Lectures 6-7

Simple Linear Regression

DSC 40A, Fall 2024

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 🤔

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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.
    - 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

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

- We chose squared loss, since it's the easiest to minimize.

Minimizing mean squared error for the simple linear model

- Our goal is to find the linear hypothesis function $H^*(x)$ that minimizes empirical risk:

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

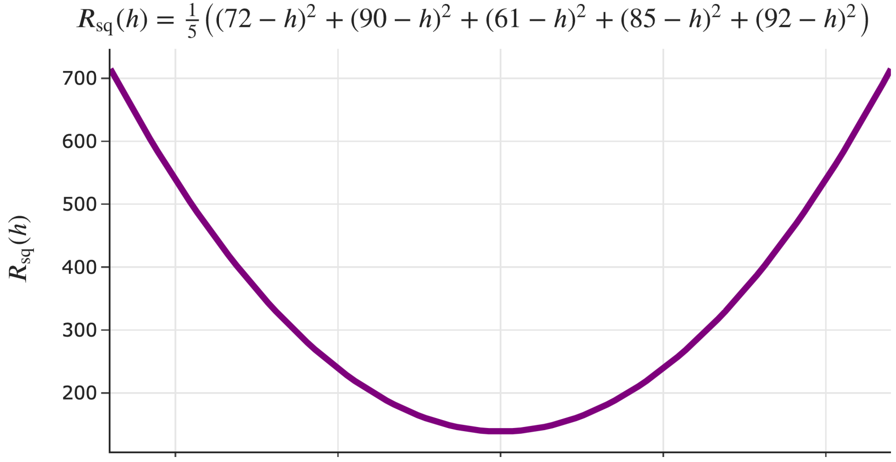
- Plugging in the linear hypothesis $H(x) = w_0 + w_1 x$, we can re-write R_{sq} as a function of w_0 and w_1:

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

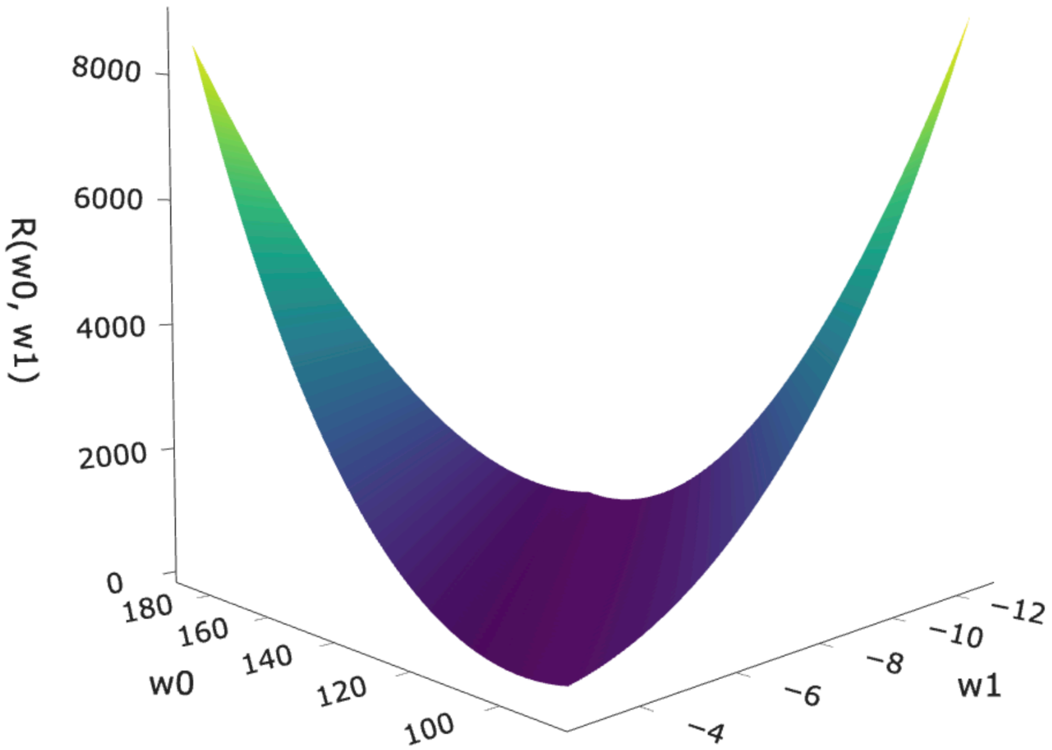
- **How do we find the parameters w_0^* and w_1^* that minimize $R_{\text{sq}}(w_0, w_1)$?**

Loss surface

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?



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).

Example

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

$$f(x, y) = x^2 - 8x + y^2 + 6y - 7$$

Minimizing mean squared error

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

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 🤔

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

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

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

$$\frac{\partial R_{\mathrm{sq}}}{\partial w_0} =$$

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

$$\frac{\partial R_{\text{sq}}}{\partial w_1} =$$

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^*

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

Solving for w_1^*

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

Least squares solutions

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

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

where:

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

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

An equivalent formula for w_1^*

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:

