Lecture 14 – Taxonomy of Machine Learning & Clustering

DSC 40A, Fall 2022 @ UC San Diego

Dr. Truong Son Hy, with help from **many others**

Announcements

- Midterm this Friday!

Agenda

- Review of feature transformation.
- Taxonomy of machine learning.
- Clustering.

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

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

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.

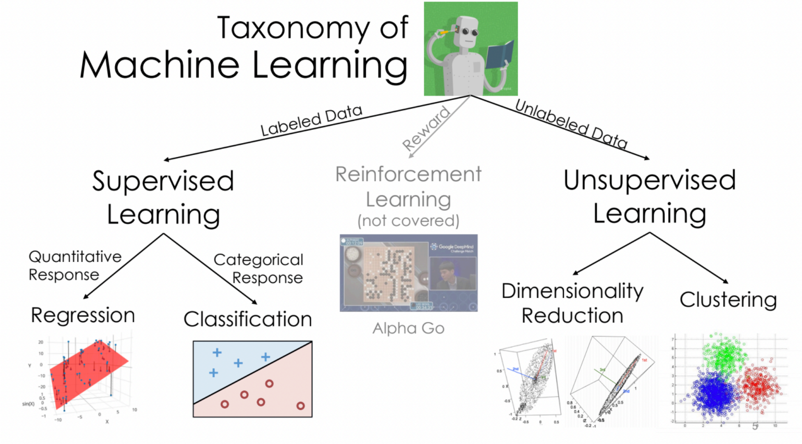
- In those cases, you'd have to resort to other methods of finding the optimal parameters.
  - For example, with $H(x) = w_0 e^{w_1 x}$, we could use gradient descent or a similar method to minimize mean squared error, $R(w_0, w_1) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - w_0 e^{w_1 x_i}\right)^2$, and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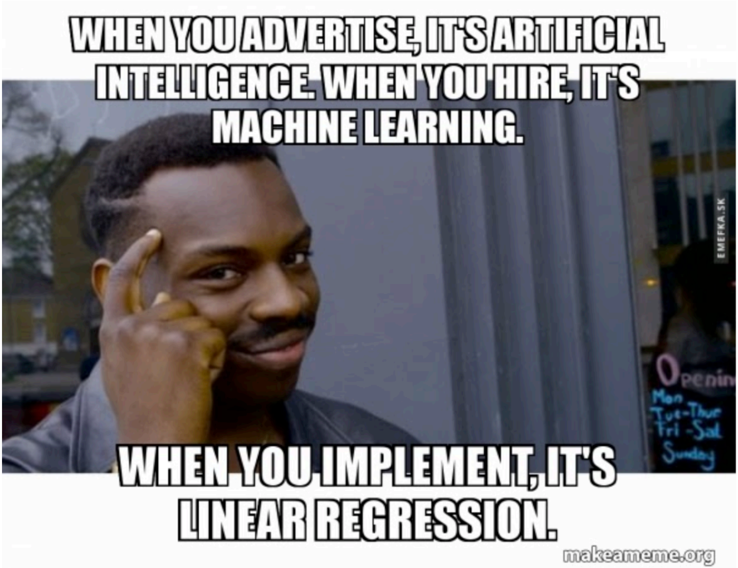
[1] taken from Joseph Gonzalez @ UC Berkeley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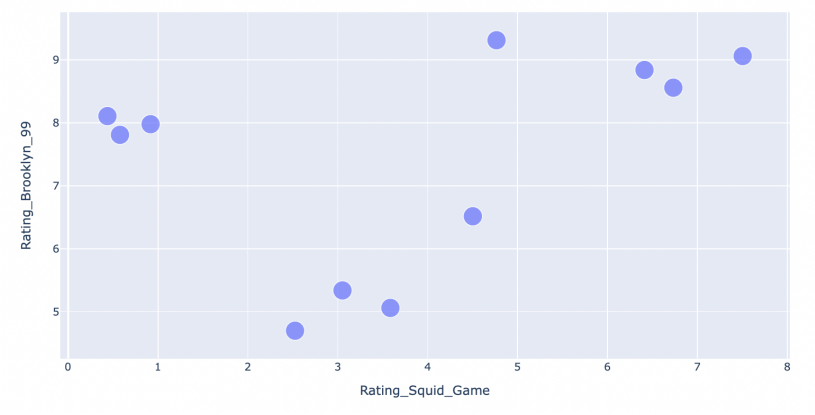
Clustering

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**:

$$\mu_1, \mu_2, ..., \mu_k$$

- 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".

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 I assign points to clusters?

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

Discussion Question

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D) k^n
E) $n \cdot k \cdot d$

Answer: 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 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://allisonhorst.com/k-means-clustering` (shared by Suraj)

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?