Lecture 6 – Simple Linear Regression

DSC 40A, Fall 2021 @ UC San Diego

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btw these large scary math symbols are just for-loops

Summation
(capital sigma)

$$\sum_{n=0}^{4} 3n$$

```
sum = 0;
for( n=0; n<=4; n++ )
   sum += 3*n;
```

Product
(capital pi)

$$\prod_{n=1}^{4} 2n$$

```
prod = 1;
for( n=1; n<=4; n++ )
   prod *= 2*n;
```

7:51 PM · 11 Sep 21 · Twitter Web App

Announcements

5 SLIP DAYS

- Homework 3 will be released after lecture, will be due on **Monday 10/18 at 11:59pm.** Will be shorter than usual.

  → NO SLIP DAYS!!!

- Groupwork 3 will be released after lecture, will be due on **Thursday 10/14 at 11:59pm**.

- **DISCUSSION SECTION ON WEDNESDAY WILL BE IN-PERSON!**
  - Wednesday, 6-6:50PM, Center Hall 113.

- Homework 1, Groupwork 1, and Groupwork 2 grades are released on Gradescope.

  SUBMIT SURVEY 2!

- Midterm is **Thursday, 10/21 during class time**.
  - **Review Session:** Tuesday 10/19, 5-8PM, PCYNH 109.
  - See `https://dsc40a.com/resources`.

Agenda

- Recap of gradient descent.
- Prediction rules.
- Minimizing mean squared error, again.

Recap: gradient descent

Gradient descent

- The goal of gradient descent is to minimize a function $R(h)$.

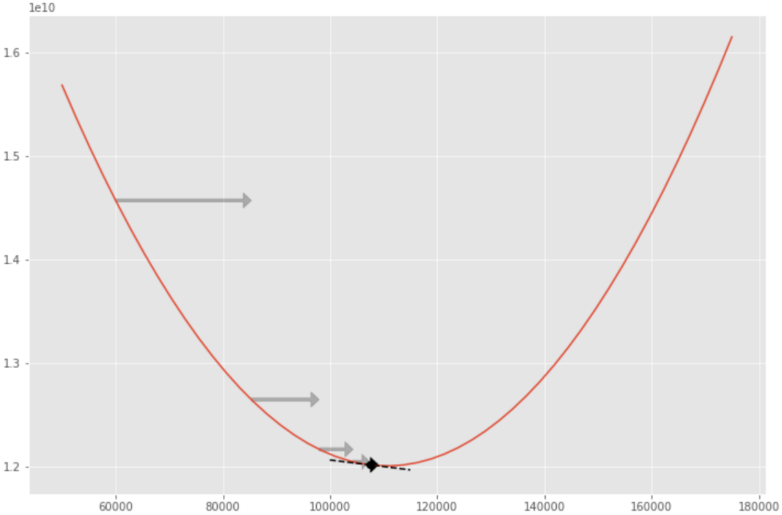
- Gradient descent starts off with an initial guess h_0 of where the minimizing input to $R(h)$ is, and on each step tries to get closer to the minimizing input h^* by moving opposite the direction of the slope:

$$\boxed{\alpha > 0} \qquad h_i = h_{i-1} - \alpha \cdot \frac{dR}{dh}(h_{i-1})$$

derivative at current guess

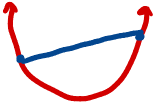
  - α is known as the learning rate, or step size. It controls how much we update our guesses by on each iteration.

- Gradient descent terminates once the guesses h_i and h_{i-1} stop changing much.

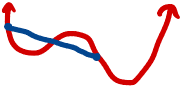


See Lecture 5’s supplemental notebook for animations.

When does gradient descent work?



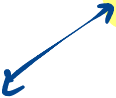
- A function f is convex if, for any two inputs a and b, the line segment connecting the two points $(a, f(a))$ and $(b, f(b))$ does not go below the function f.



