CSE/STAT 416

k-means Clustering

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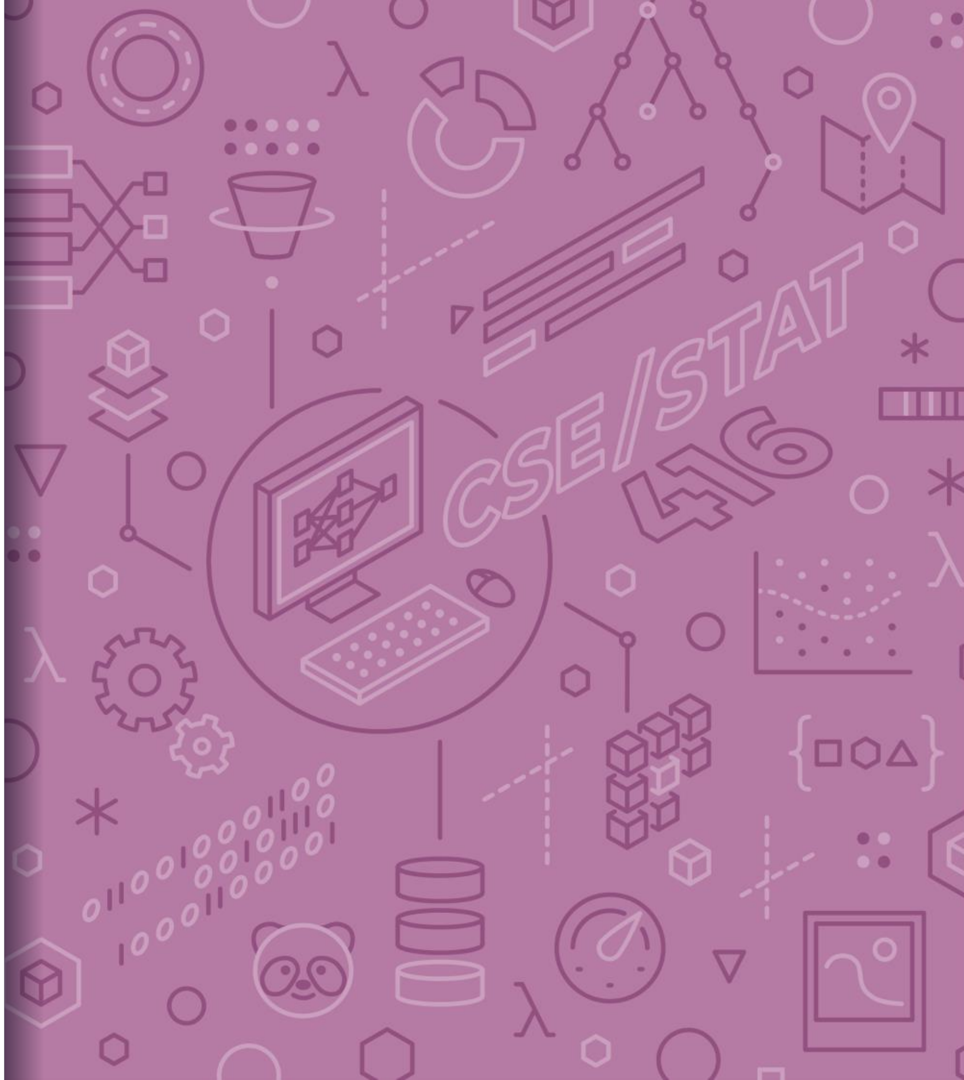
❓ **Questions?** Raise hand or **sli.do #cs416**
🎵 **Listening to:** Peach Pit



Clustering Overview

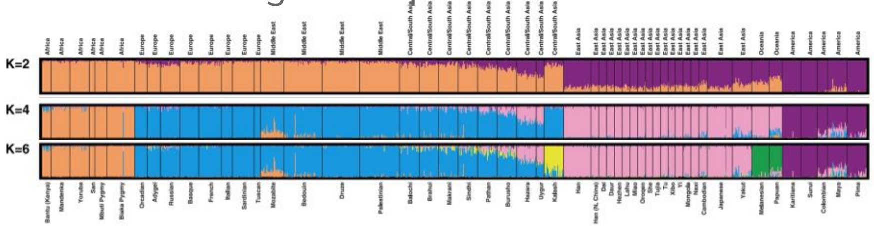
Recap

- For the past 7 weeks, we have covered different **supervised learning** algorithms
- Now, we're going to explore **unsupervised learning** methods where don't have labels / outputs in your datasets anymore.
- Note that several of the concepts you learnt for supervised learning, such as cross-validation, overfitting, bias-variance tradeoff, accuracy, error, etc. no longer apply in unsupervised learning!

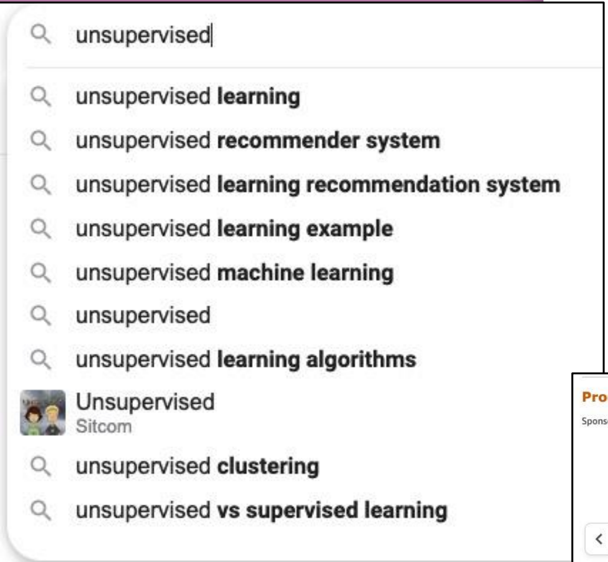
Unsupervised Learning

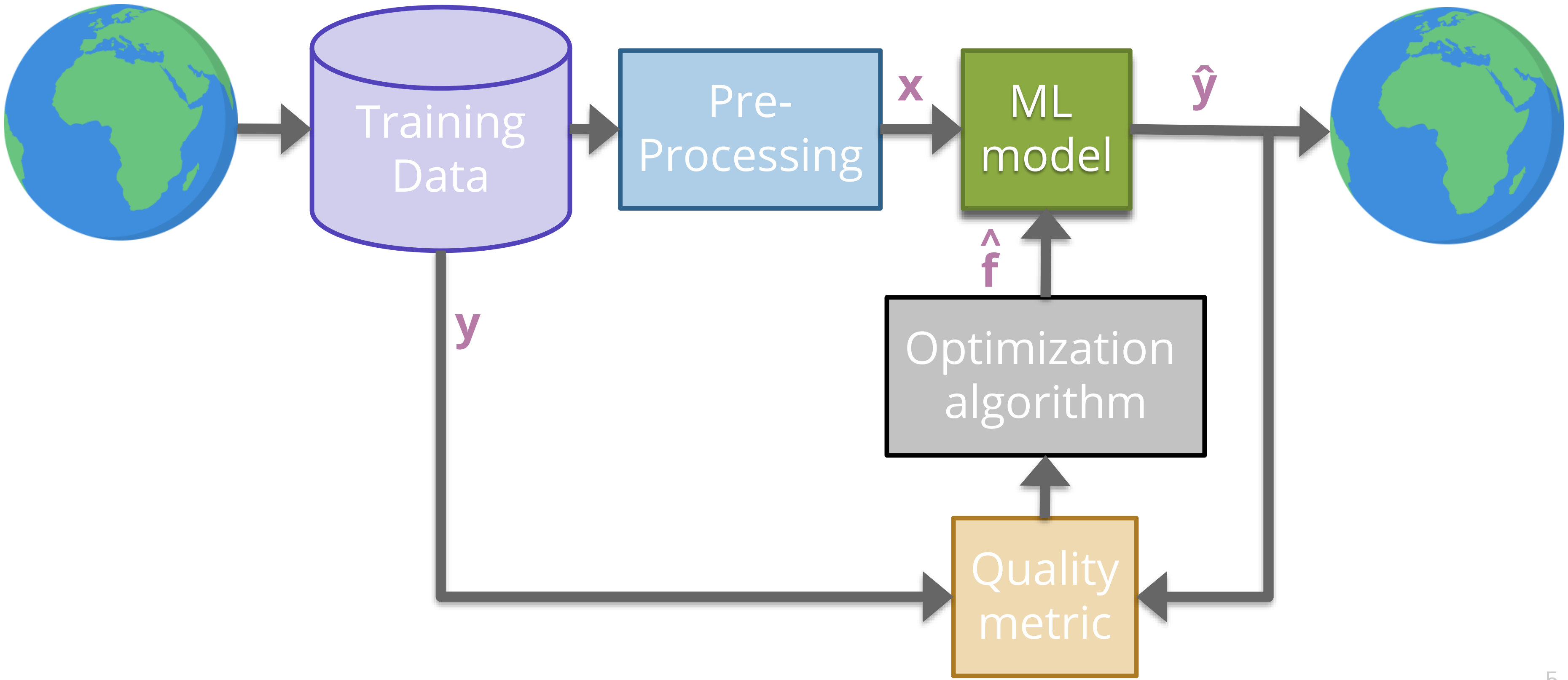
- A type of machine learning that detects underlying patterns in **unlabeled** data.
- Examples of unsupervised learning tasks:
  - Cluster similar articles together.

  - Cluster gene sequences.



  - Recommend items, searches, movies, etc.




