

DSC 40A

Theoretical Foundations of Data Science I

Question

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Lloyds Algorithm, or k-Means Clustering

1. Randomly initialize the k centroids.
2. Keep centroids fixed. Update groups.
Assign each point to the nearest centroid.
3. Keep groups fixed. Update centroids.
Move each centroid to the center of its group.
4. Repeat steps 2 and 3 until done.

Outline

- Why does k-means clustering work?
- What are some practical considerations when using this algorithm?

Why does k-means clustering work?

$\text{Cost}(\mu_1, \mu_2, \dots, \mu_k) =$ total squared distance of each data point x_i
to its nearest centroid μ_j

- Argue why updating the groups and centroids according to the algorithm reduces the cost with each iteration.
- With enough iterations, cost will be sufficiently small.

Why does k-means clustering work?

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$\text{Cost}(\mu_1, \mu_2, \dots, \mu_k) = \text{Cost}(\mu_1) + \text{Cost}(\mu_2) + \dots + \text{Cost}(\mu_k)$ where
 $\text{Cost}(\mu_j) =$ total squared distance of each data point x_i in group j to centroid μ_j

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sets initial cost
(before the
process begins)

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2. Fix the centroids. Update the groups.

consider an arbitrary iteration

Certainly $\text{Cost}(\mu_1, \mu_2, \dots, \mu_k)$ decreases in this step because
assigning each point to the **closest** centroid is best.

Why does k-means clustering work?

$\text{Cost}(\mu_1, \mu_2, \dots, \mu_k) = \text{Cost}(\mu_1) + \text{Cost}(\mu_2) + \dots + \text{Cost}(\mu_k)$ where

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3. Fix the groups. Update the centroids.

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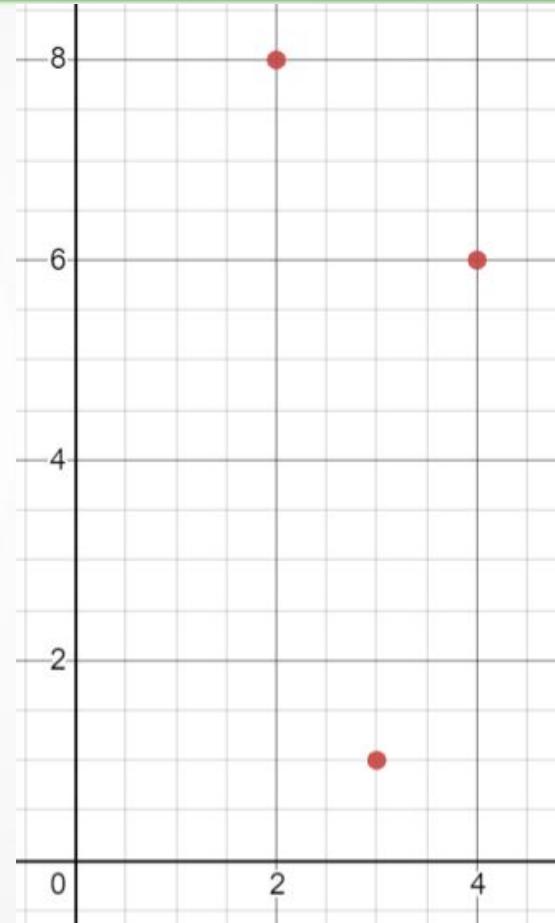
Argue that $\text{Cost}(\mu_1, \mu_2, \dots, \mu_k)$ decreases in this step because for each group j , $\text{Cost}(\mu_j)$ is minimized when we update the centroid.

Why does k-means clustering work?

$\text{Cost}(\mu_j) =$ total squared distance of each data point x_i in group j to centroid μ_j

Example: group j contains $(4, 6)$, $(2, 8)$, $(3, 1)$

How to place centroid $\mu_j = (c_1, c_2)$ to minimize cost?



