Module 12 – Multiple Linear Regression and Feature Engineering

DSC 40A, Summer 2023

Agenda

- Incorporating multiple features.
- Interpreting parameters.
- Feature engineering.

Incorporating multiple features

Last time

- We minimized the mean squared error for the prediction rule $H(x) = w_0 + w_1 x$, which was

$$R_{sq}(\vec{w}) = \frac{1}{n}||\vec{y} - X\vec{w}||^2$$

- We found that the minimizing $\vec{w}$ satisfies the **normal equations**, $X^T X\vec{w} = X^T\vec{y}$.
  - If $X^T X$ is invertible, the solution is:

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

- These same normal equations can be used to solve the **multiple linear regression** problem, where we use multiple features to predict an outcome. We simply need to adjust the design matrix X.

Multiple linear regression example

- We're want to fit a **linear** prediction rule with two features:

$$H(\text{experience}, \text{GPA}) = w_0 + w_1(\text{experience}) + w_2(\text{GPA})$$

- Collect data for each of n people:

Person #	Experience	GPA	Salary
1	3	3.7	85,000
2	6	3.3	95,000
3	10	3.1	105,000

- We represent each person with a **feature vector**:

$$\vec{x}_1 = \begin{bmatrix} 3 \\ 3.7 \end{bmatrix}, \qquad \vec{x}_2 = \begin{bmatrix} 6 \\ 3.3 \end{bmatrix}, \qquad \vec{x}_3 = \begin{bmatrix} 10 \\ 3.1 \end{bmatrix}$$

Prediction rule form determines design matrix

- When our prediction rule is

$$H(\text{experience}, \text{GPA}) = w_0 + w_1(\text{experience}) + w_2(\text{GPA}),$$

  the hypothesis vector $\vec{h} \in \mathbb{R}^n$ can be written

$$\vec{h} = \begin{bmatrix} H(\text{experience}_1, \text{GPA}_1) \\ H(\text{experience}_2, \text{GPA}_2) \\ \dots \\ H(\text{experience}_n, \text{GPA}_n) \end{bmatrix} = \begin{bmatrix} 1 & \text{experience}_1 & \text{GPA}_1 \\ 1 & \text{experience}_2 & \text{GPA}_2 \\ \dots & \dots & \dots \\ 1 & \text{experience}_n & \text{GPA}_n \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix}$$

- Notice that the rows of the design matrix are the (transposed) feature vectors, with an additional 1 in front.

Notation for multiple linear regression

- We will need to keep track of multiple[1] features for every individual in our data set.
- As before, subscripts distinguish between individuals in our data set. We have n individuals (or **training examples**).
- Superscripts distinguish between features.[2] We have d features.
  - experience = $x^{(1)}$
  - GPA = $x^{(2)}$

[1] In practice, we might use hundreds or even thousands of features.
[2] Think of them as new variable names, such as new letters.

Augmented feature vectors

- The **augmented feature vector** $\text{Aug}(\vec{x})$ is the vector obtained by adding a 1 to the front of feature vector $\vec{x}$:

$$\vec{x} = \begin{bmatrix} x^{(1)} \\ x^{(2)} \\ \vdots \\ x^{(d)} \end{bmatrix} \qquad \text{Aug}(\vec{x}) = \begin{bmatrix} 1 \\ x^{(1)} \\ x^{(2)} \\ \vdots \\ x^{(d)} \end{bmatrix} \qquad \vec{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_d \end{bmatrix}$$

- Then, our prediction rule is

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

The general problem

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

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

- We want to find a good linear prediction rule:

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

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.

Terminology for parameters

- With d features, $\vec{w}$ has $d + 1$ entries.
- w_0 is the **bias**, also known as the **intercept**.
- $w_1, \ldots, w_d$ each give the **weight**, i.e. **coefficient**, of a feature.

$$H(\vec{x}) = w_0 + w_1 x^{(1)} + \ldots + w_d x^{(d)}$$

Interpreting parameters

Example: predicting sales

- For each of 26 stores, we have:
  - net sales,
  - square feet,
  - inventory,
  - advertising expenditure,
  - district size, and
  - number of competing stores.

