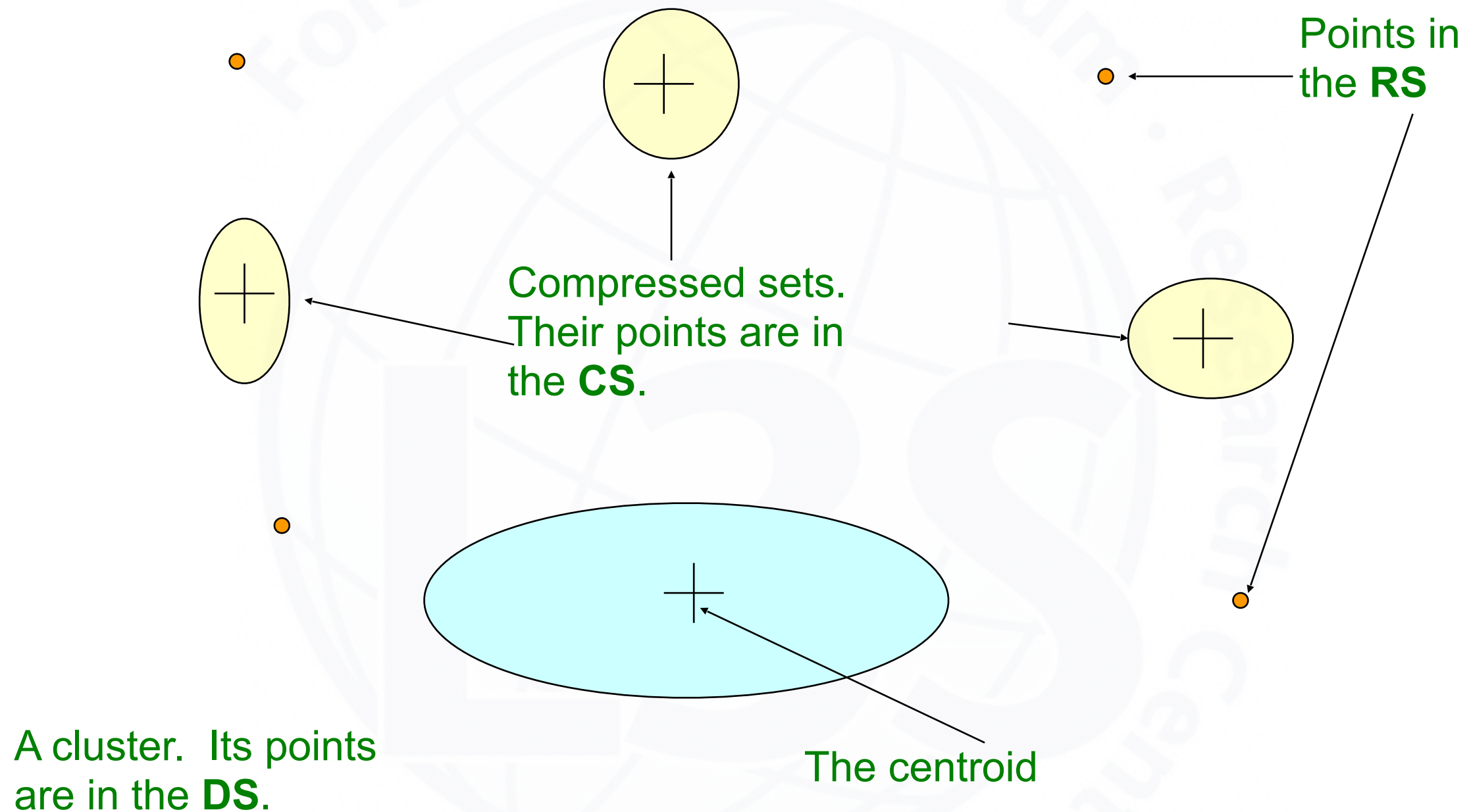
Discard set (DS): Close enough to a centroid to be summarized
Compression set (CS): Summarized, but not assigned to a cluster
Retained set (RS): Isolated points

BFR: “Galaxies” Picture



Discard set (DS): Close enough to a centroid to be summarized
Compression set (CS): Summarized, but not assigned to a cluster
Retained set (RS): Isolated points

