Lecture 10: Clustering

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https://shuaili8.github.io

https://shuaili8.github.io/Teaching/VE445/index.html

Outline

- Unsupervised learning
- Clustering
- K-means
  - Algorithm
  - How to choose K
  - Initialization
  - Properties
- Agglomerative clustering
- BFR algorithm
- CURE algorithm

Unsupervised Learning

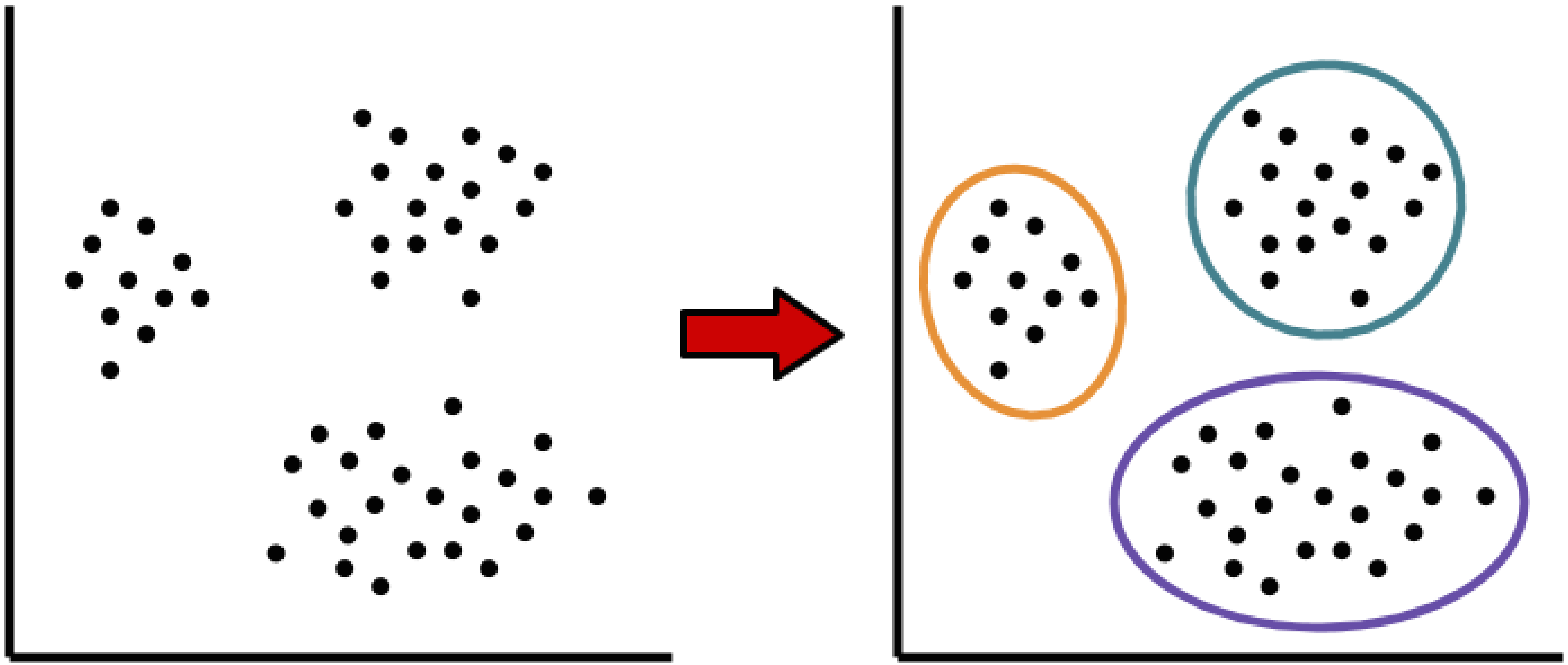
Machine learning categories

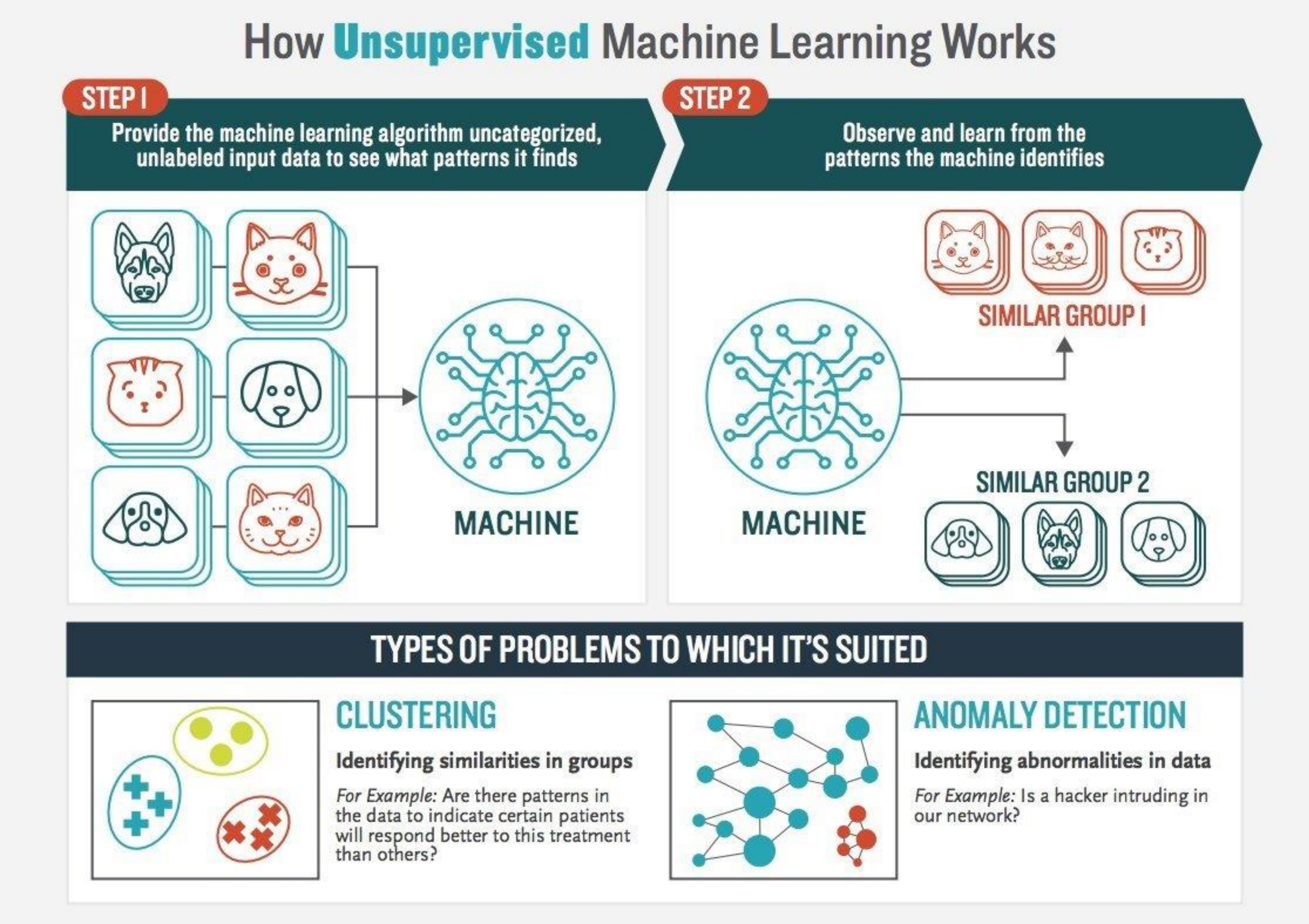
- Unsupervised learning
  - No labeled data
- Supervised learning
  - Use labeled data to predict on unseen points
- Semi-supervised learning
  - Use labeled data and unlabeled data to predict on unlabeled/unseen points
- Reinforcement learning
  - Sequential prediction and receiving feedbacks

Course outline

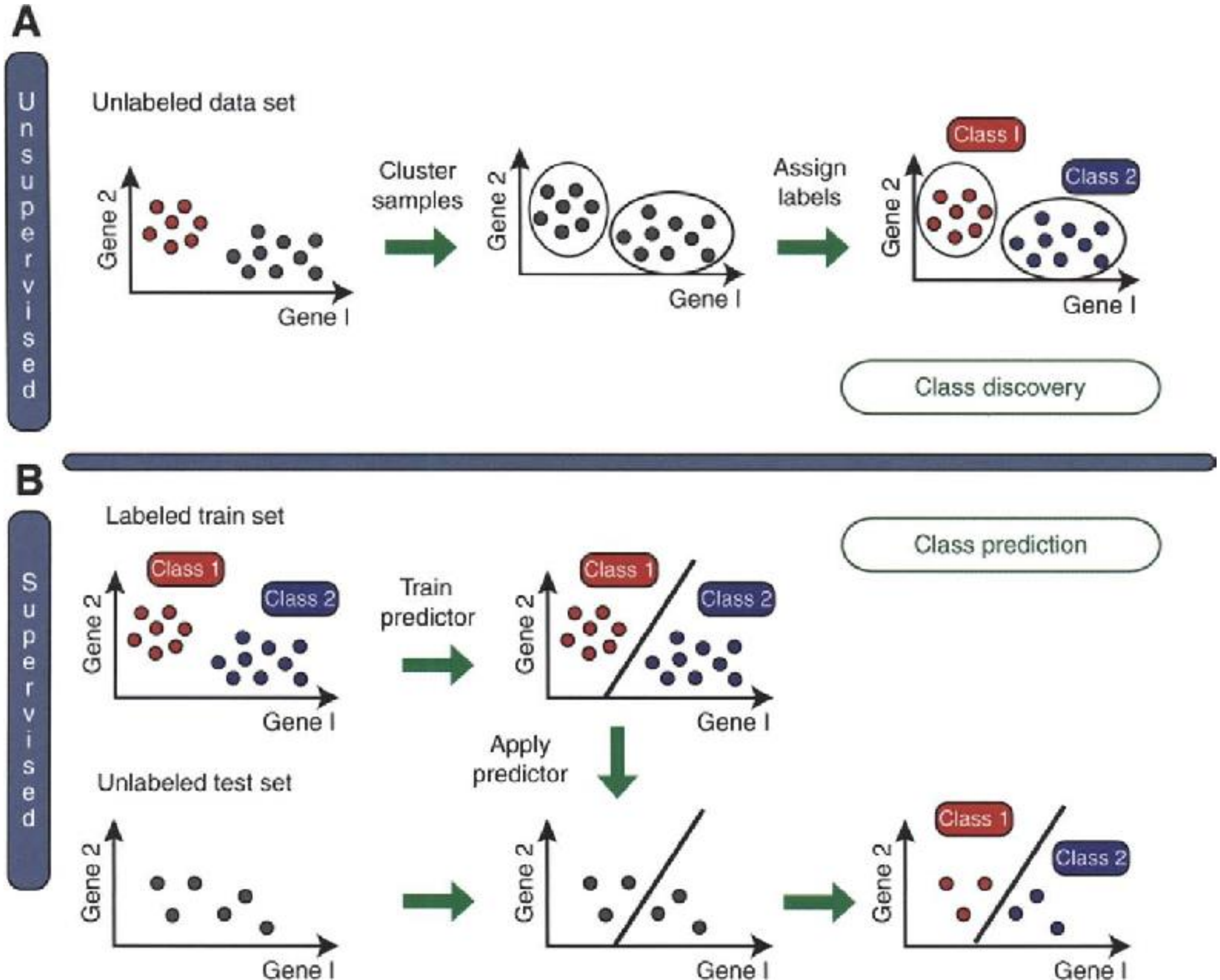
- Basics
- Supervised learning
  - Linear Regression
  - Logistic regression
  - SVM and Kernel methods
  - Decision Tree
- Deep learning
  - Neural Networks
  - Backpropagation
  - Convolutional Neural Network
  - Recurrent Neural Network
- Unsupervised learning
  - K-means, PCA, EM, GMM
- Reinforcement learning
  - Multi-armed bandits
  - MDP
  - Bellman equations
  - Q-learning
- Learning theory
  - PAC, VC-dimension, bias-variance decomposition

Unsupervised learning example




How Unsupervised Machine Learning Works
STEP 1
Provide the machine learning algorithm uncategorized, unlabeled input data to see what patterns it finds
STEP 2
Observe and learn from the patterns the machine identifies
MACHINE
SIMILAR GROUP 1
MACHINE
SIMILAR GROUP 2
TYPES OF PROBLEMS TO WHICH IT'S SUITED
CLUSTERING
Identifying similarities in groups
For Example: Are there patterns in the data to indicate certain patients will respond better to this treatment than others?
ANOMALY DETECTION
Identifying abnormalities in data
For Example: Is a hacker intruding in our network?

Supervised Learning	Unsupervised Learning
Input data is labelled	Input data is unlabeled
Uses training dataset	Uses just input dataset
Used for prediction	Used for analysis
Classification and regression	Clustering, density estimation and dimensionality reduction


A
Unsupervised
Unlabeled data set
Gene 2
Gene I
Cluster samples
Assign labels
Class I
Class 2
Class discovery
B
Supervised
Labeled train set
Class 1
Class 2
Train predictor
Class prediction
Apply predictor
Unlabeled test set

Clustering

Clustering

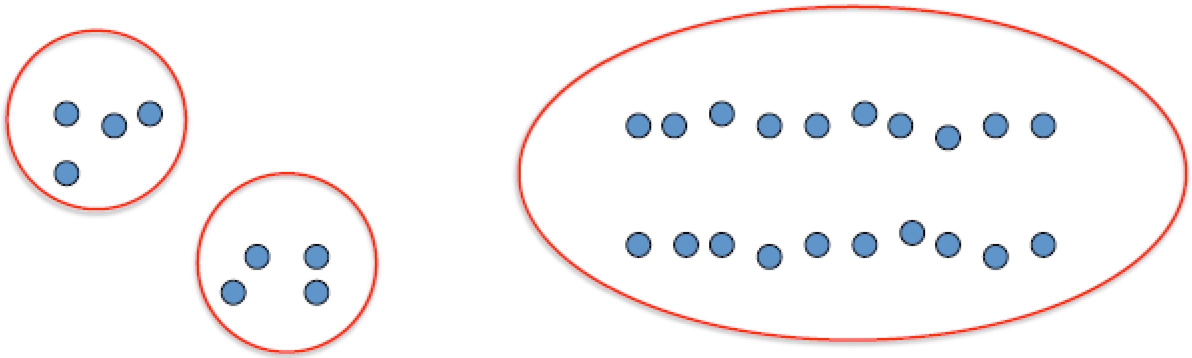
- Unsupervised learning
- Requires data, but no labels
- Detect patterns e.g. in
  - Group emails or search results
  - Customer shopping patterns
  - Regions of images
- Useful when don’t know what you’re looking for
- But: can get gibberish

Clustering (cont.)

- Goal: Automatically segment data into groups of similar points
- Question: When and why would we want to do this?
- Useful for:
  - Automatically organizing data
  - Understanding hidden structure in some data
  - Representing high-dimensional data in a low-dimensional space
- Examples: Cluster
  - customers according to purchase histories
  - genes according to expression profile
  - search results according to topic
  - Facebook users according to interests
  - a museum catalog according to image similarity

Intuition

- Basic idea: group together similar instances
- Example: 2D point patterns



Intuition (cont.)

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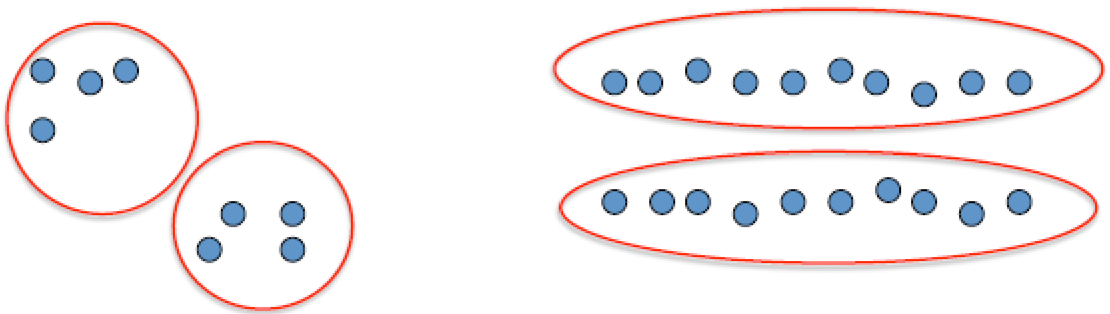
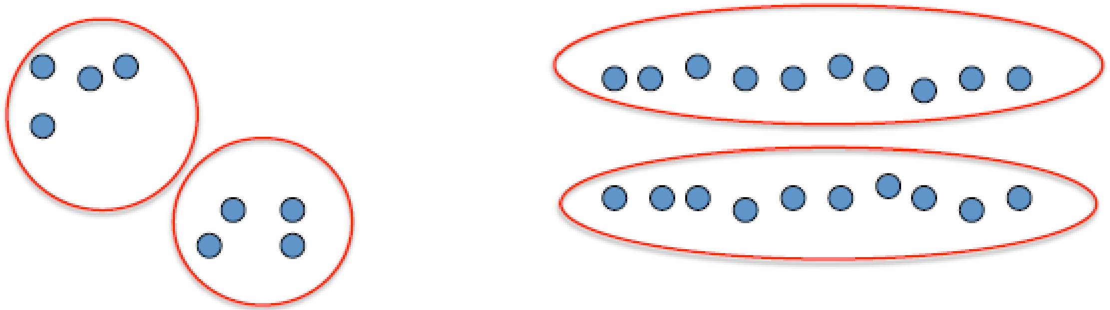


Intuition (cont.)

