Lecture 13 – Feature Engineering, Clustering

DSC 40A, Winter 2024

Announcements

- No homework due this week.
- No review session today (review session was on Monday Feb. 5)
  - But please come to OH and ask questions.

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 Course Website and 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 True/False or filling in a numerical answer.
- The exam covers Lecture 1 to Lecture 12 (HW1-3 + Linear Algebra and Multiple Linear Regression).

Midterm study strategy

- Look at annotated lecture notes.
- Review the written solutions to previous homeworks and groupworks.
- Identify which concepts are still uncertain. Re-watch podcasts, post on Campuswire, come to office hours, use resources on course website, watch Janine's lecture videos.
- Work through past exams on course website and the posted mock exam.
- Study in groups.
- Summarize key facts and formulas.

Some Tips About Midterm

- Understand the derivations we did in lecture.
  - There will be derivation problems in the midterm, but no long derivation.
  - Understand the derivation I did in lecture and some methods I used

$$\sum(x_i + y_i) = \sum x_i + \sum y_i$$

- Be able to perform simple algebra, calculus and linear algebra computation
  - Example: calculating matrix multiplication.
- Read each question carefully.
  - Example: using formal definition to prove convexity vs. using any method to prove convexity.
- Some problems are easier, some problems are harder.

Extra Credit Opportunity

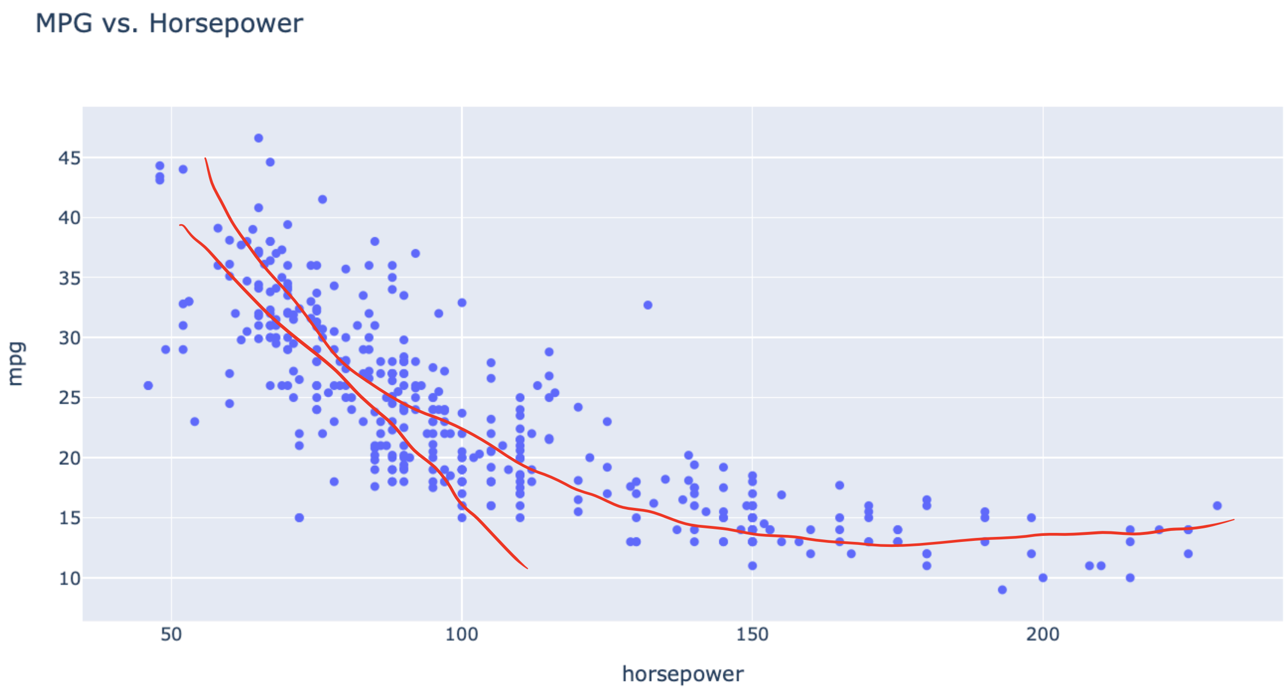
- The last problem on HW4 will be a class-wide competition on finding energies for High-Purity Germanium Detector waveforms
  - I'll explain what this is on next Monday's lecture, after the exam.
- Top predictions will get extra credit on Midterm 1.
- More detail next Monday

Agenda

- Feature engineering.
- Taxonomy of machine learning.
- Clustering.

