# Clustering

Hierarchical /Agglomerative and Point-Assignment Approaches
Measures of "Goodness" for Clusters
BFR Algorithm
CURE Algorithm

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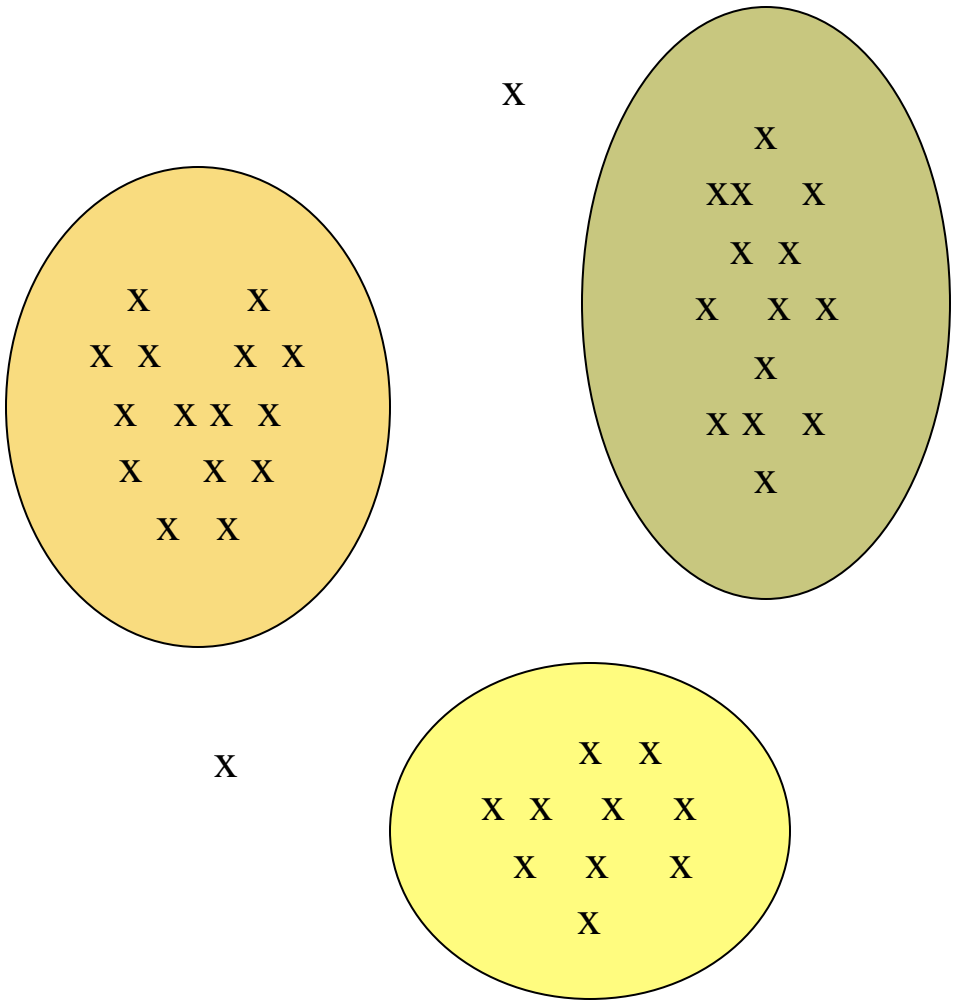
# The Problem of Clustering

- 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" to each other, while members of different clusters are "far."

# Example: Clusters



# Problems With Clustering

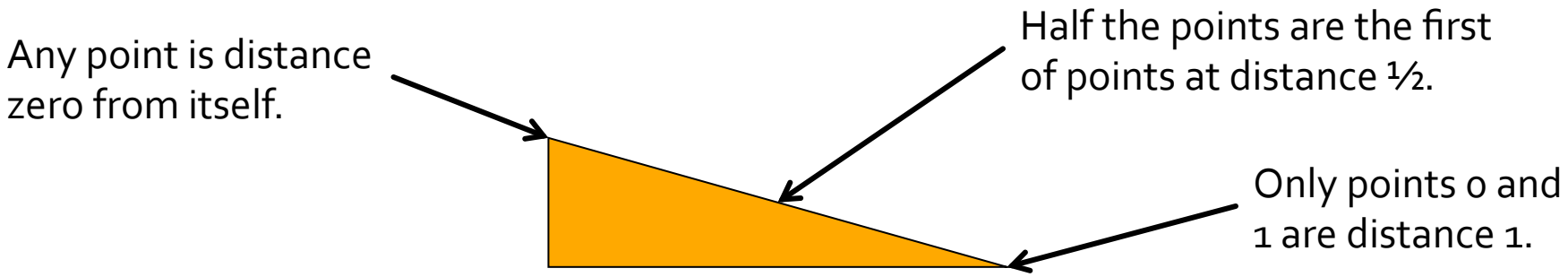
- Clustering in two dimensions looks easy.
- Clustering small amounts of data looks easy.
- And in most cases, looks are *not* deceiving.

# The Curse of Dimensionality

- 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.

# Example: Curse of Dimensionality

- Assume random points between 0 and 1 in each dimension.
- In 2 dimensions: a variety of distances between 0 and 1.41.
- In any number of dimensions, the distance between two random points in any one dimension is distributed as a triangle.



# Example – Continued

- The law of large numbers applies.
- Actual distance between two random points is the sqrt of the sum of squares of essentially the same set of differences.
  - I.e., “all points are the same distance apart.”

# Euclidean and Non-Euclidean Distances

- Euclidean spaces have dimensions, and points have coordinates in each dimension.
- Distance between points is usually the square-root of the sum of the squares of the distances in each dimension.
- Non-Euclidean spaces have a distance measure, but points do not really have a position in the space.
  - Big problem: cannot “average” points.

# Example: DNA Sequences

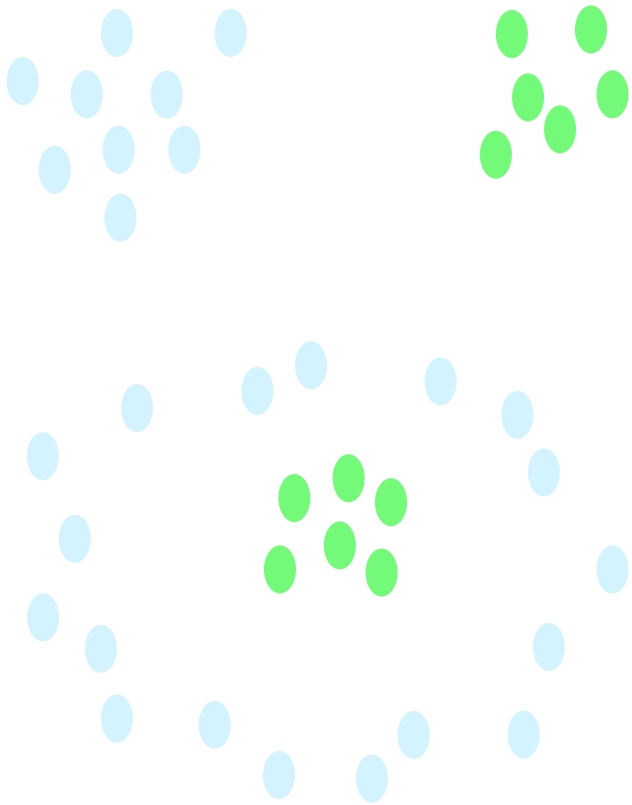
- Objects are sequences of {C,A,T,G}.
- Distance between sequences = *edit distance* = the minimum number of inserts and deletes needed to turn one into the other.
  - Notice: no way to "average" two strings.
- In practice, the distance for DNA sequences is more complicated: allows other operations like *mutations* (change of a symbol into another) or reversal of substrings.

