Lecture 5

Simple Linear Regression

DSC 40A, Fall 2024

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

- 0-1 loss
- Predictin rules using features
- Simple linear regression.
- Minimizing mean squared error for the simple linear model.

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.

Another example: 0-1 loss

Consider, for example, the **0-1 loss**:

$$L_{0,1}(y_i, h) = \begin{cases} 0 & y_i = h \\ 1 & y_i \neq h \end{cases}$$

The corresponding empirical risk is:

$$R_{0,1}(h) = \frac{1}{n} \sum_{i=1}^{n} L_{0,1}(y_i, h)$$

Question 🤔

Answer at q.dsc40a.com

$$R_{0,1}(h) = \frac{1}{n} \sum_{i=1}^{n} \begin{cases} 0 & y_i = h \\ 1 & y_i \neq h \end{cases}$$

Suppose $y_1, y_2, \ldots, y_n$ are all unique. What is $R_{0,1}(y_1)$?

- A. 0.
- B. $\frac{1}{n}$.
- C. $\frac{n-1}{n}$.
- D. 1.

Proportion of all points that aren't y_1

Minimizing empirical risk for 0-1 loss

$$R_{0,1}(h) = \frac{1}{n}\sum_{i=1}^{n}\begin{cases}0 & y_i = h\\ 1 & y_i \neq h\end{cases}$$

= proportion of all points not equal to h

1, 2, 3, 1, 4
mode is not unique

Minimized for $h = y_i$ where y_i is the most frequent value in the dataset.

$h^* = \text{mode}(y_1, y_2, \ldots, y_n)$

most common value

Summary: Choosing a loss function

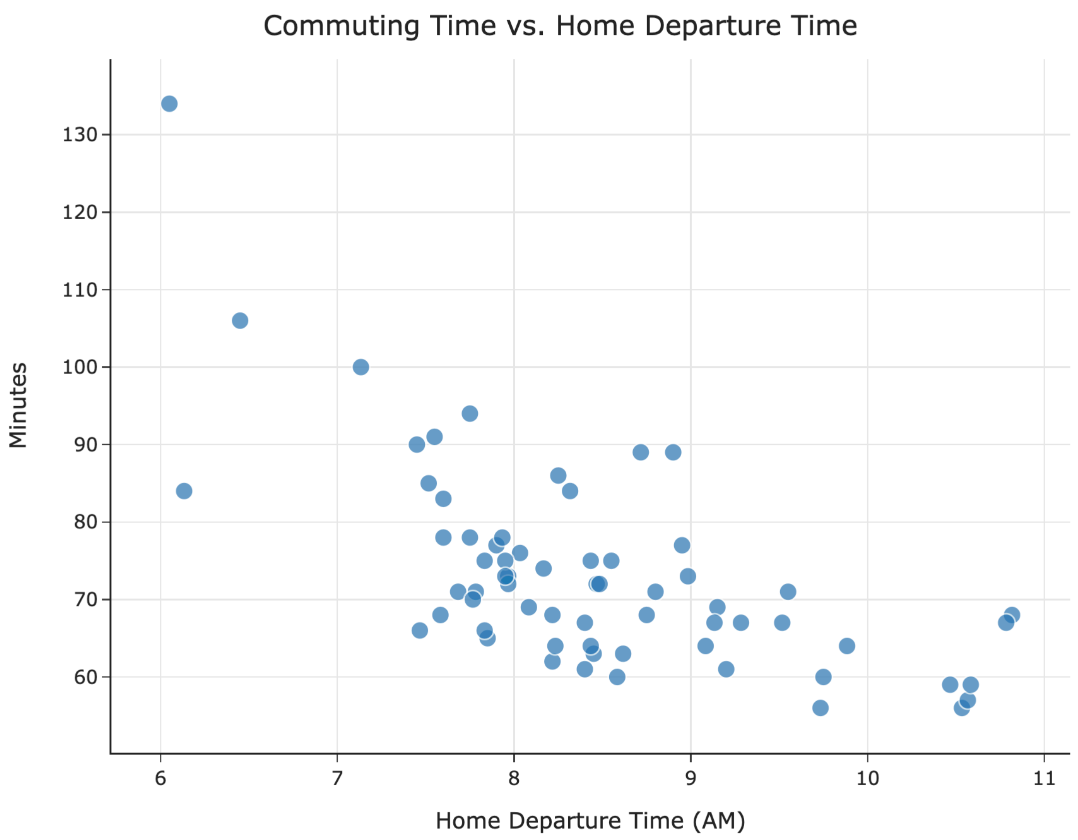
Key idea: Different loss functions lead to different best predictions, h^*!