Feature engineering

Last time: Cars



Question: Would a linear prediction rule work well on this dataset?

A quadratic prediction rule

- It looks like there's some sort of quadratic relationship between horsepower and MPG in the last scatter plot. We want to try and fit a prediction rule of the form

$$H(x) = w_0 + w_1 x + w_2 x^2$$

  - Note that while this is quadratic in horsepower, it is **linear in the parameters**!

- We can do that, by choosing our two "features" to be x_i and x_i^2, respectively.
  - In other words, $x_i^{(1)} = x_i$ and $x_i^{(2)} = x_i^2$.
  - More generally, we can create new features out of existing features.

A quadratic prediction rule

- Desired prediction rule: $H(x) = w_0 + w_1 x + w_2 x^2$.
- The resulting design matrix looks like this:

$$X = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \dots & & \\ 1 & x_n & x_n^2 \end{bmatrix}$$

- To find optimal parameter vector $\vec{w}^*$: solve the **normal equations**!

$$X^T X w^* = X^T y$$

More examples

- What if we want to use a prediction rule of the form $H(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3$?

$$\begin{bmatrix} 1 & x_i & x_i^2 & x_i^3 \\ 1 & x_i & x_i^2 & x_i^3 \\ & & \vdots & \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ w_3 \end{bmatrix}$$

- What if we want to use a prediction rule of the form $H(x) = w_1 \frac{1}{x^2} + w_2 \sin x + w_3 e^x$?

$$\begin{bmatrix} \frac{1}{x_i^2} & \sin x_i & e^{x_i} \\ & \vdots & \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix}$$

Feature engineering

- The process of creating new features out of existing information in our dataset is called **feature engineering**.
  - In this class, feature engineering will mostly be restricted to creating non-linear functions of existing features (as in the previous example).
  - In the future you'll learn how to do other things, like encode categorical information.

Non-linear functions of multiple features

- Recall our example from last lecture of predicting sales from square footage and number of competitors. What if we want a prediction rule of the form

$$
\begin{aligned}
H(\text{sqft}, \text{comp}) &= w_0 + w_1 \text{sqft} + w_2 \text{sqft}^2 \\
&\quad + w_3 \text{comp} + w_4 \text{sqft} \cdot \text{comp} \\
&= w_0 + w_1 s + w_2 s^2 + w_3 c + w_4 sc
\end{aligned}
$$

- Make design matrix:

$$
X = \begin{bmatrix} 1 & s_1 & s_1^2 & c_1 & s_1 c_1 \\ 1 & s_2 & s_2^2 & c_2 & s_2 c_2 \\ \dots & \dots & \dots & \dots & \\ 1 & s_n & s_n^2 & c_n & s_n c_n \end{bmatrix}
$$

Where s_i and c_i are square footage and number of competitors for store i, respectively.

Finding the optimal parameter vector, $\vec{w}^*$

- As long as the form of the prediction rule permits us to write $\vec{h} = X\vec{w}$ for some X and $\vec{w}$, the mean squared error is

$$R_{\text{sq}}(\vec{w}) = \frac{1}{n}\|\vec{y} - X\vec{w}\|^2$$

- Regardless of the values of X and $\vec{w}$,

$$\begin{aligned} \frac{dR_{\text{sq}}}{d\vec{w}} &= 0 \\ \implies -2X^T\vec{y} + 2X^TX\vec{w} &= 0 \\ \implies X^TX\vec{w}^* &= X^T\vec{y}. \end{aligned}$$

- The **normal equations** still hold true!

Linear in the parameters

- We can fit rules like:

$$w_0 + w_1 x + w_2 x^2 \qquad w_1 e^{-{x^{(1)}}^2} + w_2 \cos(x^{(2)} + \pi) + w_3 \frac{\log 2x^{(3)}}{x^{(2)}}$$

- This includes arbitrary polynomials.