# Methods of Clustering

- Hierarchical (Agglomerative):
  - Initially, each point in cluster by itself.
  - Repeatedly combine the two "nearest" clusters into one.
- Point Assignment:
  - Maintain a set of clusters.
  - Place points into their "nearest" cluster.
  - Possibly split clusters or combine clusters as we go.

# Which is Better?

- Point assignment good when clusters are nice, convex shapes.
- Hierarchical can win when shapes are weird.



Aside: 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.

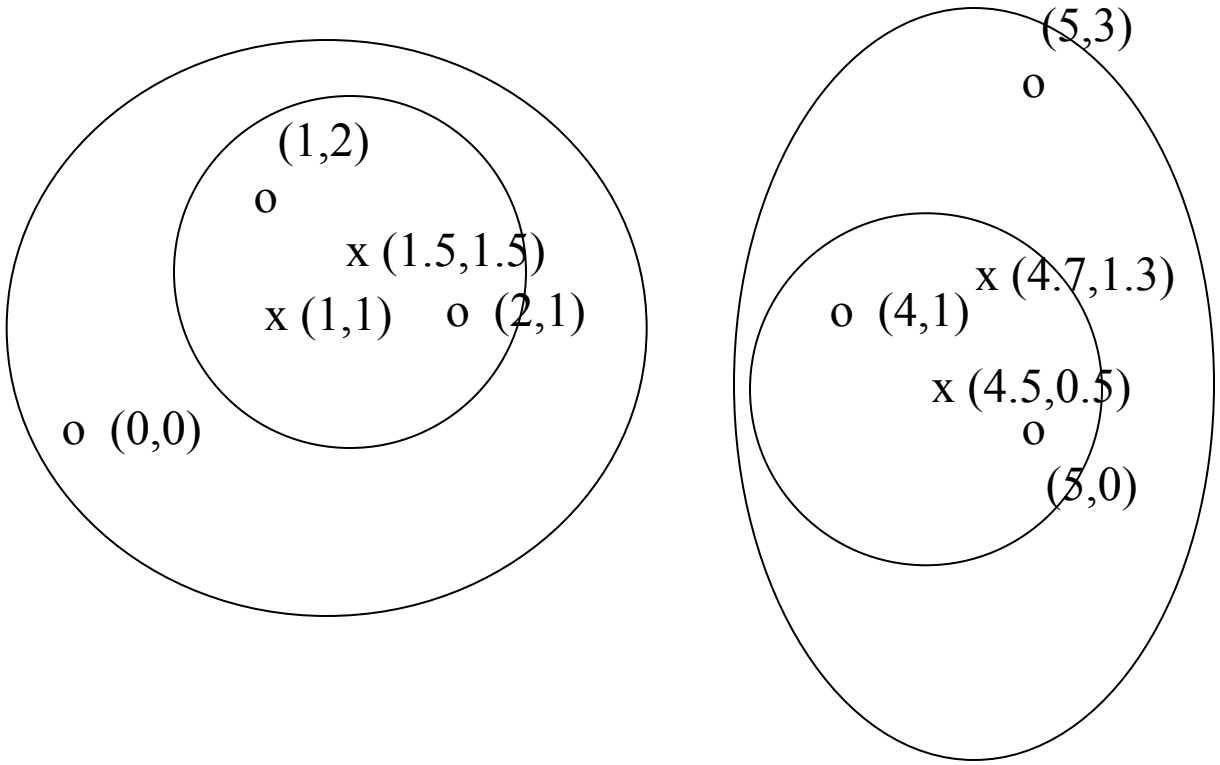
# Hierarchical Clustering

- Two important questions:
  1. How do you determine the "nearness" of clusters?
  2. How do you represent a cluster of more than one point?

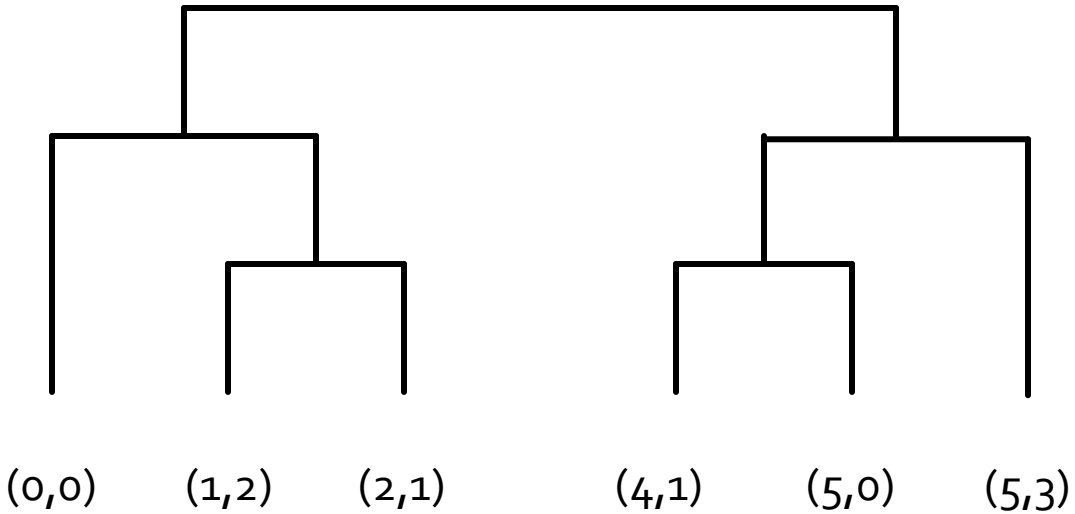
# Hierarchical Clustering – (2)

- Key problem: as you build 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 points.
  - Measure intercluster distances by distances of centroids.

# Example



# Dendrogram



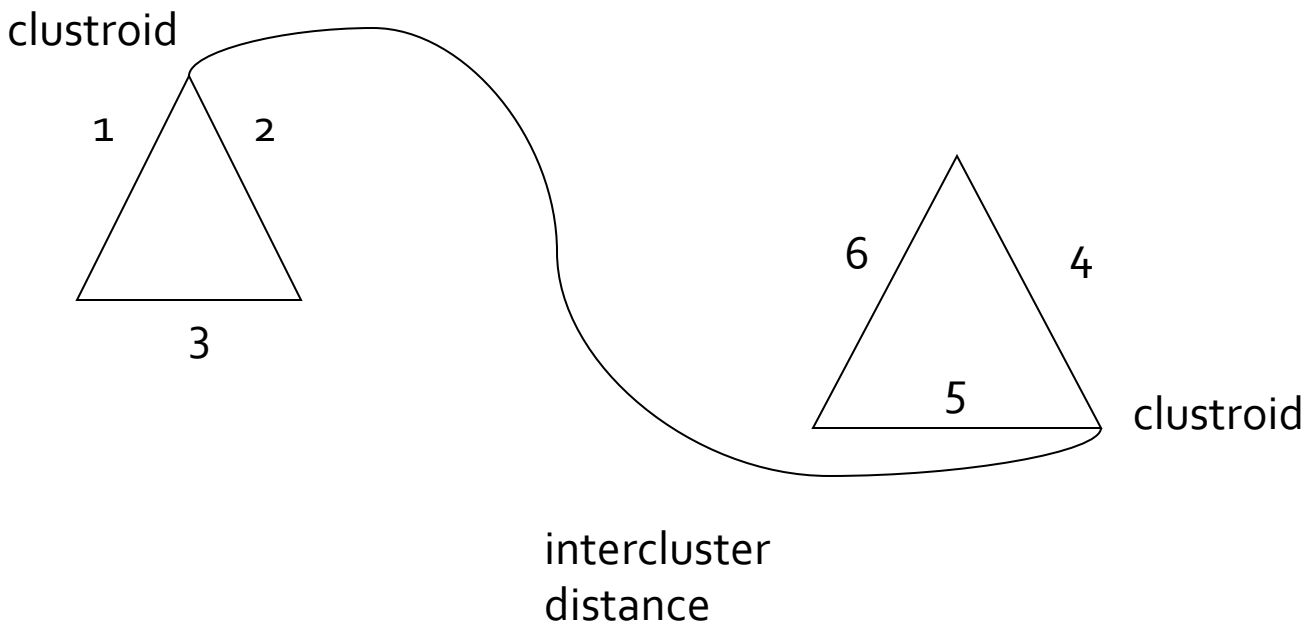
# And in the Non-Euclidean Case?

