Lecture 13

Feature engineering and transformations

DSC 40A, Fall 2024

Announcements

- Homework 3 is due today.
- Homework 2 scores will be available on Gradescope this weekend.
- Midterm logistics will be announced on Monday.
    - Additional office hours next week for the midterm.
    - Prepare by practicing with old exam problems at practice.dsc40a.com.
    - Problems are sorted by topic!

Agenda

- Feature engineering and transformations.

Question 🤔

Answer at q.dsc40a.com

Remember, you can always ask questions at q.dsc40a.com!

If the direct link doesn't work, click the "🤔 Lecture Questions" link in the top right corner of dsc40a.com.

Recap: Multiple linear regression

The general problem

- We have n data points, $(\vec{x}_1, y_1), (\vec{x}_2, y_2), \ldots, (\vec{x}_n, y_n)$, where each $\vec{x}_i$ is a feature vector of d features:

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

- We want to find a good linear hypothesis function:

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

The general solution

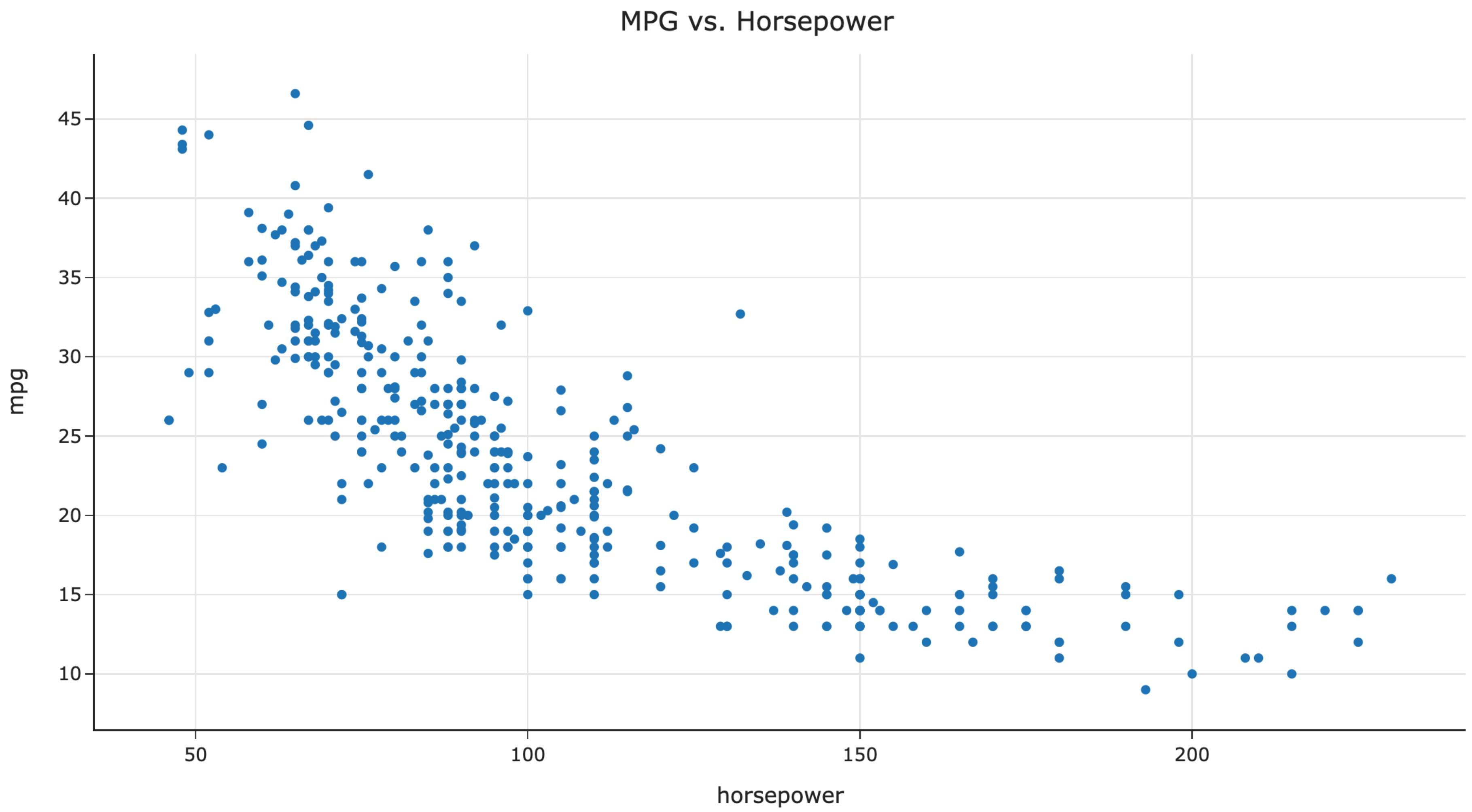
- Define the **design matrix** $X \in \mathbb{R}^{n\times(d+1)}$ and **observation vector** $\vec{y} \in \mathbb{R}^n$:

$$X = \begin{bmatrix} 1 & x_1^{(1)} & x_1^{(2)} & \dots & x_1^{(d)} \\ 1 & x_2^{(1)} & x_2^{(2)} & \dots & x_2^{(d)} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_n^{(1)} & x_n^{(2)} & \dots & x_n^{(d)} \end{bmatrix} = \begin{bmatrix} \text{Aug}(\vec{x}_1)^T \\ \text{Aug}(\vec{x}_2)^T \\ \vdots \\ \text{Aug}(\vec{x}_n)^T \end{bmatrix} \qquad \vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

- Then, solve the **normal equations** to find the optimal parameter vector, $\vec{w}^*$:

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

Feature engineering and transformations



Question: Would a linear hypothesis function work well on this dataset?

A quadratic hypothesis function

- 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 hypothesis function 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**!
  - That is, it is a **linear combination of features**.
- 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 hypothesis function

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

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

- To find the optimal parameter vector $\vec{w}^*$, we need to solve the **normal equations**!

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

More examples

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

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

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.
    - You'll be exposed to this in Homework 4, Problem 5!

Non-linear functions of multiple features

- Recall our earlier example of predicting sales from square footage and number of competitors. What if we want a hypothesis function of the form:

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

- The solution is to choose a design matrix accordingly:

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

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

- As long as the form of the hypothesis function 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 $\vec{y}$, the value of $\vec{w}^*$ that minimizes $R_{\text{sq}}(\vec{w})$ is the solution to the **normal equations**:

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

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.
  - These are all linear combinations of (just) features.

- We can't fit rules like:

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

  - These are **not** linear combinations of just features!

- We can have any number of parameters, as long as our hypothesis function 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 hypothesis function 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 hypothesis function 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.

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

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

Processors	Time (Hours)
1	8
2	4
4	3

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

Processors	Time (Hours)
1	8
2	4
4	3

How do we fit hypothesis functions that aren't linear in the parameters?

- Suppose we want to fit the hypothesis function:

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

- 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 hypothesis function that **is** linear in the parameters?

Transformations

- **Solution**: Create a new hypothesis function, $T(x)$, with parameters b_0 and b_1, where $T(x) = b_0 + b_1 x$.
- This hypothesis function 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 $\vec{w}^*$.

Once again, let's try it out! Follow along in this notebook.

Non-linear hypothesis functions in general

- Sometimes, it's just not possible to transform a hypothesis function 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, $H(x) = w_0 \sin(w_1 x)$ **can't** be transformed to be linear.
  - But, there are other methods of minimizing mean squared error:

$$R_{\text{sq}}(w_0, w_1) = \frac{1}{n} \sum_{i=1}^{n} (y_i - w_0 \sin(w_1 x))^2$$

  - One method: **gradient descent**, the topic of the next lecture!
- Hypothesis functions that are linear in the parameters are much easier to work with.

Question 🤔

Answer at q.dsc40a.com

Which hypothesis function is **not** linear in the parameters?

- A. $H(\vec{x}) = w_1(x^{(1)}x^{(2)}) + \frac{w_2}{x^{(1)}}\sin\left(x^{(2)}\right)$
- B. $H(\vec{x}) = 2^{w_1}x^{(1)}$
- C. $H(\vec{x}) = \vec{w} \cdot \text{Aug}(\vec{x})$
- D. $H(\vec{x}) = w_1\cos(x^{(1)}) + w_2 2^{x^{(2)}\log x^{(3)}}$
- E. More than one of the above.

Roadmap

- This is the end of the content that's in scope for the Midterm Exam.
- Now, we'll introduce **gradient descent**, a technique for minimizing functions that can't be minimized directly using calculus or linear algebra.
- After the Midterm Exam, we'll:
    - Switch gears to **probability**.