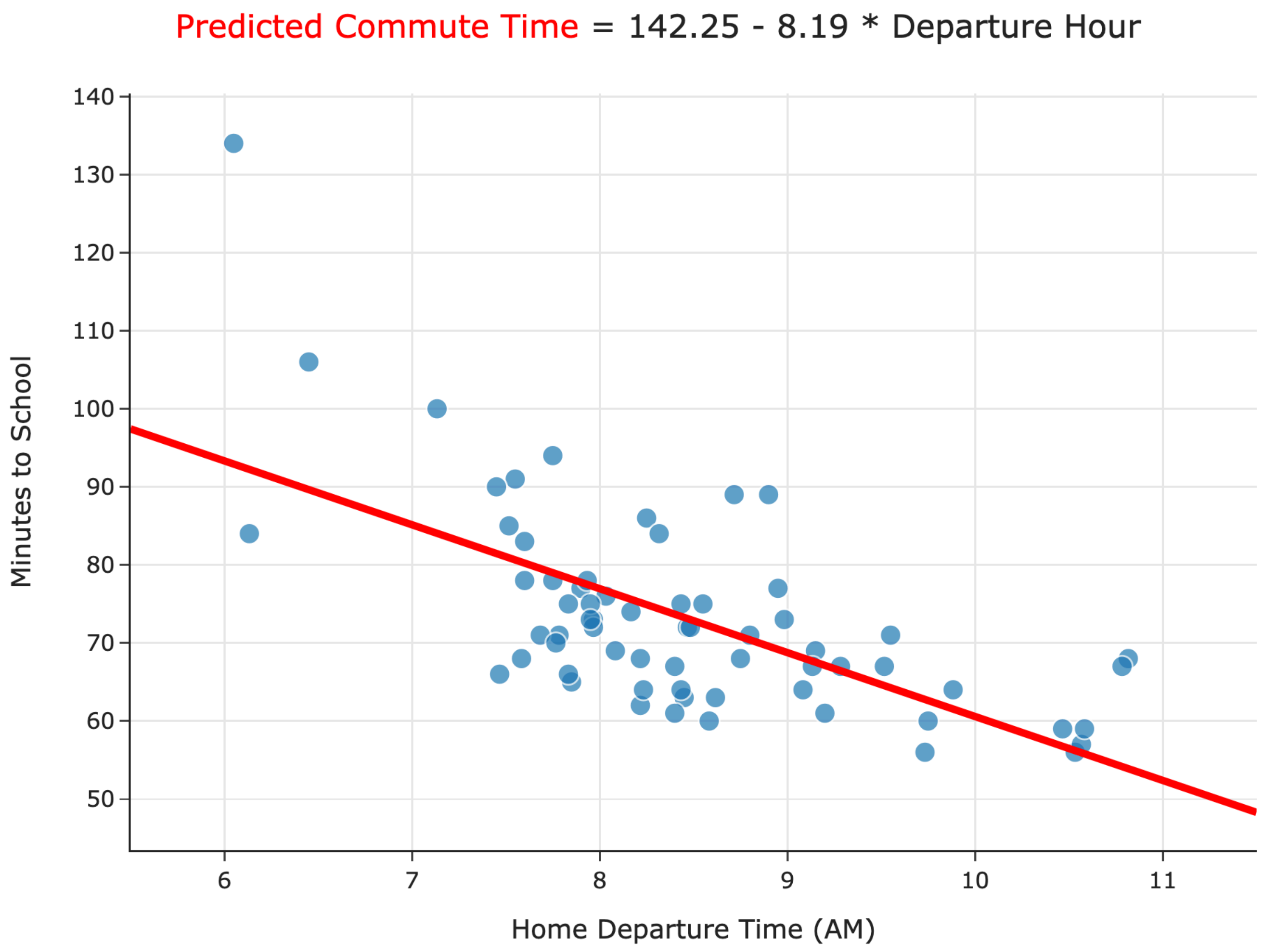
Least squares solutions

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

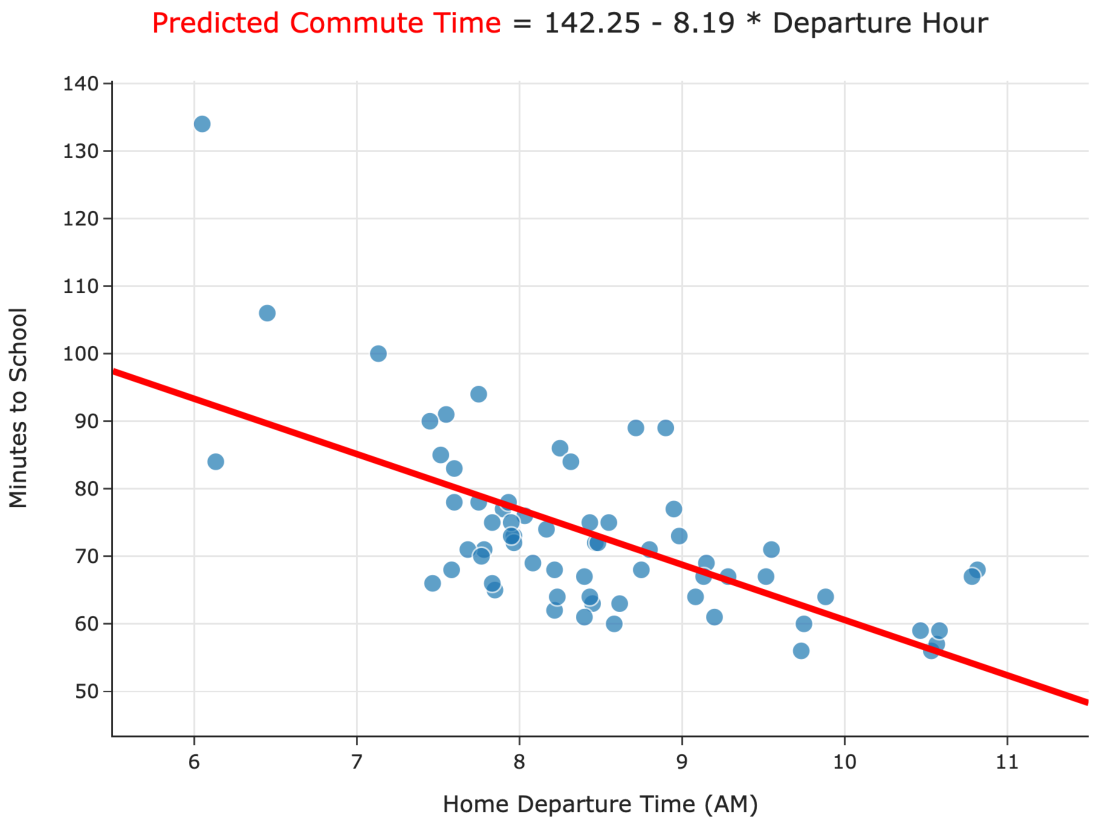
$$\boxed{w_1^* = \frac{\displaystyle\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\displaystyle\sum_{i=1}^{n}(x_i - \bar{x})^2} \qquad\qquad w_0^* = \bar{y} - w_1^*\bar{x}}$$