- The only "locations" we can talk about are the points themselves.
  - I.e., there is no "average" of two points.
- Approach 1: *clustroid* = point "closest" to other points.
  - Treat clustroid as if it were centroid, when computing intercluster distances.

# "Closest" Point?

- Possible meanings:
  1. Smallest maximum distance to the other points.
  2. Smallest average distance to other points.
  3. Smallest sum of squares of distances to other points.
  4. Etc., etc.

# Example: Intercluster Distance



# Other Approaches to Defining "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 centroid or clustroid.
  - Merge clusters whose *union* is most cohesive.

# Cohesion

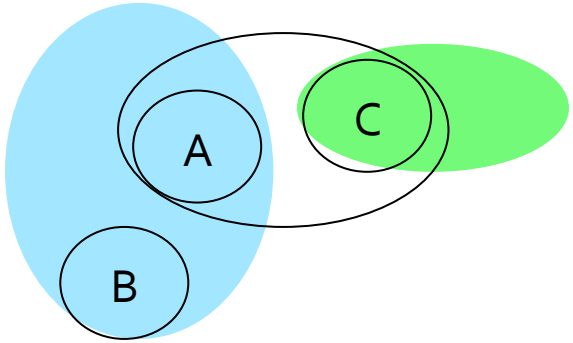
- Approach 1: Use the *diameter* of the merged cluster = maximum distance between points in the cluster.
- Approach 2: Use the average distance between points in the cluster.
- Approach 3: Density-based approach: take the diameter or average distance, e.g., and divide by the number of points in the cluster.
  - Perhaps raise the number of points to a power first, e.g., square-root.

# 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

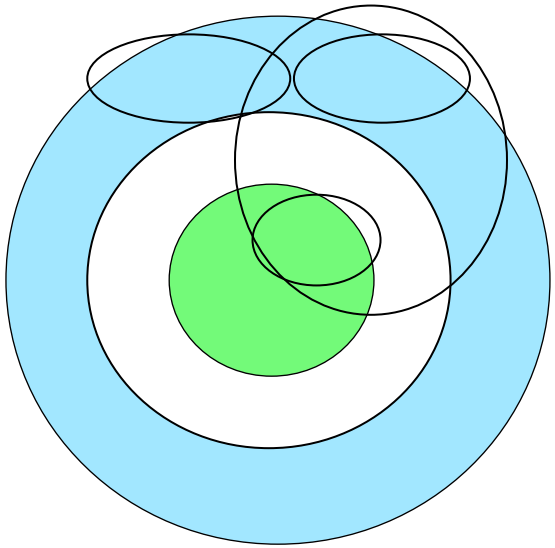
- Centroid-based merging works well.
- But merger based on closest members might accidentally merge incorrectly.




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

# Case 2: Concentric Clusters

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



# *k*–Means Algorithm(s)

- An example of point-assignment.
- Assumes Euclidean space.
- Start by picking *k*, the number of clusters.
- Initialize clusters with a *seed* (= 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, cluster them by any algorithm, and use the centroids as a seed.
- In k-means++, sample size = k times a factor that is logarithmic in the total number of points.
- Sequentially pick sample points randomly, 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.

# k-Means | |

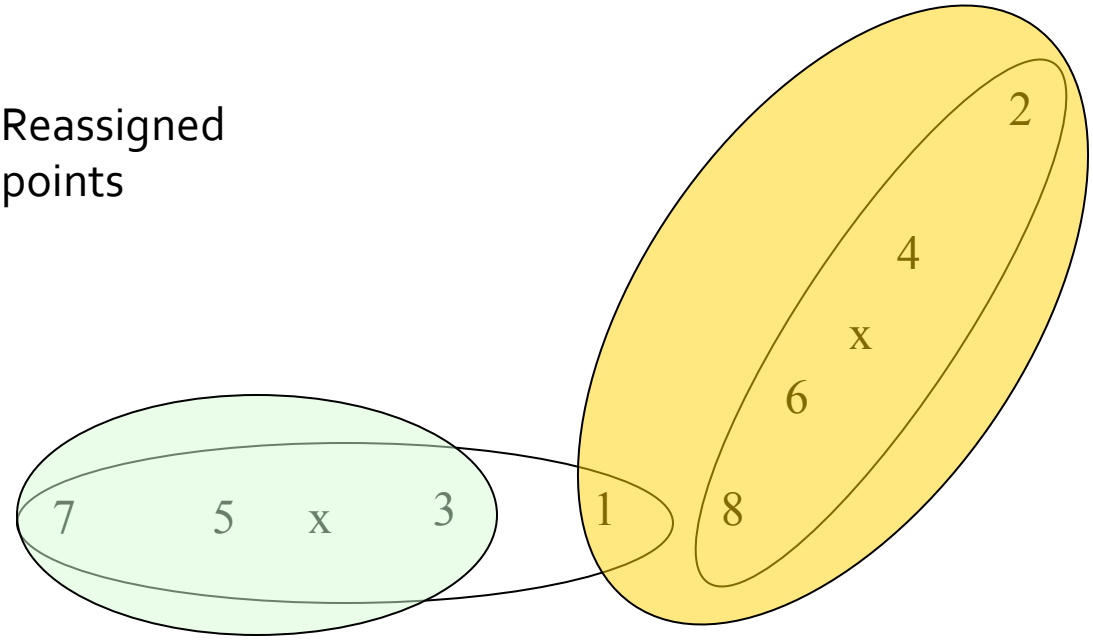
- k-means++, like other seed methods, is sequential.
  - You need to update D(p) for each unpicked p due to new point.
- Naturally parallel: many compute nodes can each handle a small set of points.
  - Each picks a few new sample points using same D(p).
- Really important and common trick: don't update after every selection; rather make many selections at one round.
  - Suboptimal picks don't really matter.

# Populating Clusters

1. For each point, place it in the cluster whose current centroid it is nearest.
2. After all points are assigned, fix the centroids of the *k* clusters.
3. Optional: reassign all points to their closest centroid.
   - Sometimes moves points between clusters.