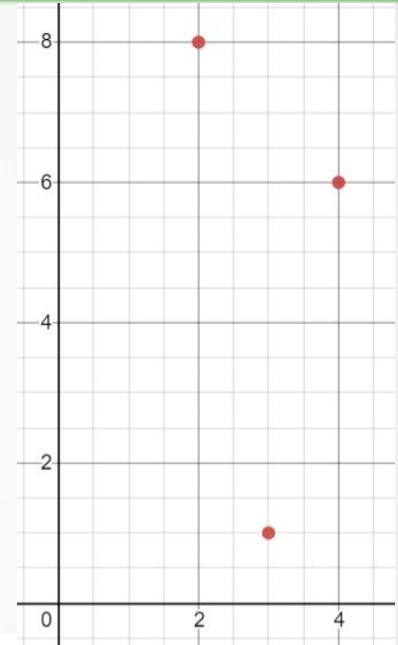
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How to place centroid $\mu_j = (c_1, c_2)$ to minimize cost?

$$\begin{aligned}\text{Cost}(\mu_j) &= \left(\sqrt{(4 - c_1)^2 + (6 - c_2)^2} \right)^2 + \left(\sqrt{(2 - c_1)^2 + (8 - c_2)^2} \right)^2 + \left(\sqrt{(3 - c_1)^2 + (1 - c_2)^2} \right)^2 \\ &= (4 - c_1)^2 + (6 - c_2)^2 + (2 - c_1)^2 + (8 - c_2)^2 + (3 - c_1)^2 + (1 - c_2)^2\end{aligned}$$



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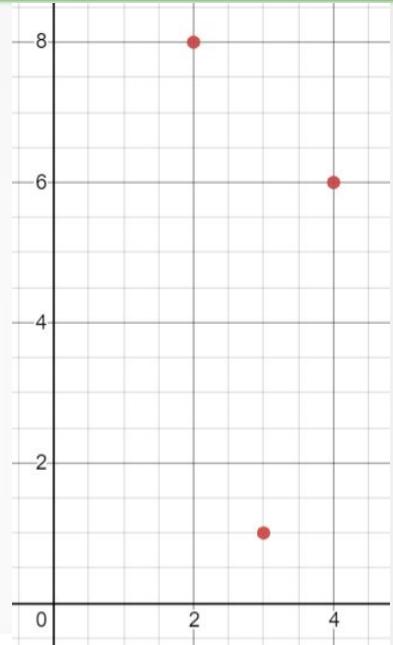
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$$\frac{\partial \text{Cost}(\mu_j)}{\partial c_1} = 2(c_1 - 4) + 2(c_1 - 2) + 2(c_1 - 3)$$

$$\frac{\partial \text{Cost}(\mu_j)}{\partial c_2} = 2(c_2 - 6) + 2(c_2 - 8) + 2(c_2 - 1)$$



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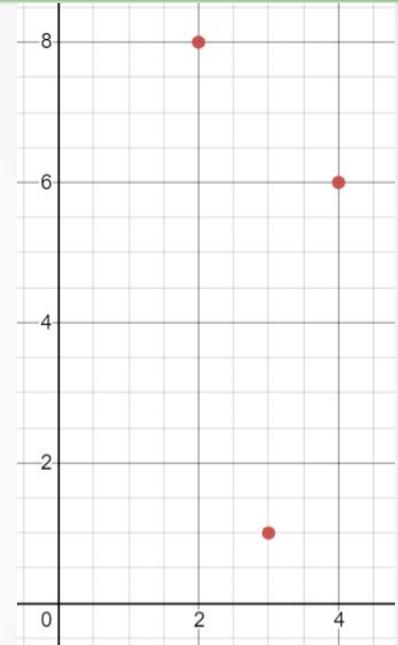
$$\frac{\partial \text{Cost}(\mu_j)}{\partial c_1} = 2(c_1 - 4) + 2(c_1 - 2) + 2(c_1 - 3)$$

