Lecture 8 – Simple Linear Regression

DSC 40A, Winter, 2024

Announcements

- **Math Warning**
  - Today's lecture is called **simple** linear regression, but it contains lots of math

  - I'll frequently stops and ask to make sure everyone catch up

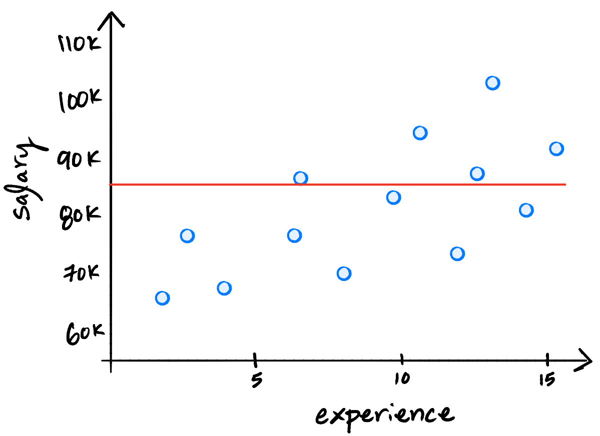
Agenda

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

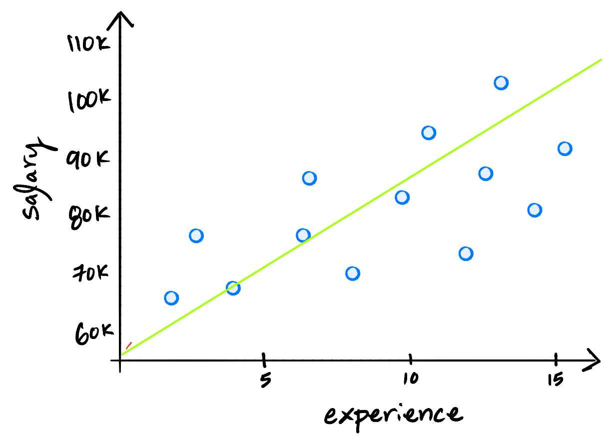
Recap of Lecture 7

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.

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

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

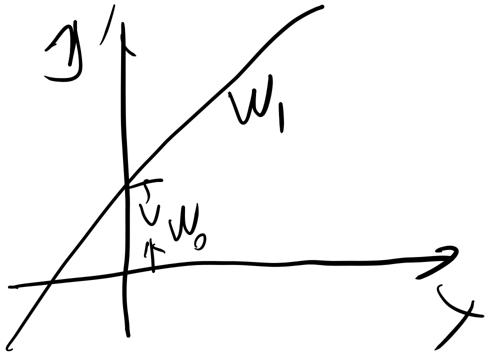
$$R_{\text{sq}}(w_0, w_1) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - (w_0 + w_1 x_i)\right)^2$$

Finding the best linear prediction rule

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

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

- **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 $\dfrac{\partial R_{sq}}{\partial w_0}$.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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^*

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

$n \cdot w_0$

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

$2 \cdot w_0$

$$-\frac{2}{n}\left[\sum_{i=1}^{n} y_i - \cancel{n} \cdot w_0 - \sum_{i=1}^{n} w_1 x_i\right]$$

$$\cancel{-}\frac{\cancel{2}}{n}\left[\sum_{i=1}^{n} y_i - \sum_{i=1}^{n} w_1 x_i\right] = \cancel{-}\cancel{2} w_0$$

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

Solve for w_1^*

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

mean$_y$ $\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$

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

$$= \bar{y} - \frac{1}{n}\sum_{i=1}^{n} w_1 x_i$$

$$-\frac{2}{n}\sum(y_i - w_0 - w_1 x_i)x_i = 0$$

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

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

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

$$-\frac{2}{n}\sum\left(y_i - \bar{y} + w_1(\bar{x} - x_i)\right)x_i = 0$$

$$-\cancel{\frac{2}{n}}\sum(y_i - \bar{y})x_i = \cancel{\frac{2}{n}}\sum w_1(\bar{x} - x_i)x_i$$

$$\sum(\bar{y} - y_i)x_i = \sum w_1(\bar{x} - x_i)x_i$$

$$w_1\sum(\bar{x} - x_i)x_i = \sum(\bar{y} - y_i)x_i$$

$$w_1^* = \frac{\sum(\bar{y} - y_i)x_i}{\sum(\bar{x} - x_i)x_i}$$

This part was on the board.

