Unsupervised Learning: Clustering

Nicholas Ruozzi
University of Texas at Dallas

Based on the slides of Vibhav Gogate

Clustering

Clustering systems:

- Unsupervised learning
- Requires data, but no labels
- Detect patterns, e.g., in
  - Group emails or search results
  - Customer shopping patterns
- Useful when don't know what you're looking for…
  - But often get gibberish

Clustering

- Want to group together parts of a dataset that are close together in some metric
  - Useful for finding the important parameters/features of a dataset

Clustering

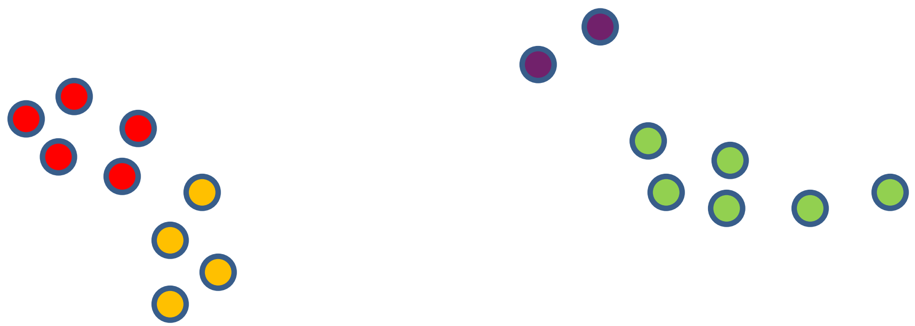
- Want to group together parts of a dataset that are close together in some metric
  - Useful for finding the important parameters/features of a dataset

Clustering

- Intuitive notion of clustering is a somewhat ill-defined problem
    - Identification of clusters depends on the scale at which we perceive the data

Clustering

- Intuitive notion of clustering is a somewhat ill-defined problem
  - Identification of clusters depends on the scale at which we perceive the data



Clustering

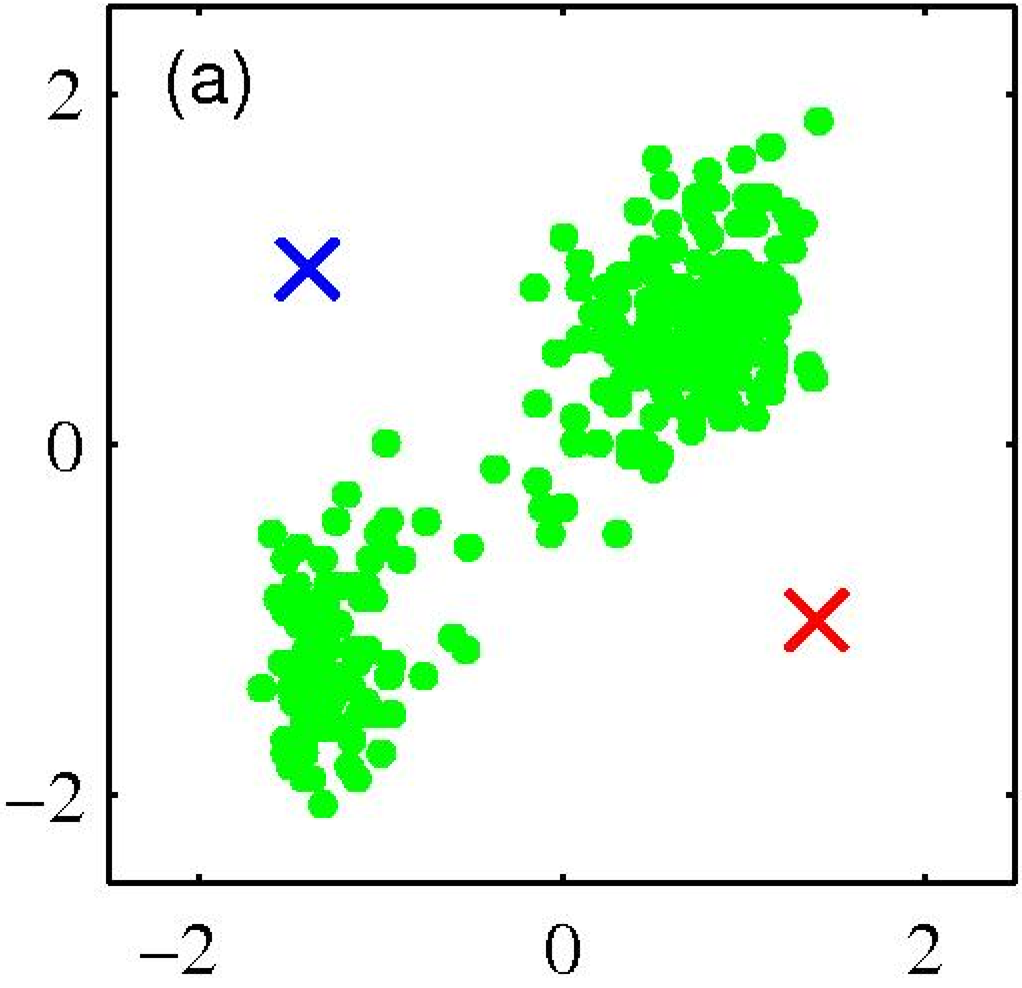
- Input: a collection of points $x^{(1)}, \ldots, x^{(m)} \in \mathbb{R}^n$, an integer k

