# Lecture 10 – Feature Engineering, Clustering

**DSC 40A, Fall 2021 @ UC San Diego**

Suraj Rampure, with help from **many others**

# Announcements

- Groupwork 4 due **Thursday at 11:59pm**.
- Homework 4 due **Tuesday(!) at 11:59pm**.
  - Remember, everyone has 5 slip days.
- Survey 4 will come out this weekend, and is also due **Tuesday at 11:59pm**.
- The office hours schedule has changed! Look at the calendar.

# Agenda

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

# Feature engineering

# The general problem

- We have $n$ data points (or **training examples**): $(\vec{x}_1, y_1), \ldots, (\vec{x}_n, y_n)$ where each $\vec{x}_i$ is a feature vector of $d$ features:

$$\vec{x}_i = \begin{bmatrix} x_i^{(1)} \\ x_i^{(2)} \\ \ldots \\ x_i^{(d)} \end{bmatrix}$$

- We want to find a good linear prediction rule:

$$\begin{aligned} H(\vec{x}) &= w_0 + w_1 x^{(1)} + w_2 x^{(2)} + \ldots + w_d x^{(d)} \\ &= \vec{w} \cdot \text{Aug}(\vec{x}) \end{aligned}$$

# The general solution

- Use design matrix

$$X = \begin{bmatrix} 1 & x_1^{(1)} & x_1^{(2)} & \dots & x_1^{(d)} \\ 1 & x_2^{(1)} & x_2^{(2)} & \dots & x_2^{(d)} \\ \dots & \dots & \dots & & \dots \\ 1 & x_n^{(1)} & x_n^{(2)} & \dots & x_n^{(d)} \end{bmatrix} = \begin{bmatrix} \text{Aug}(\vec{x}_1)^T \\ \text{Aug}(\vec{x}_2)^T \\ \dots \\ \text{Aug}(\vec{x}_n)^T \end{bmatrix}$$

  and observation vector to solve the **normal equations**

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

  to find the optimal parameter vector $\vec{w}^*$.

- **Feature engineering**: creating new features out of existing features in order to better fit the data.

# Example

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

# 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**.

## 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.

- 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.

  - See Homework 4, Question 2D and 2E.

### 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

**To answer, go to `menti.com` and enter 2657 7681.**

# Example: Amdahl's Law

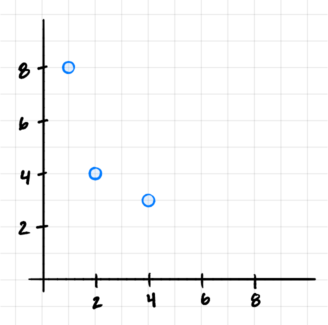
- Amdahl's Law relates the runtime of a program on $p$ processors to the time to do the sequential and nonsequential parts on one processor.

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

- 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 |

# Example: Amdahl's Law

- We found: $t_S = 1, \quad t_{NS} = \frac{48}{7} \approx 6.86$

- Therefore our prediction rule is:

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

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

# 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?

# 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 $\begin{bmatrix} \log y_1 \\ \log y_2 \\ \dots \\ \log y_n \end{bmatrix}$.

- $T(x) = b_0 + b_1 x$ 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 $\vec{w}^*$.

Follow along with the demo by clicking the **code** link on the course website next to Lecture 10.

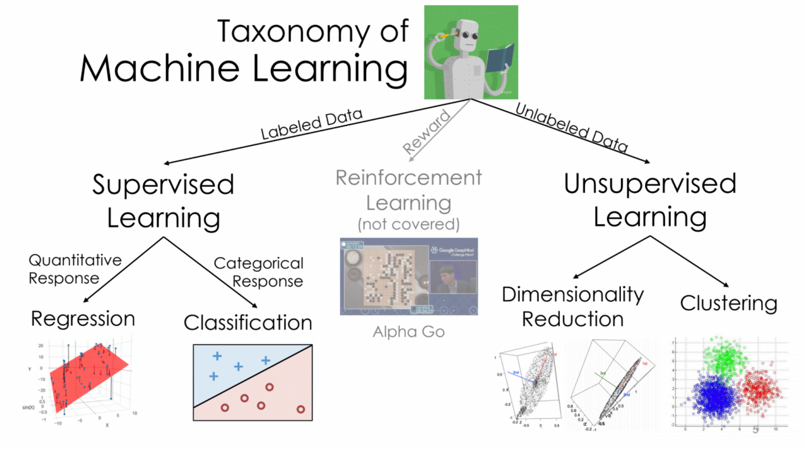
# Non-linear prediction rules in general

- 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.
  - 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.

