Lecture 7 – Linear Prediction Rules

Winter 2024

DSC 40A, ~~Spring 2023~~

Announcements

- Homework 2 is due **today at 11:59pm**.
- Homework 3 will be posted soon.
  - Last homework before Midterm 1.

Agenda

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

Recap: convexity

Convexity: Definition

- A function $f : \mathbb{R} \to \mathbb{R}$ is **convex** if for every choice of a, b and $t \in [0, 1]$:

$$(1 - t)f(a) + tf(b) \geq f((1 - t)a + tb)$$

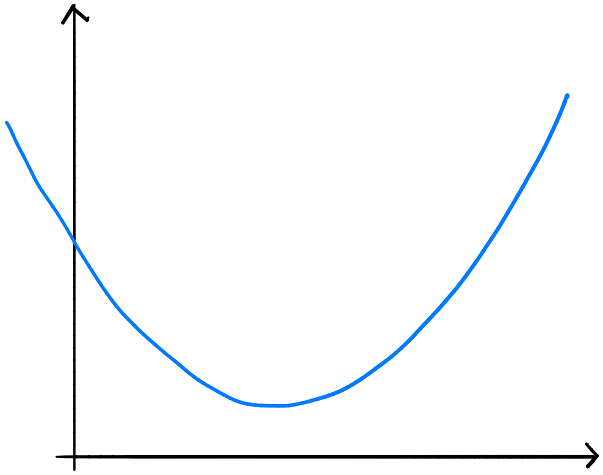
- This means that for **every** a, b in the domain of f, the line segment between

$$(a, f(a)) \qquad \text{and} \qquad (b, f(b))$$

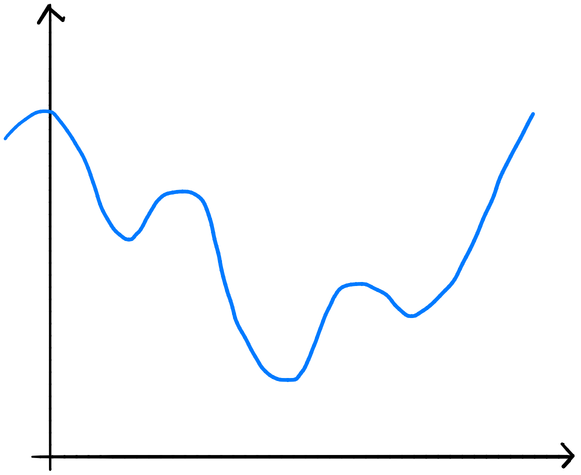
does not go below the plot of f.

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

Discussion Question

Suppose we have a function $f(x) = (x - a)^n$, which of the following statement is correct?

a) f(x) is always convex
b) f(x) is convex if n is **odd**, non-convex if n is **even**
c) f(x) is convex if n is **even**, non-convex if n is **odd**
d) f(x) is always non-convex

$$f(x) = (x-a)^n$$

$$f'(x) = n(x-a)^{n-1}$$

$$f''(x) = n(n-1)(x-a)^{n-2}$$

is $(x-3)^{24}$ convex?

Convexity and 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.
  - 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.
- For nonconvex functions, gradient descent can still be useful, but it's not guaranteed to converge to a global minimum.

Convexity of empirical risk

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

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

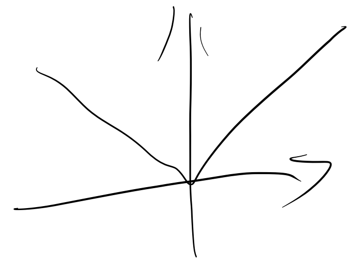
  is convex.
  - More generally, sums of convex functions are convex.

