one input variable / one output

Lectures 5-7

Simple Linear Regression

DSC 40A, Fall 2025

Announcements

- Homework 1 is due **Friday night**.
- Look at the office hours schedule here and plan to start regularly attending!
- Remember to take a look at the supplementary readings linked on the course website.

Agenda

- Simple linear regression.
- Minimizing mean squared error for the simple linear model.
- Correlation.
- Interpreting the formulas.
- Connections to related models.
- What next? Linear algebra.

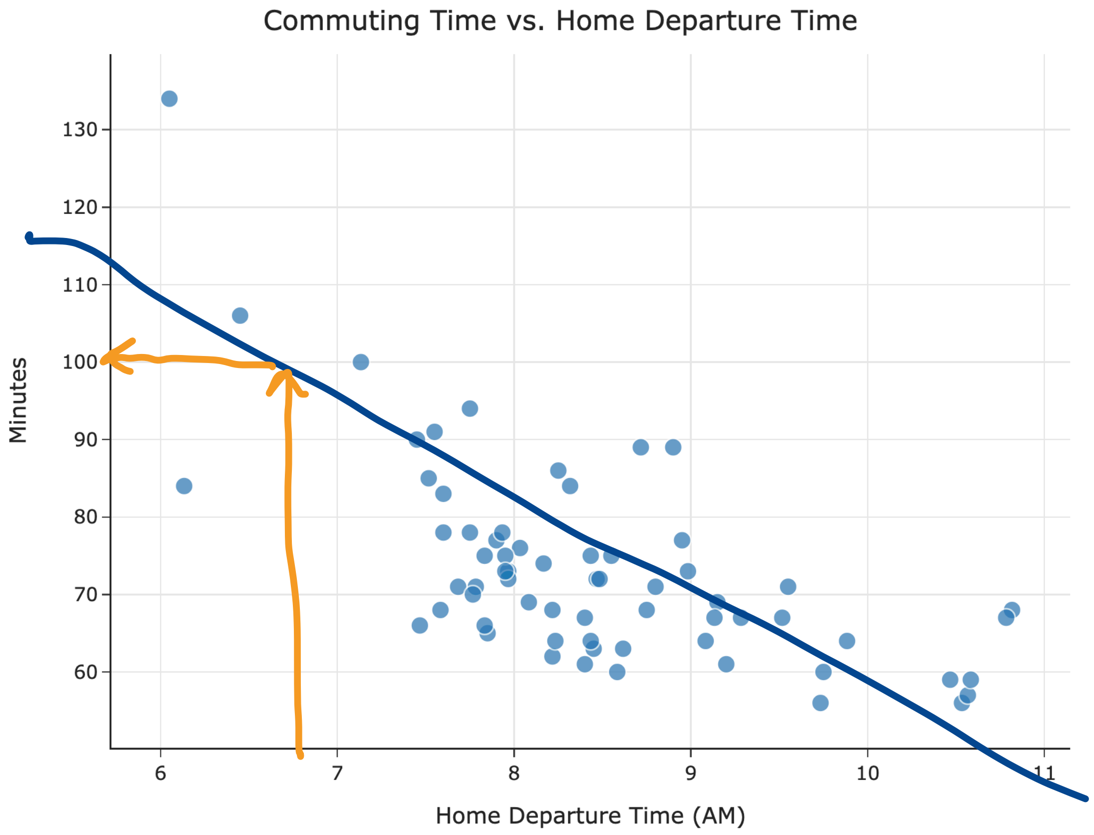
Question 🤔

Answer at q.dsc40a.com

Remember, you can always ask questions at q.dsc40a.com!

If the direct link doesn't work, click the "🤔 Lecture Questions" link in the top right corner of dsc40a.com.

Towards simple linear regression



- In Lecture 1, we introduced the idea of a hypothesis function, $H(x)$.
- We've focused on finding the best **constant model**, $H(x) = h$.
- Now that we understand the modeling recipe, we can apply it to find the best **simple linear regression model**, $H(x) = w_0 + w_1 x$.
- This will allow us to make predictions that aren't all the same for every data point.

The modeling recipe

1. Choose a model.

Before : Constant $H(x) = h$ $\longrightarrow$ Now : SLR $H(x) = w_0 + w_1 x$

2. Choose a loss function.

$L_{sq}(y_i, H(x_i)) = (y_i - H(x_i))^2$

actual

prediction

$L_{abs}(y_i, H(x_i)) = |y_i - H(x_i)|$

3. Minimize average loss to find optimal model parameters.

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

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

Finding the best linear model

- **Goal:** Out of all **linear** functions $\mathbb{R} \to \mathbb{R}$, find the function H^* with the smallest mean squared error. (MSE)
  - 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, $H^* = w_0^* + w_1^* x$ should be the linear function that minimizes

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

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

- We chose squared loss, since it's the easiest to minimize.
- **How do we find the parameters w_0^* and w_1^* that minimize $R_{\text{sq}}(w_0, w_1)$?**