BFR: “Galaxies” Picture

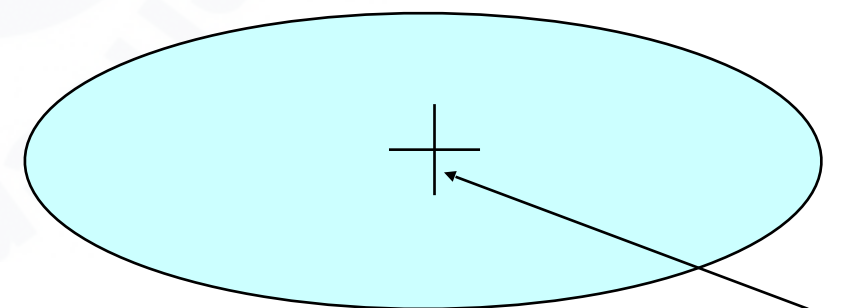


Discard set (DS): Close enough to a centroid to be summarized
Compression set (CS): Summarized, but not assigned to a cluster
Retained set (RS): Isolated points

Summarizing Sets of Points

For each cluster, the discard set (DS) is summarized by:

- The number of points, **N**
- The vector **SUM** : i^{th} component = sum of the coordinates of the points in the i^{th} dimension
- The vector **$SUMSQ$** : i^{th} component = sum of squares of coordinates in i^{th} dimension



A cluster.

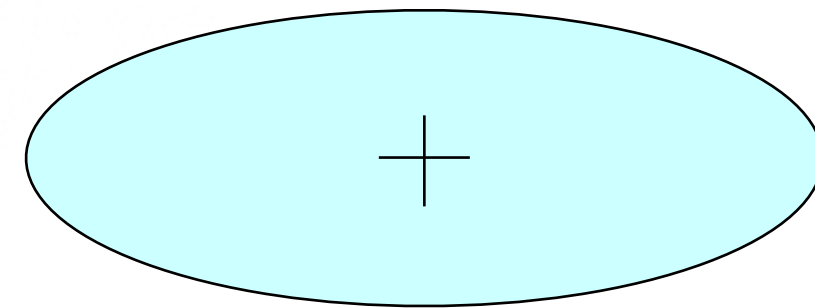
All its points are in the **DS**.

The centroid

Summarizing Points: Comments

- $2d + 1$ values represent any size cluster
 - d = number of dimensions
- Average in **each dimension** (**the centroid**) can be calculated as SUM_i / N
 - $\text{SUM}_i = i^{\text{th}}$ component of SUM
- Variance of a cluster's discard set in dimension i is: $(\text{SUMSQ}_i / N) - (\text{SUM}_i / N)^2$
 - And standard deviation is the square root of that
- **Next step: Actual clustering**

Note: Dropping the “axis-aligned” clusters assumption would require storing full covariance matrix to summarize the cluster. So, instead of **SUMSQ** being a d -dim vector, it would be a $d \times d$ matrix, which is too big!



The “Memory-Load” of Points

Processing the “Memory-Load” of points (1):

- **1)** Find those points that are “**sufficiently close**” to a cluster centroid and add those points to that cluster and the **DS**
 - These points are so close to the centroid that they can be summarized and then discarded
- **2)** Use any main-memory clustering algorithm to cluster the remaining points and the old **RS**
 - Clusters go to the **CS**; outlying points to the **RS**

Discard set (DS): Close enough to a centroid to be summarized.

Compression set (CS): Summarized, but not assigned to a cluster

Retained set (RS): Isolated points

The “Memory-Load” of Points

Processing the “Memory-Load” of points (2):