Training Data
Pre-Processing
x
ML model
ŷ
f̂
y
Optimization algorithm
Quality metric

Clustering

SPORTS

WORLD NEWS

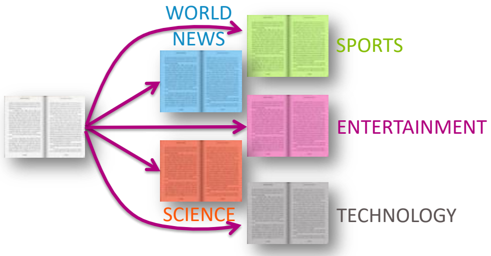
Note that we're not talking about learning user preferences (yet – come back next week ☺).

Our case study is **document retrieval**. Given that someone read a particular article, what similar articles would you recommend (without personalization)?

Labeled Data

What if the labels are known? Given labeled training data.

Can do multi-class classification methods to predict label.

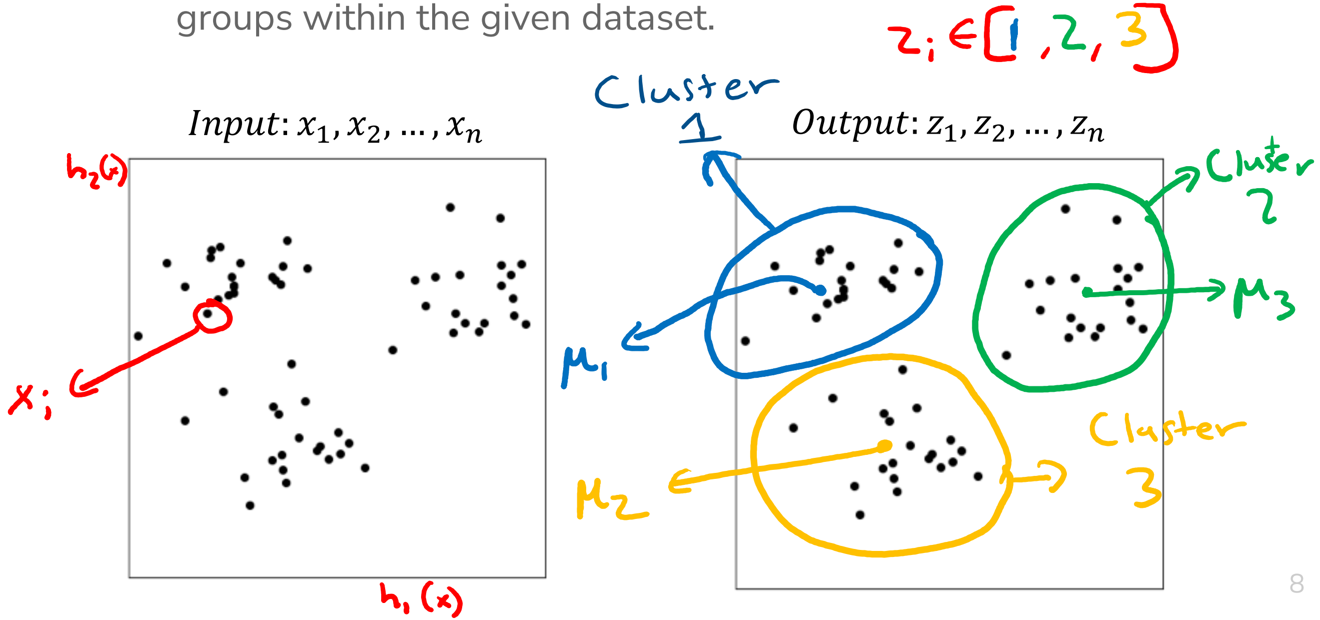


However, not all articles fit cleanly into one label.

Further, oftentimes real-world data doesn't have labels.

Unlabeled Data

- In many real world contexts, there aren't clearly defined labels so we won't be able to do classification
- We will need to come up with methods that uncover structure from the (unlabeled) input data X.
- **Clustering** is an automatic process of trying to find related groups within the given dataset.



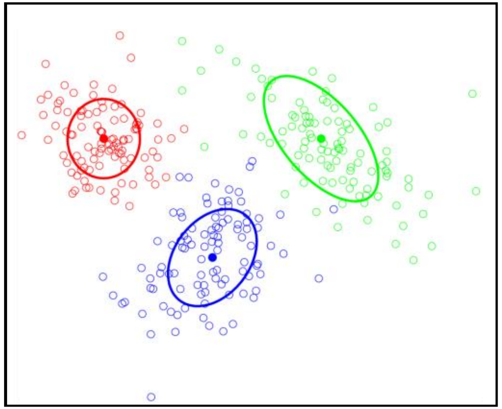
Define Clusters

In their simplest form, a **cluster** is defined by

- The location of its center (**centroid**)
- Shape and size of its **spread**

Clustering is the process of finding these clusters and **assigning** each example to a particular cluster.

- x_i gets assigned $z_i \in [1, 2, \ldots, k]$
- Usually based on closest centroid



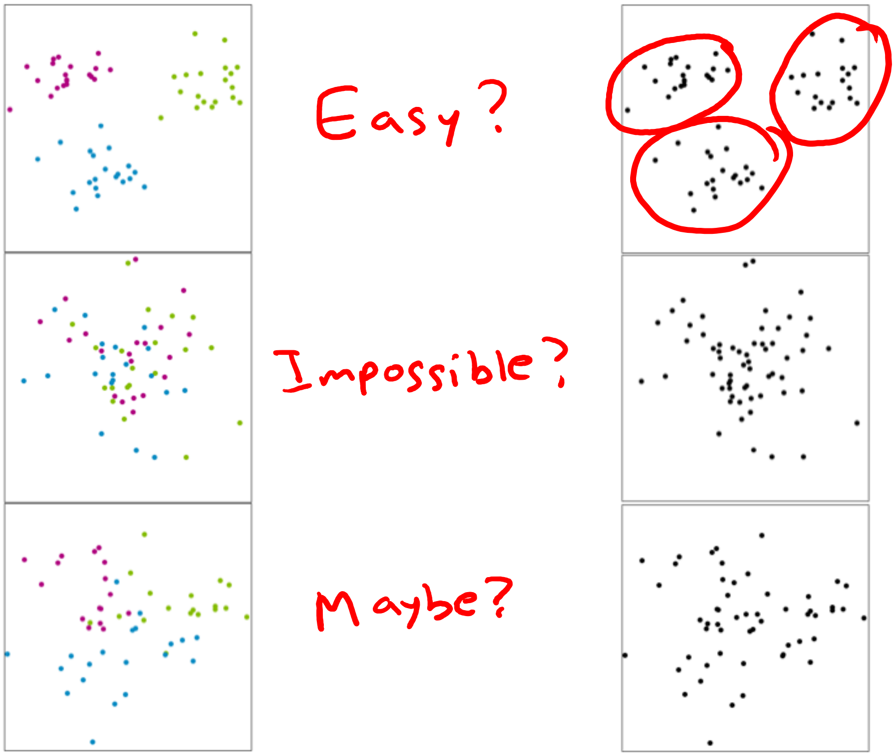
Will define some kind of objective function for a clustering that determines how good the assignments are

- Based on distance of assigned examples to each cluster.
- Close distance reflects strong similarity between datapoints.

When Might This Work?

Clustering is easy when distance captures the clusters.

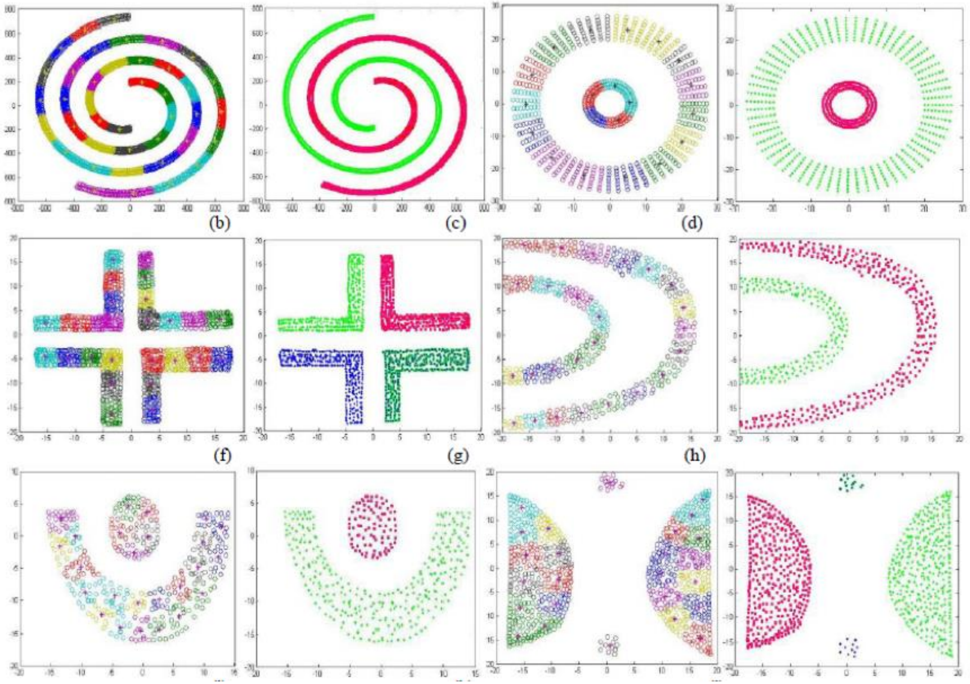
Ground Truth (not visible) Given Data



Not Always Easy

There are many clusters that are harder to learn with this setup

- Distance does not determine clusters



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Group

2 min

Think of 1-2 problems that you might want to use clustering for.

For each problem, describe:

- Why unsupervised learning is the right approach.
- What the input features are for the clustering algorithm.
- What clusters you hypothesize would emerge.