Loss	Minimizer	Always Unique?	Robust to Outliers?	Differentiable?
L_{sq}	mean	yes ✅	no ❌	yes ✅
L_{abs}	median	no ❌	yes ✅	no ❌
L_{∞}	midrange	yes ✅	no ❌	no ❌
$L_{0,1}$	mode	no ❌	yes ✅	no ❌

The optimal predictions, h^*, are all **summary statistics** that measure the **center** of the dataset in different ways.

Predictions with features

Towards simple linear regression



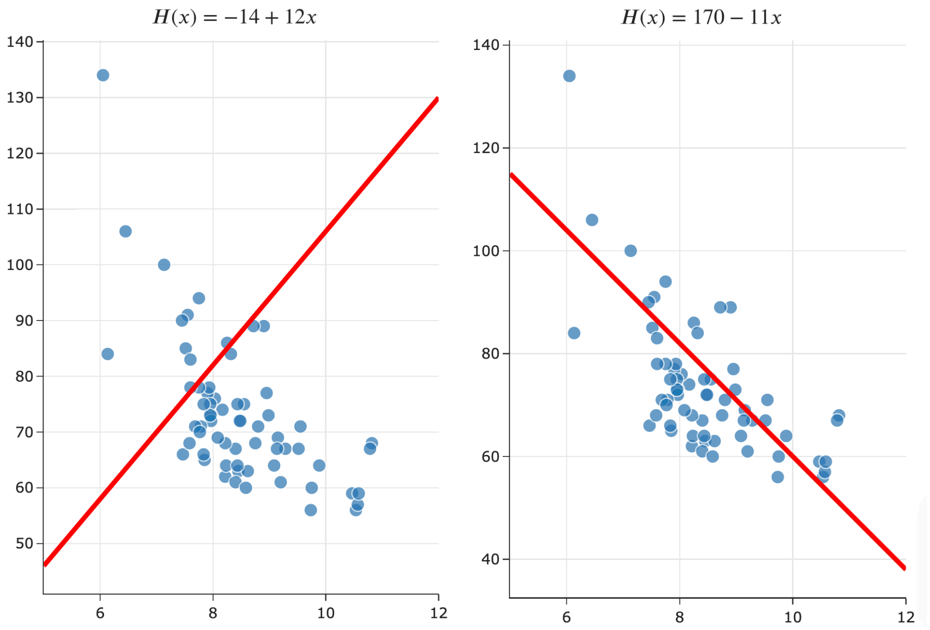
- In Lecture 1, we introduced the idea of a hypothesis function, $H(x)$.
- We've focused on finding the best **constant model**, $H(x) = h$.
- Now that we understand the modeling recipe, we can apply it to find the best **simple linear regression model**, $H(x) = w_0 + w_1 x$.
- This will allow us to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

Recap: Hypothesis functions and parameters

A hypothesis function, H, takes in an x as input and returns a predicted y.

Parameters define the relationship between the input and output of a hypothesis function.

The simple linear regression model, $H(x) = w_0 + w_1 x$, has two parameters: w_0 and w_1.



The modeling recipe

1. Choose a model.

$H(x) = h$
constant

$H(x) =$ function of x
(not constant)

$= w_0 + w_1 x$

2. Choose a loss function.

$\ell(H(x_i), y_i)$

abs

sqr

...

3. Minimize average loss to find optimal model parameters.

find w_0, w_1

Features

A **feature** is an attribute of the data – a piece of information.

- **Numerical**: maximum allowed speed, time of departure
- **Categorical**: day of week
- **Boolean**: was there a car accident on the road?

Think of features as columns in a DataFrame (i.e. table).

x_i y_i

Departure time	Day of week	Accident on route	Commute time
7:05	Monday	yes	101
8:03	Tuesday	no	87
10:20	Wednesday	yes	79
8:30	Thursday	no	76

Modeling

- We believe that commute time is a function of departure time.
- I.e., there is a function H so that:

  $$\underbrace{\text{commute time}}_{y_i} \approx H(\underbrace{\text{departure time}}_{x_i})$$

- H is called a **hypothesis function** or **prediction rule**.
- Our goal: find a good prediction rule H.

Possible Hypothesis Functions

- H_1(departure time) = 90 - 10 ·(departure time-7)
- H_2(departure time) = 90 - (departure time-8)^2
- H_3(departure time) = 20 + 6·departure time

These are all valid prediction rules.

Some are better than others.

