# Unsupervised Learning: Clustering

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Based on the slides of Vibhav Gogate

# Announcements

- Midterm (next Monday in class)
  - Closed book, closed notes, etc. (just you and a pencil)
  - Try to arrive as early as possible so as to maximize your exam taking time
  - Covers everything up to the end of boosting
  - Be prepared for theoretical questions!
  - The exam is worth a significant percentage of the grade, talk to other students and use Piazza to make sure that you are prepared!

# 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

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  - Useful for finding the important parameters/features of a dataset

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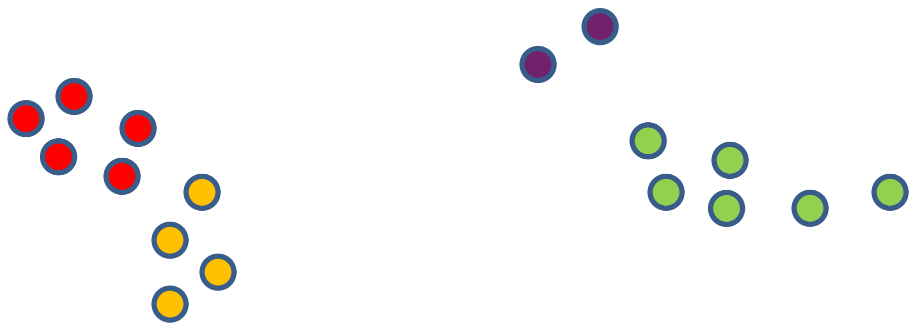


# Clustering

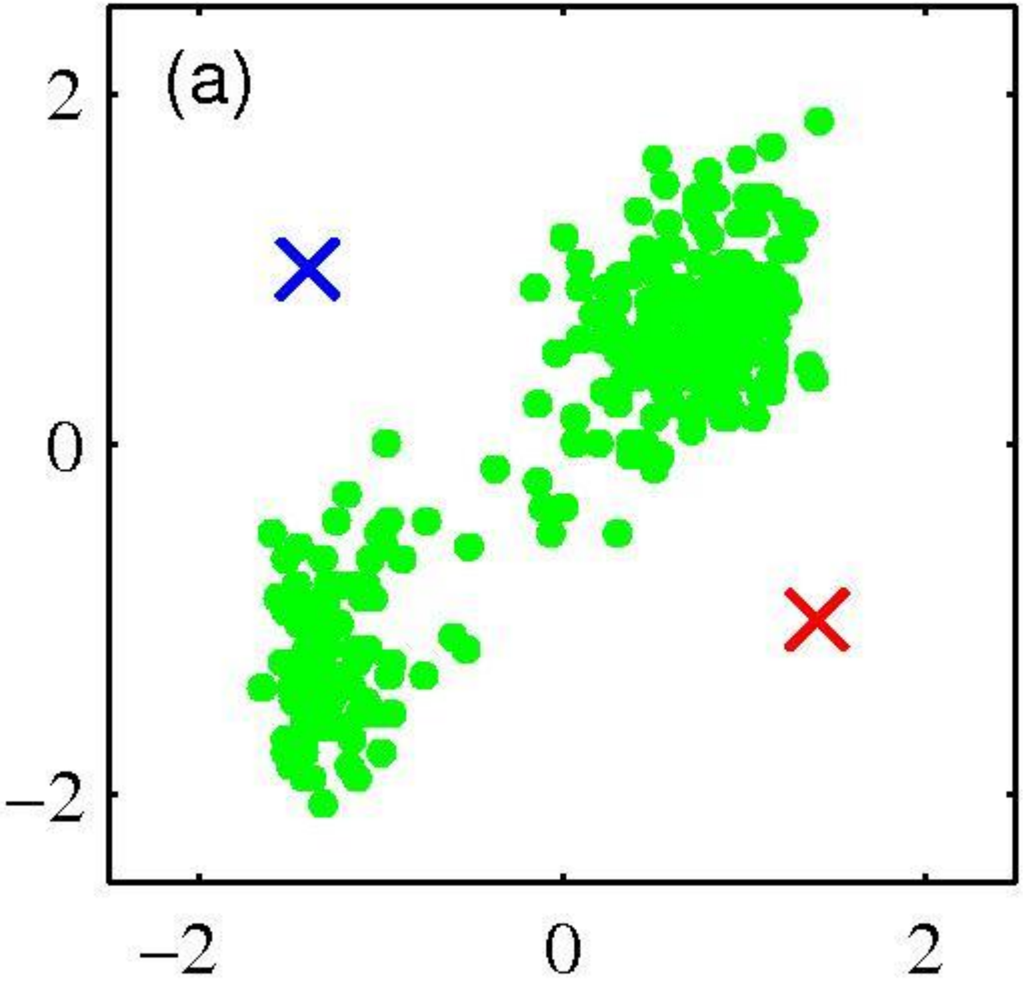
- Input: a collection of points $\mathrm{x}_1, \ldots, \mathrm{x}_\mathrm{n} \in \mathbb{R}^m$, an integer $k$