- Basic idea: group together similar instances
- Example: 2D point patterns



- What could "similar" mean?
- – One option: small Euclidean distance (squared)
- – Clustering results are crucially dependent on the measure of similarity (or distance) between "points" to be clustered

Set-up

- Given the data: $\mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$

- Each data point x is p-dimensional:

$$\mathbf{x}_n = \langle x_{n,1}, \ldots, x_{n,p} \rangle.$$

- Define a distance function between data:

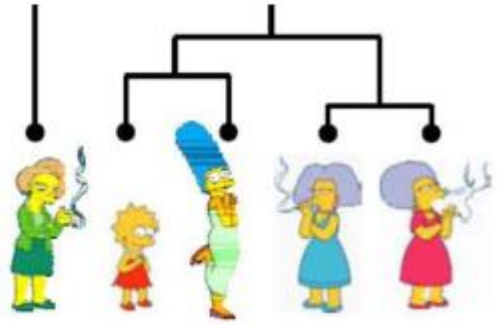
$$d(\mathbf{x}_n, \mathbf{x}_m).$$

- Goal: segment the data into K groups

Clustering algorithms

- Partition algorithms (flat clustering)
    - K-means
    - Mixture of Gaussian
    - Spectral Clustering

- Hierarchical algorithms
    - Bottom up-agglomerative
    - Top down-divisive

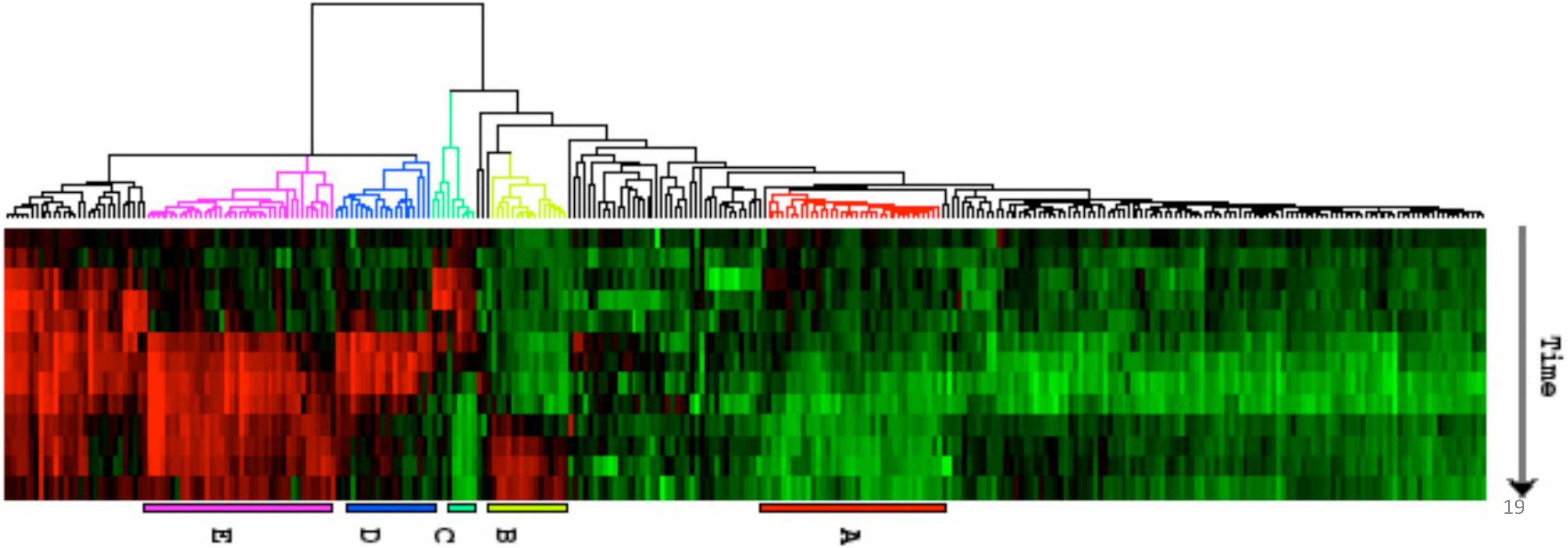


Example

- Image segmentation
- Goal: Break up the image into meaningful or perceptually similar regions

Example 2

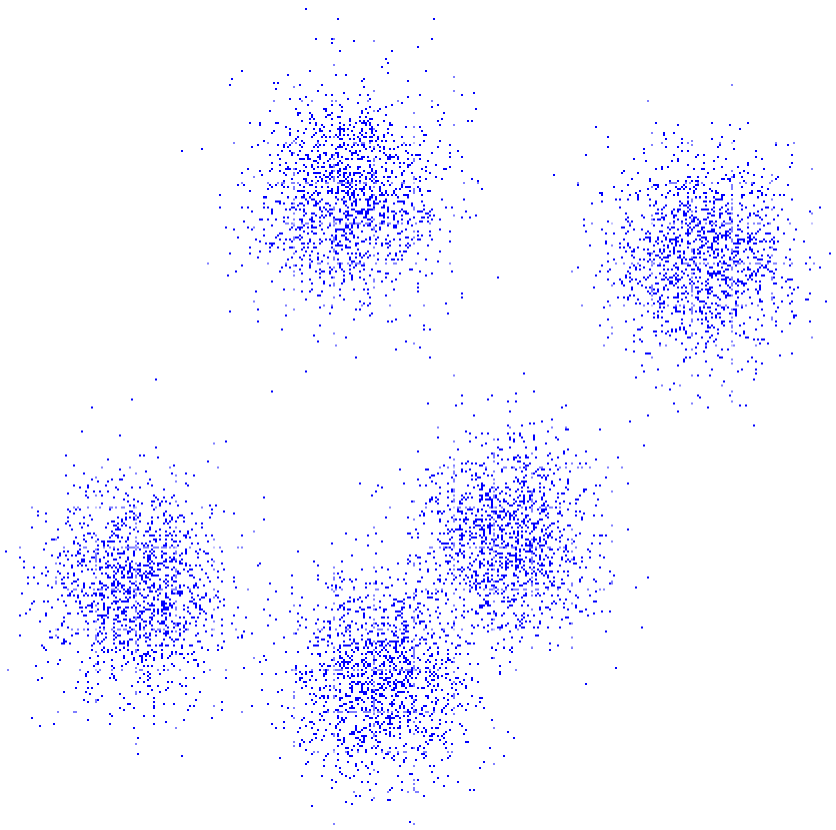
- Gene expression data clustering
  - Activity level of genes across time



K-Means

K-Means

- An iterative clustering algorithm
- Initialize: Pick K random points as cluster centers
- Alternate:
  - Assign data points to closest cluster center
  - Change the cluster center to the average of its assigned points
- Stop: when no points' assignments change



K-Means (cont.)

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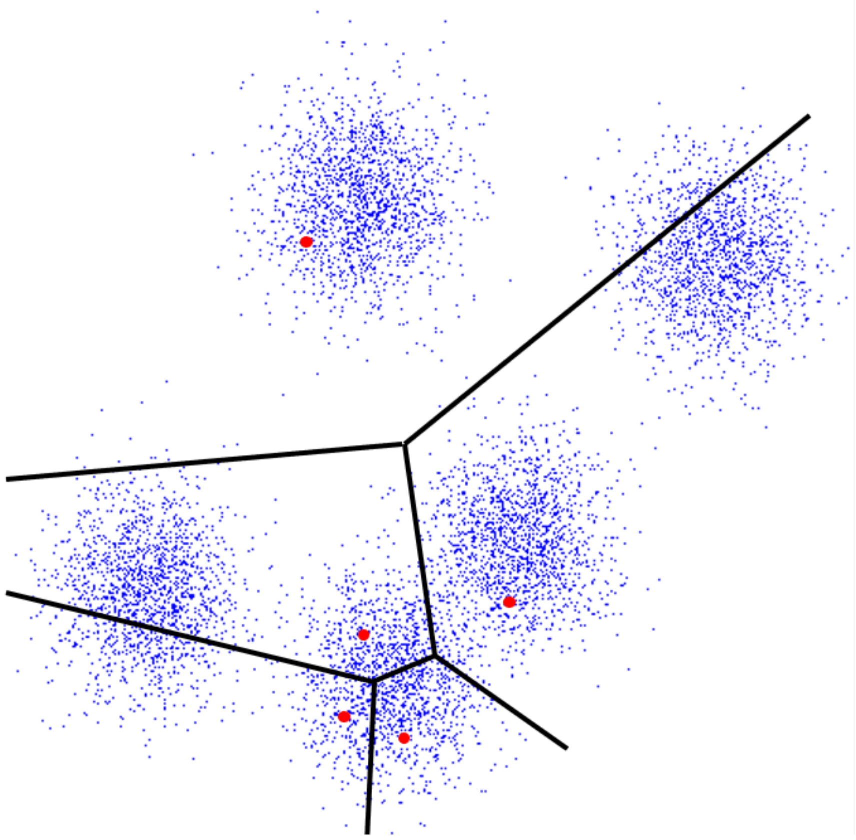

K-Means (cont.)

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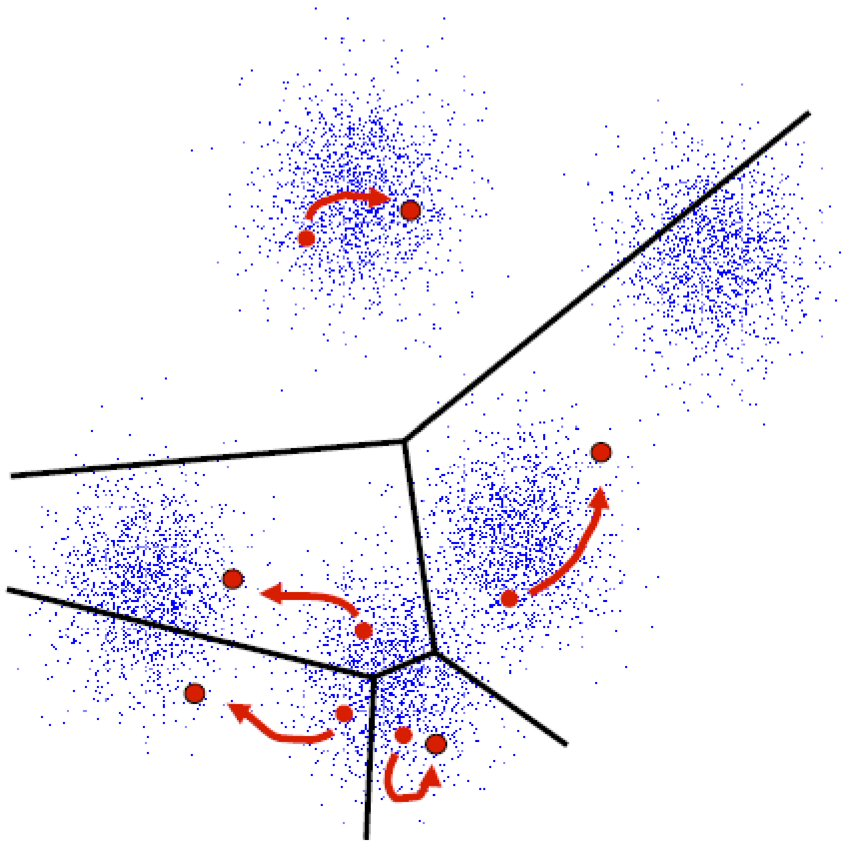
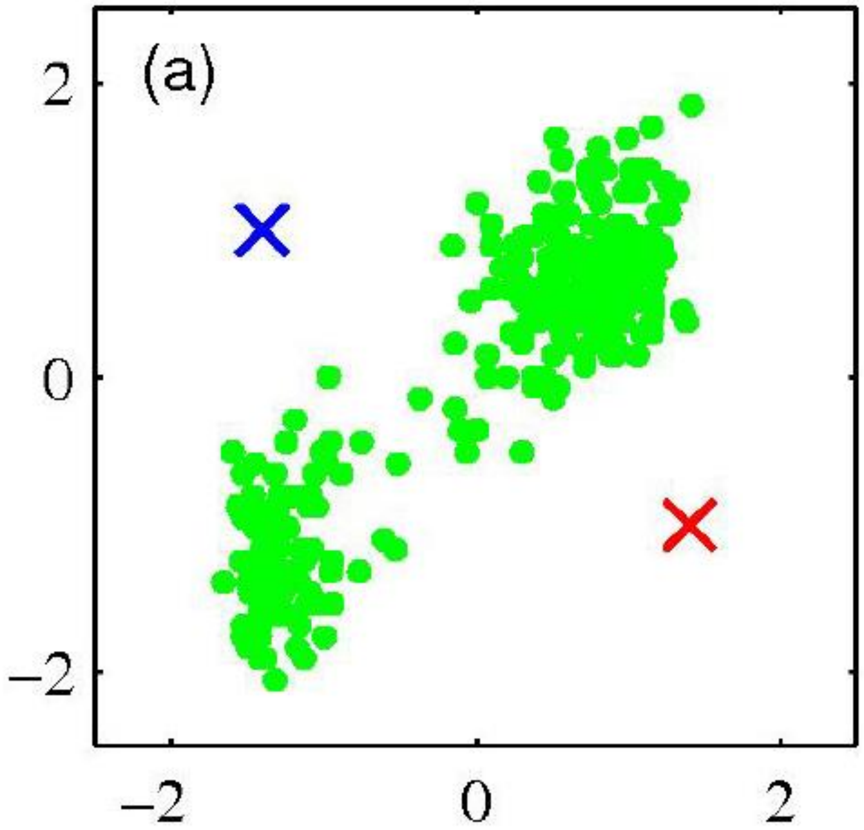


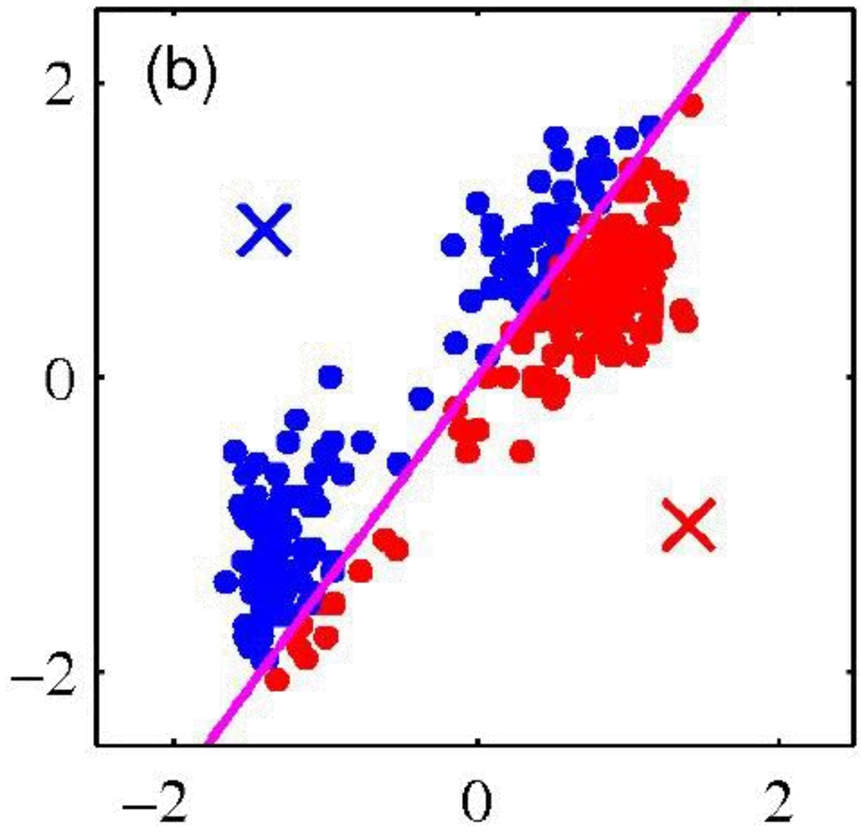
Example

- Pick K random points as cluster centers (means)
- Shown here for $K = 2$



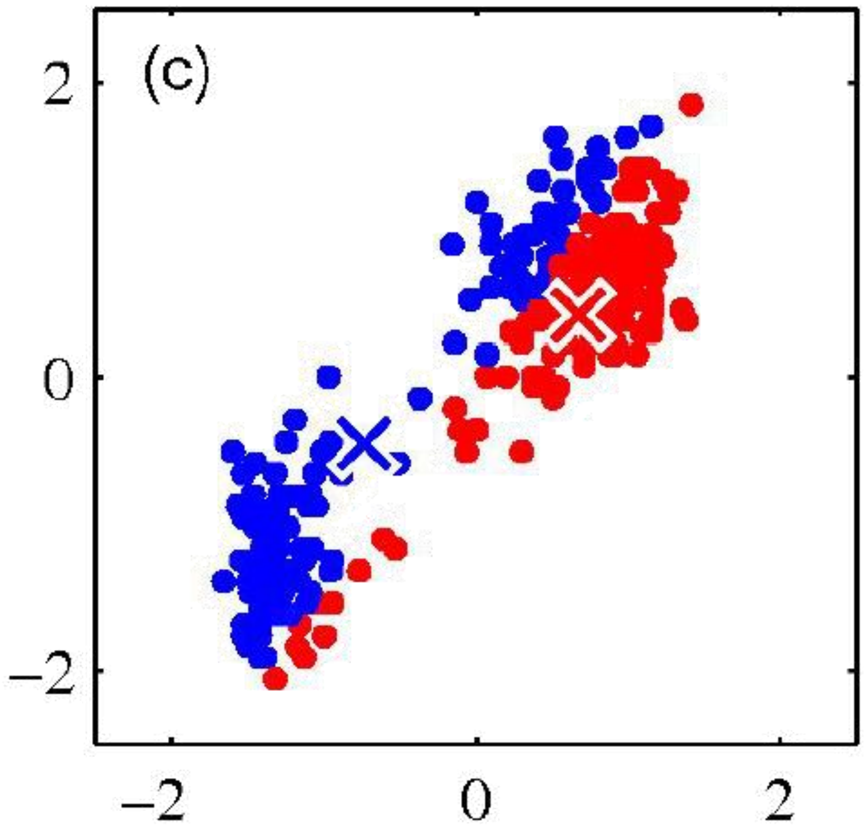
Example (cont.)