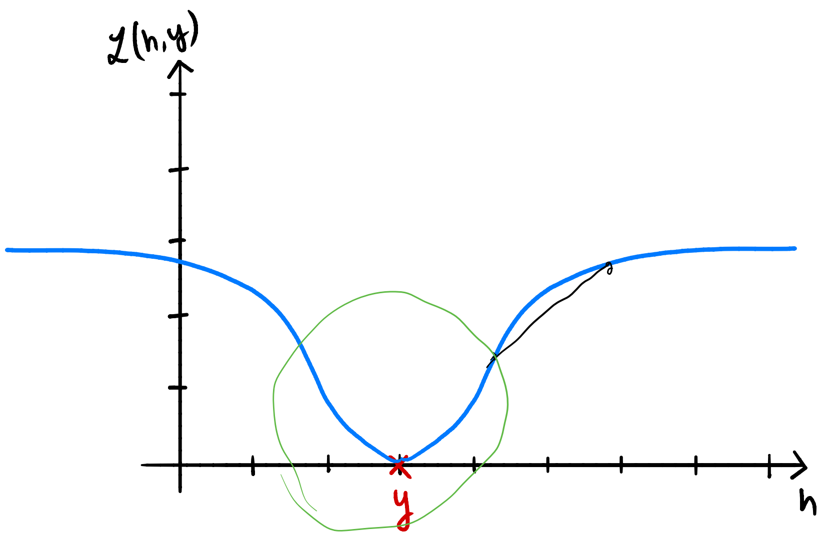
- What does this mean?
  - If a loss function is convex, then the corresponding empirical risk will also be convex.

Convexity of loss functions

$(x-a)^n$

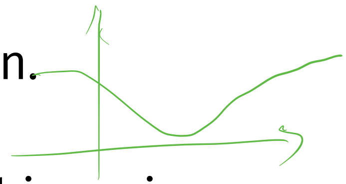
- Is $L_{sq}(h, y) = (y - h)^2$ convex? **Yes** or **No**.
- Is $L_{abs}(h, y) = |y - h|$ convex? **Yes** or **No**.
- Is $L_{ucsd}(h, y)$ convex? **Yes** or **No**.



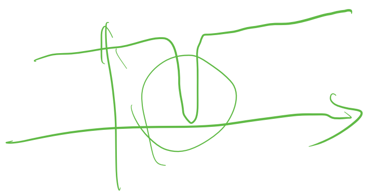


Convexity of R_{ucsd}

- A function can be convex in a region.



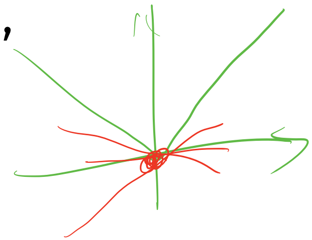
- If σ is large, $R_{ucsd}(h)$ is convex in a big region around data.
  - A large σ led to a very smooth, parabolic-looking empirical risk function with a single local minimum (which was a global minimum).
- If σ is small, $R_{ucsd}(h)$ is convex in only small regions.
  - A small σ led to a very bumpy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

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 the average loss across the entire data set (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 or 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.

