Lecture 7 – Simple Linear Regression

DSC 40A, Fall 2022 @ UC San Diego

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Announcements

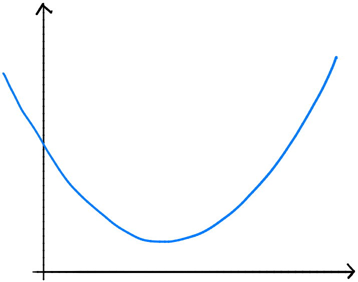
- Groupework 2 is due **Monday 10/10 at 23:59pm.**

- Midterm: 10/28 during class time.
  - Friday, 3-4PM, 4-5 PCYYNH 122.

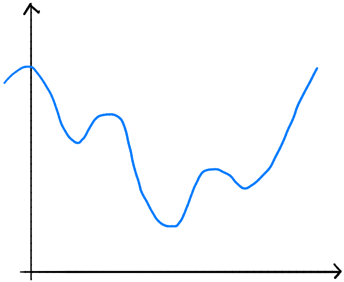
Agenda

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

Convex functions



Convex



Non-convex

Discussion Question

Which of these functions is not convex?

a) $f(x) = |x|$

b) $f(x) = e^x$

c) $f(x) = \sqrt{x-1}$

c) $f(x) = (x-3)^{24}$

To answer, go to `menti.com` **and enter the code 4821 5997.**

Why does convexity matter?

- Convex functions are (relatively) easy to minimize with gradient descent.

- **Theorem**: if $R(h)$ is convex and differentiable then gradient descent converges to a **global minimum** of R *provided* that the step size is small enough.

- **Why?**
  - If a function is convex and has a local minimum, that local minimum must be a global minimum.

  - In other words, gradient descent won't get stuck/terminate in local minimums that aren't global minimums (as happened with $R_{ucsd}(h)$ and a small σ in our demo).

Nonconvexity and gradient descent

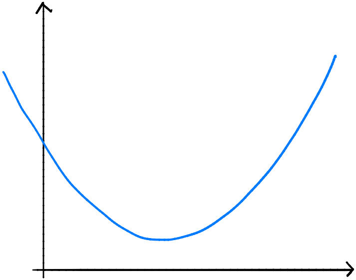
- We say a function is nonconvex if it does not meet the criteria for convexity.
- Nonconvex functions are (relatively) hard to minimize.
- Gradient descent can still be useful, but it's not guaranteed to converge to a global minimum.
  - We saw this when trying to minimize $R_{ucsd}(h)$ with a smaller σ.

Second derivative test for convexity

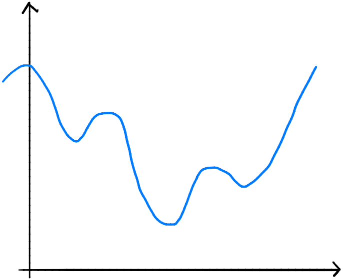
- If $f(x)$ is a function of a single variable and is twice differentiable, then:

- $f(x)$ is convex if and only if $\frac{d^2 f}{dx^2}(x) \geq 0$ for all x.

- Example: $f(x) = x^4$ is convex.



Convex



Non-convex

Convexity of empirical risk

- If $L(h, y)$ is a convex function (when y is fixed) then

$$R(h) = \frac{1}{n} \sum_{i=1}^{n} L(h, y_i)$$

  is convex.
  - Why? Because sums of convex functions are convex.

- What does this mean?
  - If a loss function is convex (for a particular type of prediction), then the corresponding empirical risk will also be convex.

Convexity of loss functions

- Is $L_{\text{sq}}(h, y) = (y - h)^2$ convex? **Yes** or **No**.

- Is $L_{\text{abs}}(h, y) = |y - h|$ convex? **Yes** or **No**.

- Is $L_{ucsd}(h, y)$ convex? **Yes** or **No**.

Convexity of R_{ucsd}

- A function can be convex in a region.

- If σ is large, $R_{ucsd}(h)$ is convex in a big region around data.
  - A large σ led to a very smooth, parabolic-looking empirical risk function with a single local minimum (which was a global minimum).

- If σ is small, $R_{ucsd}(h)$ is convex in only small regions.
  - A small σ led to a very bumpy empirical risk function with many local minimums.

Discussion Question

Recall the empirical risk for absolute loss,

$$R_{abs}(h) = \frac{1}{n} \sum_{i=1}^{n} |y_i - h|$$

Is $R_{abs}(h)$ **convex**? Is gradient descent **guaranteed** to find a global minimum, given an appropriate step size?

a) **YES** convex, **YES** guaranteed
b) **YES** convex, **NOT** guaranteed
c) **NOT** convex, **YES** guaranteed
d) **NOT** convex, **NOT** guaranteed

To answer, go to `menti.com` and enter the code 4821 5997.

Summary of gradient descent

Gradient descent

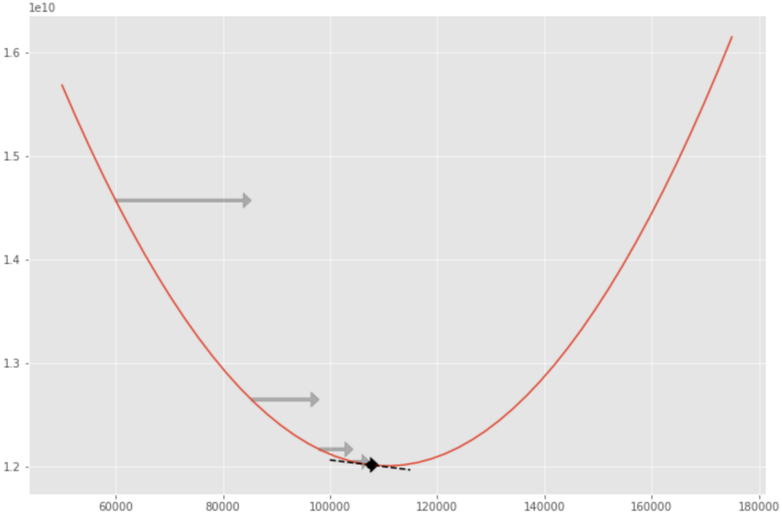
- The goal of gradient descent is to minimize a function $R(h)$.

