Extra credit for helping others on Ed

Plan project teams / idea / datasets

See new FAQ online

(if you're unsure about fit to course, talk to us)

(teams of three/four highly recommended; will all be graded the same)

Due Thu: Tell us about your project using the Team Signup Sheet on our website

Office hours: Tim's are best for lecture questions, logistics, projects, accommodations; TA office hours are best for HW and colab questions (+project if TA assigned to you)

Clustering

CS547 Machine Learning for Big Data

Tim Althoff

PAUL G. ALLEN SCHOOL OF COMPUTER SCIENCE & ENGINEERING

High Dimensional Data

High dim. data
- Locality sensitive hashing
- Clustering
- Dimensiona -lity reduction

Graph data
- Community Detection
- Spam Detection

Infinite data
- Sampling ... streams
- Filtering data streams
- Queries on streams

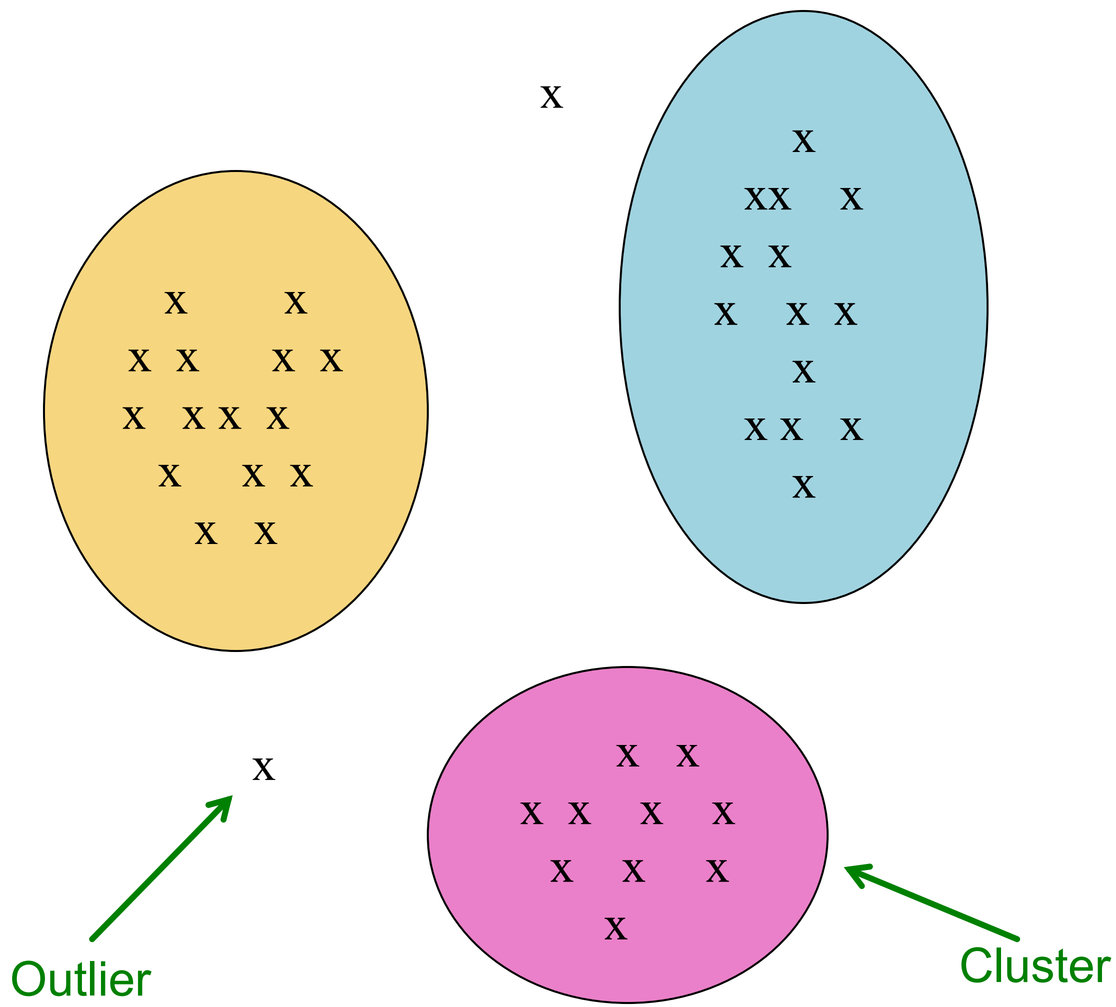
Machine learning
- Decision Trees
- Perceptron, kNN

Apps
- Recommen der systems
- Association Rules
- Duplicate document detection

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 metric
    - Euclidean, Cosine, Jaccard, edit distance, …

Example: Clusters & Outliers



Clustering Problem: Galaxies

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

Clustering Problem: Music Album

- **Intuitively: Music can be divided into categories, and customers prefer a few genres**
  - But what are categories really?
- Represent an Album by a set of customers who bought it
- Similar Albums have similar sets of customers, and vice-versa

Clustering Problem: Music Album

Space of all Albums:

- Think of a space with one dim. for each customer
  - Values in a dimension may be 0 or 1 only
  - An Album is a "point" in this space $(x_1, x_2, \ldots, x_k)$, where $x_i = 1$ iff the i^{th} customer bought the Album
- For Amazon, the dimension is 100 million plus
- **Task:** Find clusters of similar Albums

Clustering Problem: Documents

Finding topics:

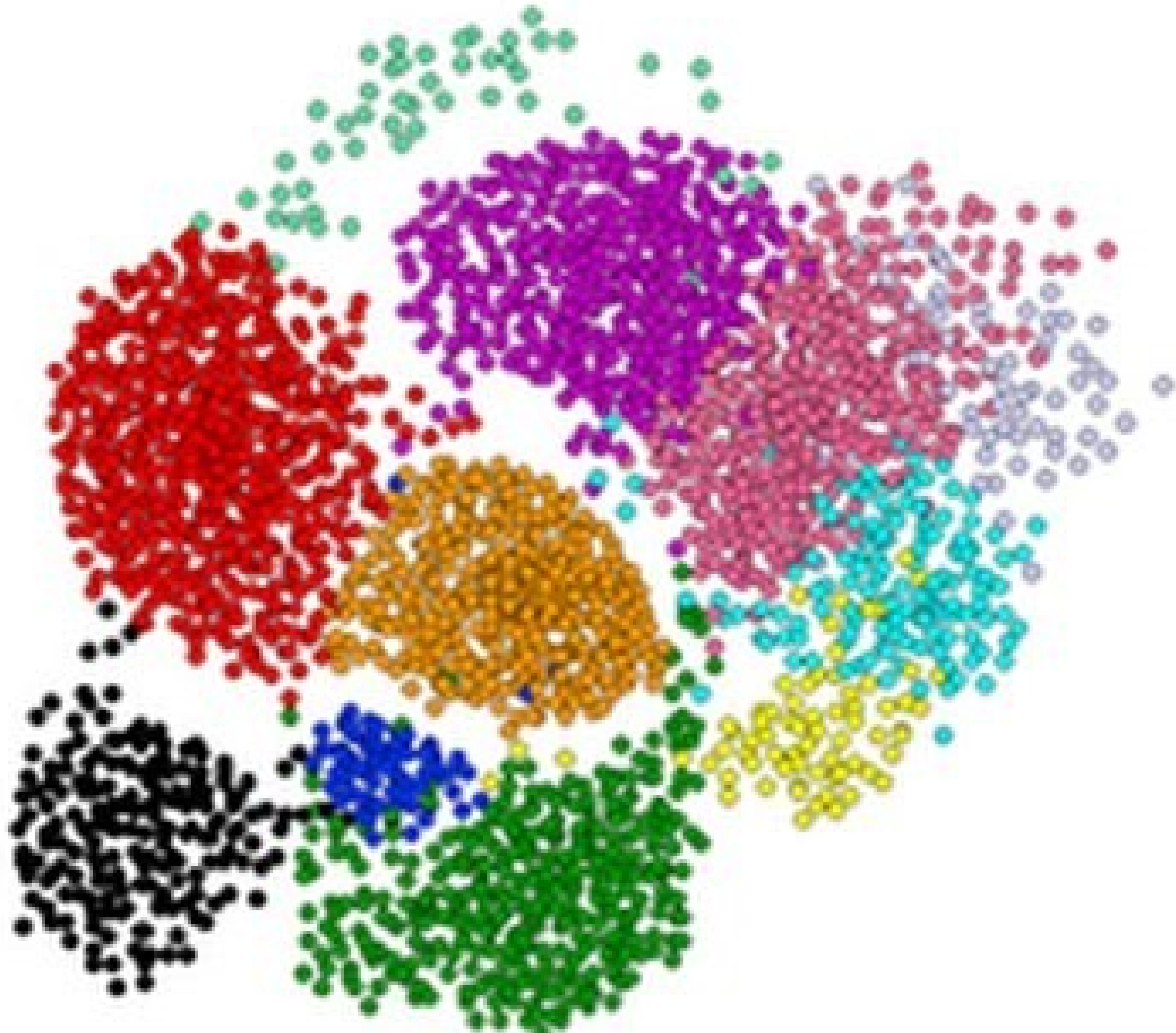
- Represent a document by a vector (x_1, x_2,…, x_k), where $x_i = 1$ iff the i th word (in some order) appears in the document

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

Cosine, Jaccard, and Euclidean

- **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**

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

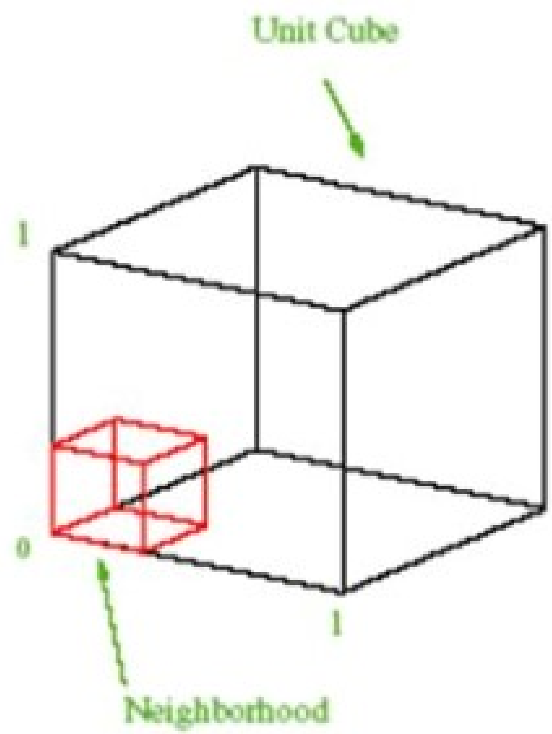
- Many applications involve not 2, but 10 or 10,000 dimensions
- **High-dimensional spaces look different:** Almost all pairs of points are very far from each other --> **The Curse of Dimensionality**

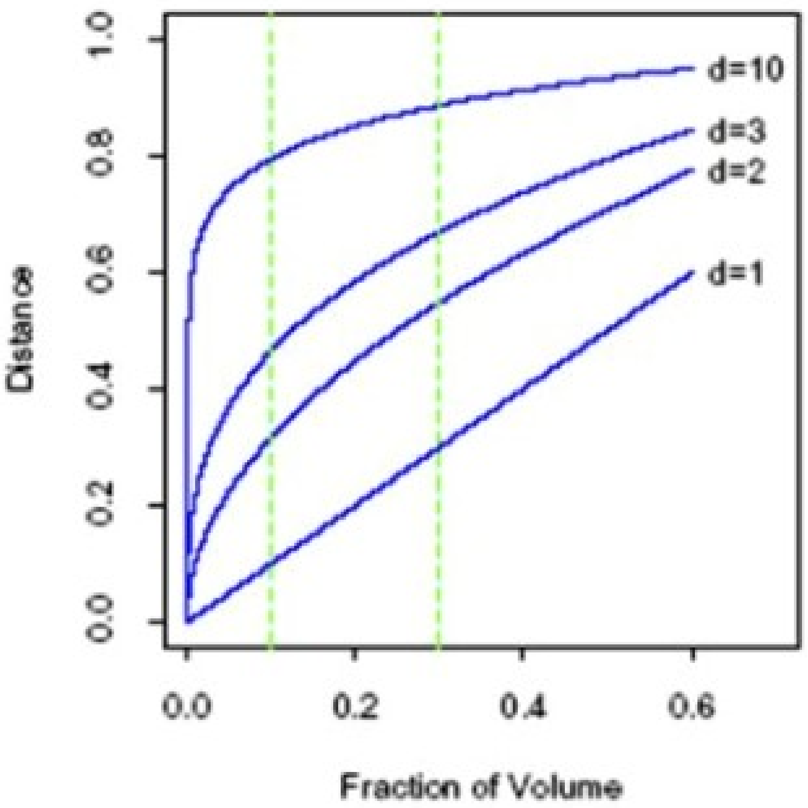
Example: Curse of Dimensionality

- **Take 10,000 uniform random points on [0,1] line. Assume query point is at the origin (0).**
- To get 10 nearest neighbors we must go to distance 10/10,000=0.001 on average
- In 2-dim we must go $\sqrt{0.001}$=0.032 to get a square that contains 0.001 volume
- In d-dim we must go $(0.001)^{\frac{1}{d}}$
- So, in 10-dim to capture 0.1% of the data we need 50% of the range.