- Iterative step 1
- Assign data points to closest cluster center



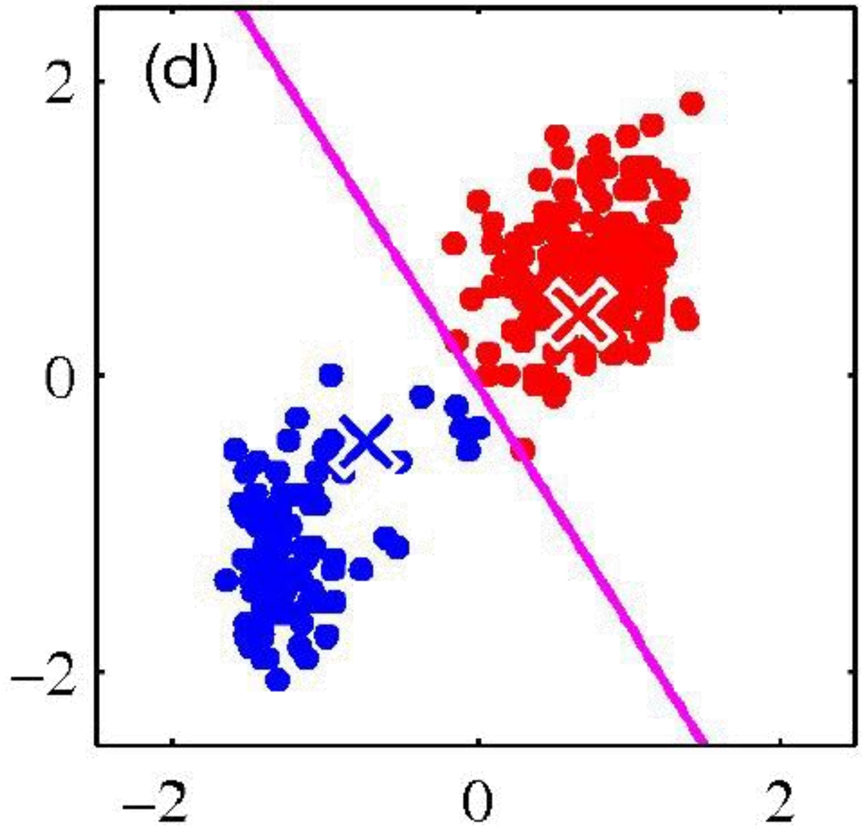
Example (cont.)

- Iterative step 2
- Change the cluster center to the average of the assigned points



Example (cont.)

- Repeat until convergence
- Convergence means that the differences of the center positions in two continuous loops is smaller than a threshold



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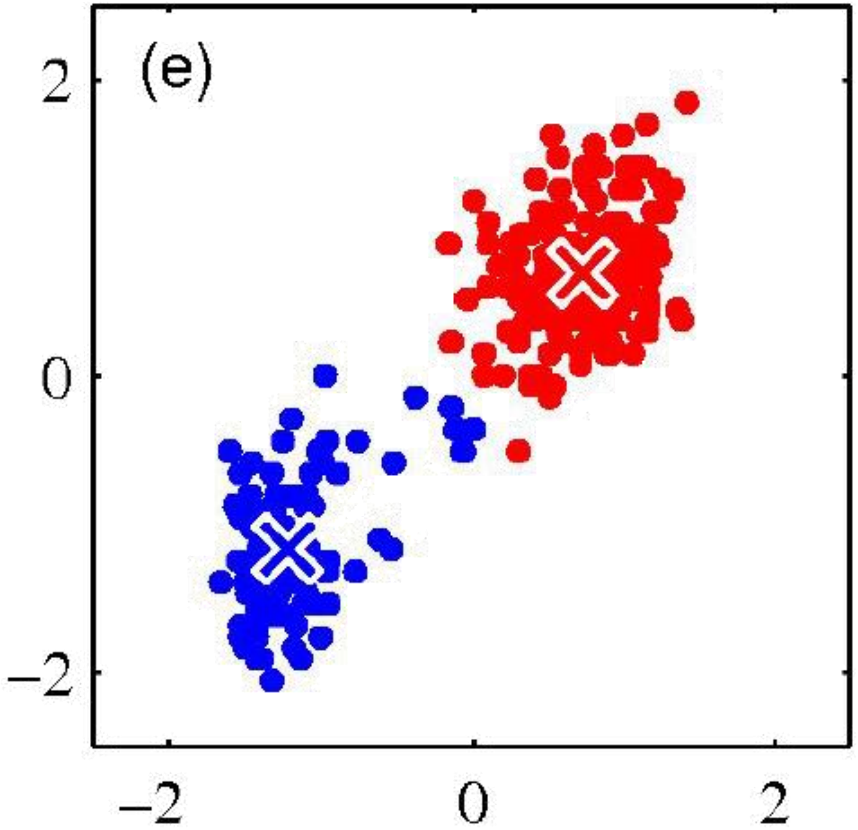

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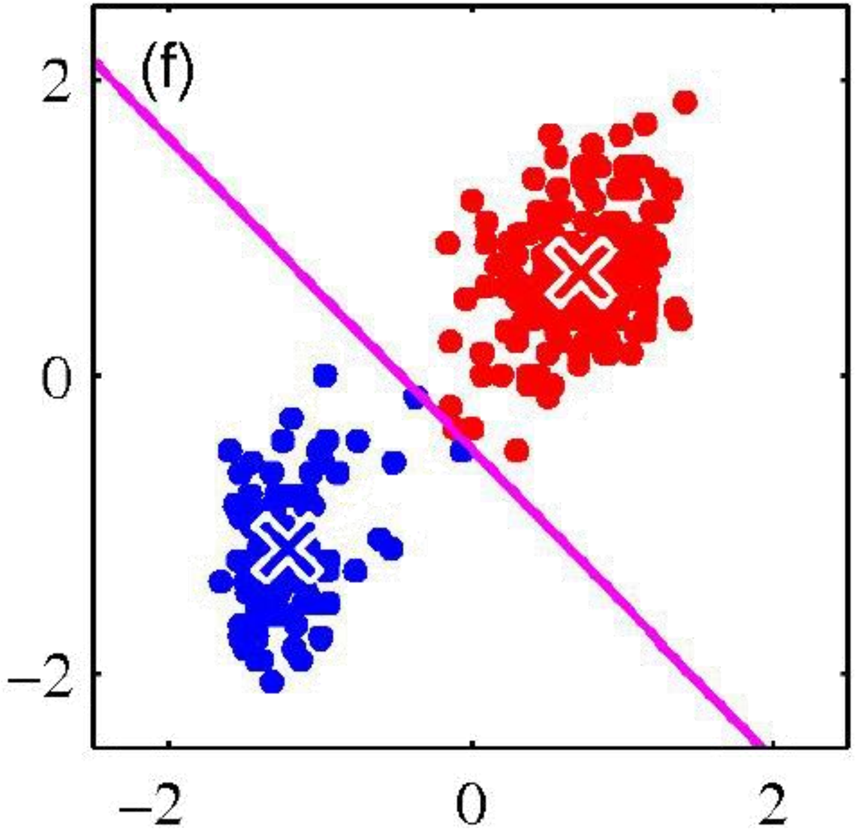
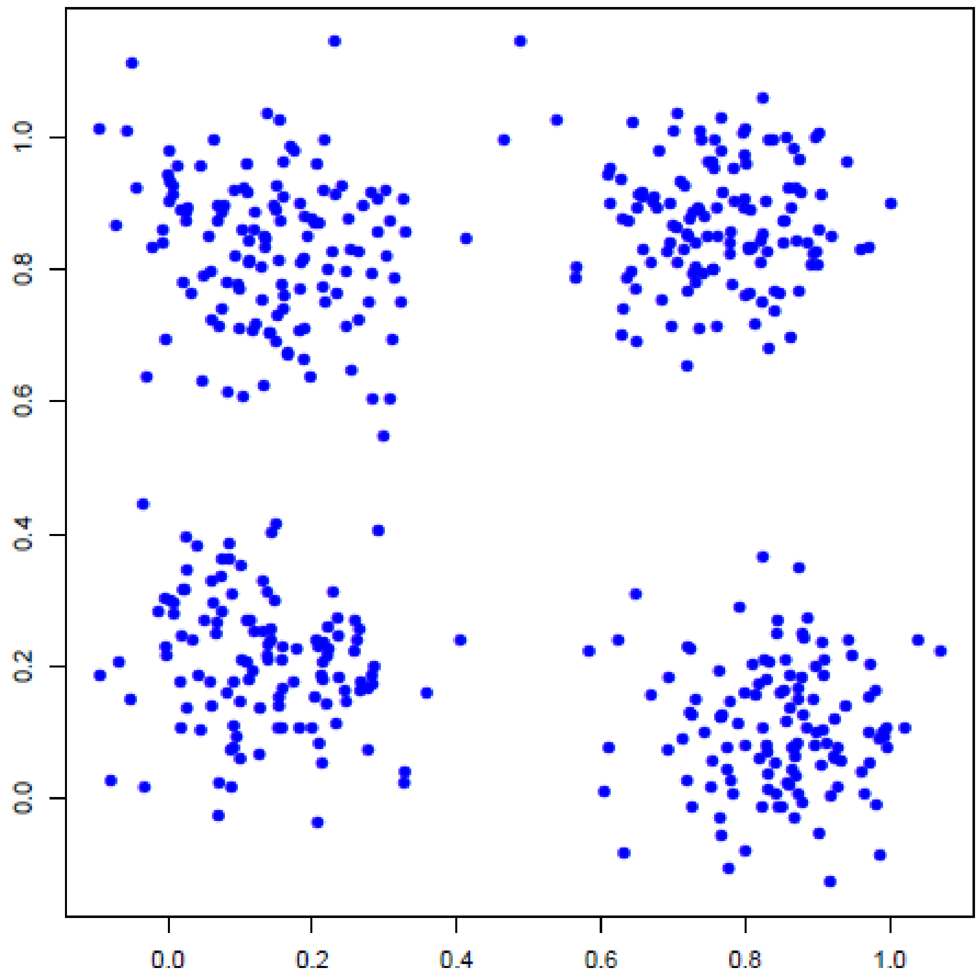


Example 2

- $K = 4$



Example 2 (cont.)

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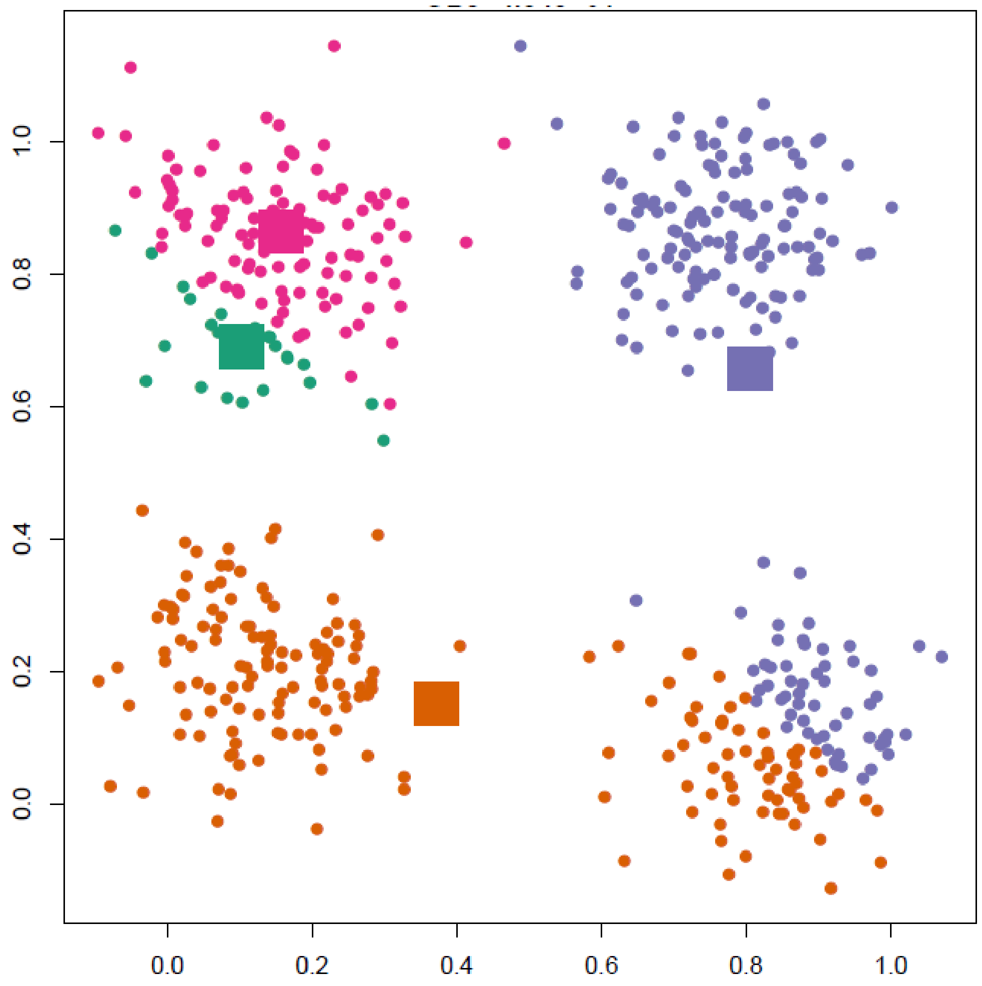

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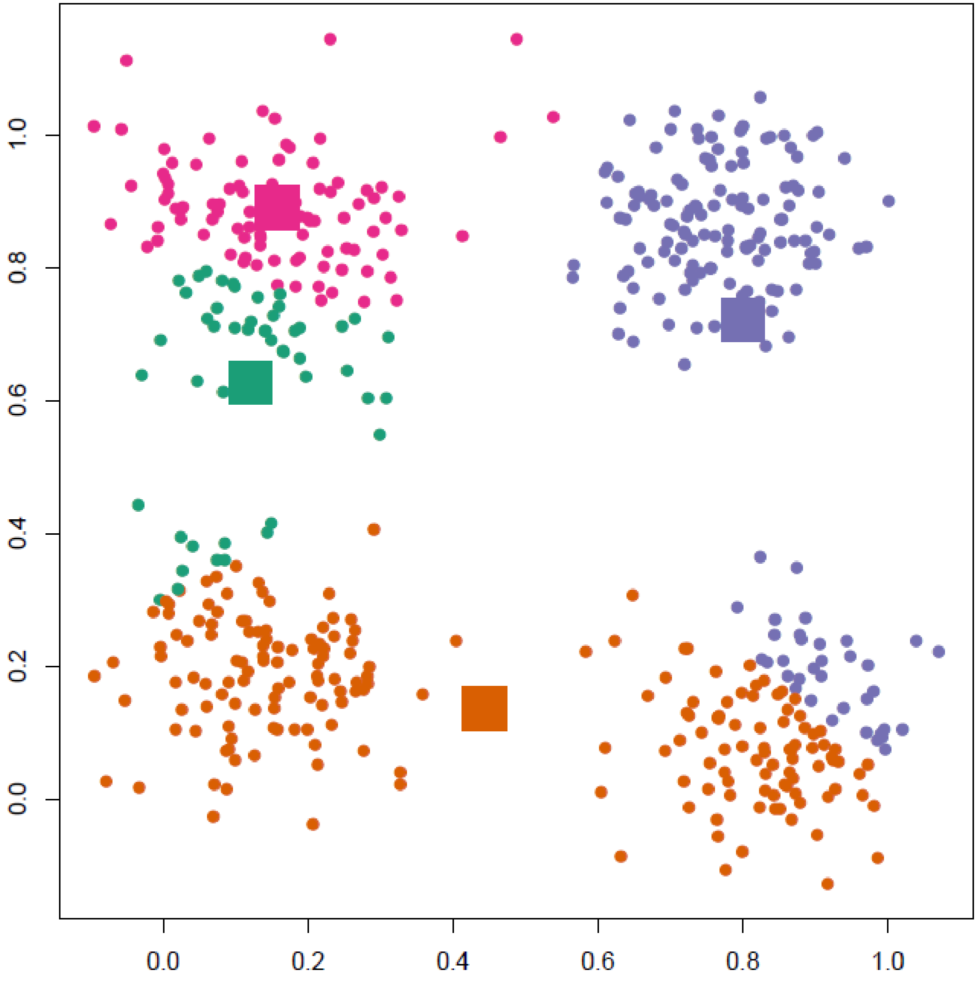