Hyperparameter

centroid

K-Means Clustering

K-Means Clustering Algorithm

- We define the criterion of assigning point to a cluster based on **its distance.**
- Shorter distance => Better Clustering

Hyper parameter

Algorithm
Given a dataset of n datapoints and a particular choice of k

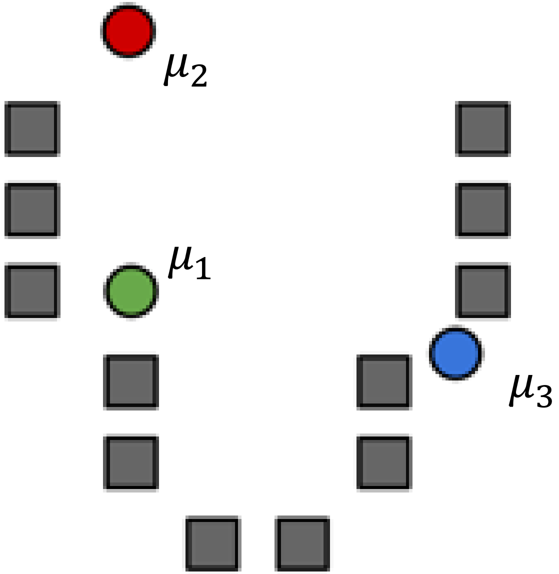
Step 0: Initialize cluster centroids randomly

Repeat until convergence:
  Step 1: Assign each example to its closest cluster centroid
  Step 2: Update the centroids to be the average of all the points assigned to that cluster

Step 0

Start by choosing the initial cluster centroids

- A common default choice is to choose centroids $\mu_1, \ldots, \mu_k$ randomly
- Will see later that there are smarter ways of initializing



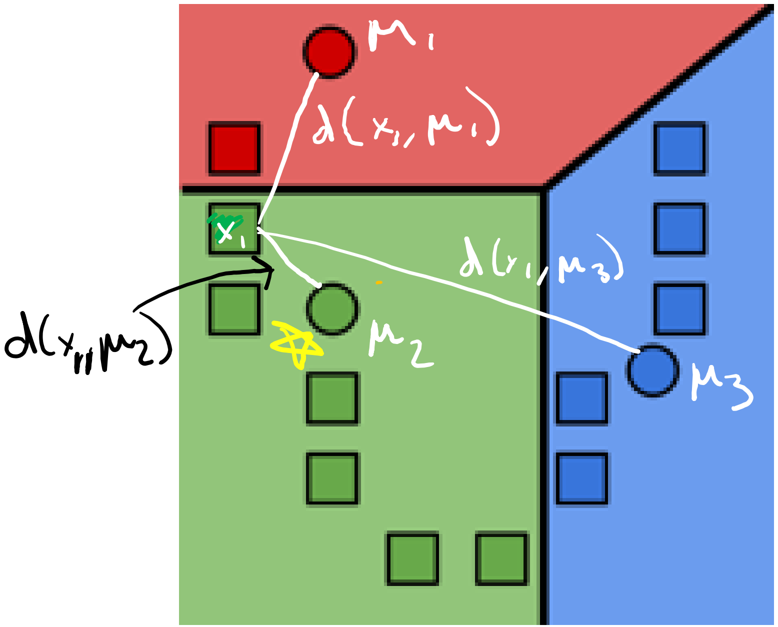
Step 1

Voronoi Tesselation

Assign each example to its closest cluster centroid

For i = 1 to n

$$z_i \leftarrow \underset{j \in [k]}{\operatorname{argmin}} \left\| \mu_j - x_i \right\|_2^2$$



Step 2

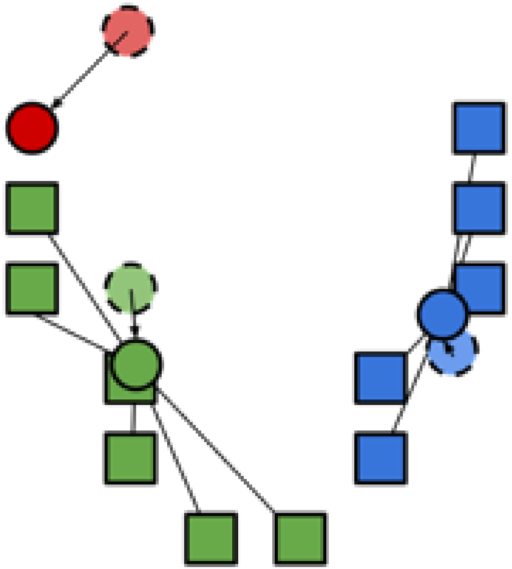
Update the centroids to be the mean of points assigned to that cluster.

$$\mu_j = \frac{\sum_{i=1}^{n} \mathbf{1}\{z_i = j\} x_i}{\sum_{i=1}^{n} \mathbf{1}\{z_i = j\}}$$

= sum of datapoints assigned to cluster j

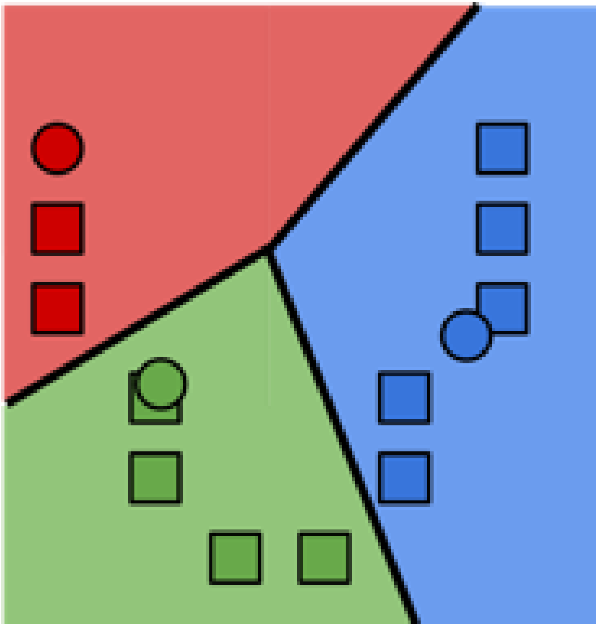
= number of datapoints assigned to cluster j

Computes center of mass for cluster!



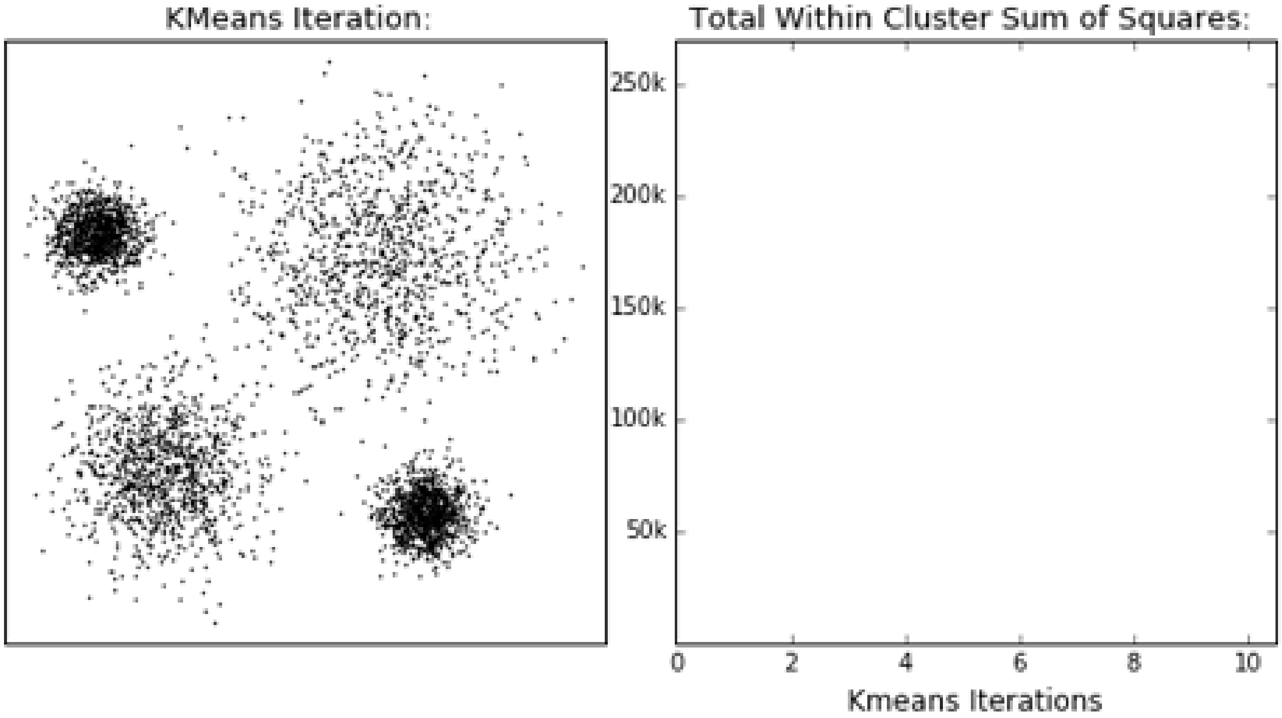
Repeat until convergence

Repeat Steps 1 and 2 until convergence



Stopping Conditions

- Cluster assignments haven't changed
- Centroids haven't changed
- Some number of max iterations have been passed



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Think

1 min

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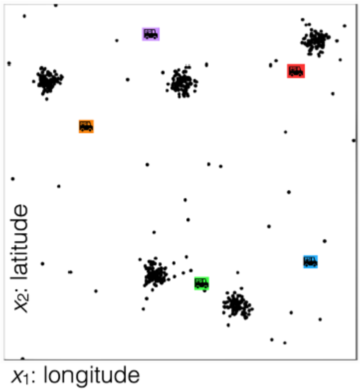
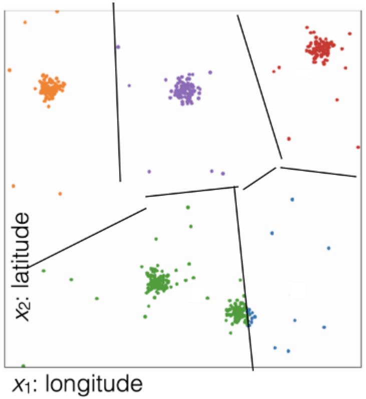
- What cluster assignment would result from these centroids?



