Module 13 – Feature Engineering, Clustering

DSC 40A, Summer 2023

Announcements

- Homework 2 is due tomorrow at 11:59pm.

- No groupwork this week during discussion. Instead, TAs will discuss extensions of linear regression to classification, classification loss metrics, and regularization.

Midterm ~~1~~ is Wednesday during lecture

- Open notes. No online calculators or generative models. No calculators with derivative capability.
- 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 everything up to the feature engineering content (but not clustering).

Midterm study strategy

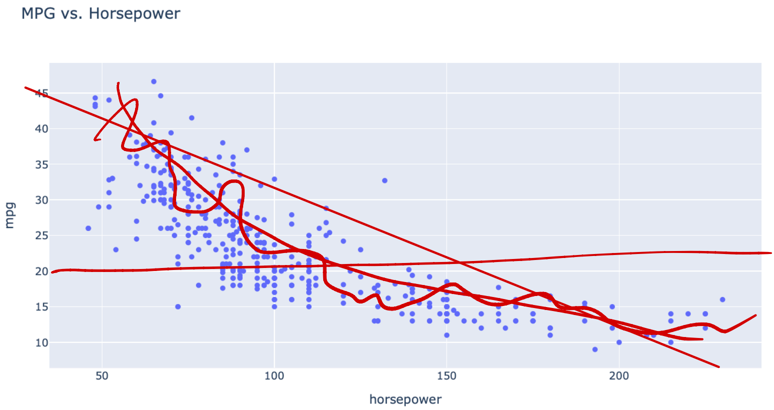
- Review the written solutions to previous homeworks and groupworks.
- Identify which concepts are still iffy. Re-watch podcasts, post on Campuswire, come to office hours, use resources on course website.
- Work through past exams on course website.
- Study in groups.
- Summarize key facts and formulas.

Agenda

- 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:

$$X = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \dots & & \\ 1 & x_n & x_n^2 \end{bmatrix} \quad \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix}$$

- 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 $H(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3$?

$$\begin{bmatrix} 1 & x & x^2 & x^3 \\ \downarrow & \downarrow & \downarrow & \downarrow \end{bmatrix} \begin{bmatrix} \\ \\ \end{bmatrix}$$

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

$$\begin{bmatrix} \frac{1}{x^2} & \sin(x) & e^x \\ \downarrow & \downarrow & \downarrow \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix}$$

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.

↳ aggregate time-series 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.
- Other times, we make a guess based on the data.

↳ or: bulk generation of features + algorithmic pruning

- 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.

non-sequential

expected runtime →

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

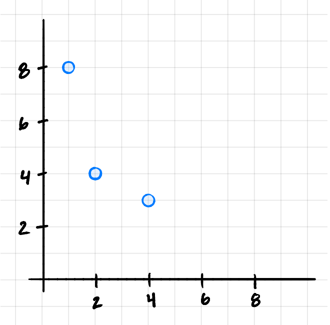
sequential

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

$H(p) = w_0 + w_1\left(\frac{1}{p}\right)$

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

$$X = \begin{bmatrix} 1 & 1/1 \\ 1 & 1/2 \\ 1 & 1/4 \end{bmatrix}$$

$$\vec{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix} \qquad \vec{y} = \begin{bmatrix} 8 \\ 4 \\ 3 \end{bmatrix}$$

$$\underbrace{\overset{2\times 3}{X^T} \overset{3\times 2}{X}}_{2\times 2} \underset{2\times 1}{\vec{w}} = \underbrace{X^T y}_{2\times 1}$$

Example: Amdahl's Law

- The solution is: $t_S = 1, \quad t_{NS} = \frac{48}{7} \approx 6.86$
- 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?

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

$$\ln(H(x)) = \underbrace{\ln(w_0)}_{\text{still not linear}} + w_1 x$$

$T(x)$

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 $T(x) = \log H(x)$.

    ln

  - $\vec{b}$ 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 $\vec{w}^*$.