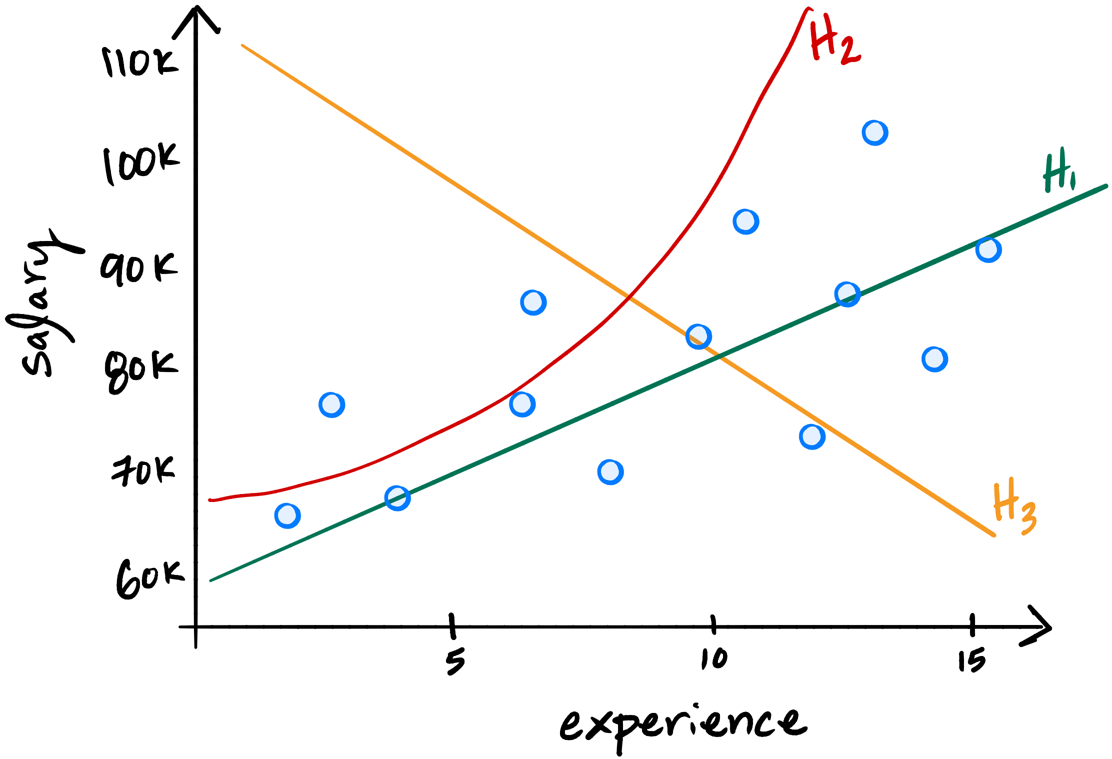
Comparing predictions

- 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:

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

- See which rule works better on data.

Example

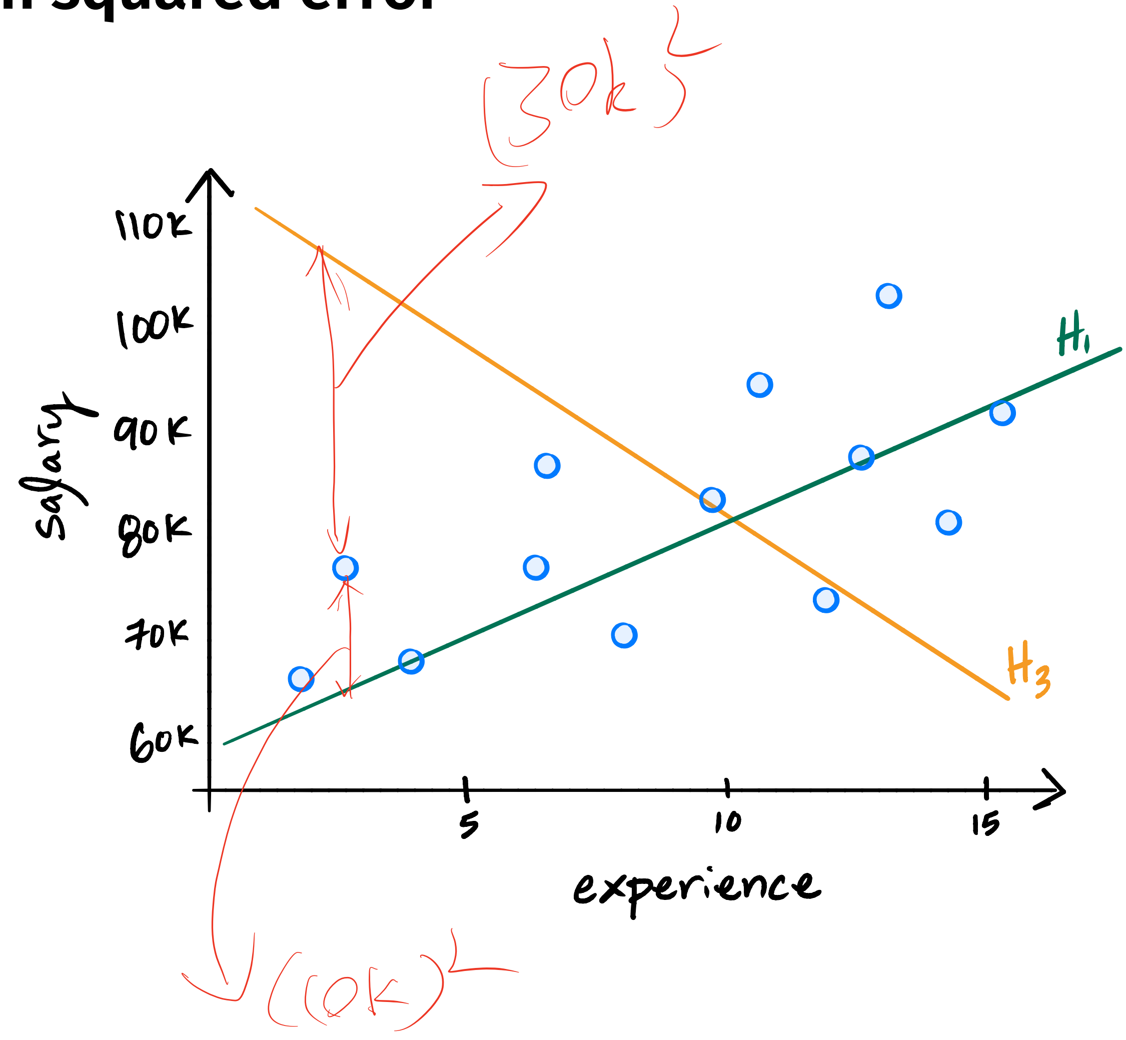


Quantifying the quality of a prediction rule H

- 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 focus on 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.