# Example: Assigning Clusters

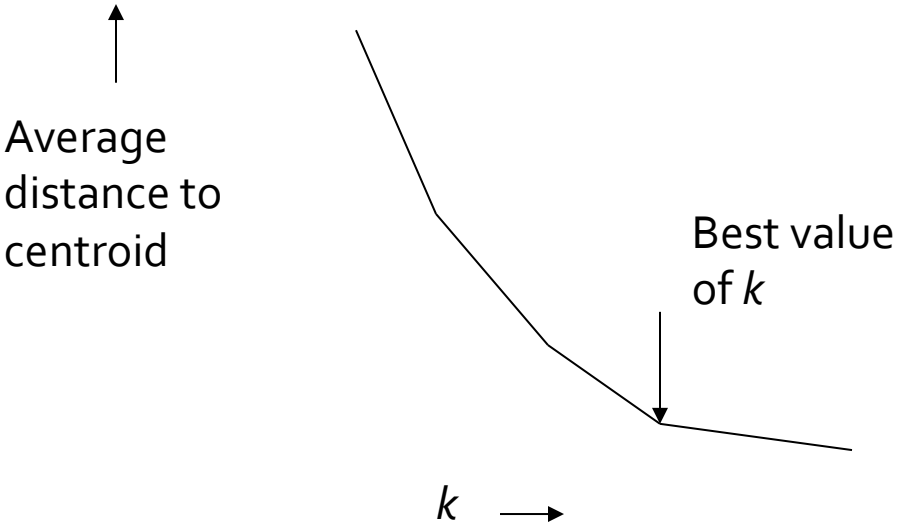
Reassigned points




Clusters after first round

# Getting *k* Right

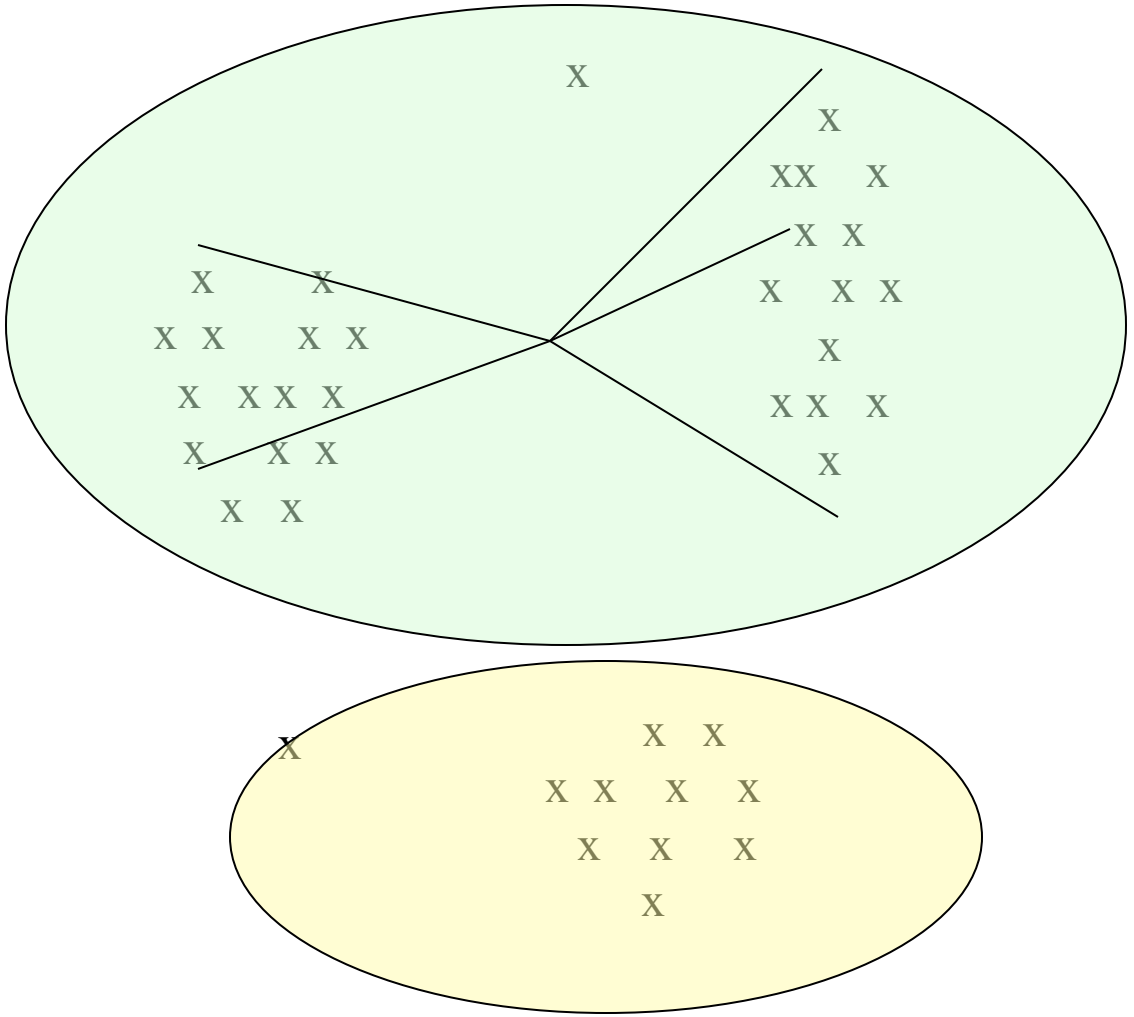
- Try different *k*, looking at the change in the average distance to centroid, as *k* increases.
- Average falls rapidly until right *k*, then changes little.




Note: binary search for k is possible.