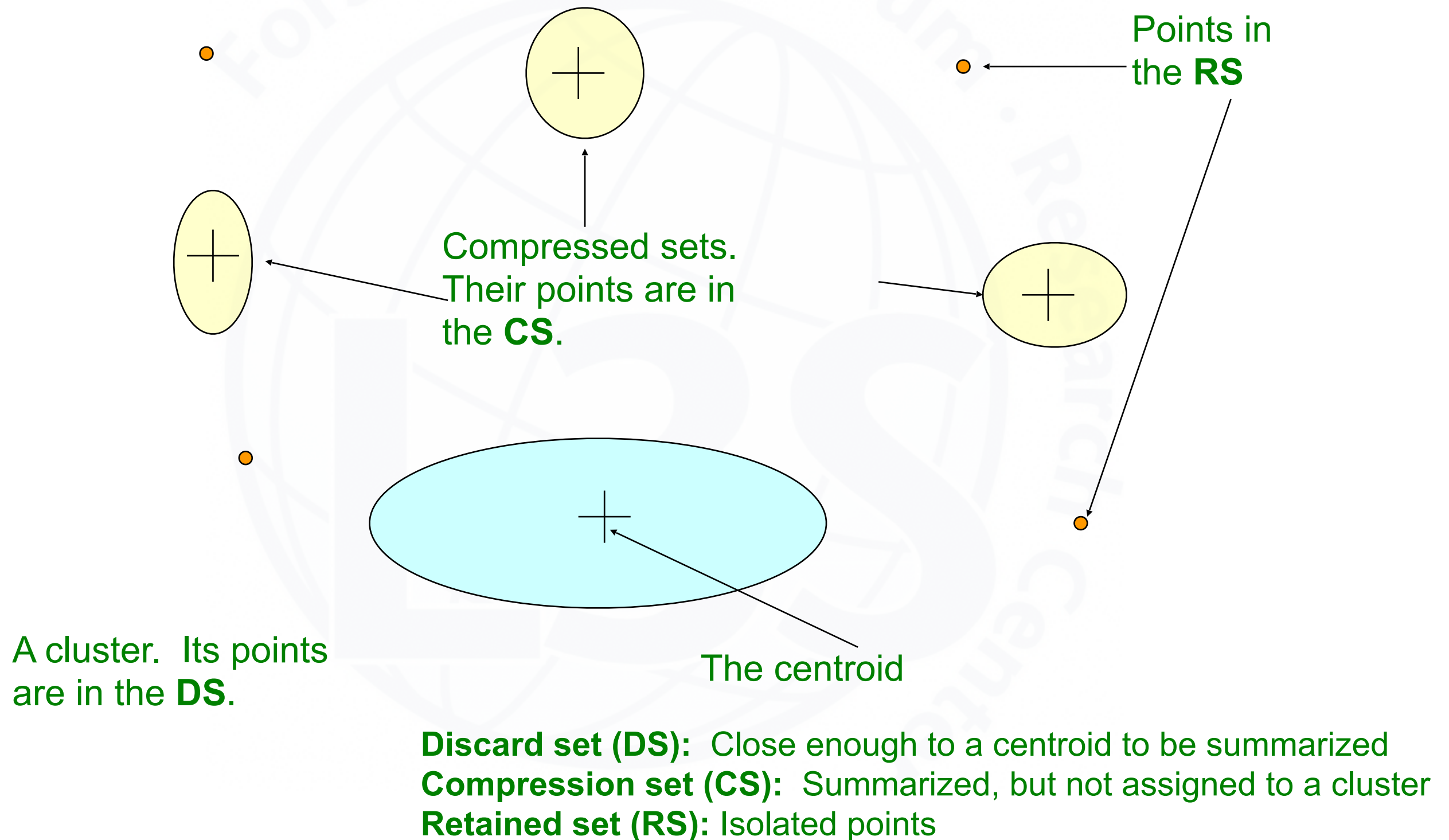
- **3) DS set:** Adjust statistics of the clusters to account for the new points
 - Add N_s , SUM_s , $SUMSQ_s$
- **4)** Consider merging compressed sets in the **CS**
- **5)** If this is the last round, merge all compressed sets in the **CS** and all **RS** points into their nearest cluster

Discard set (DS): Close enough to a centroid to be summarized.

