# DSC 40A

## Theoretical Foundations of Data Science I

# 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.

# In This Video

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

# Why does k-means clustering work?

Cost($\boldsymbol{\mu}_1$, $\boldsymbol{\mu}_2$, ... , $\boldsymbol{\mu}_k$) = total squared distance of each data point $x_i$ to its nearest centroid $\boldsymbol{\mu}_j$

- 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?

$\text{Cost}(\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \ldots, \boldsymbol{\mu}_k) =$ total squared distance of each data point $x_i$ to its nearest centroid $\boldsymbol{\mu}_j$

$\text{Cost}(\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \ldots, \boldsymbol{\mu}_k) = \text{Cost}(\boldsymbol{\mu}_1) + \text{Cost}(\boldsymbol{\mu}_2) + \ldots + \text{Cost}(\boldsymbol{\mu}_k)$ where

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1. Randomly initialize the k centroids. ← sets initial cost (before the process begins)

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2. Fix the centroids. Update the groups.

consider an arbitrary iteration

Certainly $\mathrm{Cost}(\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \ldots, \boldsymbol{\mu}_k)$ decreases in this step because assigning each point to the **closest** centroid is best.

# Why does k-means clustering work?

Cost($\boldsymbol{\mu}_1$, $\boldsymbol{\mu}_2$, ... , $\boldsymbol{\mu}_k$) = Cost($\boldsymbol{\mu}_1$) + Cost($\boldsymbol{\mu}_2$) + … + Cost($\boldsymbol{\mu}_k$) where

Cost($\boldsymbol{\mu}_j$) = total squared distance of each data point $x_i$ in group j to centroid $\boldsymbol{\mu}_j$

3. Fix the groups. Update the centroids.

consider an arbitrary iteration

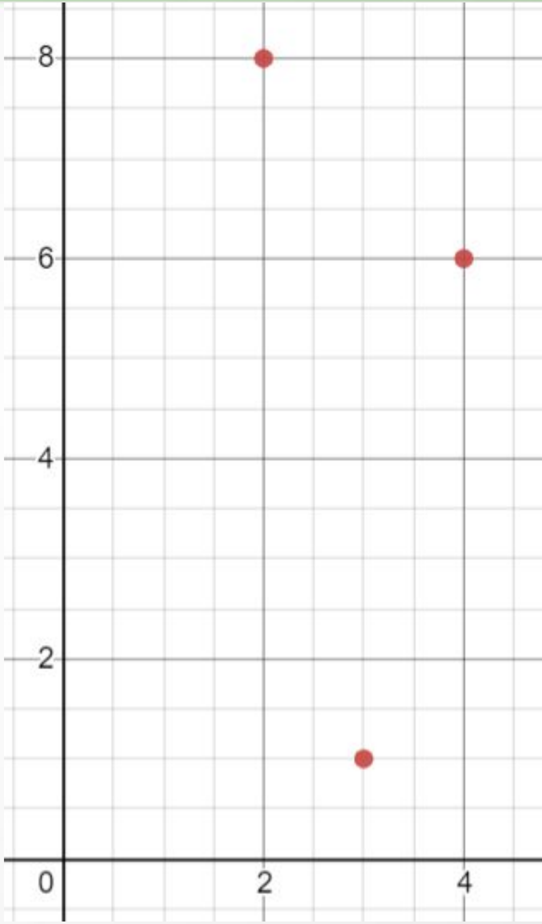
Argue that Cost($\boldsymbol{\mu}_1$, $\boldsymbol{\mu}_2$, ... , $\boldsymbol{\mu}_k$) decreases in this step because for each group j, Cost($\boldsymbol{\mu}_j$) is minimized when we update the centroid.

# Why does k-means clustering work?

Cost($\boldsymbol{\mu}_j$) = total squared distance of each data point $x_i$ in group j to centroid $\boldsymbol{\mu}_j$

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

How to place centroid $\boldsymbol{\mu}_j = (c_1, c_2)$ to minimize cost?



