DSC 40A

Theoretical Foundations of Data Science I

Announcements

- Homework 7 due 12/6.
- SET
- Final exam

Question

Answer at q.dsc40a.com

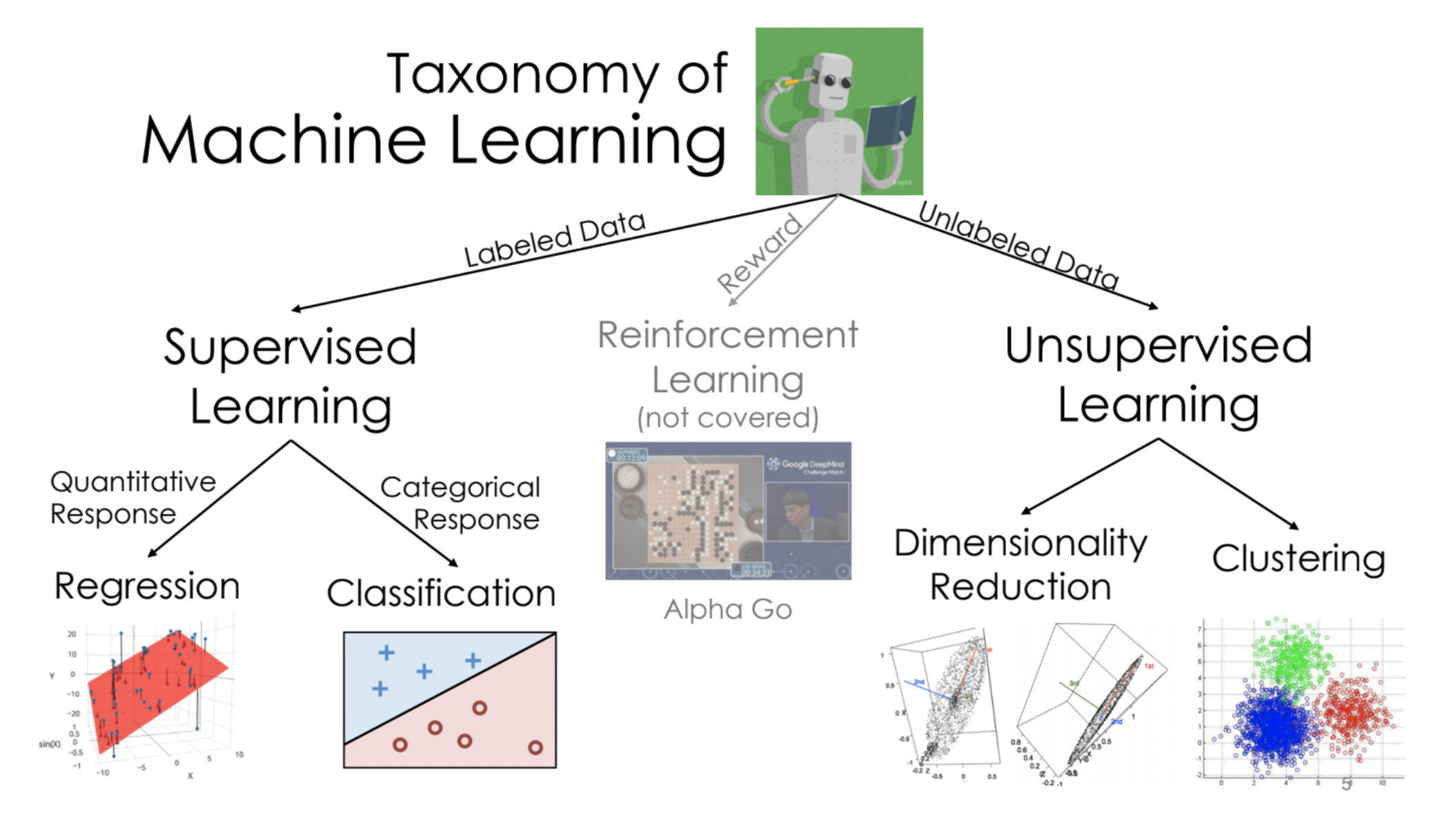
Remember, you can always ask questions at q.dsc40a.com!

If the direct link doesn't work, click the "Lecture Questions" link in the top right corner of dsc40a.com.