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

# $k$-means Clustering

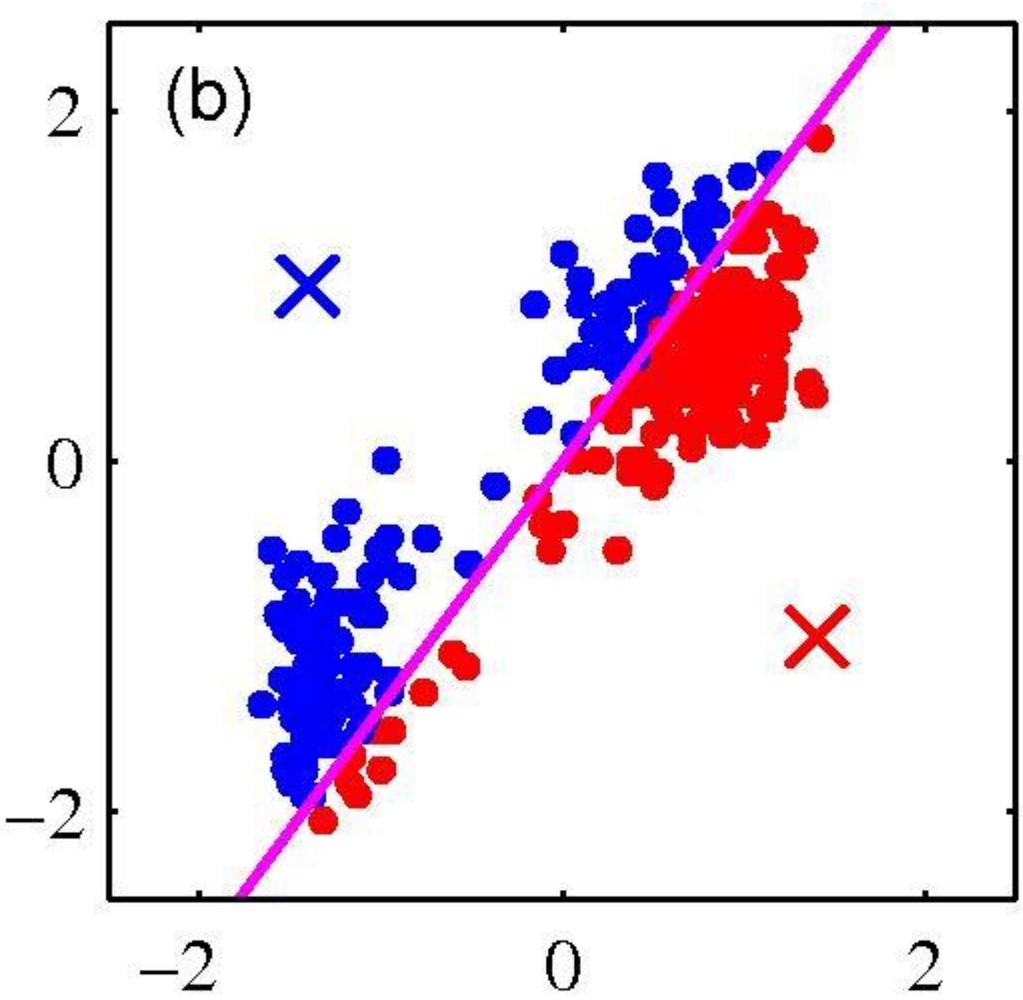
- Pick an initial set of $k$ means (usually at random)
- Repeat until the clusters do not change:
  - Partition the data points, assigning each data point to a cluster based on the mean that is closest to it
  - Update the cluster means so that the $i^{th}$ mean is equal to the average of all data points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

# $k$-means clustering: Example




Pick $k$ random points as cluster centers (means)