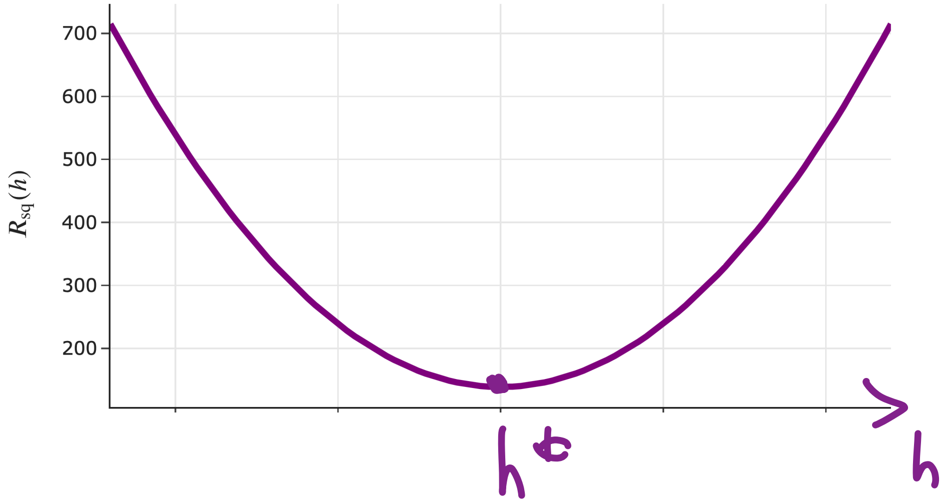
Loss surface

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

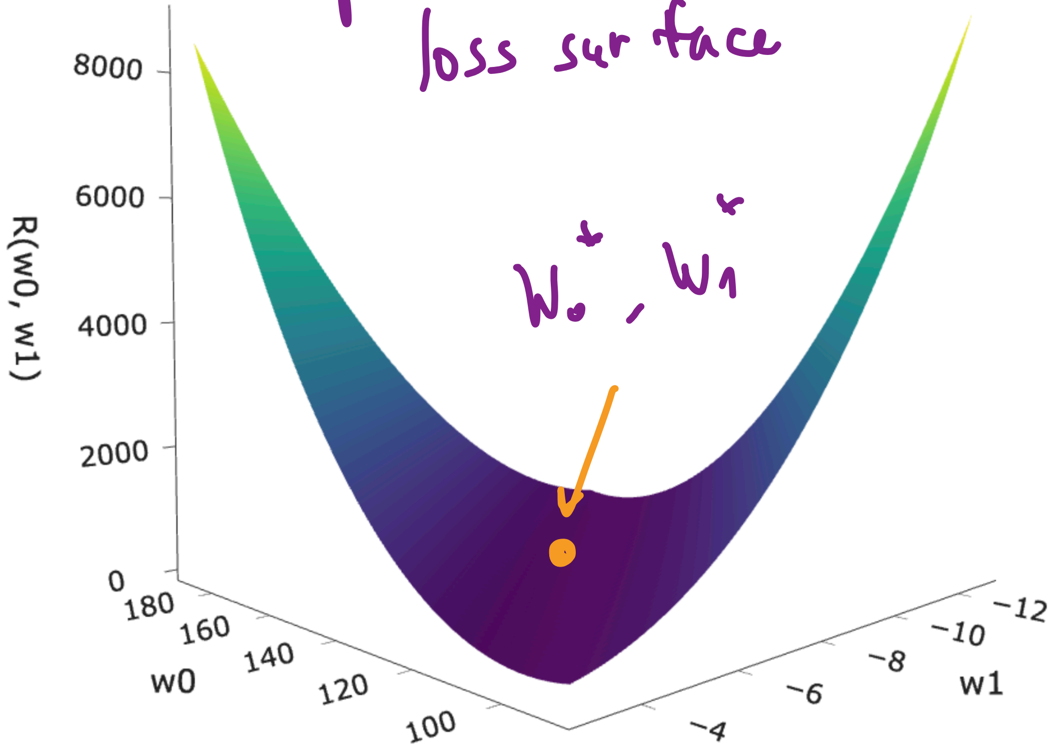
For the constant model, the graph of $R_{\text{sq}}(h)$ looked like a parabola.

What does the graph of $R_{\text{sq}}(w_0, w_1)$ look like for the simple linear regression model?

$R_{\text{sq}}(h) = \frac{1}{5}\left((72-h)^2 + (90-h)^2 + (61-h)^2 + (85-h)^2 + (92-h)^2\right)$



parabolic loss surface



Minimizing mean squared error for the simple linear model

Minimizing multivariate functions

- Our goal is to find the parameters w_0^* and w_1^* that minimize mean squared error:

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

- R_{sq} is a function of two variables: w_0 and w_1.
- To minimize a function of multiple variables:
  - Take partial derivatives with respect to each variable.
  - Set all partial derivatives to 0.
  - Solve the resulting system of equations.
  - Ensure that you've found a minimum, rather than a maximum or saddle point (using the second derivative test for multivariate functions).

$\frac{\partial R_{sq}}{\partial w_0} = 0$, $\frac{\partial R_{sq}}{\partial w_1} = 0$

R_{sq} is parabolic in w_0, w_1 → convex → single minimum

Example

Find the point (x, y, z) at which the following function is minimized.

$$f(x, y) = \underline{x^2 - 8x} + \underline{y^2 + 6y} - 7$$

complete the square
(no calculus)

$f(x,y) = (x-a)^2 + (y-b)^2 + c$
$\geq 0 \quad \geq 0$

$f(x,y) = \underbrace{x^2 - 8x + 16}-16 + \underbrace{y^2 + 6y + 9} - 9 - 7$

$= (x-4)^2 - 16 \quad (y+3)^2 - 9 \quad -7$

$= (x-4)^2 + (y+3)^2 - 32$

$\Rightarrow x^* = 4$

$y^* = -3$

$f(x^*, y^*) = -32$

calculus

$f_x = f'_x = \frac{\partial f}{\partial x}$

$\frac{\partial f(x,y)}{\partial x} = 2x - 8 = 0$

$\frac{\partial f(x,y)}{\partial y} = 2y + 6 = 0$

$\Rightarrow 2x = 8 \quad 2y = -6$

$\Rightarrow x^* = 4 \quad y^* = -3$

Minimizing multivariate functions

- Our goal is to find the parameters w_0^* and w_1^* that minimize mean squared error:

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

- R_{sq} is a function of two variables: w_0 and w_1.
- To minimize a function of multiple variables:
  - Take partial derivatives with respect to each variable.
  - Set all partial derivatives to 0.
  - Solve the resulting system of equations.
  - Ensure that you've found a minimum, rather than a maximum or saddle point (using the second derivative test for multivariate functions).

Minimizing mean squared error

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

To find the w_0^* and w_1^* that minimize $R_{\text{sq}}(w_0, w_1)$, we'll:

1. Find $\frac{\partial R_{\text{sq}}}{\partial w_0}$ and set it equal to 0.
2. Find $\frac{\partial R_{\text{sq}}}{\partial w_1}$ and set it equal to 0.
3. Solve the resulting system of equations.

Question 🤔

Answer at q.dsc40a.com

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

Which of the following is equal to $\frac{\partial R_{\text{sq}}}{\partial w_0}$?

- A. $\frac{1}{n}\sum_{i=1}^{n}(y_i - (w_0 + w_1 x_i))$
- B. $-\frac{1}{n}\sum_{i=1}^{n}(y_i - (w_0 + w_1 x_i))$
- C. $-\frac{2}{n}\sum_{i=1}^{n}(y_i - (w_0 + w_1 x_i))x_i$ $\frac{\partial R_{sq}}{\partial w_1}$
- D. $-\frac{2}{n}\sum_{i=1}^{n}(y_i - (w_0 + w_1 x_i))$ $\frac{\partial R_{sq}}{\partial w_0}$

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

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

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

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

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

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

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

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

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

Strategy

We have a system of two equations and two unknowns (w_0 and w_1):

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

To proceed, we'll:

1. Solve for w_0 in the first equation.

   The result becomes w_0^*, because it's the "best intercept."

2. Plug w_0^* into the second equation and solve for w_1.

   The result becomes w_1^*, because it's the "best slope."

Solving for w_0^*

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

$/ \cdot -\frac{n}{2}$

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

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

$$\sum_{i=1}^{n} w_0 = \underbrace{w_0 + w_0 + \dots + w_0}_{n \text{ times}} = n w_0$$

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

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

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

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

Solving for w_1^*

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

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

plug in

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

Goal: isolate w_1

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

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

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

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

Note: you cannot cancel out x_i in numerator and denominator
→ they are part of the sum

Least squares solutions

We've found that the values w_0^* and w_1^* that minimize R_{sq} are:

optimal slope

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

optimal intercept

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

where:

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

These formulas work, but let's re-write w_1^* to be a little more symmetric.

