

Lecture 7 – Linear Prediction Rules



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

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

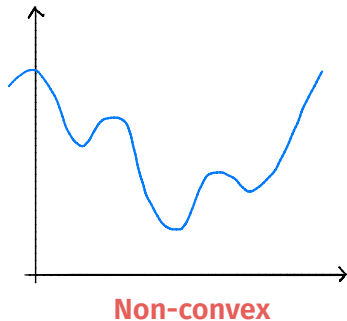
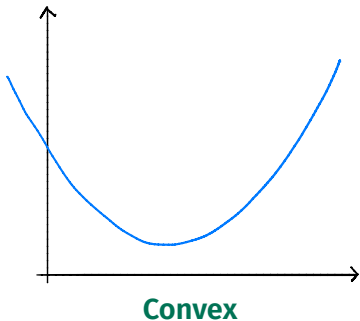
- ▶ This means that for **every** a, b in the domain of f , the line segment between

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

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 $\frac{d^2f}{dx^2}(x) \geq 0$ for all x .
- ▶ Example: $f(x) = x^4$ is 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

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

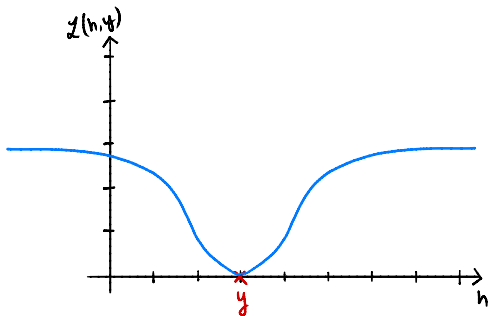
$$R(h) = \frac{1}{n} \sum_{i=1}^n L(h, y_i)$$

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

- ▶ 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 $L_{\text{ucsd}}(h, y)$ 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.

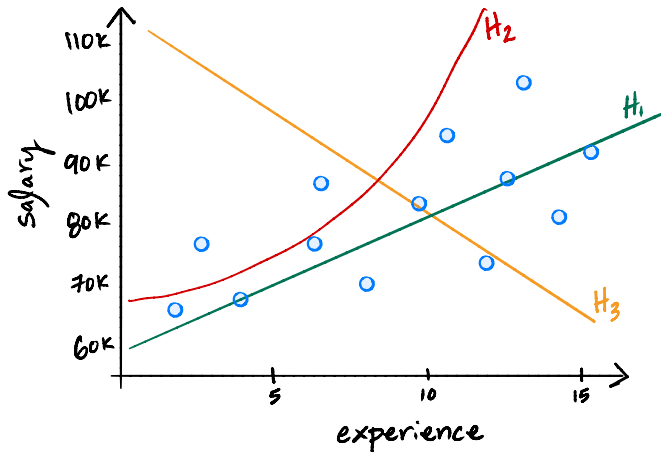
Comparing predictions

- ▶ 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:

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

- ▶ See which rule works better on data.

Example

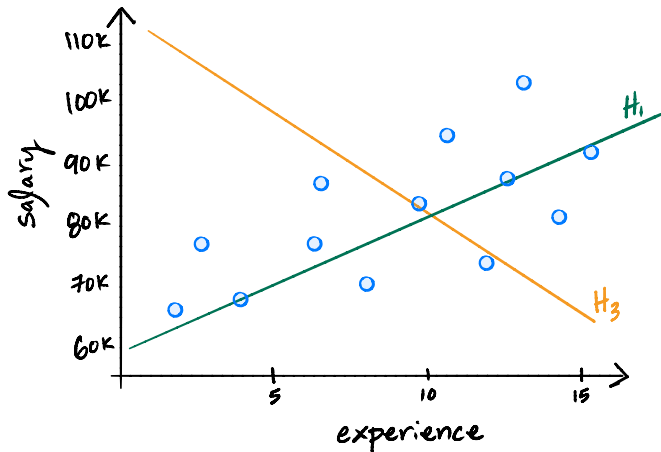


Quantifying the quality of a prediction rule H

- ▶ 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:

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

Mean squared error



Finding the best prediction rule

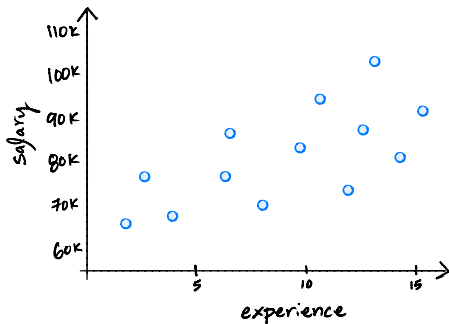
- ▶ **Goal:** out of all functions $\mathbb{R} \rightarrow \mathbb{R}$, find the function H^* with the smallest mean squared error.
- ▶ That is, H^* should be the function that minimizes

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

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**.

Solution

- ▶ Don't allow H to be just any function.
- ▶ Require that it has a certain form.
- ▶ Examples:
 - ▶ Linear: $H(x) = w_0 + w_1x$.
 - ▶ Quadratic: $H(x) = w_0 + w_1x + w_2x^2$.
 - ▶ Exponential: $H(x) = w_0e^{w_1x}$.
 - ▶ Constant: $H(x) = w_0$.

Finding the best **linear** prediction rule

- ▶ **Goal:** out of all **linear** functions $\mathbb{R} \rightarrow \mathbb{R}$, 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

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

- ▶ 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 .

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

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

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

- ▶ 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, $R_{\text{sq}}(w_0, w_1)$:

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

- ▶ 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 0 (that is, the zero vector).
 3. Solve the resulting system of equations.

Example

Discussion Question

Find the point at which the function

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

is minimized.

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:

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

- ▶ **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.