- Output: A partitioning of the input points into k sets that minimizes some metric of closeness

k-means Clustering

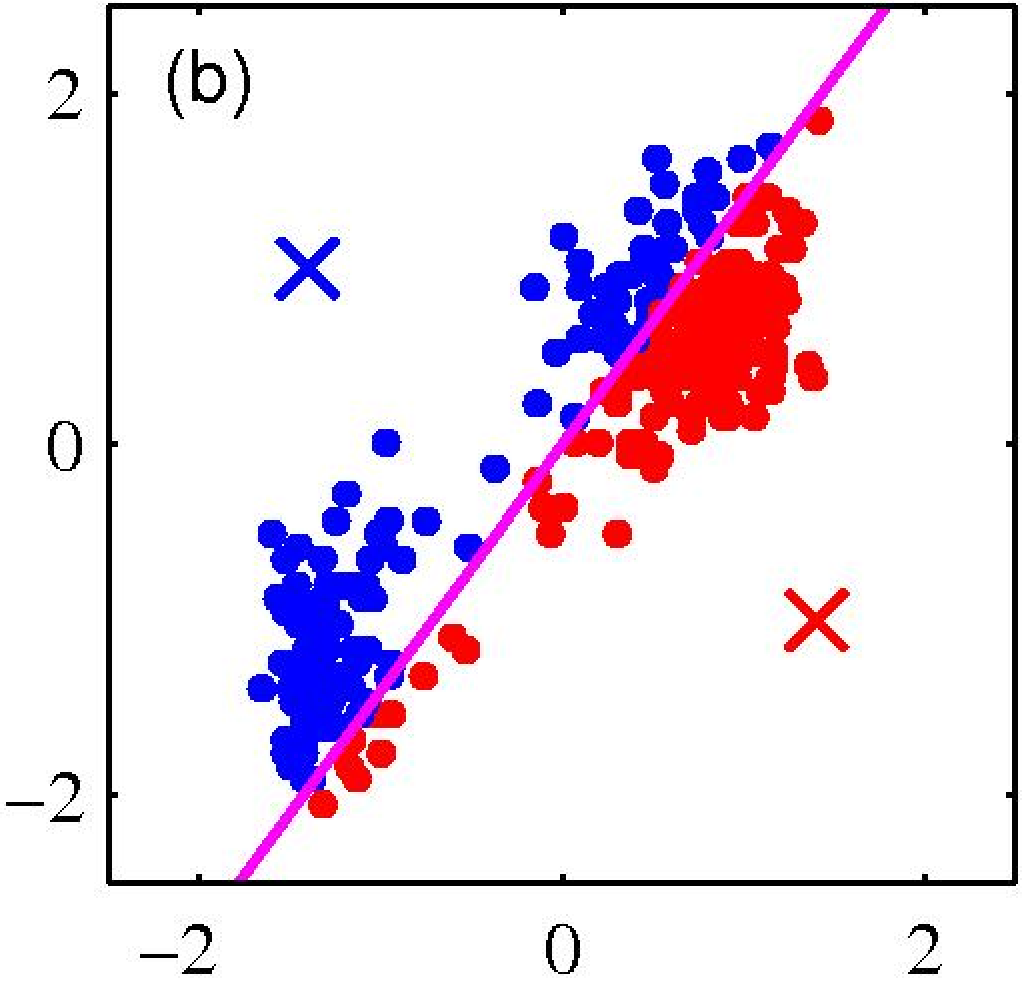
- Pick an initial set of k means (usually at random)
- Repeat until the clusters do not change:
  - Partition the data points, assigning each data point to a cluster based on the mean that is closest to it
  - Update the cluster means so that the i^{th} mean is equal to the average of all data points assigned to cluster i

k-means clustering: Example



Pick k random points as cluster centers (means)

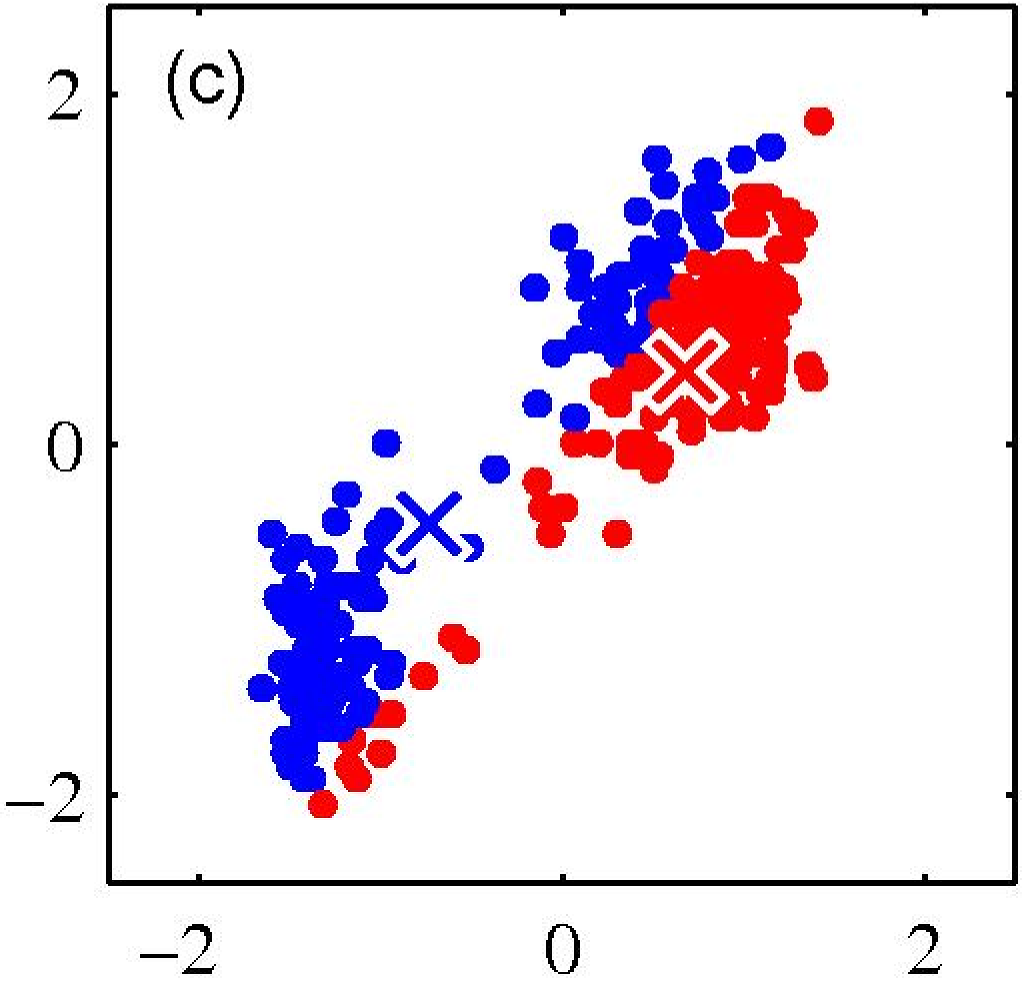
k-means clustering: Example



Iterative Step 1:

Assign data instances to closest cluster center

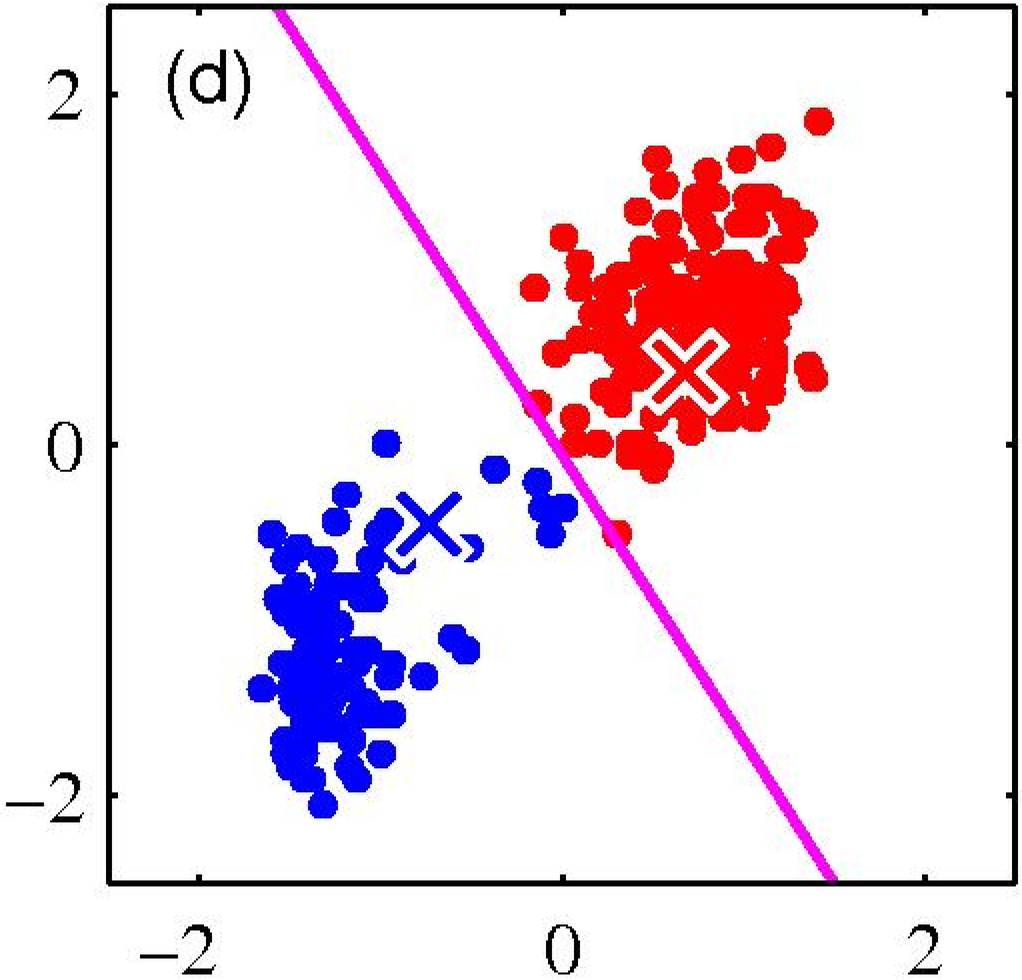
k-means clustering: Example



Iterative Step 2:

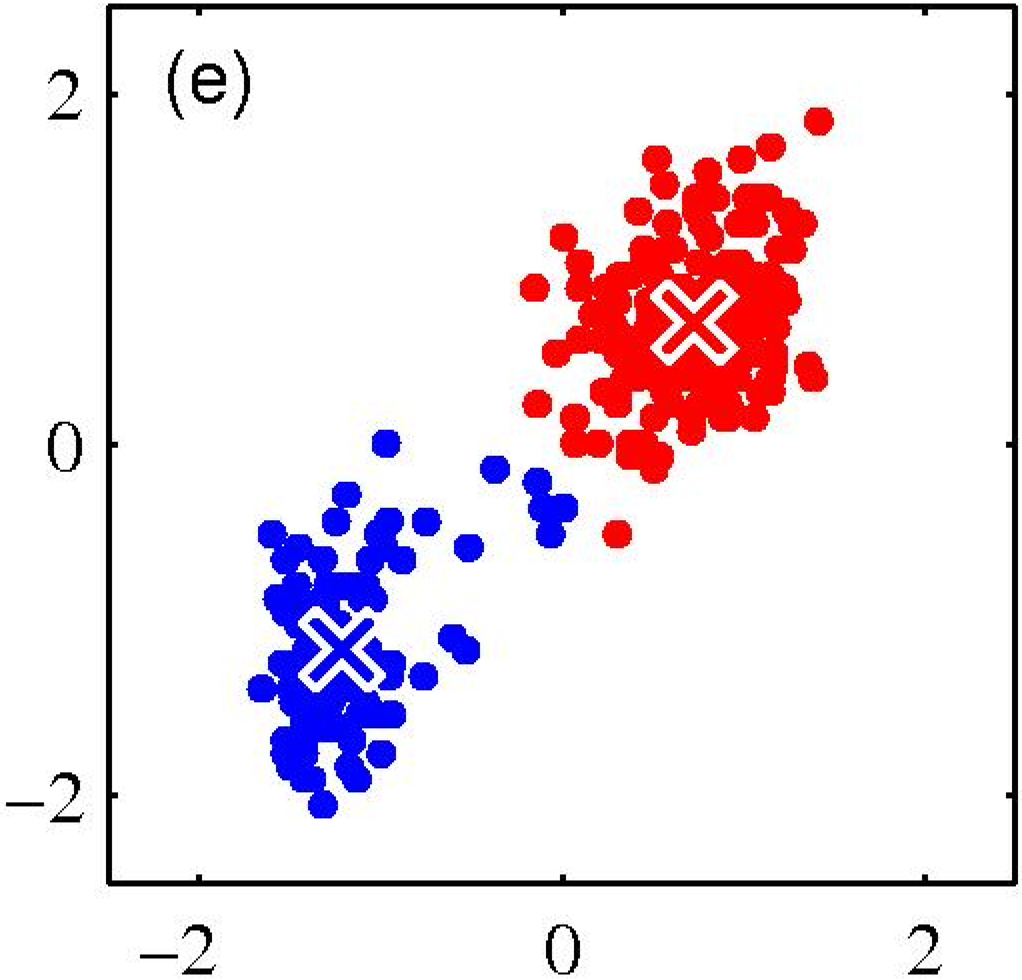
Change the cluster center to the average of the assigned points