An equivalent formula for w_1^*

$(*)\ \sum_{i=1}^{n}(y_i - \bar{y}) = \sum_{i=1}^{n} y_i - \bar{y}\underbrace{\sum_{i=1}^{n} 1}_{} =$

$= n \cdot \frac{1}{n}\sum_{i=1}^{n} y_i - n\bar{y}$

$= n\bar{y} - n\bar{y} = 0$

Claim:

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

use $\sum_{i=1}^{n}(x_i - \bar{x}) = 0$ for denominator and we're done

$\boxed{(a-b)(c-d) = a(c-d) - b(c-d)}$

Proof:

right numerator

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

$$= \sum_{i=1}^{n}(y_i - \bar{y})x_i - \bar{x}\underbrace{\sum_{i=1}^{n}(y_i - \bar{y})}_{(*) = 0?} = \boxed{\sum_{i=1}^{n}(y_i - \bar{y})x_i}$$

left numerator

strategy

need to show

1) yellow box = pink box

2) green box = cyan box

Least squares solutions

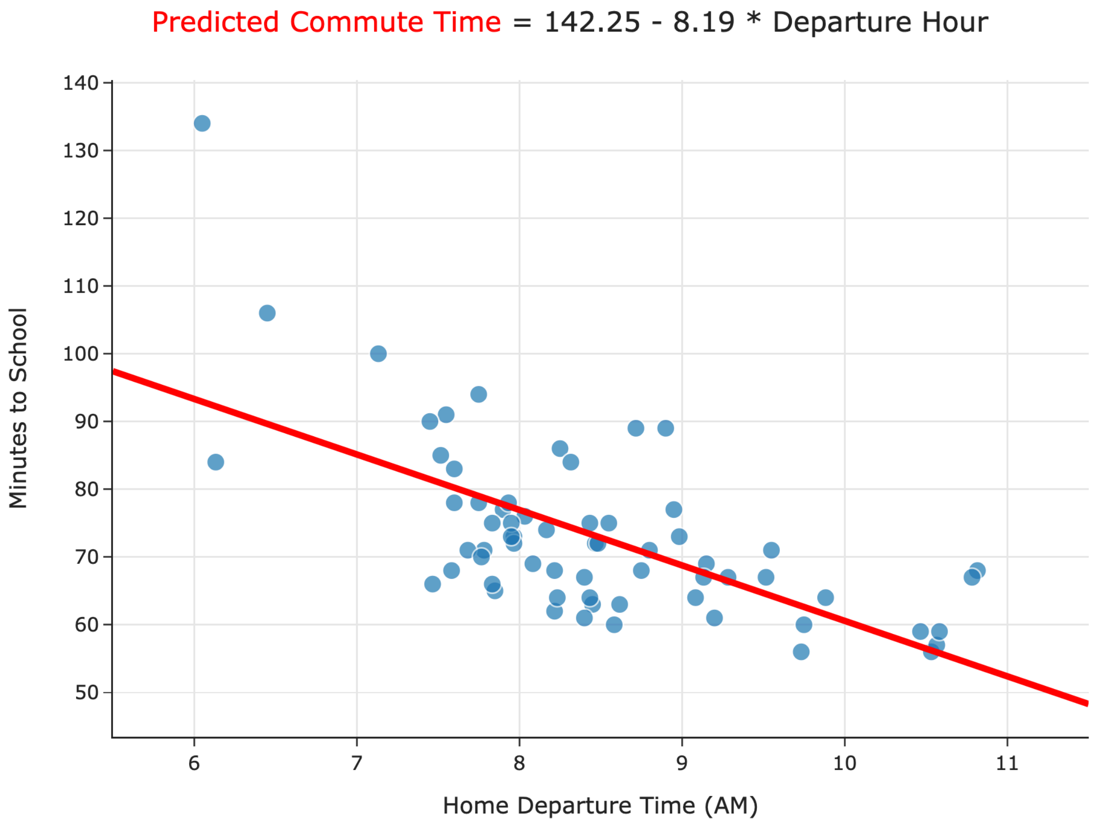
- The **least squares solutions** for the intercept w_0 and slope w_1 are:

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

- We say w_0^* and w_1^* are **optimal parameters**, and the resulting line is called the **regression line**.
- The process of minimizing empirical risk to find optimal parameters is also called "**fitting to the data.**"
- To make predictions about the future, we use $\boxed{H^*(x) = w_0^* + w_1^* x}$.

Causality

Solving for best linear model for commute



Can we conclude that leaving later **causes** you to get to school quicker?

What's next?

We now know how to find the optimal slope and intercept for linear hypothesis functions. Next, we'll:

- See how the formulas we just derived connect to the formulas for the slope and intercept of the regression line we saw in DSC 10.
    - They're the same, but we need to do a bit of work to prove that.
- Learn how to interpret the slope of the regression line.
- Discuss *causality*.
- Learn how to build regression models with **multiple inputs**.
    - To do this, we'll need linear algebra!

Agenda

- Simple linear regression.
- Correlation.
- Interpreting the formulas.
- Connections to related models.

Least squares solutions

- Our goal was to find the parameters w_0^* and $w_1{}^*$ that minimized:

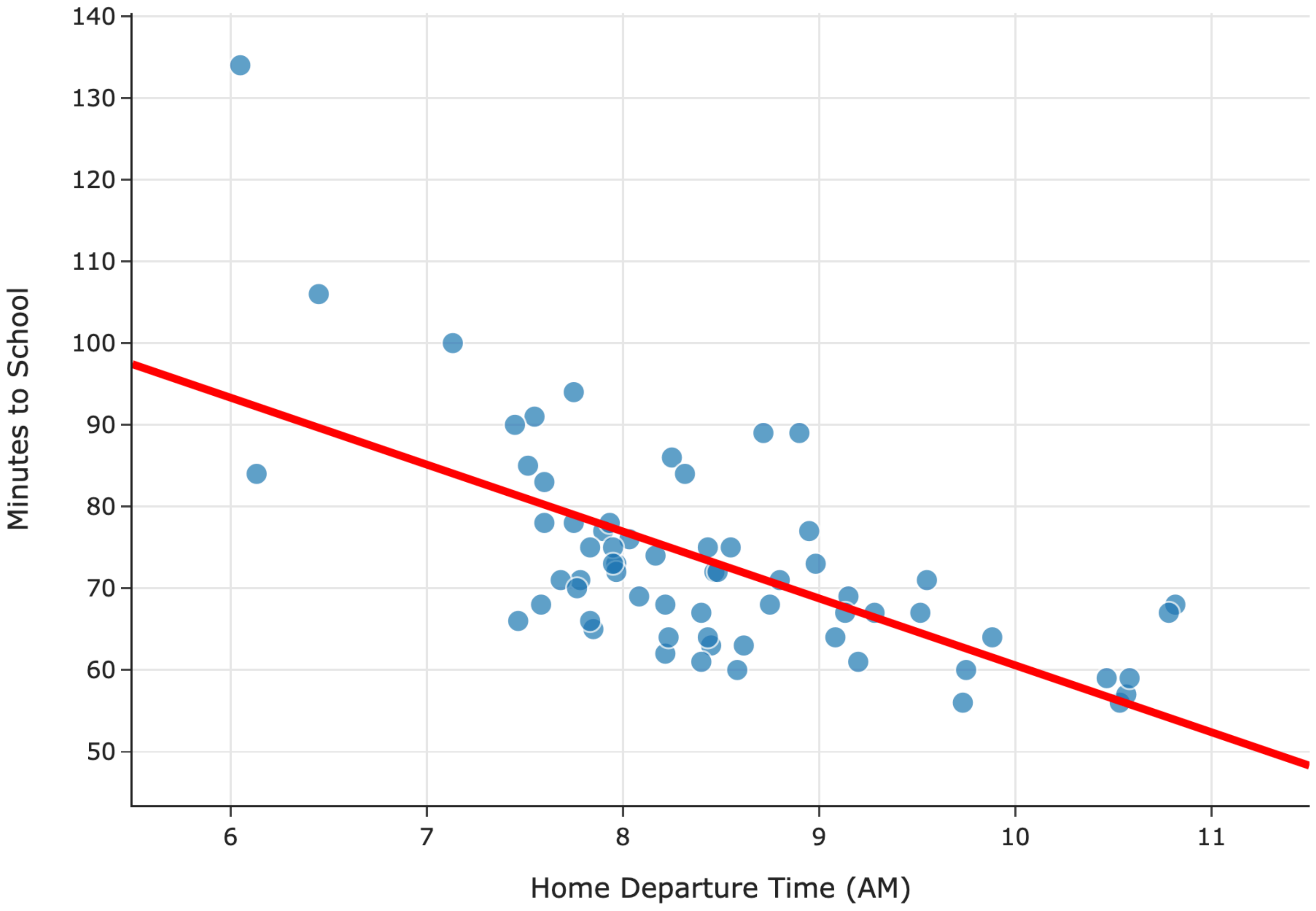
$$R_{\text{sq}}(w_0, w_1) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - (w_0 + w_1 x_i)\right)^2$$

