Module 8 – Simple Linear Regression

DSC 40A, Summer 2023

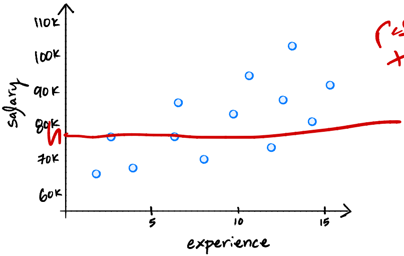
Agenda

- Recap of Module 7.
- Minimizing mean squared error for the linear prediction rule.
- Connection with correlation.

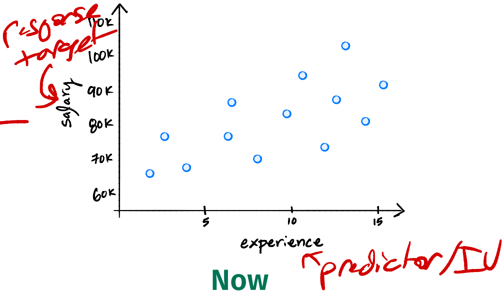
Recap of Module 7

Linear prediction rules

- **New:** Instead of predicting the same future value (e.g. salary) h for everyone, we will now use a **prediction rule** $H(x)$ that uses **features**, i.e. information about individuals, to make predictions.
- We decided to use a **linear** prediction rule, which is of the form $H(x) = w_0 + w_1 x$.
  - w_0 and w_1 are called **parameters**.



Before



Now

Finding the best linear prediction rule

- In order to find the best linear prediction rule, we need to pick a loss function and minimize the corresponding empirical risk.
  - We chose squared loss, $(y_i - H(x_i))^2$, as our loss function.
- 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 $H(x_i) = w_0 + w_1 x_i$.

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

Finding the best linear prediction rule

- **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:** To minimize $R(w_0, w_1)$, compute the gradient (vector of partial derivatives), set it equal to zero, and solve.

Minimizing mean squared error for the linear prediction rule

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

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

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

$$\frac{\partial R_{sq}}{\partial w_0} = \frac{1}{n}\sum_{i=1}^{n} \frac{dR_{sq}}{dw_0}\left(y_i - (w_0 + w_1 x_i)\right)^2$$

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

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

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

$$\frac{\partial R_{sq}}{\partial w_1} = \frac{1}{n}\sum_{i=1}^{n} \frac{dR_{sq}}{dw_1}\left(y_i - (w_0 + w_1 x_i)\right)^2$$

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

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

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^*

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

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

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

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

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

$$w_0 = \underbrace{\frac{1}{n}\sum_{i=1}^{n} y_i}_{\leftarrow \text{mean } y} - w_1 \cdot \underbrace{\frac{1}{n}\sum_{i=1}^{n} x_i}_{\leftarrow \text{mean } x}$$

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

Solve for w_1^*

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

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

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

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

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

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

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

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

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:

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

$$n \cdot \bar{x} - n \cdot \bar{x}$$

$$= 0$$

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

Least squares solutions

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

most common →

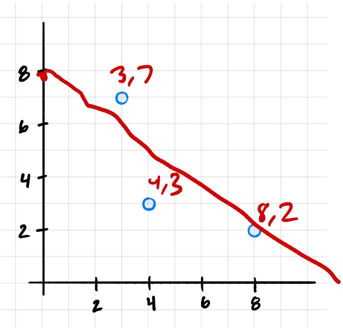
$$w_1^* = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \qquad w_0^* = \bar{y} - w_1\bar{x}$$