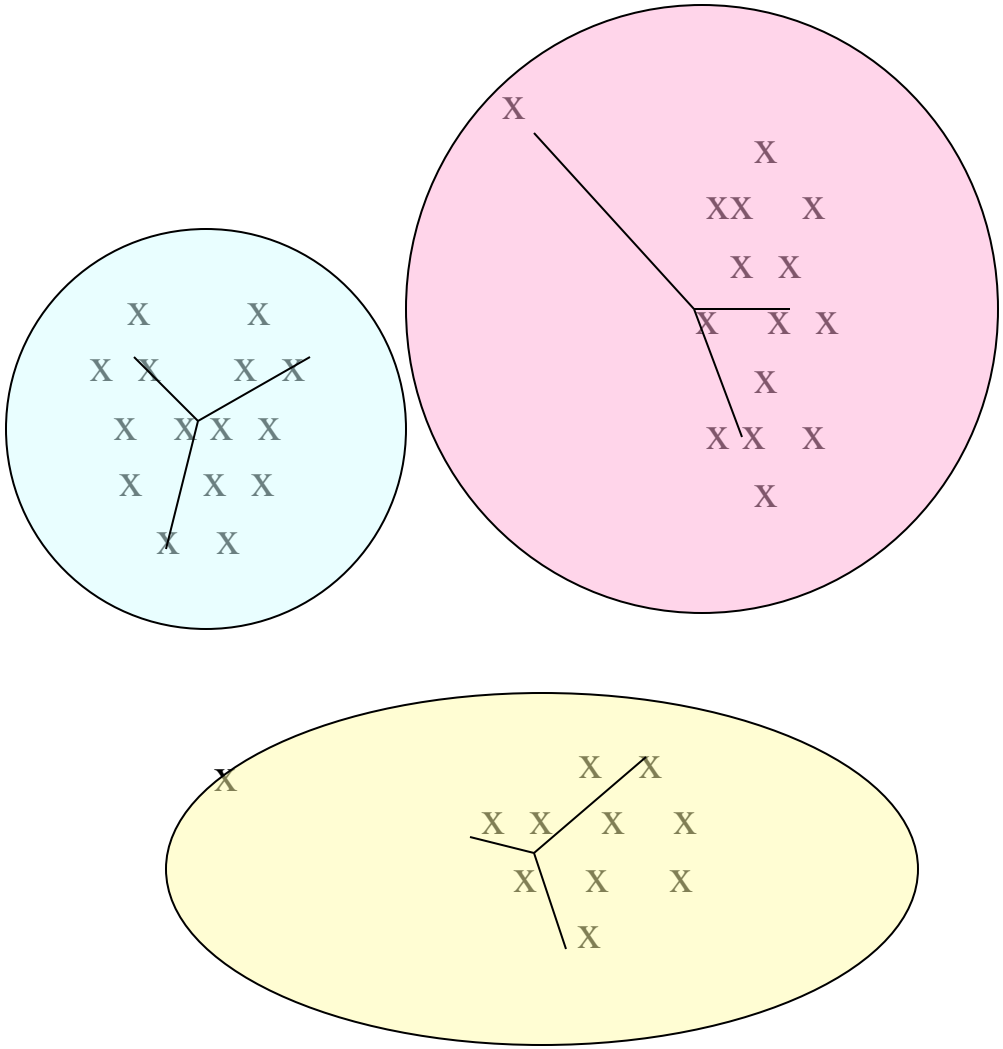
# Example: Picking *k*

Too few;
many long
distances
to centroid.



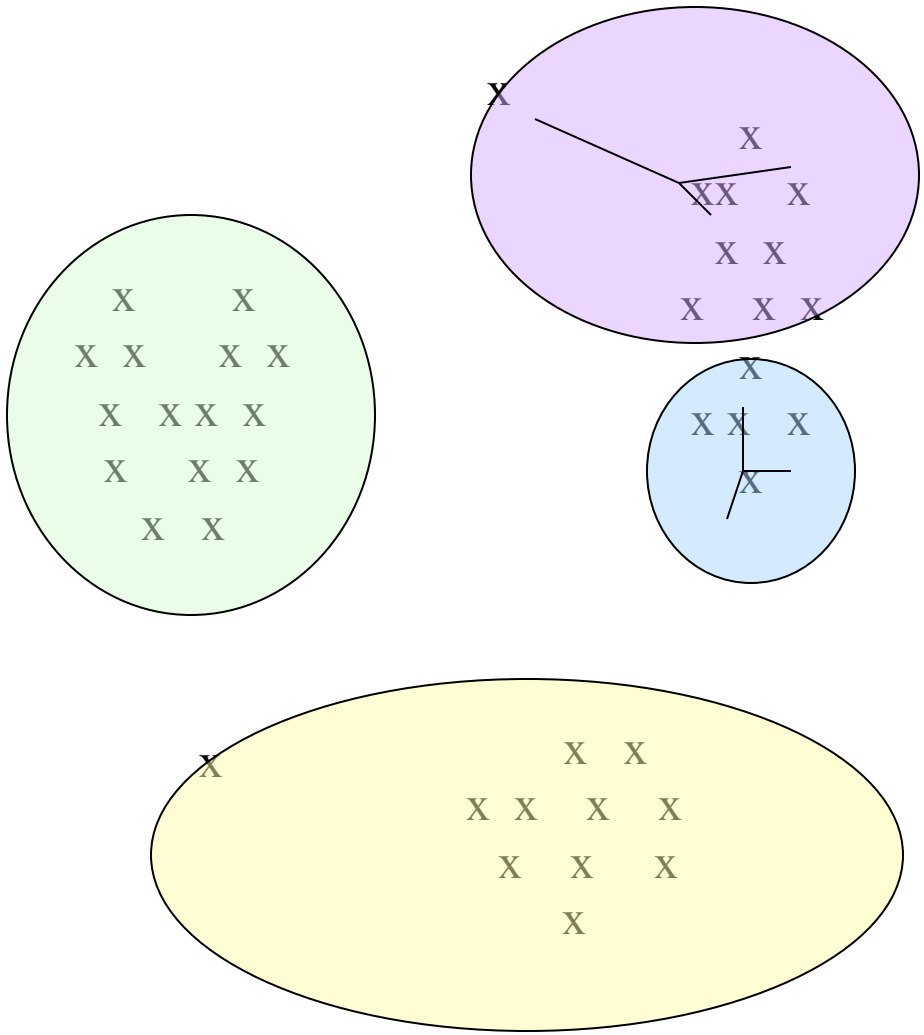
# Example: Picking *k*

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.
- It assumes that clusters are normally distributed around a centroid in a Euclidean space.
  - Standard deviations in different dimensions may vary.

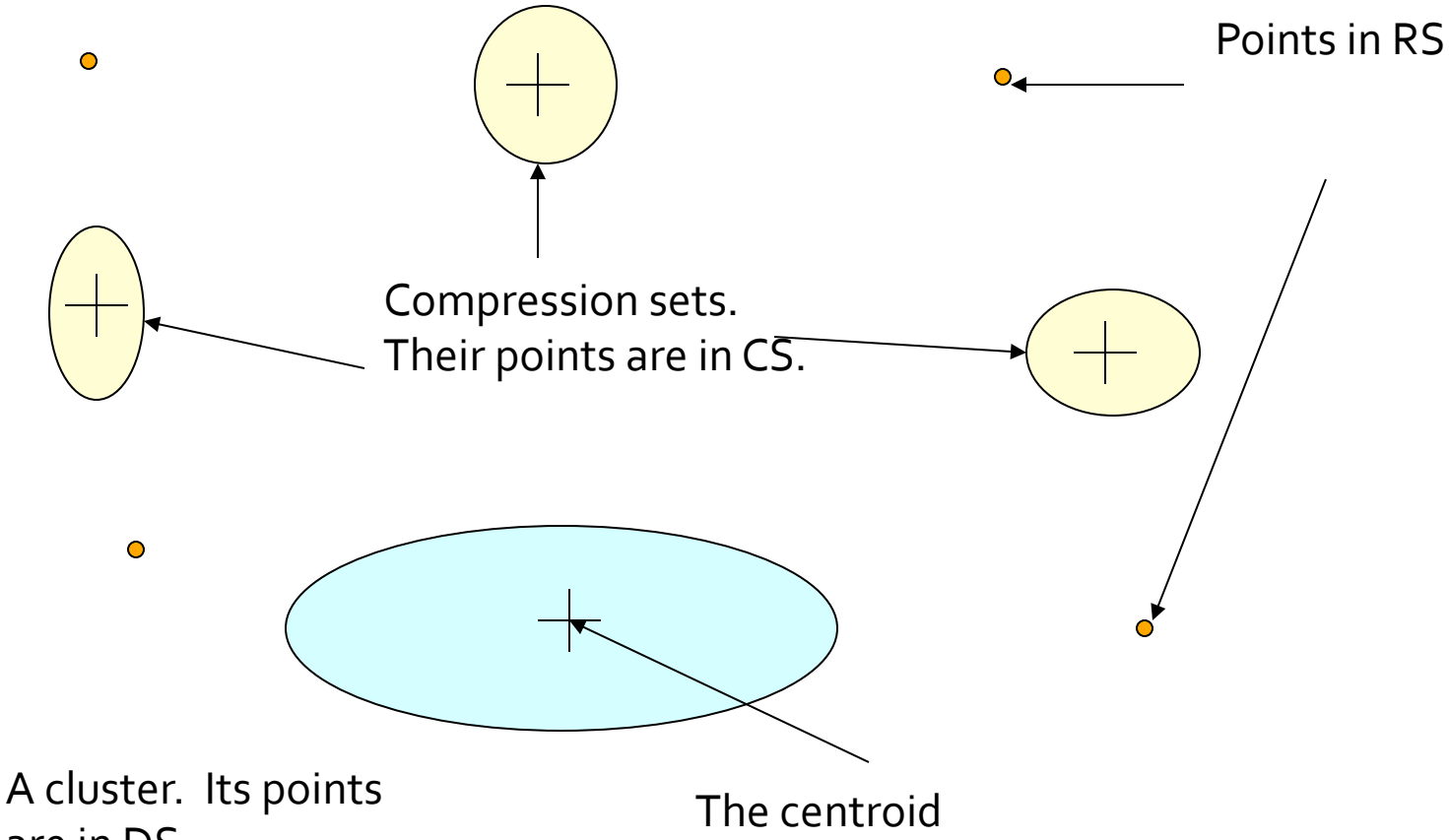
# BFR – (2)

- Points are read one main-memory-full at a time.
- Most points from previous memory loads are summarized by simple statistics.
  - Also kept in main memory, which limits how many points can be read in one “memory load.”
- To begin, from the initial load we select the initial *k* centroids by some sensible approach.