- To do so, we used calculus, and we found that the minimizing values are:

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

- We say w_0^* and w_1^* are **optimal parameters**, and the resulting line is called the **regression line**.

Predicted Commute Time = 142.25 - 8.19 * Departure Hour



Now what?

We've found the optimal slope and intercept for linear hypothesis functions using squared loss (i.e. for the regression line). Now, we'll:

- See how the formulas we just derived connect to the formulas for the slope and intercept of the regression line we saw in DSC 10.
  - They're the same, but we need to do a bit of work to prove that.
- Learn how to interpret the slope of the regression line.
- Understand connections to other related models.
- Learn how to build regression models with **multiple inputs**.
  - To do this, we'll need linear algebra!

Question 🤔

Answer at q.dsc40a.com

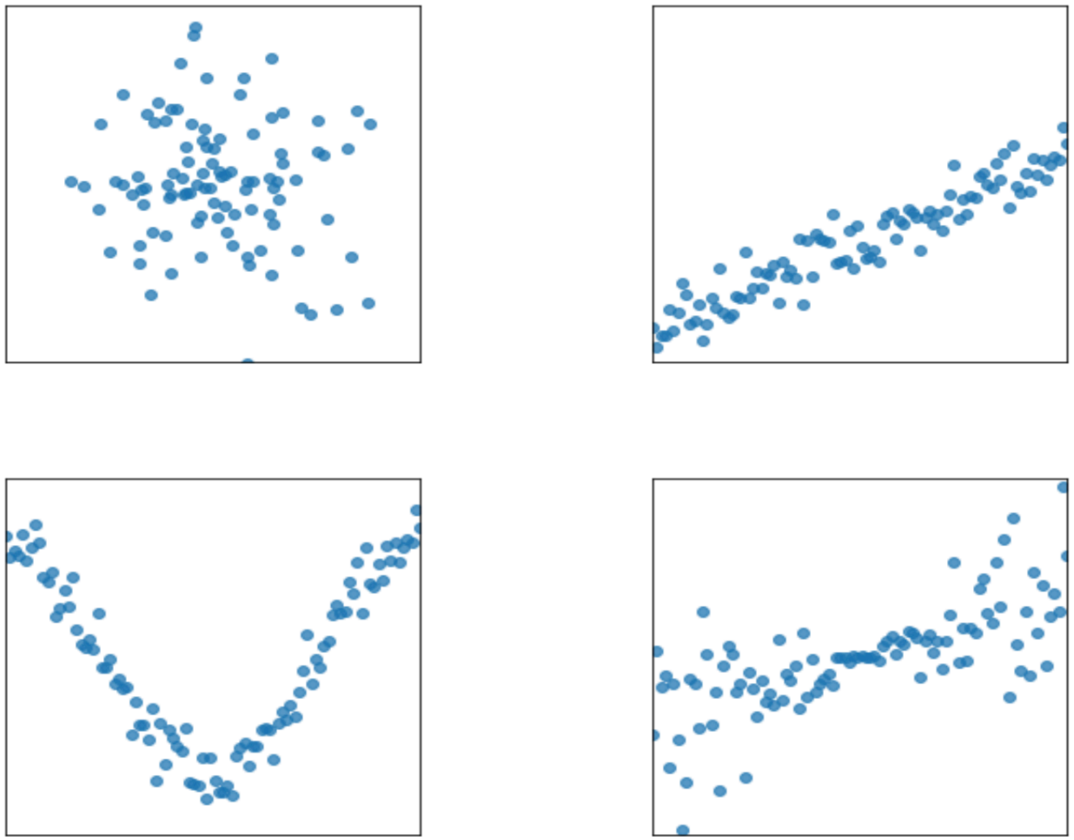
Consider a dataset with just two points, $(2, 5)$ and $(4, 15)$. Suppose we want to fit a linear hypothesis function to this dataset using squared loss. What are the values of w_0^* and w_1^* that minimize empirical risk?

- A. $w_0^* = 2$, $w_1^* = 5$
- B. $w_0^* = 3$, $w_1^* = 10$
- C. $w_0^* = -2$, $w_1^* = 5$
- D. $w_0^* = -5$, $w_1^* = 5$

Correlation

Quantifying patterns in scatter plots

- In DSC 10, you were introduced to the idea of the **correlation coefficient**, r.
- 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.