  - $R_{abs}(h) = \frac{1}{n}\sum_{i=1}^{n} |y_i - h|$: convex.
  - $R_{sq}(h) = \frac{1}{n}\sum_{i=1}^{n} (y_i - h)^2$: convex.

  - $R_{ucsd}(h) = \frac{1}{n}\sum_{i=1}^{n} \left[1 - e^{-(y_i-h)^2/\sigma^2}\right]$: not convex.

- **Theorem:** If $R(h)$ is convex and differentiable then gradient descent converges to a **global minimum** of R given an appropriate step size.



Prediction rules

How do we predict someone's salary?

After collecting salary data, we...

1. Choose a loss function.

   average of loss function over my dataset!

2. Find the best prediction by minimizing empirical risk.

- So far, we've been predicting future salaries without using any information about the individual (e.g. GPA, years of experience, number of LinkedIn connections).

- **New focus:** How do we incorporate this information into our prediction-making process?

Features

A **feature** is an attribute – a piece of information.

- **Numerical**: age, height, years of experience
- **Categorical**: college, city, education level
- **Boolean**: knows Python?, had internship?

Think of features as columns in a DataFrame (i.e. table).

	YearsExperience	Age	FormalEducation	Salary
0	6.37	28.39	Master's degree (MA, MS, M.Eng., MBA, etc.)	120000.0
1	0.35	25.78	Some college/university study without earning ...	120000.0
2	4.05	31.04	Bachelor's degree (BA, BS, B.Eng., etc.)	70000.0
3	18.48	38.78	Bachelor's degree (BA, BS, B.Eng., etc.)	185000.0
4	4.95	33.45	Master's degree (MA, MS, M.Eng., MBA, etc.)	125000.0

Variables

inputs

- The features, x, that we base our predictions on are called **predictor variables**.

outputs

- The quantity, y, that we're trying to predict based on these features is called the **response variable**.

y is not a "feature"

- We'll start by predicting salary based on years of experience.

Prediction rules

- We believe that salary is a function of experience.
- In other words, we think that there is a function H such that:
$$\text{salary} \approx H(\text{years of experience})$$
- H is called a **hypothesis function** or **prediction rule**.
- **Our goal**: find a good prediction rule, H.

Possible prediction rules

$$H_1(\text{years of experience}) = \underline{\$50{,}000} + \underline{\$2{,}000} \times \underline{(\text{years of experience})}$$

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

$$H_3(\text{years of experience}) = \$100{,}000 - \$5{,}000 \times (\text{years of experience})$$

probably bad

- These are all valid prediction rules.
- Some are better than others.

Comparing predictions

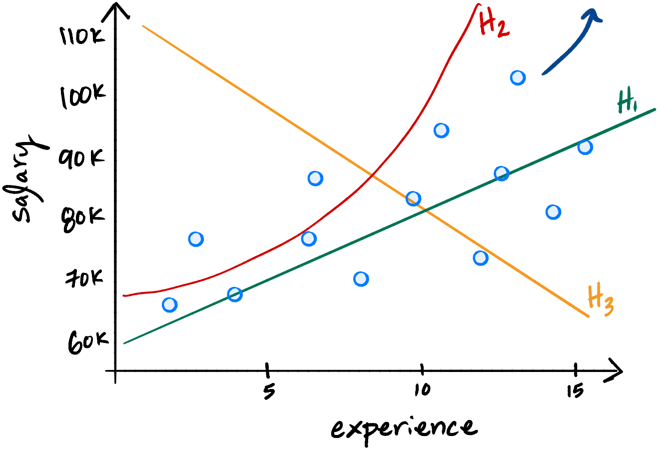
- How do we know which prediction rule is best: H_1, H_2, H_3?
- We gather data from n people. Let x_i be experience, y_i be salary:

$$\begin{matrix} (\text{Experience}_1, \text{Salary}_1) \\ (\text{Experience}_2, \text{Salary}_2) \\ \dots \\ (\text{Experience}_n, \text{Salary}_n) \end{matrix} \quad \rightarrow \quad \begin{matrix} (x_1, y_1) \\ (x_2, y_2) \\ \dots \\ (x_n, y_n) \end{matrix}$$

- See which rule works better on data.