k-means clustering: Example

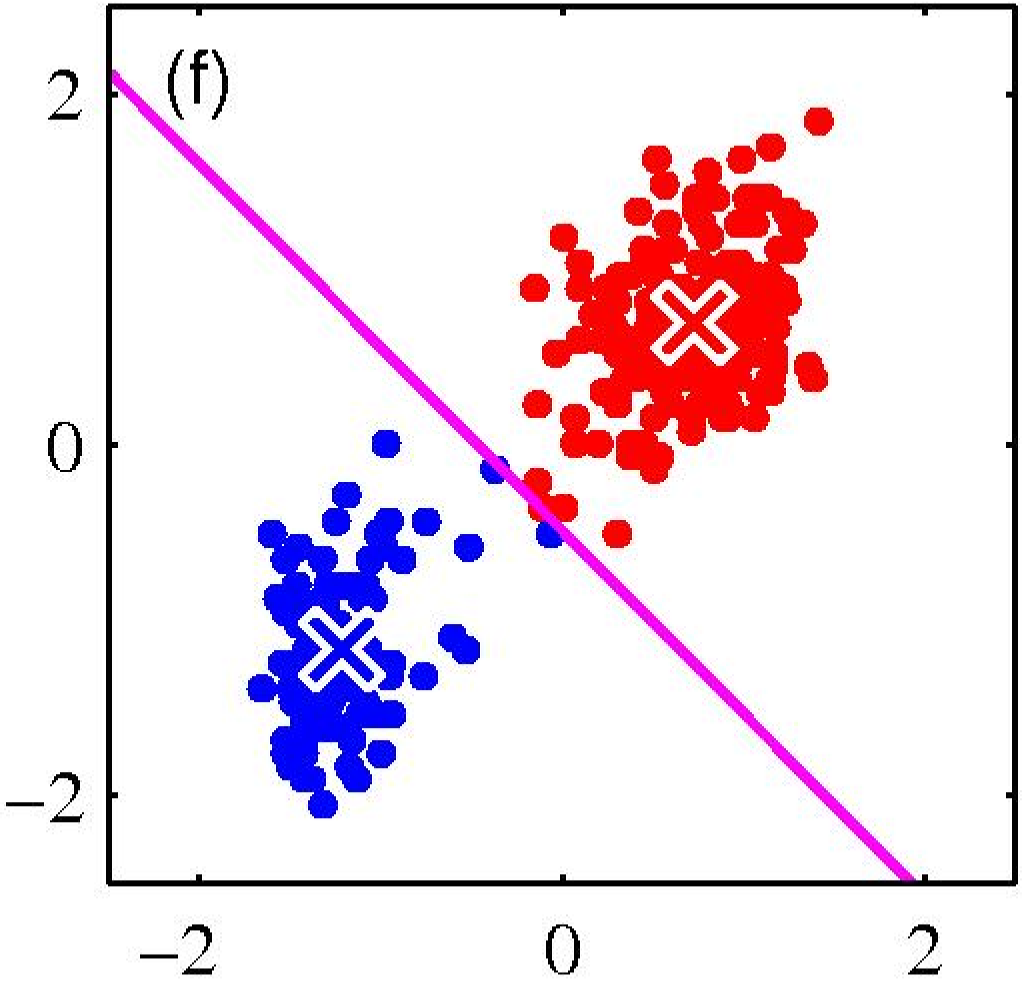


Repeat until convergence

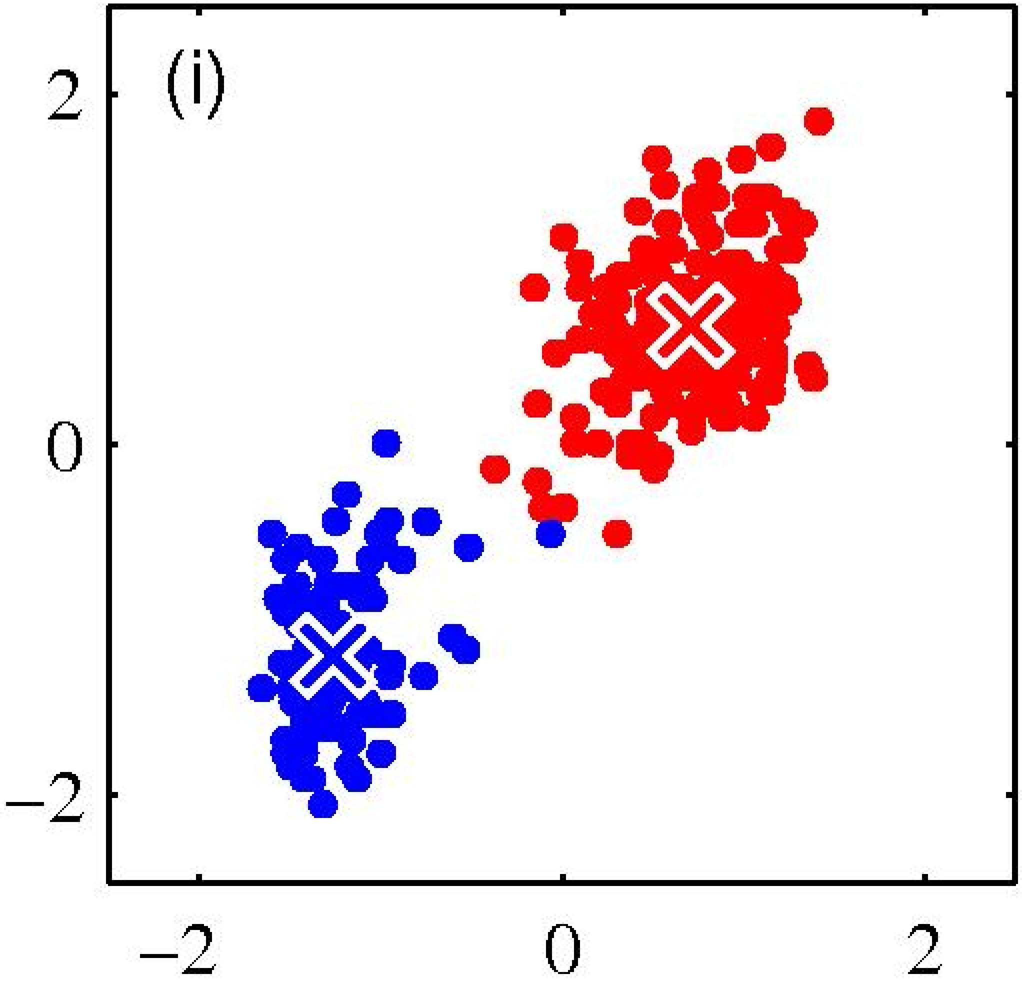
k-means clustering: Example



k-means clustering: Example



k-means clustering: Example