Outline

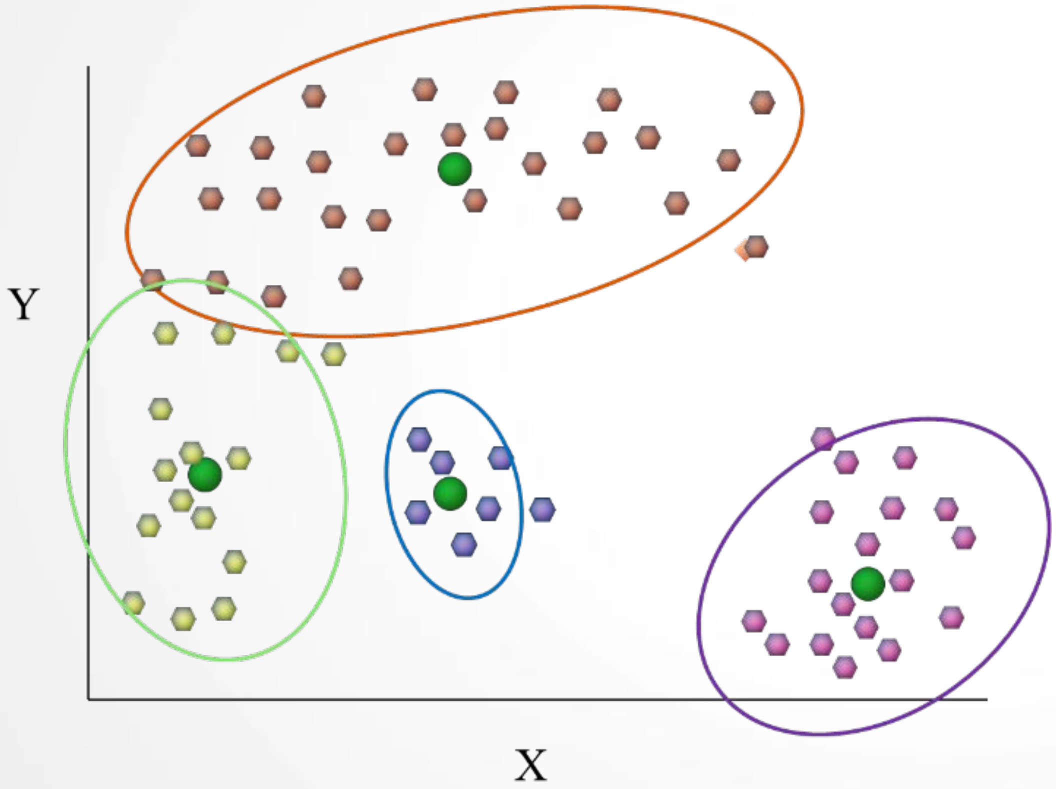
- We’ll look at the clustering problem in machine learning and an algorithm that solves this problem.
- Look out for connections to loss functions and risk minimization!

Today



Taxonomy of
Machine Learning
Labeled Data
Reward
Unlabeled Data
Supervised Learning
Reinforcement Learning
(not covered)
Unsupervised Learning
Quantitative Response
Categorical Response
Regression
Classification
Alpha Go
Dimensionality Reduction
Clustering

Clustering: Applications



- Bot detection
- Marketing to different subpopulations
- Discovering structure:
  - strains of viruses
  - new species
  - communities in a social network
  - chemicals properties

Clustering: Problem Statement

Given a list of n data points (or vectors) in R^d

$$x_1, x_2, \dots, x_n$$

and a positive integer, k,

group the data points into k groups (clusters) of nearby points.

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Given a list of n data points (or vectors) in R^d

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and a positive integer, k,

group the data points into k groups (clusters) of nearby points.

Which of these inequalities should be true?

A. $d < n$
B. $n < d$
C. $k < n$
D. $n < k$

How to define groups?

Pick k cluster centers (centroids),

$$\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \dots, \boldsymbol{\mu}_k$$

These k centroids define the k groups, by placing each data point in the group corresponding to the nearest centroid.

How to define centroids?

Choose the k cluster centers (centroids) to minimize a cost function.

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

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.

Step 1: Randomly initialize the k centroids.

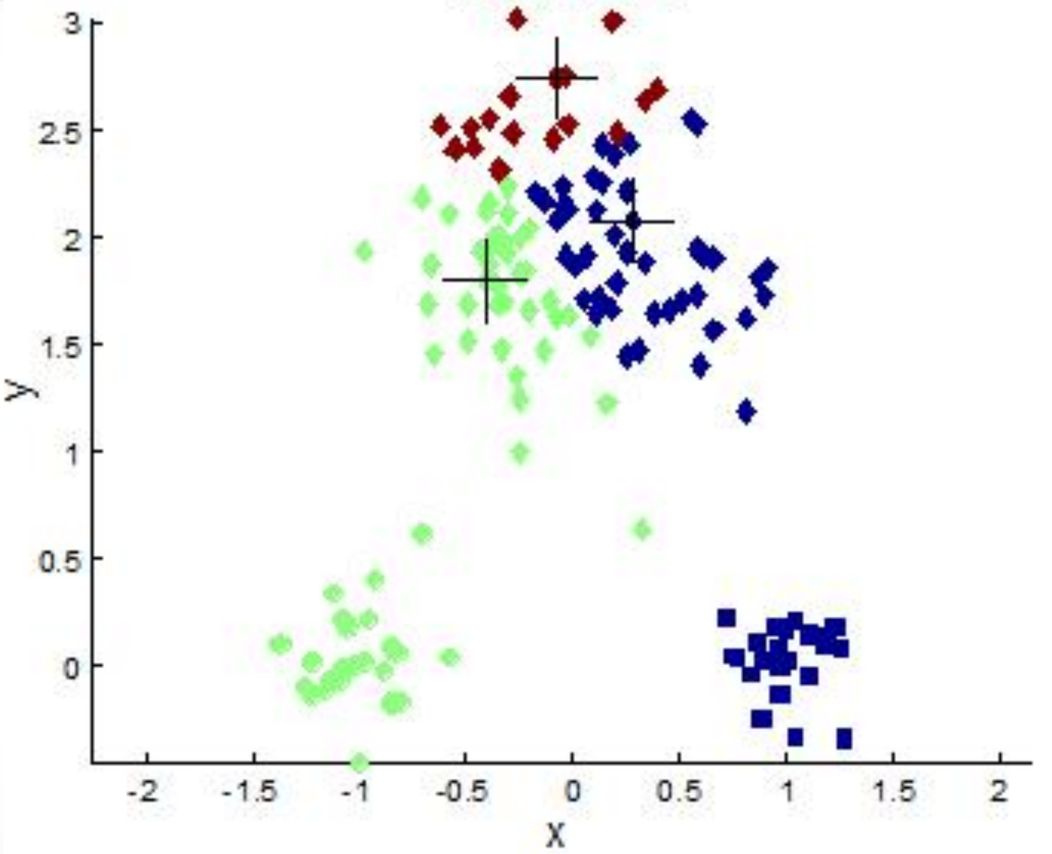
Two common strategies:

- Randomly select k of the data points x_i.
- Randomly assign each data point to one of k groups. Set the centroid of each group to be the center of the points assigned to that group.

