Lecture 12 – Multiple Linear Regression and Feature Engineering

DSC 40A, Fall 2022 @ UC San Diego

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Agenda

Wed OH 5–6 PM
SDSC 2nd floor

- Recap of Lecture 11.
- Using multiple features.
- Practical demo.
- Interpreting weights.

Recap of Lecture 11

Regression and linear algebra

- Last time, we used linear algebra to fit a prediction rule of the form

$$H(x) = w_0 + w_1 x$$

- To do so, we first defined a **design matrix** X, **parameter vector** $\vec{w}$, and **observation vector** $\vec{y}$ as follows:

unseen data

$$\begin{bmatrix} 1 & x_1' \\ 1 & x_2' \\ \vdots & \end{bmatrix}$$

$$X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \dots & \dots \\ 1 & x_n \end{bmatrix}, \qquad \vec{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}, \qquad \vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ \dots \\ y_n \end{bmatrix}$$

- We also re-wrote our prediction rule as a matrix-vector multiplication, defining the **hypothesis vector** $\vec{h}$ as

$X = [1 \quad x]$

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

prediction on dataset

Minimizing mean squared error

- With our new linear algebra formulation of regression, our mean squared error now looks like:

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

- To find $\vec{w}^*$, the optimal parameter vector, we took the gradient of $R_{sq}(\vec{w})$ with respect to $\vec{w}$, set it equal to 0, and solved.
- The result is the **normal equations**:

$$A\vec{w} = \vec{b}$$

$$\underbrace{X^TX}_{A}\underbrace{\vec{w}^*}_{\vec{w}} = \underbrace{X^T\vec{y}}_{\vec{b}}$$

- When X^TX is invertible, an equivalent form is

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

  - This gives the same w_0^* and w_1^* as our formulas from Lecture 9.

Using multiple features

Using multiple features

- How do we predict salary given **multiple** features?
- We believe salary is a function of experience *and* GPA.
- In other words, we believe there is a function H so that:

$$\text{salary} \approx H(\text{years of experience}, \text{GPA})$$

- Recall: H is a **prediction rule**.
- **Our goal**: find a good prediction rule, H.

Example prediction rules

$$H_1(\text{experience}, \text{GPA}) = \$2,000 \times (\text{experience}) + \$40,000 \times \frac{\text{GPA}}{4.0}$$

$$H_2(\text{experience}, \text{GPA}) = \$60,000 \times 1.05^{(\text{experience}+\text{GPA})}$$

$$H_3(\text{experience}, \text{GPA}) = \cos(\text{experience}) + \sin(\text{GPA})$$

Linear prediction rules

$w_0 + w_1 x_1^{(1)} + w_2 x_2^{(2)} + \cdots$

- We'll restrict ourselves to **linear** prediction rules:

$w_0 + w_1 \square + w_2 \square \cdots$

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

$f(x) = x + 2$

$f(x_1) = y_1$

$f(x_2) = y_2$

- This is called **multiple linear regression.**

$x = 1 : 3$

$x = 2 : 4$

- Note that H is **linear in the parameters** w_0, w_1, w_2.
  - H is a linear combination of features (1, experience, GPA) with ws as the coefficients (w_0, w_1, and w_2).

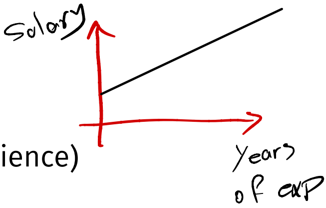
$f(1+2) = 3 + 2 = 5 \neq 7$

- As a result, we can solve the **normal equations** to find w_0^*, w_1^*, and w_2^*!

- Linear regression with multiple features is called **multiple linear regression**.