# Three Classes of Points

1. The *discard set* (*DS*): points close enough to a centroid to be summarized.
2. The *compression set* (*CS*): groups of points that are close together but not close to any centroid. They are summarized, but not assigned to a cluster.
3. The *retained set* (*RS*): isolated points.

# "Galaxies" Picture



# Summarizing Sets of Points

- Each cluster in the discard set and each compression set is summarized by:
  1. The number of points, *N*.
  2. The vector SUM, whose *i* th component is the sum of the coordinates of the points in the *i* th dimension.
  3. The vector SUMSQ: *i* th component = sum of squares of coordinates in *i* th dimension.

# Comments

- $2d + 1$ values represent any number of points.
  - $d$ = number of dimensions.
- Averages in each dimension (centroid coordinates) can be calculated easily as $SUM_i / N$.
  - $SUM_i$ = $i^{th}$ component of SUM.
- Variance in dimension $i$ can be computed by: $(SUMSQ_i / N) - (SUM_i / N)^2$
  - And the standard deviation is the square root of that.

# Processing a "Memory-Load" of Points

1. Find those points that are "sufficiently close" to a cluster centroid; add those points to that cluster and the DS.
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.

# Processing – (2)

3. Adjust statistics of the clusters to account for the new points.
   - Consider merging compressed sets in the CS.
4. If this is the last round, merge all compressed sets in the CS and all RS points into their nearest cluster.

# A Few Details . . .

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

# How Close is Close Enough?

- We need a way to decide whether to put a new point into a cluster.
- BFR suggest two ways:
  1. The *Mahalanobis distance* is less than a threshold.
  2. Low likelihood of the currently nearest centroid changing.

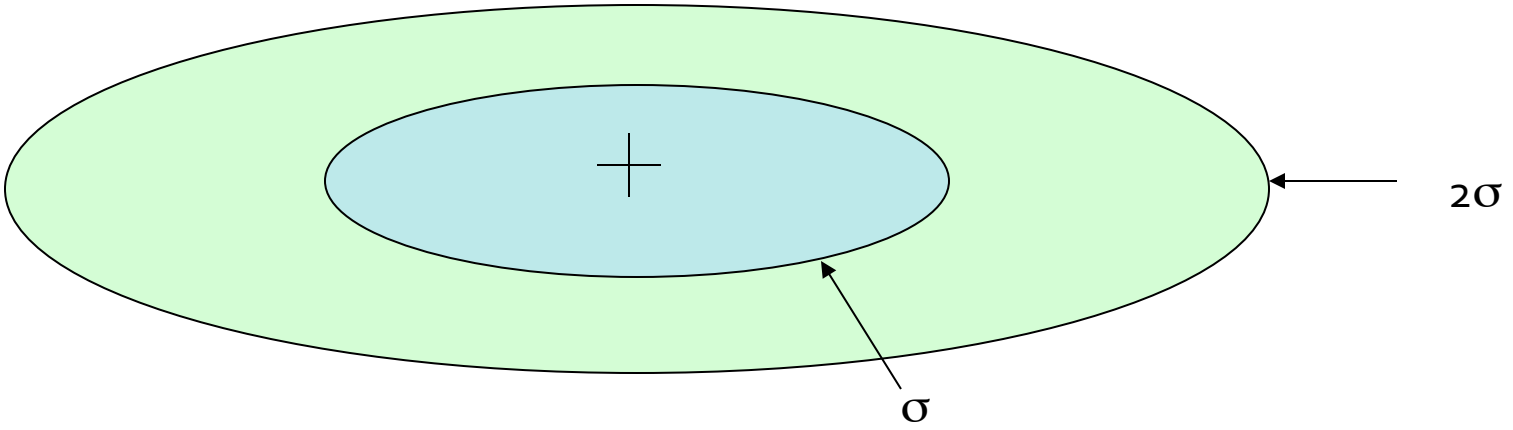
# Mahalanobis Distance

- Normalized Euclidean distance from centroid.
- For point $(x_1, \ldots, x_k)$ and centroid $(c_1, \ldots, c_k)$:
  1. Normalize in each dimension: $y_i = (x_i - c_i)/\sigma_i$
     - $\sigma_i$ = standard deviation in $i^{th}$ dimension for this cluster.
  2. Take sum of the squares of the $y_i$'s.
  3. Take the square root.

# Mahalanobis Distance – (2)

- If clusters are normally distributed in $d$ dimensions, then after transformation, one standard deviation = $\sqrt{d}$.
  - I.e., 70% 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. 4 standard deviations.