$$0 = 2(c_1 - 4) + 2(c_1 - 2) + 2(c_1 - 3)$$

$$0 = c_1 - 4 + c_1 - 2 + c_1 - 3$$

$$3c_1 = 4 + 2 + 3$$

$$c_1 = \frac{4 + 2 + 3}{3}$$



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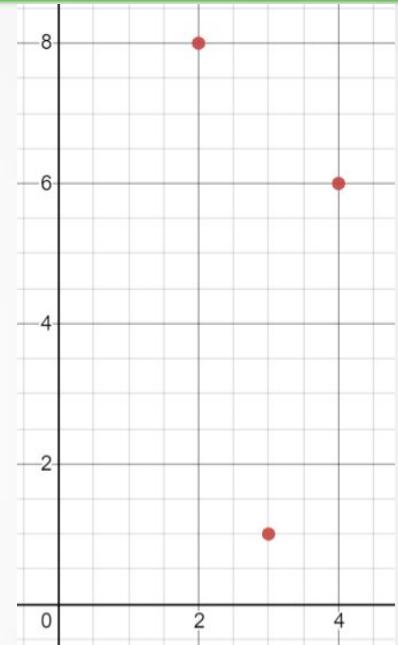
$$\frac{\partial \text{Cost}(\mu_j)}{\partial c_2} = 2(c_2 - 6) + 2(c_2 - 8) + 2(c_2 - 1)$$

$$0 = 2(c_2 - 6) + 2(c_2 - 8) + 2(c_2 - 1)$$

$$0 = c_2 - 6 + c_2 - 8 + c_2 - 1$$

$$3c_2 = 6 + 8 + 1$$

$$c_2 = \frac{6 + 8 + 1}{3}$$



Why does k-means clustering work?

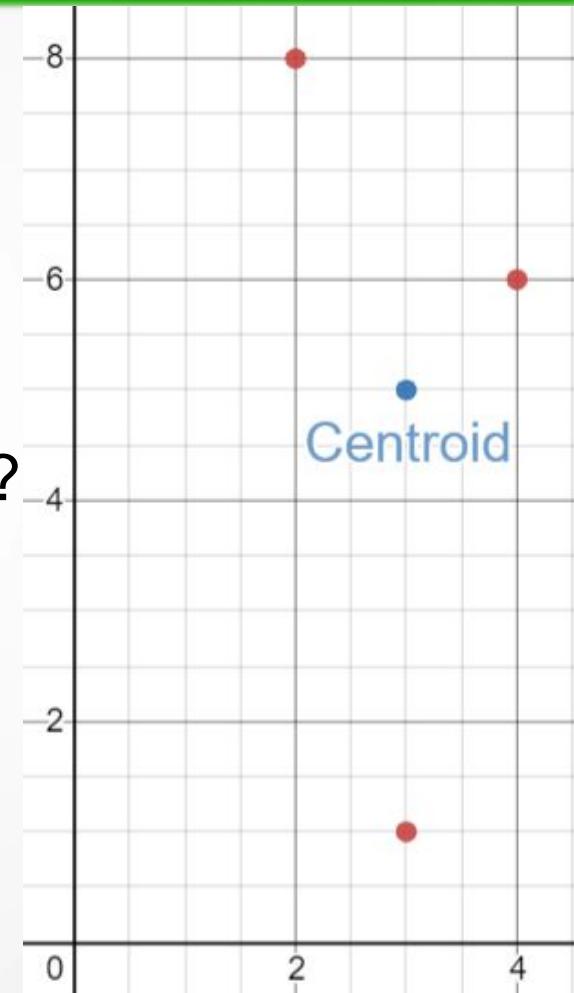
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Example: group j contains $(4, 6)$, $(2, 8)$, $(3, 1)$

How to place centroid $\mu_j = (c_1, c_2)$ to minimize cost?

$$(c_1, c_2) = \left(\frac{4+2+3}{3}, \frac{6+8+1}{3} \right) = (3, 5)$$

Minimize cost by averaging in each coordinate.