Example: Curse of Dimensionality

Curse of Dimensionality: All points are very far from each other

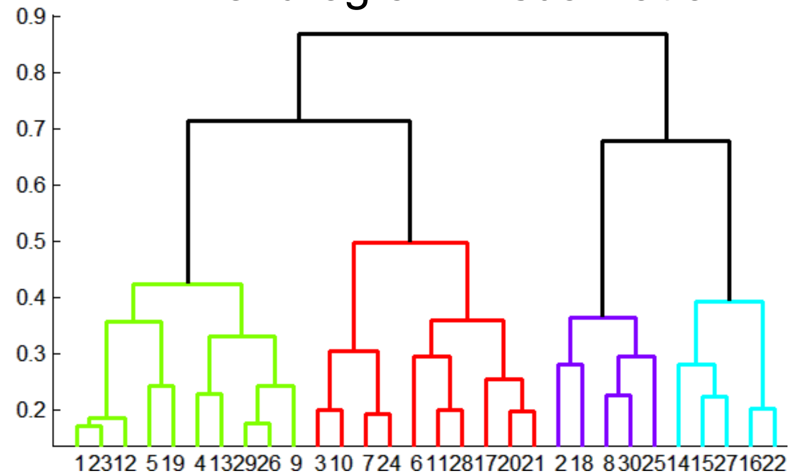




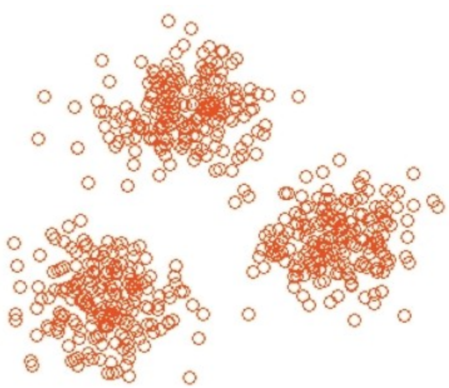
Overview: Methods of Clustering

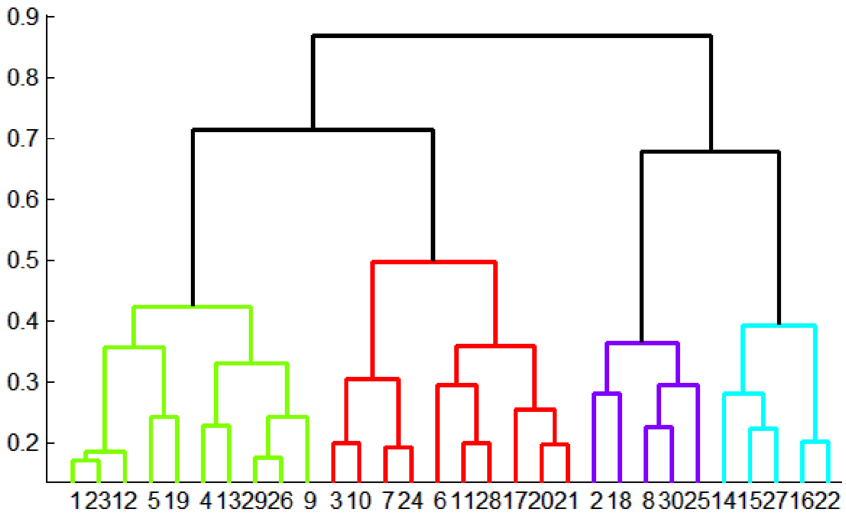
- **Hierarchical:**
  - **Agglomerative** (bottom up):
    - Initially, each point is a cluster
    - Repeatedly combine the two "nearest" clusters into one
  - **Divisive** (top down):
    - Start with one cluster and recursively split it

Dendrogram Visualization



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

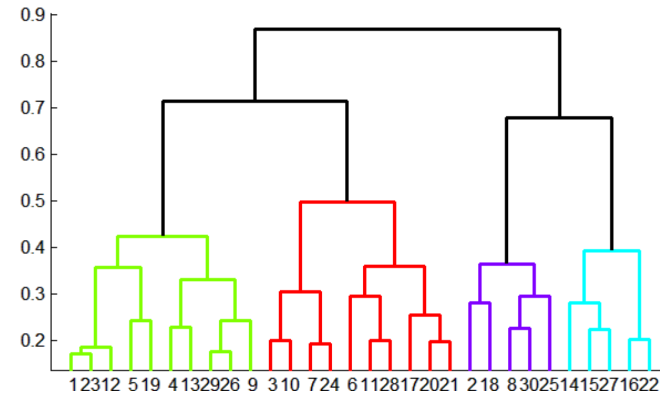




Hierarchical Clustering

Hierarchical Clustering

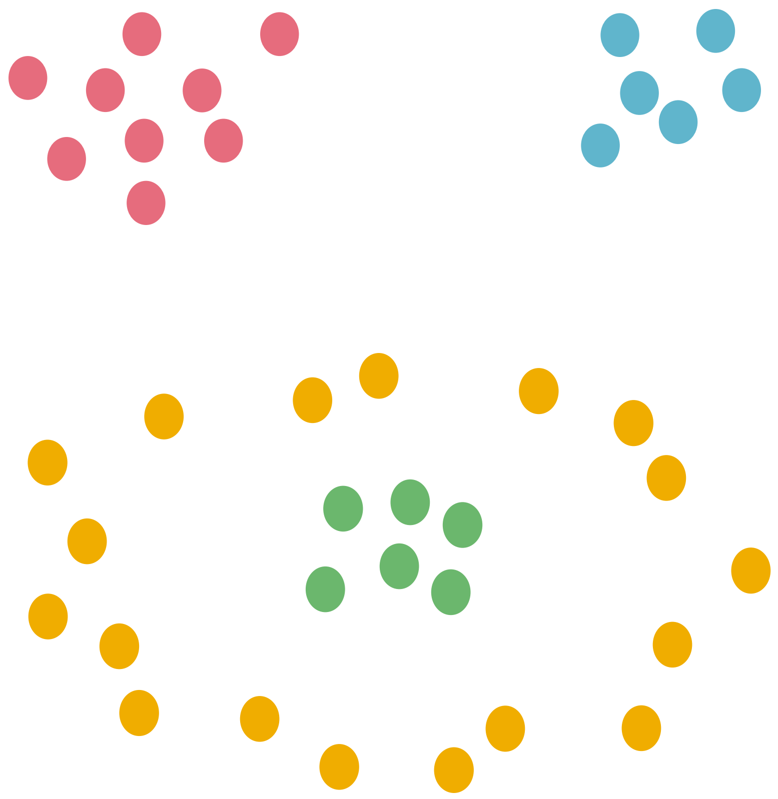
- **Key operation:**
  Repeatedly combine two nearest clusters



- **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?

Which is Better?

- Point assignment good when clusters are nice, convex shapes:
- Hierarchical can win when shapes are weird:
  - Note both clusters have essentially the same centroid.

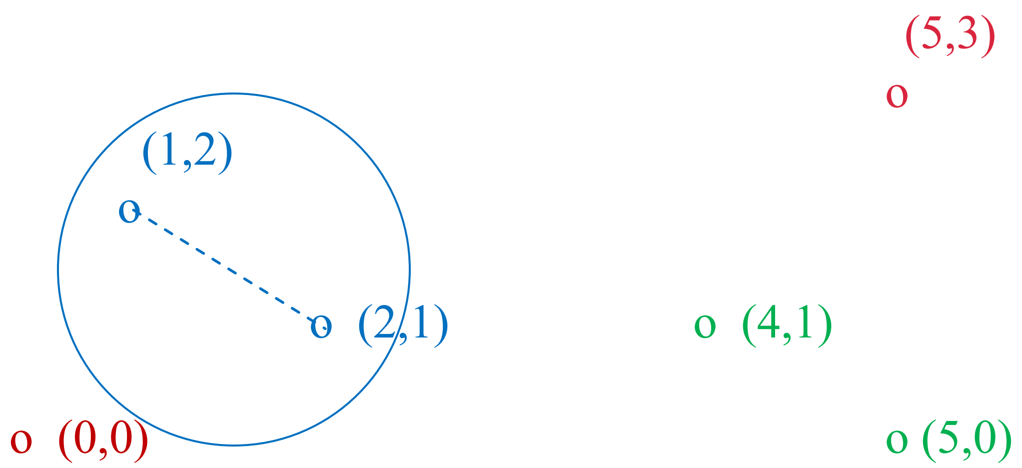


Note: if you realized you had concentric clusters, you could map points based on distance from center, and turn the problem into a simple, one-dimensional case.