Compression set (CS): Summarized, but not assigned to a cluster

Retained set (RS): Isolated points

BFR: “Galaxies” Picture

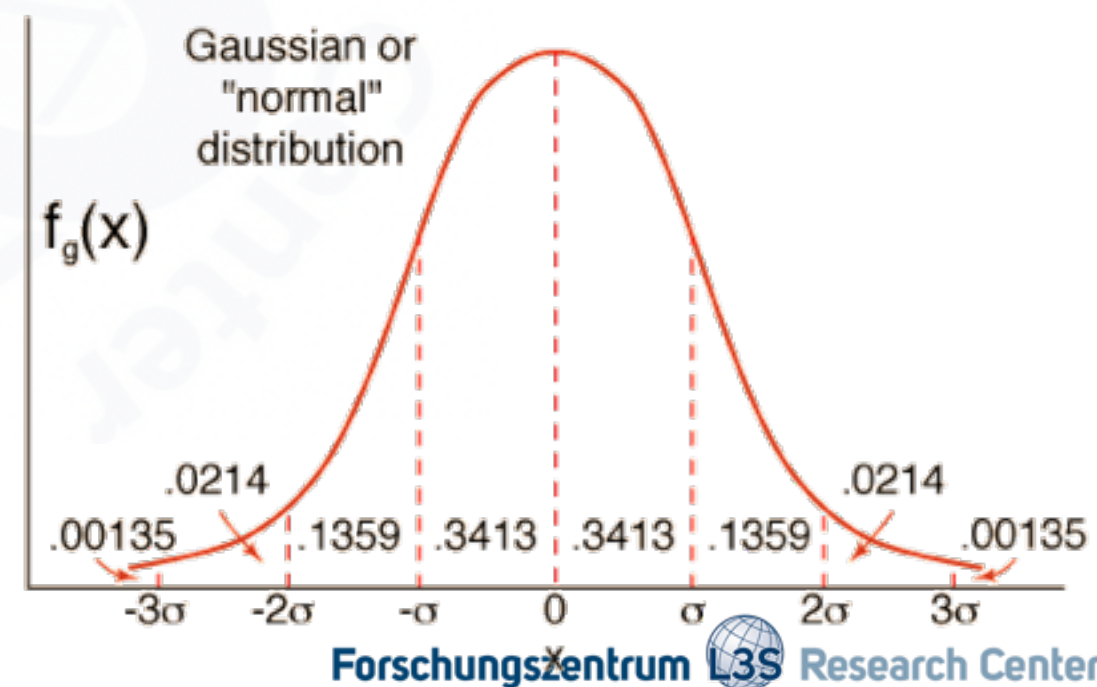


A Few Details...

- **Q1) How do we decide if a point is “close enough” to a cluster that we will add the point to that cluster?**
- **Q2) How do we decide whether two compressed sets (CS) deserve to be combined into one?**

How Close is Close Enough?

- Q1) We need a way to decide whether to put a new point into a cluster (and discard)
- BFR suggests two ways:
 - The **Mahalanobis distance** is less than a threshold
 - High likelihood of the point belonging to currently nearest centroid



Mahalanobis Distance

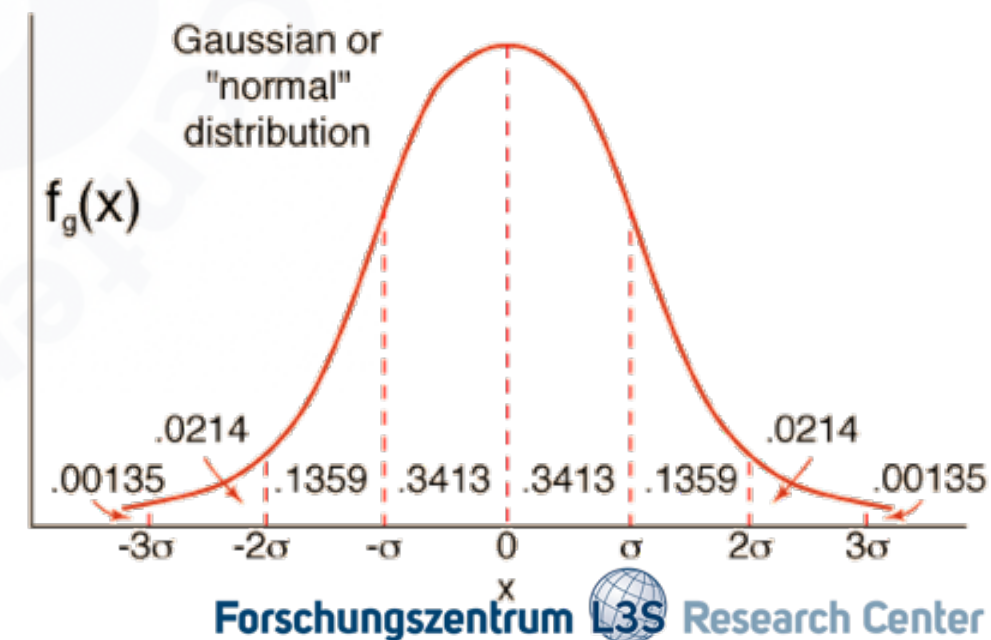
- **Normalized Euclidean distance from centroid**
- For point (x_1, \dots, x_d) and centroid (c_1, \dots, c_d)
 1. Normalize in each dimension: $y_i = (x_i - c_i) / \sigma_i$
 2. Take sum of the squares of the y_i
 - 3. Take the square root

