Lecture 14 – Clustering

DSC 40A, Spring 2023

Announcements

- Midterm 1 is Friday during lecture.

- No groupwork tonight. Instead, TA and tutors will host a mock exam and review session **today from 7-9pm in FAH 1301**.
    - Note the room change (same building).

    - You'll take the midterm from Winter 2022, when I last taught this class.

    - **Bring paper.** Formula sheet and exam questions provided.

Midterm 1 is Friday during lecture

- Formula sheet will be provided for you. No other notes.
- No calculators. This implies no crazy calculations.
- Assigned seats will be posted on Campuswire.
- We will not answer questions during the exam. State your assumptions if anything is unclear.
- The exam will include long-answer homework-style questions, as well as short-answer questions such as multiple choice or filling in a numerical answer.
- The exam covers Homeworks 1 through 4, which includes Monday's lecture, but not clustering.

Midterm study strategy

- Review the written solutions to previous homeworks and groupworks.

- Identify which concepts are still iffy. Re-watch podcasts, post on Campuswire, come to office hours, use resources on course website.

- Work through past exams on course website.

- Study in groups.

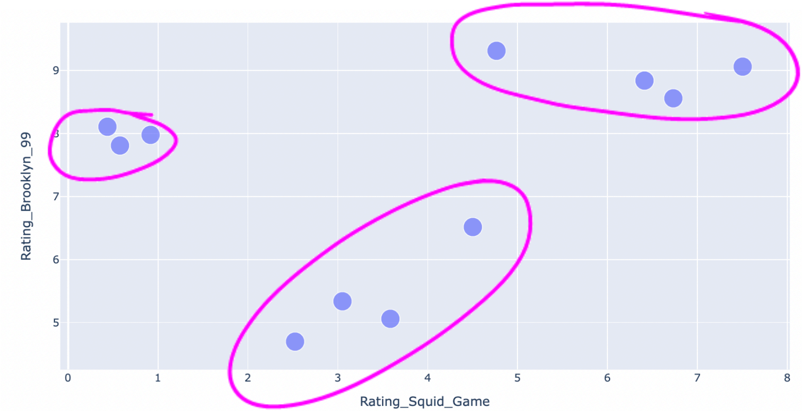
- Summarize key facts and formulas.

Agenda

- The clustering problem.
- k-Means Clustering algorithm.
- Why does k-Means work?
- Practical considerations.

The clustering problem

Question: how might we "cluster" these points into groups?



$n = 11, \; d = 2, \; k = 3$

Problem statement: clustering

Goal: Given a list of n data points, stored as vectors in $\mathbb{R}^d$, $\vec{x}_1, \vec{x}_2, ..., \vec{x}_n$, and a positive integer k, **place the data points into k groups of nearby points**.

n = # data pts
d = dimension

- These groups are called "clusters".
- Think about groups as **colors**.
  - i.e., the goal of clustering is to assign each point a color, such that points of the same color are close to one another.
- Note, unlike with regression, there is no "right answer" that we are trying to predict — there is no y!
  - Clustering is an **unsupervised** method.

How do we define a group?

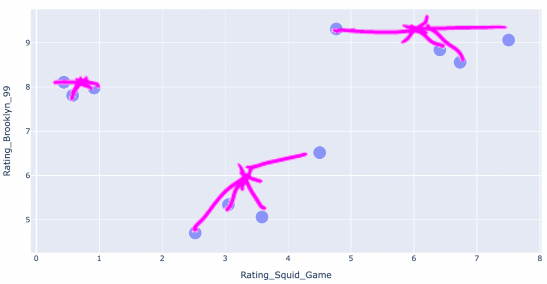
- One solution: pick k cluster centers, i.e. **centroids**:

$$\vec{\mu}_1, \vec{\mu}_2, \ldots, \vec{\mu}_k \text{ in } \mathbb{R}^d$$

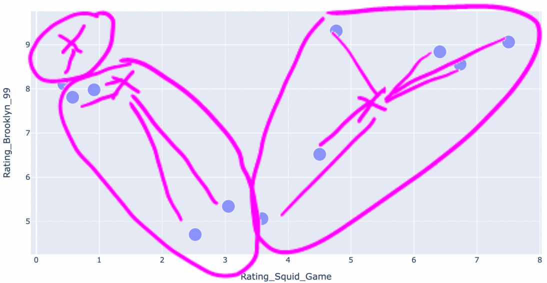
- These k centroids define the k groups.

- Each data point “belongs” to the group corresponding to the nearest centroid.

- This reduces our problem from being “find the best group for each data point” to being “find the best locations for the centroids”.



good-
short
lines



bad-
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How do we pick the centroids?