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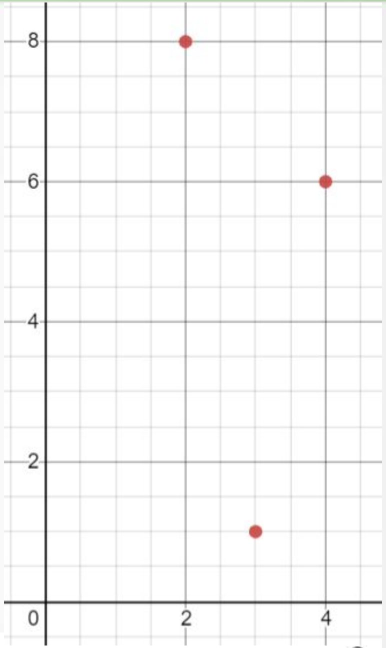


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$$\begin{aligned}\text{Cost}\ (\mu_j) &= \left(\sqrt{(4-c_1)^2+(6-c_2)^2}\right)^2 + \left(\sqrt{(2-c_1)^2+(8-c_2)^2}\right)^2 + \left(\sqrt{(3-c_1)^2+(1-c_2)^2}\right)^2 \\ &= (4-c_1)^2+(6-c_2)^2+(2-c_1)^2+(8-c_2)^2+(3-c_1)^2+(1-c_2)^2\end{aligned}$$

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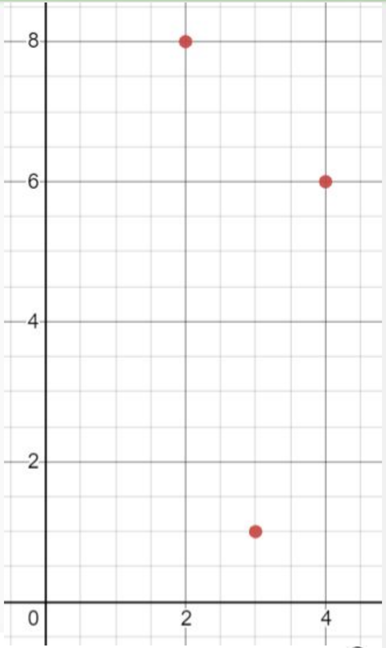


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$$\frac{\partial \text{Cost}(\mu_j)}{\partial c_1} = 2(c_1-4)+2(c_1-2)+2(c_1-3)$$

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

# Why does k-means clustering work?

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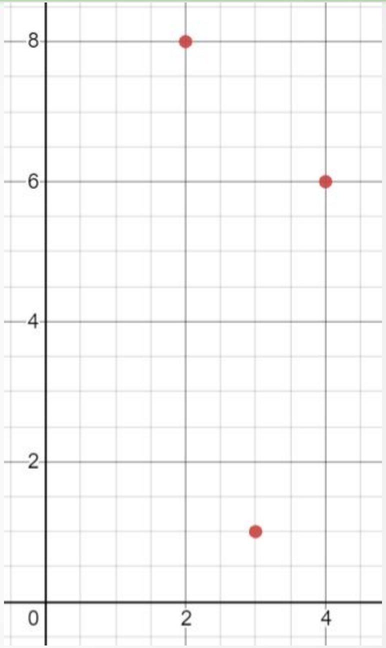
Example: group j contains (4, 6), (2, 8), (3,1)

How to place centroid $\boldsymbol{\mu}_j = (c_1, c_2)$ to minimize cost?

$$\frac{\partial \mathrm{Cost}(\mu_j)}{\partial c_1} = 2(c_1 - 4) + 2(c_1 - 2) + 2(c_1 - 3)$$
$$0 = 2(c_1 - 4) + 2(c_1 - 2) + 2(c_1 - 3)$$
$$0 = c_1 - 4 + c_1 - 2 + c_1 - 3$$
$$3c_1 = 4 + 2 + 3$$
$$c_1 = \frac{4 + 2 + 3}{3}$$



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How to place centroid $\boldsymbol{\mu}_j$ = ($c_1$, $c_2$) to minimize cost?