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:

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

$$= \sum x_i - n \cdot \bar{x}$$

$$= \sum x_i - n \cdot \left[\frac{1}{n}\sum x_i\right]$$

$$= \sum x_i - \sum x_i = 0$$

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:

$$\sum(x_i - \bar{x}) = 0, \quad \sum(y_i - \bar{y}) = 0 \Rightarrow \sum(x_i - \bar{x})\cdot\bar{x} = 0, \quad \sum(y_i - \bar{y})\bar{x} = 0$$

Pull these out

$$w_1^* = \frac{\sum(y_i - \bar{y})x_i - 0}{\sum(x_i - \bar{x})x_i - 0} = \frac{\sum(y_i - \bar{y})x_i - \sum(y_i - \bar{y})\bar{x}}{\sum(x_i - \bar{x})x_i - \sum(x_i - \bar{x})\bar{x}}$$

Pull these out

$$= \frac{\sum(y_i - \bar{y})(x_i - \bar{x})}{\sum(x_i - \bar{x})(x_i - \bar{x})} = \frac{\sum(y_i - \bar{y})(x_i - \bar{x})}{\sum(x_i - \bar{x})^2}$$

Least squares solutions

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

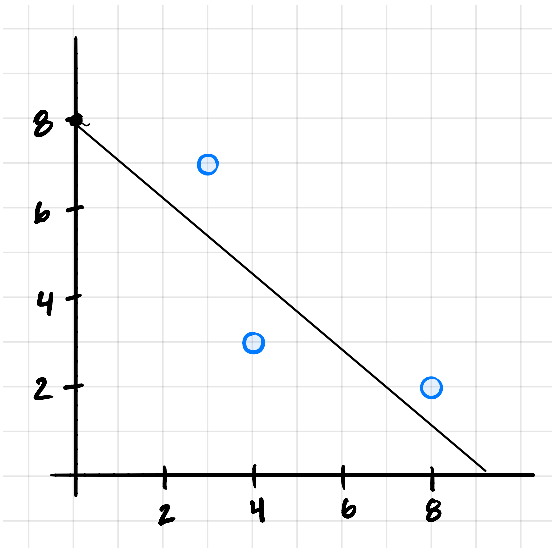
$$w_1^* = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \qquad w_0^* = \bar{y} - w_1\bar{x}$$

  - 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



$\bar{x} = 5$

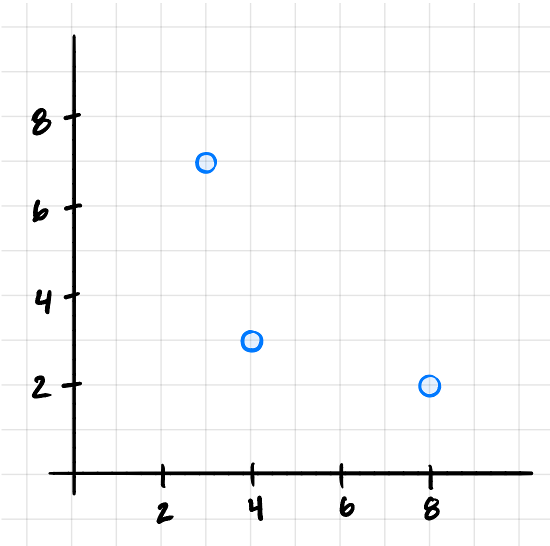
$\bar{y} = 4$

$$w_1^* = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} = \frac{-6-6+1}{4+1+9} = \frac{-11}{14}$$

$$w_0^* = \bar{y} - w_1\bar{x} = 4 + \frac{11}{14}\cdot 5 = \frac{56+55}{14} = \frac{111}{14} \approx 8$$

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

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				

Terminology

- x: **features**.
- y: **response variable**.
- 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**.