- Let's come up with an **cost function**, C, which describes how good a set of centroids is.
  - Cost functions are a generalization of empirical risk functions.

- One possible cost function:

$$C(\underbrace{\mu_1, \mu_2, \ldots, \mu_k}_{\text{set of centroids}}) = \text{total squared distance of each data point } \vec{x}_i \text{ to its closest centroid } \mu_j$$

- This C has a special name, **inertia**.

- Lower values of C lead to "better" clusterings.
  - **Goal:** Find the centroids $\mu_1, \mu_2, \ldots, \mu_k$ that minimize C.

Discussion Question

Suppose we have n data points, $\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_n$, each of which are in $\mathbb{R}^d$.

Suppose we want to cluster our dataset into k clusters.

How many ways can we assign points to clusters?

a) $d \cdot k$

b) d^k

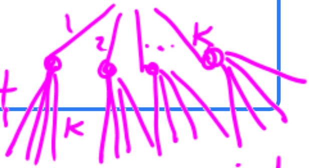
c) n^k

[✓ d) k^n]

e) $n \cdot k \cdot d$

first point $\vec{x}_1$

second point x_2



ways to color n points with one of k colors

How do we minimize inertia?

- **Problem**: there are exponentially many possible clusterings. It would take too long to try them all.
- **Another Problem**: we can't use calculus or algebra to minimize C, since to calculate C we need to know which points are in which clusters.
- We need another solution.

k-Means Clustering

k-Means Clustering, i.e. Lloyd’s Algorithm

Here’s an algorithm that attempts to minimize inertia:

1. Pick a value of *k* and randomly initialize *k* centroids.

   picks k data points

2. Keep the centroids fixed, and update the groups.
   - Assign each point to the nearest centroid.
3. Keep the groups fixed, and update the centroids.
   - Move each centroid to the center of its group.

     (average coordinates)
4. Repeat steps 2 and 3 until the centroids stop changing.

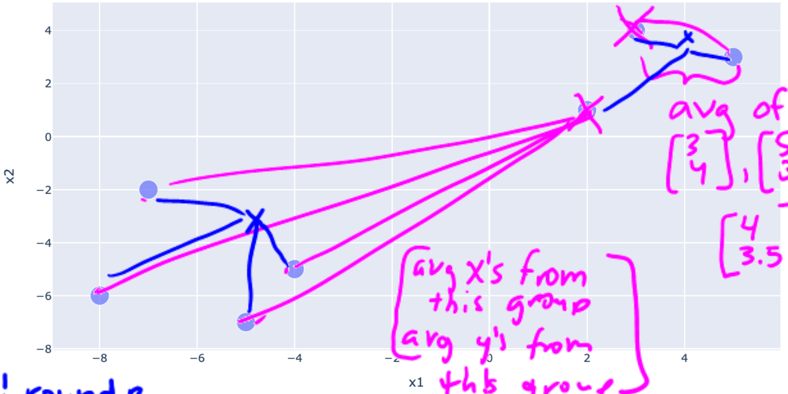
Example

See the following site for an interactive visualization of k-Means Clustering: `https://tinyurl.com/40akmeans`

An example by hand

Suppose we choose the initial centroids $\mu_1 = \begin{bmatrix}2\\1\end{bmatrix}$ and $\mu_2 = \begin{bmatrix}3\\4\end{bmatrix}$.

Where will the centroids move to after one iteration of k-Means Clustering?



avg of $\begin{bmatrix}3\\4\end{bmatrix}, \begin{bmatrix}5\\3\end{bmatrix}$

$\begin{bmatrix}4\\3.5\end{bmatrix}$

$\left[\begin{array}{l}\text{avg x's from this group}\\ \text{avg y's from this group}\end{array}\right]$

blue! round 2

Demo

Let’s see k-Means Clustering in action. Follow along here.

Why does k-Means work?

What is the goal of k-Means Clustering?

- Recall, our goal is to find the centroids $\mu_1, \mu_2, \ldots, \mu_k$ that minimize inertia:

  $C(\mu_1, \mu_2, \ldots, \mu_k) =$ total squared distance of each data point $\vec{x}_i$ to its closest centroid μ_j

- Let's argue that each step of the k-Means Clustering algorithm reduces inertia.
  - After enough iterations, inertia will be small enough.

Why does k-Means work? (Step 1)

Step 1: Pick a value of k and randomly initialize k centroids.

- After initializing our k centroids, we have an initial value of inertia. We are going to argue that this only decreases.

Why does k-Means work? (Step 2)

Step 2: Keep the centroids fixed, and update the groups by assigning each point to the nearest centroid.