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

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

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

Example



$\bar{x} = 5$

$\bar{y} = 4$

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

$$w_0^* = \bar{y} - w_1\bar{x} = 4 - \frac{-11}{14}\cdot 5$$

$$\approx 8$$

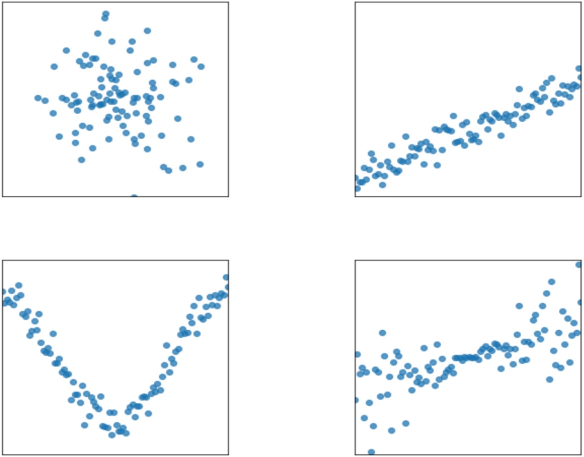
x_i	y_i	$(x_i - \bar{x})$	$(y_i - \bar{y})$	$(x_i - \bar{x})(y_i - \bar{y})$	$(x_i - \bar{x})^2$
3	7	-2	3	-6	4
4	3	-1	-1	1	1
8	2	3	-2	-6	9
				-11	14

Terminology

- x: **features**. years exp
- y: **response variable**. salary
- w_0, w_1: **parameters**.
- w_0^*, w_1^*: **optimal parameters**.
  - Optimal because they minimize mean squared error.
- The process of finding the optimal parameters for a given prediction rule and dataset is called "**fitting to the data**".
- $R_{sq}(w_0, w_1) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - (w_0 + w_1 x_i)\right)^2$: **mean squared error**, **empirical risk**.

Connection with correlation

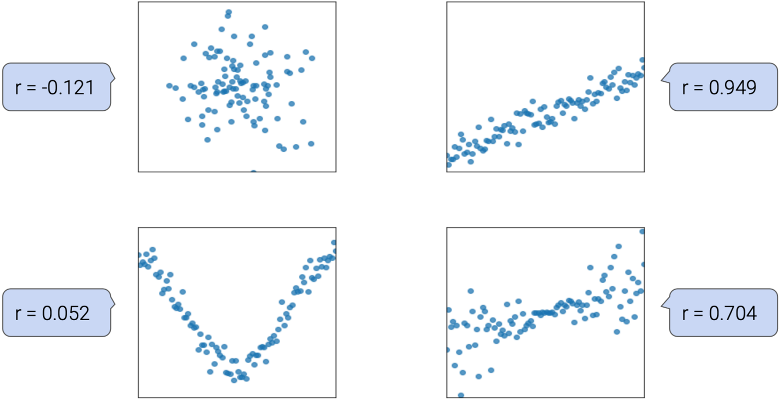
Patterns in scatter plots



Correlation coefficient

- In DSC 10, you were introduced to the idea of correlation.
  - It is a measure of the strength of the **linear association** of two variables, x and y.
  - Intuitively, it measures how tightly clustered a scatter plot is around a straight line.
  - It ranges between -1 and 1.

Patterns in scatter plots



Definition of correlation coefficient

- The correlation coefficient, r, is defined as **the average of the product of x and y, when both are in standard units**.
  - Let σ_x be the standard deviation of the x_i's, and $\bar{x}$ be the mean of the x_i's.
  - x_i in standard units is $\dfrac{x_i - \bar{x}}{\sigma_x}$.
  - The correlation coefficient is

$$r = \frac{1}{n} \sum_{i=1}^{n} \left(\frac{x_i - \bar{x}}{\sigma_x} \right) \left(\frac{y_i - \bar{y}}{\sigma_y} \right)$$

Another way to express w_1^*

- It turns out that w_1^*, the optimal slope for the linear prediction rule, can be written in terms of r!

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

- It's not surprising that r is related to w_1^*, since r is a measure of linear association.

- Concise way of writing w_0^* and w_1^*:

$$w_1^* = r\frac{\sigma_y}{\sigma_x} \qquad w_0^* = \bar{y} - w_1^*\bar{x}$$