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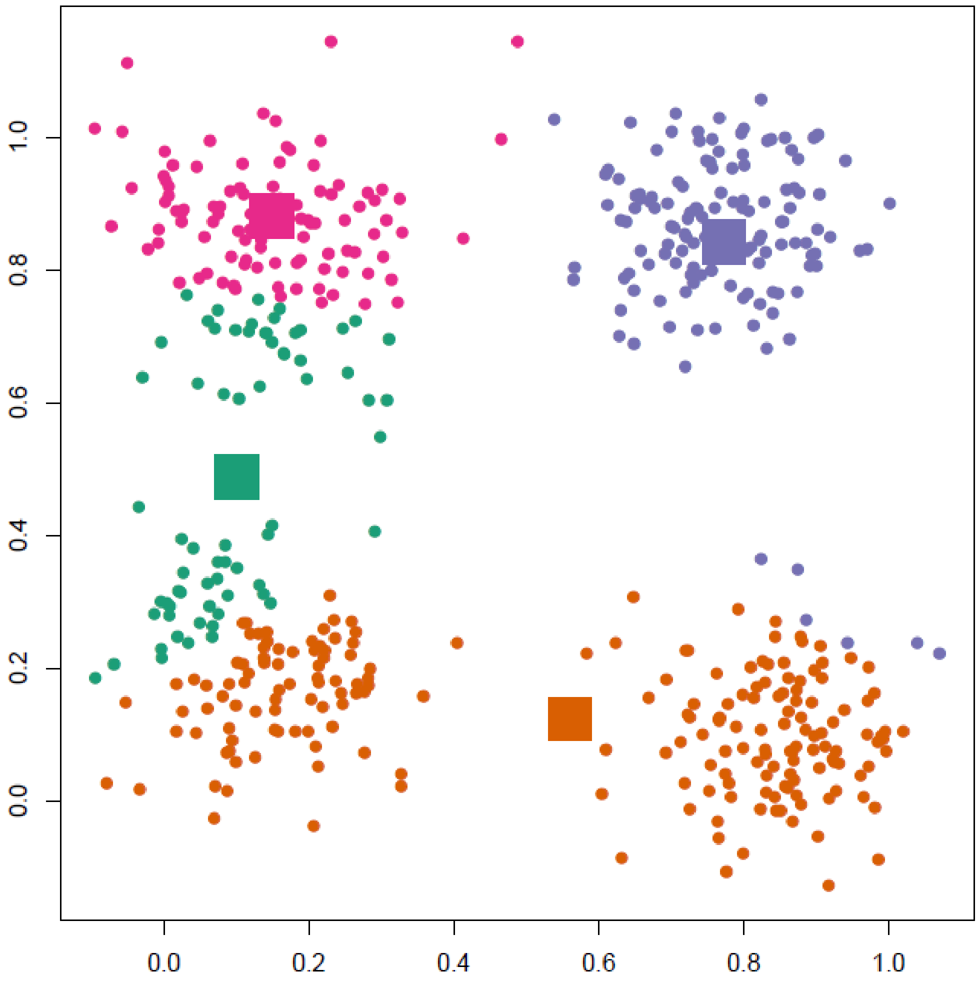

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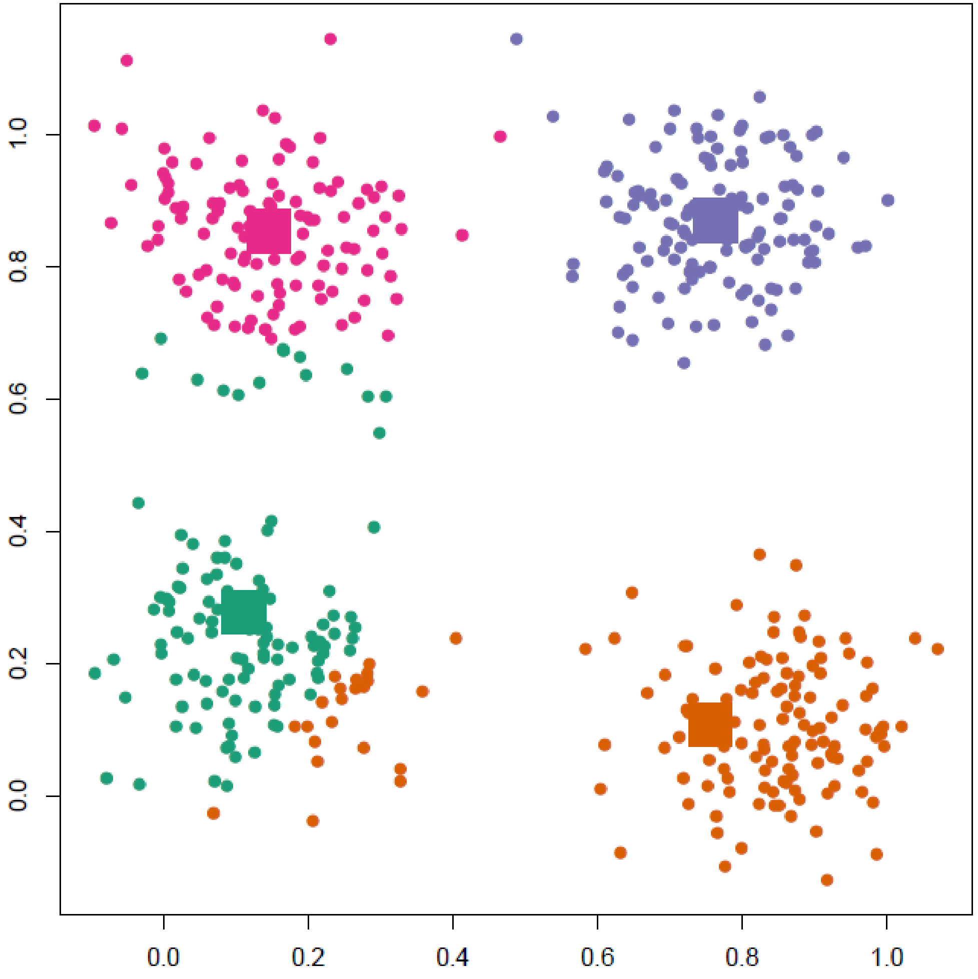

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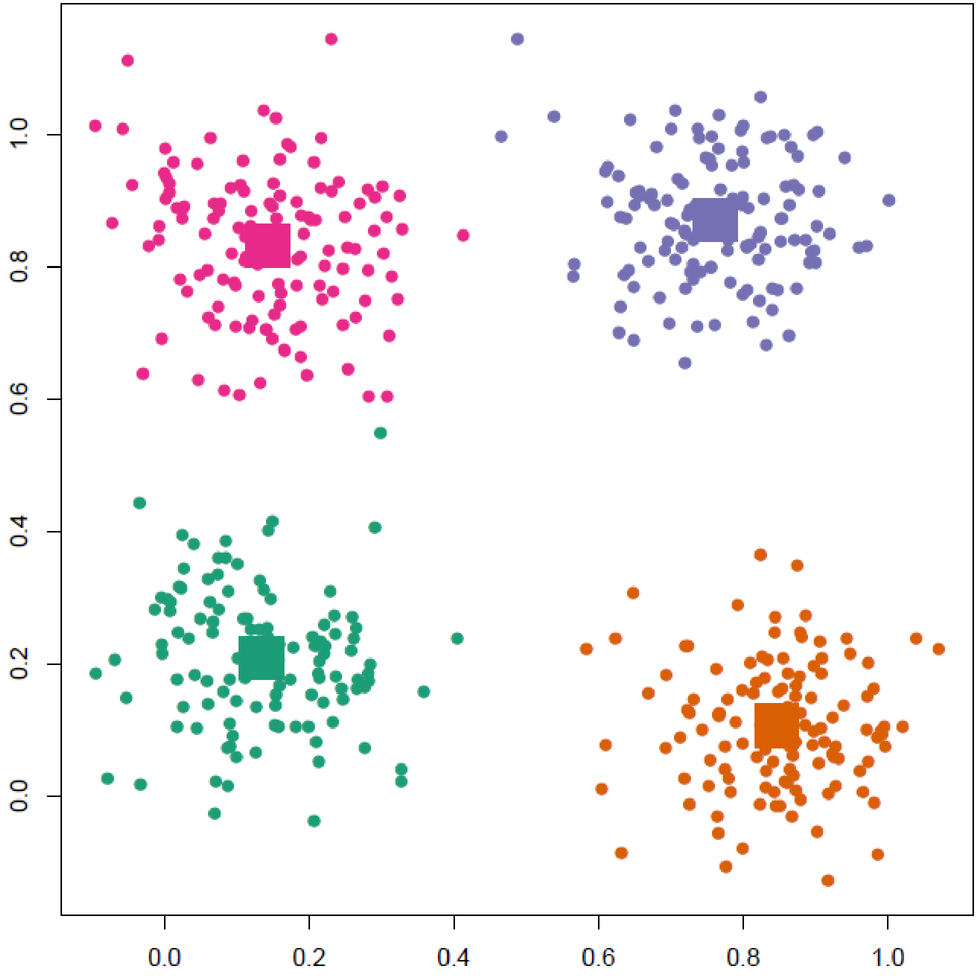


Remained Questions in K-Means

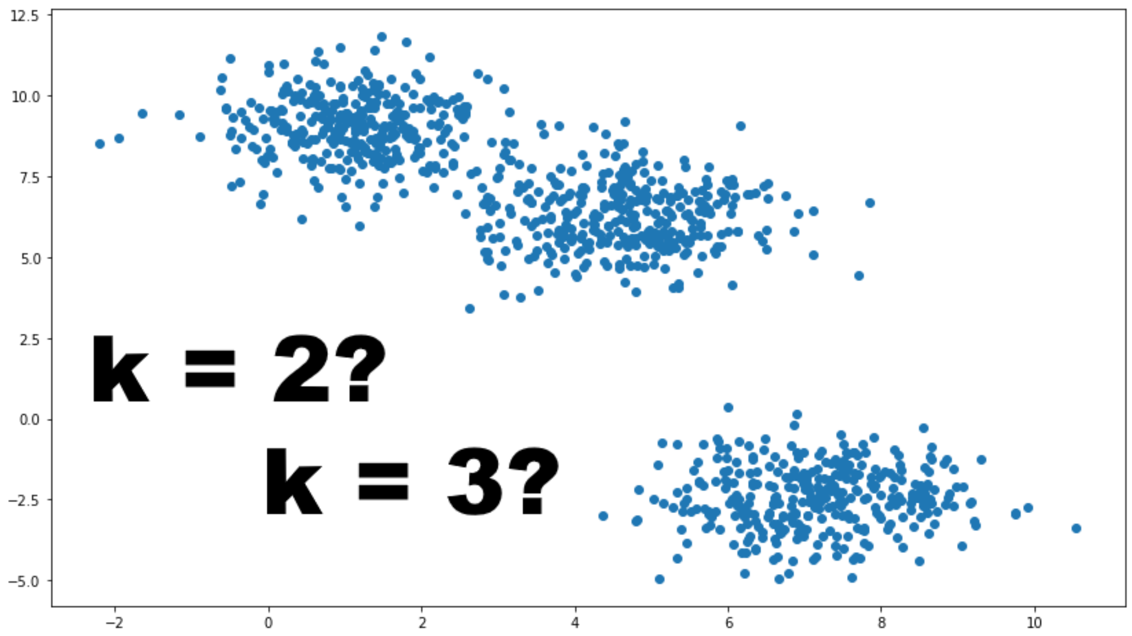
Remained questions in K-means

- Although the workflow of K-means is straight forward, there are some important questions that need to be discussed

- How to choose the hyper-parameter K?
- How to initialize?

How to choose K?

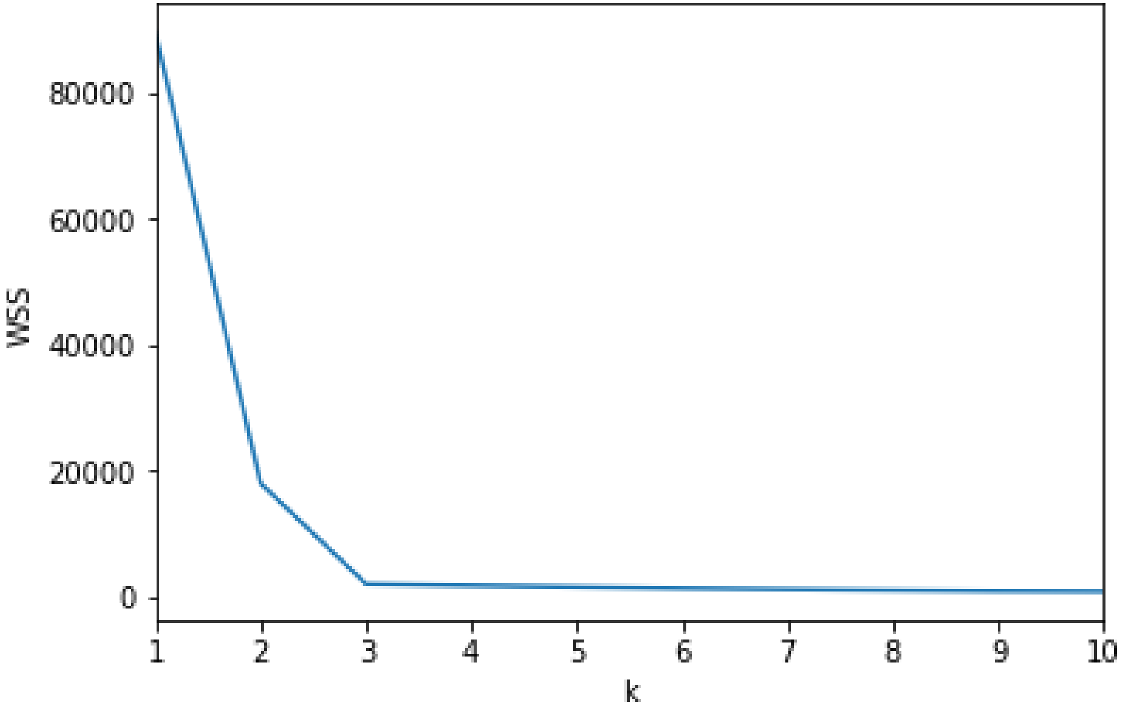
- K is the most important hyper-parameter in K-means which strongly affects its performance. In some situation, it’s not an easy task to find the proper K
- The solution includes:
  - The elbow method
  - The silhouette method



The elbow method

- Calculate the Within-Cluster-Sum of Squared Errors (WSS) for different values of K, and choose the K ***for which WSS stops dropping significantly***. In the plot of WSS-versus-k, this is visible as an elbow

- Example: $K = 3$



The silhouette method

- The problem of the elbow method is that in many situations the most suitable K cannot be unambiguously identified. So we need the silhouette method

- The silhouette value measures how similar a point is to its own cluster (cohesion) compared to other clusters (separation). The range of the silhouette value is between +1 and -1. A high value is desirable and indicates that the point is placed in the correct cluster

The silhouette method (cont.)