Discussion Question

Consider a dataset with just two points, $(2, 5)$ and $(4, 15)$. Suppose we want to fit a linear prediction rule to this dataset by minimizing mean squared error. What are the values of w_0^* and w_1^* that minimize mean squared error?

a) $w_0^* = 2, w_1^* = 5$

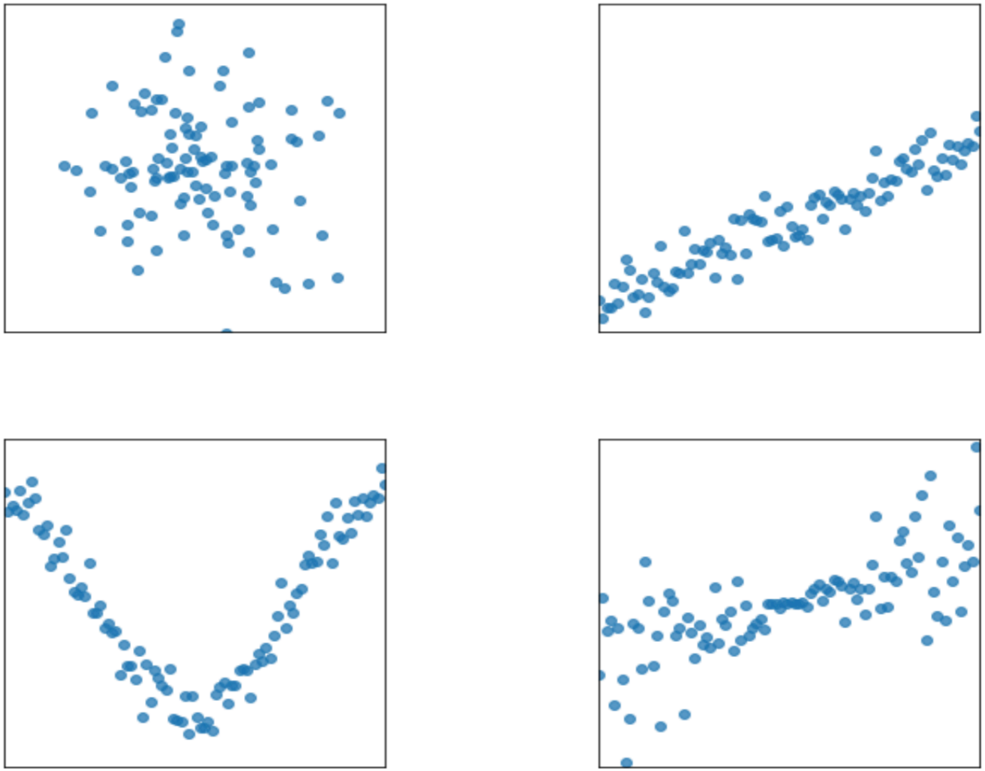
b) $w_0^* = 3, w_1^* = 10$

c) $w_0^* = -2, w_1^* = 5$

d) $w_0^* = -5, w_1^* = 5$

Connection with correlation

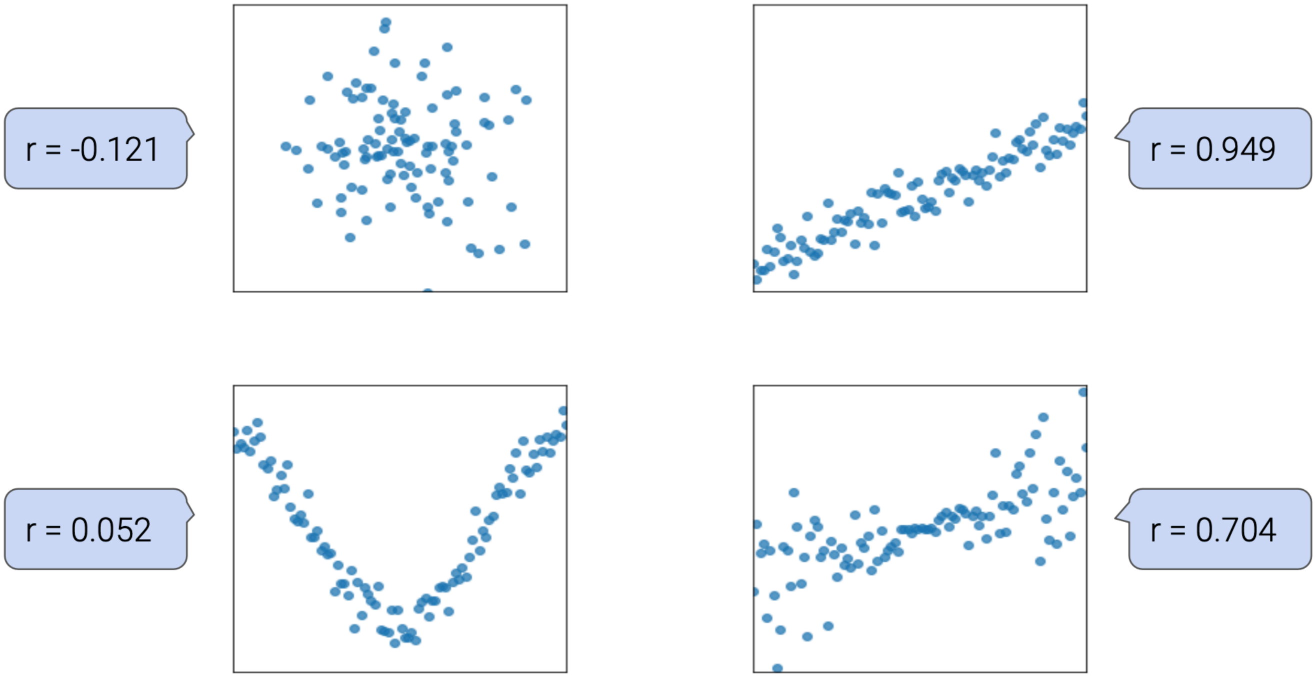
Patterns in scatter plots



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.

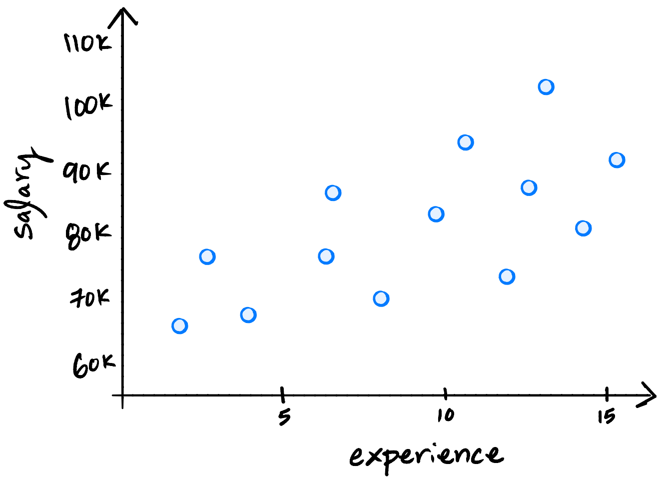
- Concise way of writing w_0^* and w_1^*:

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

Proof that $w_1^* = r\frac{\sigma_y}{\sigma_x}$

Interpreting the slope