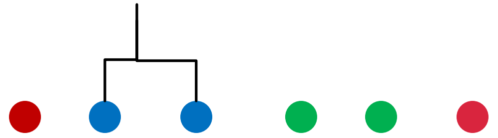
Hierarchical Clustering

- **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

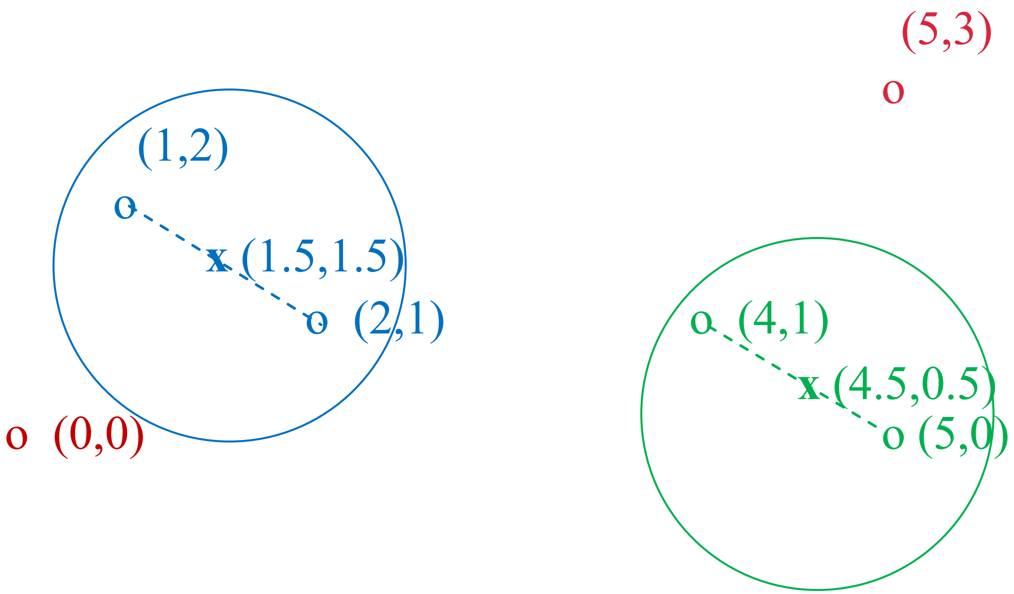


Data:
o … data point
x … centroid

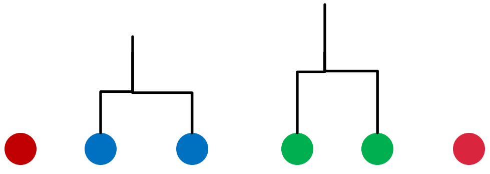


Dendrogram

Example: Hierarchical clustering

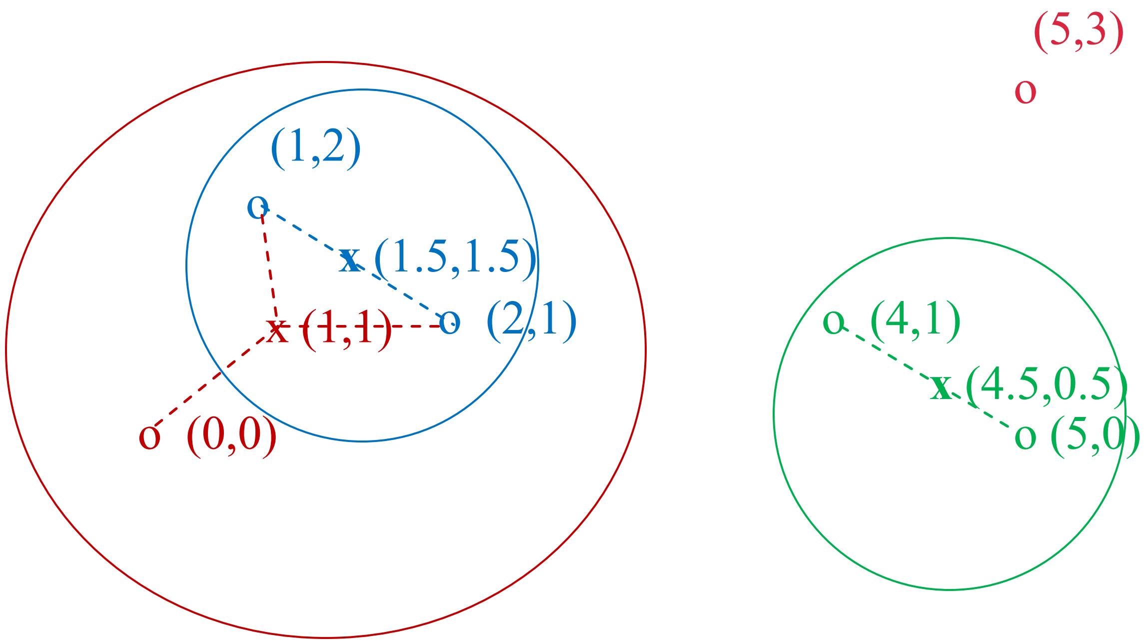


Data:
o … data point
x … centroid

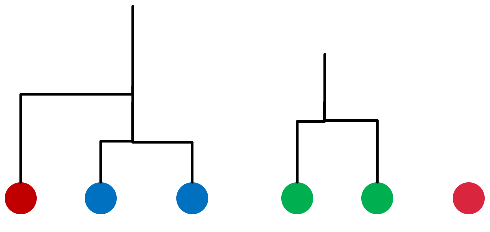


Dendrogram

Example: Hierarchical clustering

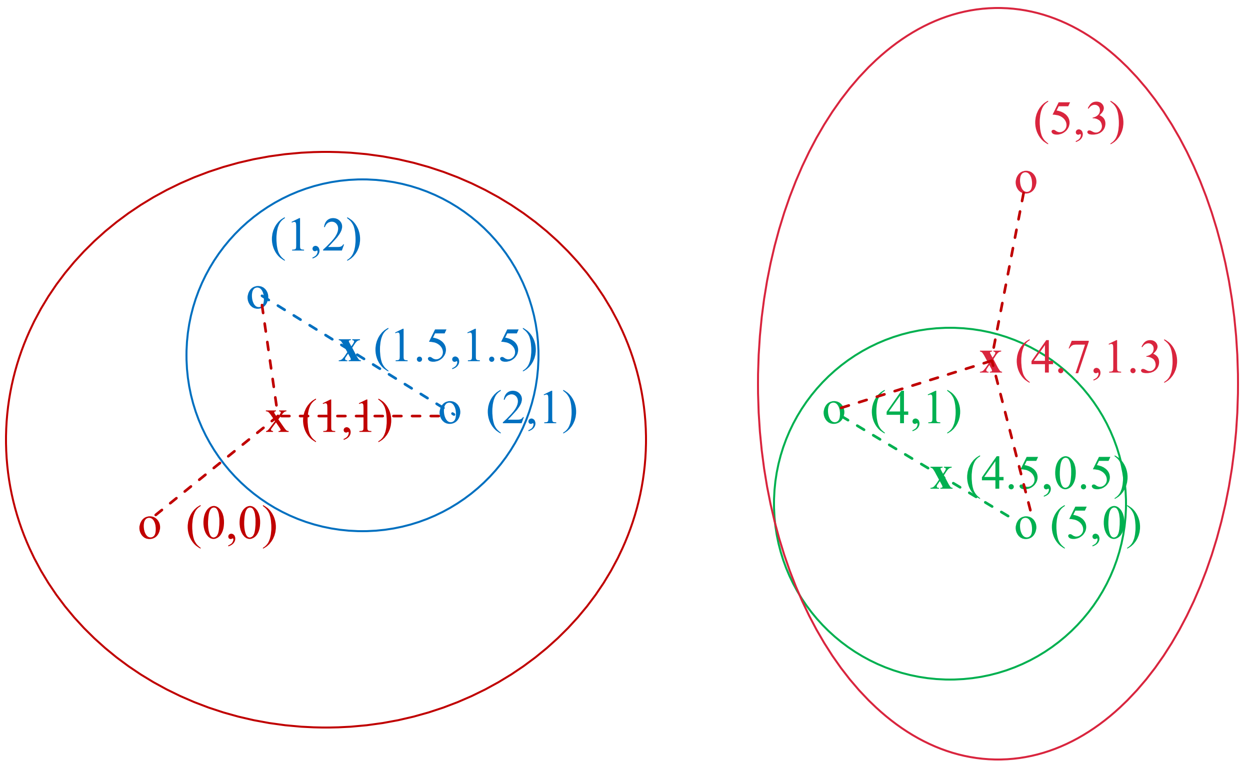


Data:
o … data point
x … centroid

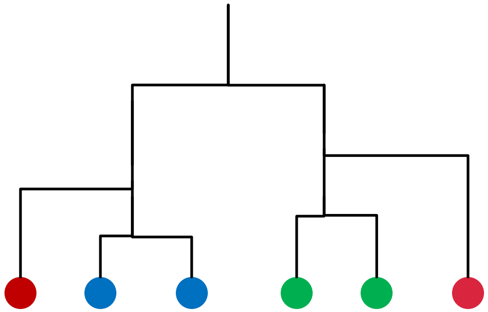


Dendrogram

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 (e.g. sets)

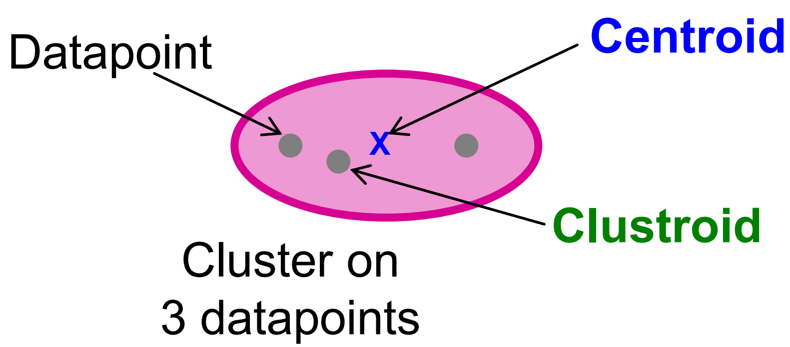
- **Approach 1:**
  - **(1.1) How to represent a cluster of many points?** ***clustroid*** = (data)point "***closest***" to other points
  - **(1.2) How do you determine the "nearness" of clusters?** Treat clustroid as if it were centroid, when computing inter-cluster distances

"Closest" Point?

(1.1) 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

(1.2) How do you determine the "nearness" of clusters? Treat clustroid as if it were centroid, when computing intercluster distances.

Approach 2: No centroid, just define distance directly between clusters

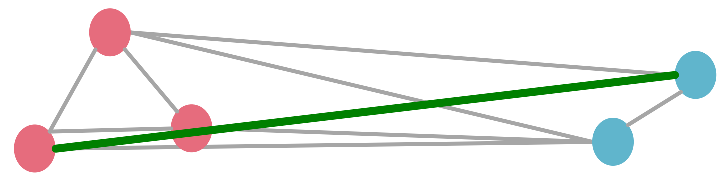
Intercluster distance = minimum of the distances between any two points, one from each cluster

Cohesion

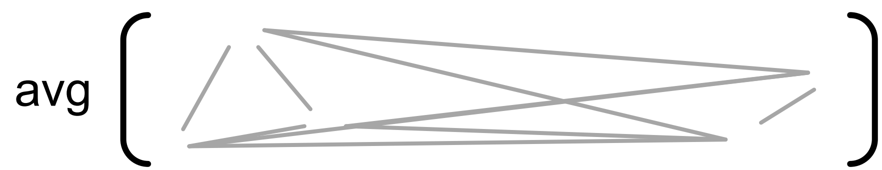
Approach 3: Pick a notion of **cohesion** of clusters

- Merge clusters whose *union* is most cohesive

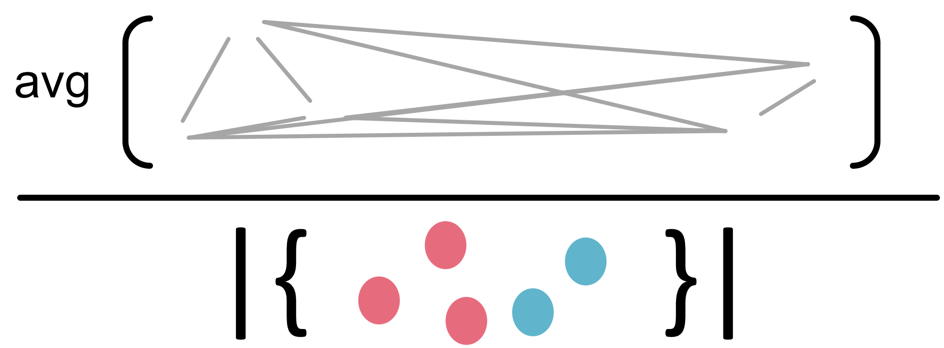
3.1: diameter of the merged cluster = maximum distance between points in the cluster



3.2: average distance between points in the cluster



3.3: density-based approach
Take the diameter or avg. distance, and divide by the number of points in the cluster



When to stop?

When do we stop merging clusters?

- When some number k of clusters are found (assumes we know the number of clusters)
- When stopping criterion is met
  - Stop if diameter exceeds threshold
  - Stop if density is below some threshold
  - Stop if merging clusters yields a bad cluster
    - E.g., diameter suddenly jumps
- Keep merging until there is only 1 cluster left

Which is Best?

- It really depends on the shape of clusters.
  - Which you may not know in advance.

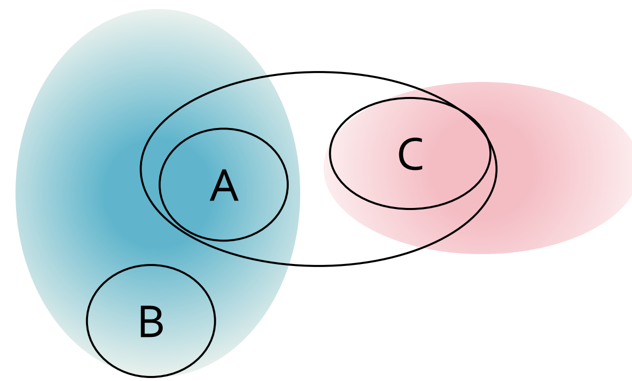
Which is Best?

- It really depends on the shape of clusters.
  - Which you may not know in advance.

- **Example:** We'll compare two approaches:
  1. Merge clusters with smallest distance between centroids (or clustroids for non-Euclidean)
  2. Merge clusters with the smallest distance between two points, one from each cluster

Case 1: Convex Clusters

- Centroid-based merging works well.
- But merger based on closest members might accidentally merge incorrectly.

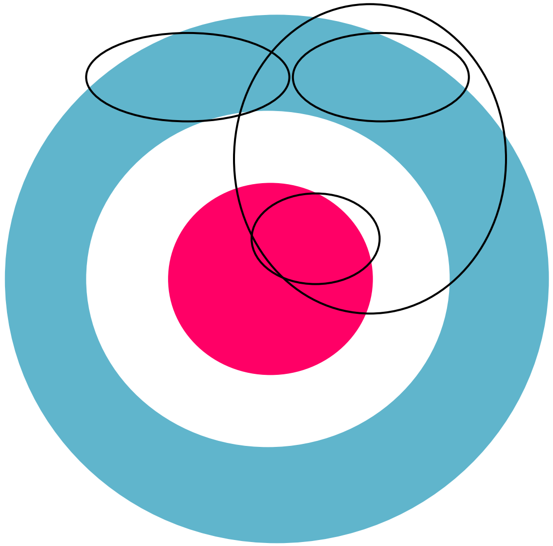


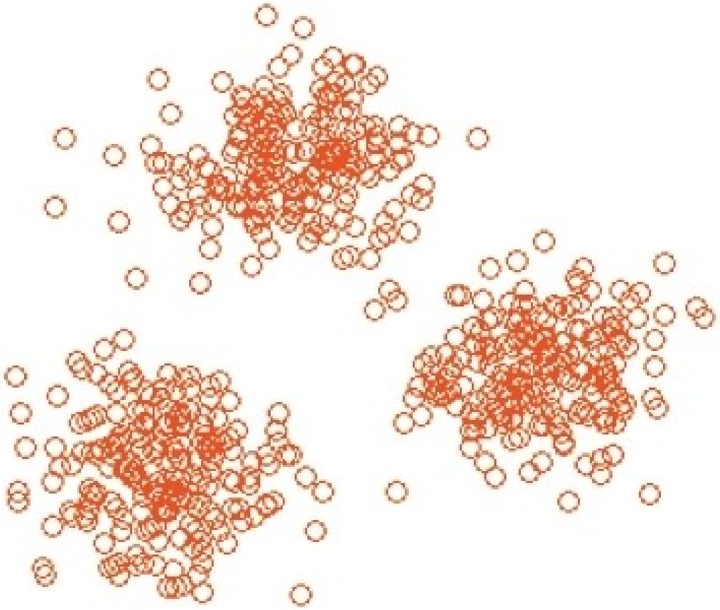
A and B have closer centroids than A and C, but closest points are from A and C.