Centroids



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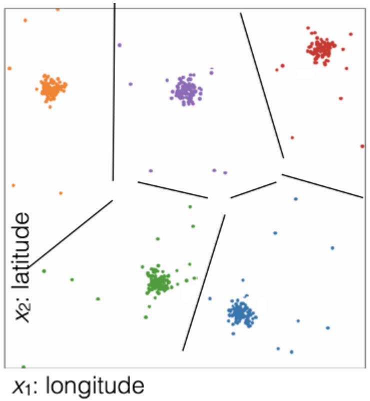

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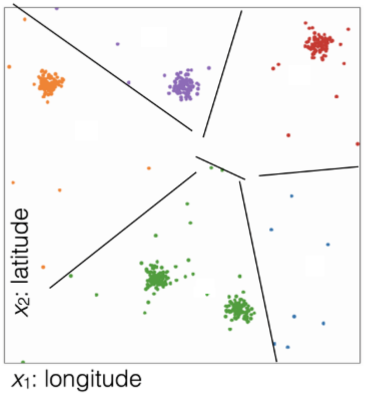

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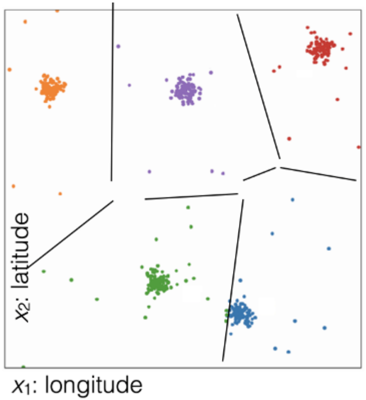

(C)

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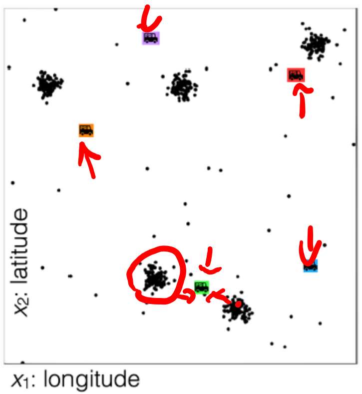
Group

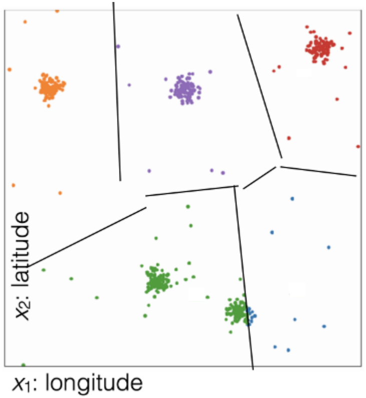
~~1~~ min
1.5 min

sli.do #cs416

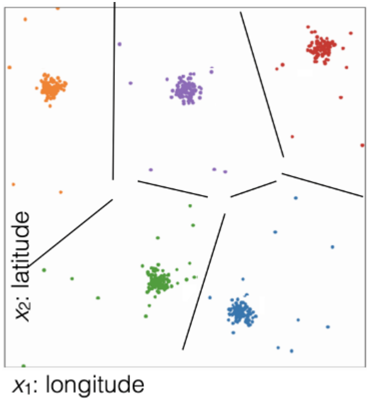
- What cluster assignment would result from these centroids?



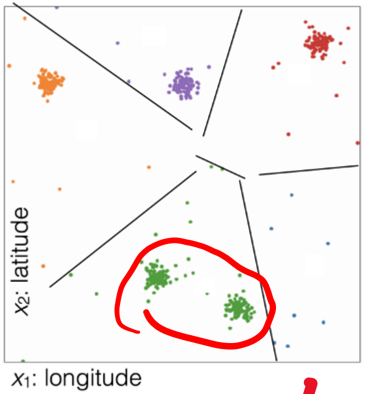
Centroids



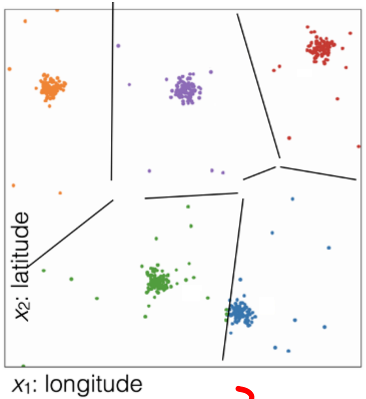
(D)



(A)



(B) ?



(C) ?

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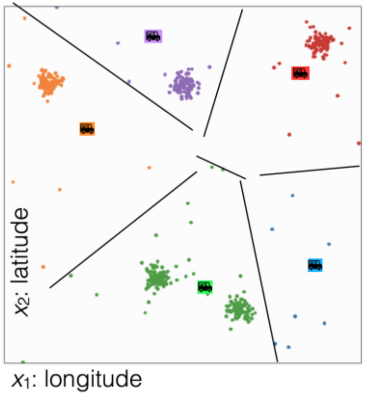
Think

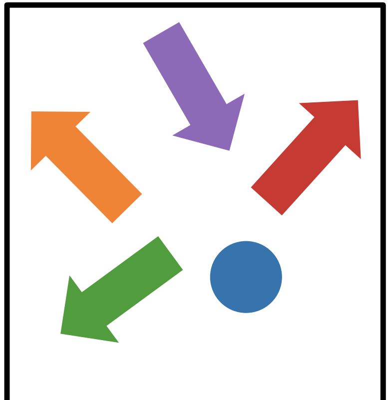
1 min

sli.do #cs416

- In what direction would each of the centroids (roughly) move?



Cluster Assignments



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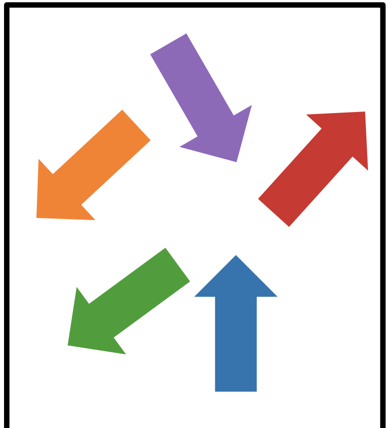
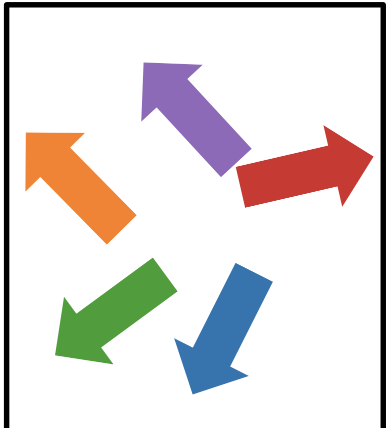


(A)



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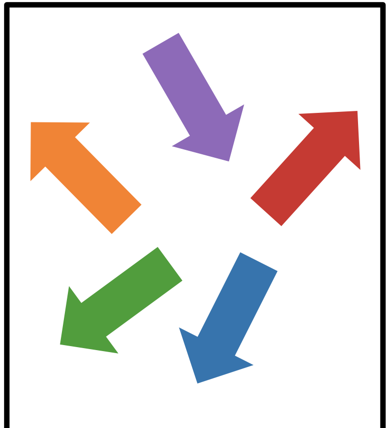

(C)

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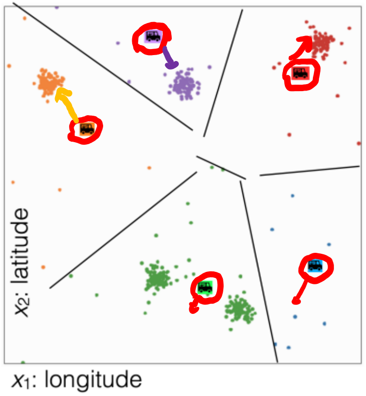
Group

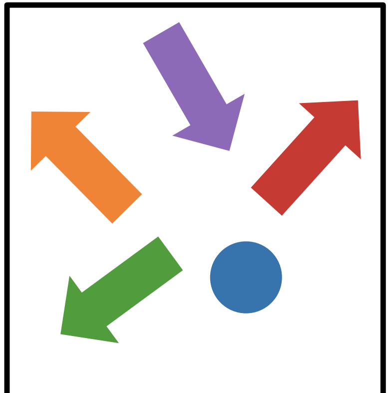
~~2~~ min
1 min

sli.do #cs416

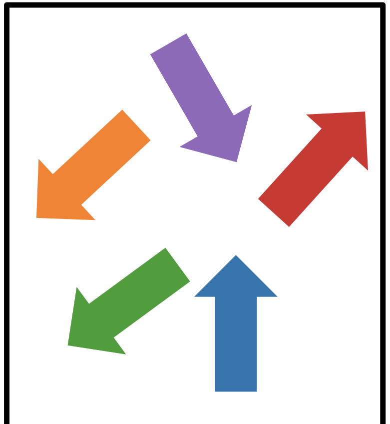
- In what direction would each of the centroids (roughly) move?