Demo

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

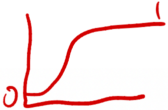
Non-linear prediction rules in general

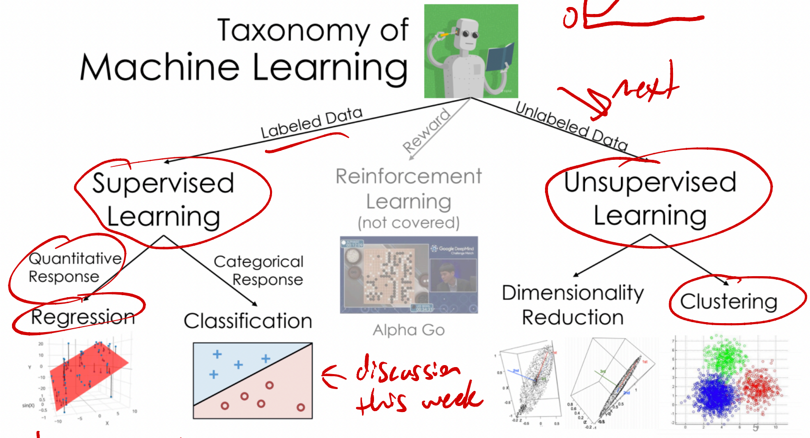
- Sometimes, it's just not possible to transform a prediction rule to be linear in terms of some parameters.
- In those cases, you'd have to resort to other methods of finding the optimal parameters.
  - For example, with $H(x) = w_0 e^{w_1 x}$, we could use gradient descent or a similar method to minimize 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.
  - 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.



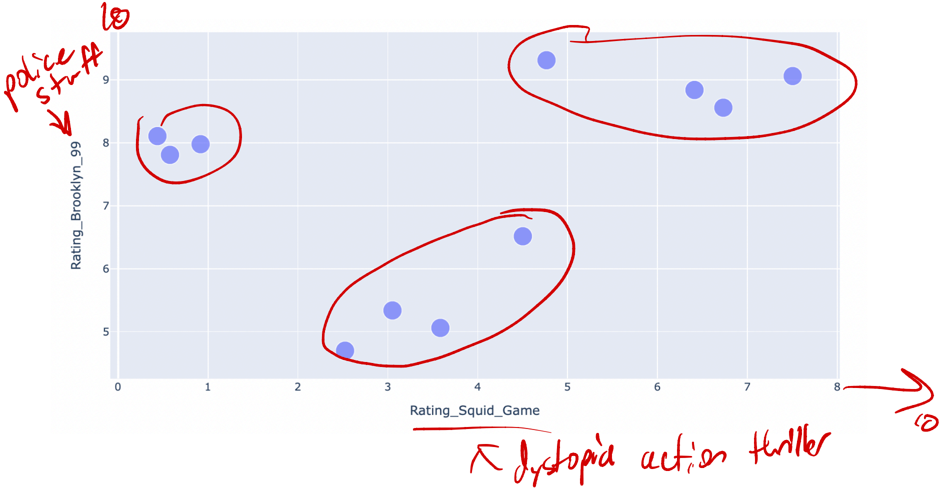


1 ↳ all concepts discussed generalize to classification

[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 $\mathbb{R}^d$,
samples
$\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_n$, and a positive integer k, **place the data points into k groups of nearby points**.

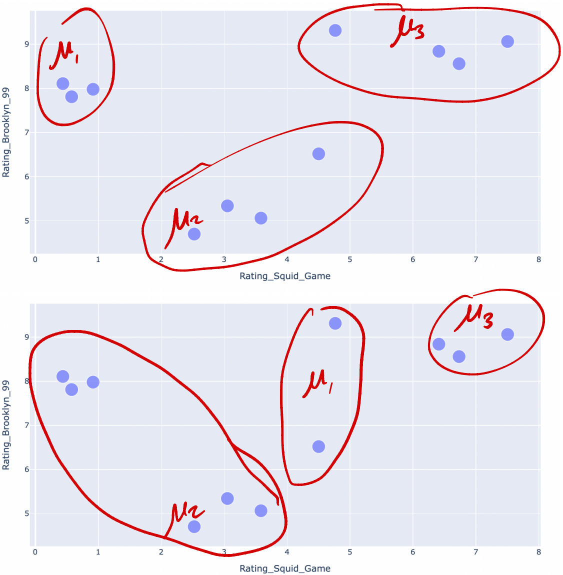
- These groups are called "clusters".
- Think about groups as **types**.
  - i.e., the goal of clustering is to assign each point a type, such that points of the same type are close to one another.
- Note, unlike with regression, there is no "right answer" that we are trying to predict — there is no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