Data density

Case 2: Concentric Clusters

- Linking based on closest members works well
- But Centroid-based linking might cause errors





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
    - OK, as long as there are no *outliers* (points that are far from any reasonable cluster)

k-Means++

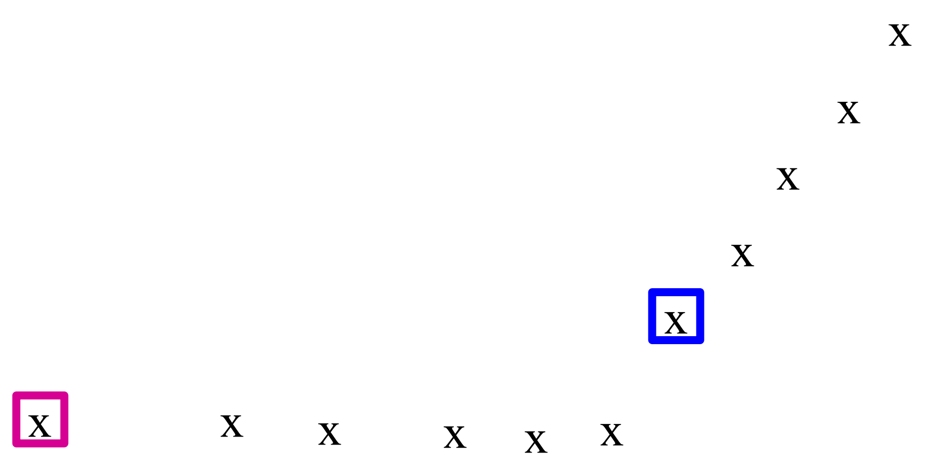
- **Basic idea:** Pick a small sample of points S, cluster them by any algorithm, and use the centroids as a seed
- In **k-means++,** sample size $|S|$ = k times a factor that is logarithmic in the total number of points

- **How to pick sample points:** Visit points in random order, but the probability of adding a point p to the sample is proportional to $D(p)^2$.
  - $D(p)$ = distance between p and the nearest picked point.

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

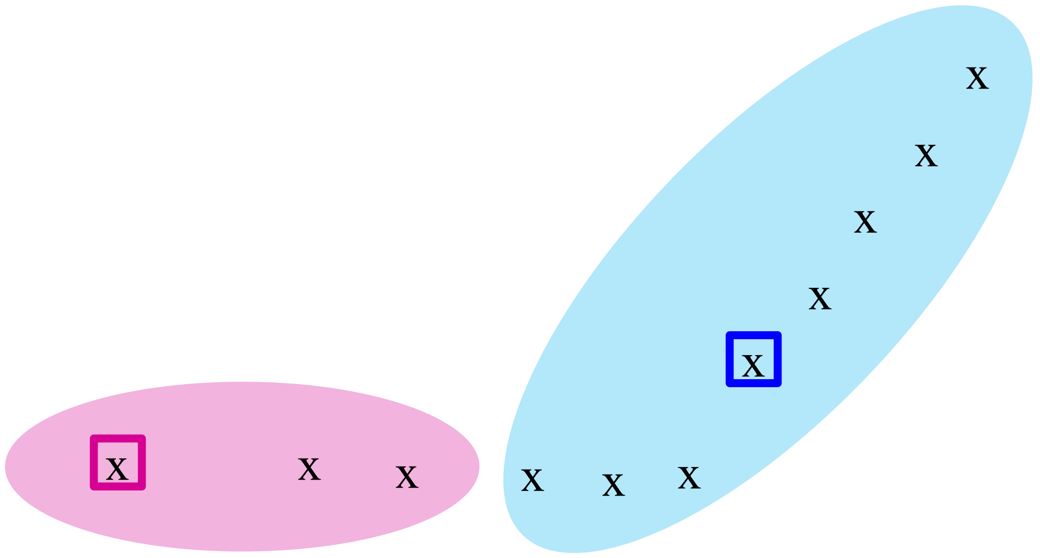


x … data point

… centroid

Clusters after round 1

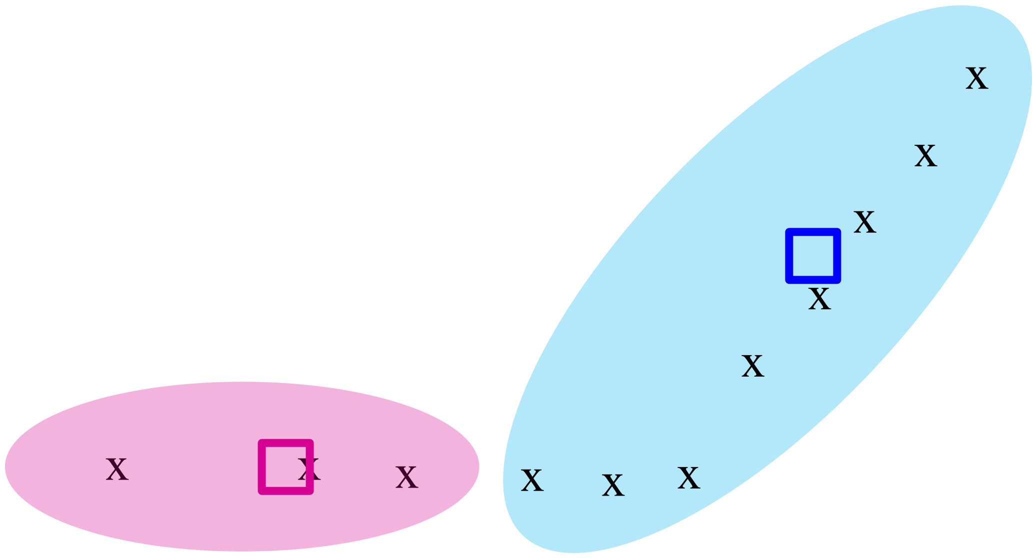
Example: Assigning Clusters



x … data point
… centroid

Clusters after round 1

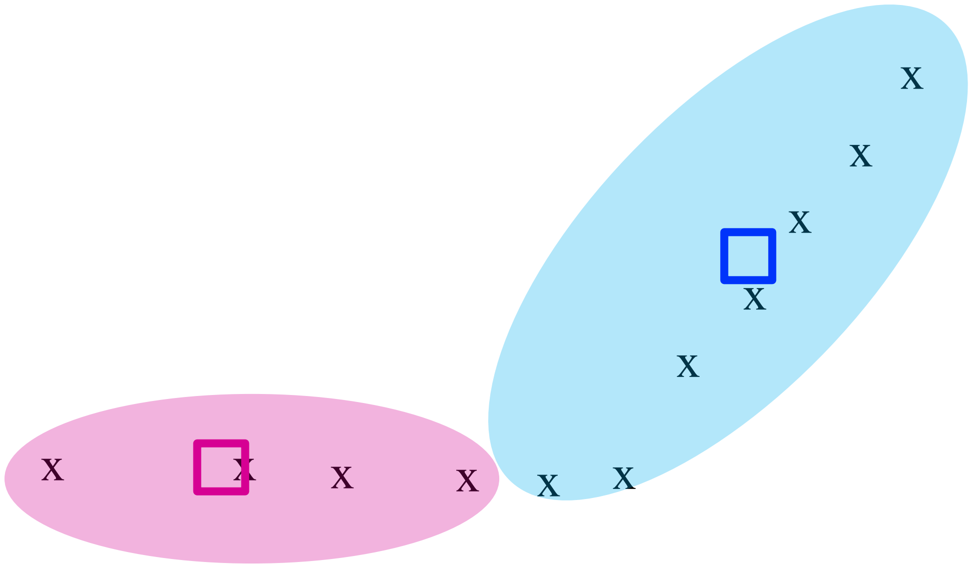
Example: Assigning Clusters



x … data point
… centroid

Clusters after round 2

Example: Assigning Clusters



x … data point

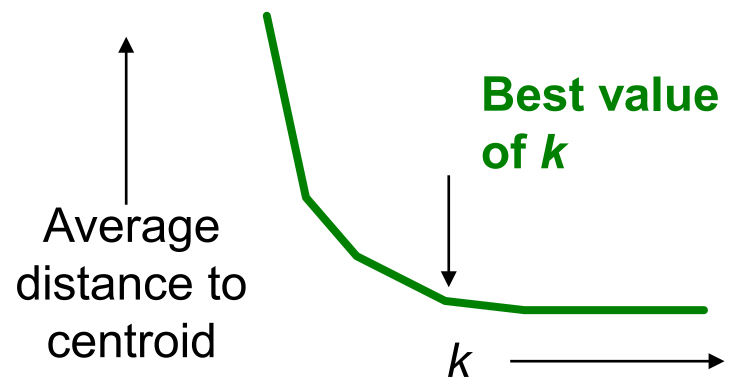
… centroid

Clusters after round 2

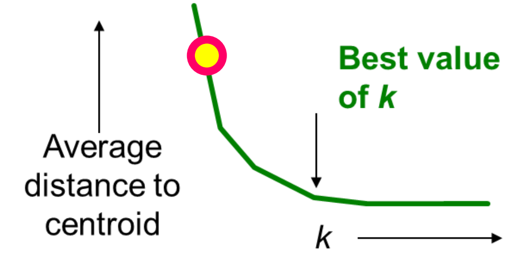
Getting the *k* right

How to select *k*?

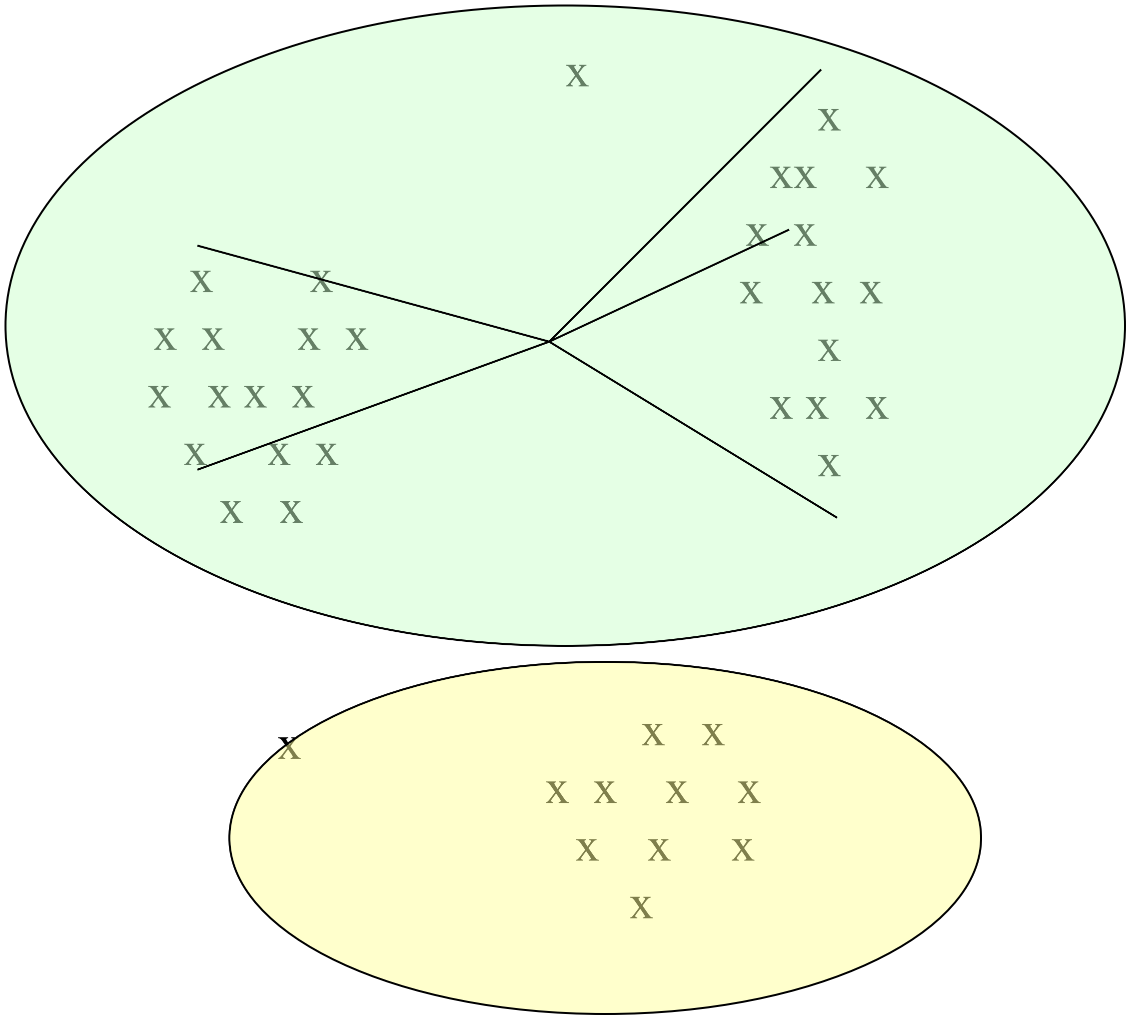
- Try different **k**, looking at the change in the average distance to centroid as **k** increases
- Average falls rapidly until right **k**, then changes little