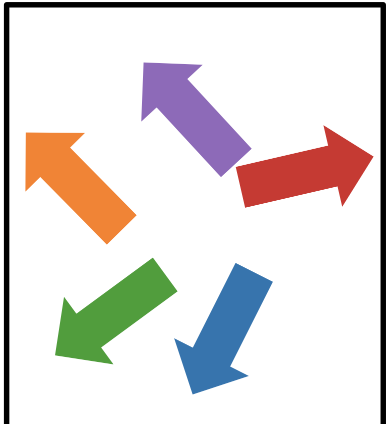
Cluster Assignments



(D) ?



(A)



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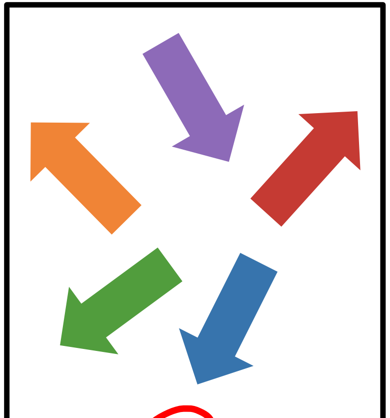
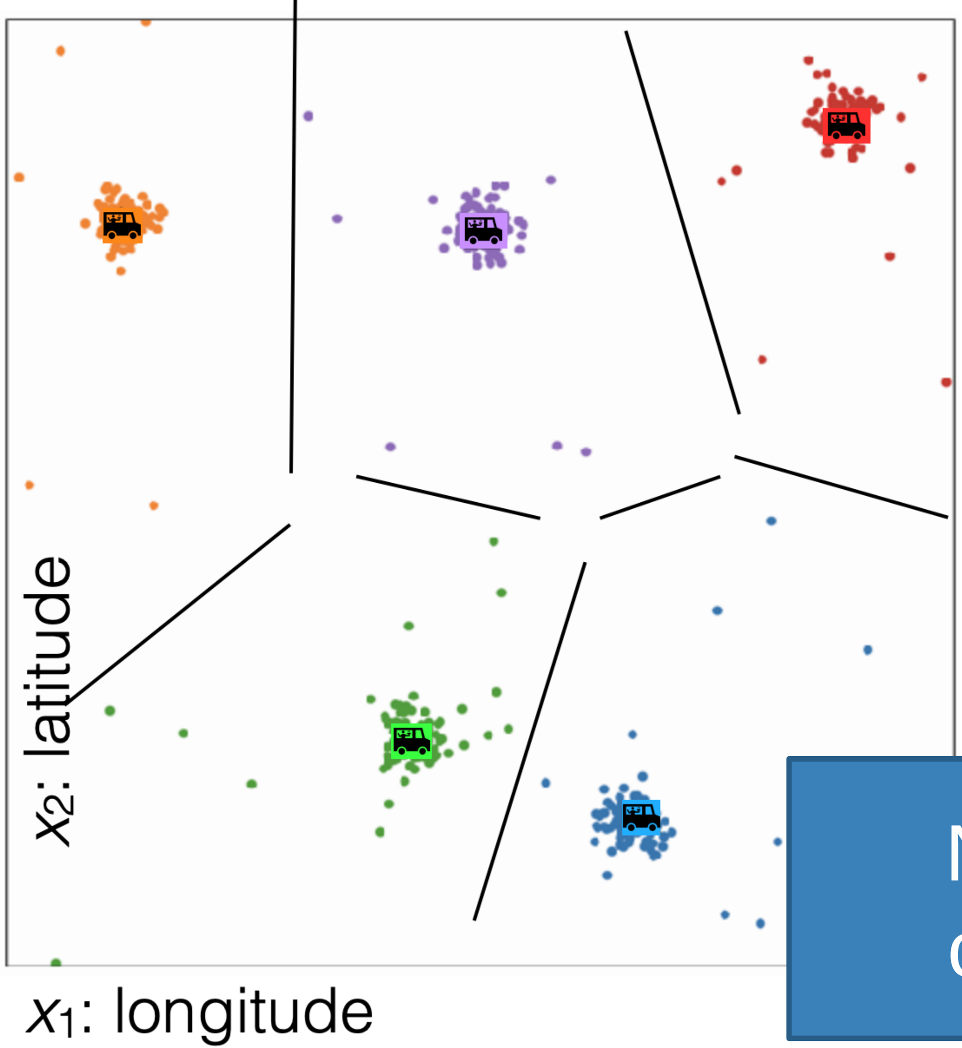


(C) ?