- For each data point $i \in C_k$, let $a(i)$ be its mean distance to all other points in the same cluster

$$a(i) = \frac{1}{|C_k| - 1} \sum_{j \in C_k, i \neq j} d(i, j)$$

- And let $b(i)$ be the smallest mean distance to other clusters

$$b(i) = \min_{l \neq k} \frac{1}{|C_l|} \sum_{j \in C_l} d(i, j)$$

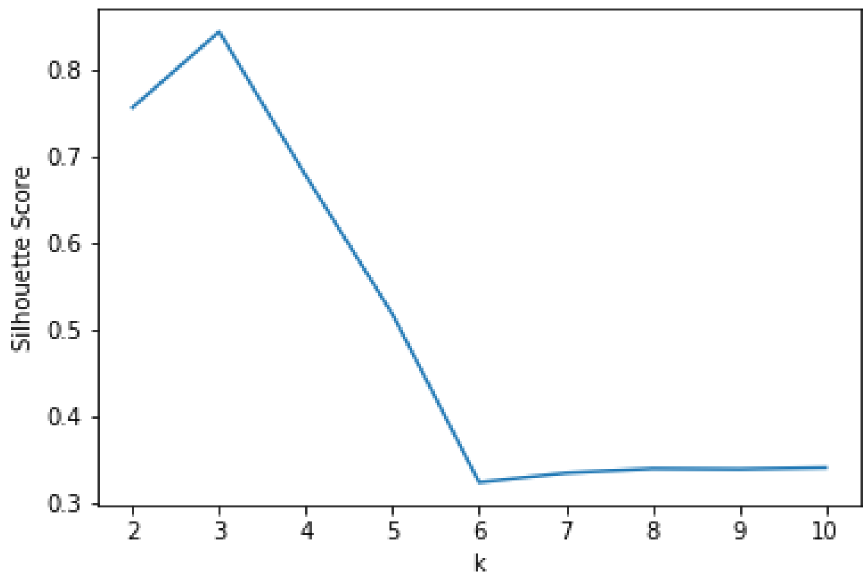
The silhouette method (cont.)

- The silhouette value of $i \in C_k$ is defined as:

$$s(i) = \begin{cases} \dfrac{b(i) - a(i)}{\max\{a(i), b(i)\}}, & if\ |C_k| > 1 \\ 0, & if\ |C_k| = 1 \end{cases}$$

- The silhouette score is the average of $s(i)$ among all data

- Choose the k with the maximal silhouette score



How to initialize center positions?

- The positions of the centers in the stage of initialization are also very important in K-means algorithms. In some situations it can produce totally different clustering results
- Example:

How to initialize center positions? (cont.)

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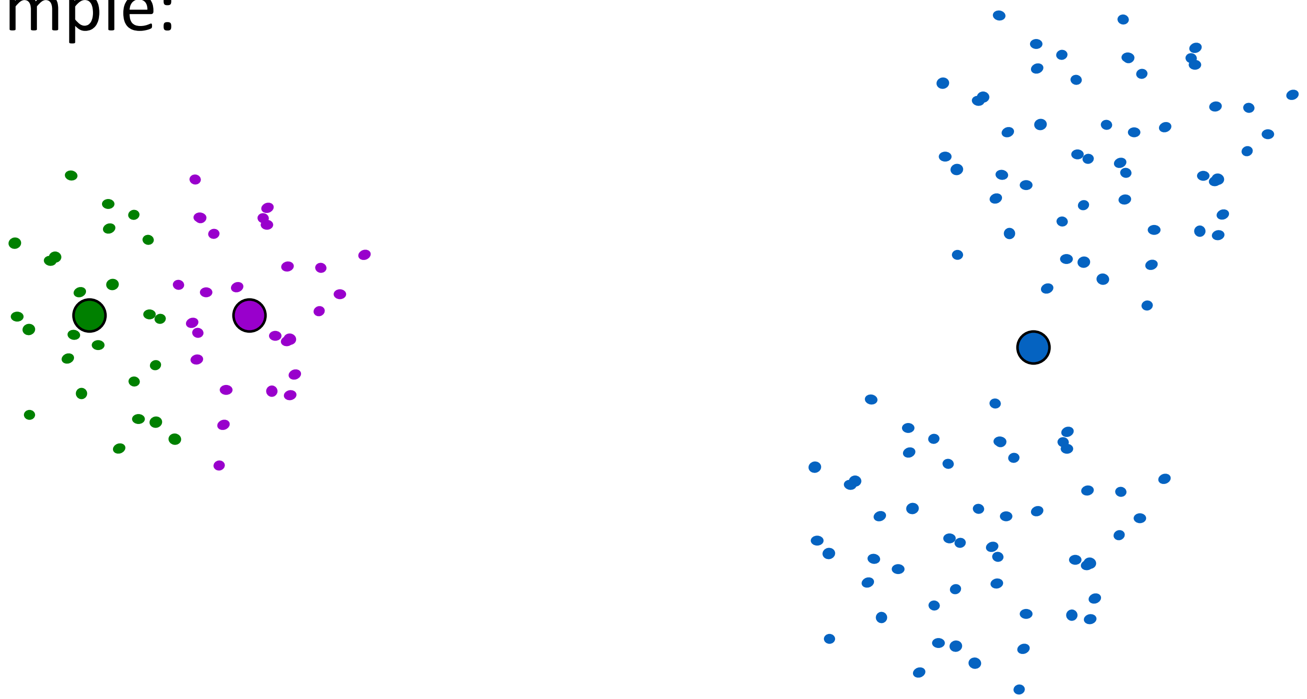
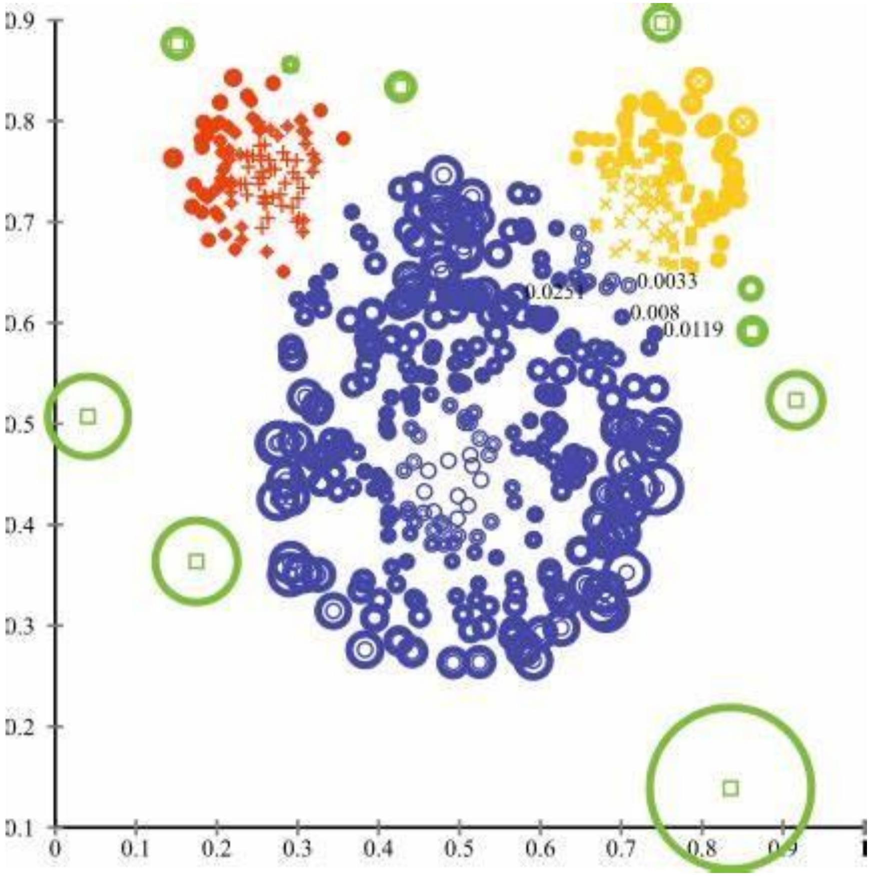
- Example:



A possible solution

- 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++

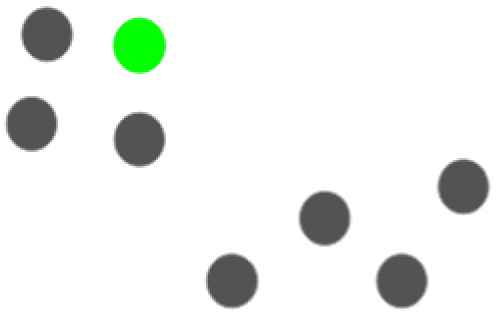
1. The first centroid is chosen uniformly at random from the data points that we want to cluster. This is similar to what we do in K-Means, but instead of randomly picking all the centroids, we just pick one centroid here
2. Next, we compute the distance d_x is the nearest distance from data point x to the centroids that have already been chosen
3. Then, choose the new cluster center from the data points with the probability of x being proportional to d_x^2
4. We then repeat steps 2 and 3 until K clusters have been chosen

Example

- Suppose we have the following points and we want to make 3 clusters here:

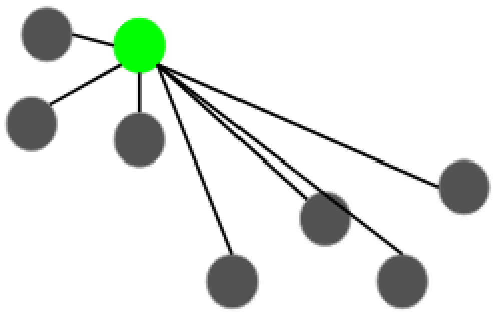
Example (cont.)

- First step is to randomly pick a data point as a cluster centroid:



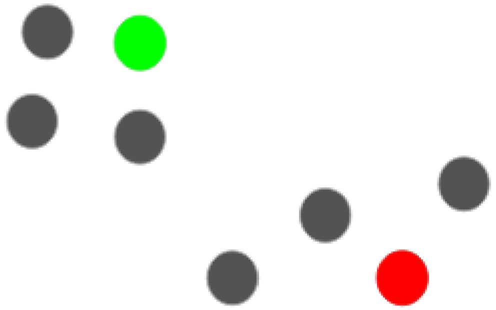
Example (cont.)

- Calculate the distance d_x of each data point with this centroid:



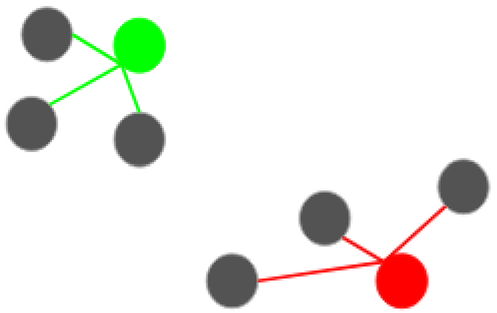
Example (cont.)

- The next centroid will be sampled with the probability proportional to d_x^2
- Say the sampled is the red one



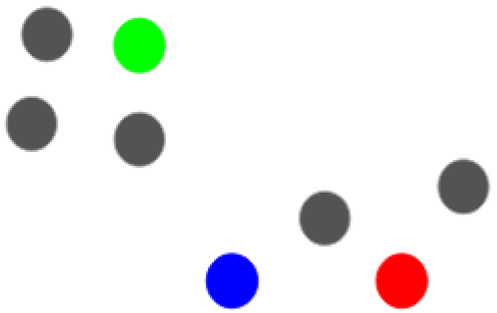
Example (cont.)

- To select the last centroid, compute d_x, which is the distance to its closest centroid



Example (cont.)

- Sample the one with the probability proportional to d_x^2
- Say, the blue one



Properties of K-Means

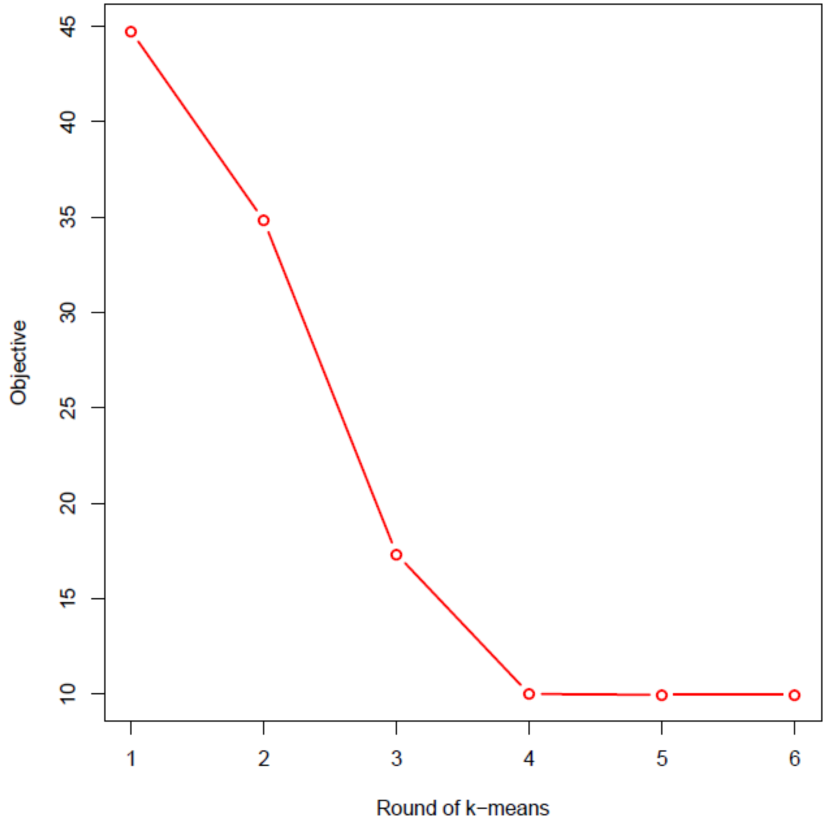
How to measure the performance

- K-means can be evaluated by the sum of distance from points to corresponding centers, or the WSS

number of clusters   number of cases   centroid for cluster *j*   case *i*

$$\text{objective function} \leftarrow J = \sum_{j=1}^{k}\sum_{i=1}^{n} \underbrace{\left\| x_i^{(j)} - c_j \right\|^2}_{\text{Distance function}}$$

- The loss will approach zero when increase K



Properties of the K-means algorithm

- Guaranteed to converge in a finite number of iterations

- Running time per iteration:
  1. Assign data points to closest cluster center
     O(KN) time
  2. Change the cluster center to the average of its assigned points
     O(N)

Distance

- Distance is of crucial importance in K-means. So what kind of properties should the distance measure have?

- Symmetric
  - $D(A, B) = D(B, A)$

- Positivity, and self-similarity
  - $D(A, B) \geq 0$, and $D(A, B) = 0$ iff $A = B$

- Triangle inequality
  - $D(A, B) + D(B, C) \geq D(A, C)$

Convergence of K-means

Objective

$$\min_{\mu}\min_{C}\sum_{i=1}^{k}\sum_{x\in C_i}|x-\mu_i|^2$$

1. Fix μ, optimize C:

$$\min_{C}\sum_{i=1}^{k}\sum_{x\in C_i}|x-\mu_i|^2=\min_{c}\sum_{i}^{n}\left|x_i-\mu_{x_i}\right|^2$$

Step 1 of kmeans

2. Fix C, optimize μ:

$$\min_{\mu}\sum_{i=1}^{k}\sum_{x\in C_i}|x-\mu_i|^2$$

 – Take partial derivative of μ_i and set to zero, we have

$$\mu_i=\frac{1}{|C_i|}\sum_{x\in C_i}x$$

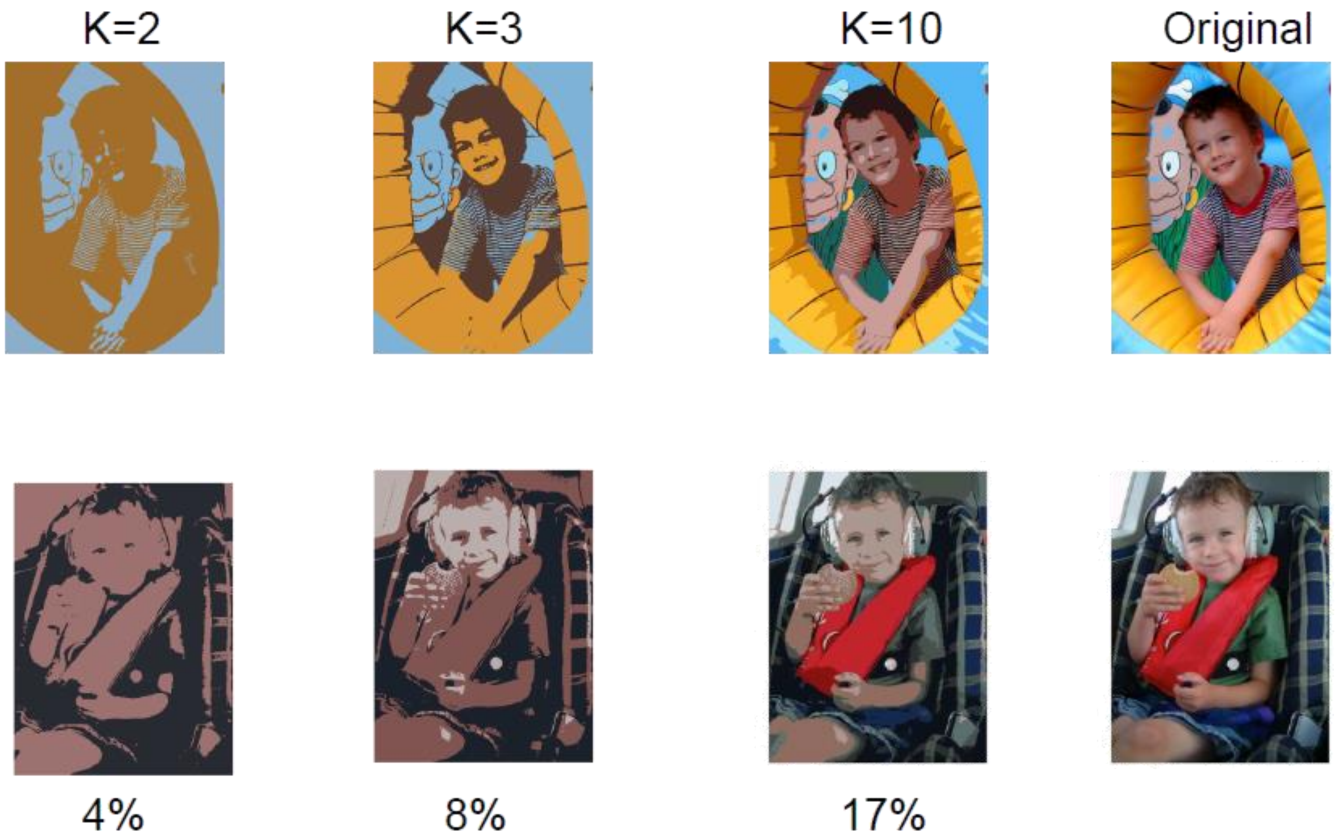
Step 2 of kmeans

Not guaranteed to converge to optimal

Kmeans takes an alternating optimization approach, each step is guaranteed to decrease the objective – thus guaranteed to converge

