Lecture 14 – Feature Engineering, Clustering

DSC 40A, Fall 2022 @ UC San Diego

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Announcements

- Midterm on Oct 28.
- **Groupwork 4 due Monday Oct. 31, at 11:59pm**.
- **Homework 4 due Friday Nov. 4 at 2:00pm**.
- Office hours: Wednesdays 5-6, SDSC, first floor room 152E.
  - Zoom link: `https://umich.zoom.us/j/93336146754`.
  - Password=123456.
  - Review secession: Monday (Discussion) and Wednesday (Lecture).

Agenda

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

Feature engineering

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.

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.

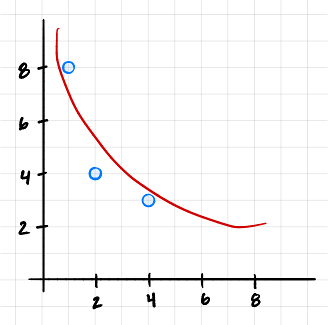
$$H(p) = t_S + \frac{t_{NS}}{p} \sim H(x) = W_0 + \frac{W_1}{x}$$

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

Processors	Time (Hours)
1	8
2	4
4	3

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

$$\vec{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}$$



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

new feature: $\frac{1}{x_i}$

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

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

Normal Eqs.

x_i	y_i
1	8
2	4
4	3

$$\vec{w}^* = (X^TX)^{-1}X^T\vec{y}$$

$$\cancel{(X^T)^{-1}}\,\cancel{X^T}X\vec{w}^* =$$

$$X^{-1}$$

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?

$H(x) = w_0 + w_1 x$ $\rightsquigarrow$ $H(x) = w_0 + \frac{w_1}{x}$

- 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

$\ln(\cdot) = \log_e(\cdot)$

$\ln(ab) = \ln(a) + \ln(b)$ *

$\log(a^b) = b\log(a)$

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

$$H(x) = w_0 e^{w_1 x} \xRightarrow{\ln(\,)} \ln(H(x)) = \underbrace{\ln(w_0) + \ln(e^{w_1 x})}_{*}$$

$$= \ln(w_0) + w_1 x \overbrace{\ln(e)}^{1} = \underbrace{\ln(w_0)}_{b_0} + \underbrace{w_1}_{b_1} x$$

$\ln(H(x))$

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

find b_0^*, b_1^*

transform back them to w_0^* w_1^*

not obs. vec. $\cancel{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}} \rightsquigarrow \begin{bmatrix} T(y_1) \\ \vdots \\ T(y_n) \end{bmatrix}$ new obs. vec.

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 $\vec{w}^*$.

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

Non-linear prediction rules in general

~~$\log(a+b) \neq \log a + \log b$~~

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

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

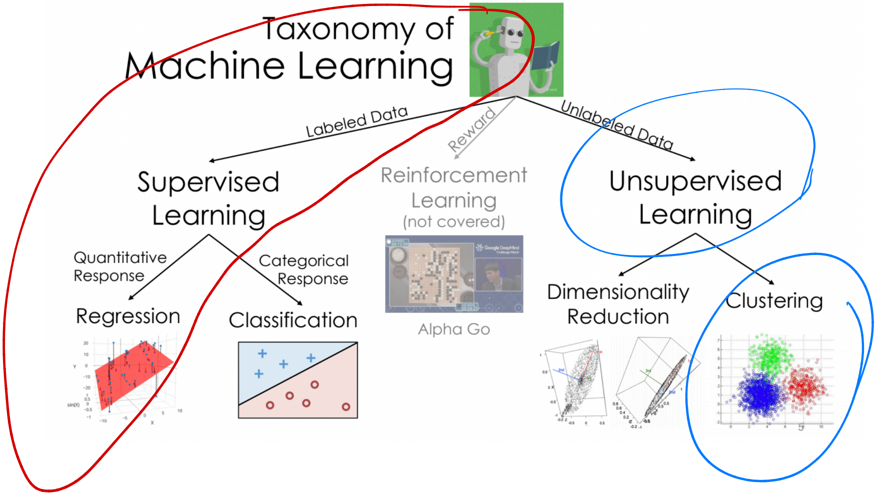
- In those cases, you'd have to resort to other methods of finding the optimal parameters.
  - For example, with $H(x) = w_0 e^{w_1 x}$, we could use gradient descent or a similar method to minimize mean squared error, $R(w_0, w_1) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - w_0 e^{w_1 x_i}\right)^2$, and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