Cost, Loss, and Risk

The cost of placing the centroid at (c_1, c_2) is

$$\begin{aligned}\text{Cost } (\mu_j) &= \left(\sqrt{(4 - c_1)^2 + (6 - c_2)^2} \right)^2 + \left(\sqrt{(2 - c_1)^2 + (8 - c_2)^2} \right)^2 + \left(\sqrt{(3 - c_1)^2 + (1 - c_2)^2} \right)^2 \\ &= (4 - c_1)^2 + (6 - c_2)^2 + (2 - c_1)^2 + (8 - c_2)^2 + (3 - c_1)^2 + (1 - c_2)^2\end{aligned}$$

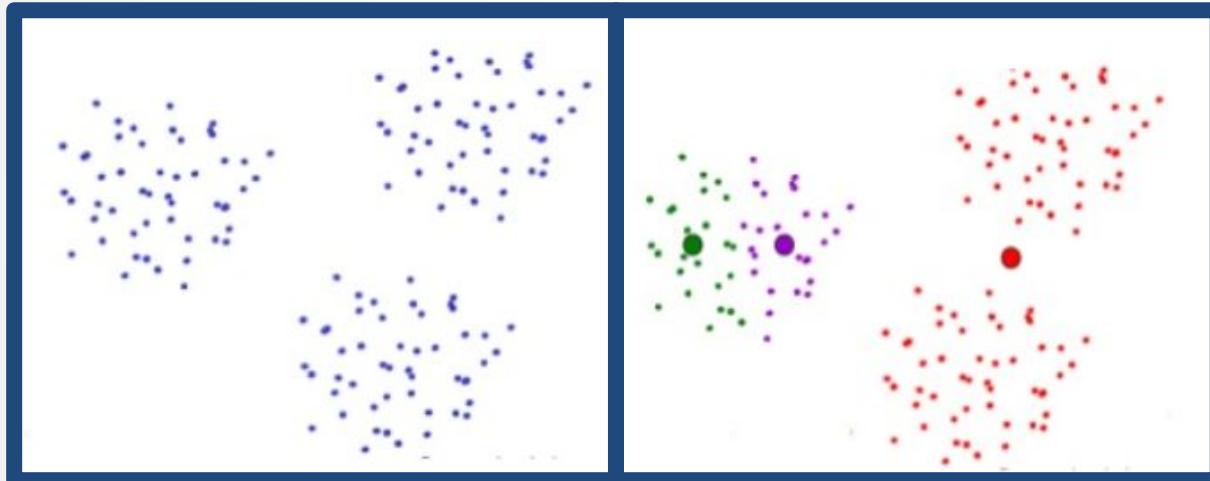
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- Argue why updating the groups and centroids according to the algorithm reduces the cost with each iteration.
- With enough iterations, cost will be sufficiently small.

k-Means Clustering in Practice: Initialization

Can get unlucky with random initialization.