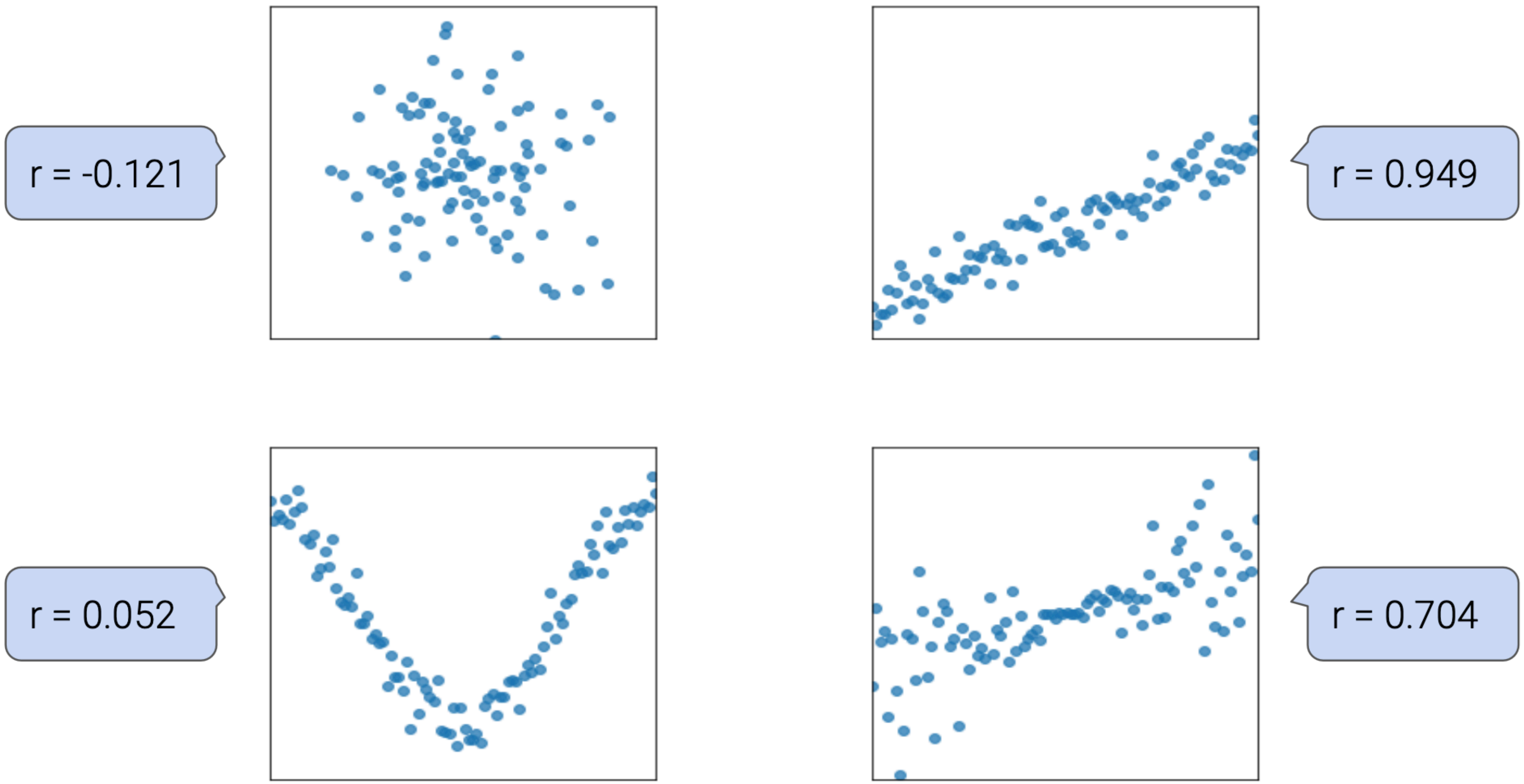


The correlation coefficient

- 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_is, and $\bar{x}$ be the mean of the x_is.
- x_i in standard units is $\frac{x_i - \bar{x}}{\sigma_x}$.
- The correlation coefficient, then, is:

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

The correlation coefficient, visualized



Another way to express w_1^*

- It turns out that w_1^*, the optimal slope for the linear hypothesis function when using squared loss (i.e. the regression line), can be written in terms of r!

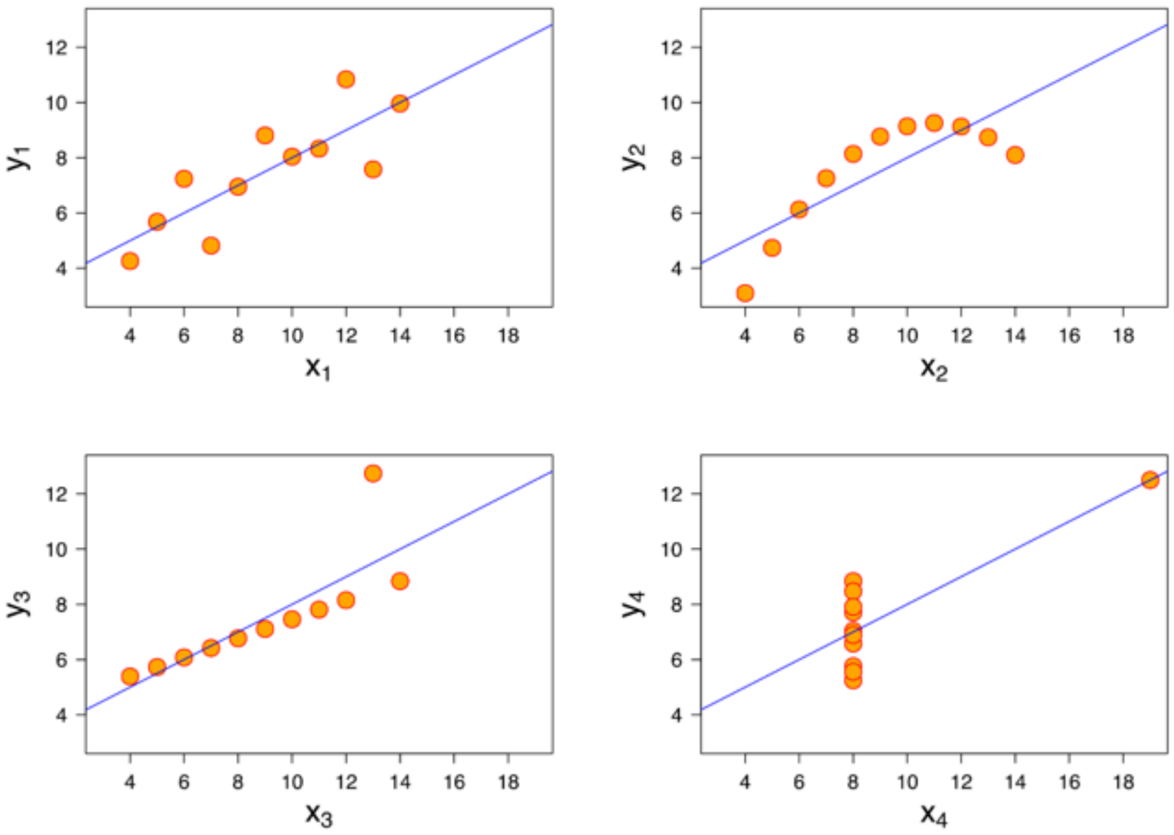
$$w_1^* = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} = r\frac{\sigma_y}{\sigma_x}$$

- 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^*:

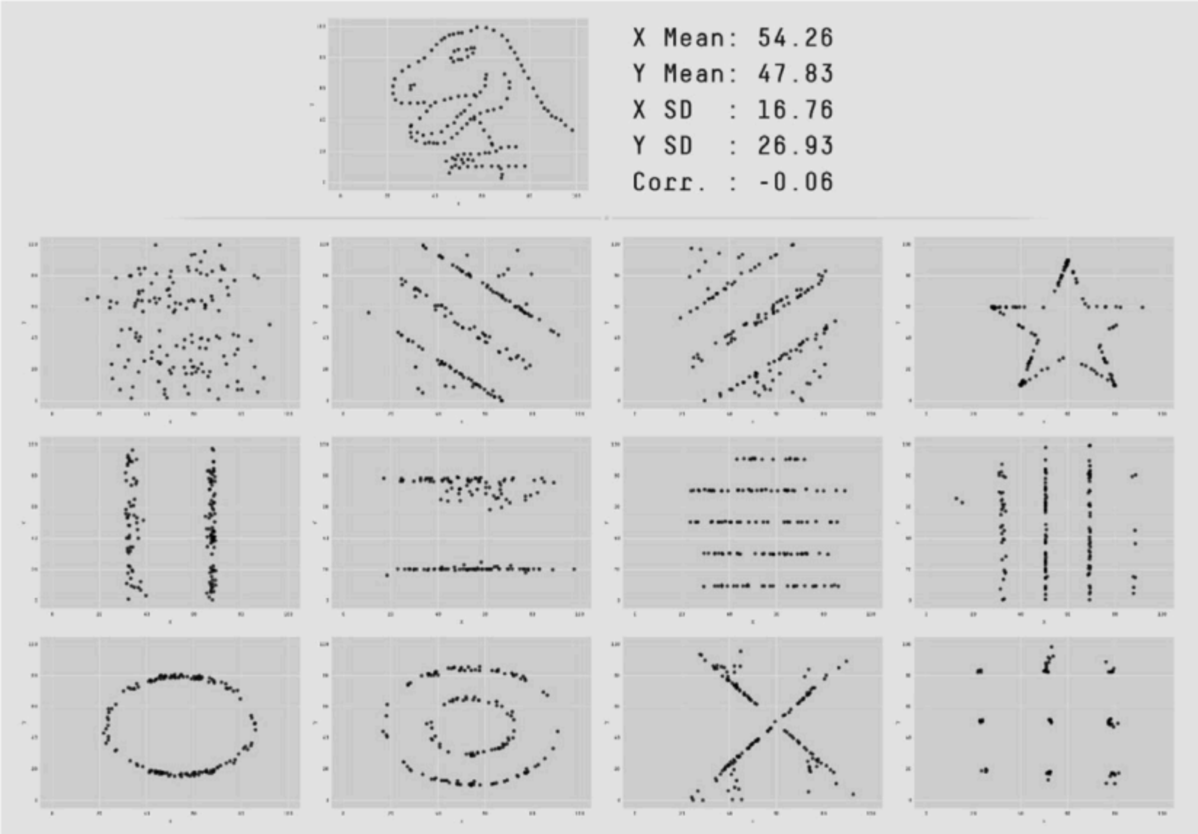
$$w_1^* = r\frac{\sigma_y}{\sigma_x} \qquad w_0^* = \bar{y} - w_1^*\bar{x}$$

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

Dangers of correlation



Dangers of correlation



Interpreting the formulas

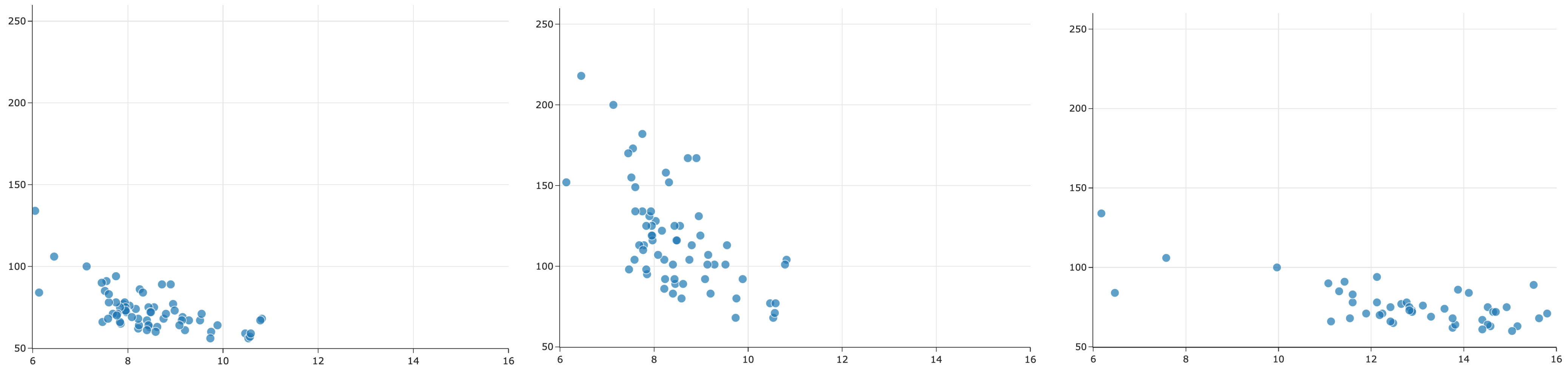
Interpreting the slope

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

- The units of the slope are **units of y per units of x**.
- In our commute times example, in $H(x) = 142.25 - 8.19x$, our predicted commute time **decreases by 8.19 minutes per hour**.

Interpreting the slope

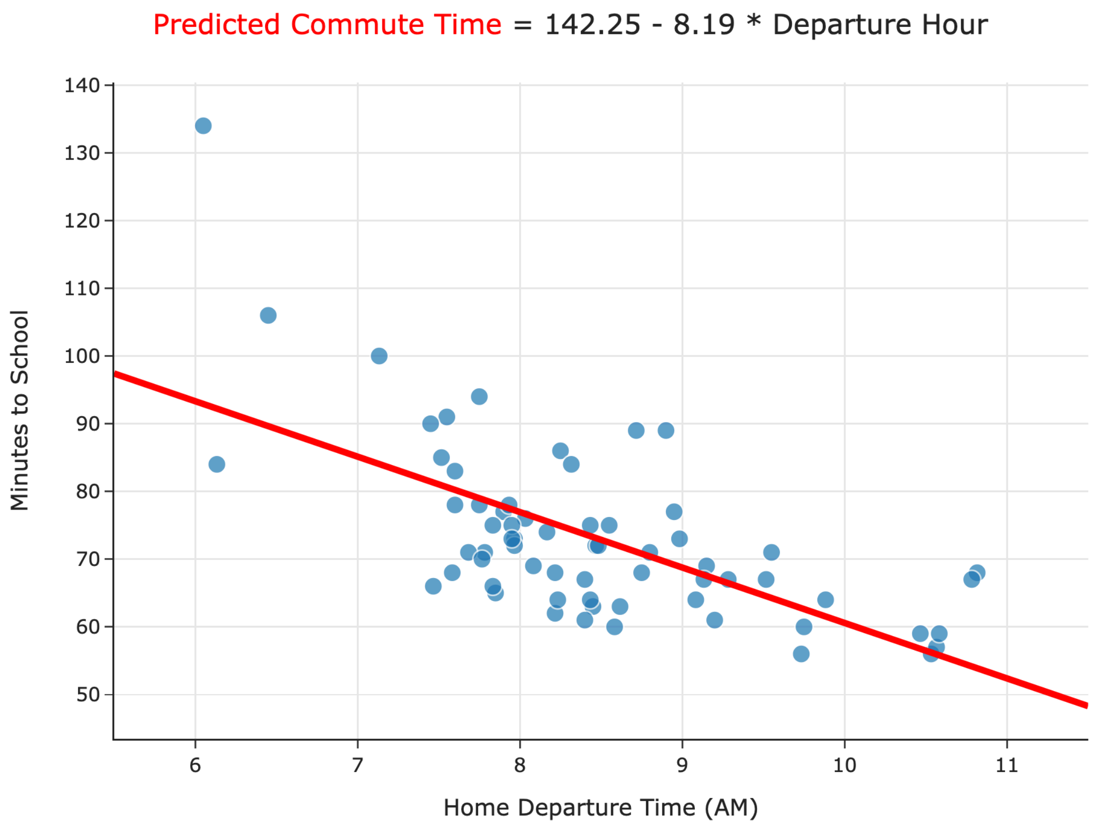
$$w_1^* = r\frac{\sigma_y}{\sigma_x}$$



- Since $\sigma_x \geq 0$ and $\sigma_y \geq 0$, the slope's sign is r's sign.
- As the y values get more spread out, σ_y increases, so the slope gets steeper.
- As the x values get more spread out, σ_x increases, so the slope gets shallower.