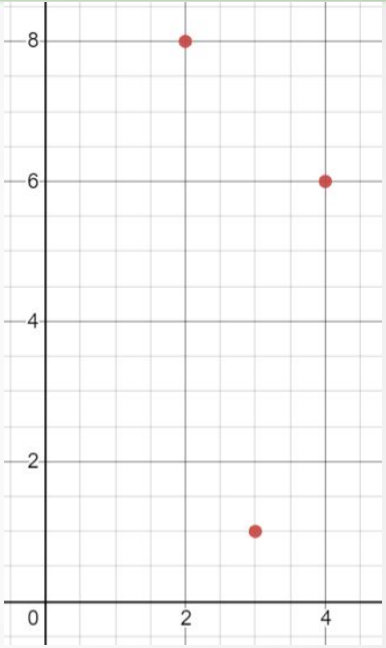
$$\frac{\partial \text{Cost}(\mu_j)}{\partial c_2} = 2(c_2 - 6) + 2(c_2 - 8) + 2(c_2 - 1)$$

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

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

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

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



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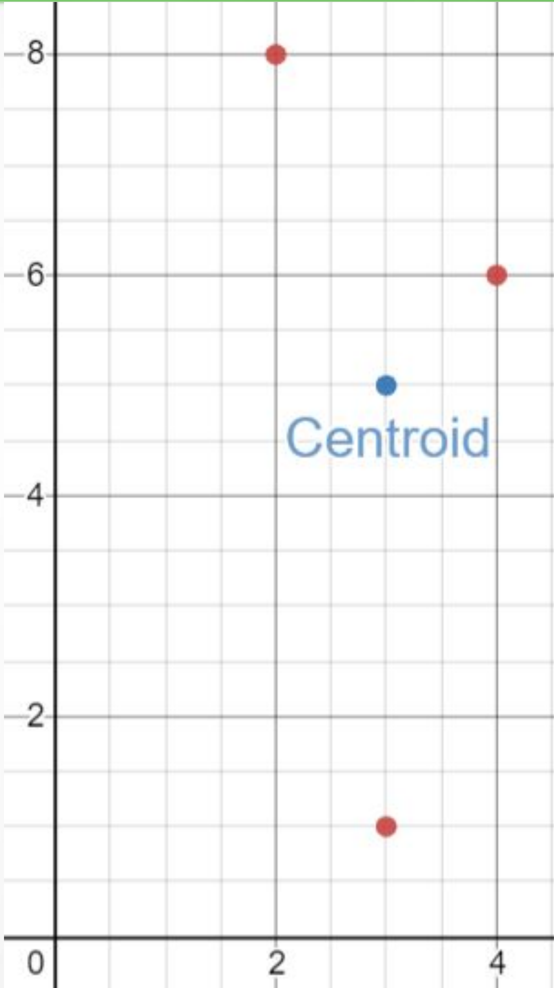
How to place centroid $\boldsymbol{\mu}_j = (c_1, c_2)$ to minimize cost?

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

Minimize cost by averaging in each coordinate.