Step 2: Keep centroids fixed. Update groups.

For each point,

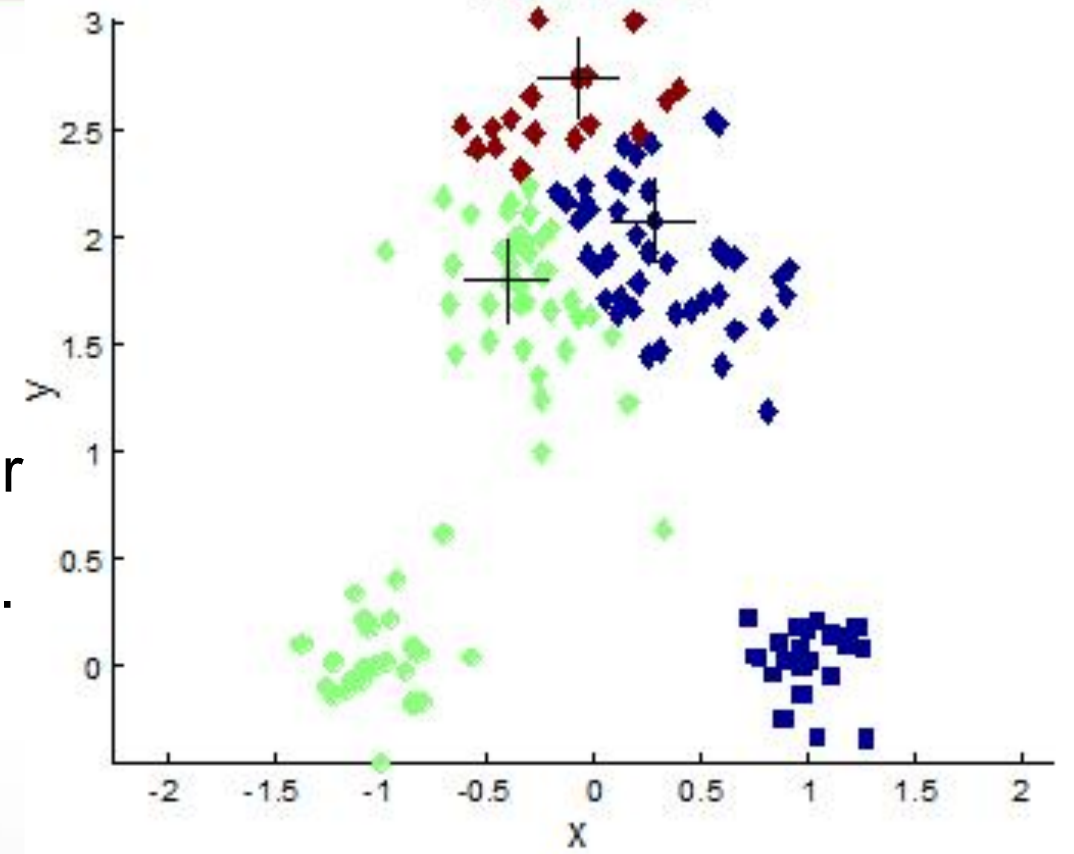
- find the nearest centroid and
- add the point to a group corresponding to that nearest centroid.



Step 3: Keep groups fixed. Update centroids.

For each centroid,

- average the coordinates of all data points in the group, and
- move the centroid to this center point with average coordinates.



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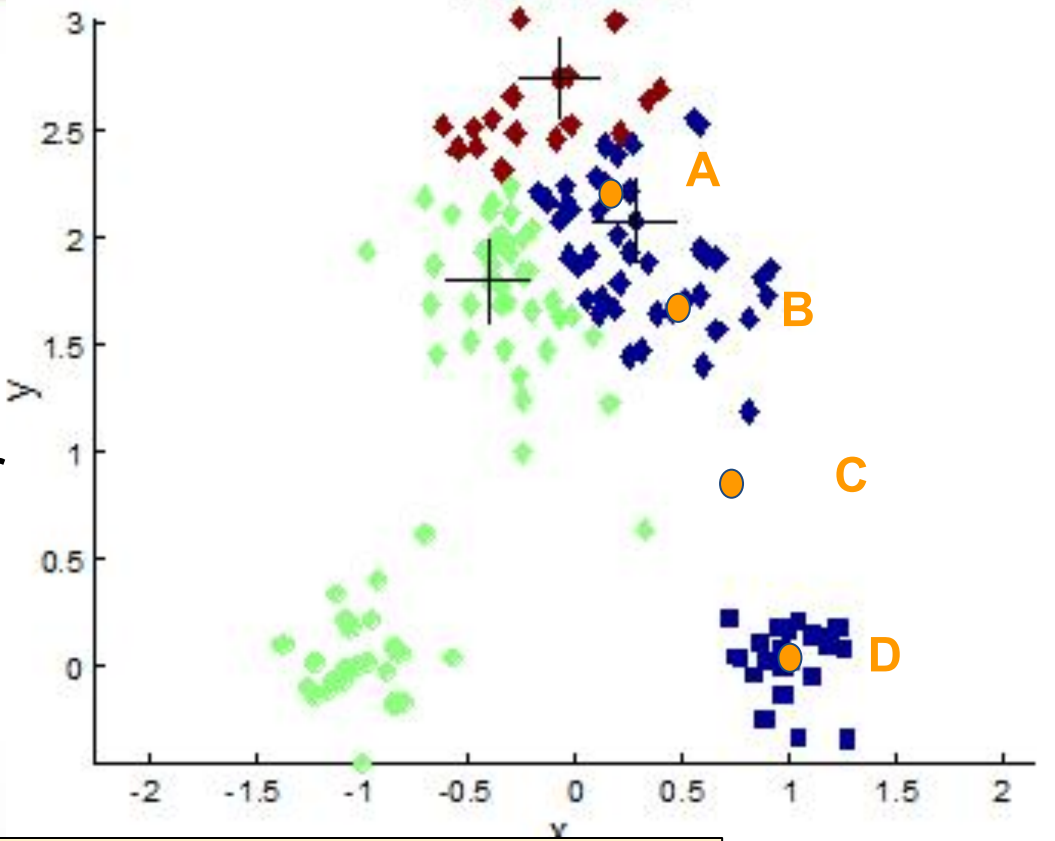