- Assuming the centroids are fixed, for each $\vec{x}_i$ we have a choice — which group should it be a part of?
- Whichever group we choose, inertia will be calculated using the squared distance between $\vec{x}_i$ and that group's centroid.
- Thus, to minimize inertia, we assign each $\vec{x}_i$ to the group corresponding to the closest centroid.

Note that this analysis holds every time we're at Step 2, not just the first time.

Why does k-Means work? (Step 3)

Step 3: Keep the groups fixed, and update the centroids by moving each centroid to the center of its group (by averaging coordinates).

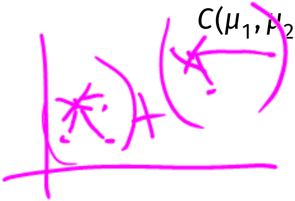
- Before we justify why this is optimal, let’s revisit inertia.

Aside: separating inertia

- Inertia:

$$C(\mu_1, \mu_2, \dots, \mu_k) = \text{total squared distance of each data point } \vec{x}_i \text{ to its closest centroid } \mu_j$$

- Note that an equivalent way to write inertia is



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

$$C(\mu_j) = \text{total squared distance of each data point } \vec{x}_i \text{ in group } j \text{ to centroid } \mu_j$$

- What's the point?

Why does k-Means work? (Step 3)

$C(\mu_1, \mu_2, \ldots, \mu_k) = C(\mu_1) + C(\mu_2) + \ldots + C(\mu_k)$ where

$C(\mu_j)$ = total squared distance of each data point $\vec{x}_i$ in group j to centroid μ_j

Step 3: Keep the groups fixed, and update the centroids by moving each centroid to the center of its group (by averaging coordinates).

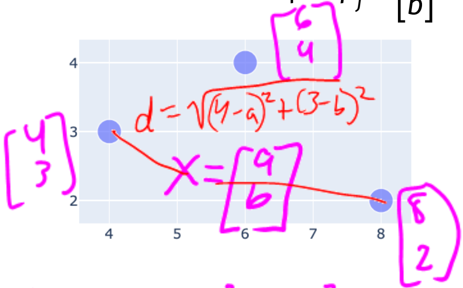
- Let's argue why this minimizes $C(\mu_j)$, for each group j.

Why does k-Means work? (Step 3)

$C(\mu_j)$ = total squared distance of each data point $\vec{x}_i$ in group j to centroid μ_j

Suppose group j contains the points $(4, 3)$, $(6, 4)$, and $(8, 2)$.

Where should we put $\mu_j = \begin{bmatrix} a \\ b \end{bmatrix}$ to minimize $C(\mu_j)$?



$\begin{bmatrix} 6 \\ 4 \end{bmatrix}$ $\begin{bmatrix} 4 \\ 3 \end{bmatrix}$ $\begin{bmatrix} 8 \\ 2 \end{bmatrix}$

$d = \sqrt{(4-a)^2 + (3-b)^2}$

$x = \begin{bmatrix} a \\ b \end{bmatrix}$

we'll place centroid in location that has lowest cost

$C(a,b) = (4-a)^2 + (3-b)^2 + (8-a)^2 + (2-b)^2 + (6-a)^2 + (4-b)^2$

Why does k-Means work? (Step 3)

$$C(a,b) = (4-a)^2 + (3-b)^2 + (8-a)^2 + (2-b)^2 + (6-a)^2 + (4-b)^2$$

$$\frac{\partial C}{\partial a} = -2(4-a) - 2(8-a) - 2(6-a) = 0$$

$$4-a+8-a+6-a=0$$

$$3a = 4+8+6$$

$$a^* = \frac{4+8+6}{3} = \text{the mean of first coordinates}$$

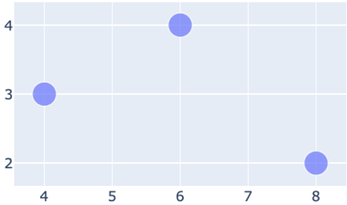
similarly for $\frac{\partial C}{\partial b} = 0 \Rightarrow b^* = \frac{3+2+4}{3} = \text{mean}$

Why does k-Means work? (Step 3)

$C(\mu_j)$ = total squared distance of each data point $\vec{x}_i$
in group j to centroid μ_j

Suppose group j contains the points $(4, 3)$, $(6, 4)$, and $(8, 2)$.