- 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 $\boxed{H^*(x) = w_0^* + w_1^* x}$.

Let's test these formulas out in code! Follow along here.



Causality



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!

Least squares solutions

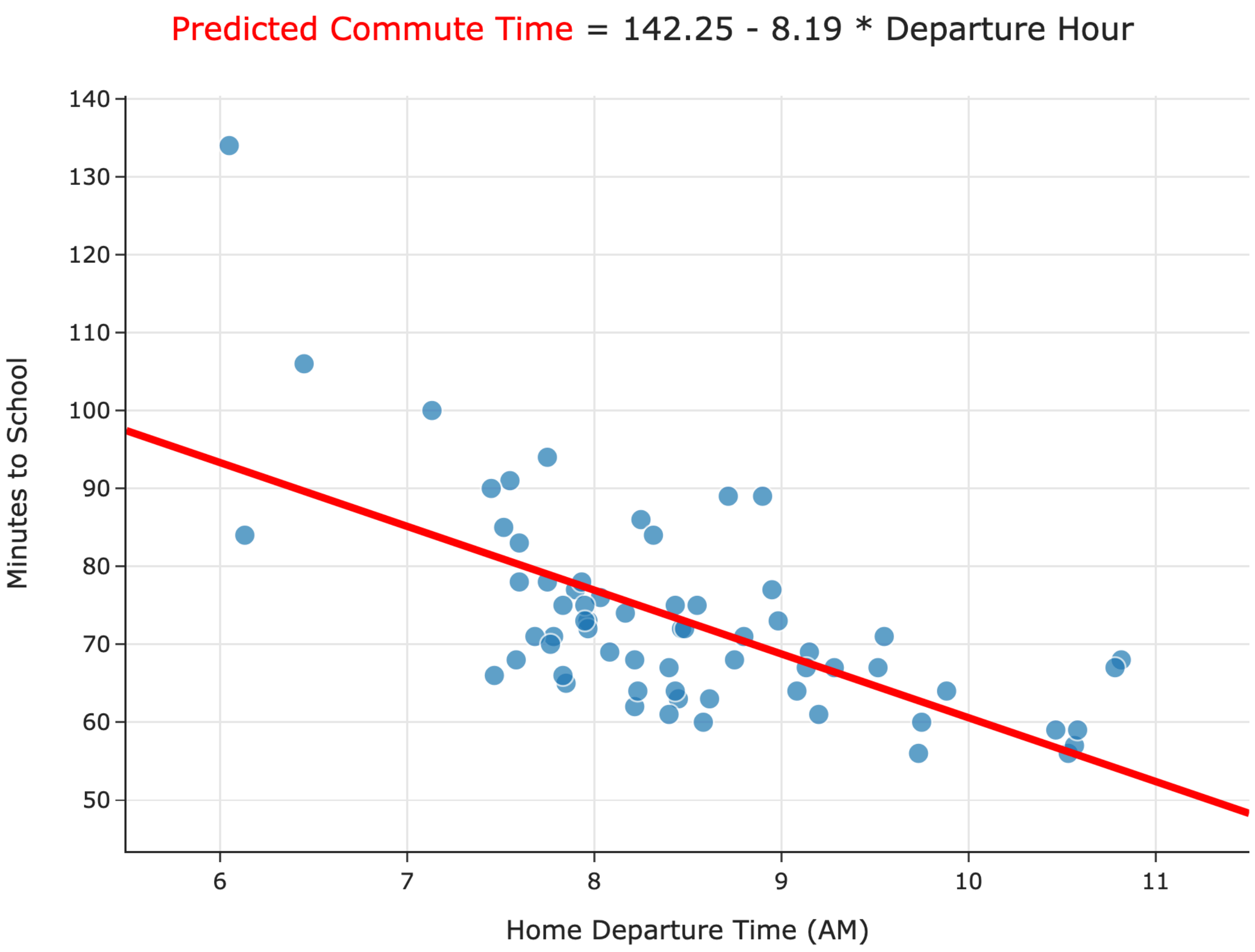
- Our goal was to find the parameters w_0^* and $w_1{}^*$ that minimized:

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

- 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
Minutes to School
140
130
120
110
100
90
80
70
60
50
6
7
8
9
10
11
Home Departure Time (AM)

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

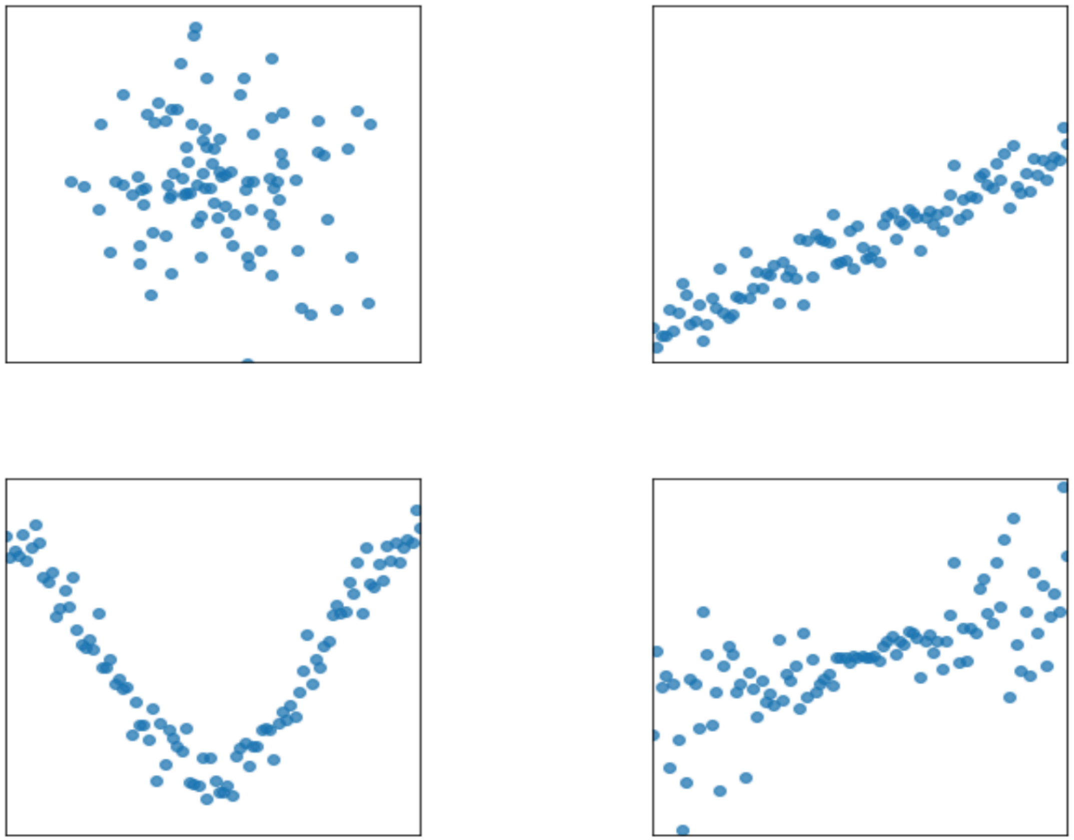
Consider a dataset with just two points, $(2, 5)$ and $(4, 15)$. Suppose we want to fit a linear hypothesis function to this dataset using squared loss. What are the values of w_0^* and w_1^* that minimize empirical risk?

- 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.