# Picture: Equal M.D. Regions



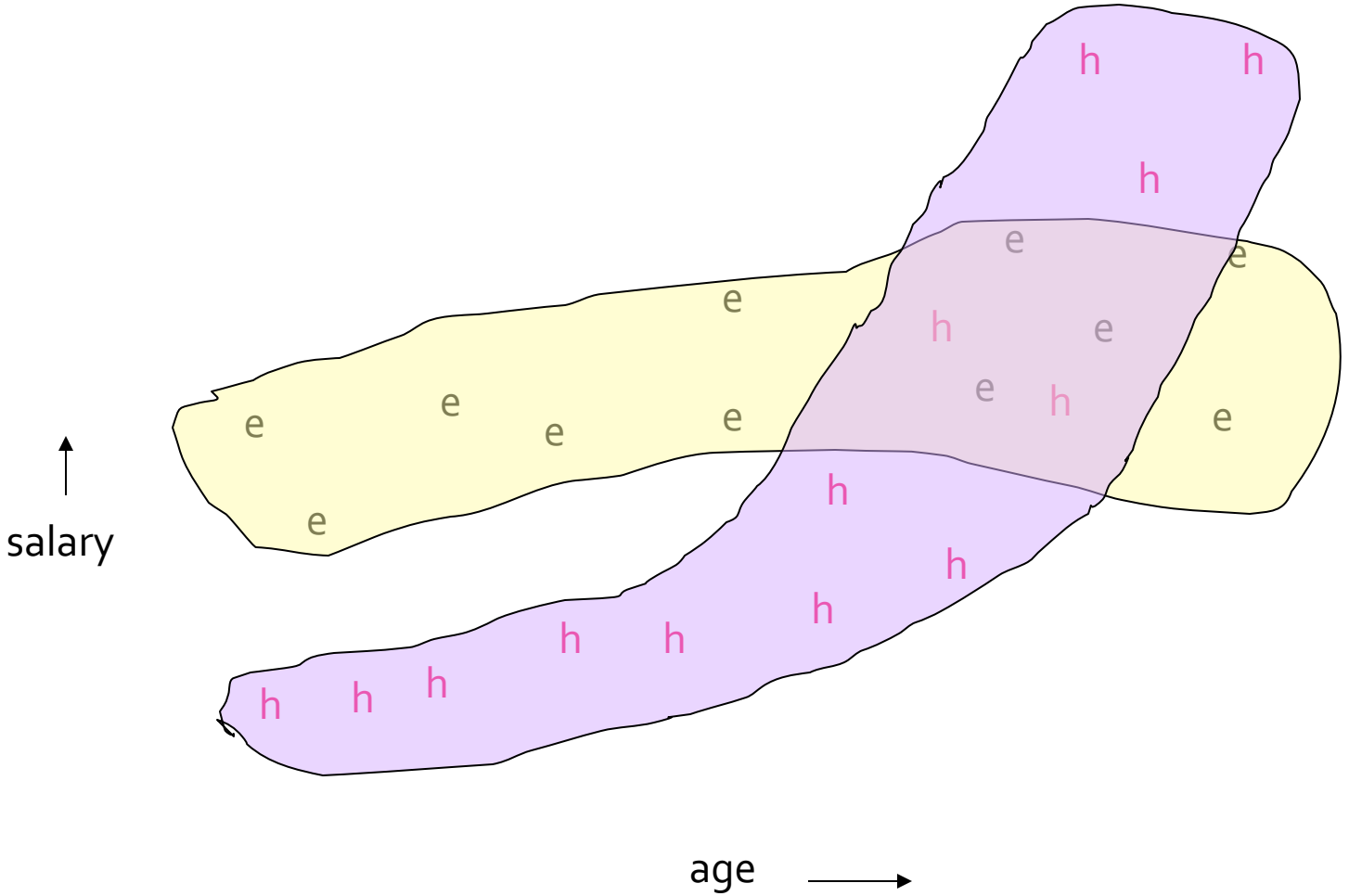
# Should Two CS Subclusters Be Combined?

- Similar to measuring cohesion. For example:
- Compute the variance of the combined subcluster, in each dimension.
  - *N*, SUM, and SUMSQ allow us to make that calculation quickly.
- Combine if the variance is below some threshold.
- Many alternatives: treat dimensions differently, consider density.

# 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.
- CURE:
  - Assumes a Euclidean distance.
  - Allows clusters to assume any shape.