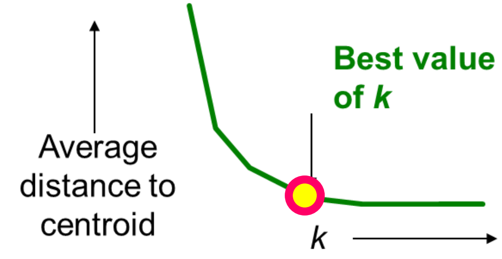
Example: Picking *k*



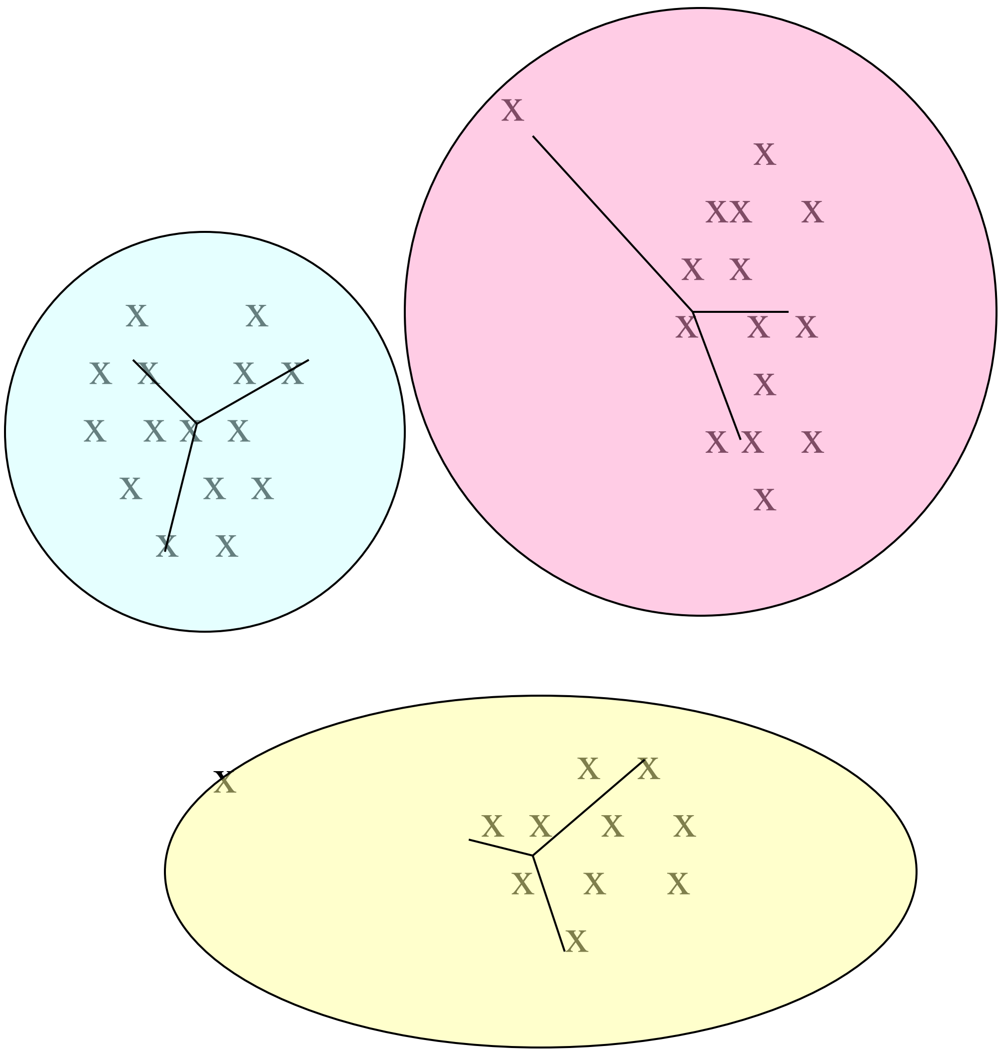
Too few;
many long distances to centroid



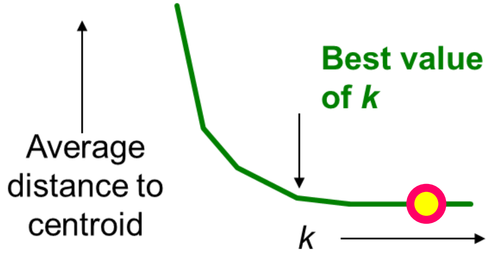
Example: Picking *k*



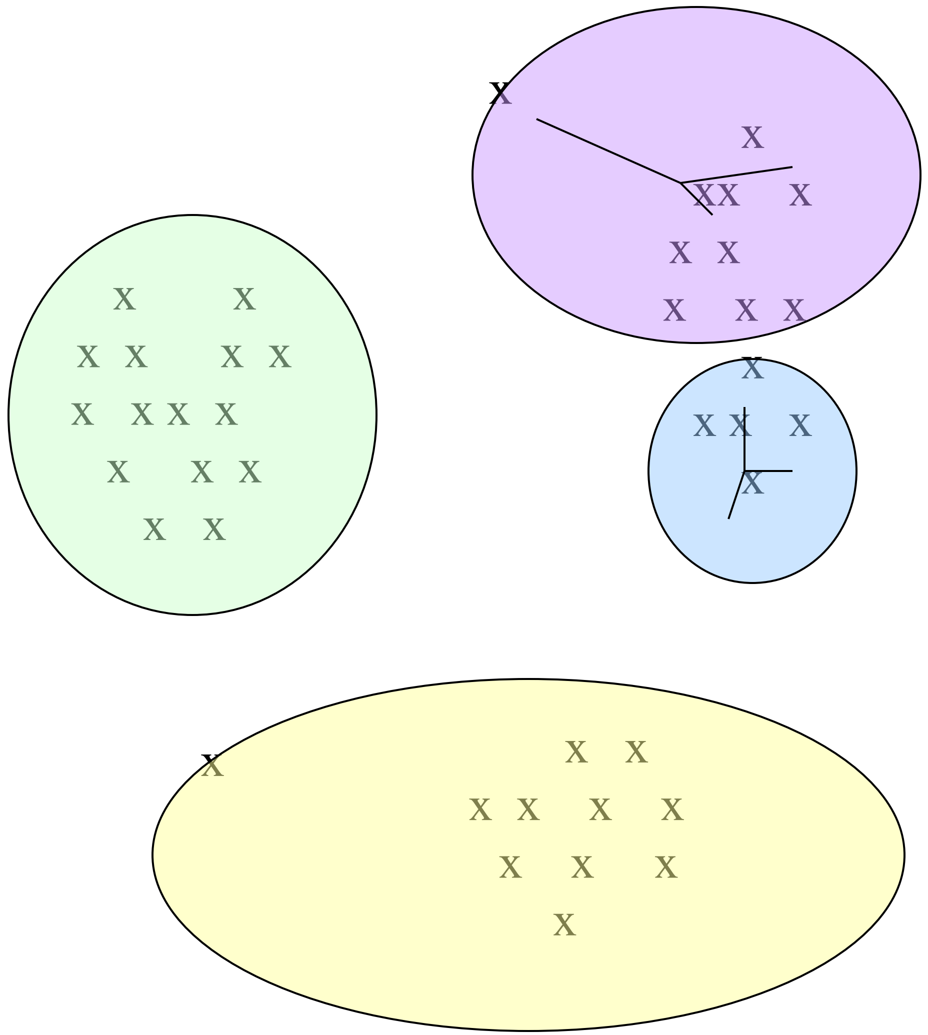
Just right;
distances rather short



Example: Picking *k*

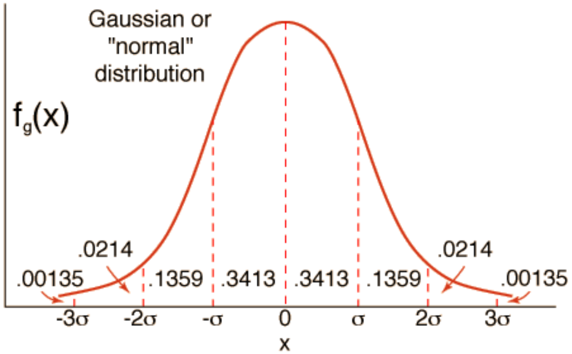


Too many;
little improvement in average distance



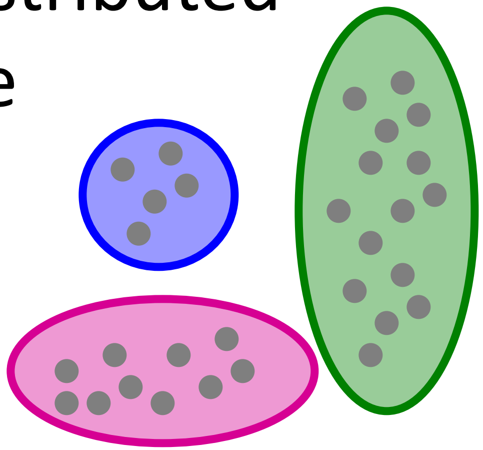
The BFR Algorithm

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



- Goal is to find cluster centroids; point assignment can be done in a second pass through the data.

BFR Overview

- **Efficient way to summarize clusters:** Want memory required O(clusters) and not O(data)
- **IDEA: Rather than keeping points, BFR keeps summary statistics of groups of points**
  - **3 sets: Cluster summaries, Outliers, Points to be clustered**
- **Overview of the algorithm:**
  - **1.** Initialize *K* clusters/centroids
  - **2.** Load in a bag of points from disk
  - **3.** Assign new points to one of the *K* original clusters, if they are within some distance threshold of the cluster
  - **4.** Cluster the remaining points, and create new clusters
  - **5.** Try to merge new clusters from step 4 with any of the existing clusters
  - **6.** Repeat steps 2-5 until all points are examined

BFR Algorithm

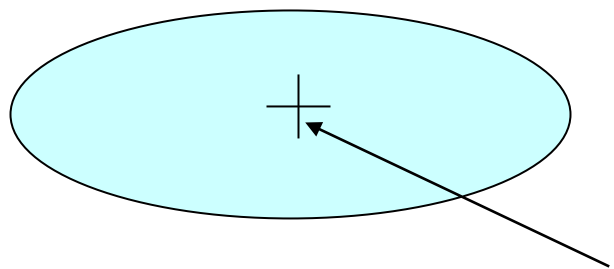
- **Points are read from disk one main-memory-full at a time**
- **Most points from previous memory loads are summarized by simple statistics**
- **Step 1)** From the initial load we select the initial ***k*** centroids by some sensible approach:
  - Take ***k*** random points
  - Take a small random 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