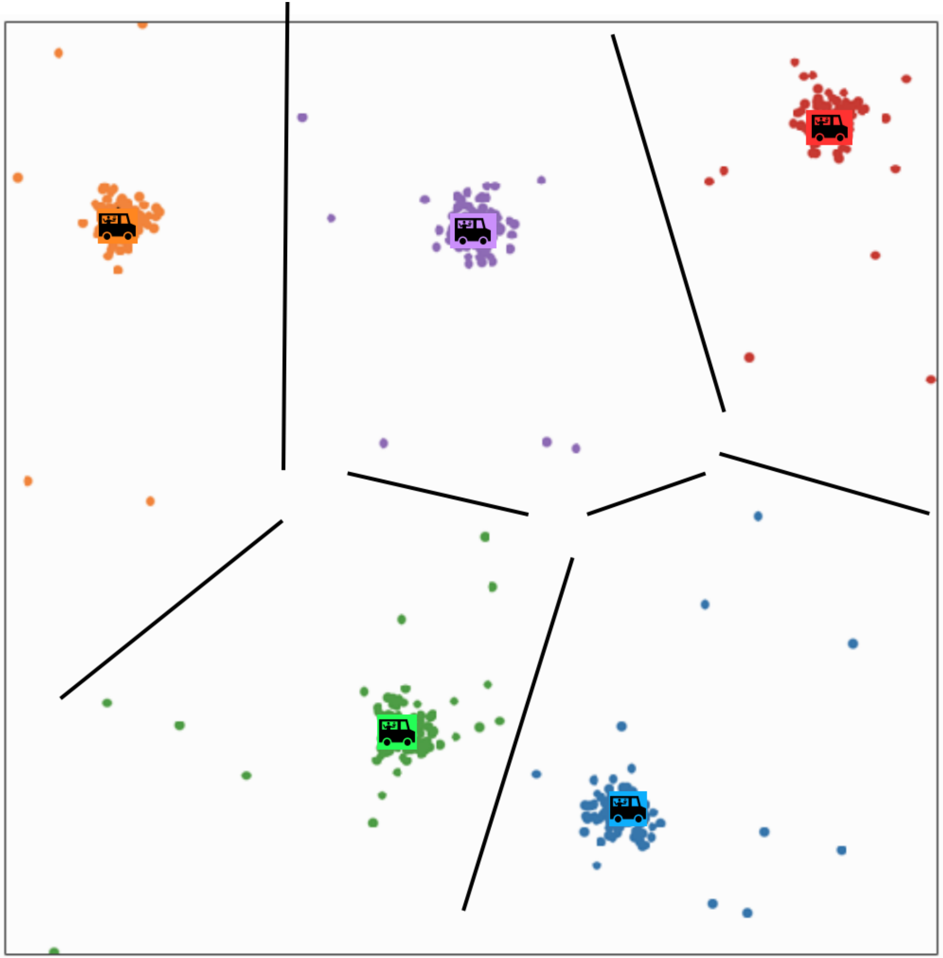


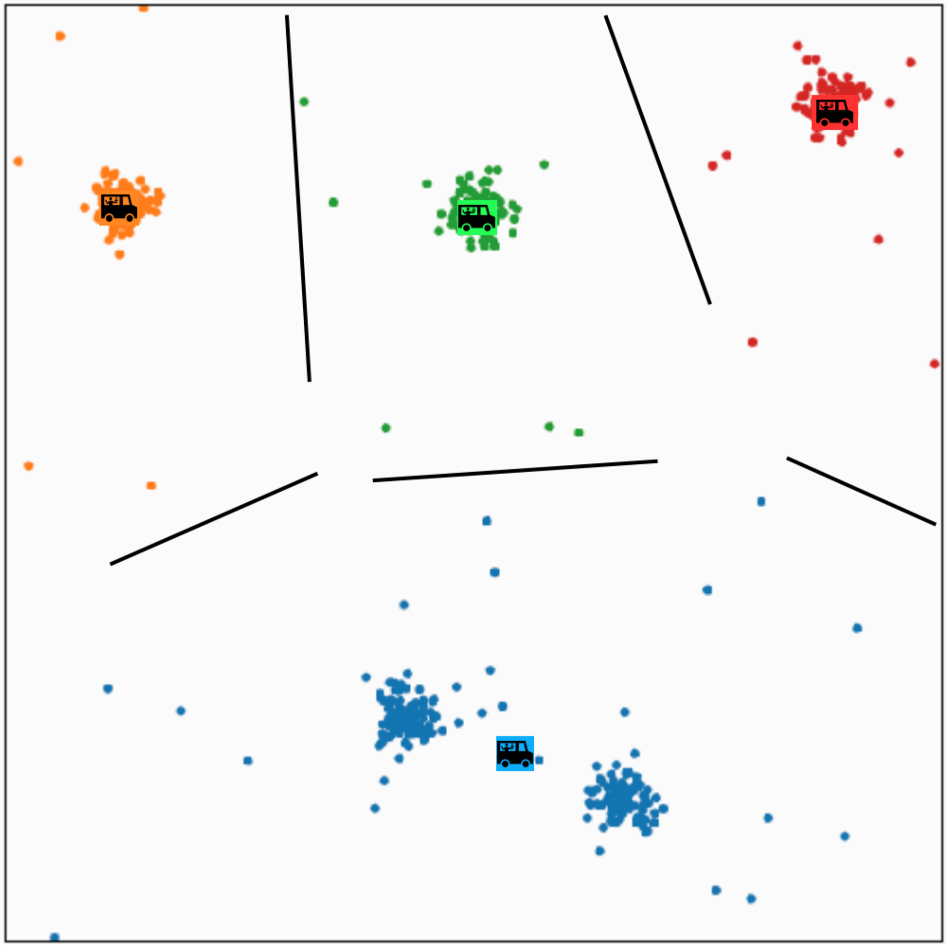
No more changes

Different k gives different results

K=5

K=4





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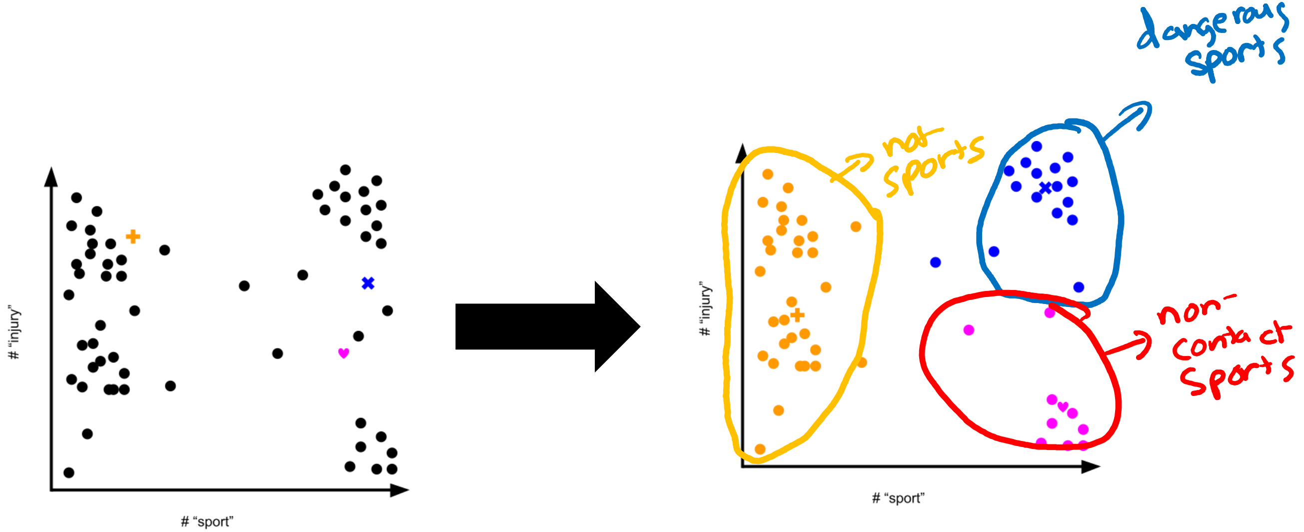
Group

1.5 min

- You are clustering news articles using the features "# sport" and "# injury." How would you interpret these clusters?
- "This is a cluster of ...[some characterization]... articles."



Brain Break

Effect of Initialization

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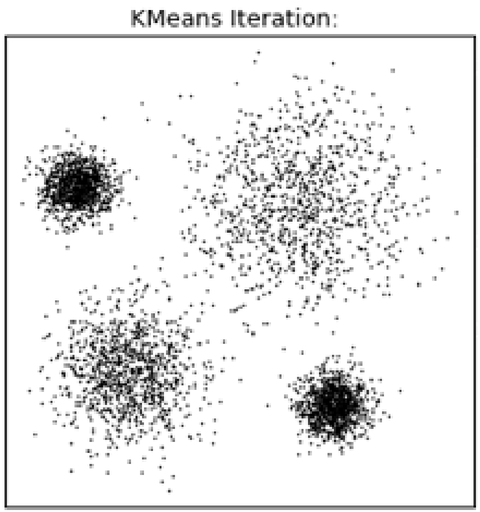
Group

1.5 min

sli.do #cs416

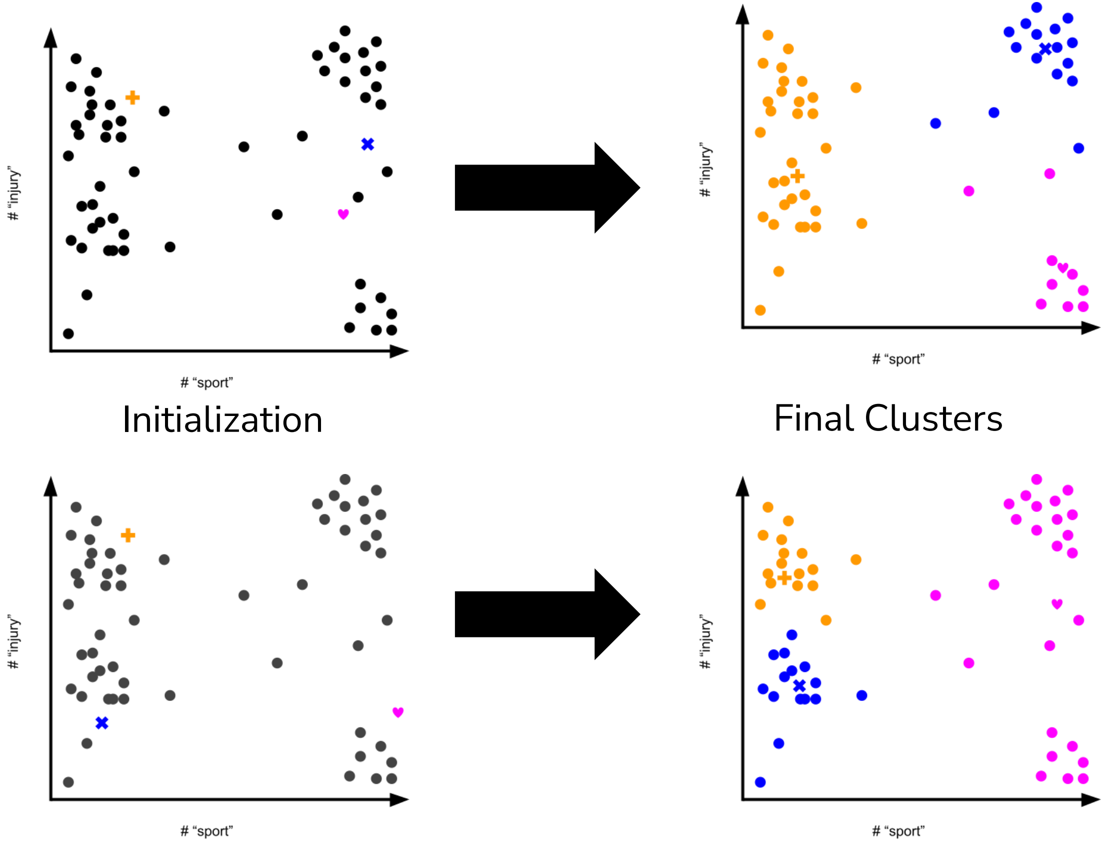
What convergence guarantees do you think we will have with k-means?

- Converges to the global optimum
- ✓ Converges to a local optima
- None



Effects of Initialization

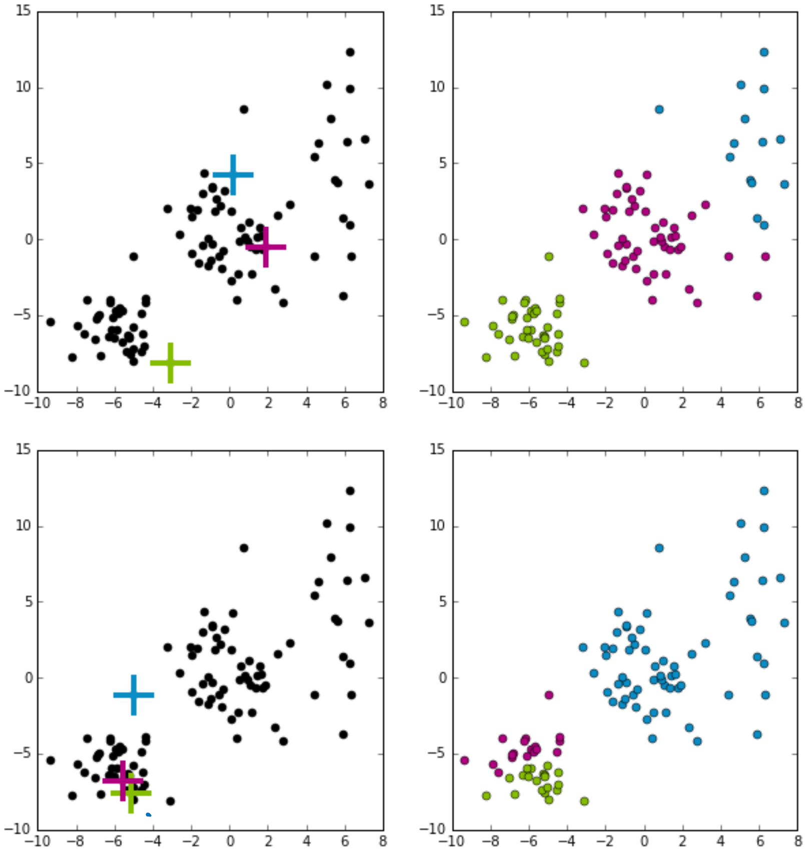
Results **heavily depend** on initial centroids



Effect of initialization

What does it mean for something to converge to a local optima?

- Some initialization can be bad and affect the quality of clustering
- Initialization will greatly impact results!



