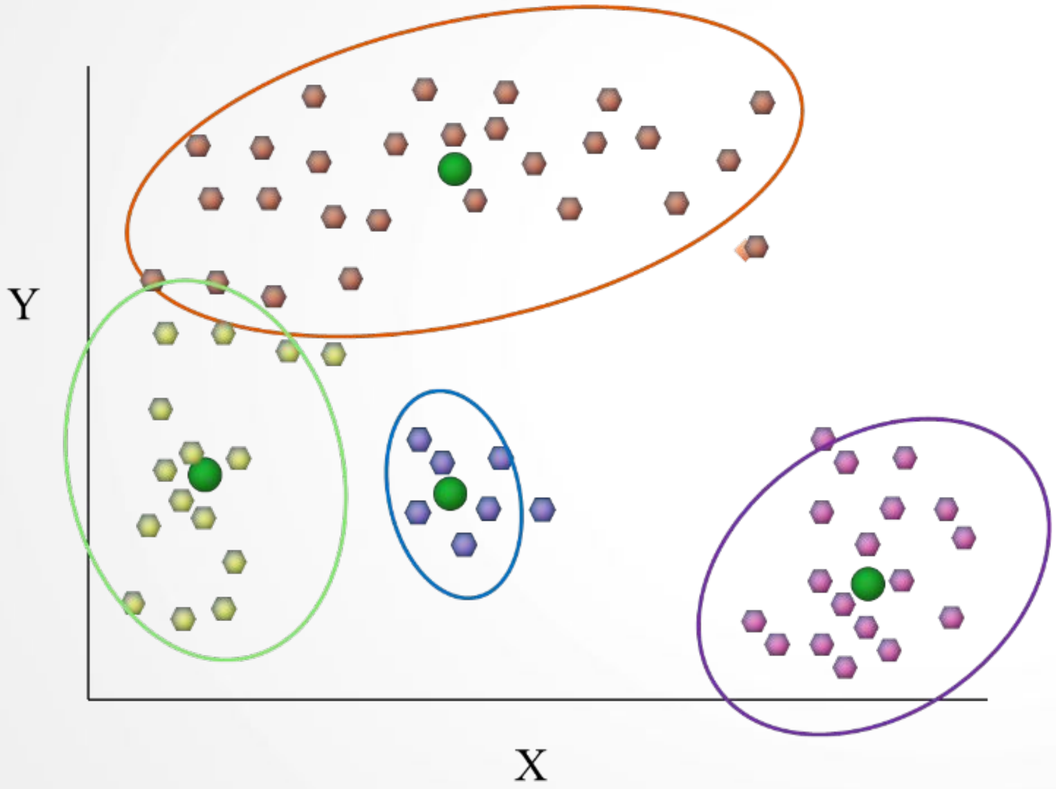
DSC 40A

Theoretical Foundations of Data Science I

In This Video

- 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!

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

$$x_1, x_2, \ldots, x_n$$

and a positive integer, k,

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

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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.

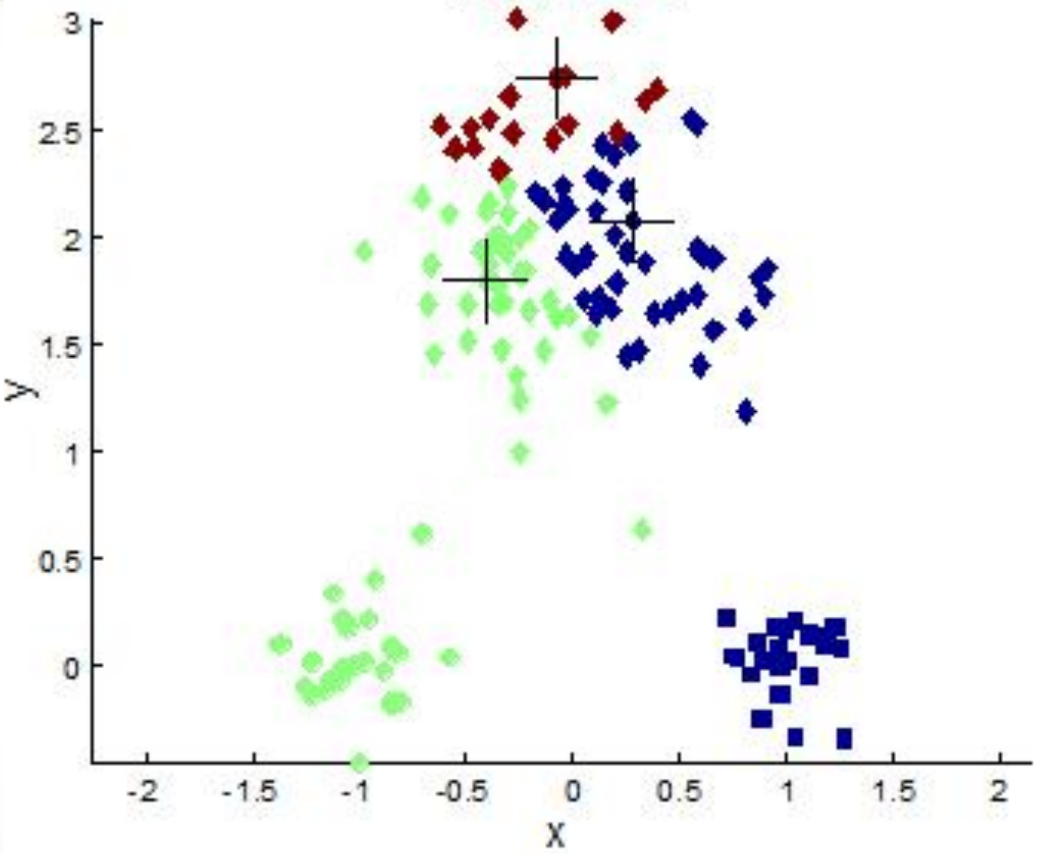
Two common strategies:

- 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,

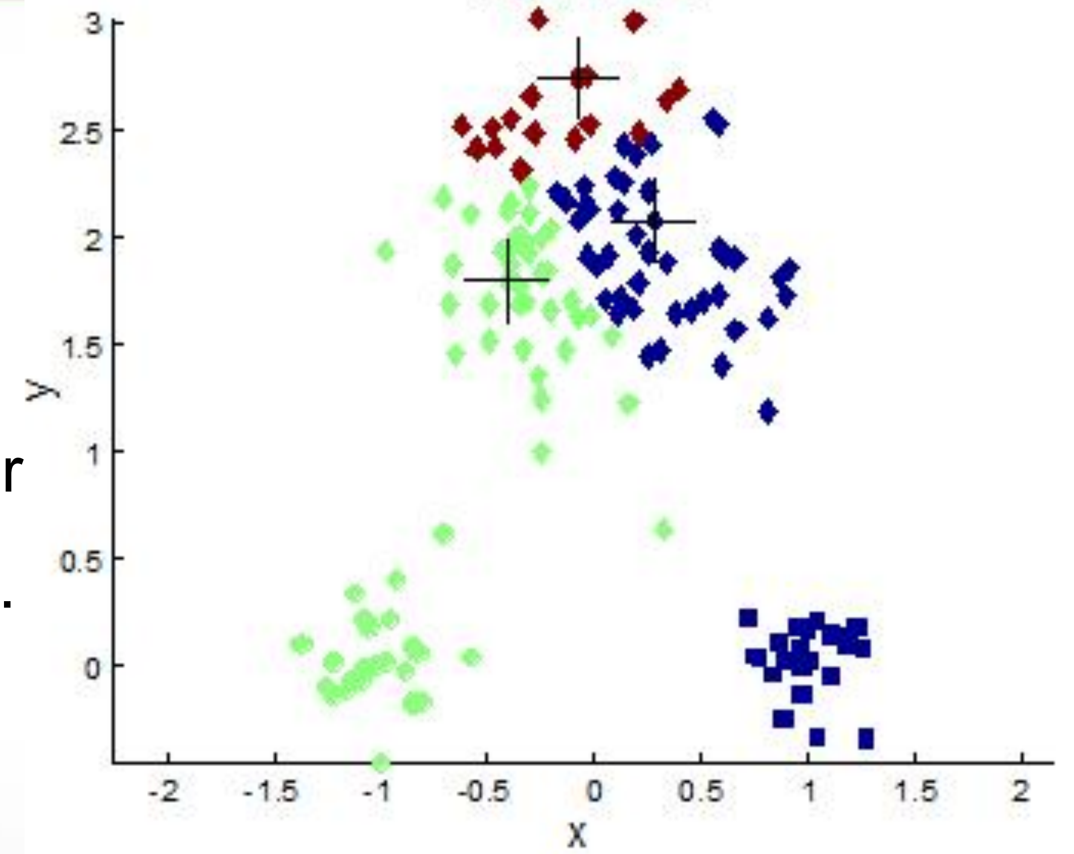
- find the nearest centroid and
- add the point to a group corresponding to that nearest centroid.