# Cost, Loss, and Risk

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

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

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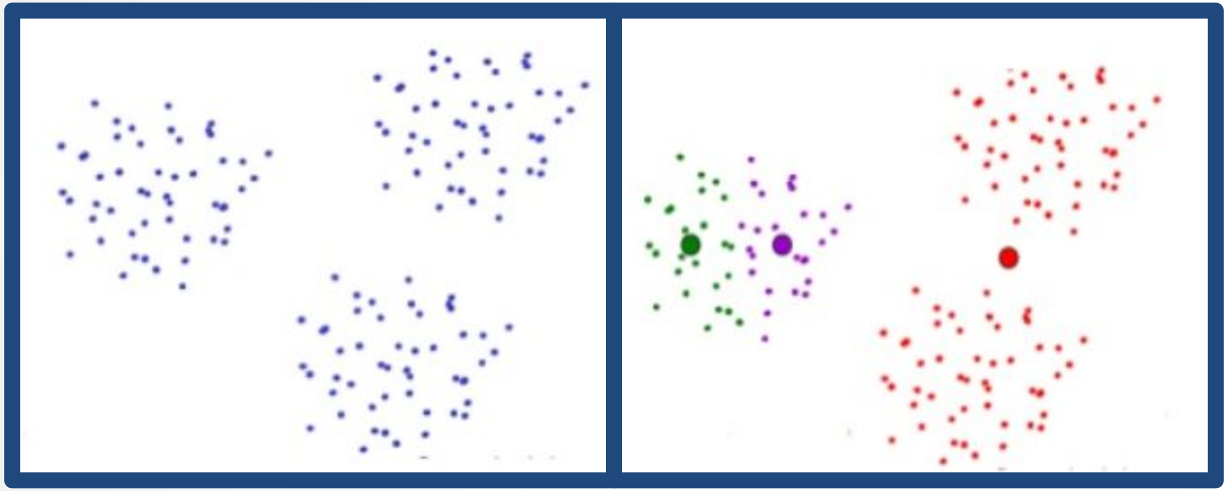
- Argue why updating the groups and centroids according to the algorithm reduces the cost with each iteration.
- With enough iterations, cost will be sufficiently small.

# 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

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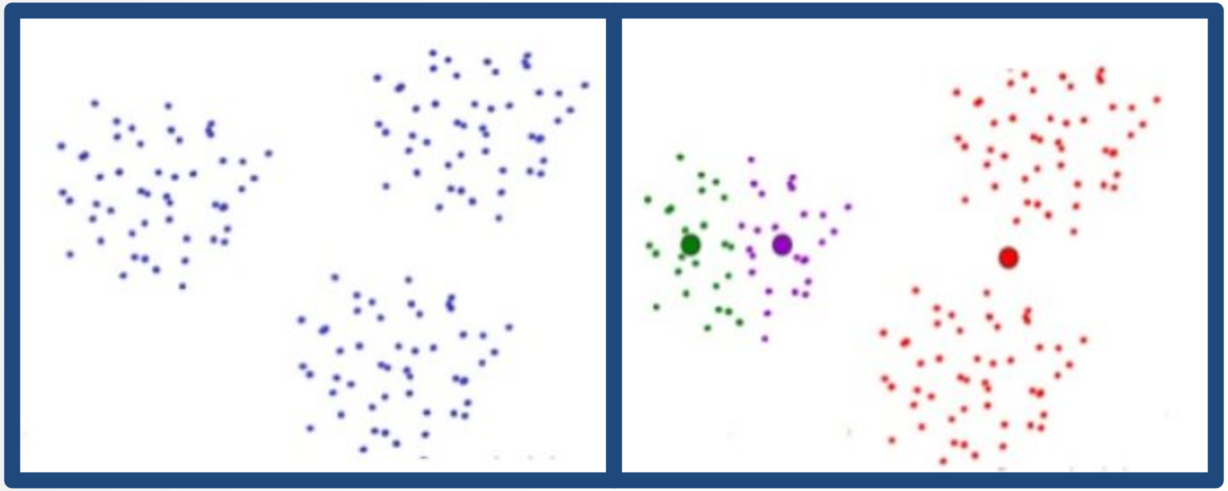

In general, how do we assess which result is the best?

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.