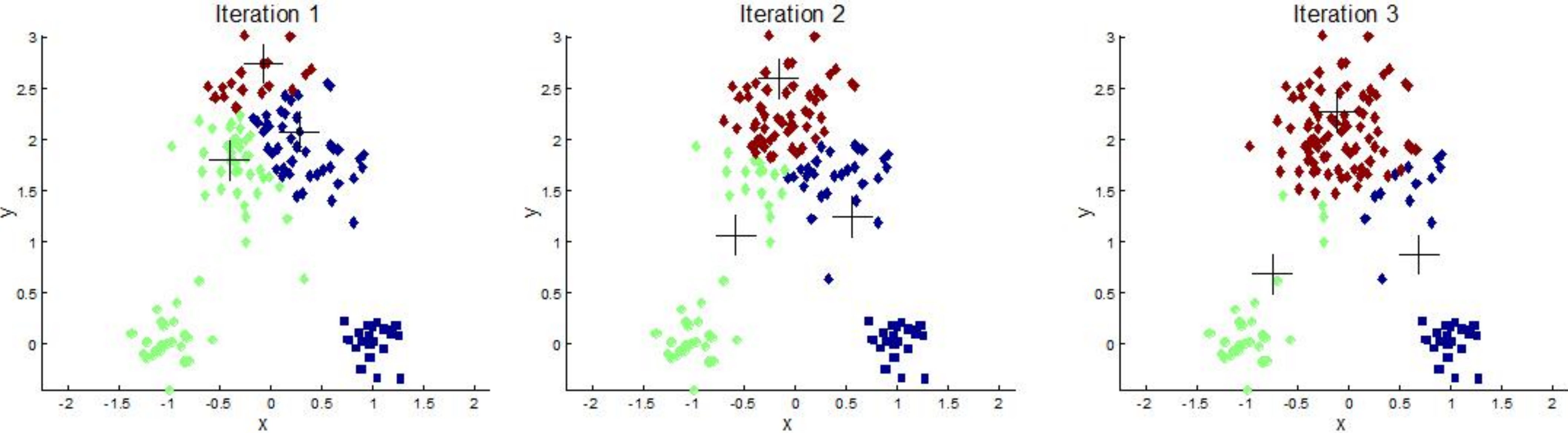
For the blue group of points, approximately where will the centroid move to?

Step 4: Repeat steps 2 and 3 until done.

Done when:

- max number of iterations is reached, or
- centroids don’t move (at all, or very much), or
- groups don’t change (at all, or very much)

k-Means Clustering Example



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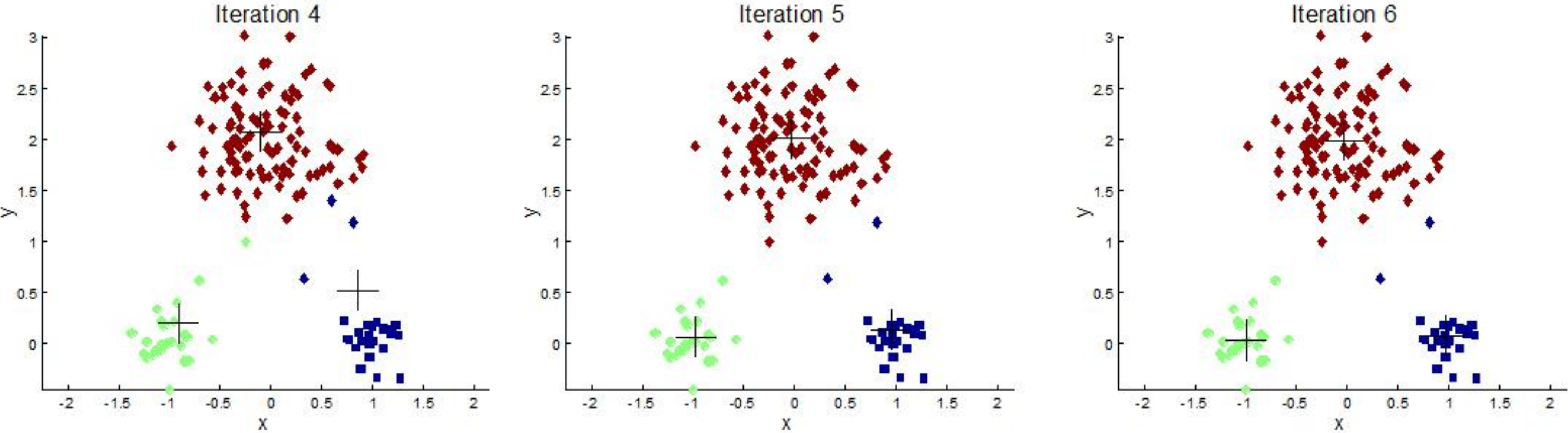

Summary

- We described the clustering problem and the k-means algorithm, which solves this problem.
- **Next time:** We'll see that updating the centroids according to this algorithm reduces the cost with each iteration.