Smart Initializing w/ k-means++

Making sure the initialized centroids are “good” is critical to finding quality local optima. Our purely random approach was wasteful since it’s very possible that initial centroids start close together.

Idea: Try to select a set of points farther away from each other.

k-means++ does a slightly smarter random initialization

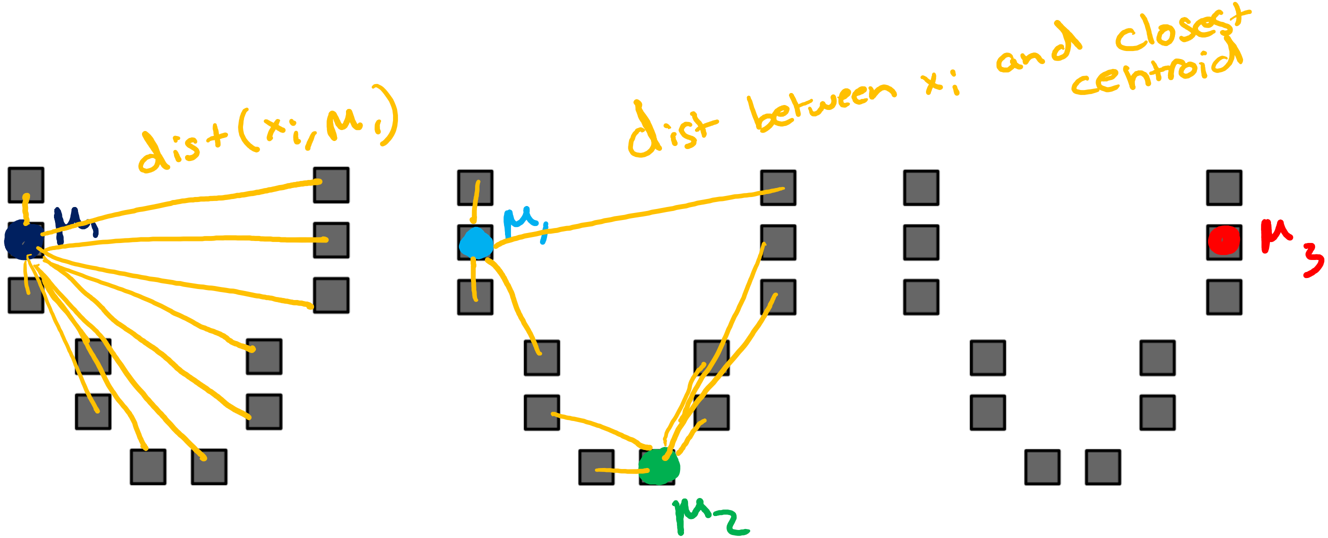
1. Choose first cluster μ_1 from the data uniformly at random
2. For each datapoint x_i, compute the distance between x_i and the closest centroid from the current set of centroids (starting with just μ_i). Denote that distance $d(x_i)$.
3. Choose a new centroid from the remaining data points, where the probability of x_i being chosen is proportional to $d(x_i)^2$.
4. Repeat 2 and 3 until we have selected k centroids.

k-means++ Example

Start by picking a point at random

Then pick points proportional to their distances to their centroids

This tries to maximize the spread of the centroids!



k-means++ Pros / Cons

Pros

- Improves quality of local minima
- Faster convergence to local minima

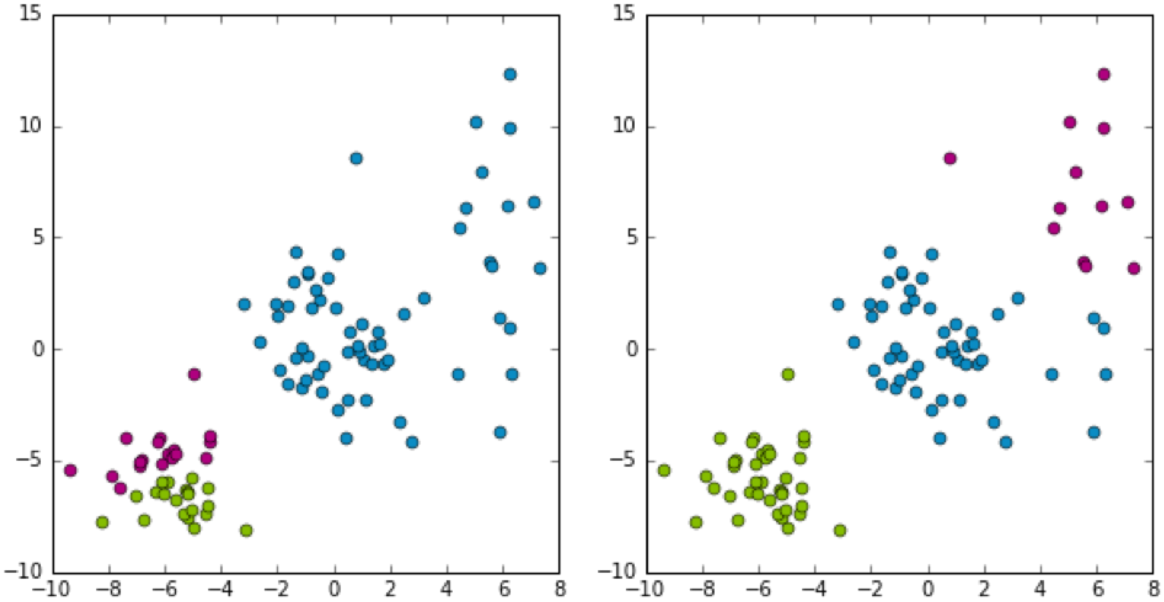
Cons

- Computationally more expensive at beginning when compared to simple random initialization

Assessing Performance

Which Cluster?

Which clustering would I prefer?

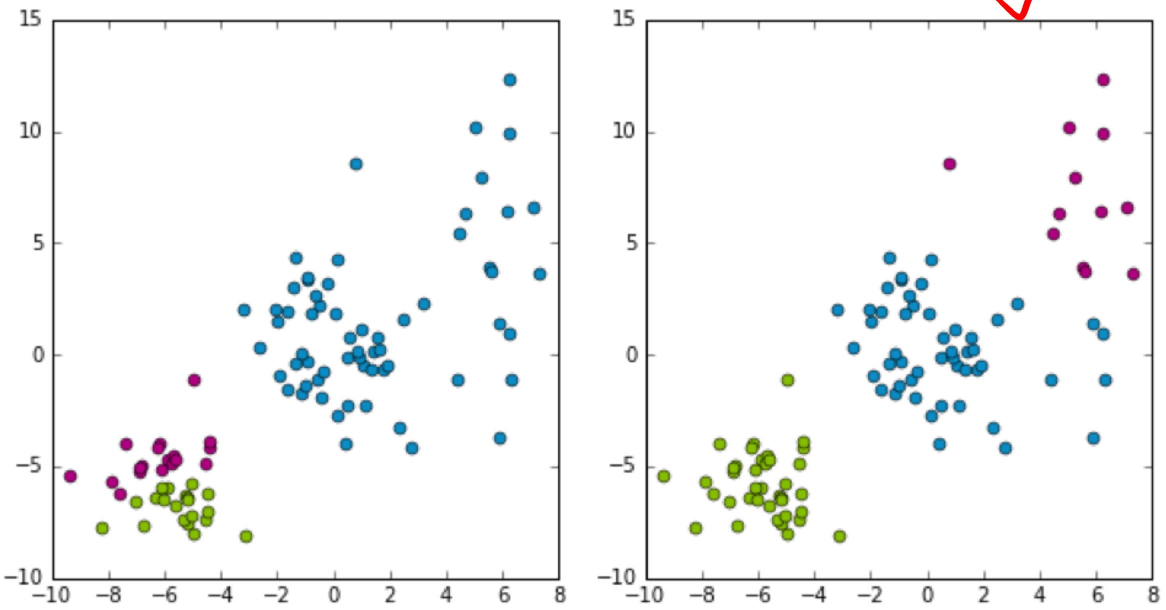


Don’t know, there is no “right answer” in clustering 🤷 .

Depends on the practitioner’s domain-specific knowledge and interpretation of results!

Which Cluster?

Which clustering does k-means prefer?



k-means is trying to optimize the **heterogeneity** objective

$$\underset{z,\mu}{\operatorname{argmin}} \underbrace{\sum_{j=1}^{k}}_{\text{sum over clusters}} \underbrace{\sum_{i=1}^{n} \mathbf{1}\{z_i = j\} \left|\left|\mu_j - x_i\right|\right|_2^2}_{\text{total distance between points in that cluster and the centroid}}$$

sum over clusters

total distance between points in that cluster and the centroid

Coordinate Descent

k-means is trying to minimize the heterogeneity objective

$$\underset{z,\mu}{\operatorname{argmin}} \sum_{j=1}^{k} \sum_{i=1}^{n} \mathbf{1}\{z_i = j\} \left|\left|\mu_j - x_i\right|\right|_2^2$$

Step 0: Initialize cluster centers

Repeat until convergence: fix μ, minimize z

Step 1: Assign each example to its closest cluster centroid

Step 2: Update the centroids to be the mean of all the points assigned to that cluster fix z, minimize μ

Coordinate Descent alternates how it updates parameters to find minima. On each of iteration of Step 1 and Step 2, heterogeneity decreases or stays the same.