$$d(x, c) = \sqrt{\sum_{i=1}^d \left(\frac{x_i - c_i}{\sigma_i} \right)^2}$$

σ_i ... standard deviation of points in the cluster in the i^{th} dimension

Mahalanobis Distance

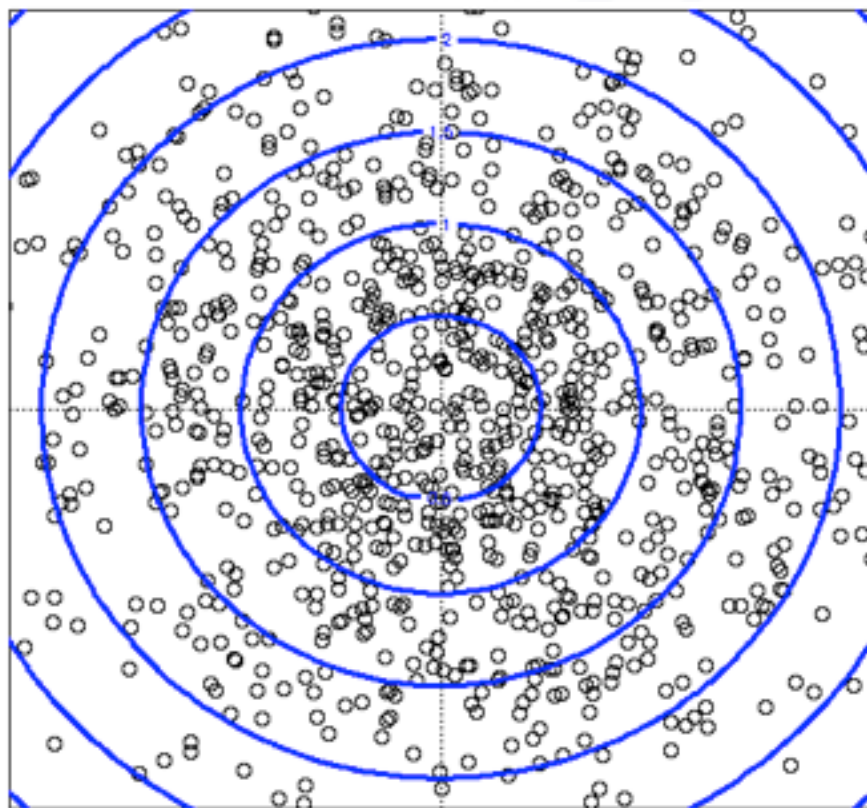
- If clusters are normally distributed in d dimensions, then after transformation, one standard deviation = \sqrt{d}
 - i.e., 68% of the points of the cluster will have a Mahalanobis distance $< \sqrt{d}$
-
- Accept a point for a cluster if its M.D. is $<$ some threshold, e.g. **2** standard deviations