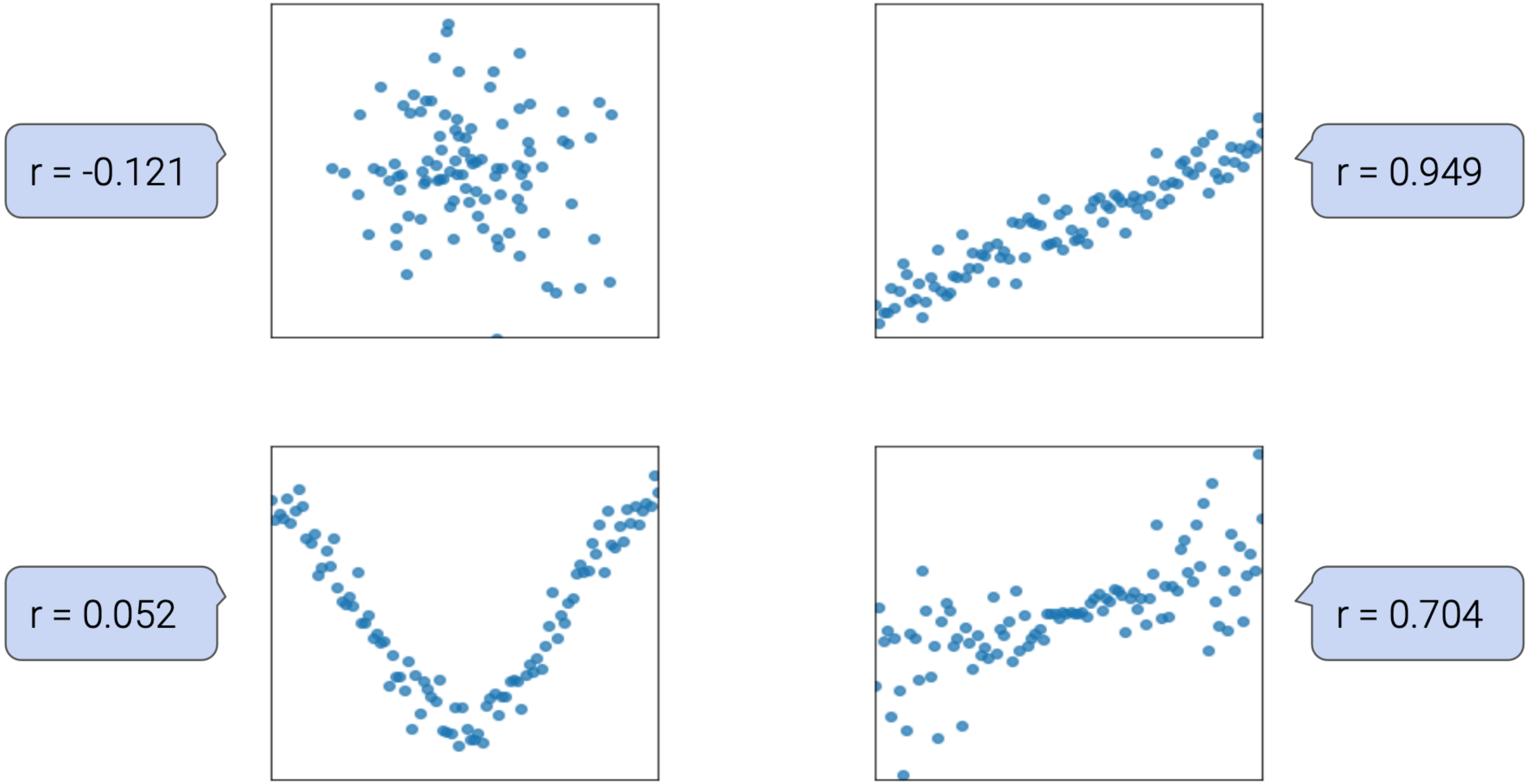


The correlation coefficient

- 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!

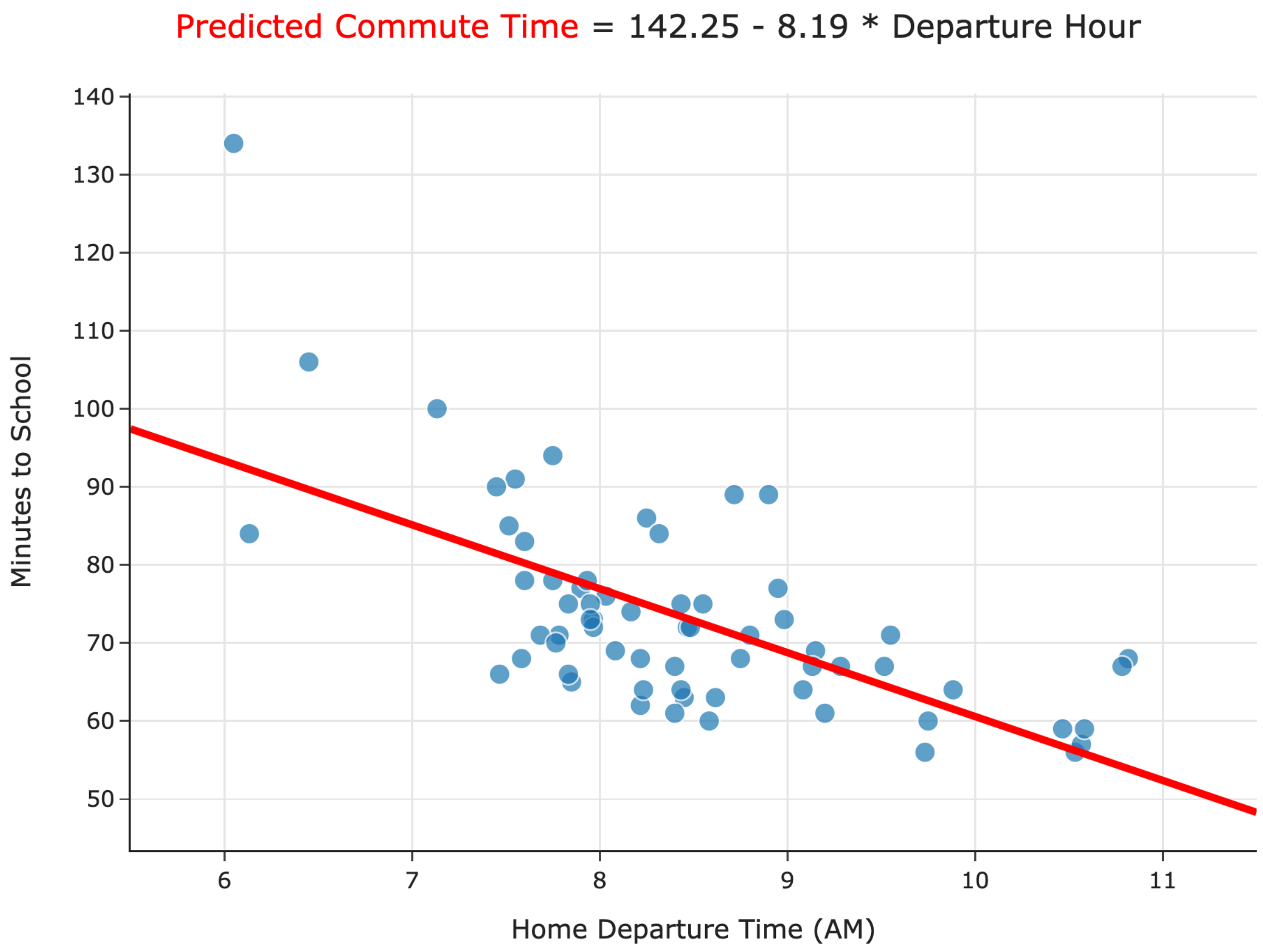
$$w_1^* = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} = r\frac{\sigma_y}{\sigma_x}$$

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

Let's test these new formulas out in code! Follow along here.