k-Means for Segmentation

$k = 2$

Original

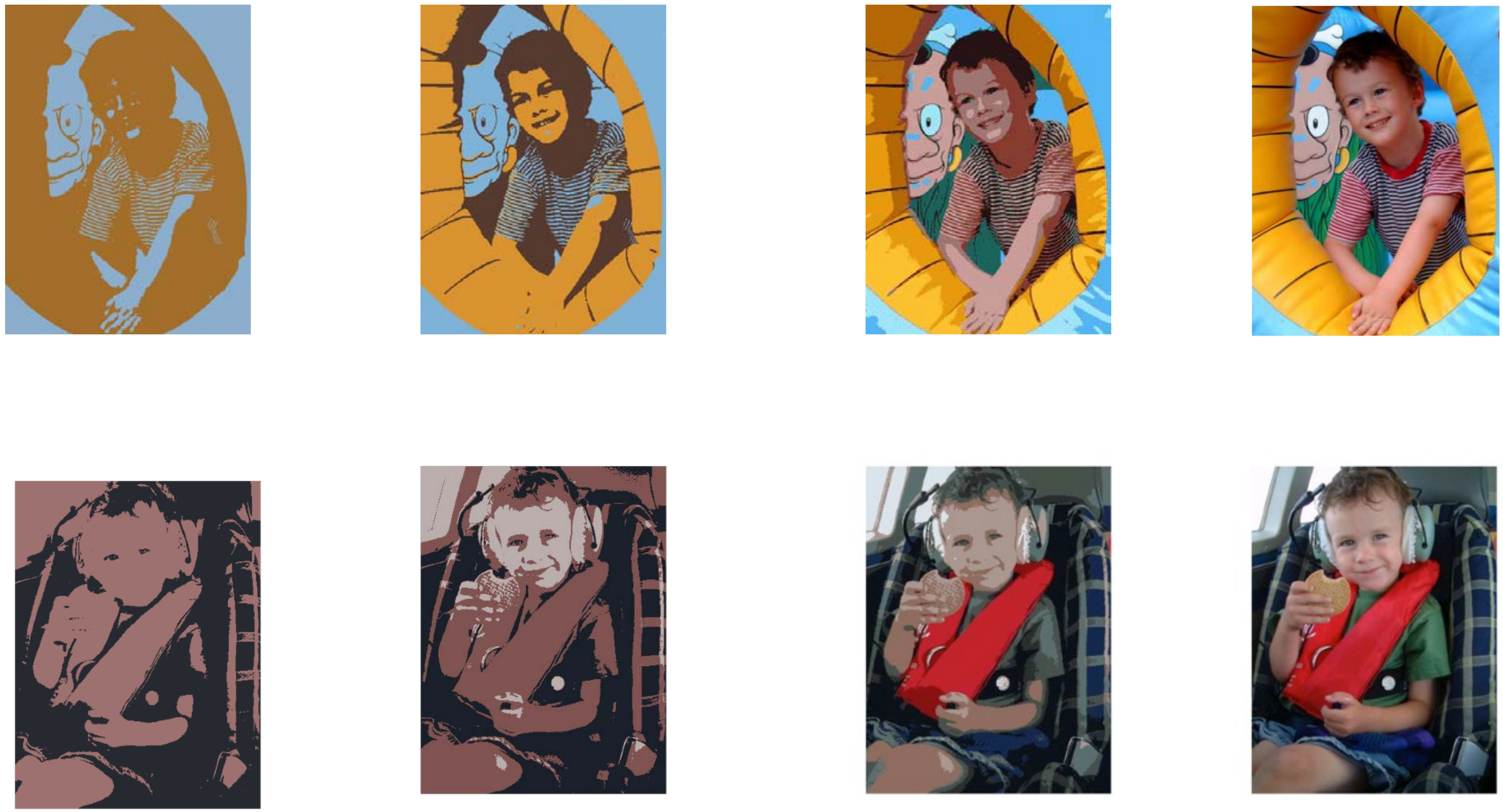
Goal of Segmentation is to partition an image into regions, each of which has reasonably homogenous visual appearance