Example

blue: data points



Quantifying the quality of a prediction rule H

- Our prediction for person i's salary is $H(x_i)$.
- As before, we'll use a **loss function** to quantify the quality of our predictions.
  - Absolute loss: $|y_i - H(x_i)|$. → |actual − predicted|
  - Squared loss: $(y_i - H(x_i))^2$. → (actual − predicted)^2

very similar to before!

- We'll use squared loss, since it's differentiable.
- Using squared loss, the **empirical risk** (mean squared error) of the prediction rule H is:

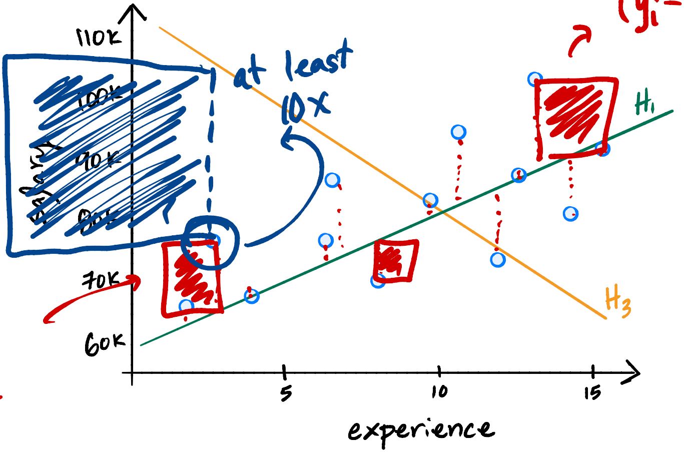
$$\boxed{R_{sq}(H) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - H(x_i)\right)^2}$$

h

Mean squared error

good prediction rule
= low MSE $(R_{sq}(H))$

$(y_i - H(x_i))^2$



squared error

Finding the best prediction rule

- **Goal:** out of all functions $\mathbb{R} \to \mathbb{R}$, find the function H^* with the smallest mean squared error.
- That is, H^* should be the function that minimizes

$$R_{sq}(H) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - H(x_i)\right)^2$$

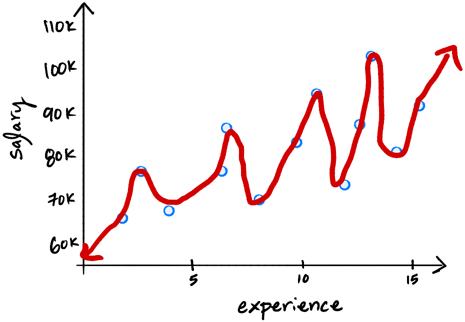
- There's a problem.

Discussion Question

Given the data below, is there a prediction rule H which has **zero** mean squared error?

a) Yes b) No

To answer, go to `menti.com` **and enter the code 8851 5429.**



Problem

- We can make mean squared error very small, even zero!
- But the function will be weird.
- This is called **overfitting**.
- Remember our real goal: make good predictions on data **we haven't seen**.

Solution

- Don't allow H to be just any function.
- Require that it has a certain form.
- Examples:
  - Linear: $H(x) = w_0 + w_1 x$. $y = mx + b$
  - Quadratic: $H(x) = w_0 + w_1 x_1 + w_2 x^2$.
  - Exponential: $H(x) = w_0 e^{w_1 x}$.
  - Constant: $H(x) = w_0$.