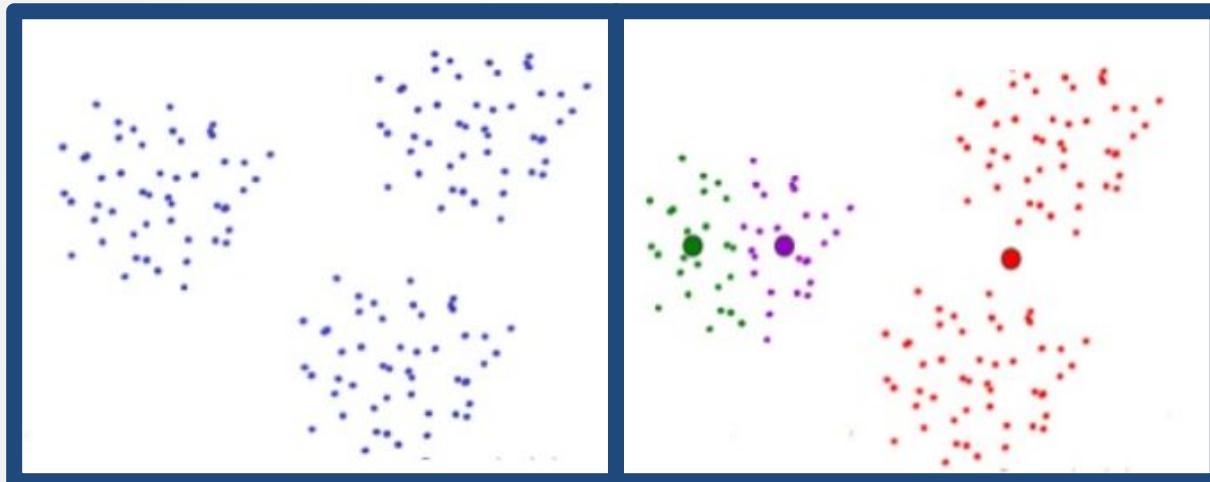


In general, how do we assess which result is the best?

- A. Clusters appear how we expect them to
- B. Clusters are evenly sized
- C. Cost function is lowest

k-Means Clustering in Practice: Initialization

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In general, how do we assess which result is the best?

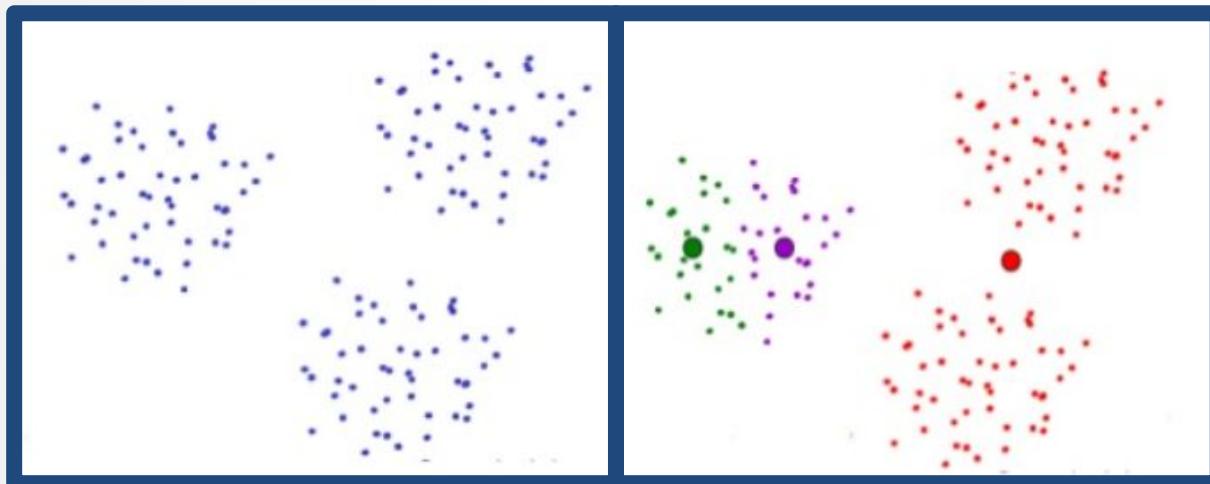
- A. Clusters appear how we expect them to
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Solution?

- Try algorithm several times, pick the best result.
- Similar approach used in gradient descent.