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

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Outline

- 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)

Why does k-means clustering work?

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

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

2. Fix the centroids. Update the groups.

consider an arbitrary iteration

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

Why does k-means clustering work?

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

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3. Fix the groups. Update the centroids.

consider an arbitrary iteration

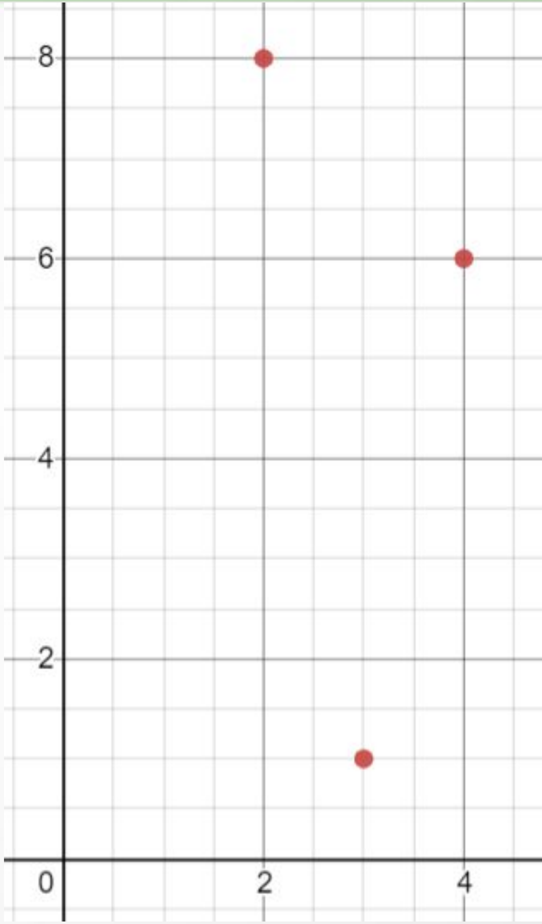
Argue that $\text{Cost}(\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \ldots, \boldsymbol{\mu}_k)$ decreases in this step because for each group j, $\text{Cost}(\boldsymbol{\mu}_j)$ is minimized when we update the centroid.

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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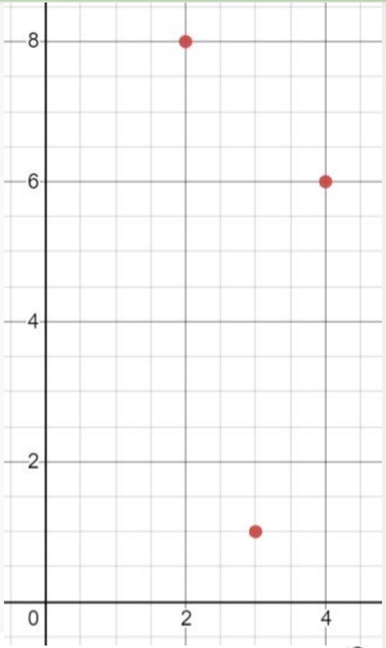

$$\begin{aligned}\text{Cost}\,(\mu_j) &= \left(\sqrt{(4-c_1)^2+(6-c_2)^2}\right)^2 + \left(\sqrt{(2-c_1)^2+(8-c_2)^2}\right)^2 + \left(\sqrt{(3-c_1)^2+(1-c_2)^2}\right)^2 \\ &= (4-c_1)^2+(6-c_2)^2+(2-c_1)^2+(8-c_2)^2+(3-c_1)^2+(1-c_2)^2\end{aligned}$$

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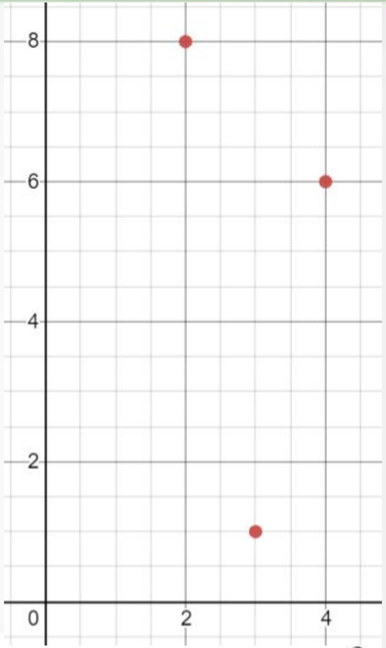

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$$\frac{\partial \text{Cost}(\mu_j)}{\partial c_1} = 2(c_1-4)+2(c_1-2)+2(c_1-3)$$

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

Why does k-means clustering work?

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?

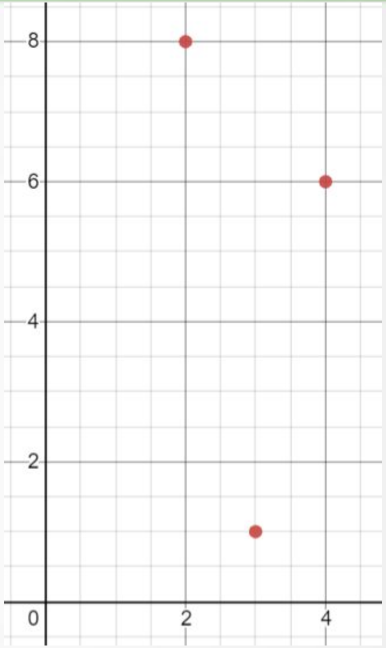
$$\frac{\partial \text{Cost}(\mu_j)}{\partial c_1} = 2(c_1 - 4) + 2(c_1 - 2) + 2(c_1 - 3)$$