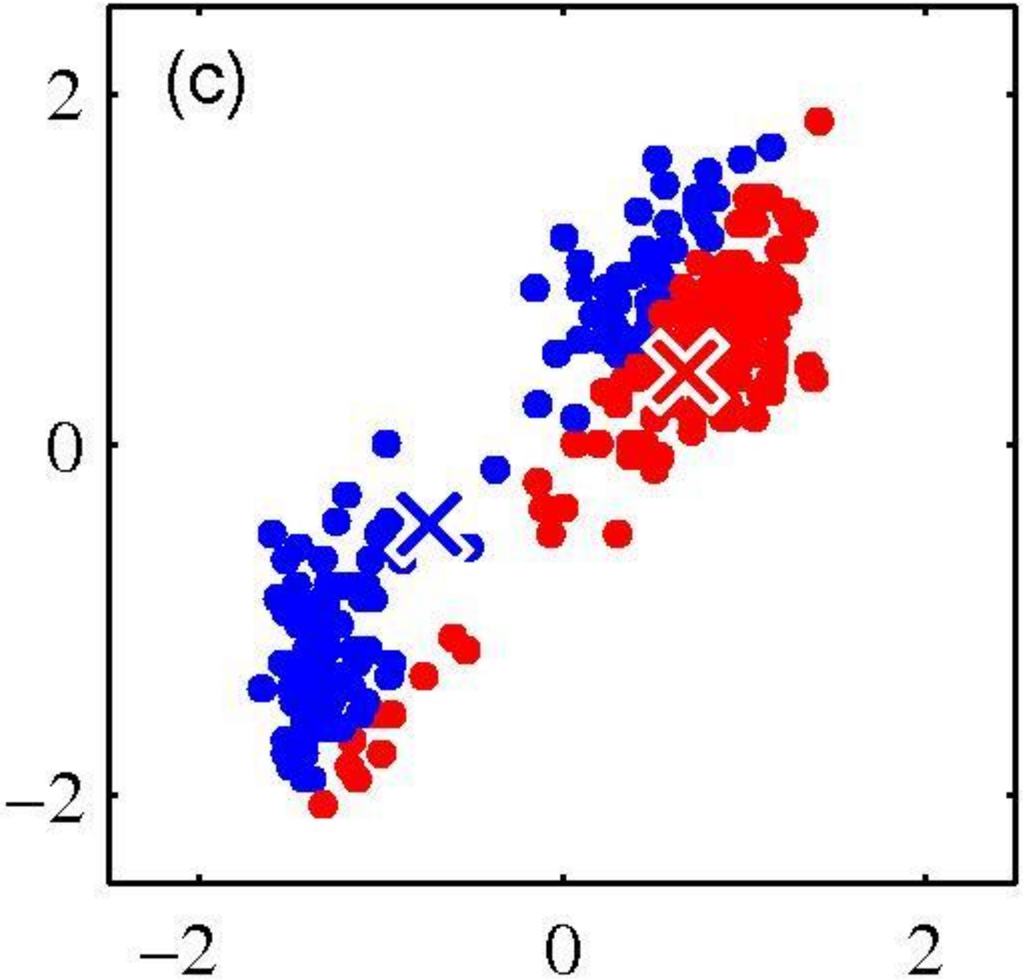
# $k$-means clustering: Example




Iterative Step 1:

Assign data instances to closest cluster center

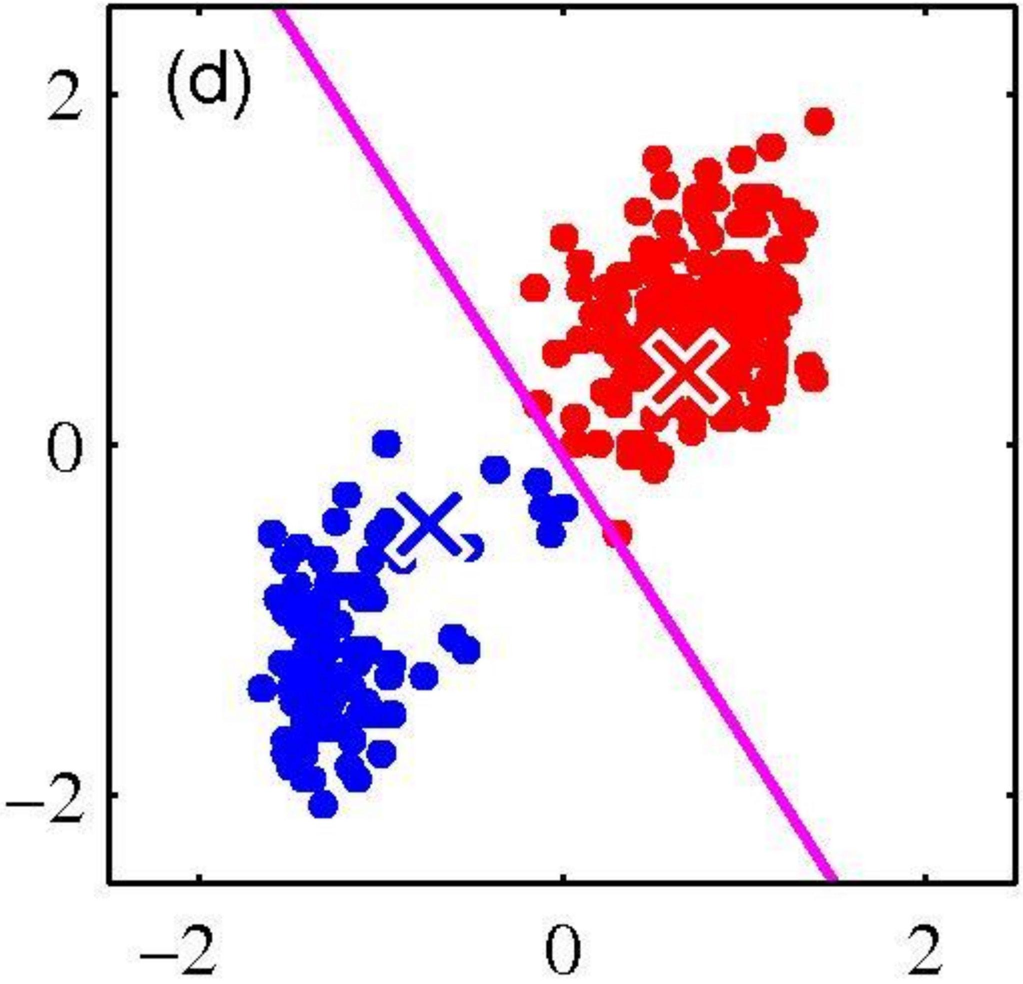
# $k$-means clustering: Example




Iterative Step 2:

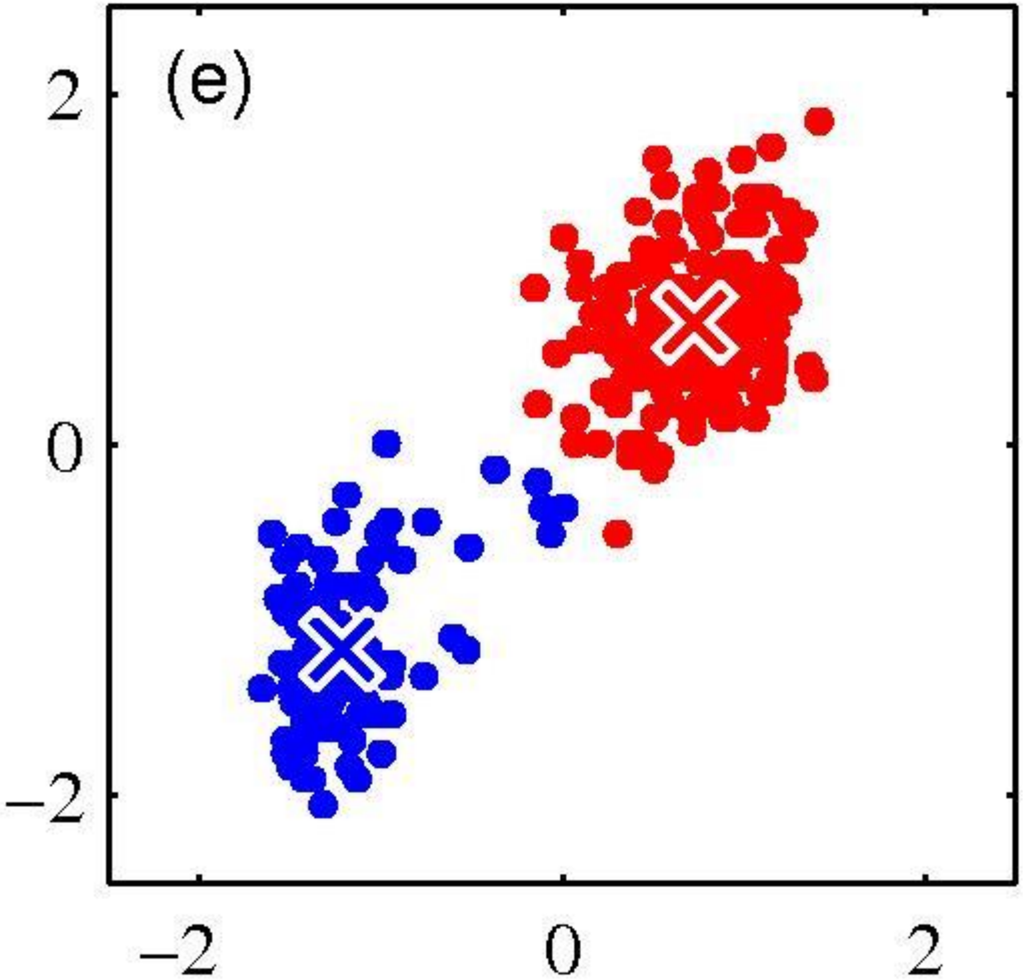
Change the cluster center to the average of the assigned points