Finding the best linear prediction rule

- **Goal:** out of all $\boxed{\text{linear}}$ functions $\mathbb{R} \to \mathbb{R}$, find the function H^* with the smallest mean squared error.
  - Linear functions are of the form $\underbrace{H(x) = w_0 + w_1 x}_{y=mx+b}$.
  - They are defined by a slope (w_1) and intercept (w_0).
- That is, H^* should be the linear function that minimizes

$$R_{sq}(H) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - H(x_i)\right)^2$$

- This problem is called **least squares regression**.
  - "Simple linear regression" refers to linear regression with a single predictor variable.

Minimizing mean squared error for the linear prediction rule

Minimizing the mean squared error

- The MSE is a function R_{sq} of a function H.

$R_{sq}(h)$

$$\boxed{R_{\text{sq}}(H) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - H(x_i)\right)^2}$$

- But since H is linear, we know $H(x_i) = w_0 + w_1 x_i$.

$$R_{\text{sq}}(w_0, w_1) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - (w_0 + w_1 x_i)\right)^2$$

used to be just h!

different slope/intercept ⇒ different MSE

- Now R_{sq} is a function of w_0 and w_1.
- We call w_0 and w_1 **parameters**.
  - Parameters define our prediction rule.

Updated goal

- Find the slope w_1^* and intercept w_0^* that minimize the MSE, $R_{\text{sq}}(w_0, w_1)$:

$$R_{\text{sq}}(w_0, w_1) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - (w_0 + w_1 x_i)\right)^2$$

- Strategy: multivariable calculus.

Recall: the gradient

- If $f(x, y)$ is a function of two variables, the **gradient** of f at the point (x_0, y_0) is a **vector** of **partial derivatives**:

$f(x,y) = x^2 - 2xy + y^4$

$\frac{\partial f}{\partial x} = 2x - 2y$

$\frac{\partial f}{\partial y} = -2x + 4y^3$

$$\nabla f(x_0, y_0) = \begin{pmatrix} \frac{\partial f}{\partial x}(x_0, y_0) \\ \frac{\partial f}{\partial y}(x_0, y_0) \end{pmatrix}$$

- **Key Fact #1**: The derivative is to the tangent line as the gradient is to the tangent plane.

- **Key Fact #2**: The gradient points in the direction of the biggest increase.

- **Key Fact #3**: The gradient is zero at critical points.

Strategy

To minimize $R(w_0, w_1)$: compute the gradient, set it equal to zero, and solve.

$$R_{sq}(w_0, w_1) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - (w_0 + w_1 x_i)\right)^2$$

inputs are w_0, w_1

$$\frac{\partial R}{\partial w_0} = 0 \qquad \frac{\partial R}{\partial w_1} = 0$$

$$R_{\text{sq}}(w_0, w_1) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - (w_0 + w_1 x_i)\right)^2$$

Discussion Question

Choose the expression that equals $\frac{\partial R_{\text{sq}}}{\partial w_0}$.

a) $\frac{1}{n} \sum_{i=1}^{n} \left(y_i - (w_0 + w_1 x_i)\right)$

b) $-\frac{1}{n} \sum_{i=1}^{n} \left(y_i - (w_0 + w_1 x_i)\right)$

c) $-\frac{2}{n} \sum_{i=1}^{n} \left(y_i - (w_0 + w_1 x_i)\right) x_i$

d) $-\frac{2}{n} \sum_{i=1}^{n} \left(y_i - (w_0 + w_1 x_i)\right)$

Go to `menti.com` and enter the code 8851 5429.