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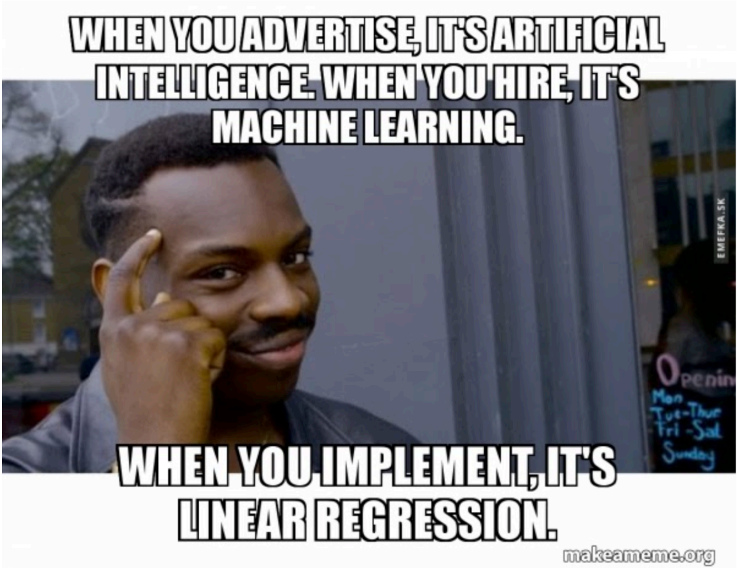
[1]taken from Joseph Gonzalez @ UC Berkeley


WHEN YOU ADVERTISE, IT'S ARTIFICIAL INTELLIGENCE. WHEN YOU HIRE, IT'S MACHINE LEARNING.
WHEN YOU IMPLEMENT, IT'S LINEAR REGRESSION.
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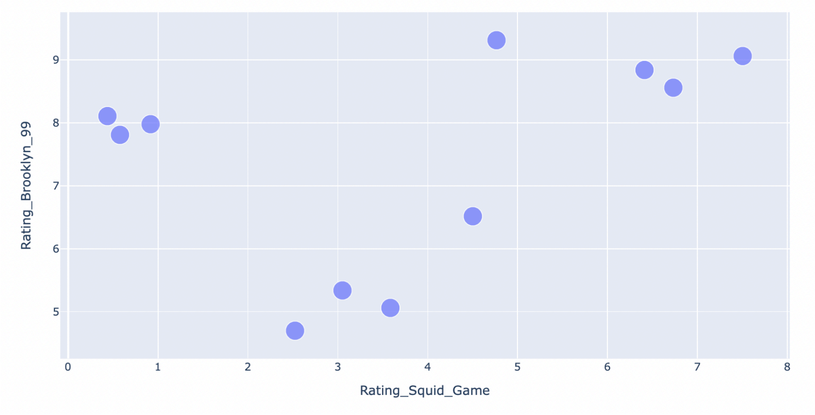
# Clustering

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



# Problem statement: clustering

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

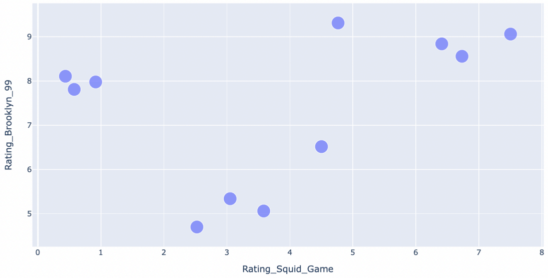
- These groups are called "clusters".
- Think about groups as **colors**.
  - i.e., the goal of clustering is to assign each point a color, such that points of the same color are close to one another.
- Note, unlike with regression, there is no "right answer" that we are trying to predict — there is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

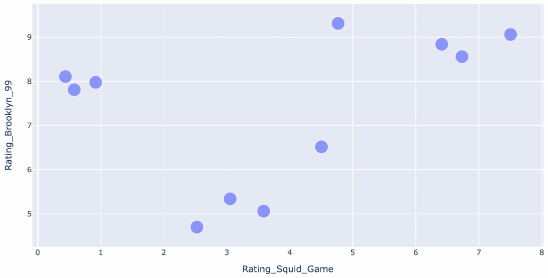
# How do we define a group?

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

$$\mu_1, \mu_2, \ldots, \mu_k$$

- 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”.


Rating_Brooklyn_99
Rating_Squid_Game
0 1 2 3 4 5 6 7 8
5 6 7 8 9


Rating_Brooklyn_99
Rating_Squid_Game
0 1 2 3 4 5 6 7 8
5 6 7 8 9

# 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 $\mu_j$

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

- Lower values of $C$ lead to "better" clusterings.
  - **Goal:** Find the centroids $\mu_1, \mu_2, ..., \mu_k$ 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 I assign points to clusters?

A) $d \cdot k$
B) $d^k$
C) $n^k$
D) $k^n$
E) $n \cdot k \cdot d$

**To answer, go to `menti.com` and enter 2657 7681.**

## 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 attemps 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 $w_0, w_1, ..., w_d$, 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?