# $k$-means clustering: Example




Repeat until convergence

# $k$-means clustering: Example



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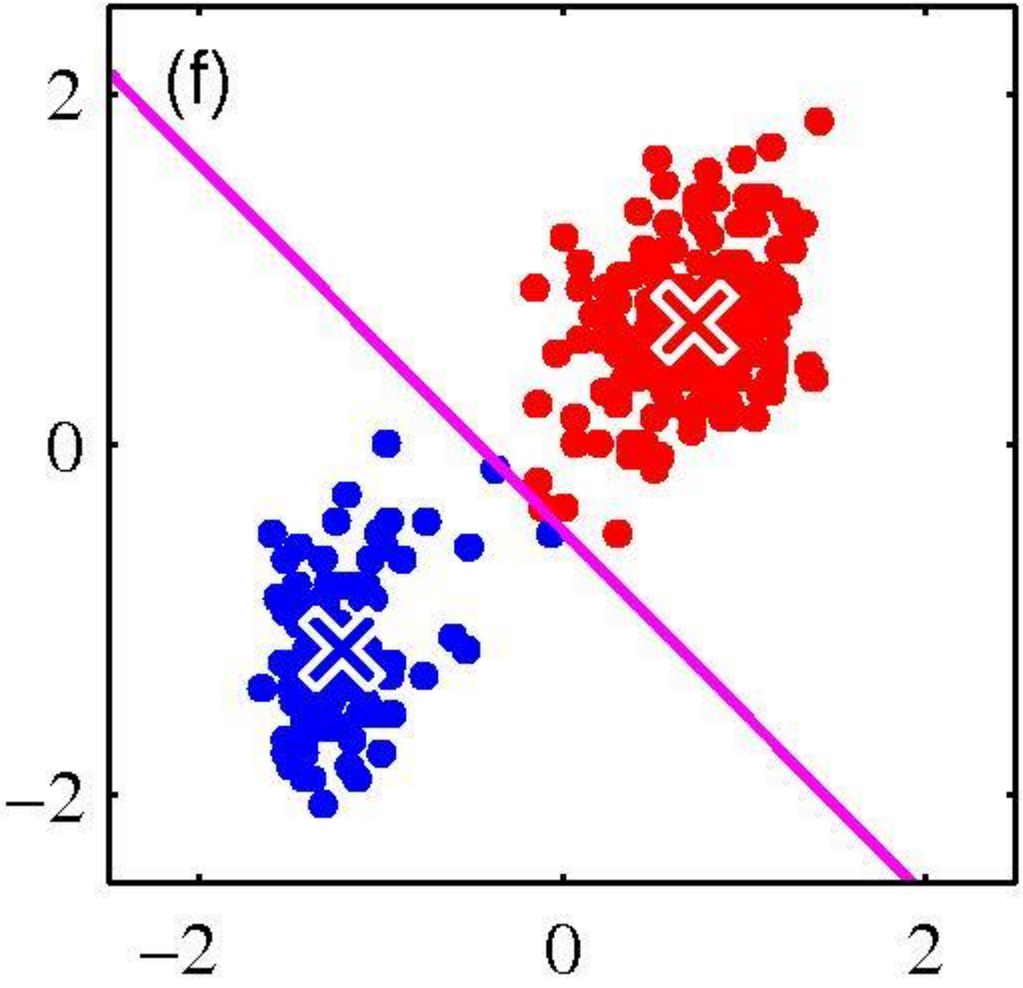

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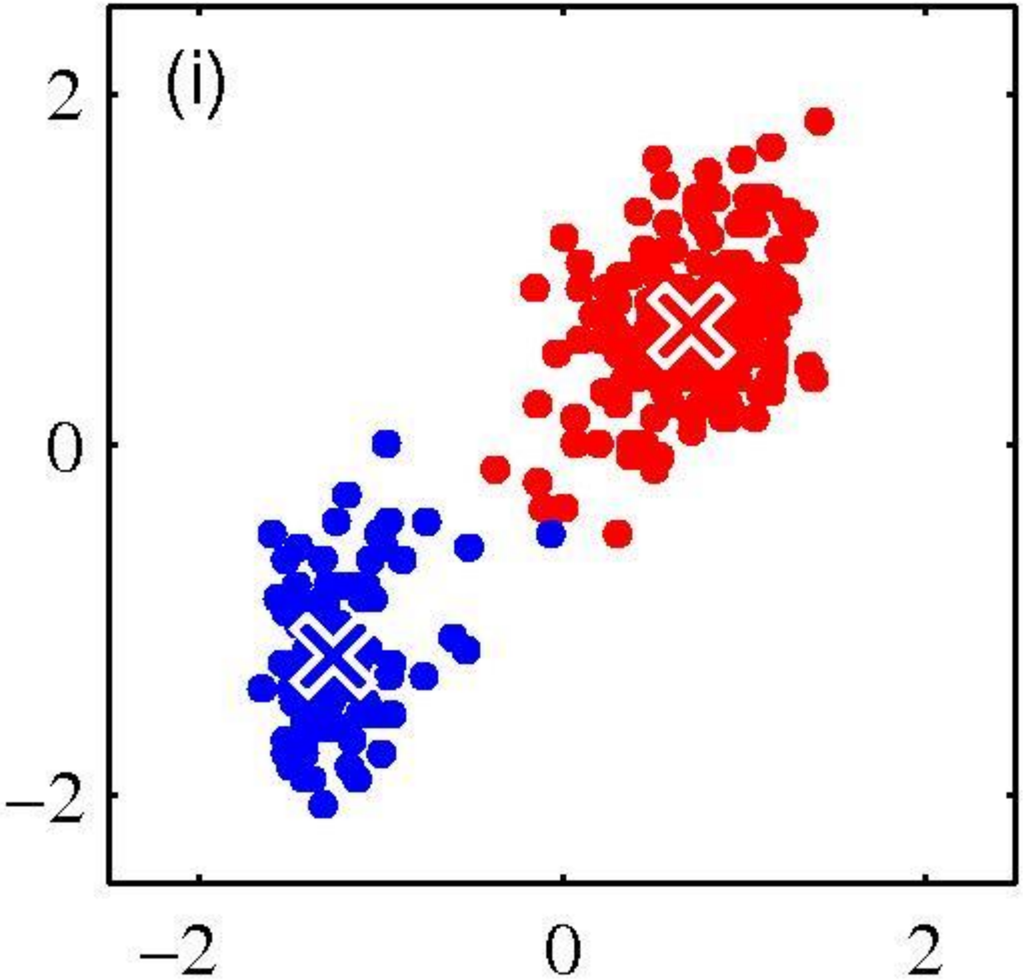