Application: Segmentation

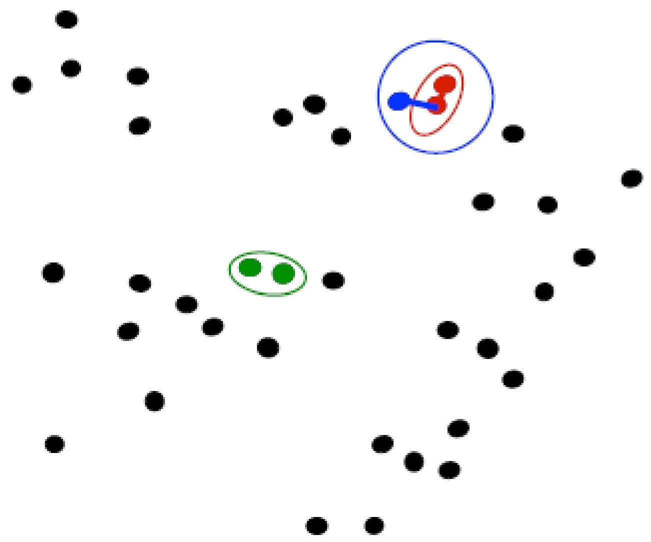
- Goal of segmentation is to partition an image into regions each of which has reasonably homogenous visual appearance
- Cluster the colors



Agglomerative Clustering

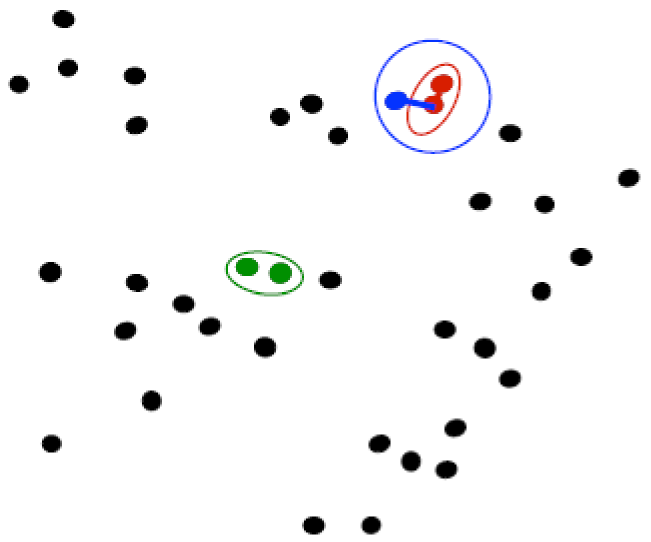
Agglomerative clustering

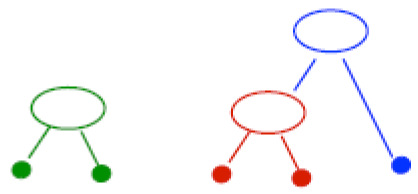
- Agglomerative clustering:
  - First merge very similar instances
  - Incrementally build larger clusters out of smaller clusters
- Algorithm:
  - Maintain a set of clusters
  - Initially, each instance in its own cluster
  - Repeat:
    - Pick the two closest clusters
    - Merge them into a new cluster
    - Stop when there’s only one cluster left



Agglomerative clustering

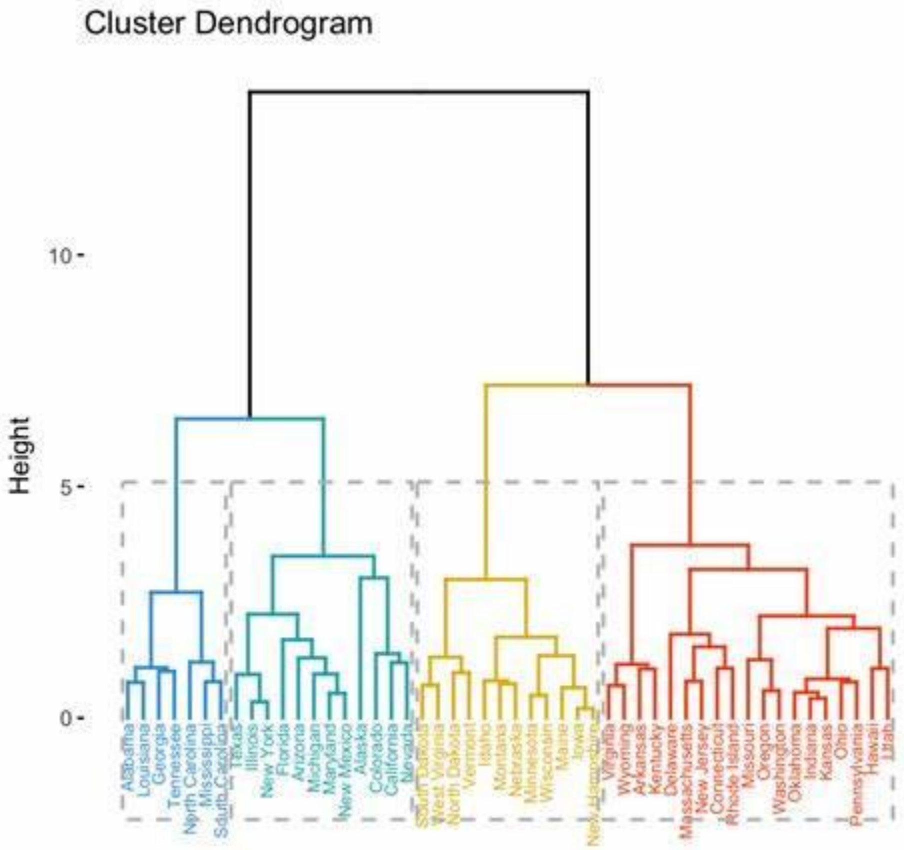
- Produces not one clustering, but a family of clusterings represented by a dendrogram





Example

- Different heights give different clustering

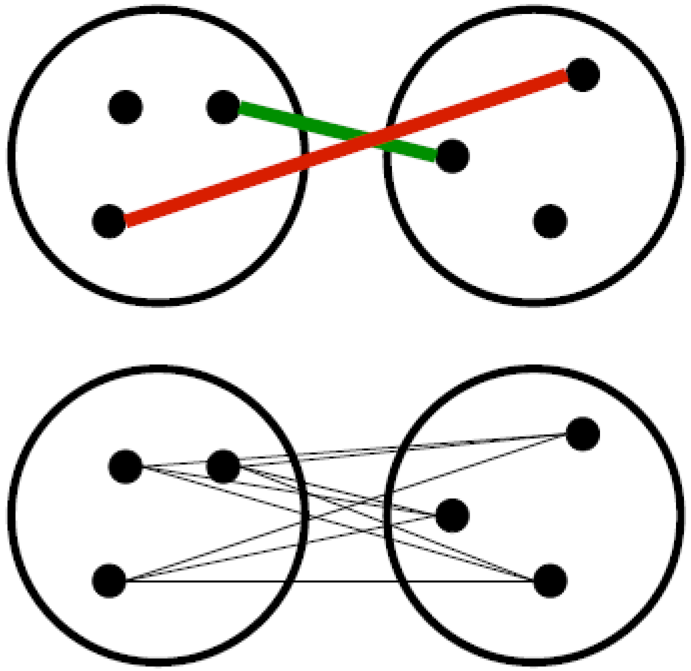


Closeness

- How should we define “closest” for clusters with multiple elements?

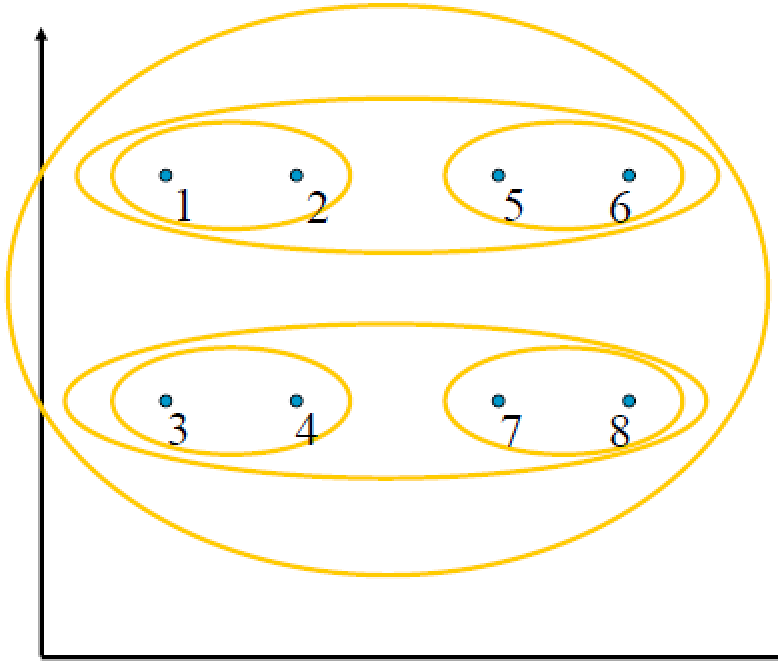
- Many options:
  - Closest pair (single-link clustering)
  - Farthest pair (complete-link clustering)
  - Average of all pairs

- Different choices create different clustering behaviors

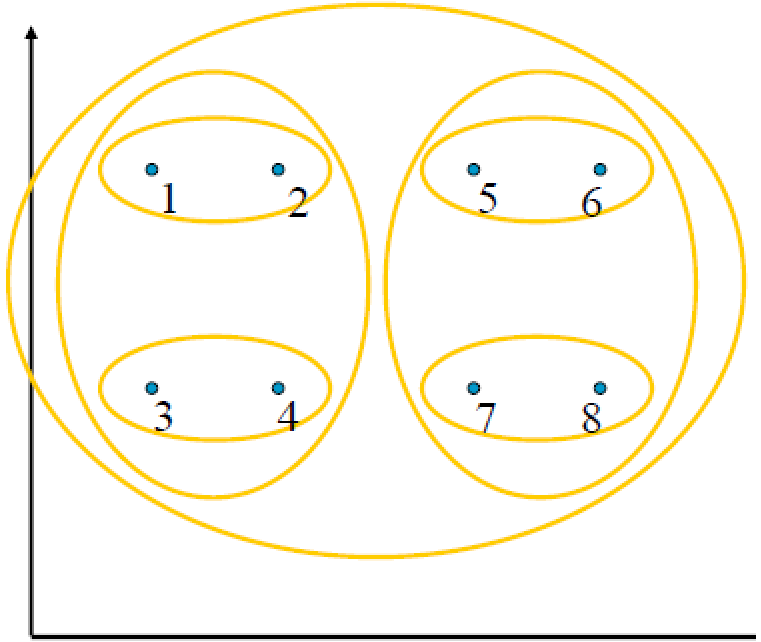


Closeness example

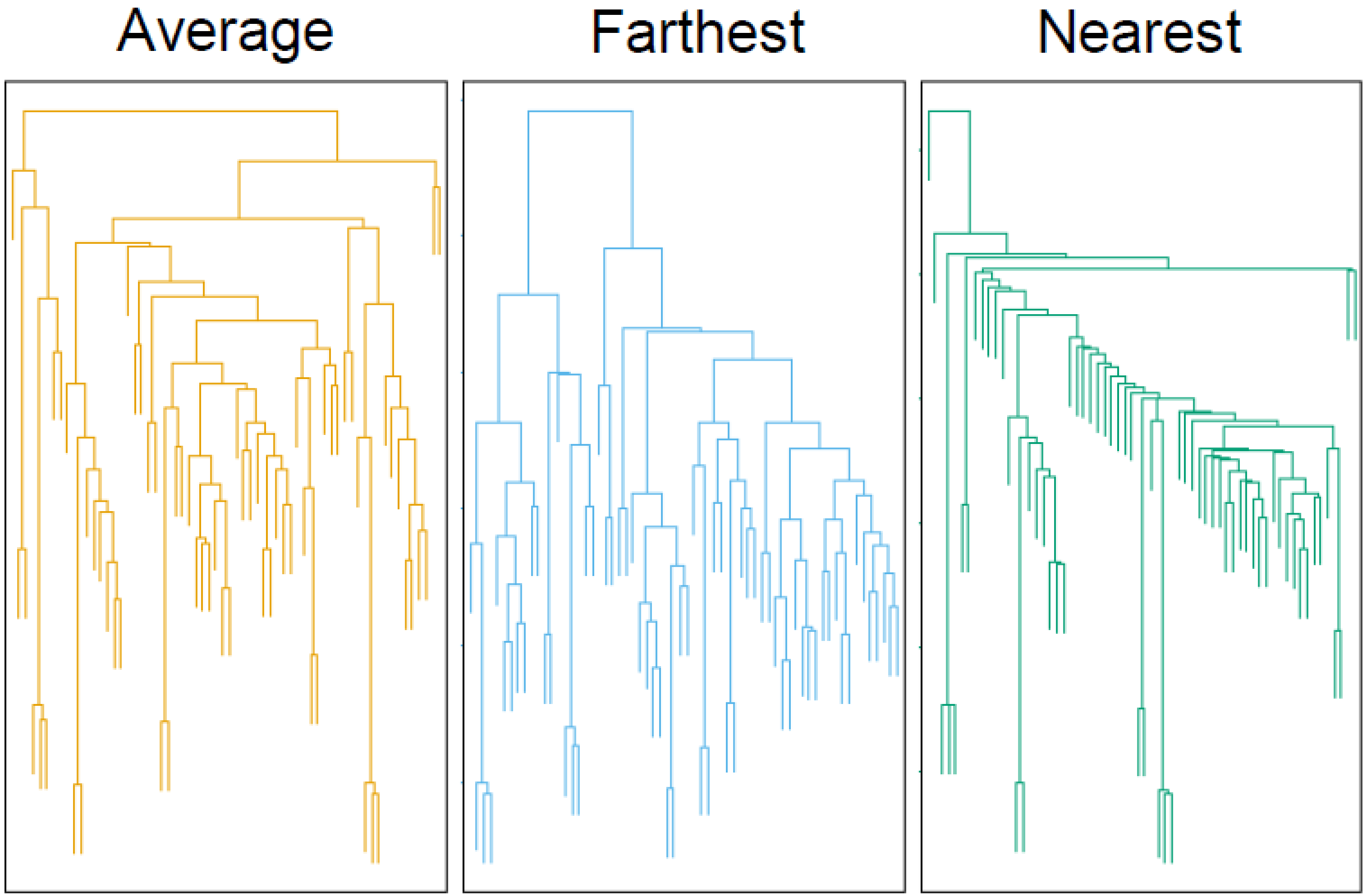
Closest pair
(single-link clustering)



Farthest pair
(complete-link clustering)



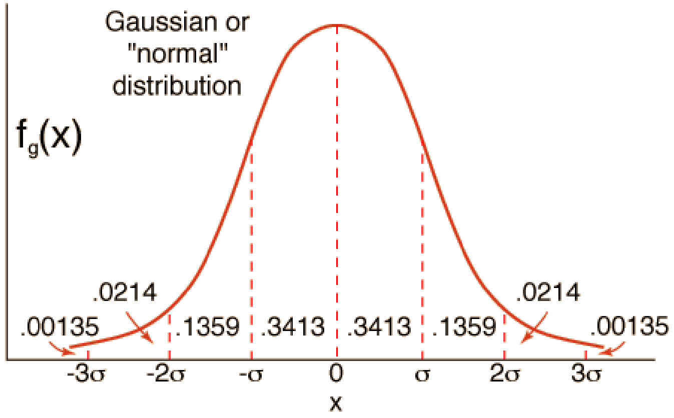
Closeness example 2



The BFR Algorithm

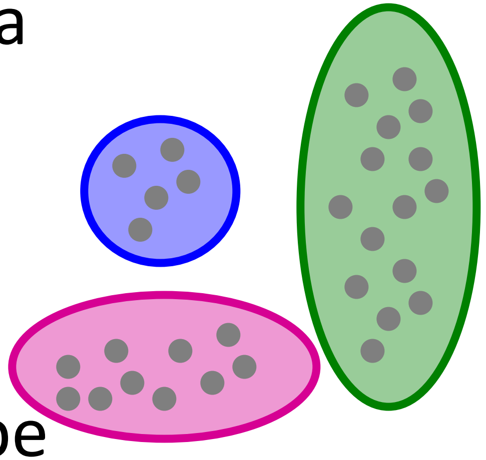
Extension of K-Means to large data

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 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