$$R_{sq}(w_0, w_1) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - (w_0 + w_1 x_i)\right)^2$$

$$\frac{\partial R_{sq}}{\partial w_0} = \frac{1}{n} \sum_{i=1}^{n} \frac{\partial}{\partial w_0} \left(y_i - (w_0 + w_1 x_i)\right)^2$$

$$= \frac{1}{n} \sum_{i=1}^{n} 2\left(y_i - (w_0 + w_1 x_i)\right)(-1)$$

$$= \boxed{-\frac{2}{n} \sum_{i=1}^{n} \left(y_i - (w_0 + w_1 x_i)\right)}$$

$$R_{sq}(w_0, w_1) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - (w_0 + w_1 x_i)\right)^2$$

$$\frac{\partial R_{sq}}{\partial w_1} = \frac{1}{n} \sum_{i=1}^{n} 2\left(y_i - (w_0 + w_1 x_i)\right)(-x_i)$$

$$= -\frac{2}{n} \sum_{i=1}^{n} \left(y_i - (w_0 + w_1 x_i)\right) x_i$$

Strategy

$\frac{\partial R}{\partial w_0} = 0$ ✓

$$-\frac{2}{n}\sum_{i=1}^{n}\left(y_i - (w_0 + w_1 x_i)\right) = 0 \qquad -\frac{2}{n}\sum_{i=1}^{n}\left(y_i - (w_0 + w_1 x_i)\right) x_i = 0$$

1. Solve for w_0 in first equation.
   - The result becomes w_0^*, since it is the "best intercept".

2. Plug w_0^* into second equation, solve for w_1.
   - The result becomes w_1^*, since it is the "best slope".

Solve for w_0^*

$$\left(-\frac{n}{2}\right) -\frac{2}{n}\sum_{i=1}^{n}\left(y_i - (w_0 + w_1 x_i)\right) = 0 \left(-\frac{n}{2}\right)$$

$$\sum_{i=1}^{n}\left(y_i - (w_0 + w_1 x_i)\right) = 0$$

$$w_0 + w_0 + \dots + w_0$$

$$\sum_{i=1}^{n} y_i - \sum_{i=1}^{n} w_0 - \sum_{i=1}^{n} w_1 x_i = 0$$

$$\sum_{i=1}^{n} y_i - n w_0 - w_1 \sum_{i=1}^{n} x_i = 0$$

$$\sum_{i=1}^{n} y_i - w_1 \sum_{i=1}^{n} x_i = n w_0$$

$$w_0 = \frac{1}{n}\sum_{i=1}^{n} y_i - w_1 \frac{1}{n}\sum_{i=1}^{n} x_i$$

$$\boxed{w_0^* = \bar{y} - w_1 \bar{x}}$$

Solve for w_1^*

$$\bar{y} - w_1 \bar{x}$$

$$\left(-\frac{n}{2}\right) -\frac{2}{n}\sum_{i=1}^{n}\left(y_i - (w_0 + w_1 x_i)\right)x_i = 0 \left(-\frac{n}{2}\right)$$

only 1 unknown!

$$\sum_{i=1}^{n}\left(y_i - (\bar{y} - w_1\bar{x} + w_1 x_i)\right)x_i = 0$$

$$\sum_{i=1}^{n}\left[(y_i - \bar{y}) - w_1(x_i - \bar{x})\right]x_i = 0$$

$$\sum_{i=1}^{n}\left[(y_i - \bar{y})x_i - w_1(x_i - \bar{x})x_i\right] = 0$$

$$\sum_{i=1}^{n}(y_i - \bar{y})x_i = w_1 \sum_{i=1}^{n}(x_i - \bar{x})x_i$$

$$w_1^* = \frac{\sum_{i=1}^{n}(y_i - \bar{y})x_i}{\sum_{i=1}^{n}(x_i - \bar{x})x_i}$$

Least squares solutions

- We've found that the values w_0^* and w_1^* that minimize the function $R_{sq}(w_0, w_1) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - (w_0 + w_1 x_i)\right)^2$ are

best slope

best intercept

$$w_1^* = \frac{\displaystyle\sum_{i=1}^{n}(y_i - \bar{y})x_i}{\displaystyle\sum_{i=1}^{n}(x_i - \bar{x})x_i} \qquad\qquad w_0^* = \bar{y} - w_1^*\bar{x}$$

where

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n}x_i \qquad\qquad \bar{y} = \frac{1}{n}\sum_{i=1}^{n}y_i$$

- Let's re-write the slope w_1^* to be a bit more symmetric.