k-Means Clustering in Practice: Initialization

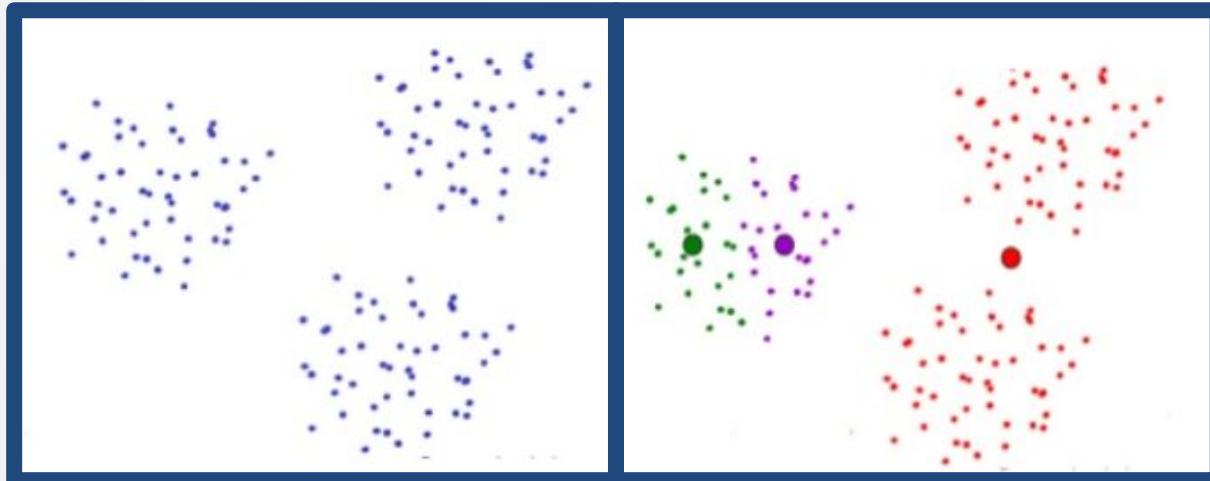
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- No guarantees of a satisfactory solution with this algorithm.
- Brute force algorithm would try all assignments of points to clusters and choose the one with the lowest cost.

k-Means Clustering in Practice: Initialization

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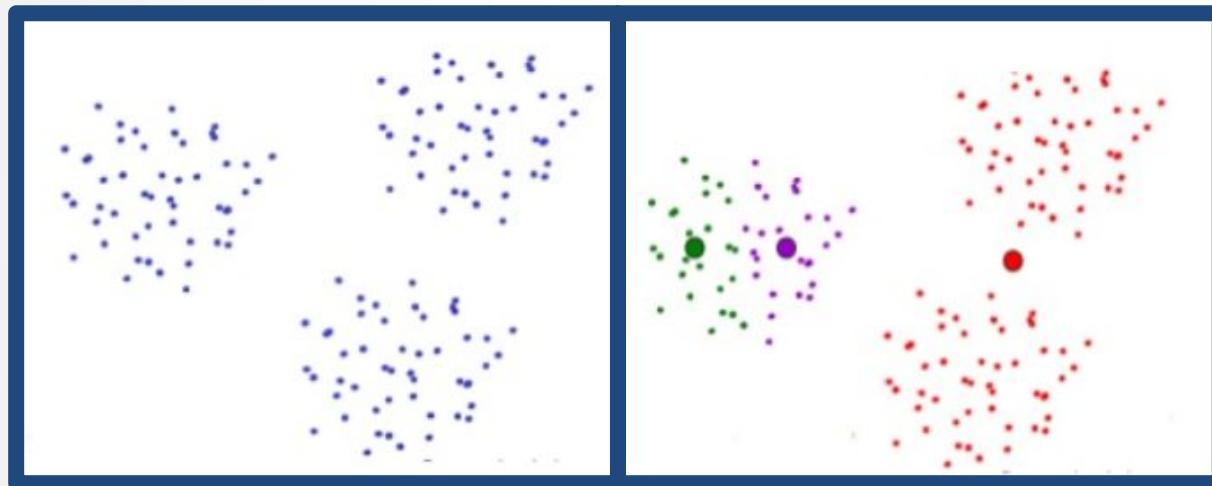


How many ways to assign n points to k clusters?

- No guarantees of a satisfactory solution with this algorithm.
- Brute force algorithm would try all assignments of points to clusters and choose the one with the lowest cost.