Interpreting the formulas

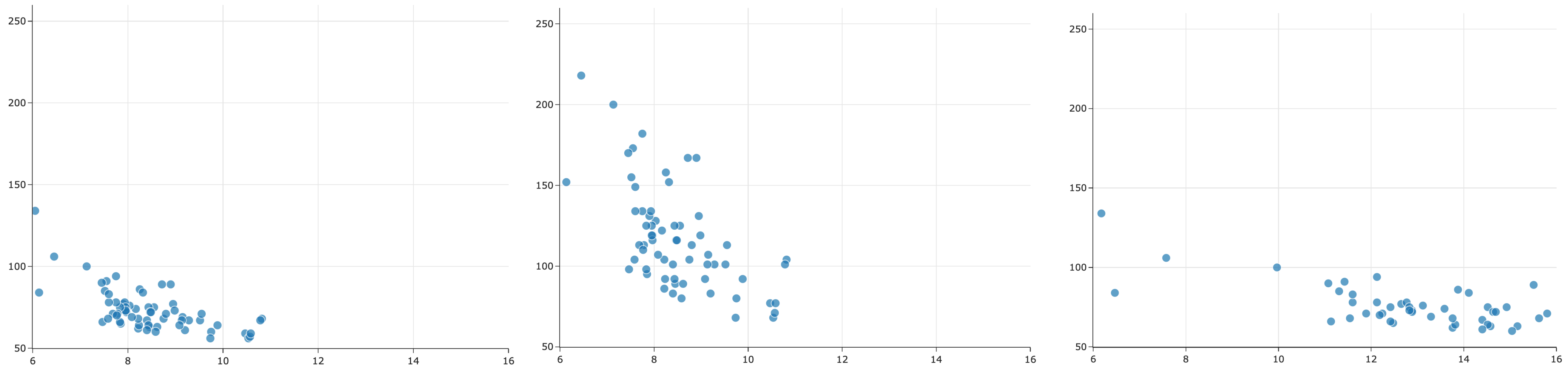
Interpreting the slope

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

- 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

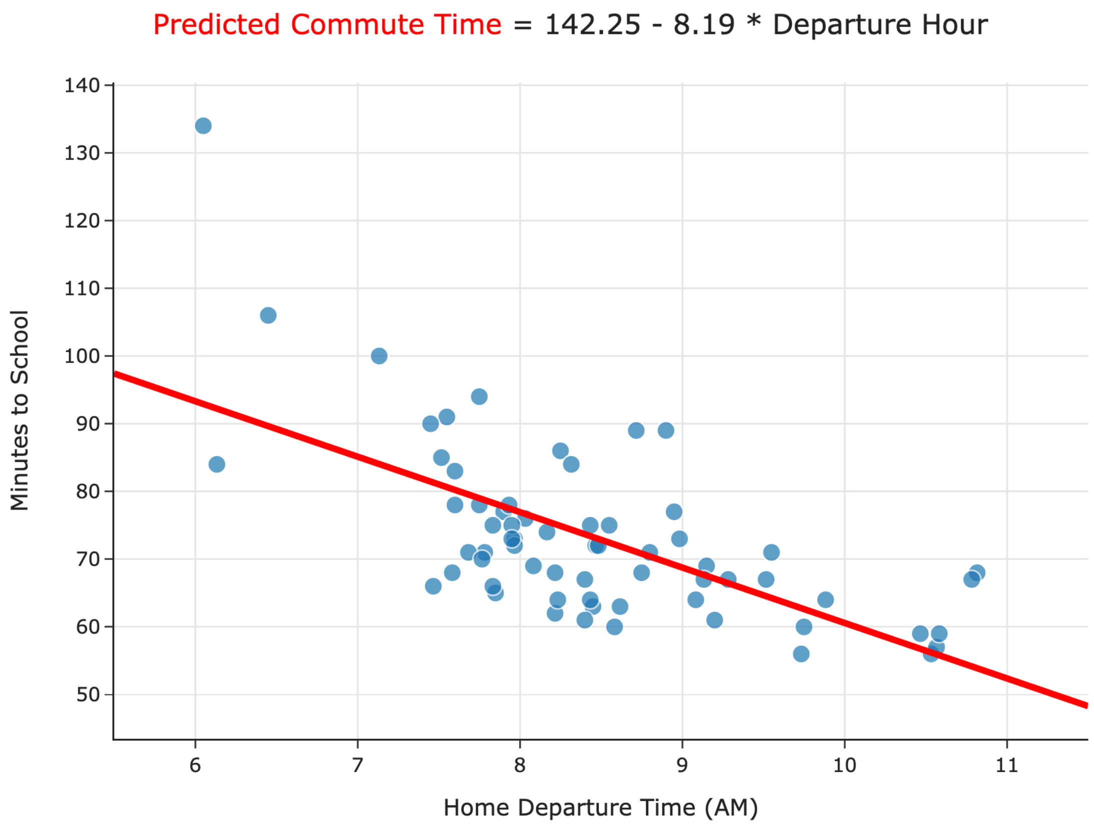
$$w_1^* = r\frac{\sigma_y}{\sigma_x}$$



- 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^*?