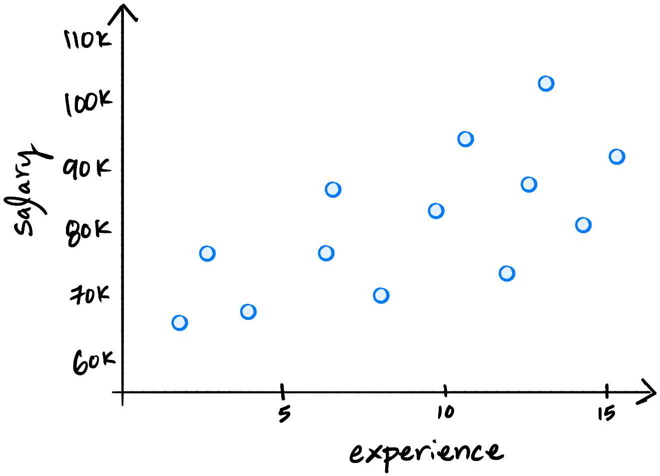
$$w_1^* = r\frac{\sigma_y}{\sigma_x}$$



- σ_y and σ_x are always non-negative. As a result, the sign of the slope is determined by the sign of r.
- As the y values get more spread out, σ_y increases and so does the slope.
- As the x values get more spread out, σ_x increases and the slope decreases.

Interpreting the intercept

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



- What is $H^*(\bar{x})$?

Discussion Question

We fit a linear prediction rule for salary given years of experience. Then everyone gets a \$5,000 raise. Which of these happens?

a) slope increases, intercept increases

b) slope decreases, intercept increases

c) slope stays same, intercept increases

d) slope stays same, intercept stays same