# $k$-Means for Segmentation

$k = 2$

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

– $S_i \subseteq \{1, \ldots, n\}$ is the $i^{th}$ cluster

– $S_i \cap S_j = \emptyset$ for $i \neq j$, $\cup_i S_i = \{1, \ldots, n\}$

– $\mu_i$ is the centroid of the $i^{th}$ cluster

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



UTD

# $k$-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

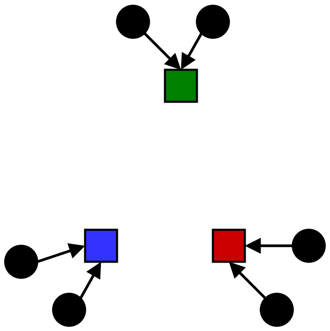
- Consider the $k$-means objective function

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

points

cluster assignments

cluster means



- Two stages each iteration
  - Update cluster assignments: fix means $\mu$, change assignments $S$
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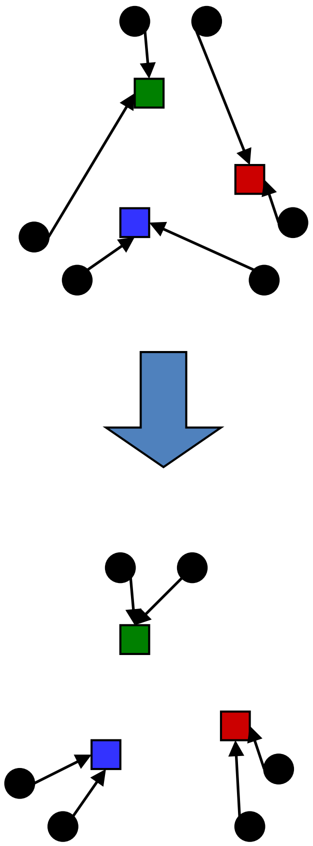
# Phase I: Update Assignments

- 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 $\phi$ as the sum of the distances of all points to their respective means must decrease**

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

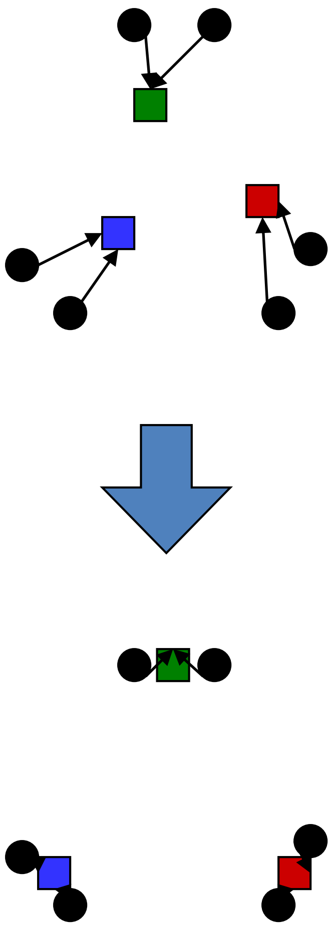


# Phase II: Update Means

- 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?



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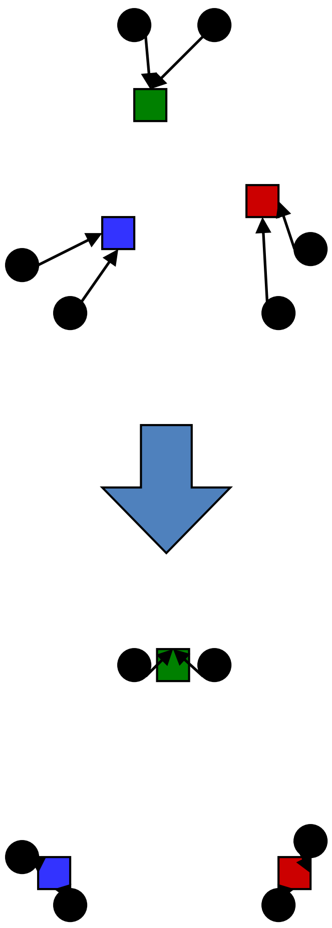
- Also can only decrease total distance…
  - The point $y$ with minimum squared Euclidean distance to a set of points is their mean