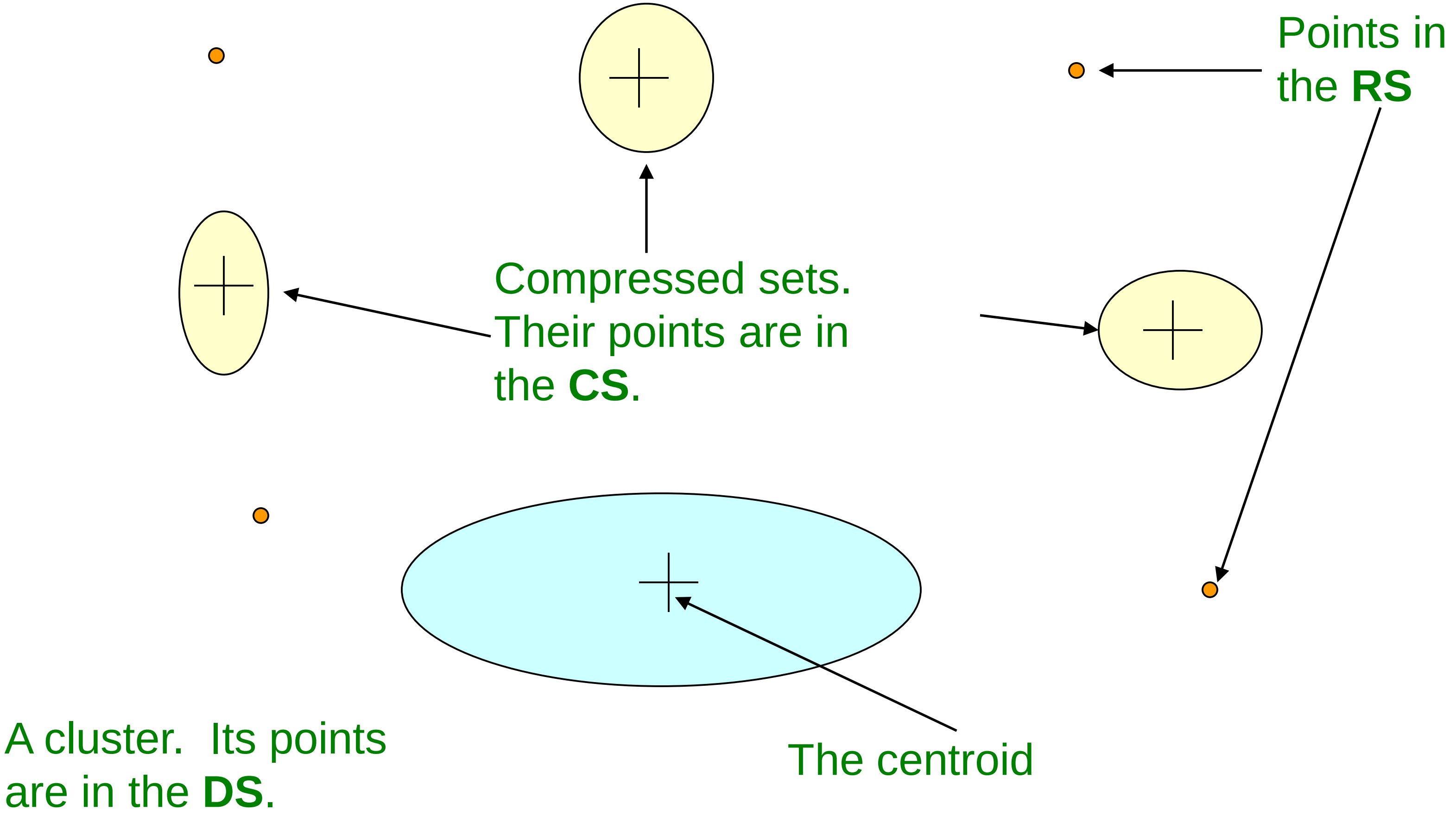
- Points are read from disk one main-memory-full at a time
- Most points from previous memory loads are summarized by simple statistics
- Step 1) From the initial load we select the initial *k* centroids by some sensible approach, which can be
  - Take ***k*** random points
  - Take a small random sample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

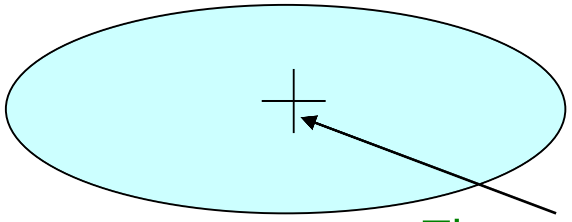


Discard set (DS): Close enough to a centroid to be summarized
Compression set (CS): Summarized, but not assigned to a cluster
Retained set (RS): Isolated points

Summarizing sets of points

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

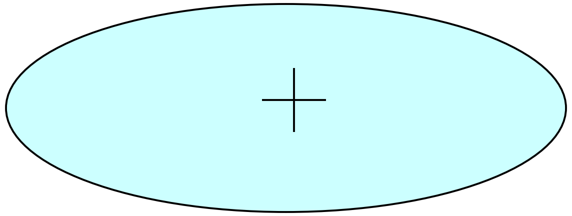
- The number of points, N
- The vector SUM, whose i^{th} component is the sum of the coordinates of the points in the i^{th} dimension
- The vector $SUMSQ$: i^{th} component = sum of squares of coordinates in i^{th} dimension



Summarizing points: Comments

- $2d + 1$ values represent any size cluster
  - d = number of dimensions
- Average in each dimension (the centroid) can be calculated as SUM_i / N
  - SUM_i = i^{th} component of SUM
- Variance of a cluster's discard set in dimension *i* is: $(\mathrm{SUMSQ}_i / N) - (\mathrm{SUM}_i / N)^2$
  - 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 2-5) 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 2-5) 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.
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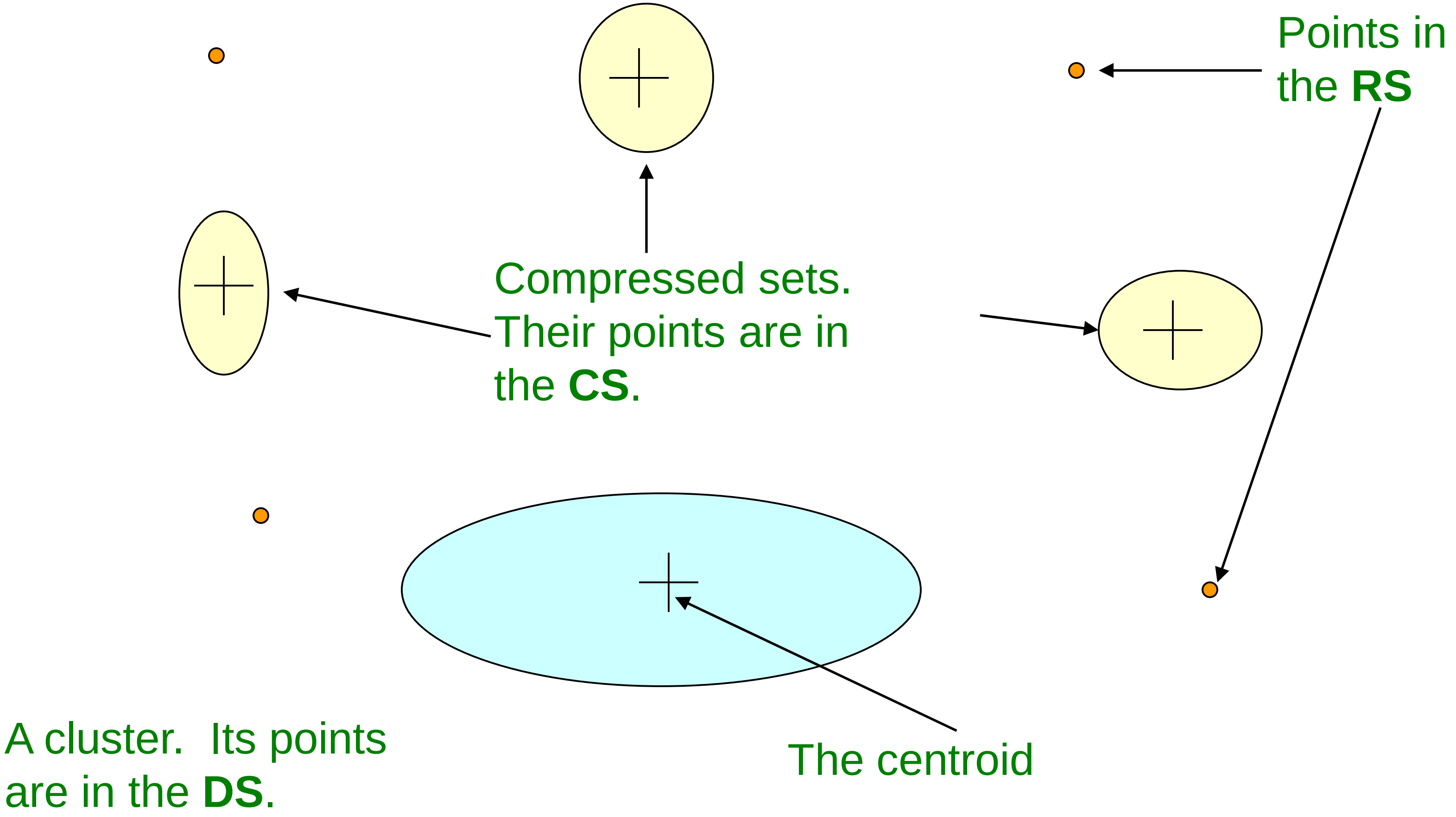
BFR: “Galaxies” picture



Discard set (DS): Close enough to a centroid to be summarized
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A few details …

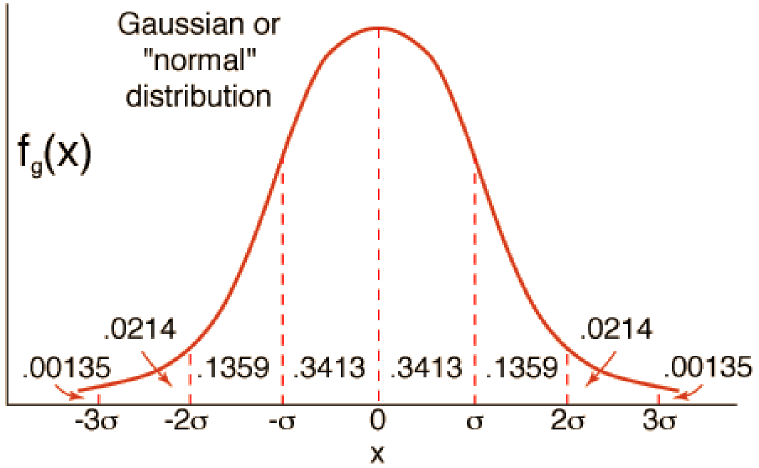
- Q1) How do we decide if a point is “close enough” to a cluster that we will add the point to that cluster?

- 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

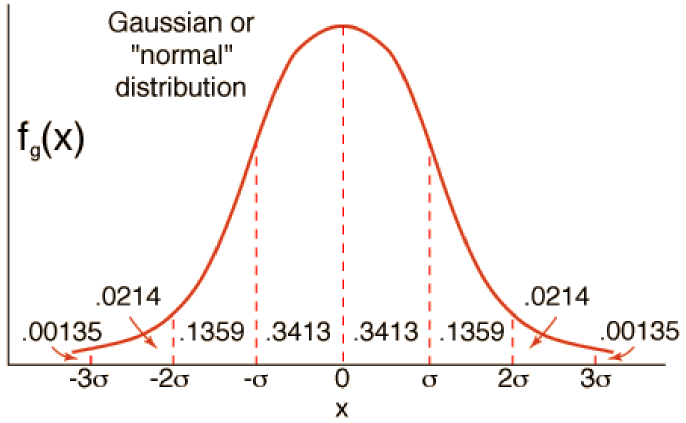
$$d(x, c) = \sqrt{\sum_{i=1}^{d} \left(\frac{x_i - c_i}{\sigma_i} \right)^2}$$

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

Mahalanobis distance (cont.)

- 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 $< \sqrt{d}$

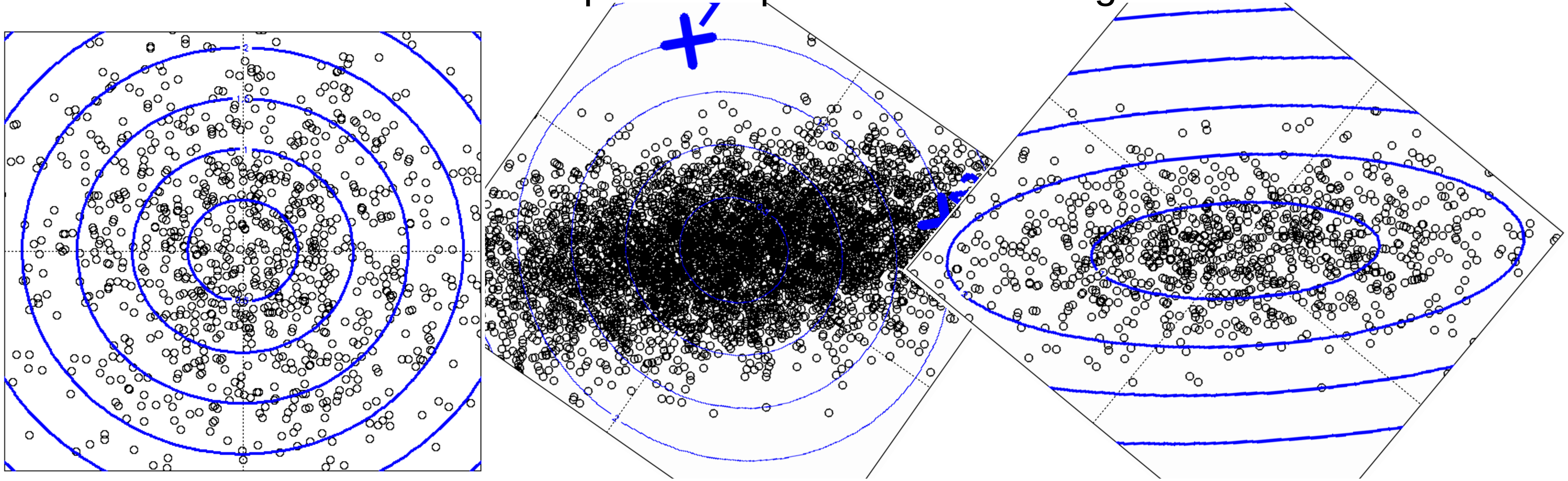
- Accept a point for a cluster if its M.D. is < some threshold, e.g. 2 standard deviations



Picture: Equal M.D. regions

- Euclidean vs. Mahalanobis distance

Contours of equidistant points from the origin



Uniformly distributed points, Euclidean distance

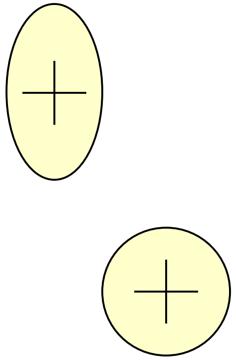
Normally distributed points, Euclidean distance

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



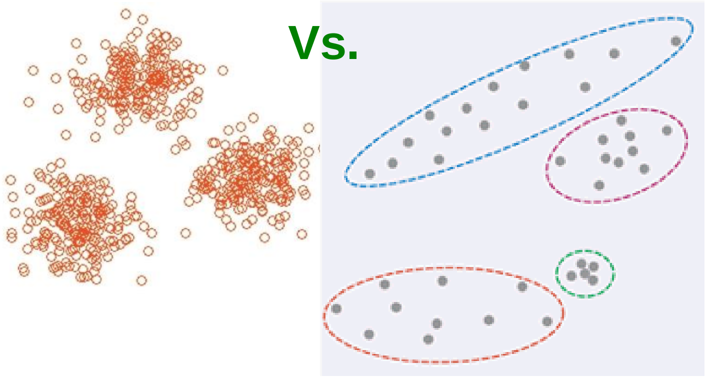
- Many alternatives: Treat dimensions differently, consider density