Key fact

[3, 5, 7]

mean : 5

$(3-5)+(5-5)+(7-5)$

The **sum of deviations from the mean** for any dataset is 0.

deviation

$$\sum_{i=1}^{n}(x_i - \bar{x}) = 0 \qquad \sum_{i=1}^{n}(y_i - \bar{y}) = 0$$

Proof:

$$\sum_{i=1}^{n}(x_i - \bar{x}) = \sum_{i=1}^{n} x_i - \sum_{i=1}^{n} \bar{x}$$

$$= \sum_{i=1}^{n} x_i - n\bar{x}$$

$$= n \cdot \frac{1}{n}\sum_{i=1}^{n} x_i - n\bar{x}$$

$$= n\bar{x} - n\bar{x} = \boxed{0}$$

Equivalent formula for w_1^*

Claim

$$w_1^* = \frac{\sum_{i=1}^{n}(y_i - \bar{y})x_i}{\sum_{i=1}^{n}(x_i - \bar{x})x_i} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

Proof:

$$\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y}) = \sum_{i=1}^{n}\Big[(y_i - \bar{y})x_i - (y_i - \bar{y})\underset{\text{constant}}{\bar{x}}\Big]$$

$$= \sum_{i=1}^{n}(y_i - \bar{y})x_i - \bar{x}\underbrace{\sum_{i=1}^{n}(y_i - \bar{y})}_{0}$$

$$= \sum_{i=1}^{n}(y_i - \bar{y})x_i \quad \checkmark$$

I proved that the numerators are the same.

Proof for denominators is very similar.

Least squares solutions

- The **least squares solutions** for the slope w_1^* and intercept w_0^* are:

$$\boxed{w_1^* = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \qquad w_0^* = \bar{y} - w_1^*\bar{x}}$$

  - We also say that w_0^* and w_1^* are **optimal parameters**.

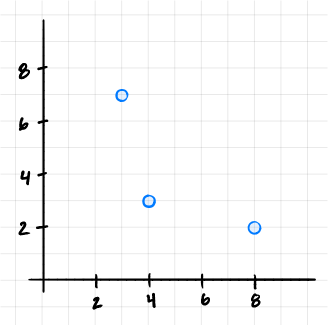
"best" bc they minimize MSE

- To make predictions about the future, we use the prediction rule

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

Example

⇒ Will repeat Thursday.



$$\bar{x} = \frac{3+4+8}{3} = 5$$

$$\bar{y} = \frac{7+3+2}{3} = 4$$

$$w_1^* = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} = -\frac{11}{14}$$

$$w_0^* = \bar{y} - w_1^* \bar{x} = 4 - \left(-\frac{11}{14}\right)\cdot 5 \approx 7.92$$

x_i	y_i	$(x_i - \bar{x})$	$(y_i - \bar{y})$	$(x_i - \bar{x})(y_i - \bar{y})$	$(x_i - \bar{x})^2$
3	7	−2	3	−6	4
4	3	−1	−1	1	1
8	2	3	−2	−6	9
				total = −11	total = 14

Summary

Summary, next time

- We introduced the linear prediction rule, $H(x) = w_0 + w_1 x$.

- To determine the best choice of slope (w_1) and intercept (w_0), we chose the squared loss function $(y_i - H(x_i))^2$ and minimized empirical risk $R_{sq}(w_0, w_1)$:

$$R_{sq}(w_0, w_1) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - (w_0 + w_1 x_i)\right)^2$$

- After solving for w_0^* and w_1^* through partial differentiation, we have a prediction rule $H^*(x) = w_0^* + w_1^* x$ that we can use to make predictions about the future.

- **Next time**: Revisiting correlation from DSC 10. Revisiting gradient descent. Introducing a linear algebraic formulation of linear regression.