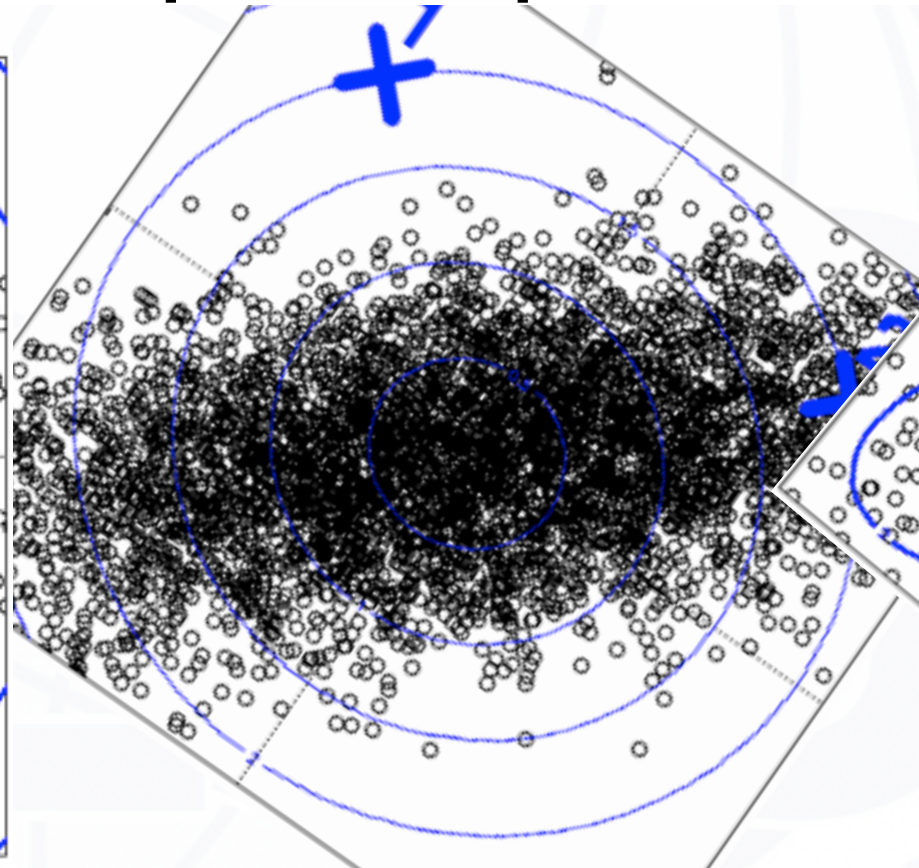
Picture: Equal M.D. Regions

- Euclidean vs. Mahalanobis distance

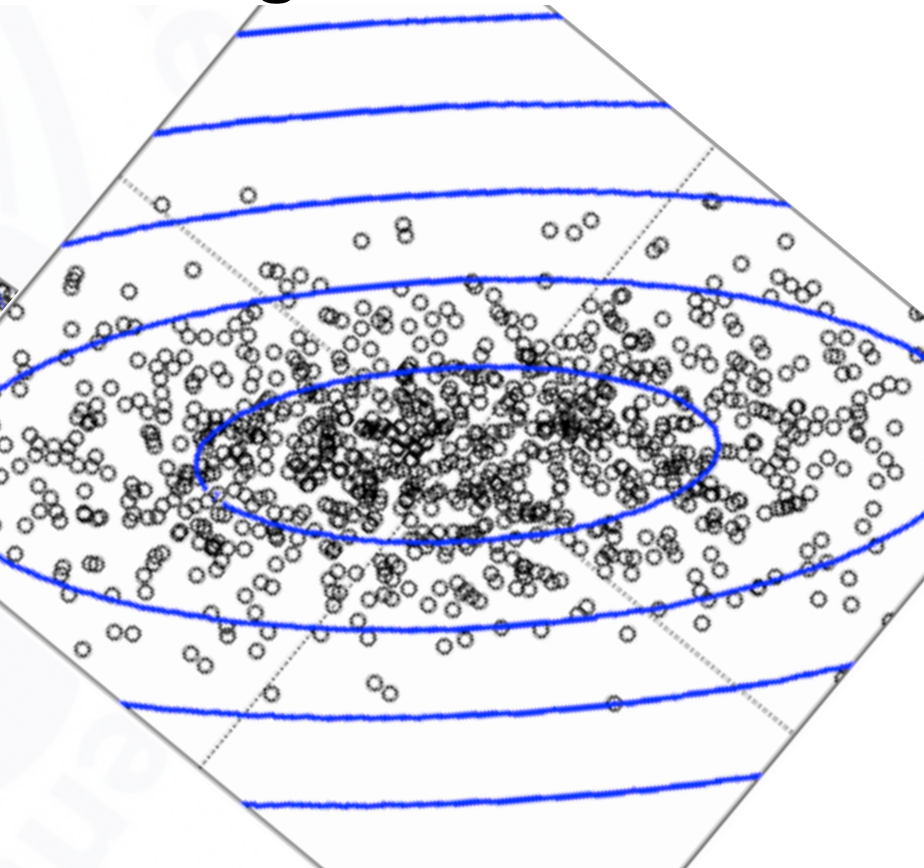
Contours of equidistant points from the origin



Uniformly distributed points,
Euclidean distance



Normally distributed points,
Euclidean distance

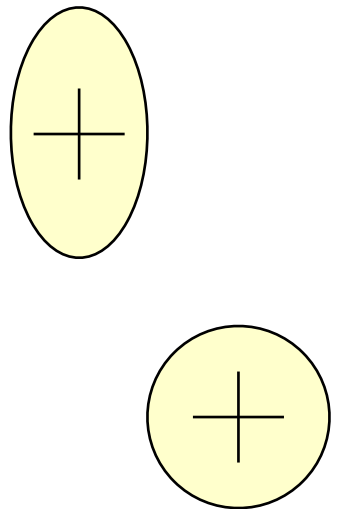


Normally distributed points,
Mahalanobis distance

Should 2 CS clusters be combined?

Q2) Should 2 CS subclusters be combined?

- Compute the variance of the combined subcluster
 - **N** , **SUM** , and **$SUMSQ$** allow us to make that calculation quickly
- Combine if the combined variance is below some threshold
- **Many alternatives:** Treat dimensions differently, consider density



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*
 - **BFR**: Large scale clustering