- Goal: predict net sales given these features

- To begin:

$$H(\text{square feet}, \text{competitors}) = w_0 + w_1(\text{square feet}) + w_2(\text{competitors})$$

Example: predicting sales

$$H(\text{square feet}, \text{competitors}) = w_0 + w_1(\text{square feet}) + w_2(\text{competitors})$$

Discussion Question

What will be the sign of w_1^* and w_2^*?

a) $w_1^* = +, \quad w_2^* = -$
b) $w_1^* = +, \quad w_2^* = +$
c) $w_1^* = -, \quad w_2^* = -$
d) $w_1^* = -, \quad w_2^* = +$

Example: predicting sales

$H(\text{square feet}, \text{competitors}) = w_0 + w_1(\text{square feet}) + w_2(\text{competitors})$

Discussion Question

What will be the sign of w_1^* and w_2^*?

a) $w_1^* = +$, $\quad w_2^* = -$
b) $w_1^* = +$, $\quad w_2^* = +$
c) $w_1^* = -$, $\quad w_2^* = -$
d) $w_1^* = -$, $\quad w_2^* = +$

Let's try it out ourselves. Follow along here.

Which features are most "important"?

Discussion Question

Which feature has the greatest effect on the outcome?

a) square feet: $w_1^* = 16.202$
b) competitors: $w_2^* = -5.311$
c) inventory: $w_2^* = 0.175$
d) advertising: $w_3^* = 11.526$
e) district size: $w_4^* = 13.580$

Which features are most "important"?

- The most important feature is **not necessarily** the feature with largest weight.

- Features are measured in different units, scales.
  - Suppose I fit one prediction rule, H_1, with sales in dollars, and another prediction rule, H_2, with sales in thousands of dollars.
  - Sales is just as important in both prediction rules.
  - But the weight of sales in H_1 will be 1000 times smaller than the weight of sales in H_2.
  - Intuitive explanation: $5 \times 45000 = (5 \times 1000) \times 45$.

- **Solution**: before doing regression, **standardize** each feature, i.e. convert each feature to standard units.

Standard units

- Recall: to convert a feature $x_1, x_2, ..., x_n$ to standard units, we use the formula

$$x_i \text{ in standard units} = \frac{x_i - \bar{x}}{\sigma_x}$$

- Example: 1, 7, 7, 9
  - Mean:
  - Standard deviation:
  - Standardized data:

Standard units for multiple linear regression

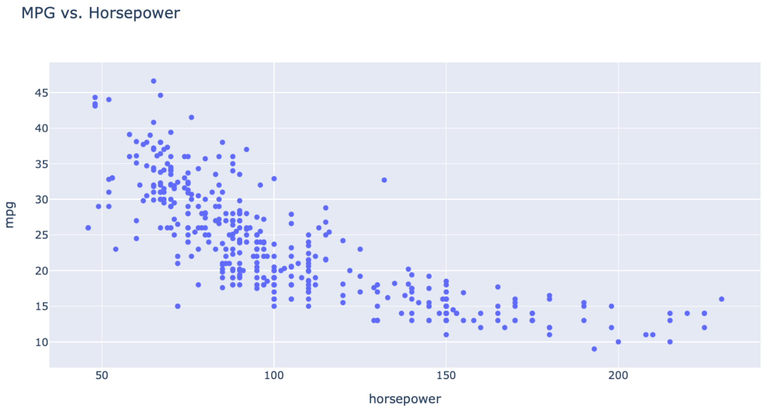
- The result of standardizing each feature (separately!) is that the units of each feature are on the same scale.
  - There's no need to standardize the outcome (net sales), since it's not being compared to anything.

- Then, solve the normal equations. The resulting $w_0^*, w_1^*, \ldots, w_d^*$ are called the **standardized regression coefficients**.

- Standardized regression coefficients can be directly compared to one another.

Let's try it out in our demo notebook.

Feature engineering



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:

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

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

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

Feature engineering

- More generally, we can create new features out of existing information in our dataset. This process 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.

Summary

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- The normal equations can be used to solve the **multiple linear regression** problem, where we use multiple features to predict an outcome.

- We can interpret the parameters as weights. The signs of weights give meaningful information, but we can only compare weights if our features are standardized.

- We can create non-linear features out of existing features. This process is called **feature engineering**.
  - A prediction rule only needs to be a **linear function of the parameters** for us to use linear regression. It does not need to be a linear function of the features.