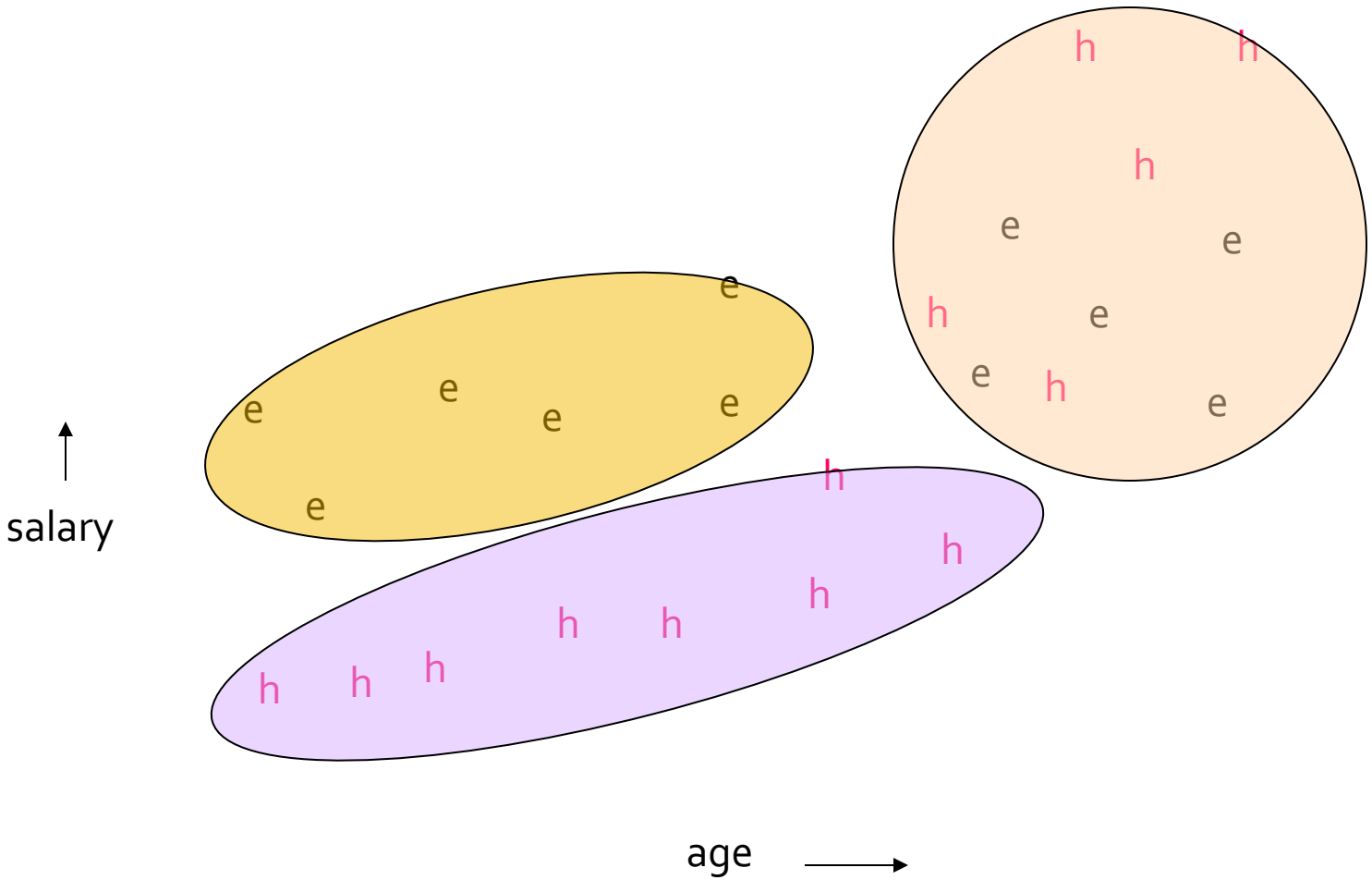
# Example: Stanford Faculty Salaries



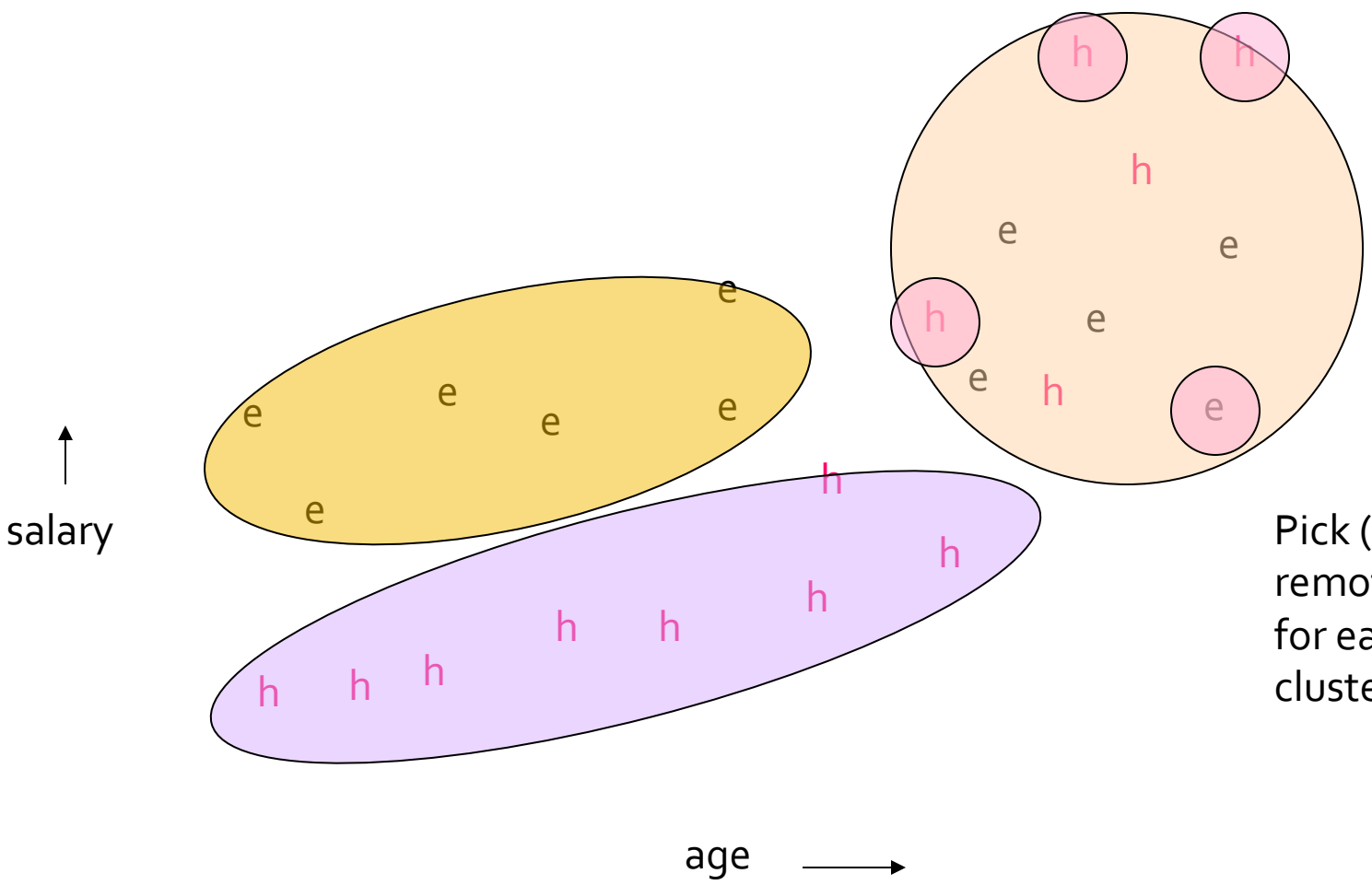
# Starting CURE

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

# Example: Initial Clusters

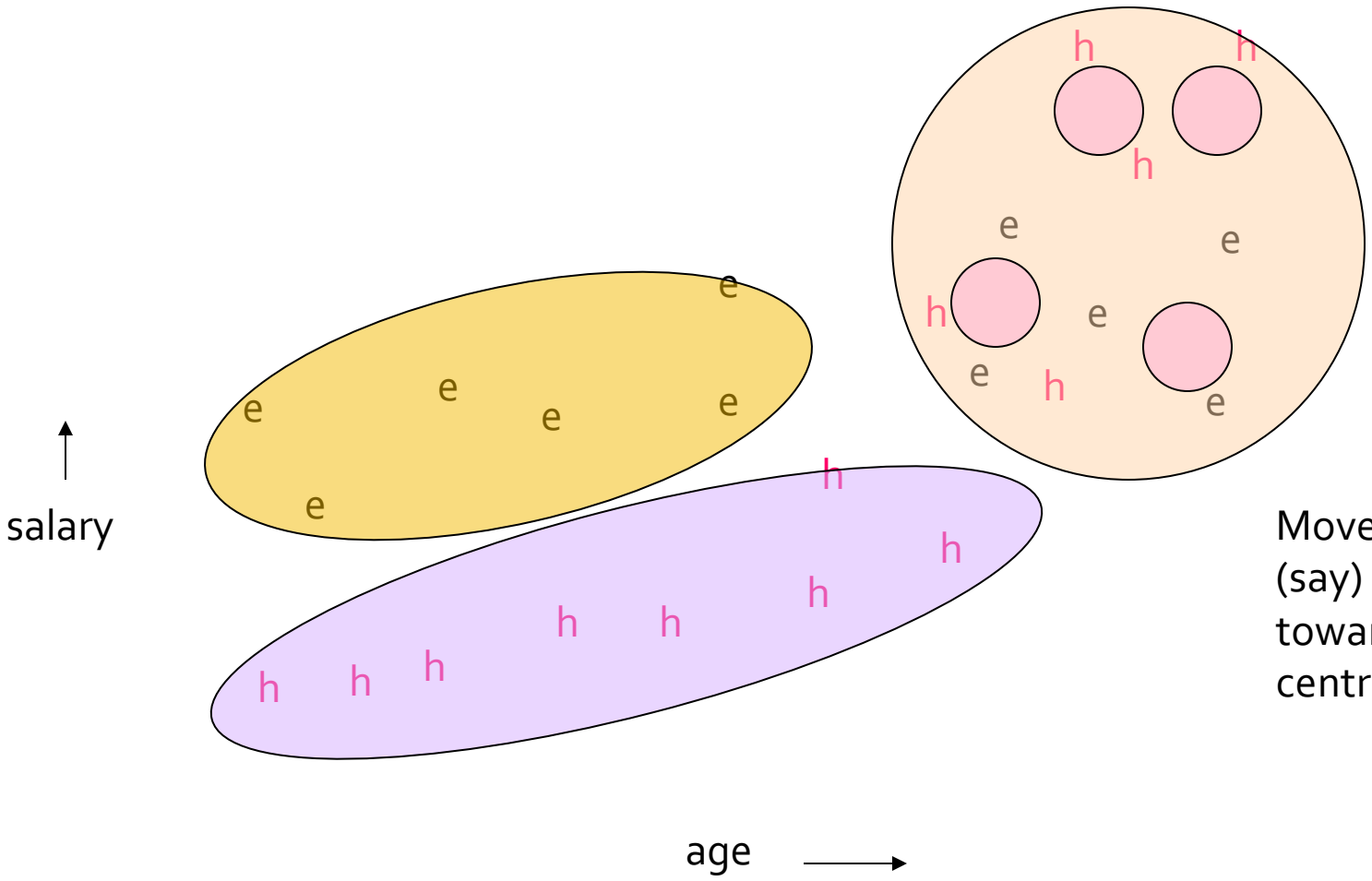


# Example: Pick Dispersed Points




Pick (say) 4 remote points for each cluster.

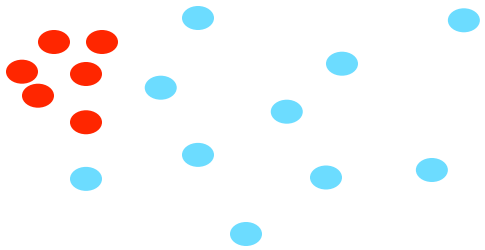
# Example: Pick Dispersed Points




Move points (say) 20% toward the centroid.

# Why the 20% Move Inward?

- 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.



# Finishing CURE

- Now, visit each point *p* in the data set.
- Place it in the "closest cluster."
  - Normal definition of "closest": that cluster with the closest (to *p*) among all the sample points of all the clusters.