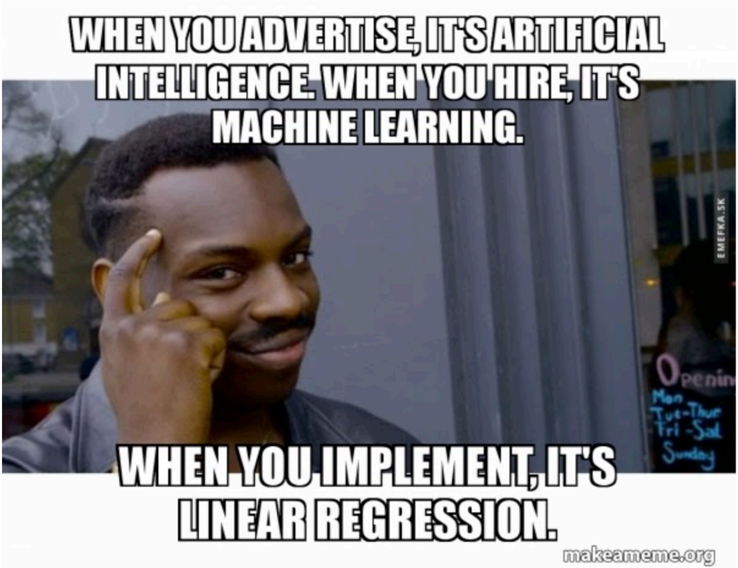
What is machine learning?

- **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.



[1]

[1]taken from Joseph Gonzalez @ UC Berkeley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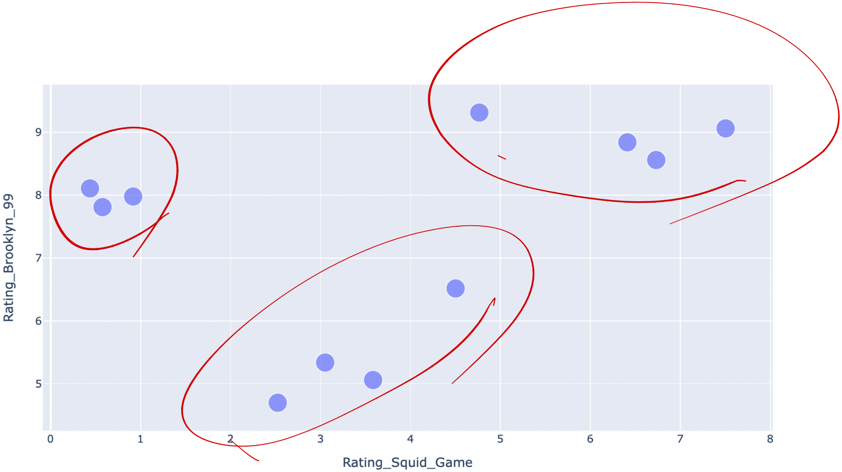
Clustering

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

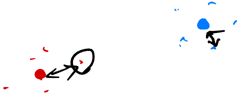


Problem statement: clustering

Goal: Given a list of n data points, stored as vectors in $\mathbb{R}^d$, $\vec{x}_1, \vec{x}_2, ..., \vec{x}_n$, 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.

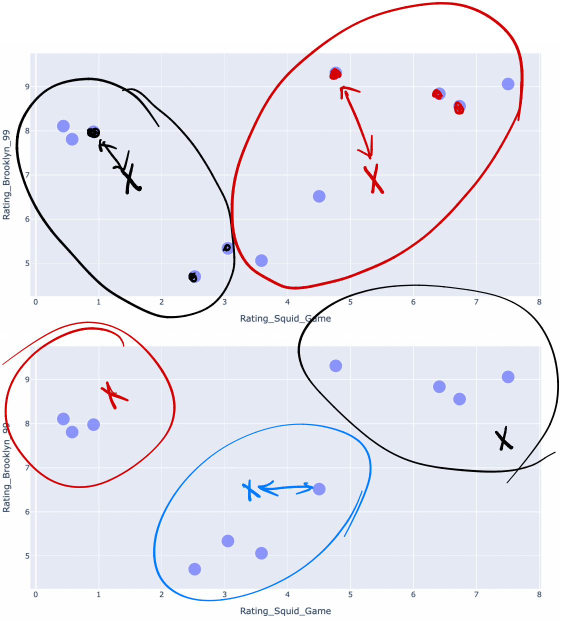
How do we define a group?



- 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

K=2

K=3

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:

absolute

$C(\mu_1, \mu_2, ..., \mu_k) =$ 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.

(empty cluster is valid) Cluster can have zero member!

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 8482 5148.

$$\underset{\vec{x}_1}{\underline{k}} \quad \underset{\vec{x}_2}{\underline{k}} \quad \cdots \quad \underset{\vec{x}_n}{\underline{k}} = k^n$$

3^{100} large

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.

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

- 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?