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

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

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

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



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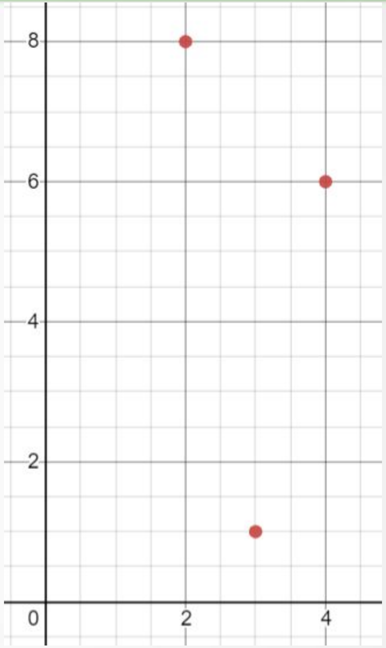
How to place centroid $\boldsymbol{\mu}_j = (c_1, c_2)$ to minimize cost?

$$\frac{\partial \mathrm{Cost}(\mu_j)}{\partial c_2} = 2(c_2 - 6) + 2(c_2 - 8) + 2(c_2 - 1)$$
$$0 = 2(c_2 - 6) + 2(c_2 - 8) + 2(c_2 - 1)$$
$$0 = c_2 - 6 + c_2 - 8 + c_2 - 1$$
$$3c_2 = 6 + 8 + 1$$
$$c_2 = \frac{6+8+1}{3}$$



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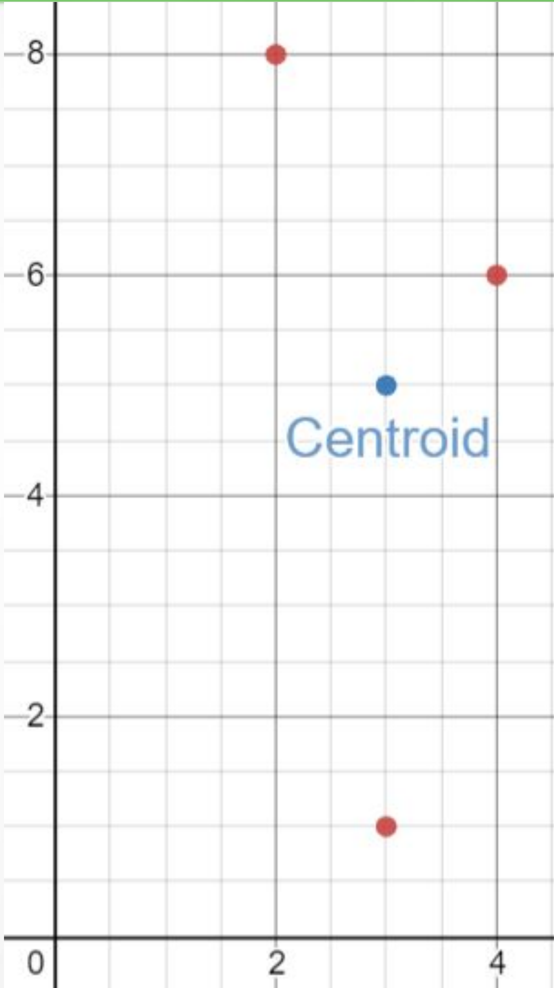
How to place centroid $\boldsymbol{\mu}_j = (c_1, c_2)$ to minimize cost?

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

Minimize cost by averaging in each coordinate.



Cost, Loss, and Risk

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

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

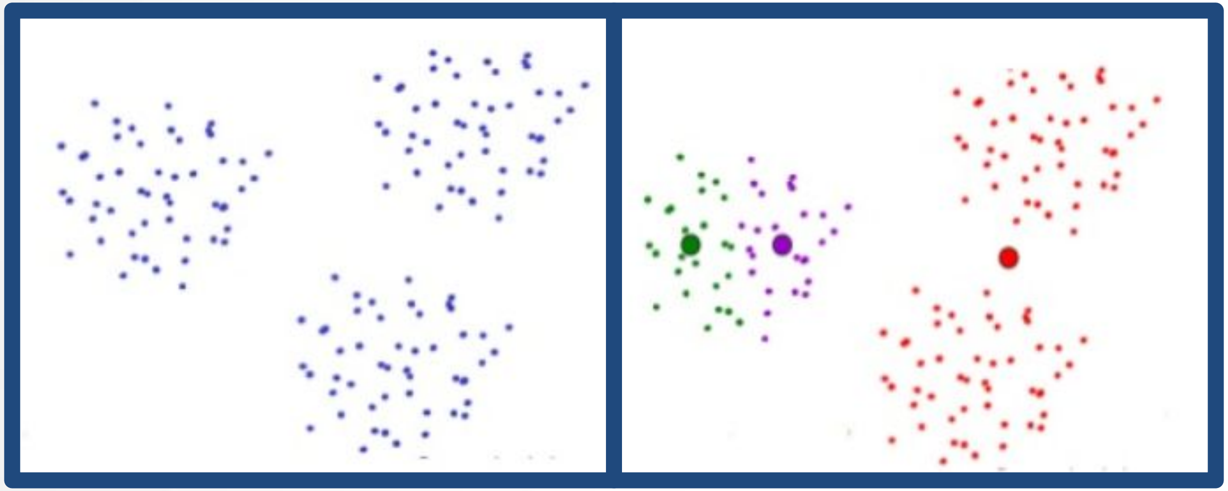
Why does k-means clustering work?