=> Will converge in finite time

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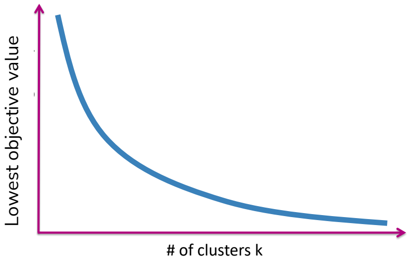
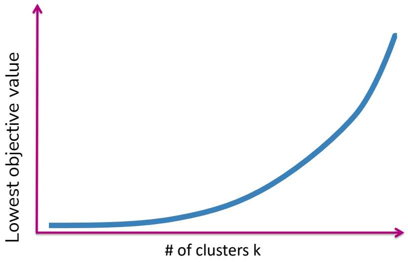
Think

1 min

Consider training k-means to convergence for different values of k. Which of the following graphs shows how the heterogeneity objective will change based on the value of k?



A



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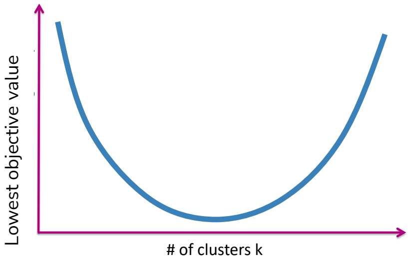

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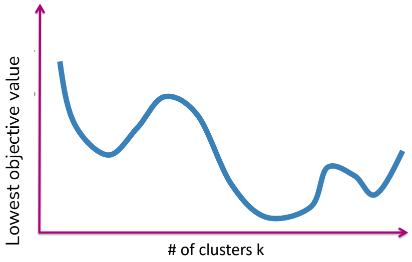

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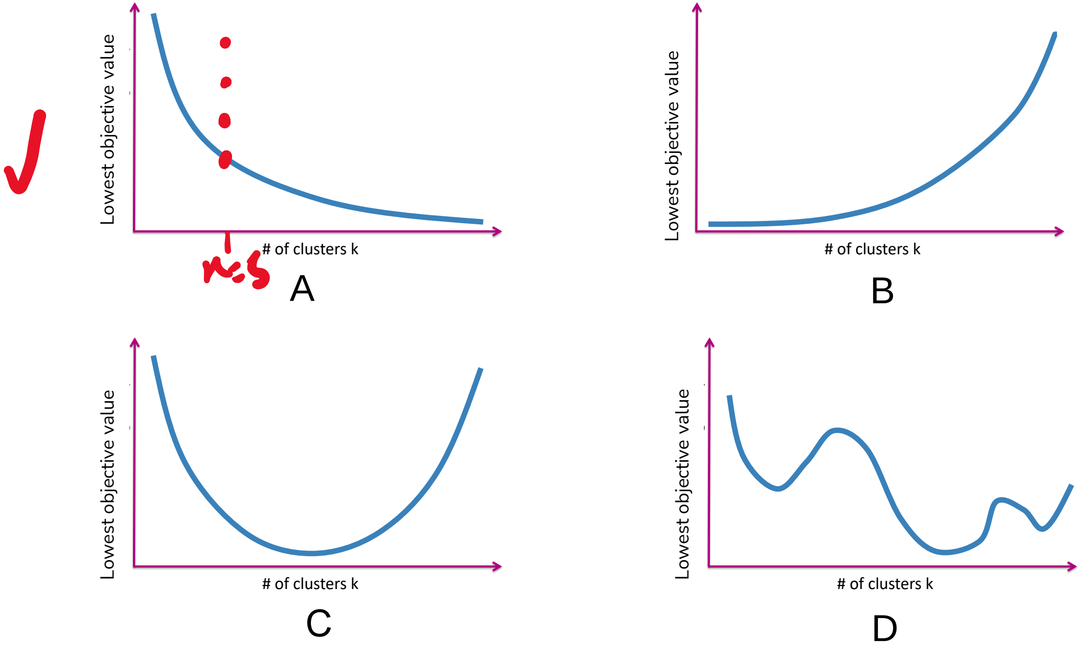
Group

2 mins

Need many trials to find opt per k

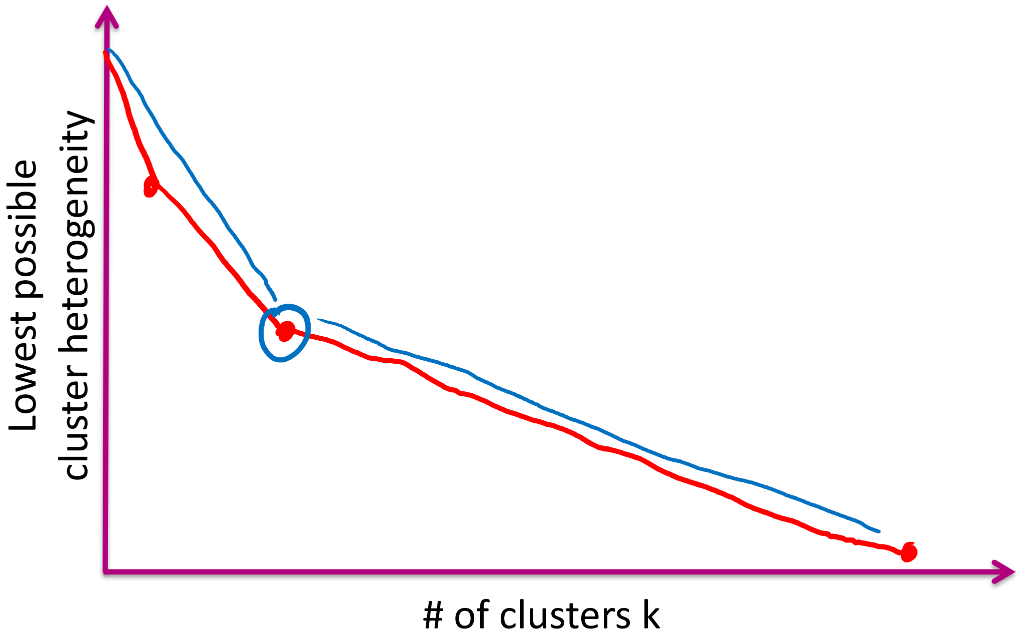
Consider training k-means to convergence for different values of k. Which of the following graphs shows how the heterogeneity objective will change based on the value of k?



How to Choose k?

No right answer! Depends on your application.

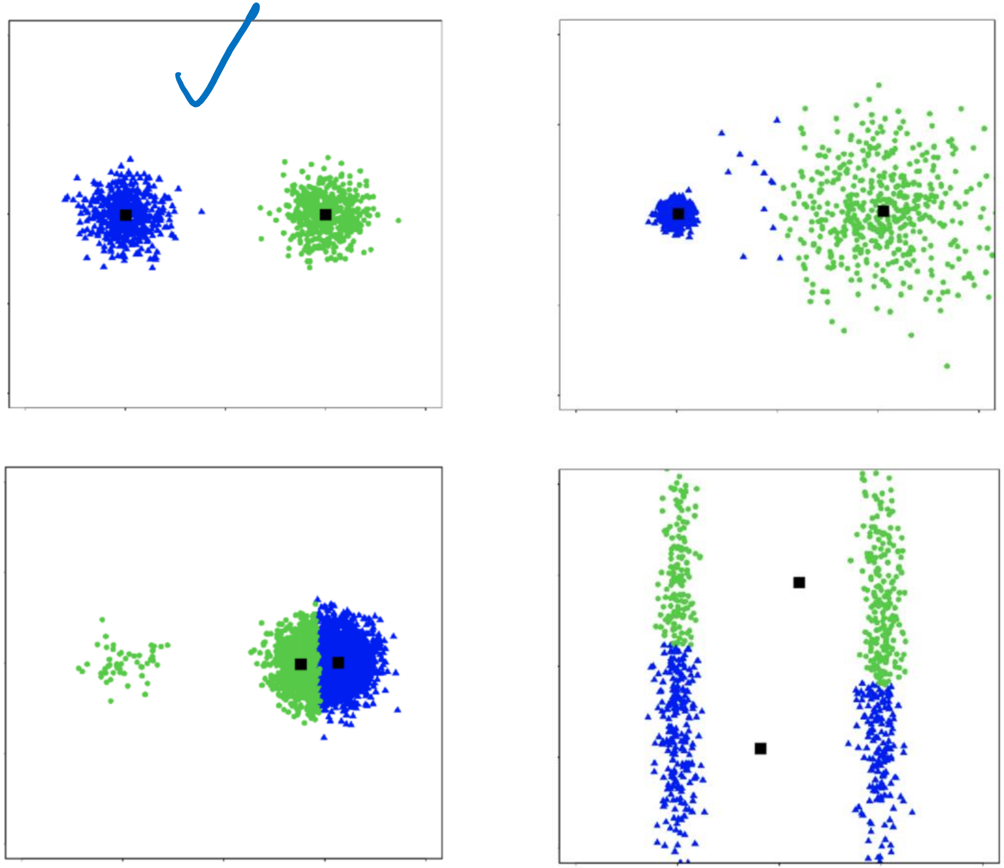
- General, look for the “elbow” in the graph



Note: You will usually have to run k-means multiple times for each k

Cluster shape

- k-means works well for well-separated **hyper-spherical** clusters of the same size



Clustering vs Classification

- Clustering looks like we assigned labels (by coloring or numbering different groups) but we didn't use any **labeled** data.
- In clustering, the "labels" don't have meaning. To give meaning to the labels, human inputs is required
- Classification learns from minimizing the error between a prediction and an actual **label**.
- Clustering learns by minimizing the distance between points in a cluster.
- Classification quality metrics (accuracy / loss) do not apply to clustering (since there is no label).
- You can't use validation set / cross-validation to choose the best choice of k for clustering.

Recap

- Differences between classification and clustering
- What types of clusters can be formed by k-means
- K-means algorithm
- Convergence of k-means
- How to choose k
- Better initialization using k-means++