- We can't fit rules like:

$$w_0 + e^{w_1 x} \qquad w_0 + \sin(w_1 x^{(1)} + w_2 x^{(2)})$$

- We can have any number of parameters, as long as our prediction rule is **linear in the parameters**, or linear when we think of it as a function of the parameters.

Determining function form

- How do we know what form our prediction rule should take?
- Sometimes, we know from *theory*, using knowledge about what the variables represent and how they should be related.

data-driven

- Other times, we make a guess based on the data.
- Generally, start with simpler functions first.
  - Remember, the goal is to find a prediction rule that will generalize well to unseen data.

Discussion Question

Suppose you collect data on the height, or position, of a freefalling object at various times t_i. Which form should your prediction rule take to best fit the data?

a) constant, $H(t) = w_0$

b) linear, $H(t) = w_0 + w_1 t$

c) quadratic, $H(t) = w_0 + w_1 t + w_2 t^2$

d) no way to know without plotting the data

$g = 9.8 m/s^2$

$v = -gt + V_0$ → Initial Velocity

$h = -\frac{1}{2} g t^2 + V_0 t + h_0 = W_2 t^2 + W_1 t + W_0$

→ initial position

Example: Amdahl’s Law

- Amdahl’s Law relates the runtime of a program on p processors to the time to do the sequential and nonsequential parts on one processor.

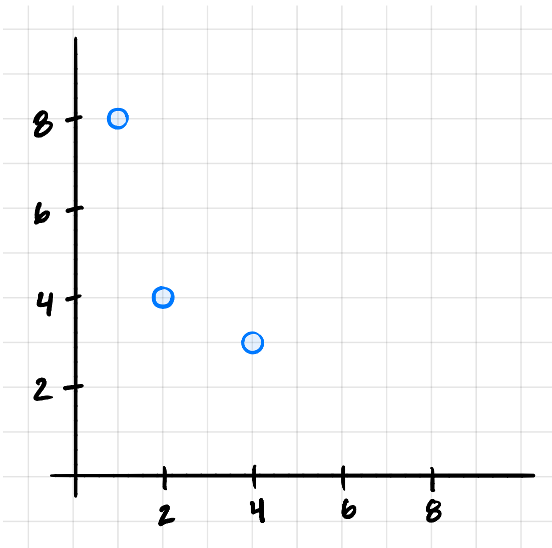
parallel

$$H(p) = t_S + \frac{t_{NS}}{p}$$

- Collect data by timing a program with varying numbers of processors:

Processors	Time (Hours)
1	8
2	4
4	3

Example: fitting $H(x) = w_0 + w_1 \cdot \frac{1}{x}$



x_i	y_i
1	8
2	4
4	3

$$X = \begin{bmatrix} 1 & \frac{1}{x_1} \\ 1 & \frac{1}{x_2} \\ 1 & \frac{1}{x_3} \end{bmatrix} \qquad \vec{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 1 \\ 1 & \frac{1}{2} \\ 1 & \frac{1}{4} \end{bmatrix} \qquad \vec{y} = \begin{bmatrix} 8 \\ 4 \\ 3 \end{bmatrix}$$

$$X^T X \vec{w} = X^T \vec{y}$$

Example: Amdahl's Law

- The solution is: $t_{\text{S}} = 1, \quad t_{\text{NS}} = \frac{48}{7} \approx 6.86$
- Therefore our prediction rule is:

$$H(p) = t_{\text{S}} + \frac{t_{\text{NS}}}{p}$$

$$= 1 + \frac{6.86}{p}$$

Transformations

How do we fit prediction rules that aren't linear in the parameters?

- Suppose we want to fit the prediction rule

$$H(x) = w_0 e^{w_1 x}$$

  This is **not** linear in terms of w_0 and w_1, so our results for linear regression don't apply.

- **Possible Solution:** Try to apply a **transformation**.

Transformations

- **Question:** Can we re-write $H(x) = w_0 e^{w_1 x}$ as a prediction rule that **is** linear in the parameters?