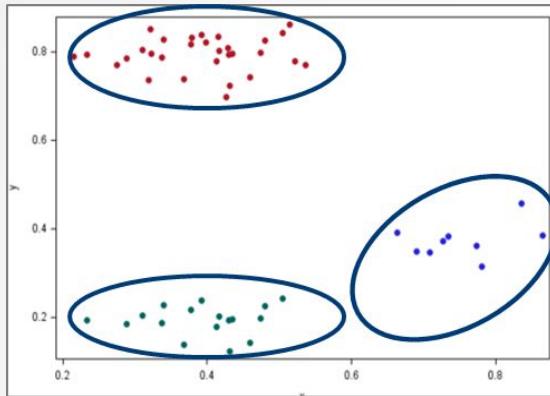
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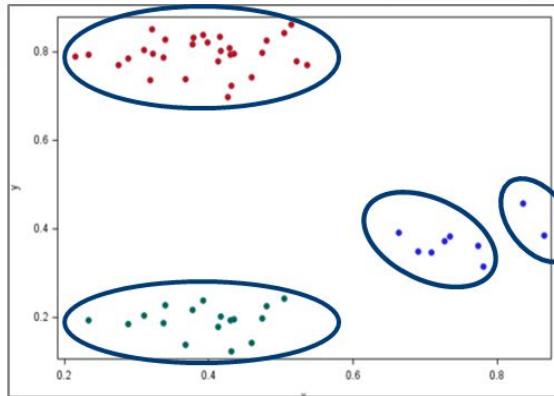


- No guarantees of a satisfactory solution with this algorithm.
- Any algorithm that is guaranteed to find the best coloring of data points takes exponential time (computationally infeasible).

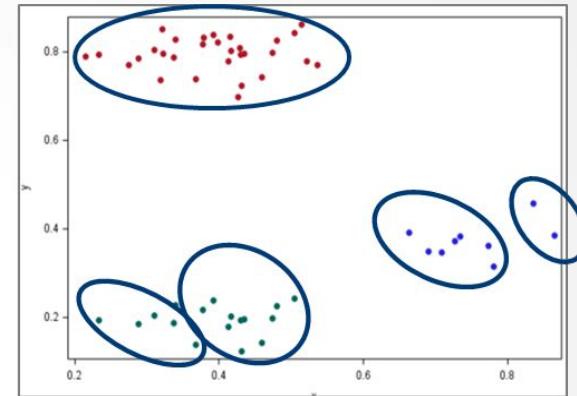
k-Means Clustering in Practice: Choosing k



k=3

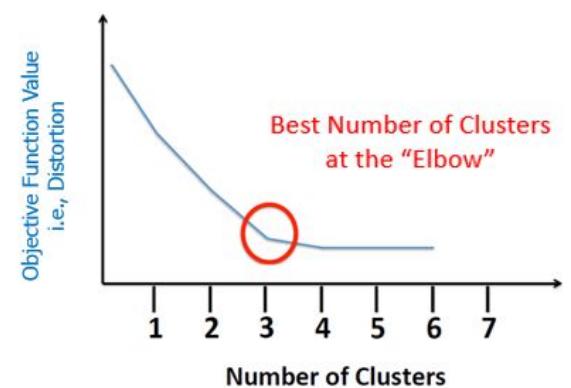


k=4



k=5

- Most commonly done by hand (visualizations, trial and error)
- Elbow method
- Context or domain knowledge
- Use a different clustering algorithm



What if a centroid has no points in its group?

What should we do if a centroid has no points in its group?

- A. Terminate the algorithm.
- B. Wait for points get added to the group in a subsequent iteration.
- C. Set the centroid to be a data point, chosen at random.
- D. Set the centroid to be one of the other centroids, chosen at random.

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Two options:

- Eliminate that centroid and find $k-1$ clusters instead
- Randomly re-initialize that centroid

Summary

- We saw that k-means clustering works because each step of the algorithm reduces the cost function, which measures the quality of a set of centroids.
- We discussed some practical considerations, including random initialization and choice of k.