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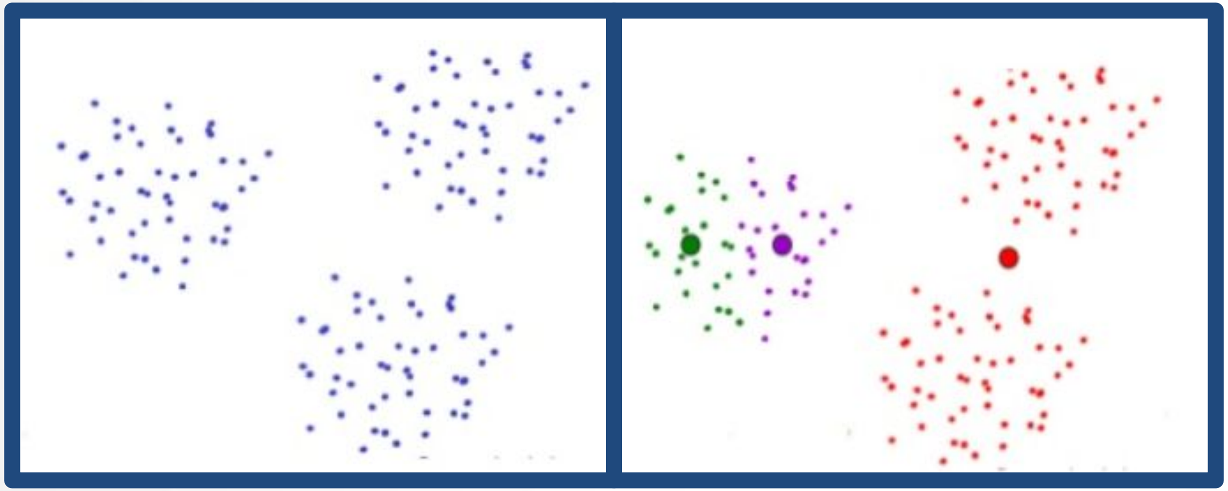

- No guarantees of a satisfactory solution with this algorithm.
- Brute force algorithm would try all assignments of points to clusters and choose the one with the lowest cost.

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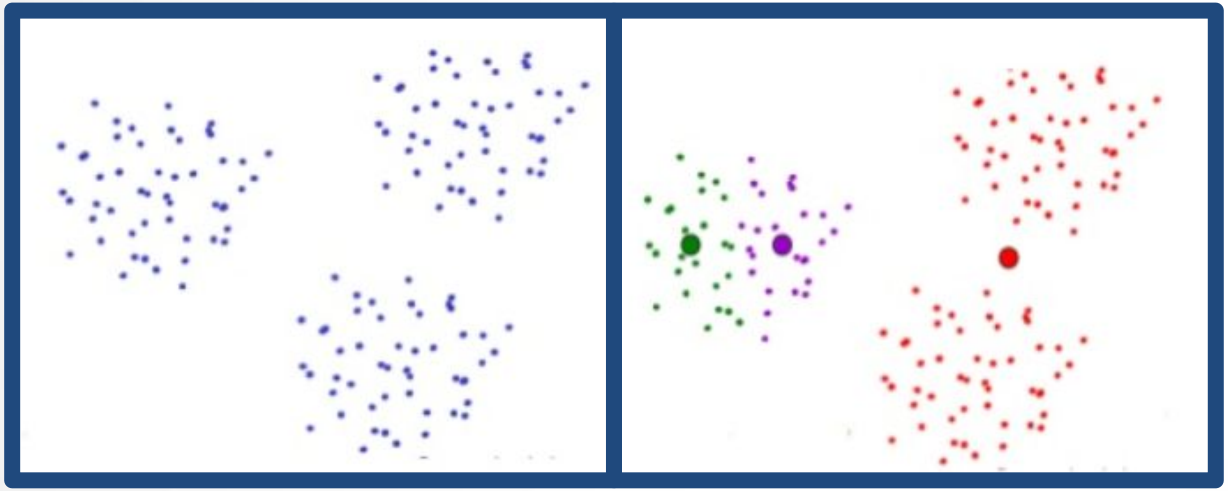

How many ways to assign n points to k clusters?