k-Means for Segmentation

$k=2$	$k=3$	Original
		
		

k-Means for Segmentation

$k = 2$ | $k = 3$ | $k = 10$ | Original



k-means Clustering as Optimization

- Minimize the distance of each input point to the mean of the cluster/partition that contains it

$$\min_{S_1,\ldots,S_k} \sum_{i=1}^{k} \sum_{j \in S_i} \left\| x^{(j)} - \mu_i \right\|^2$$

where

- $S_i \subseteq \{1, \ldots, M\}$ is the i^{th} cluster
- $S_i \cap S_j = \emptyset$ for $i \neq j$, $\cup_i S_i = \{1, \ldots, n\}$
- μ_i is the centroid of the i^{th} cluster

k-means Clustering as Optimization

- Minimize the distance of each input point to the mean of the cluster/partition that contains it

$$\min_{S_1,\ldots,S_k} \sum_{i=1}^{k} \sum_{j \in S_i} \left\| x^{(j)} - \mu_i \right\|^2$$

where

- $S_i \subseteq \{1, \ldots, M\}$ is the i^{th} cluster
- $S_i \cap S_j = \emptyset$ for $i \neq j$, $\cup_i S_i = \{1, \ldots, n\}$
- μ_i is the centroid of the i^{th} cluster

Exactly minimizing this function is NP-hard (even for $k = 2$)

k-means Clustering

- The k-means clustering algorithm performs a block coordinate descent on the objective function

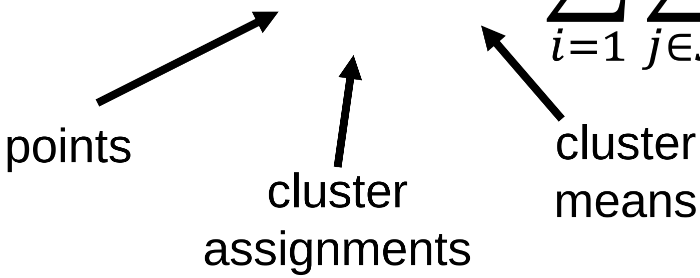
$$\sum_{i=1}^{k} \sum_{j \in S_i} \left\| x^{(j)} - \mu_i \right\|^2$$

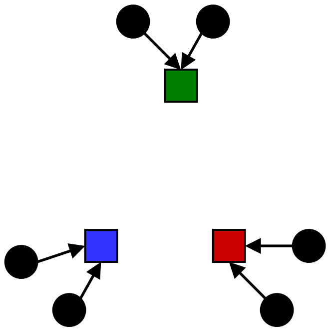
- This is not a convex function: could get stuck in local minima

k-Means as Optimization

- Consider the k-means objective function

$$\phi(x, S, \mu) = \sum_{i=1}^{k} \sum_{j \in S_i} \left\| x^{(j)} - \mu_i \right\|^2$$





- Two stages each iteration
  - Update cluster assignments: fix means μ, change assignments S
  - Update means: fix assignments S, change means μ

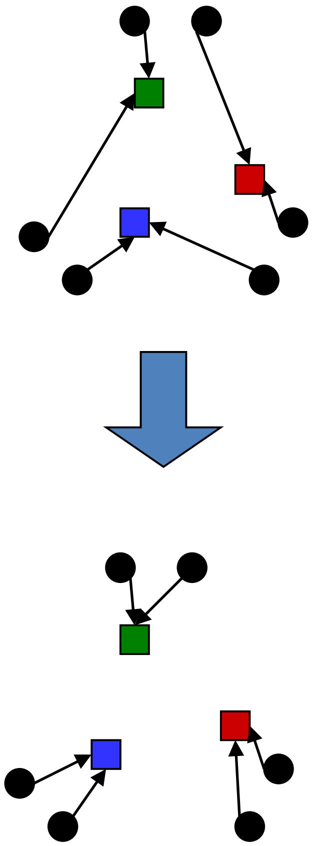
Phase I: Update Assignments

- For each point, re-assign to closest mean, $x^{(j)} \in S_i$ if

$$j \in \arg\min_i \left\| x^{(j)} - \mu_i \right\|^2$$

- Can only decrease ϕ as the sum of the distances of all points to their respective means must decrease

$$\phi(x, S, \mu) = \sum_{i=1}^{k} \sum_{j \in S_i} \left\| x^{(j)} - \mu_i \right\|^2$$

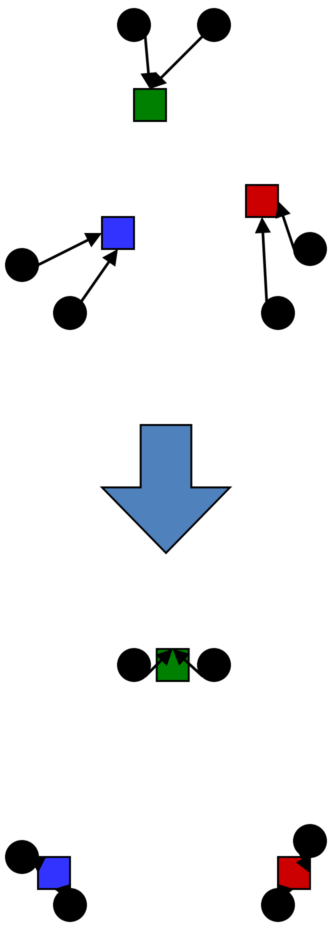


Phase II: Update Means

- Move each mean to the average of its assigned points

$$\mu_i = \sum_{j \in S_i} \frac{x^{(j)}}{|S_i|}$$

- Also can only decrease total distance…
  - Why?