- 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:

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

  - 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.

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

- The features, x, that we base our predictions on are called **predictor variables**.
- The quantity, y, that we're trying to predict based on these features is called the **response variable**.
- 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

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

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

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

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

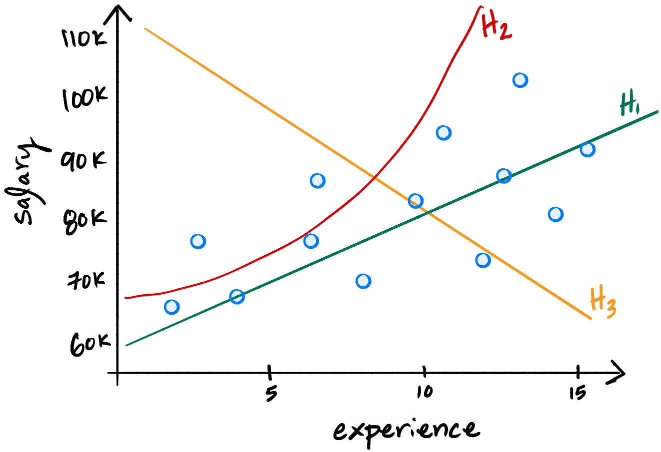
Comparing predictions

- 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:

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

- See which rule works better on data.

Example

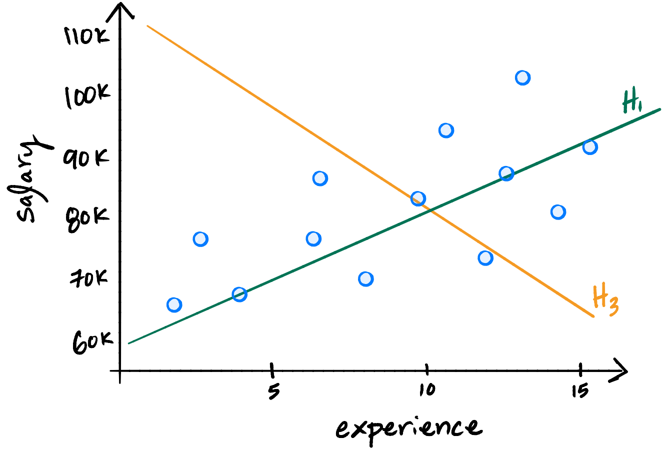


Quantifying the quality of a prediction rule H

- 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: $|y_i - H(x_i)|$.
  - Squared loss: $(y_i - H(x_i))^2$.
- We'll use squared loss, since it's differentiable.
- Using squared loss, the **empirical risk** (mean squared error) of the prediction rule H is:

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

Mean 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

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

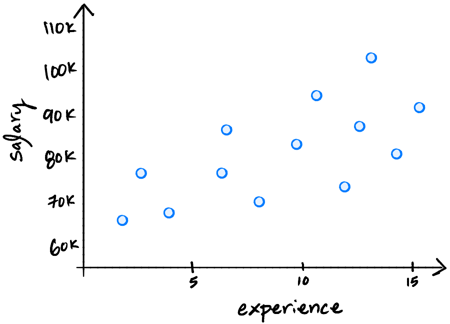
- There's a problem.

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 4821 5997.**



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: $H(x) = w_0 + w_1 x$.
  - 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 linear functions $\mathbb{R} \to \mathbb{R}$, find the function H^* with the smallest mean squared error.
  - Linear functions are of the form $H(x) = w_0 + w_1 x$.
  - 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.

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

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

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

- 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**:

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

- **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.

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

Discussion Question

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

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

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

$$\frac{\partial R_{\text{sq}}}{\partial w_0} =$$

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

$$\frac{\partial R_{\text{sq}}}{\partial w_1} =$$

Strategy

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

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^*

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

Solve for w_1^*

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

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

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

where

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

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

Key fact

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

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

Proof:

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:

Least squares solutions

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

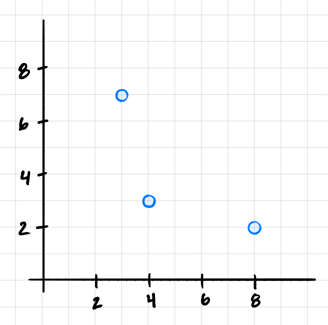
$$w_1^* = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \qquad\qquad w_0^* = \bar{y} - w_1\bar{x}$$

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

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

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

Example



$\bar{x} =$

$\bar{y} =$

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

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

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				
4	3				
8	2				

Summary

- Gradient descent is a general tool used to minimize differentiable functions.

- Gradient descent updates guesses for h^* by using the update rule

$$h_i = h_{i-1} - \alpha \cdot \left(\frac{dR}{dh}(h_{i-1}) \right)$$

- Convex functions are (relatively) **easy** to optimize with gradient descent.

- We introduced prediction rule framework to incorporate features in our predictions.

- 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.