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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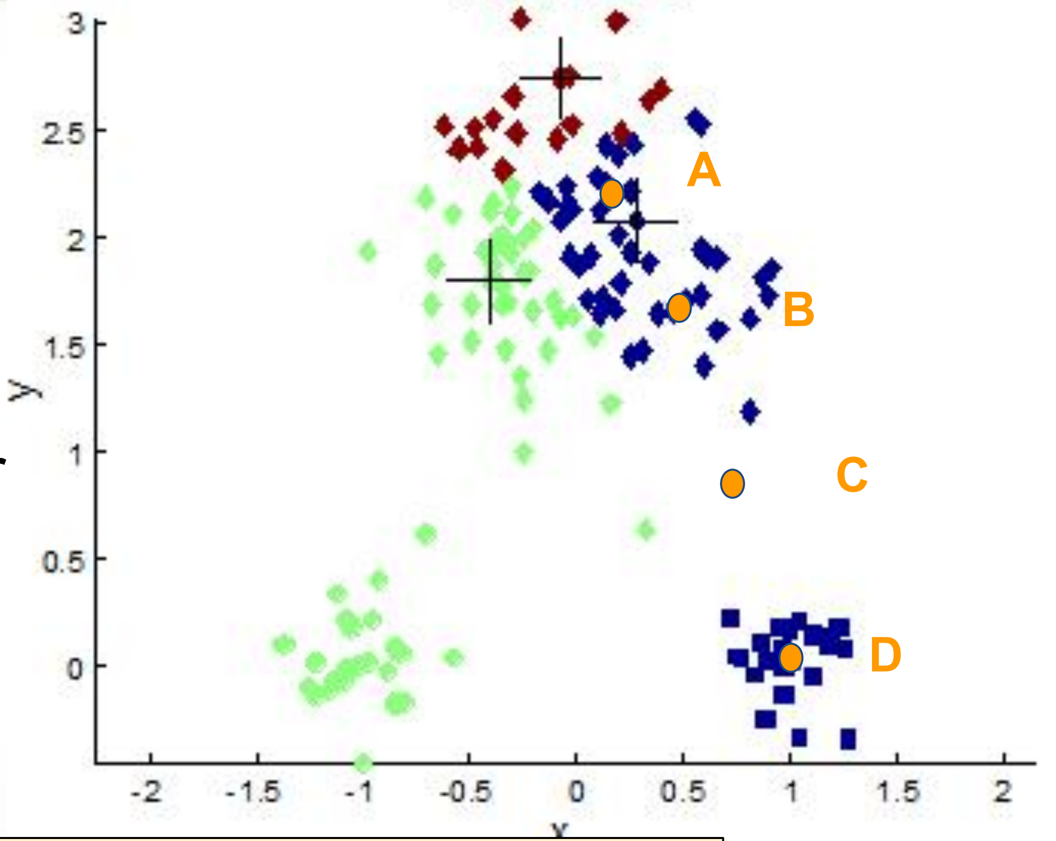


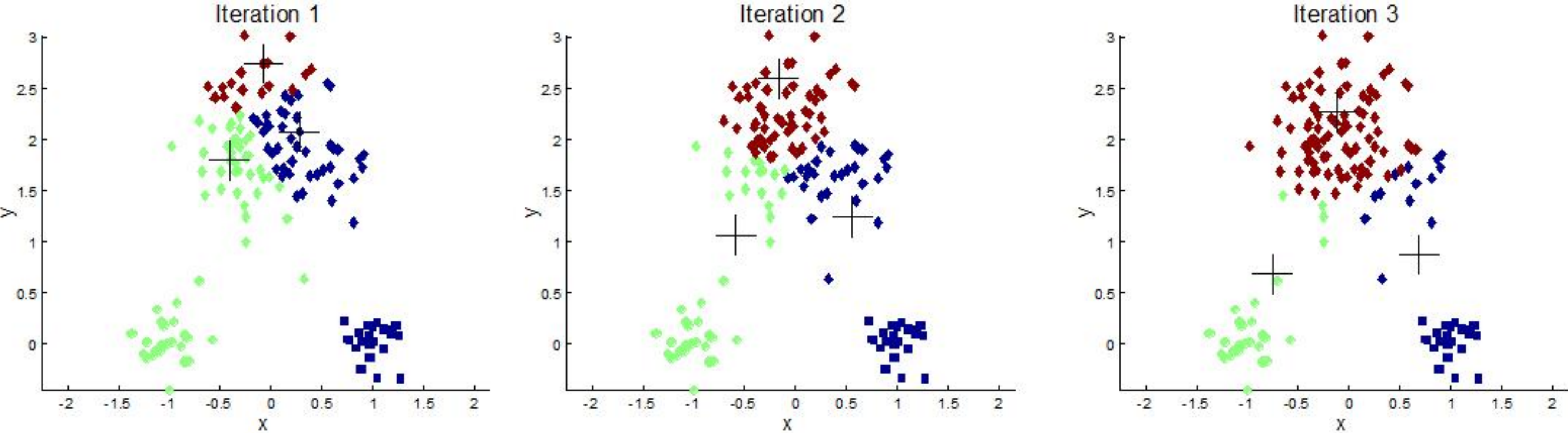
For the blue group of points, approximately where will the centroid move to?