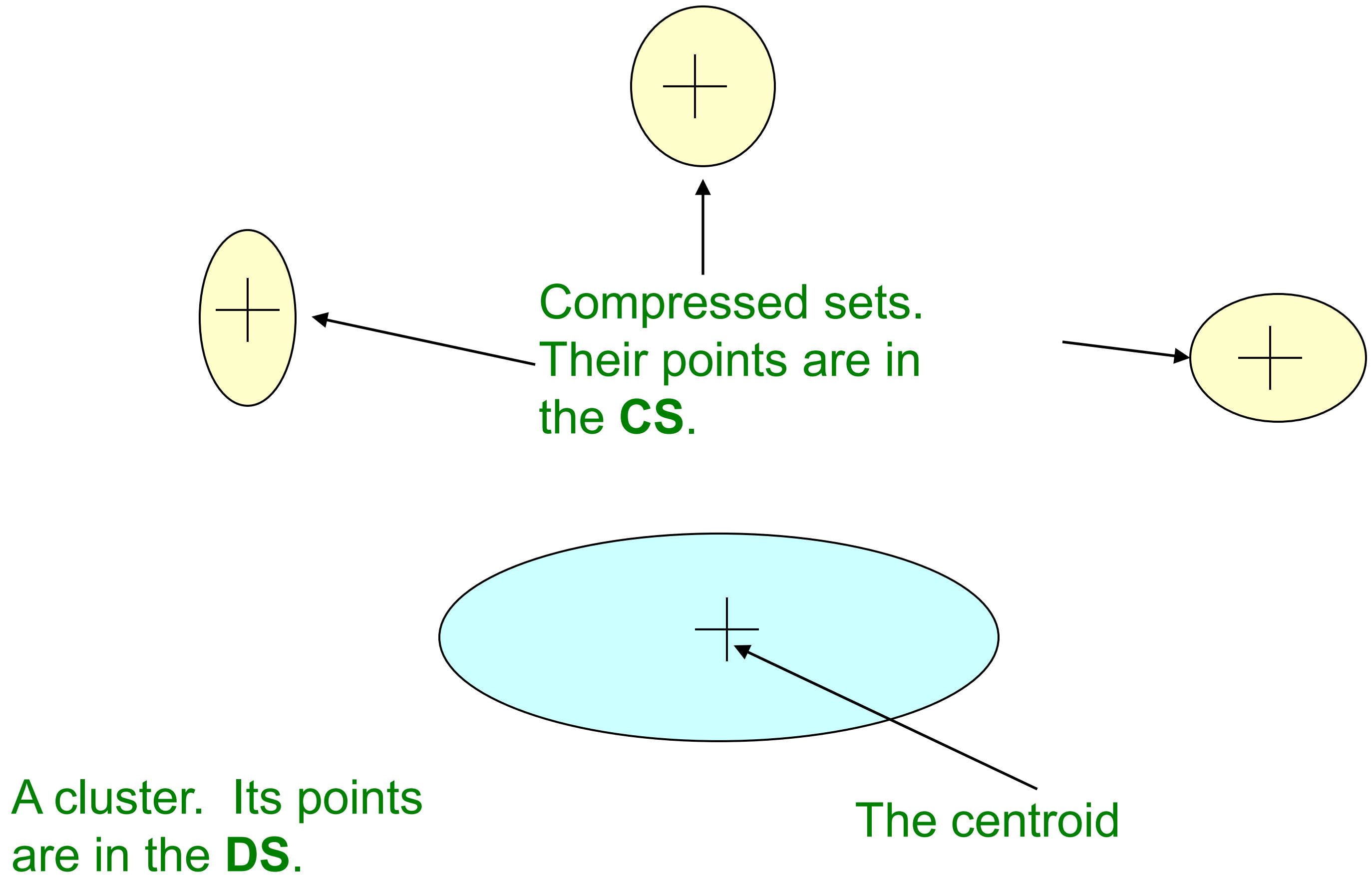


A cluster. Its points are in the **DS**.

The centroid

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



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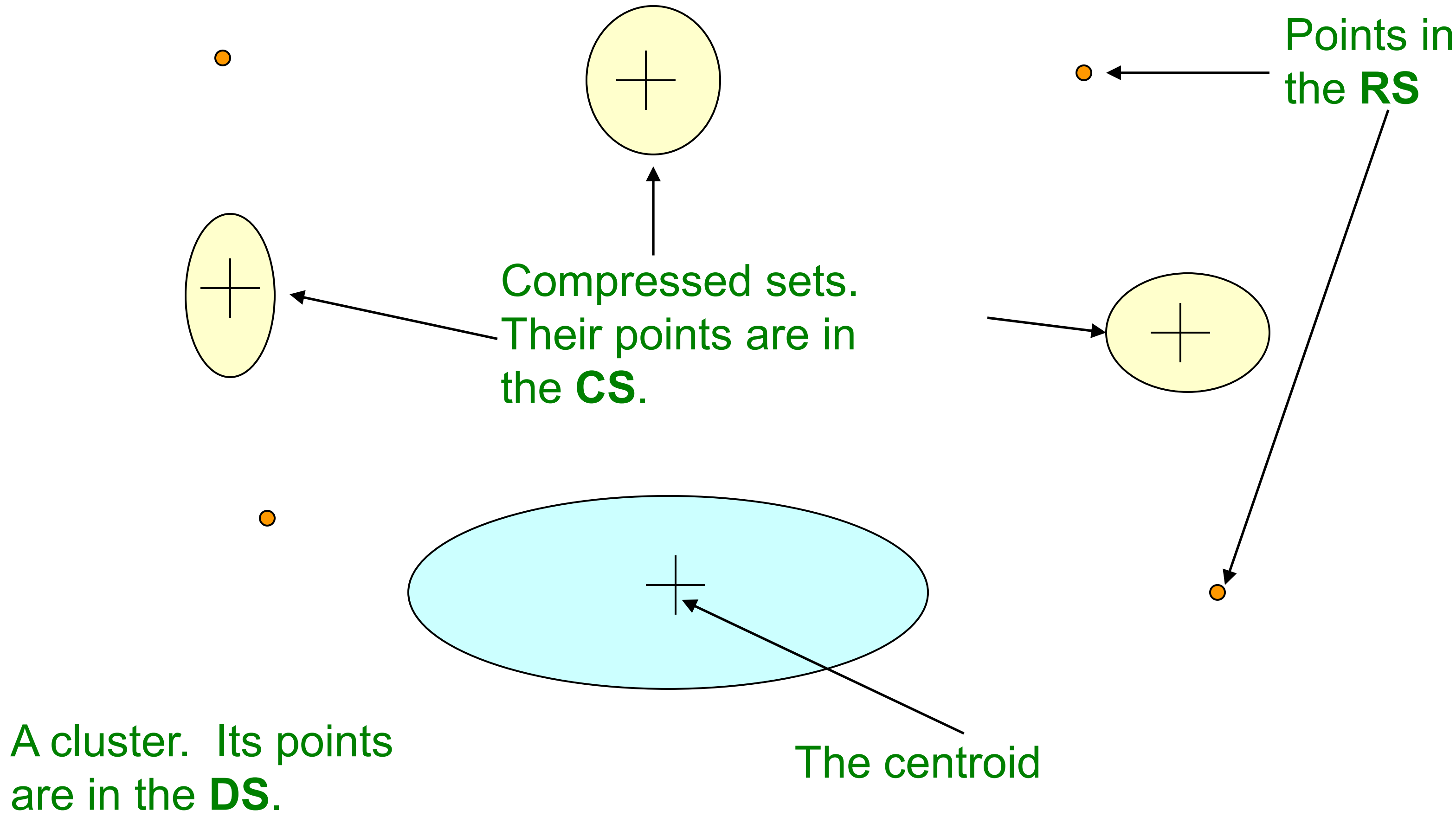
BFR: "Galaxies" Picture

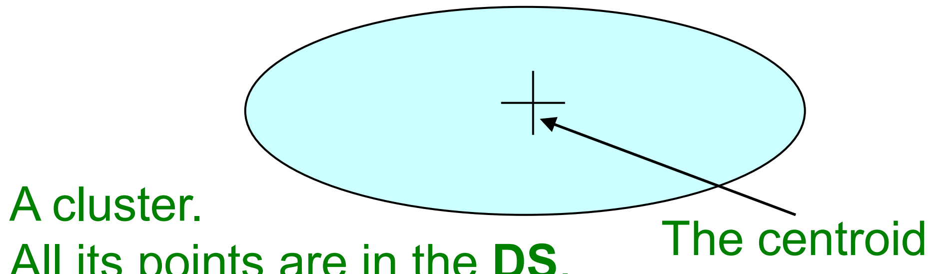


Discard set (DS): Close enough to a centroid to be summarized
Compression set (CS): Summarized, but not assigned to a cluster
Retained set (RS): Isolated points

Summarizing Sets of Points

For each cluster, the discard set (DS) is <u>summarized</u> by:

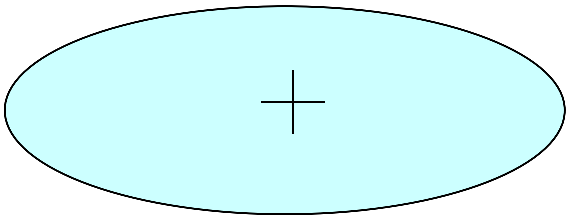
- The number of points, ***N***
- The vector ***SUM***, whose i^{th} component is the sum of the coordinates of the points in the i^{th} dimension
- The vector ***SUMSQ***: i^{th} component = sum of squares of coordinates in i^{th} dimension



Summarizing Points: Comments

- **2*d* + 1** values represent any size cluster
  - ***d*** = number of dimensions
- Average in **each dimension** (**the centroid**) can be calculated as $\mathbf{SUM}_i\,/\,N$
  - $\mathbf{SUM}_i = i^{th}$ component of SUM
- Variance of a cluster's discard set in dimension i is: $\mathbf{(SUMSQ_i\,/\,N) - (SUM_i\,/\,N)^2}$
  - 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 x d*** matrix, which is too big!



The "Memory-Load" of Points

Steps 3-5) Processing "Memory-Load" of points:

- **Step 3)** 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
- **Step 4)** Use any in-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

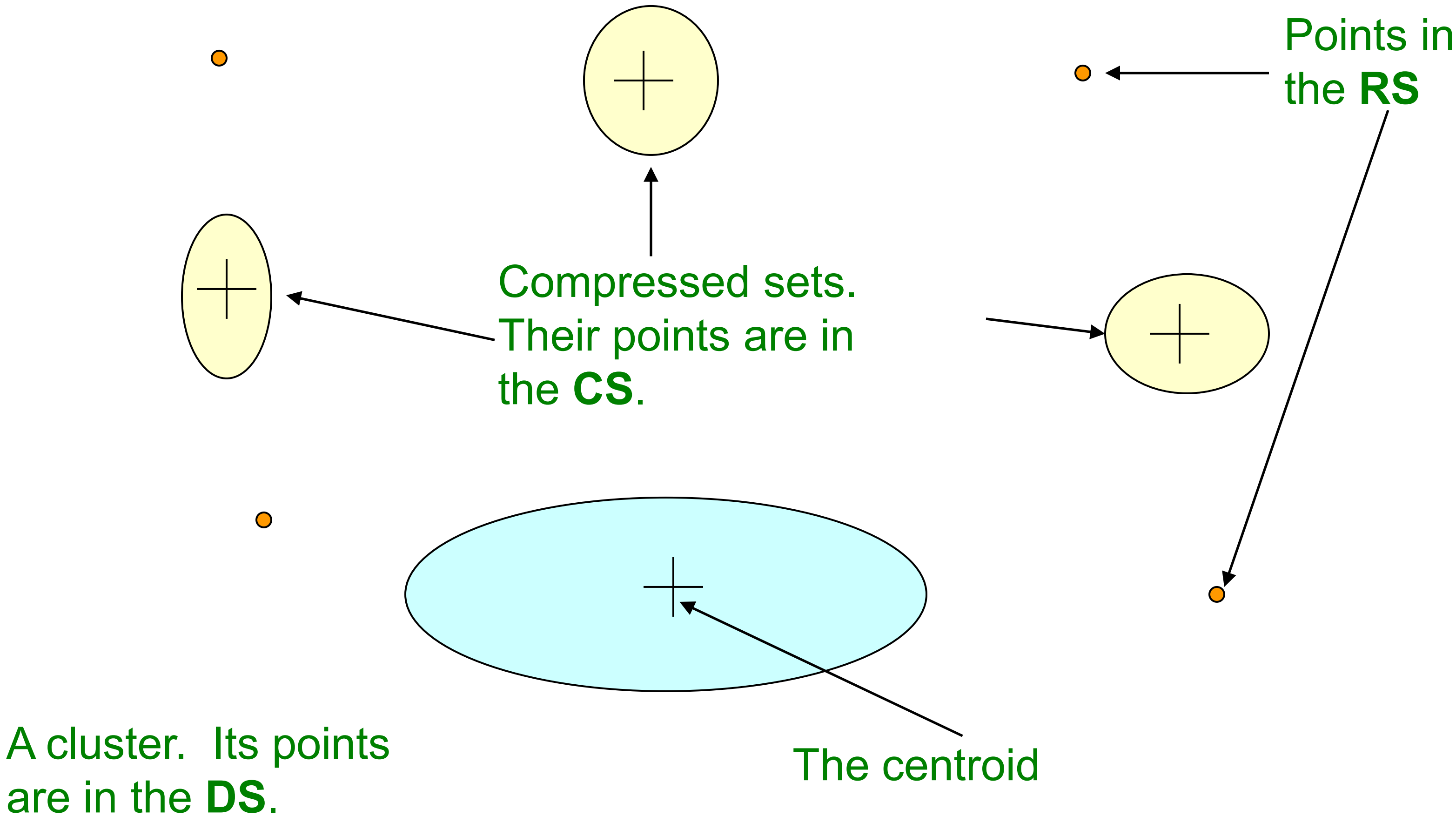
The "Memory-Load" of Points

Steps 3-5) Processing "Memory-Load" of points:

- **Step 5) DS set:** Adjust statistics of the clusters to account for the new points
  - Add ***N***s, ***SUM***s, ***SUMSQ***s
  - Consider merging compressed sets in the **CS**
- **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



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

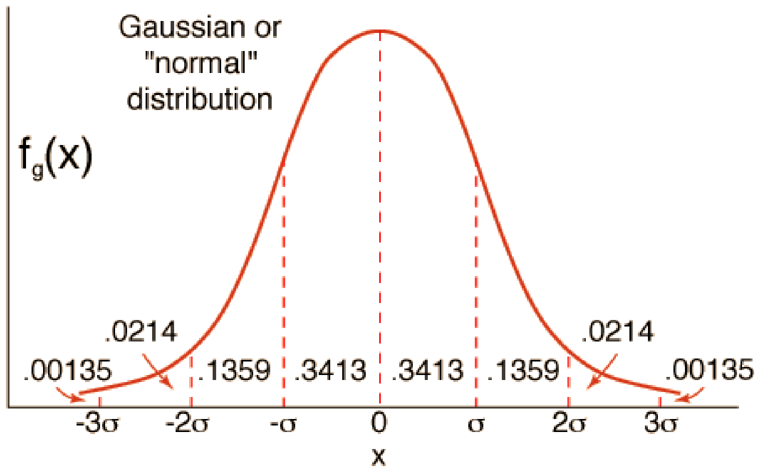
A Few Details…

- **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**

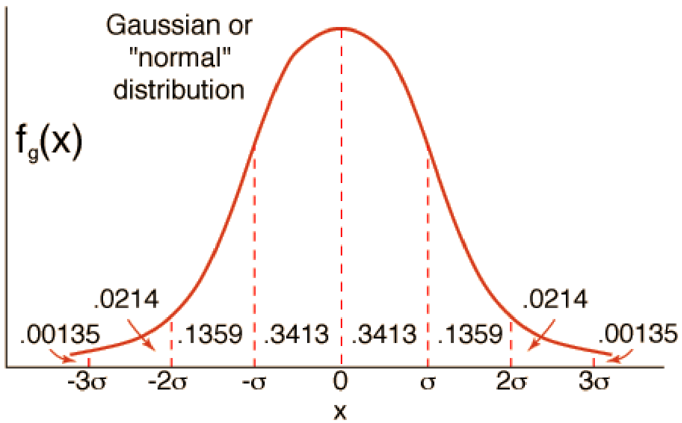
- For point $(x_1, \ldots, x_d)$ and centroid $(c_1, \ldots, c_d)$
  1. Normalize in each dimension: $y_i = (x_i - c_i) / \sigma_i$
  2. Take sum of the squares of the y_i
  3. Take the square root

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

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

Mahalanobis Distance

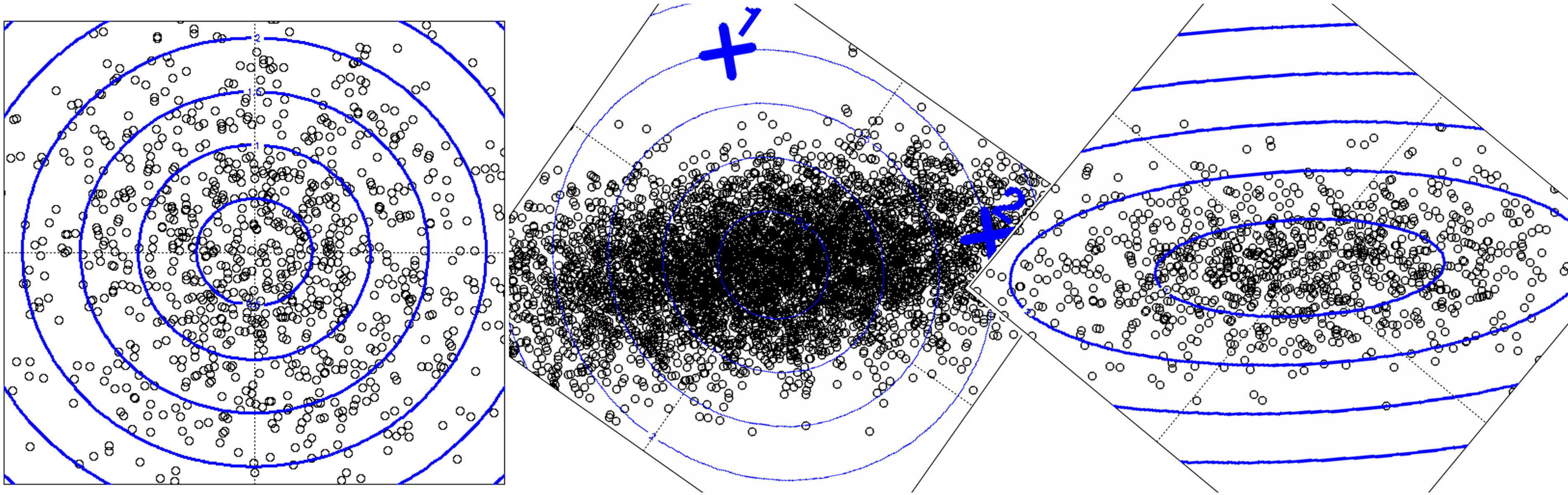
- If clusters are normally distributed in $\boldsymbol{d}$ dimensions, then after transformation, one standard deviation **=>** Distance $\sqrt{\boldsymbol{d}}$
  - i.e., 68% of the points of the cluster will have a Mahalanobis distance $< \sqrt{\boldsymbol{d}}$
- Accept a point for a cluster if its 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

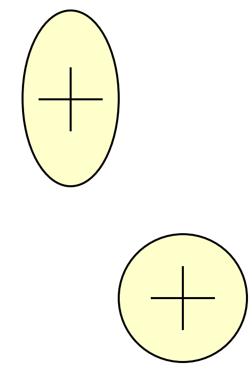


Uniformly distributed points, Euclidean distance	**Normally distributed points, Euclidean distance**	**Normally distributed points, Mahalanobis distance**

Should 2 CS clusters be combined?

Q2) Should 2 CS clusters 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

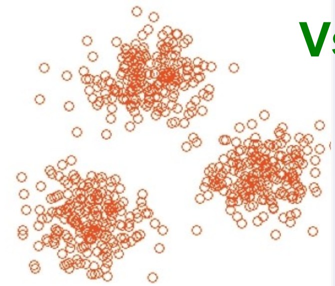


- **Many alternatives:** Treat dimensions differently, consider density

The CURE Algorithm

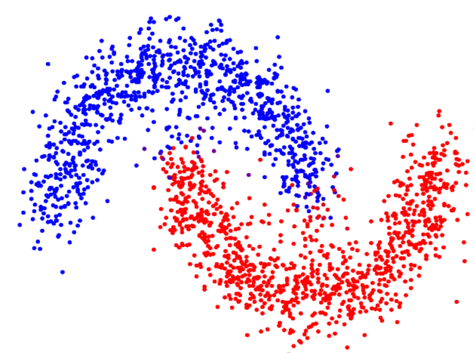
The CURE Algorithm

- **Problem with BFR/*k*-means:**
  - Assumes clusters are normally distributed in each dimension
  - And axes are fixed – ellipses at an angle are ***not OK***

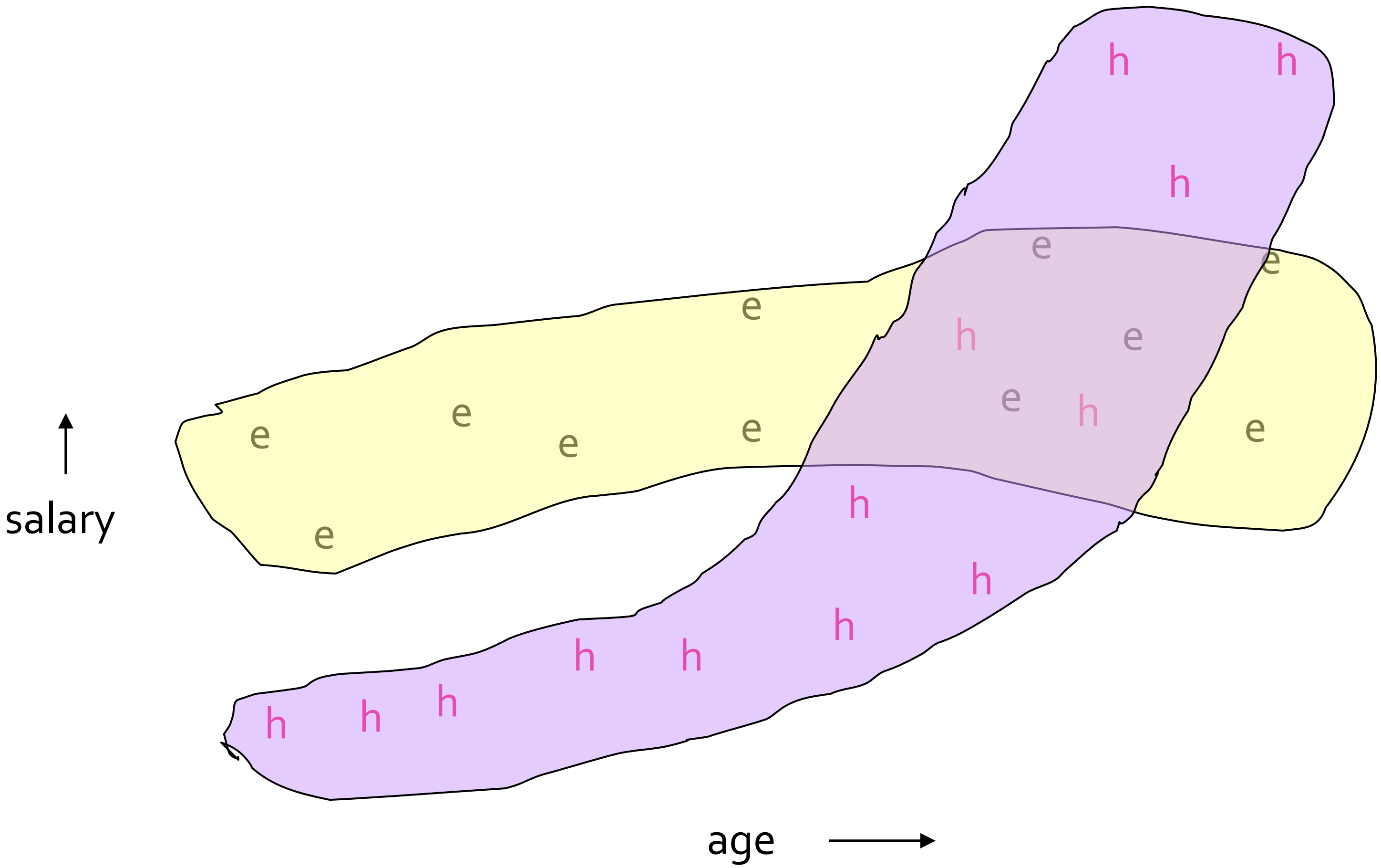


Vs.