Key: take ln on both side

$$\ln H(x) = \ln w_0 e^{w_1 x}$$

$$= \ln(w_0) + \ln(e^{w_1 x})$$

$$= \ln(w_0) + w_1 x$$

$$T(x) = b_0 + b_1 x$$

$\ln a \cdot b = \ln a + \ln b$

$\ln e^{z} = z$

Transformations

- **Solution:** Create a new prediction rule, $T(x)$, with parameters b_0 and b_1, where $T(x) = b_0 + b_1 x$.
  - This prediction rule is related to $H(x)$ by the relationship $T(x) = \log H(x)$.
  - $\vec{b}$ is related to $\vec{w}$ by $b_0 = \log w_0$ and $b_1 = w_1$.
  - Our new observation vector, $\vec{z}$, is $\begin{bmatrix} \log y_1 \\ \log y_2 \\ \ldots \\ \log y_n \end{bmatrix}$.
- $T(x) = b_0 + b_1 x$ is linear in its parameters, b_0 and b_1.
- Use the solution to the normal equations to find $\vec{b}^*$, and the relationship between $\vec{b}$ and $\vec{w}$ to find $\vec{w}^*$.

Demo

Let's try this out in a Jupyter notebook. Follow along here.

Non-linear prediction rules in general

- Sometimes, it's just not possible to transform a prediction rule to be linear in terms of some parameters.

- In those cases, you'd have to resort to other methods of finding the optimal parameters.
  - For example, with $H(x) = w_0 e^{w_1 x}$, we could use gradient descent or a similar method to minimize mean squared error, $R(w_0, w_1) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - w_0 e^{w_1 x_i}\right)^2$, and find w_0^*, w_1^* that way.

- Prediction rules that are linear in the parameters are much easier to work with.

Taxonomy of machine learning

What is machine learning?

- **One definition:** Machine learning is about getting a computer to find patterns in data.
- Have we been doing machine learning in this class? **Yes.**
  - Given a dataset containing salaries, predict what my future salary is going to be.

    Empirical Risk Minimization
  - Given a dataset containing years of experience, GPAs, and salaries, predict what my future salary is going to be given my years of experience and GPA.

    regression

given the "answer" for training data

(GPA, Exp, ...)

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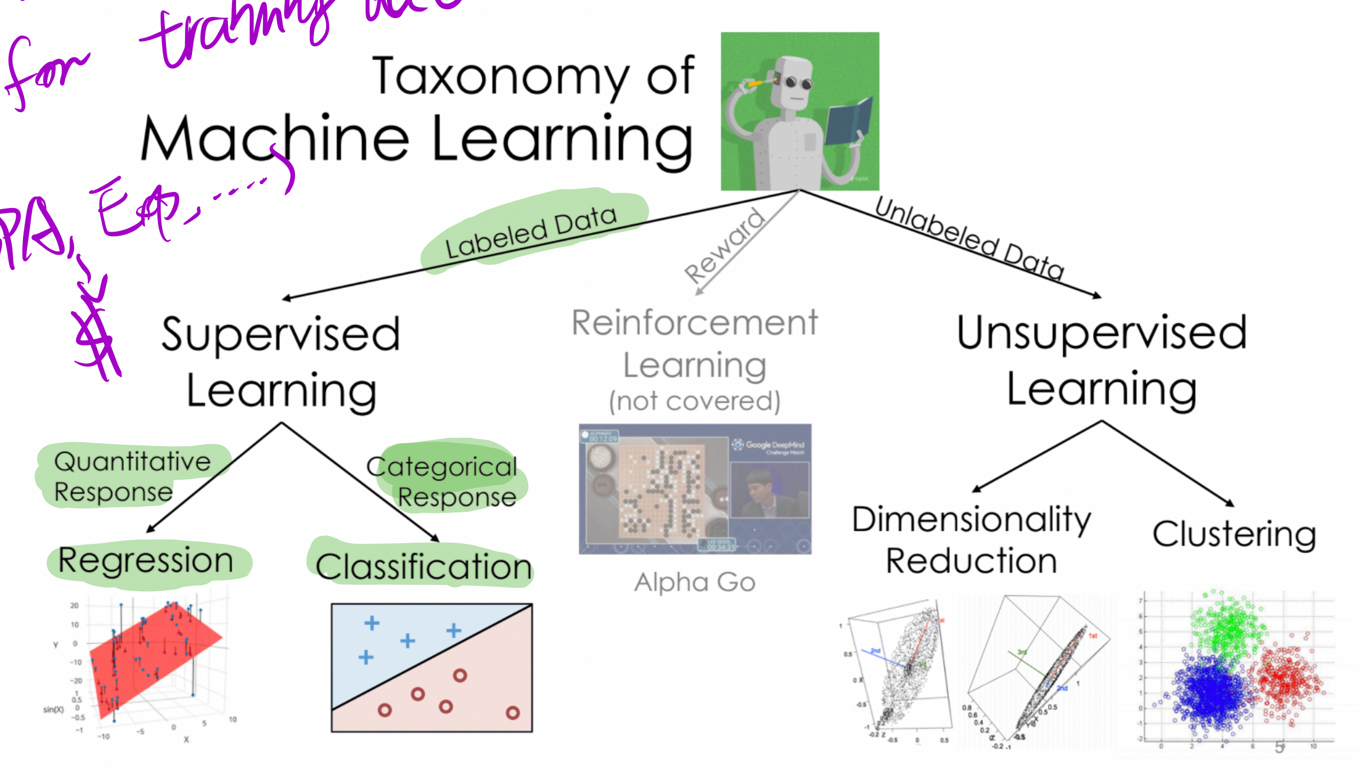