Interpreting the intercept

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



- What are the units of the intercept?
- What is the value of $H^*(\bar{x})$?

Question 🤔

Answer at q.dsc40a.com

We fit a regression line to predict commute times given departure hour. Then, we add 75 minutes to all commute times in our dataset. What happens to the resulting regression line?

- A. Slope increases, intercept increases.
- B. Slope decreases, intercept increases.
- C. Slope stays the same, intercept increases.
- D. Slope stays the same, intercept stays the same.

Correlation and mean squared error

- **Claim**: Suppose that w_0^* and w_1^* are the optimal intercept and slope for the regression line. Then,

$$R_{\text{sq}}(w_0^*, w_1^*) = \sigma_y^2(1 - r^2)$$

- That is, the mean squared error of the regression line's predictions and the correlation coefficient, r, always satisfy the relationship above.
- Even if it's true, why do we care?
  - In machine learning, we often use both the mean squared error and r^2 to compare the performances of different models.
  - If we can prove the above statement, we can show that **finding models that minimize mean squared error** is equivalent to **finding models that maximize** r^2.

Proof that $R_{\text{sq}}(w_0^*, w_1^*) = \sigma_y^2(1 - r^2)$

Connections to related models

Question 🤔

Answer at q.dsc40a.com

Suppose we chose the model $H(x) = w_1 x$ and squared loss.

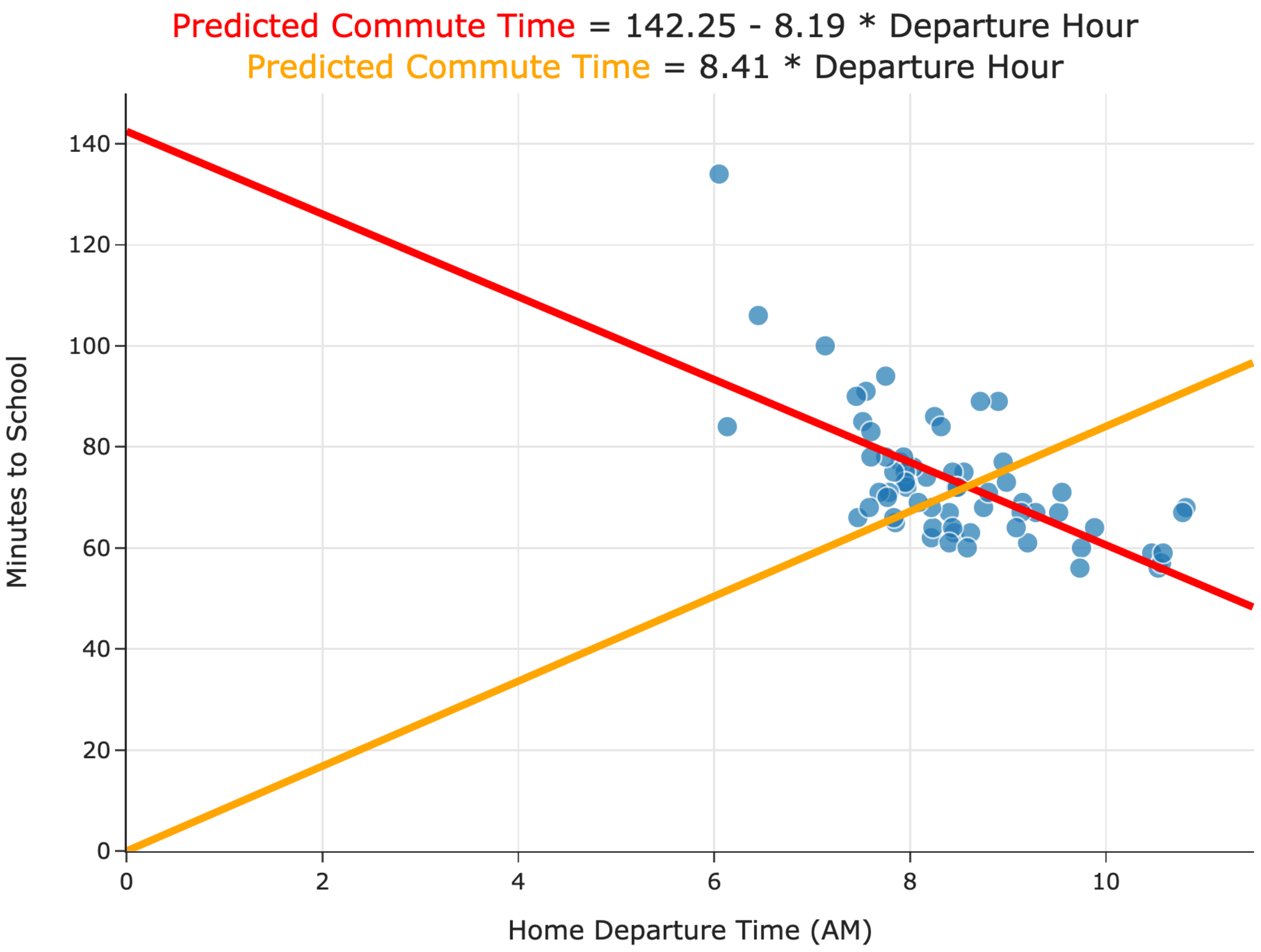
What is the optimal model parameter, w_1^*?

- A. $\dfrac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}$
- B. $\dfrac{\sum_{i=1}^n x_i y_i}{\sum_{i=1}^n x_i^2}$
- C. $\dfrac{\sum_{i=1}^n x_i y_i}{\sum_{i=1}^n x_i^2}$
- D. $\dfrac{\sum_{i=1}^n y_i}{\sum_{i=1}^n x_i}$

Exercise

Suppose we chose the model $H(x) = w_1 x$ and squared loss.

What is the optimal model parameter, w_1^*?


Predicted Commute Time = 142.25 - 8.19 * Departure Hour
Predicted Commute Time = 8.41 * Departure Hour
Minutes to School
0
20
40
60
80
100
120
140
0
2
4
6
8
10
Home Departure Time (AM)

Exercise

Suppose we choose the model $H(x) = w_0$ and squared loss.

What is the optimal model parameter, w_0^*?