The CURE Algorithm

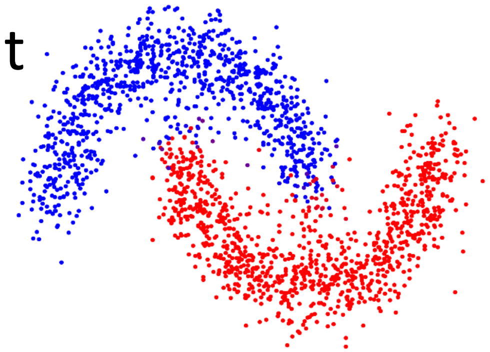
Extension of k-means to clusters of arbitrary shapes

The CURE algorithm

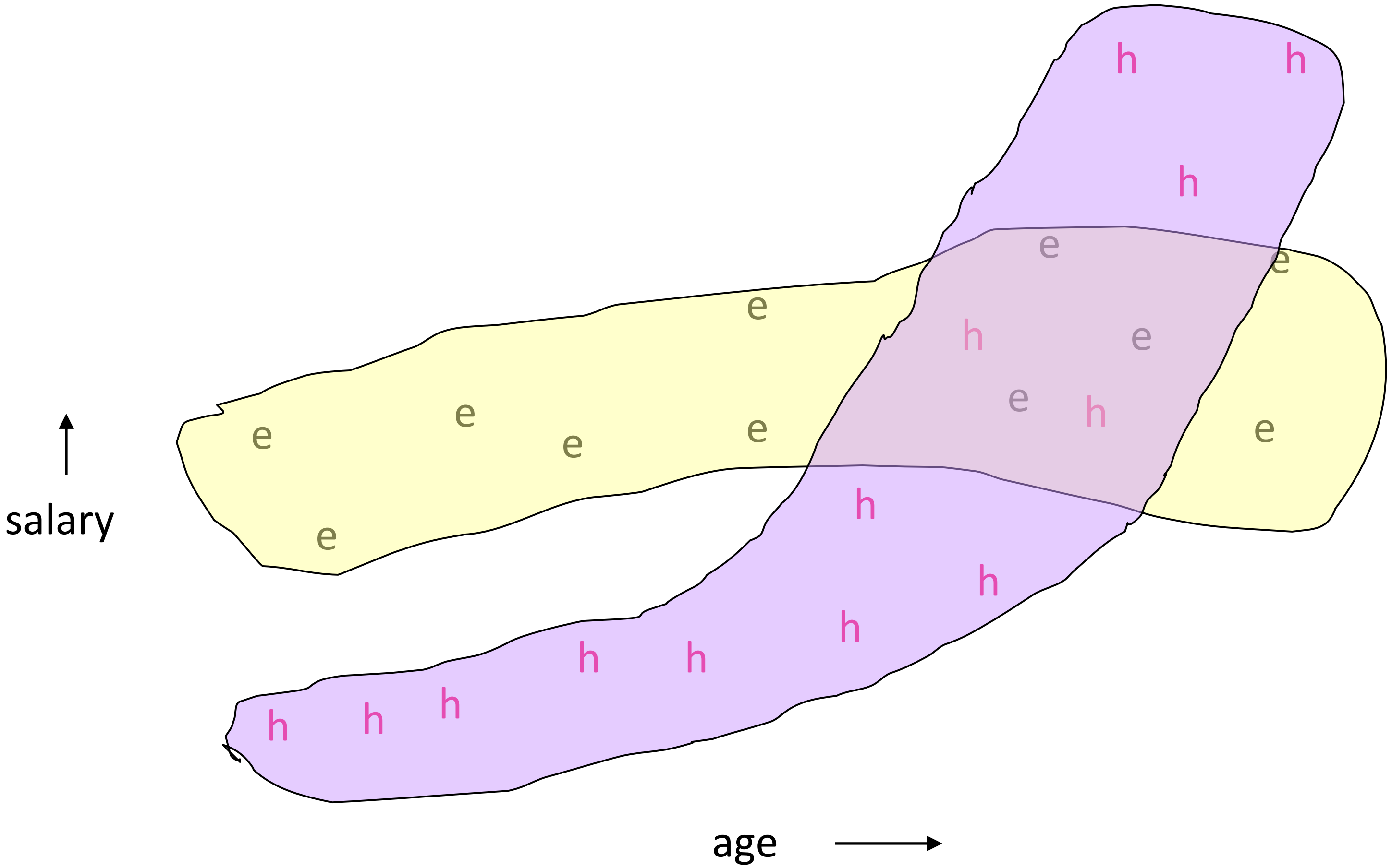
- Problem with BFR/*k*-means:
  - Assumes clusters are normally distributed in each dimension
  - And axes are fixed – ellipses at an angle are ***not OK***



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



Example: Stanford salaries

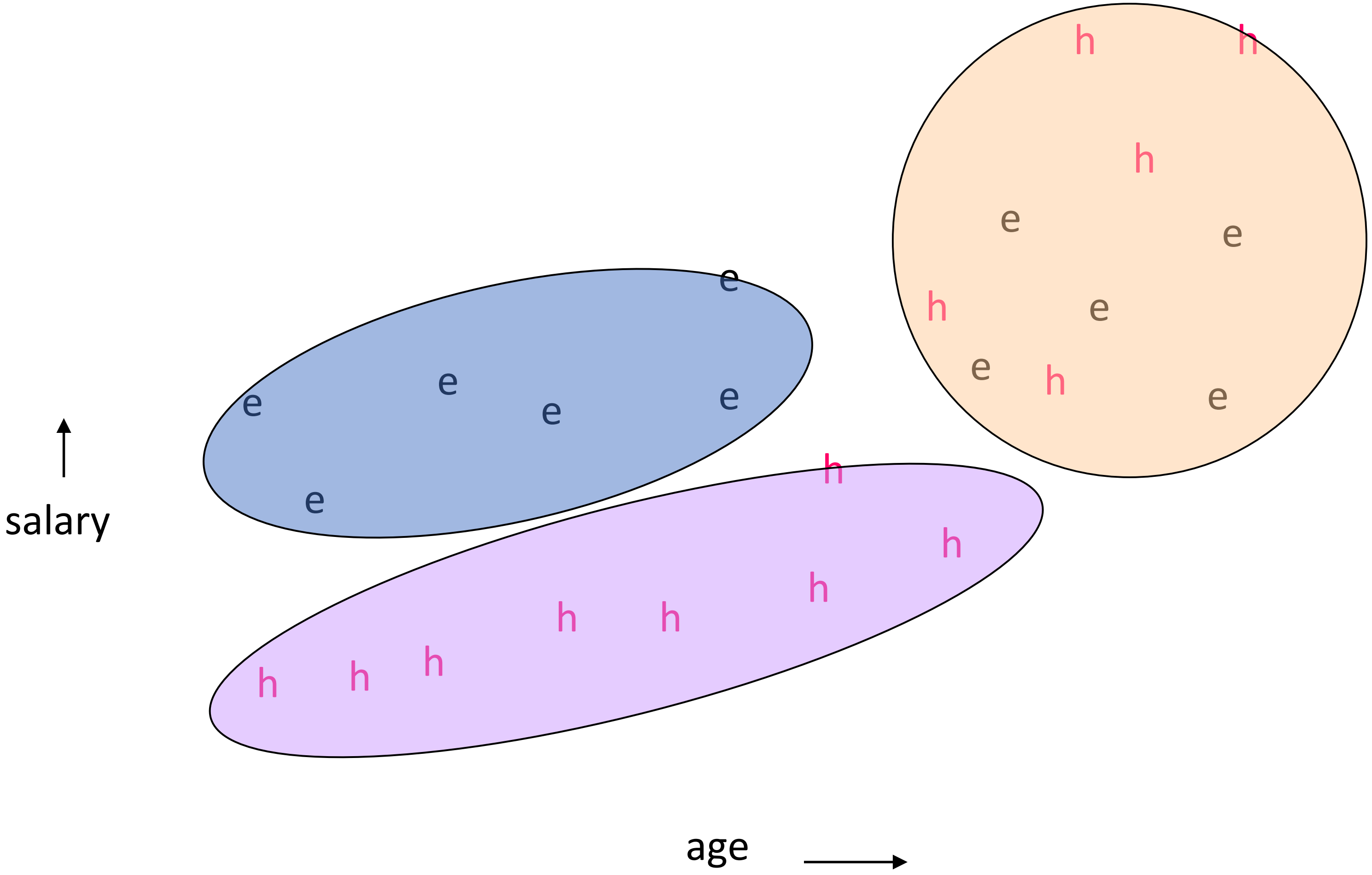


Starting CURE

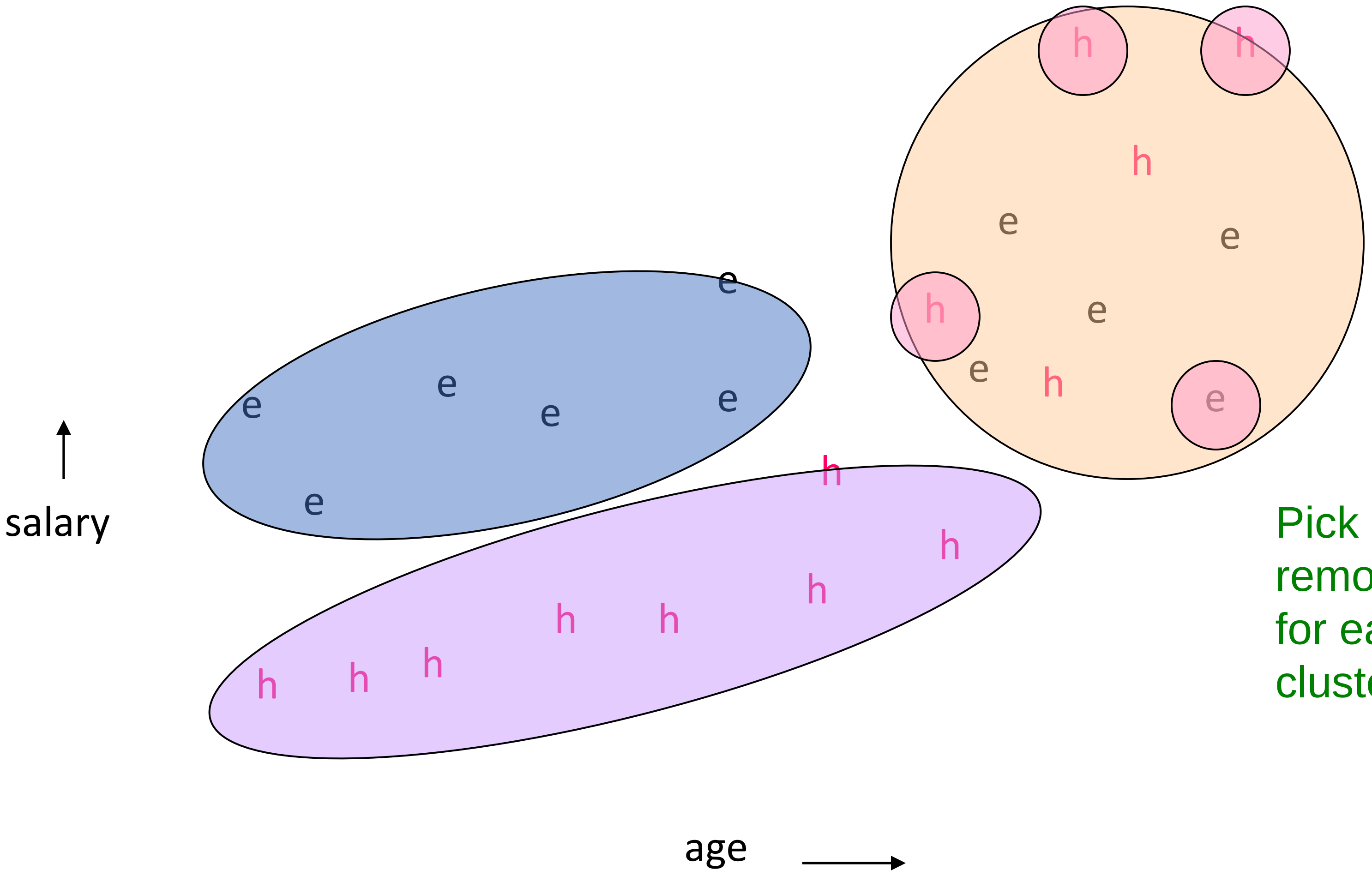
2 Pass algorithm. Pass 1:

- 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

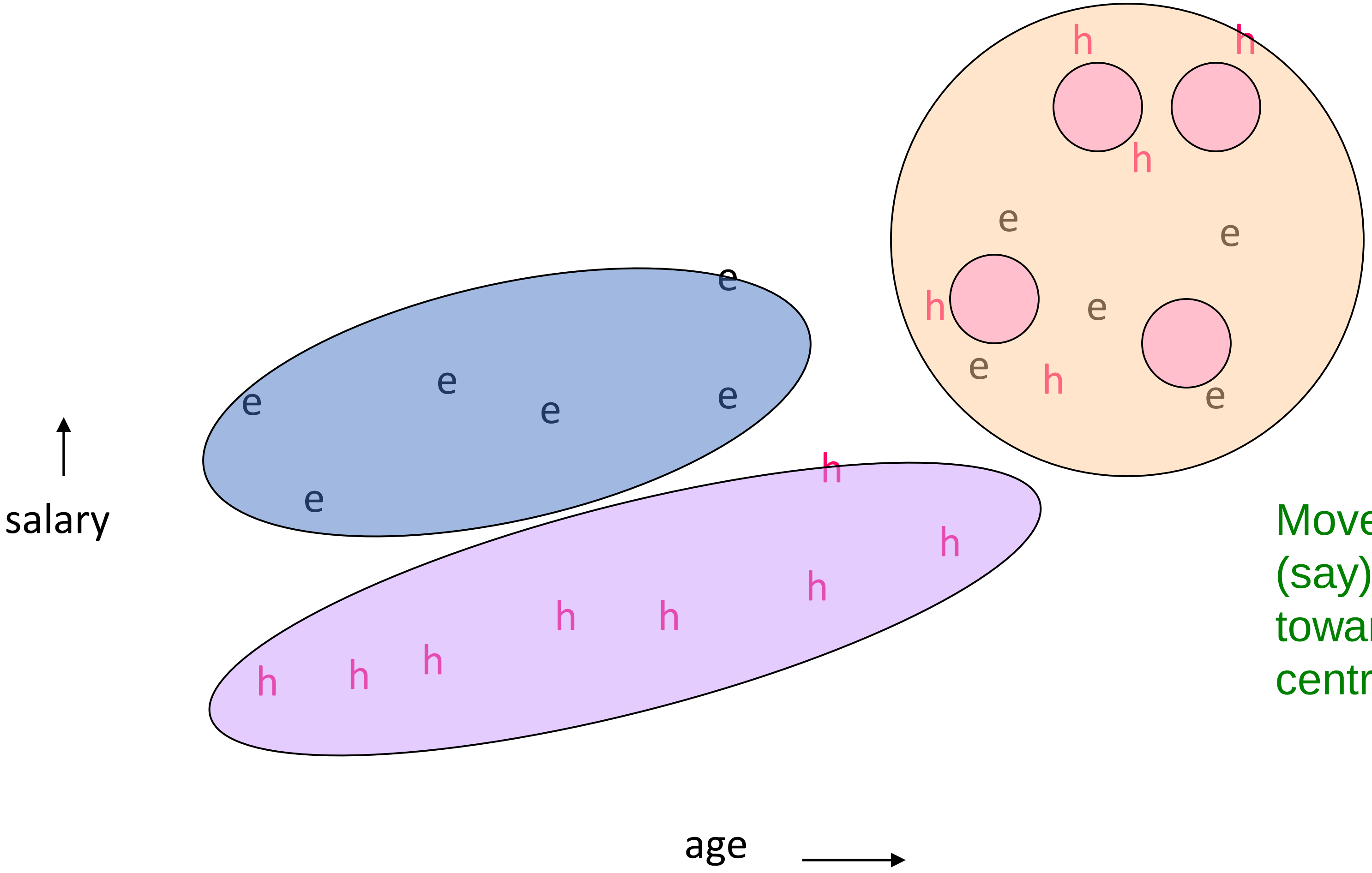


Example: Pick dispersed points



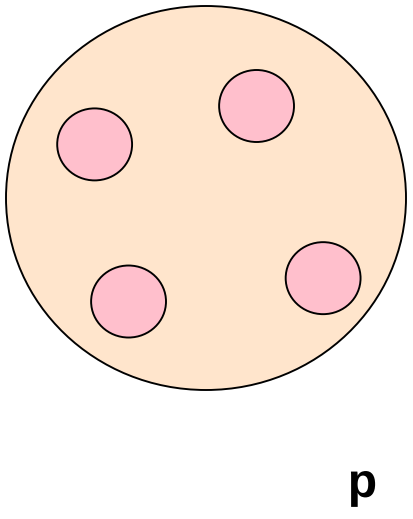
Pick (say) 4 remote points for each cluster.

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 to ***p*** and assign it to representative's cluster

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