$\forall \alpha, \beta : f(\alpha x_1 + \beta x_2) = \alpha y_1 + \beta y_2$

Geometric interpretation



Question: The prediction rule

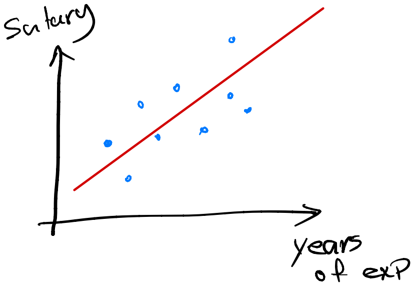
$$H(\text{experience}) = w_0 + w_1(\text{experience})$$

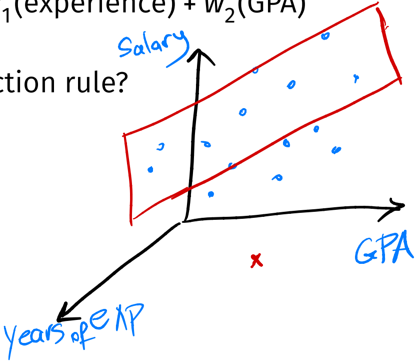
looks like a line in 2D.

1. How many dimensions do we need to graph

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

2. What is the shape of the prediction rule?





Example dataset

- For each of n people, collect each feature, plus salary:

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**:

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

The hypothesis vector

- 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

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

Design matrix

$$\begin{bmatrix} 1 & x_1 & G_1 \\ 1 & x_2 & G_2 \\ \vdots & \vdots & \vdots \\ 1 & & \end{bmatrix}$$

$$w_0 + w_1(\text{exp}_1) + w_2(\text{GPA}_1)$$

How do we find $\vec{w}^*$?

- To find the best parameter vector, $\vec{w}^*$, we can use the design matrix and observation vector

$\vec{x}_1^T$

$$X = \begin{bmatrix} 1 & \text{experience}_1 & \text{GPA}_1 \\ 1 & \text{experience}_2 & \text{GPA}_2 \\ \dots & \dots & \dots \\ 1 & \text{experience}_n & \text{GPA}_n \end{bmatrix}, \vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ \dots \\ y_n \end{bmatrix}$$

and solve the **normal equations**

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

- 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 = $x^{(2)}$

$x_1^{(1)}$ $\quad x_1^{(2)}$ $\quad x_1^2$

[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 $\vec{x}$:

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

$\to$ d-dim

$\to$ $d+1$-dim

$d+1$-dim

- Then, our prediction rule is

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

The general problem

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

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

- We want to find a good linear prediction rule:

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

The general solution

- Use design matrix

$\mathrm{Aug}(\vec{x}_1)^T$

$\vec{x} = \begin{bmatrix} \\ \\ \end{bmatrix}$

$$X = \begin{bmatrix} 1 & x_1^{(1)} & x_1^{(2)} & \dots & x_1^{(d)} \\ 1 & x_2^{(1)} & x_2^{(2)} & \dots & x_2^{(d)} \\ \dots & \dots & \dots & & \dots \\ 1 & x_n^{(1)} & x_n^{(2)} & \dots & x_n^{(d)} \end{bmatrix} = \begin{bmatrix} \mathrm{Aug}(\vec{x}_1)^T \\ \mathrm{Aug}(\vec{x}_2)^T \\ \dots \\ \mathrm{Aug}(\vec{x}_n)^T \end{bmatrix}$$

$\mathrm{Aug}(\vec{x}) = \begin{bmatrix} \vdots \end{bmatrix}$

Design

and observation vector to solve the **normal equations**

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

to find the optimal parameter vector.

Interpreting the 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.

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

- The sign of w_i tells us about the relationship between ith feature and the output of our prediction rule.

Practical demo

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 square footage, inventory, etc.

- 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) $w_1^* = -, \quad w_2^* = +$

To answer, go to `menti.com` **and enter 8482 5148.**

Follow along with the demo by clicking the **code** link on the course website next to Lecture 12.

Interpreting weights

Discussion Question

Which feature has the greatest effect on the outcome?

A) square feet: $w_1^* = 16.202$
B) competing stores: $w_2^* = -5.311$
C) inventory: $w_3^* = 0.175$
D) advertising: $w_4^* = 11.526$
E) district size: $w_5^* = 13.580$

To answer, go to `menti.com` and enter 8482 5148.

Which features are most "important"?

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

$ $H(x) = w_0 + w_1 x + w_2 z$

$\frac{\$}{ft^2}$ ft^2 $\frac{\$}{kg}$ kg

- 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: $5 \times 45000 = (5 \times 1000) \times 45.$ K\$

w_1

- **Solution**: we should **standardize** each feature, i.e. convert each feature to standard units.

Summary

Summary

- 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.