Where should we put $\mu_j = \begin{bmatrix} a \\ b \end{bmatrix}$ to minimize $C(\mu_j)$?



a^* = mean of 1st coords

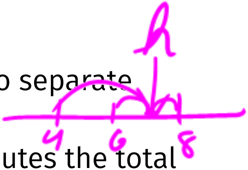
b^* = mean of 2nd coords

Cost and empirical risk

- On the previous slide, we saw a function of the form

$$\begin{aligned} C(\mu_j) = C(a, b) &= (4 - a)^2 + (3 - b)^2 \\ &+ (6 - a)^2 + (4 - b)^2 \\ &+ (8 - a)^2 + (2 - b)^2 \end{aligned}$$

- $C(a, b)$ can be thought of as the sum of two separate functions, $f(a)$ and $g(b)$.
  - $f(a) = (4 - a)^2 + (6 - a)^2 + (8 - a)^2$ computes the total squared distance of each x_1 coordinate to a.
  - From earlier in the course, we know that $a^* = \frac{4+6+8}{3} = 6$ minimizes $f(a)$.

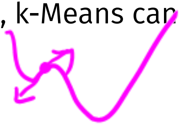


Connection to squared loss / risk

Practical considerations

Initialization

- Depending on our initial centroids, k-Means may “converge” to a clustering that doesn’t actually have the lowest possible inertia.
  - In other words, like gradient descent, k-Means can get caught in a **local minimum**.



- Some solutions:
  - Run k-Means several times, each with different randomly chosen initial centroids. Keep track of the inertia of the final result in each attempt. Choose the attempt with the lowest inertia.
  - **k-Means++**: choose one initial centroid at random, and place other centroids far from all other centroids.

Choosing *k*

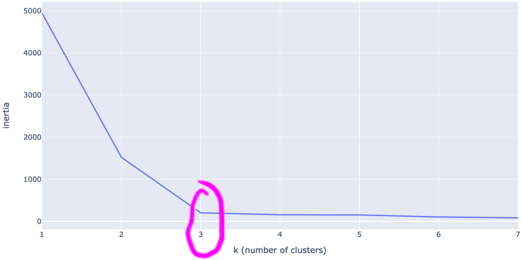
- Note that as *k* increases, inertia decreases.
  - Intuitively, as we add more centroids, the distance between each point and its closest centroid will drop.

- But the goal of clustering is to put data points into groups, and having a large number of groups may not be meaningful.

- This suggests a tradeoff between *k* and inertia.

The "elbow" method

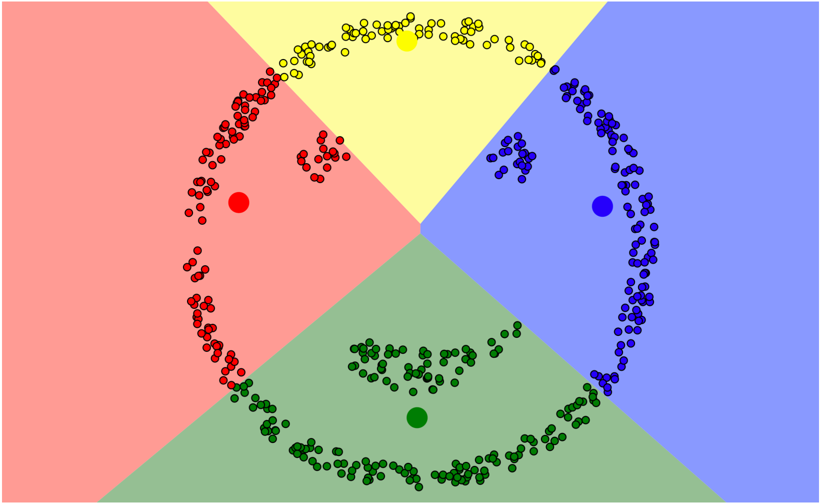
- Strategy: run k-Means Clustering for many choices of k (e.g. $k = 1, 2, 3, ..., 8$).
- Compute the value of inertia for each resulting set of centroids.
- Plot a graph of inertia vs k.
- Choose the value of k that appears at an "elbow".



See the notebook for a demo.

Low inertia isn't everything!

- Even if k-Means works as intended and finds the choice of centroids that minimize inertia, the resulting clustering may not look "right" to us humans.
  - Recall, inertia measures the total squared distance to centroids.
  - This metric doesn't always match our intuition.
- Let's look at some examples at `https://tinyurl.com/40akmeans`.
  - Go to "I'll Choose" and "Smiley Face". Good luck!



Other clustering techniques

- k-Means Clustering is just one way to cluster data.
- There are many others, each of which work differently and produce different kinds of results.
- Another common technique: **agglomerative clustering**.
  - High level: start out with each point being in its own cluster. Repeatedly combine clusters until only *k* are left.
- Check out this chart.

Summary

- k-Means Clustering attempts to minimize inertia.
    - We showed that it minimizes inertia at each step, but it's possible that it converges to a local minimum.
    - Different initial centroids can lead to different clusterings.
- To choose k, the number of clusters, we can use the elbow method.
- Next time: switching gears to probability and combinatorics.