Step 4: Repeat steps 2 and 3 until done.

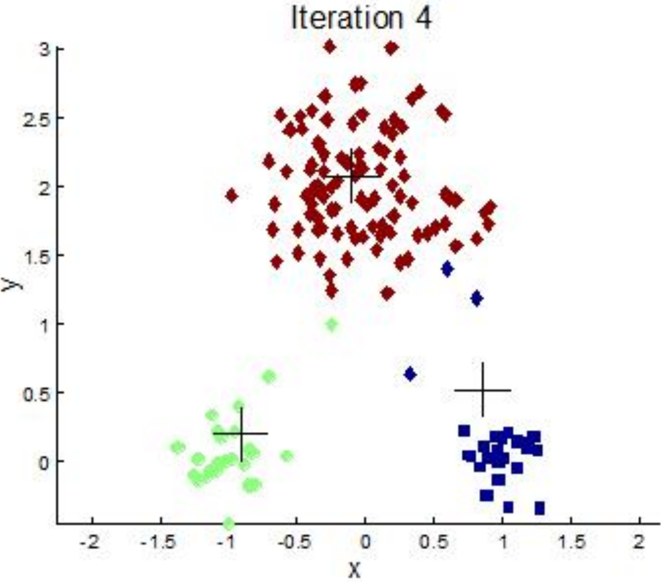
Done when:

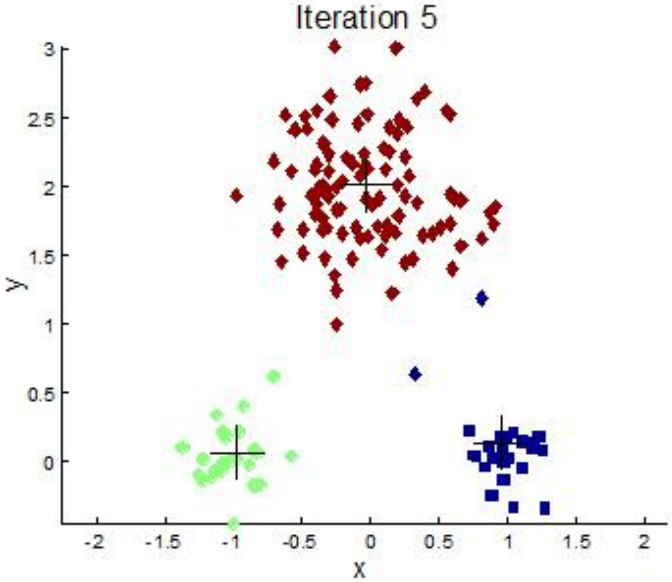
- max number of iterations is reached, or
- centroids don’t move (at all, or very much), or
- groups don’t change (at all, or very much)

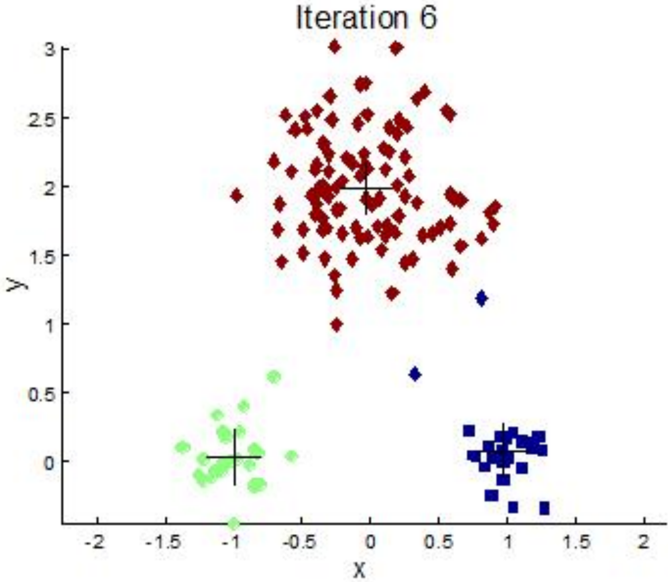
k-Means Clustering Example



k-Means Clustering Example







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 $\boldsymbol{\mu}_j$