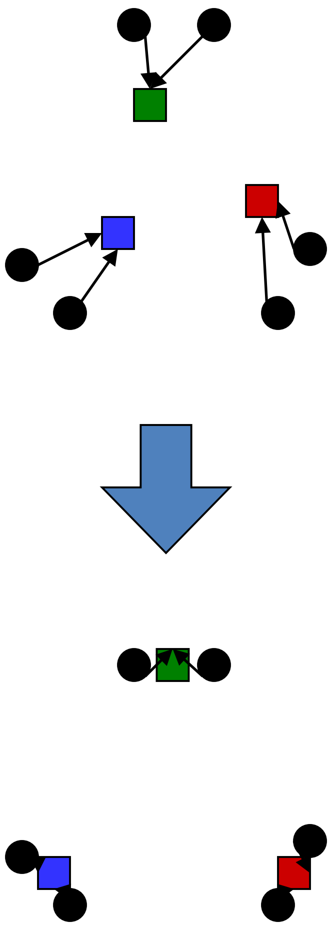


Phase II: Update Means

- Move each mean to the average of its assigned points

$$\mu_i = \sum_{j \in S_i} \frac{x^{(j)}}{|S_i|}$$

- Also can only decrease total distance…
  - The point y with minimum squared Euclidean distance to a set of points is their mean

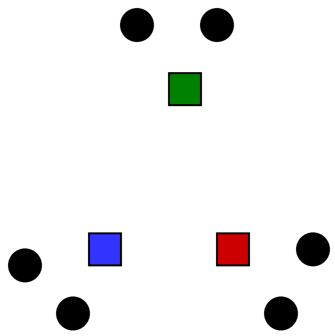


Initialization

- K-means is sensitive to initialization
  - It does matter what you pick!
  - What can go wrong?

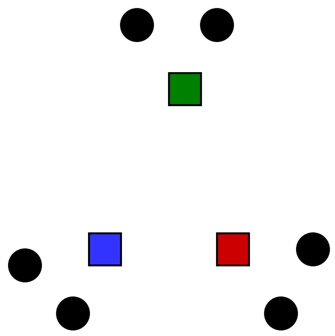
Initialization

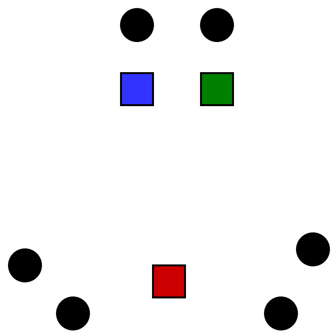
- K-means is sensitive to initialization
  - It does matter what you pick!
  - What can go wrong?



Initialization

- K-means is sensitive to initialization
  - It does matter what you pick!
  - What can go wrong?
    - Various schemes to help alleviate this problem: initialization heuristics

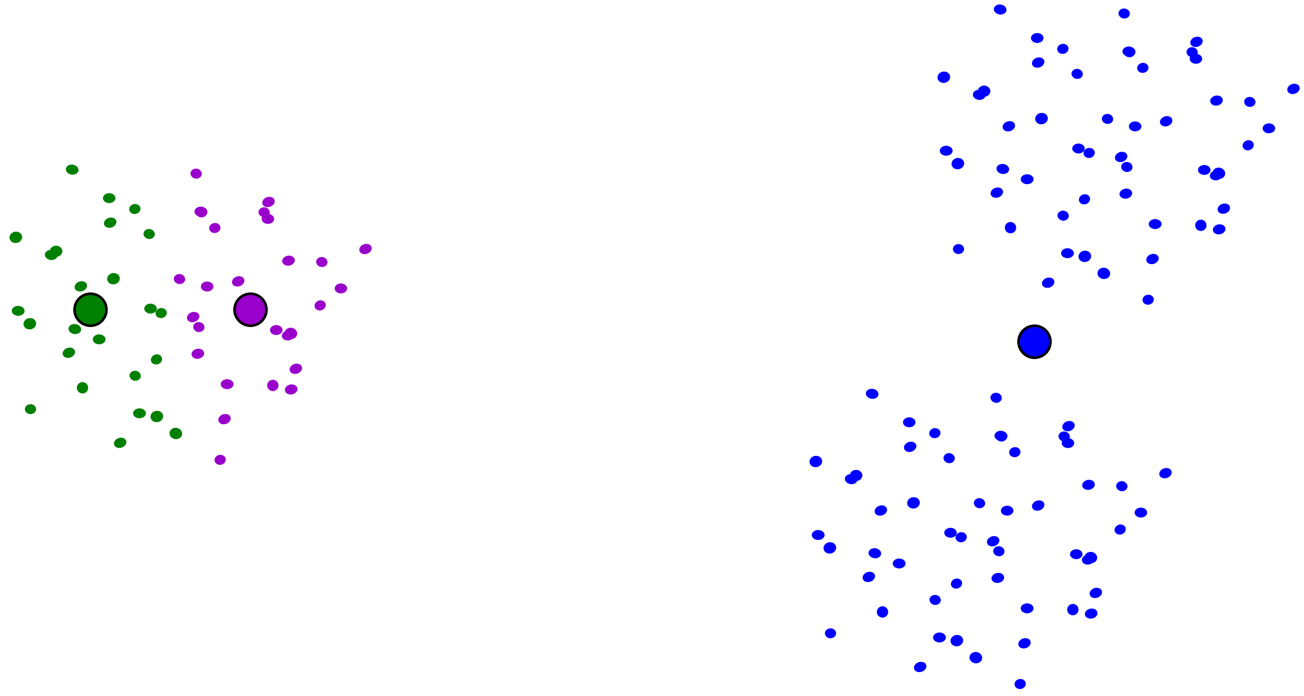




k-means Clustering

- Not clear how to figure out the "best" k in advance
- Want to choose k to pick out the interesting clusters, but not to overfit the data points
  - Large k doesn't necessarily pick out interesting clusters
  - Small k can result in large clusters than can be broken down further