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.

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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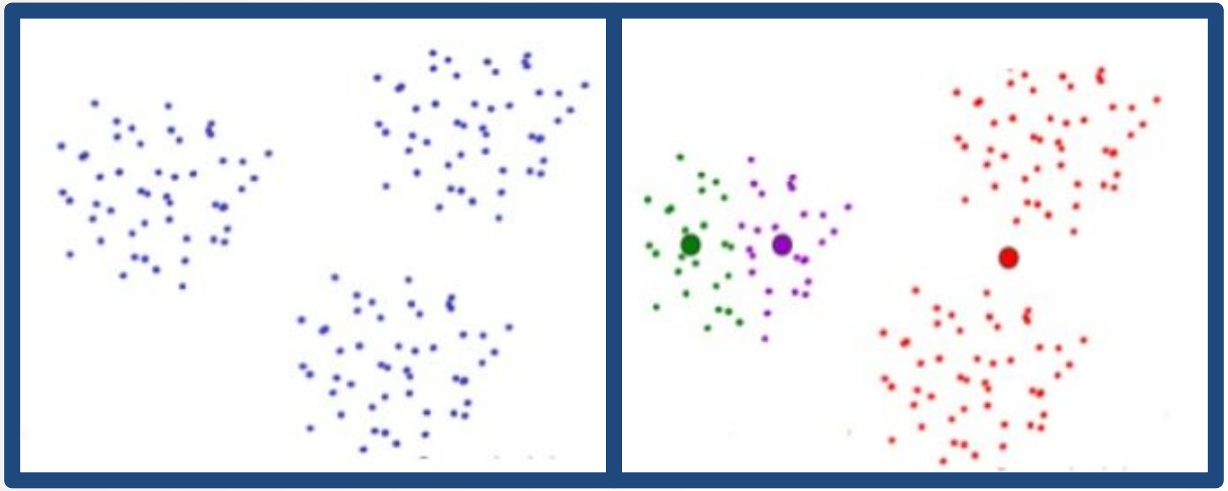

In general, how do we assess which result is the best?

A. Clusters appear how we expect them to
B. Clusters are evenly sized
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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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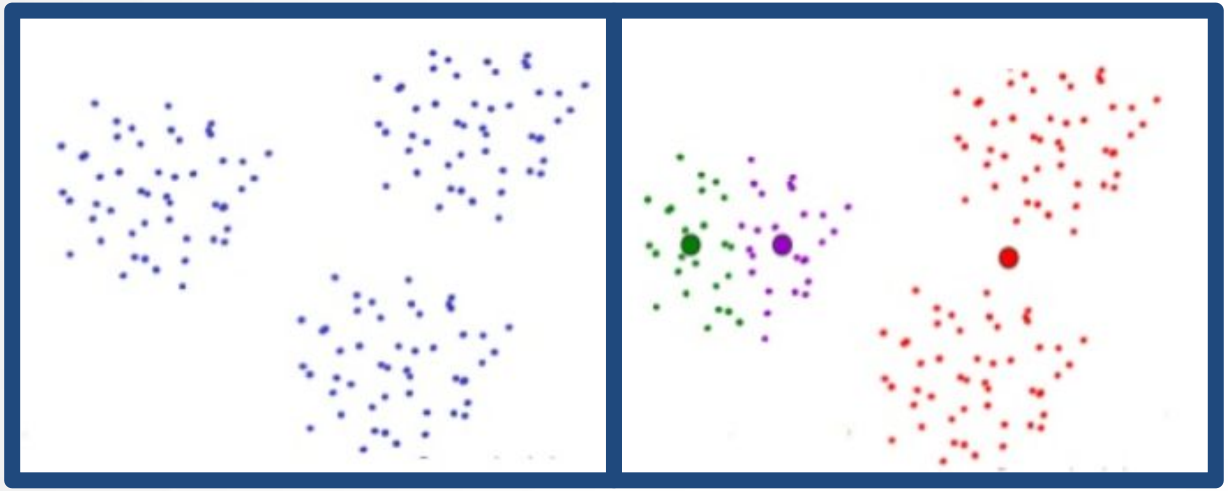

- No guarantees of a satisfactory solution with this algorithm.
- Brute force algorithm would try all assignments of points to clusters and choose the one with the lowest cost.

k-Means Clustering in Practice: Initialization

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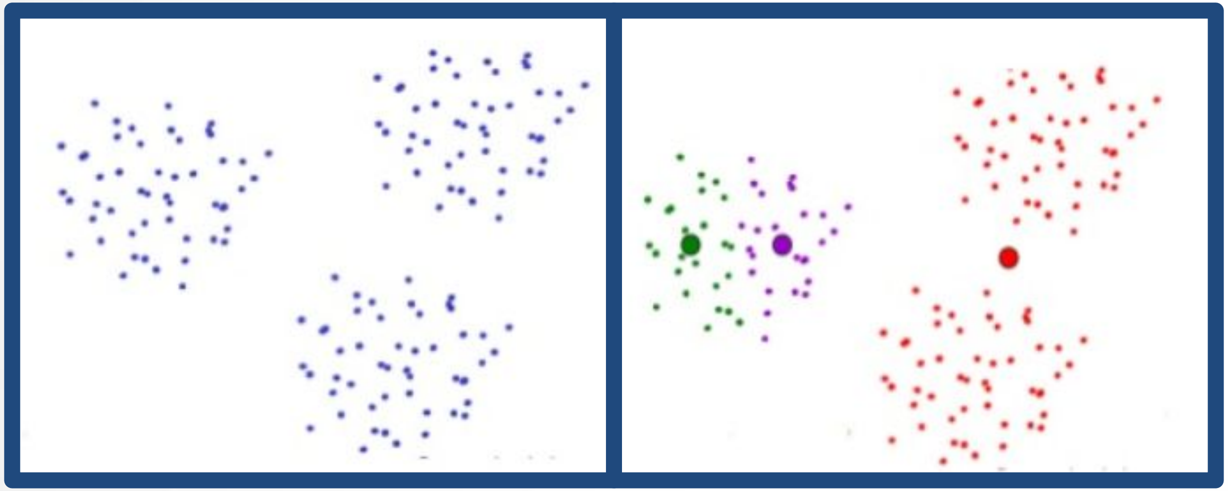

How many ways to assign n points to k clusters?