- **CURE (Clustering Using REpresentatives):**
  - Assumes a Euclidean distance
  - Allows clusters to assume any shape
  - **Uses a collection of representative points to represent clusters**



Example: University Salaries

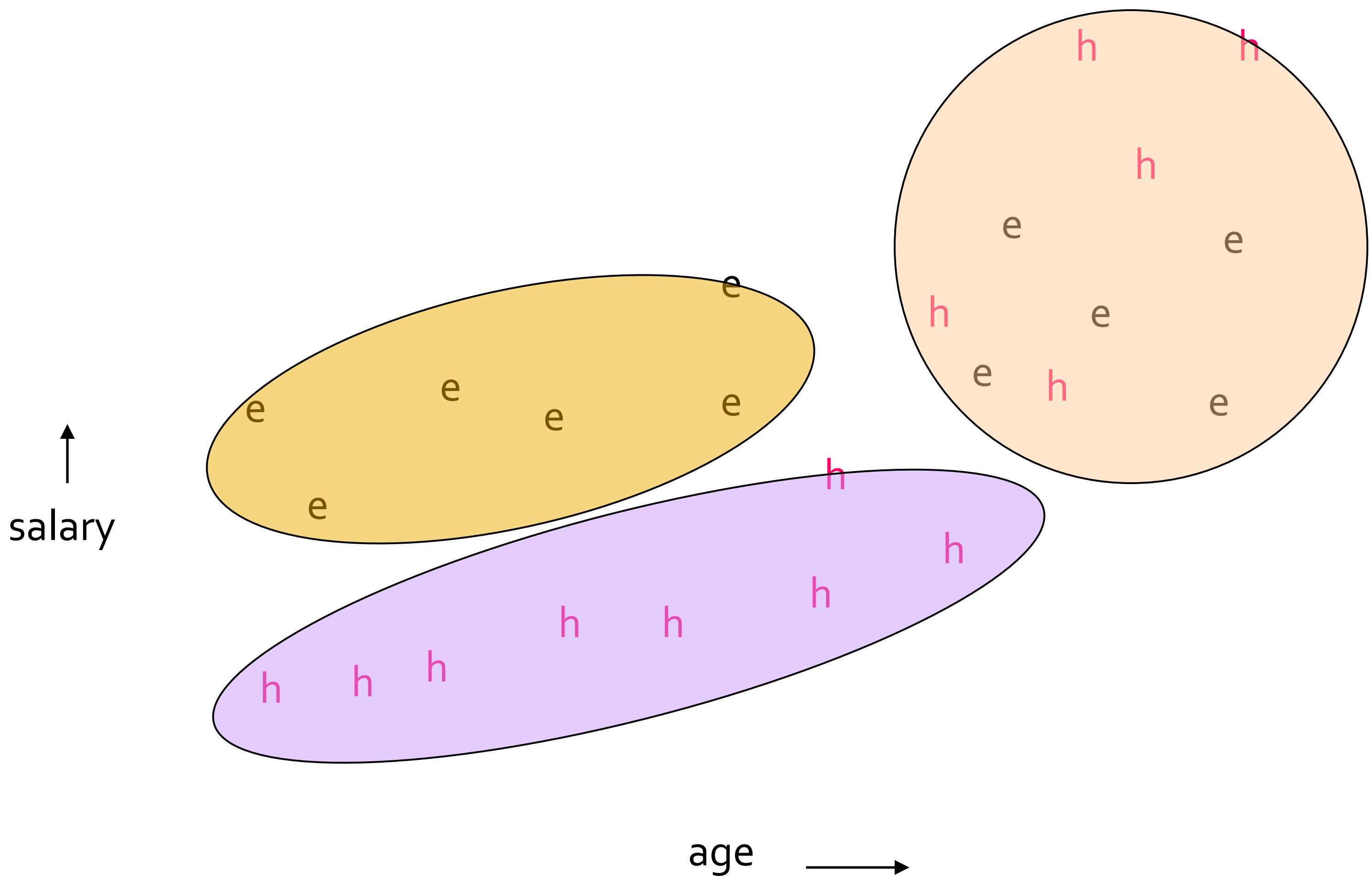


Starting CURE

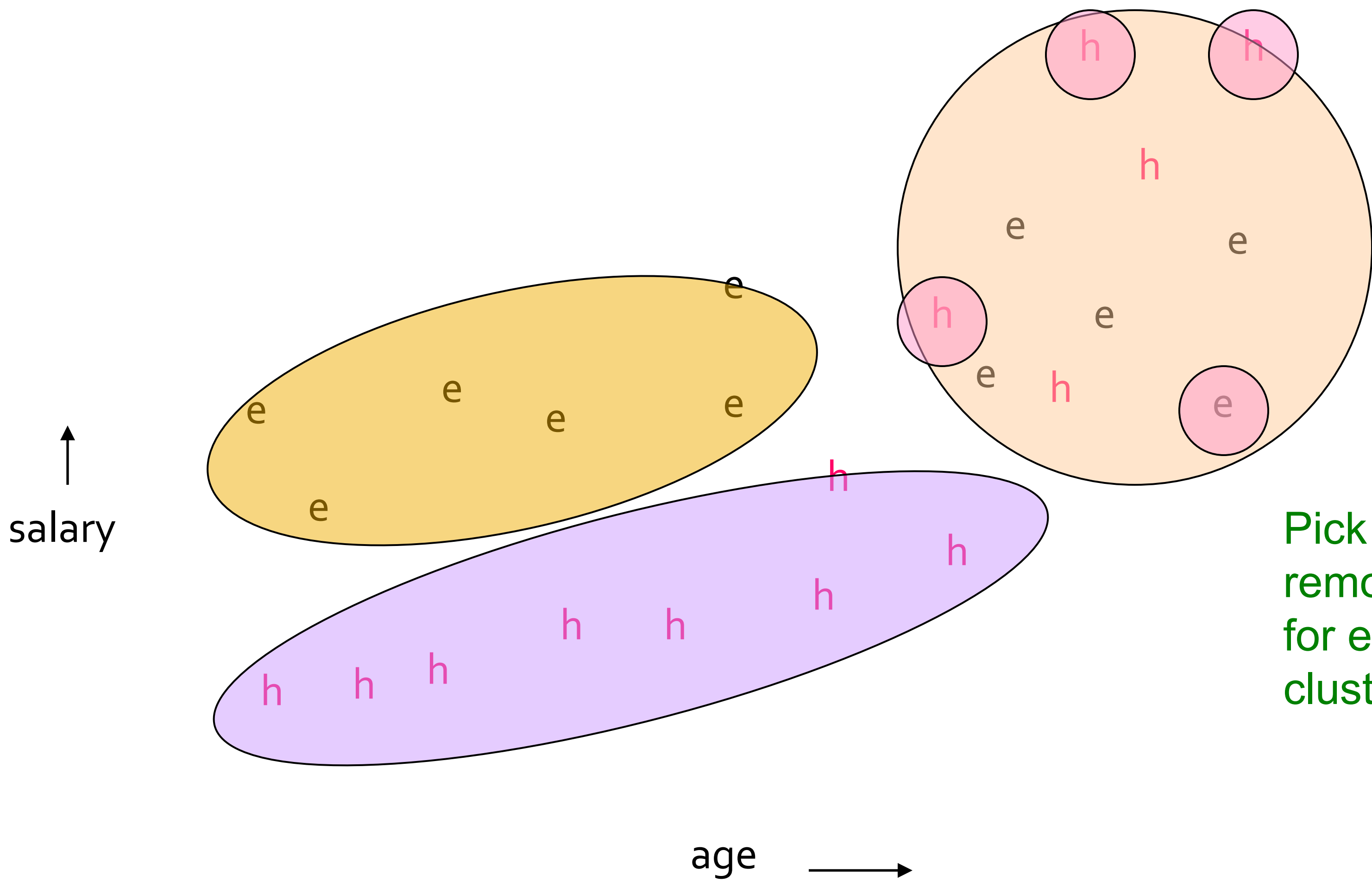
<u>**2 Pass algorithm. Pass 1:**</u>

- **0) Pick a random sample of points that fit in main memory**
- **1) Initial clusters:**
  - Cluster these points hierarchically – group nearest points/clusters
- **2) Pick representative points:**
  - For each cluster, pick a sample of points, as dispersed as possible
  - From the sample, pick representatives by moving them (say) 20% toward the centroid of the cluster

Example: Initial Clusters

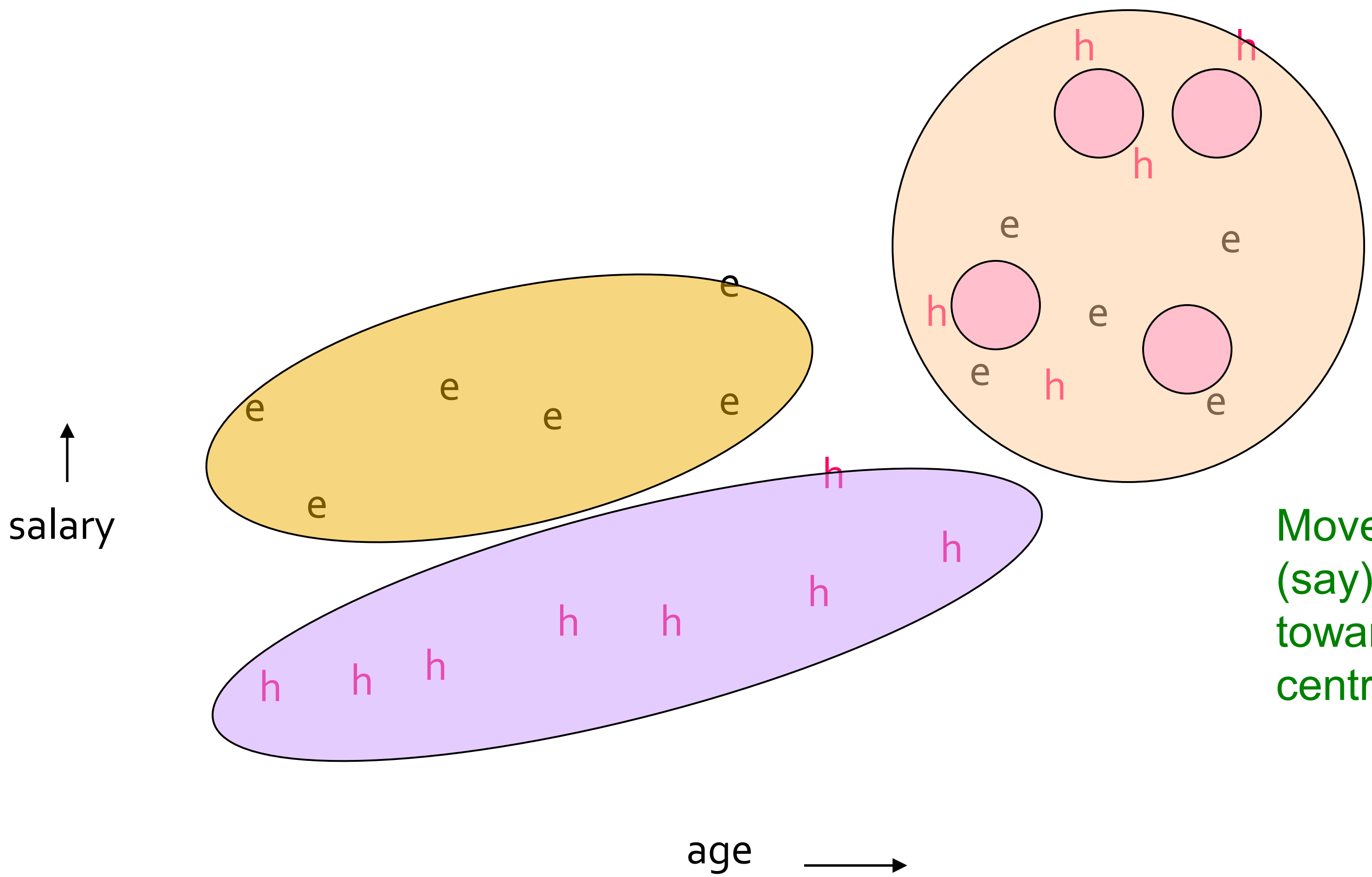


Example: Pick Dispersed Points



Pick (say) 4 remote points for each cluster.

Example: Pick Dispersed Points

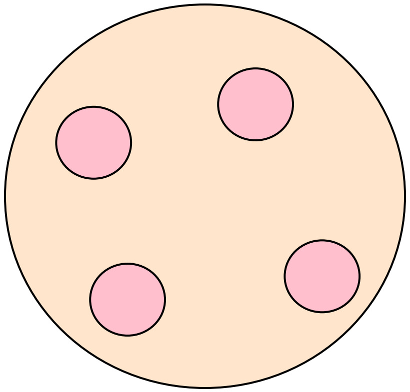


Move points (say) 20% toward the centroid.

Finishing CURE

Pass 2:

- Now, rescan the whole dataset and visit each point ***p*** in the data set



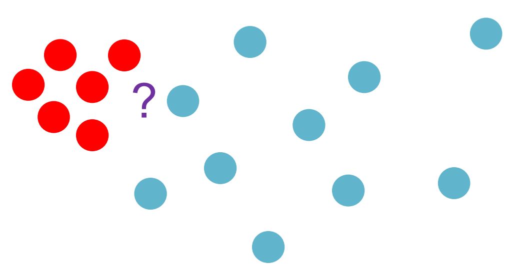
- **Place it in the "closest cluster"**
  - Normal definition of "closest":
    Find the closest representative point to ***p*** and assign it to representative's cluster

p

Why the 20% Move Inward?

Intuition:

- A large, dispersed cluster will have large moves from its boundary
- A small, dense cluster will have little move.
- Favors a small, dense cluster that is near a larger dispersed cluster



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**
  - **CURE**

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