Local Optima

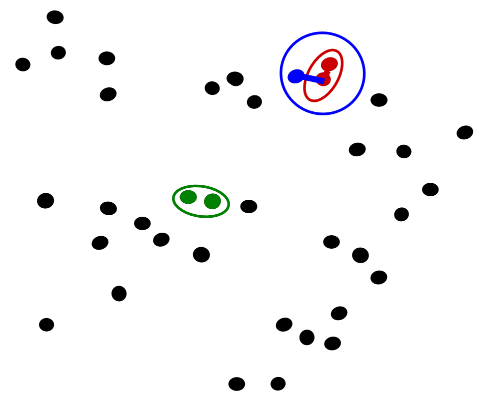


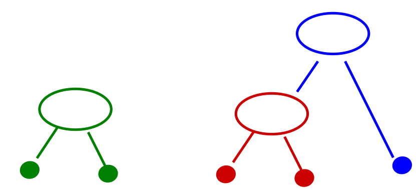
k-Means Summary

- Guaranteed to converge
  - But not to a global optimum
- Choice of k and initialization can greatly affect the outcome
- Runtime: $O(kM)$ per iteration
- Popular because it is fast, though there are other clustering methods that may be more suitable depending on your data

Hierarchical Clustering

- Agglomerative clustering
  - 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 is only one cluster left

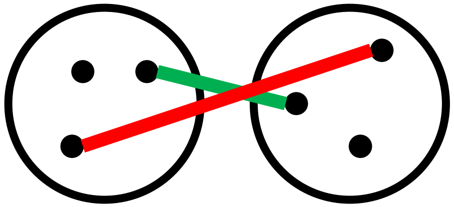




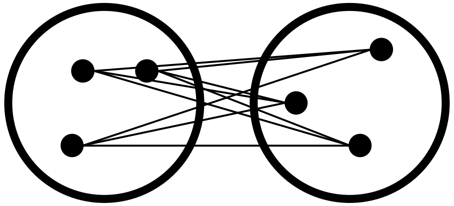
- Produces not one clustering, but a family of clusterings represented by a dendrogram

Agglomerative Clustering

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



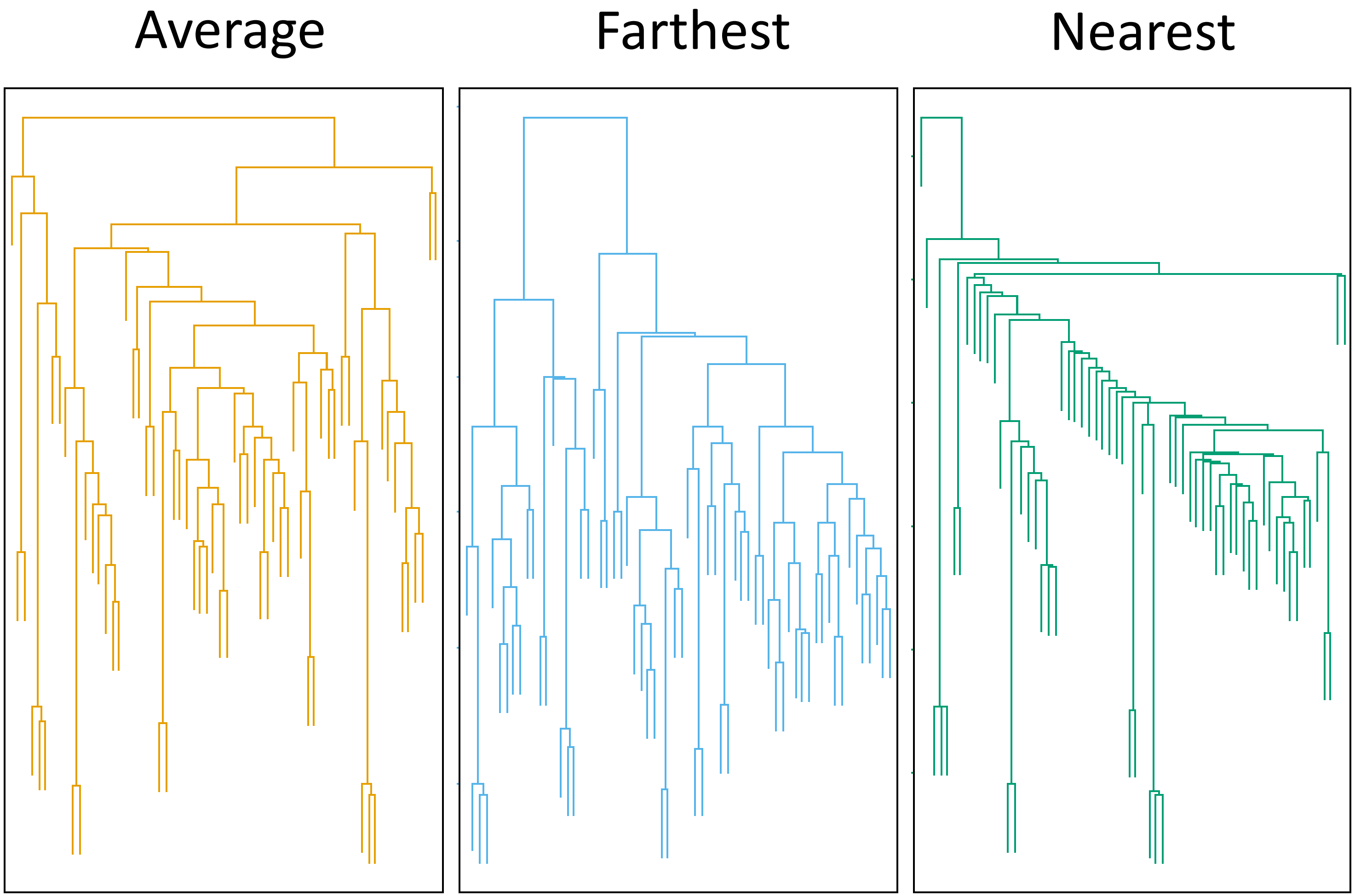
Closest / farthest pair



Average of all pairs

- Many more choices, each produces a different clustering...

Clustering Behavior



Mouse tumor data from [Hastie]