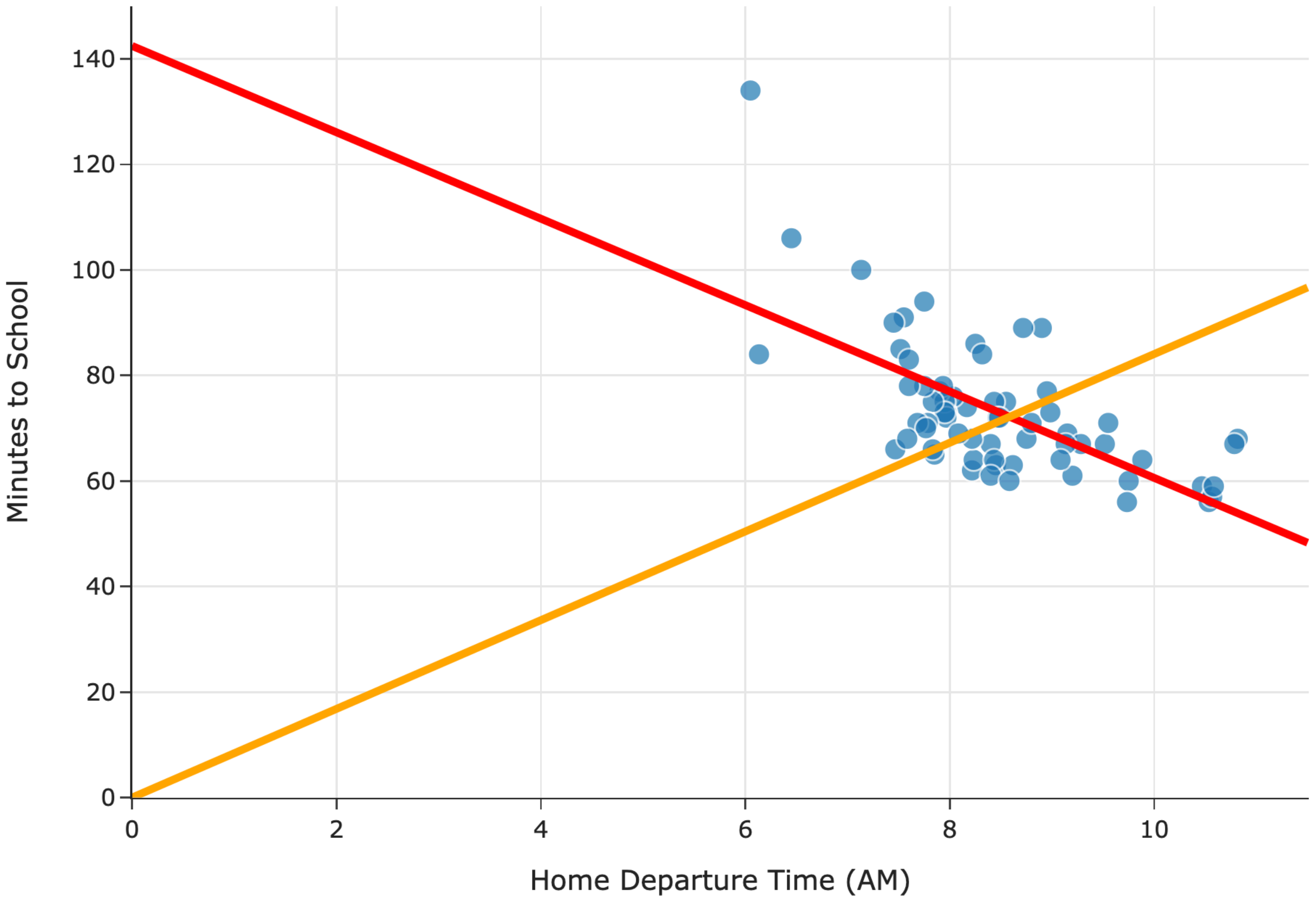
- A. $\dfrac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}$
- B. $\dfrac{\sum_{i=1}^n x_i y_i}{\sum_{i=1}^n x_i^2}$
- C. $\dfrac{\sum_{i=1}^n x_i y_i}{\sum_{i=1}^n x_i^2}$
- D. $\dfrac{\sum_{i=1}^n y_i}{\sum_{i=1}^n x_i}$