- 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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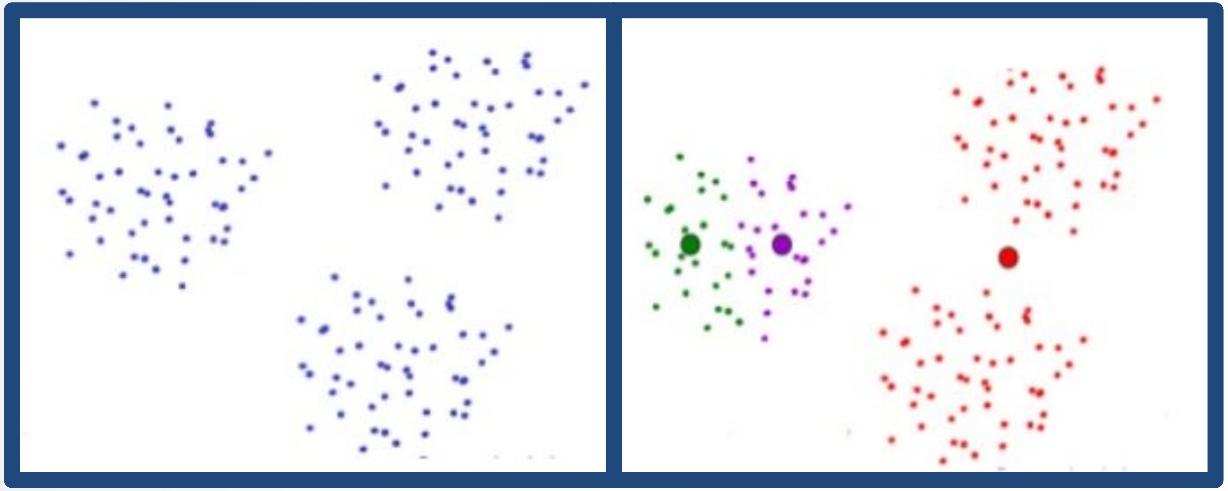
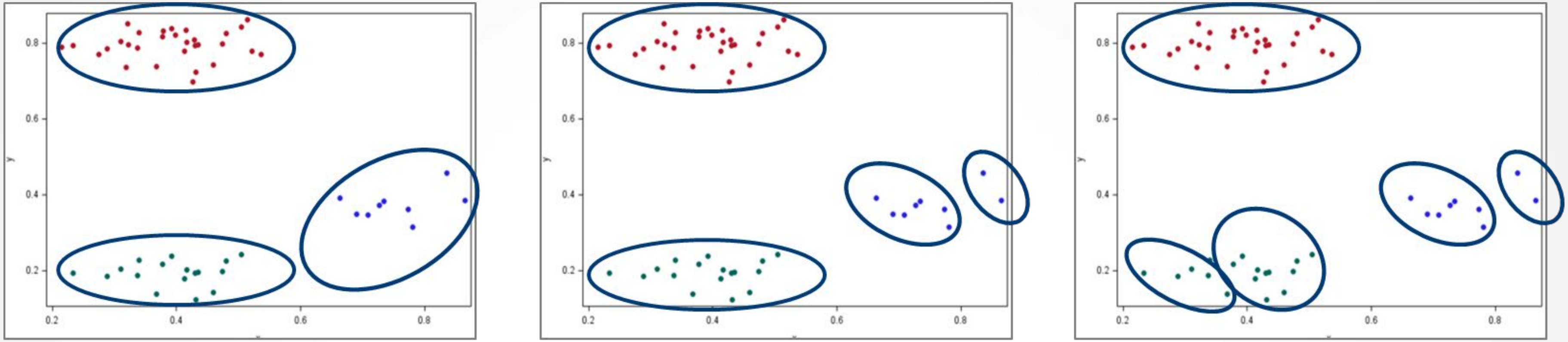


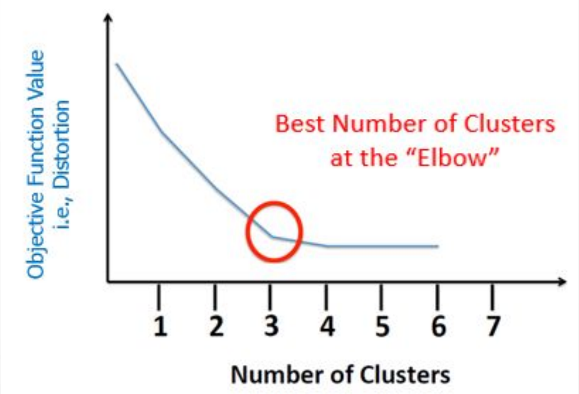
- No guarantees of a satisfactory solution with this algorithm.
- Any algorithm that is guaranteed to find the best coloring of data points takes exponential time (computationally infeasible).

# 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.