Comparing mean squared errors

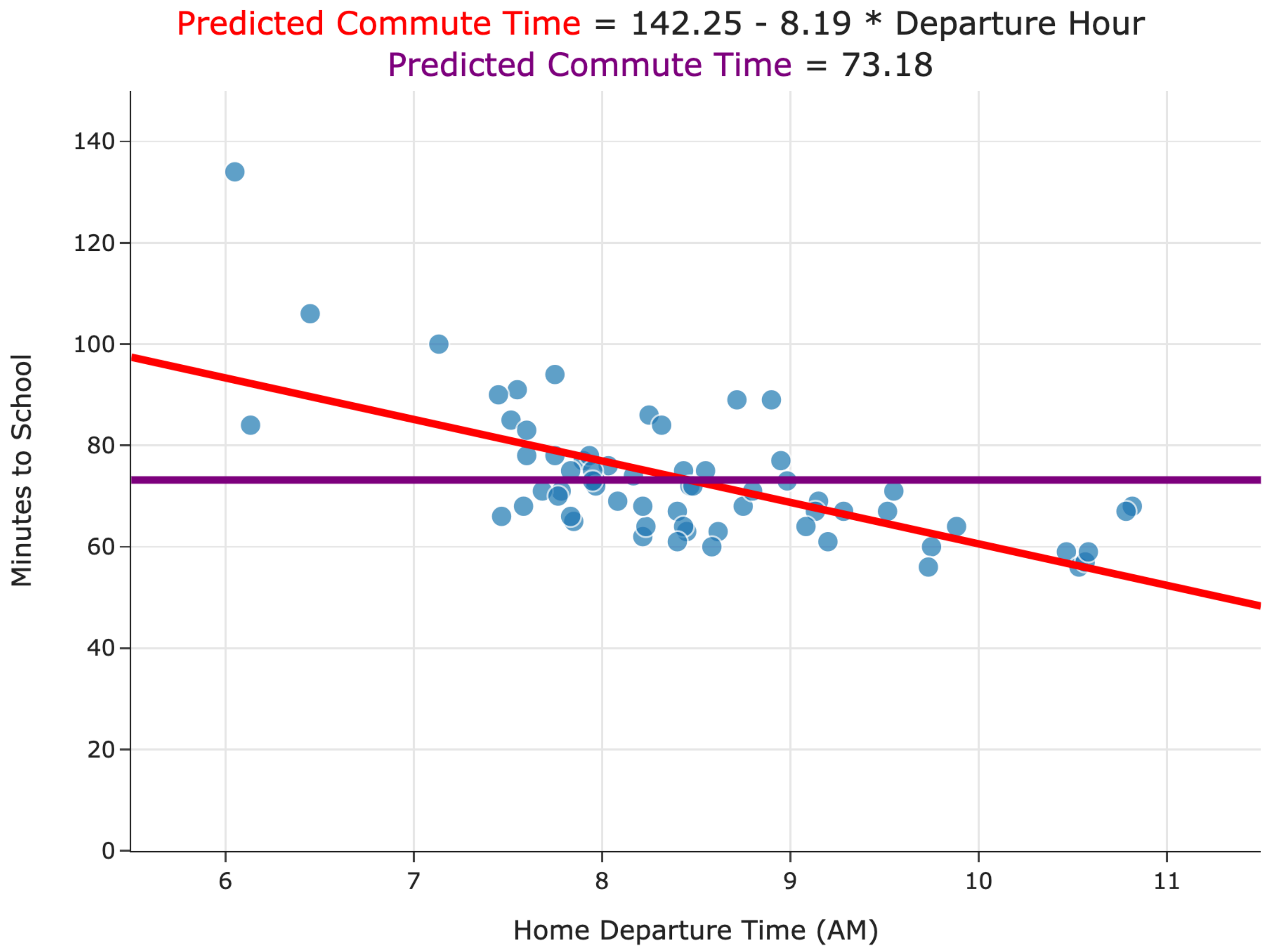
- With both:
  - the constant model, $H(x) = h$, and
  - the simple linear regression model, $H(x) = w_0 + w_1 x$,

  when we chose squared loss, we minimized mean squared error to find optimal parameters:

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

- **Which model minimizes mean squared error more?**

Comparing mean squared errors



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

- The MSE of the best simple linear regression model is ≈ 97.
- The MSE of the best constant model is ≈ 167.
- The simple linear regression model is a more flexible version of the constant model.

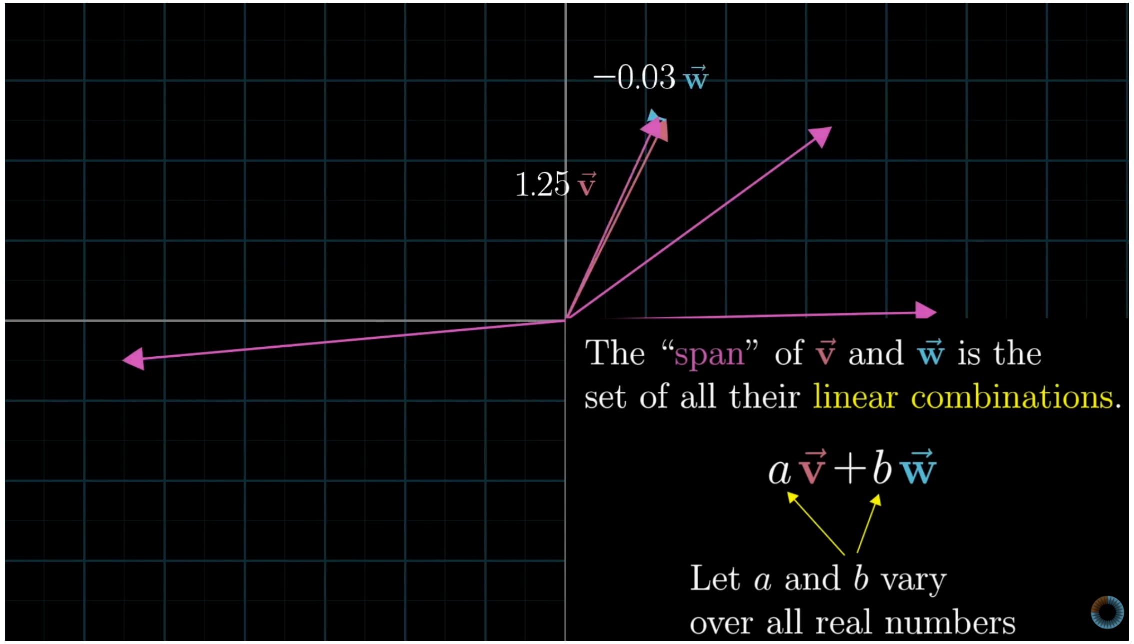
Linear algebra review

Wait... why do we need linear algebra?

- Soon, we'll want to make predictions using more than one feature.
    - Example: Predicting commute times using departure hour and temperature.
- Thinking about linear regression in terms of **matrices and vectors** will allow us to find hypothesis functions that:
    - Use multiple features (input variables).
    - Are non-linear, e.g. $H(x) = w_0 + w_1 x + w_2 x^2$.
- Before we dive in, let's review.

Spans of vectors

- One of the most important ideas you'll need to remember from linear algebra is the concept of the **span** of two or more vectors.
- To jump start our review of linear algebra, let's start by watching 🎥 this video by 3blue1brown.



Next time

- We'll review the necessary linear algebra prerequisites.
- We'll then start to formulate the problem of minimizing mean squared error for the simple linear regression model **using matrices and vectors**.
- We'll send some relevant linear algebra review videos on Ed.