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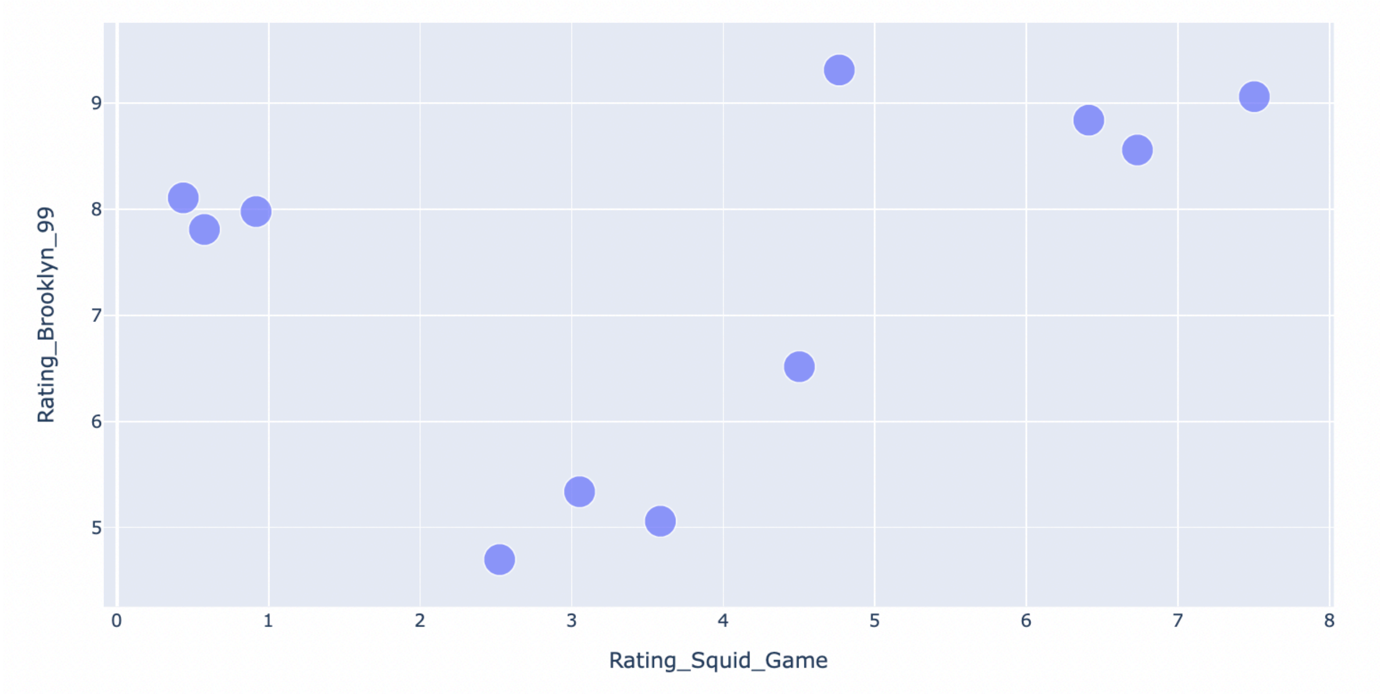
[1] taken from Joseph Gonzalez at UC Berkeley

Clustering

Question: how might we “cluster” these points into groups?