# Initialization

- K-means is sensitive to initialization
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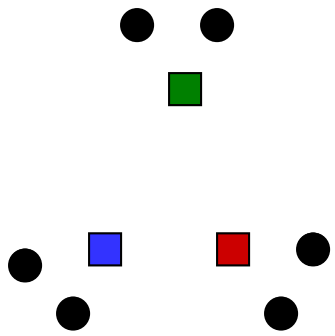
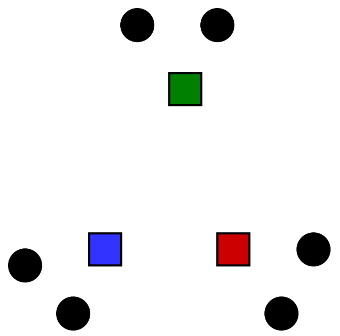
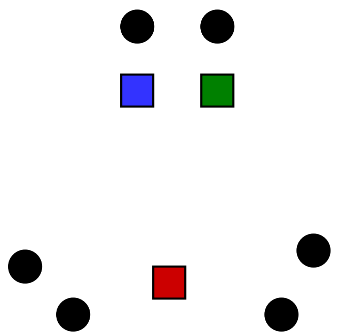


# Initialization

- 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

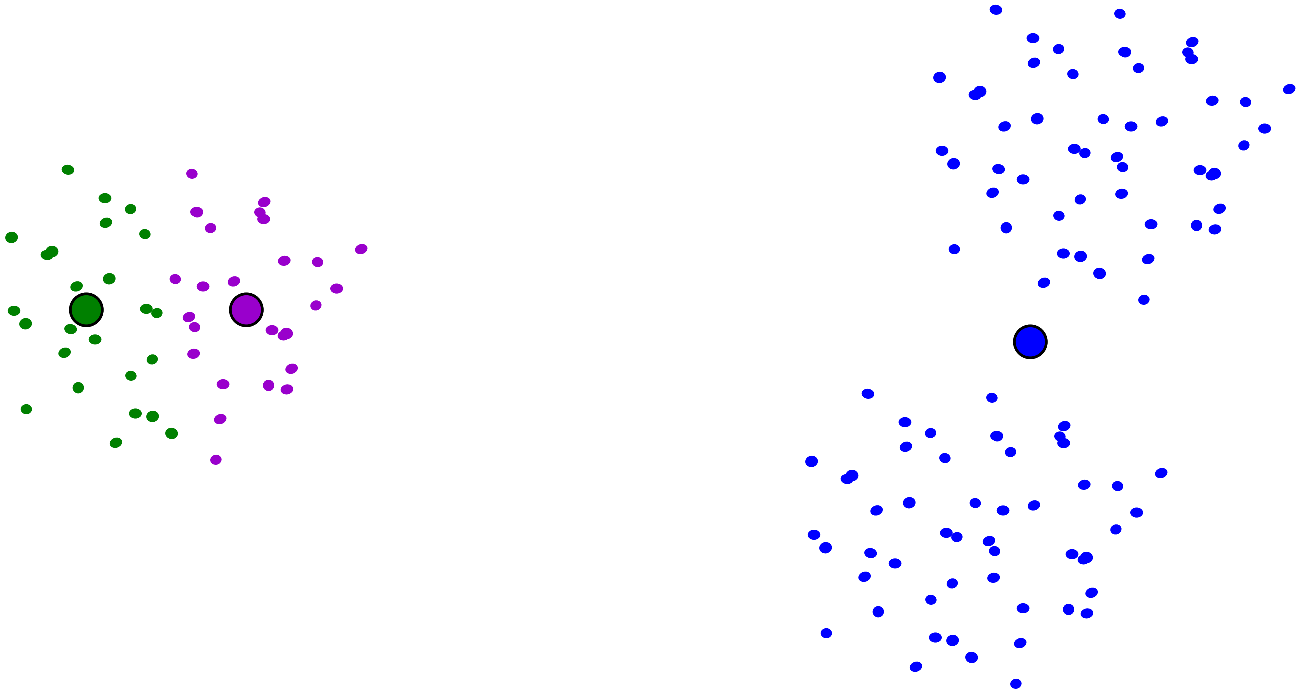




# $k$-means Clustering

- Not clear how to figure out the "best" $k$ in advance
- Want to choose $k$ to pick out the interesting clusters, but not to over fit 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

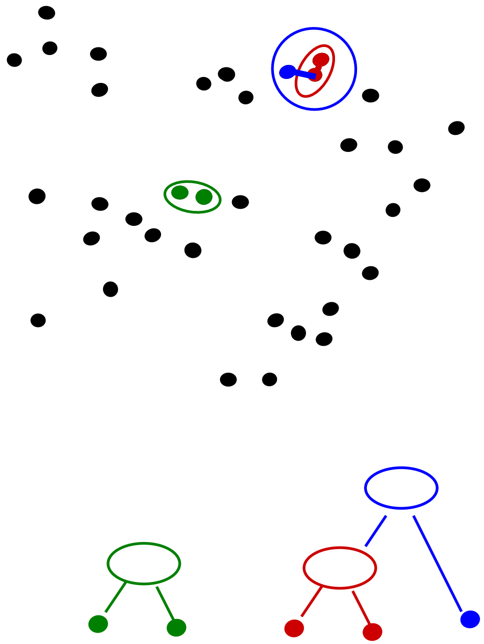


# $k$-Means Summary

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

# Hierarchical Clustering

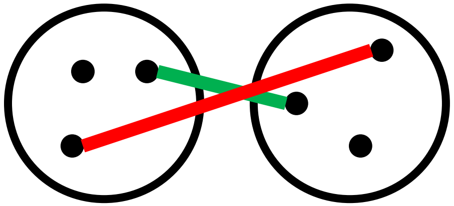
- Agglomerative clustering
  - Incrementally build larger clusters out of smaller clusters
- Algorithm:
  - Maintain a set of clusters
  - Initially, each instance in its own cluster
  - Repeat:
    - Pick the two closest clusters
    - Merge them into a new cluster
    - Stop when there is only one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