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



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

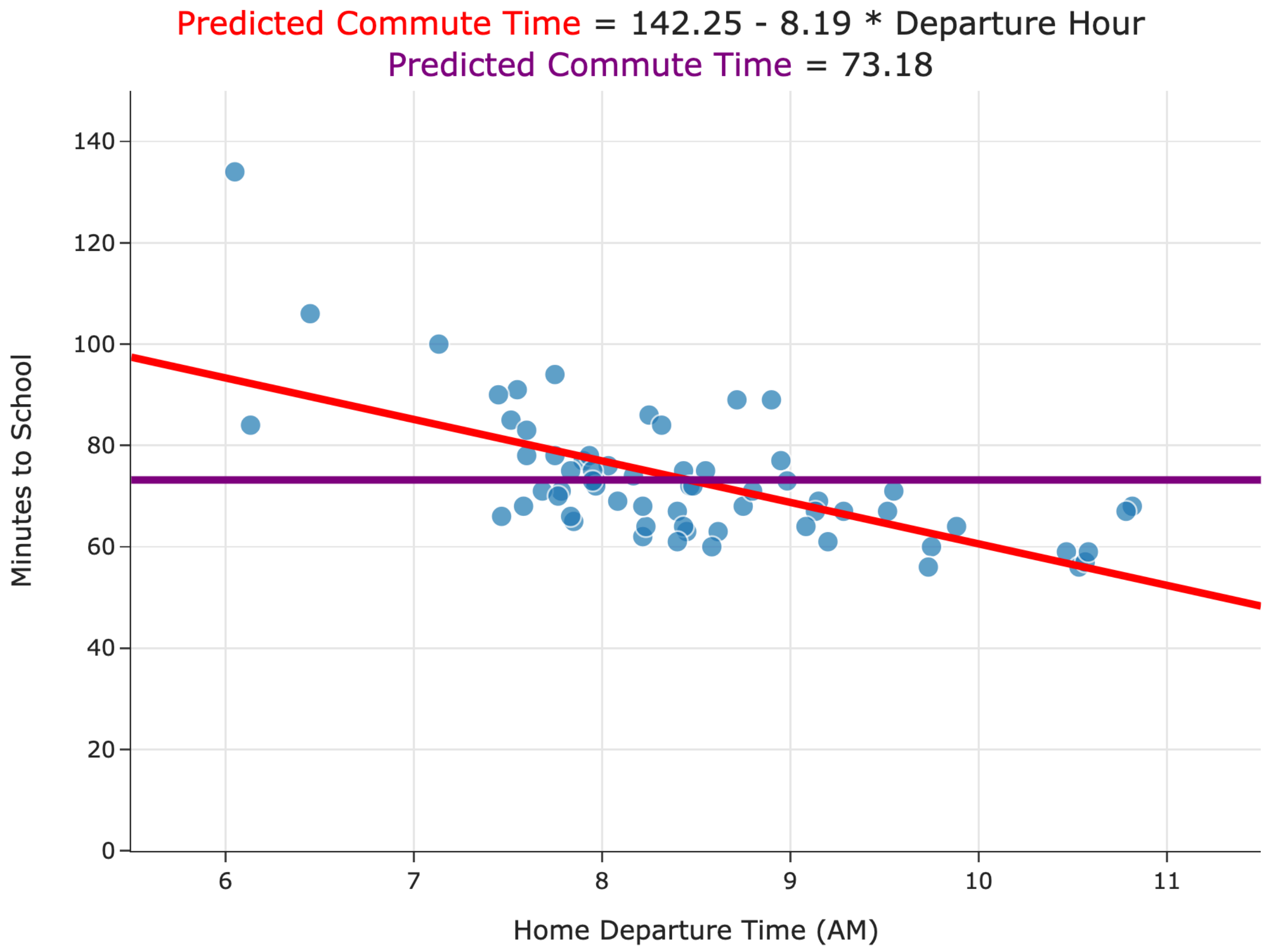
- With both:
  - the constant model, $H(x) = h$, and
  - the simple linear regression model, $H(x) = w_0 + w_1 x$,

  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.

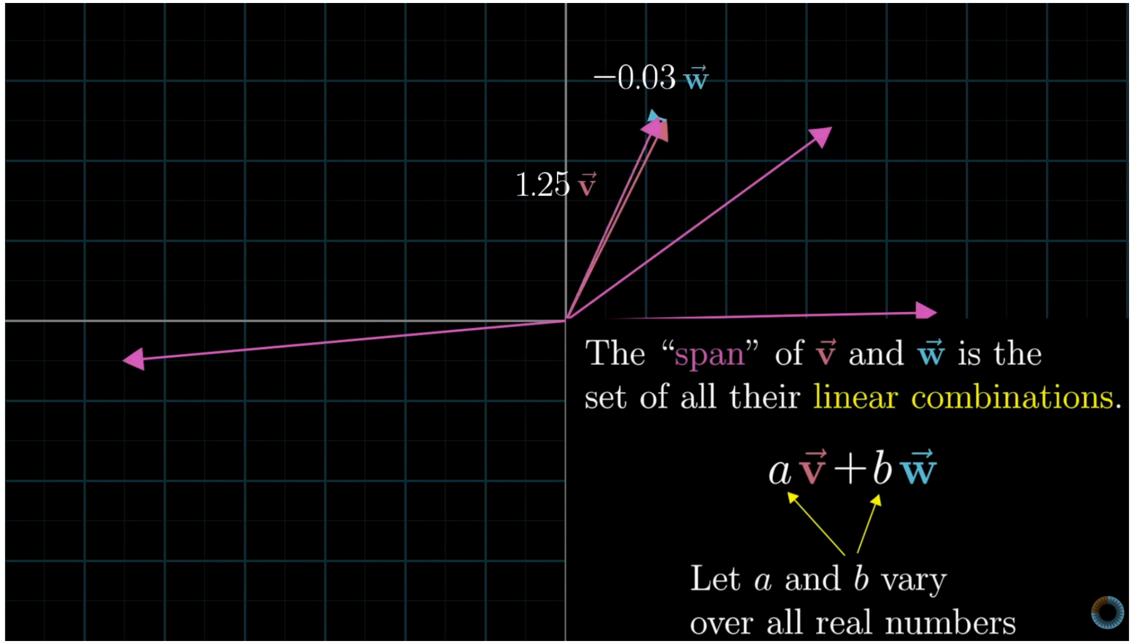
Linear algebra review

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.