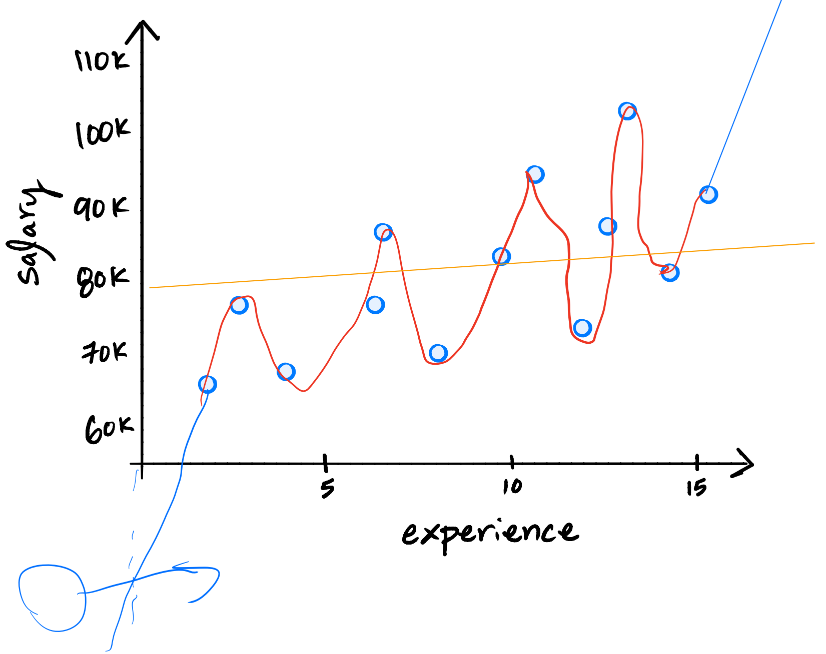
- That is, H^* should be the function that minimizes

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

Discussion Question

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

a) Yes   b) No



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**.

Out-of-Sample Data

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: $H(x) = w_0 + w_1 x + w_2 x^2$.
  - 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 **linear regression**.
  - **Simple** linear regression refers to linear regression with a single predictor variable, x.

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, $R_{\text{sq}}(w_0, w_1)$:

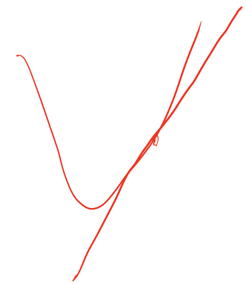
$$R_{\text{sq}}(w_0, w_1) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - (w_0 + w_1 x_i) \right)^2$$

- Strategy: multivariable calculus.

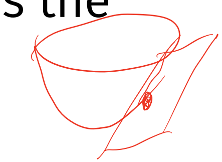
Recall: the **gradient**

- 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.

Minimizing multivariable functions

- From calculus, to optimize a multivariable differentiable function:
  1. Calculate the gradient vector, or vector of partial derivatives.
  2. Set the gradient equal to to 0 (that is, the zero vector).
  3. Solve the resulting system of equations.

$$\begin{pmatrix} \frac{\partial f}{\partial x}(x_0, y_0) \\ \frac{\partial f}{\partial y}(x_0, y_0) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Example

Discussion Question

Find the point at which the function

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

is minimized.

$$\begin{cases} \dfrac{\partial f}{\partial x} = 2x + 0 - 2 - 0 = 0 \\ \dfrac{\partial f}{\partial y} = 0 + 2y - 0 - 4 = 0 \end{cases} \qquad \begin{cases} 2x - 2 = 0 \\ 2y - 4 = 0 \end{cases} \Rightarrow \begin{cases} x = 1 \\ y = 2 \end{cases}$$

Summary

Summary, next time

- We introduced the linear prediction rule, $H(x) = w_0 + w_1 x$.
- To determine the best linear prediction rule, we'll use the squared loss and choose the one that minimizes the empirical risk, or mean squared error:

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

- **Next time**: We'll use calculus to minimize the mean squared error and find the best linear prediction rule.
  - Spoiler alert: it's the regression line, as we saw in DSC 10.