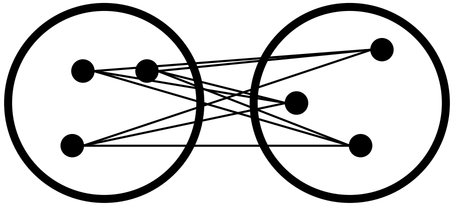
- Produces not one clustering, but a family of clusterings represented by a dendrogram

# Agglomerative Clustering

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



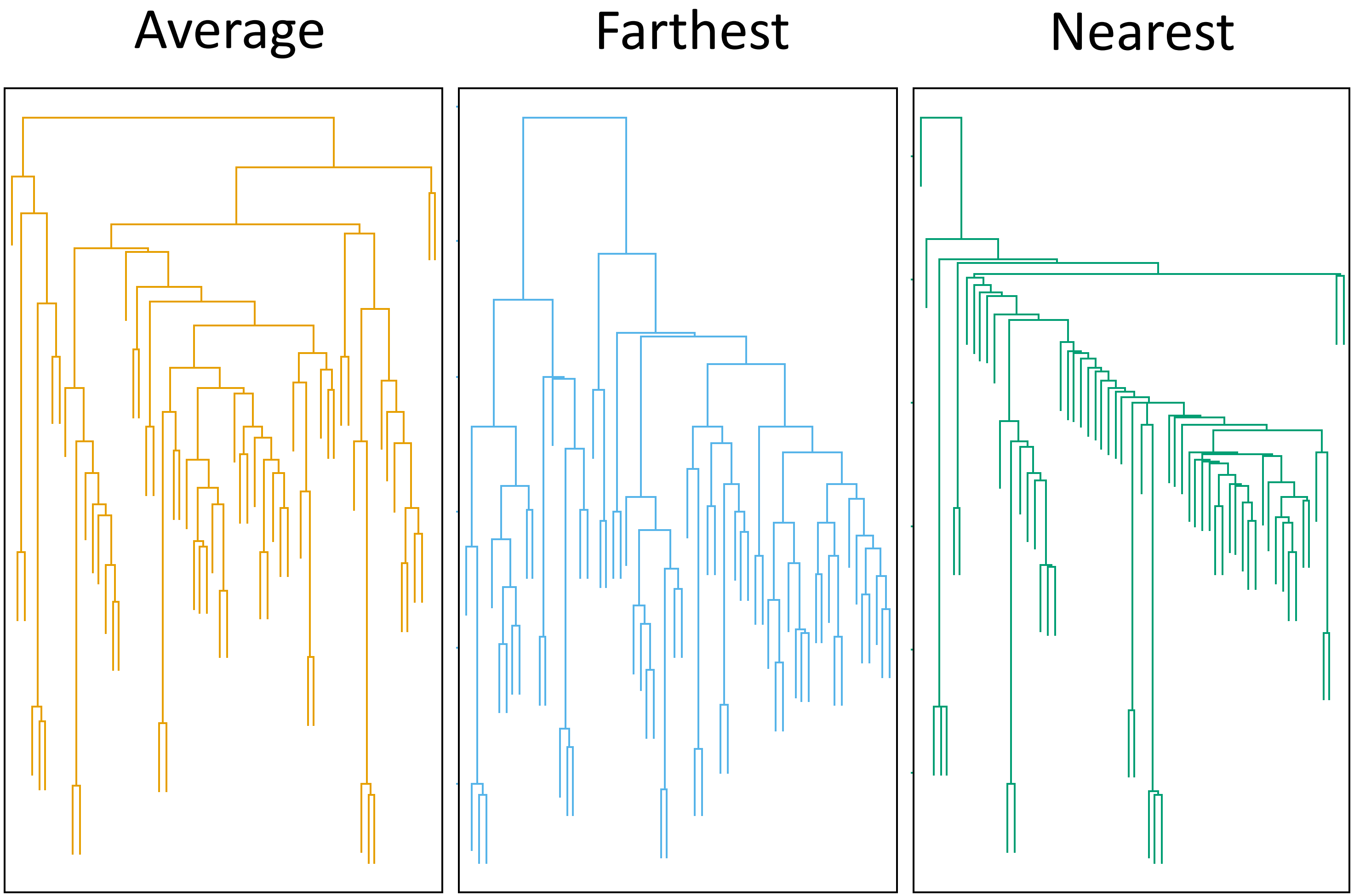
Closest / farthest pair



Average of all pairs

- Many more choices, each produces a different clustering…

# Clustering Behavior




Mouse tumor data from [Hastie]