- No guarantees of a satisfactory solution with this algorithm.
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k-Means Clustering in Practice: Initialization

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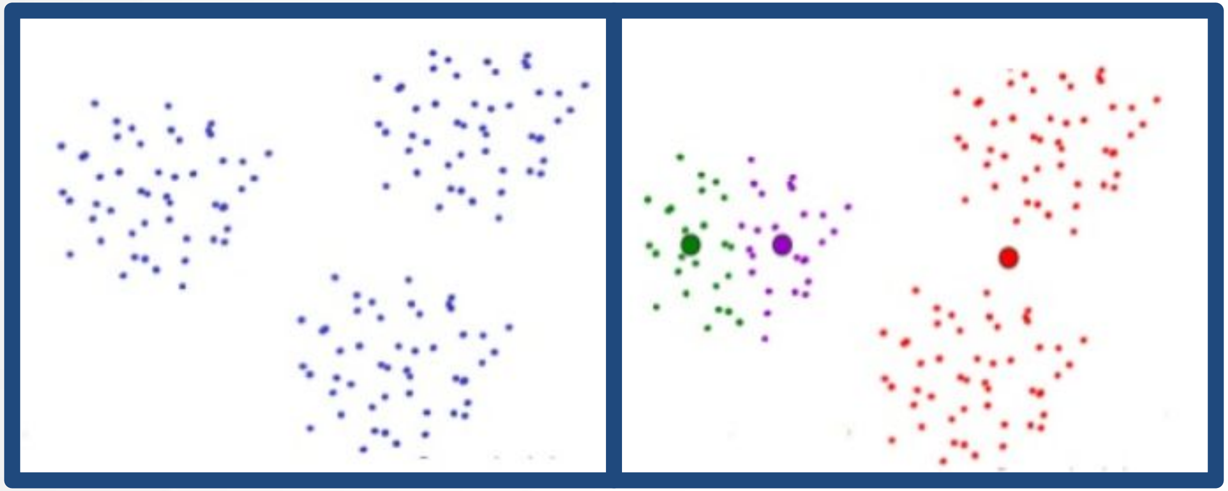
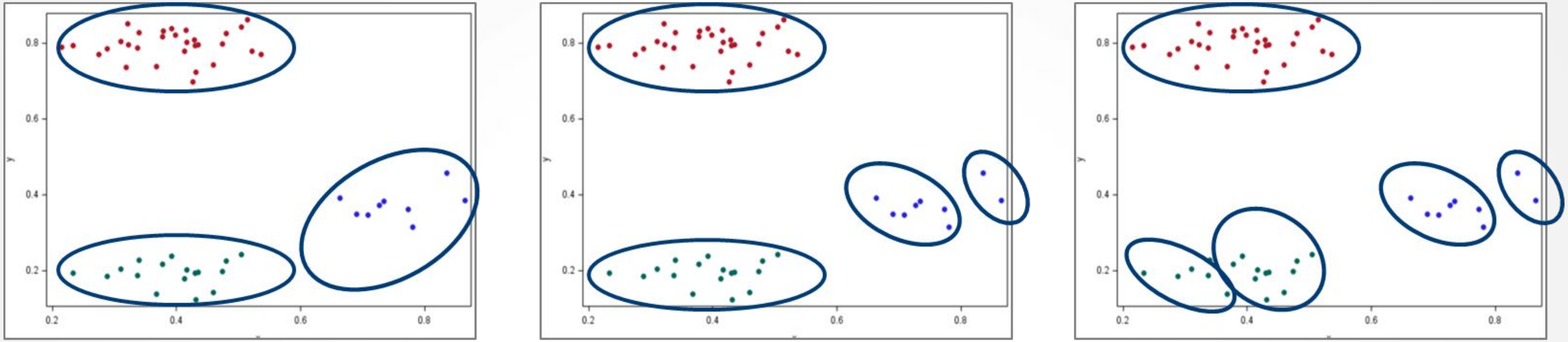


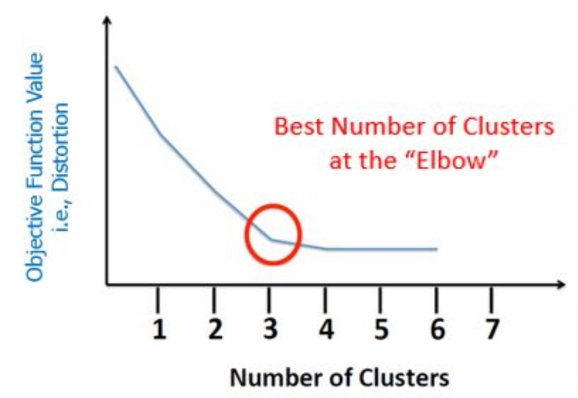
- No guarantees of a satisfactory solution with this algorithm.
- Any algorithm that is guaranteed to find the best coloring of data points takes exponential time (computationally infeasible).

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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D. Set the centroid to be one of the other centroids, chosen at random.

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.