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**.

- 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?

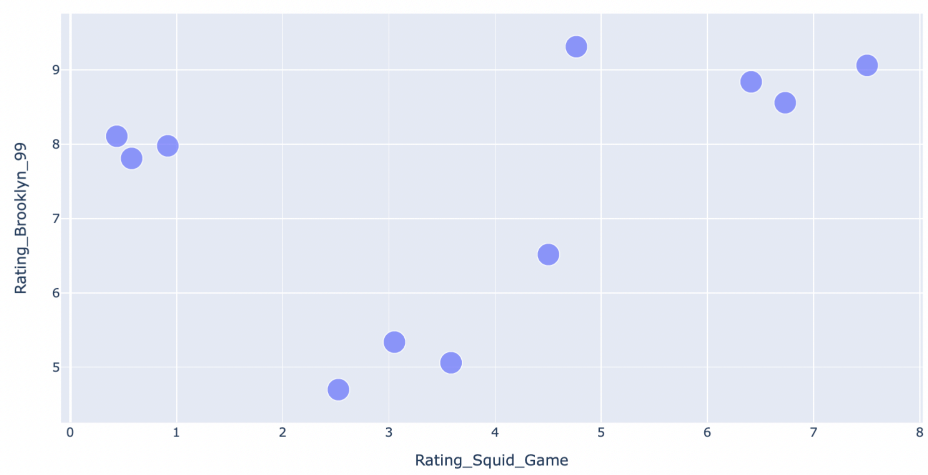
- One solution: pick k cluster centers, i.e. **centroids**:

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

- 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".



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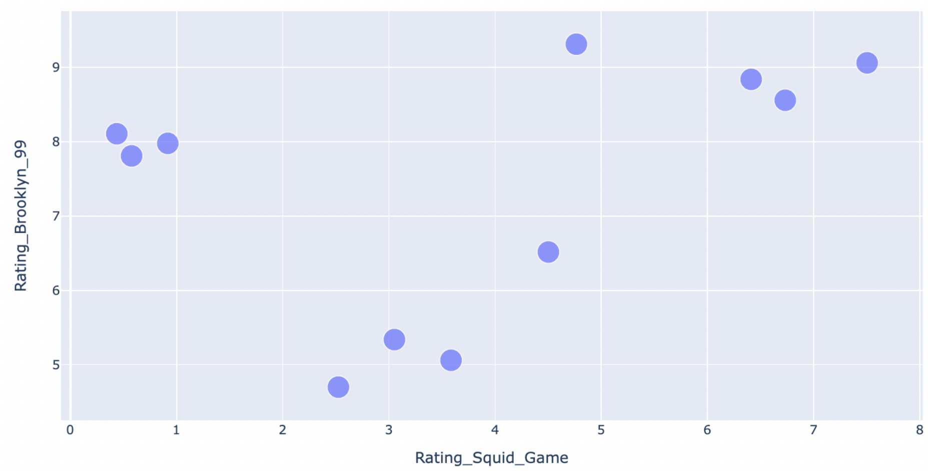

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How do we pick the centroids?

- 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:

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

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

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

Discussion Question

Suppose we have n data points, $\vec{x}_1, \vec{x}_2, ..., \vec{x}_n$, 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) $n \cdot k \cdot d$

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, 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.
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.
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`

Summary, next time

Summary

- The process of creating new features is called feature engineering.
- As long as our prediction rule is linear in terms of its parameters $w_0, w_1, \ldots, w_d$, we can use the solution to the normal equations to find $\vec{w}^*$.
  - Sometimes it's possible to transform a prediction rule into one that is linear in its parameters.
- Linear regression is a form of supervised machine learning, while clustering is a form of unsupervised learning.
- Clustering aims to place data points into "groups" of points that are close to one another. k-means clustering is one method for finding clusters.

Next time

- How does k-means clustering attempt to minimize inertia?
- How do we choose good initial centroids?
- How do we choose the value of k, the number of clusters?