Comparing predictions

- How do we know which hyppthesis is best: $H_1,\ H_2,\ H_3$?
- We gather data from n days of commute. Let x_i be departure time, y_i be commute time:

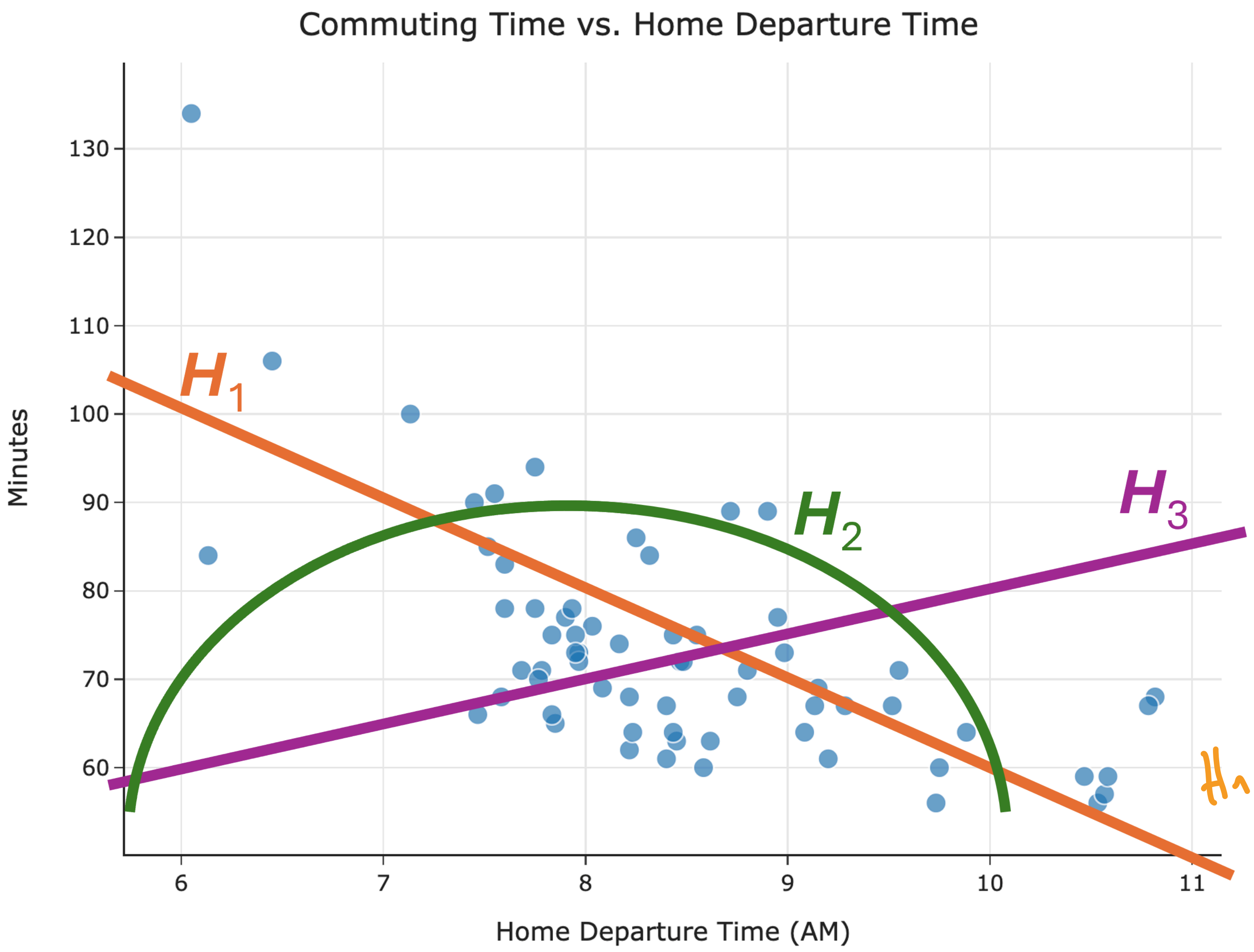
(departure time$_1$, commute time$_1$) $\quad (x_1, y_1)$

(departure time$_2$, commute time$_2$) $\quad (x_2, y_2)$

$\dots \quad \rightarrow$

(departure time$_n$, commute time$_n$) $\quad (x_n, y_n)$

- See which rule works better on data.



H_1 seems the best
but how do we know?

Quantifying the performance of a model

- Reminder: one loss function, which measures how far $H(x_i)$ is from y_i, is **absolute loss.** $|H(x_i)-y_i|$
- The mean absolute error of $H(x)$ is

predicted commute

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

departure time

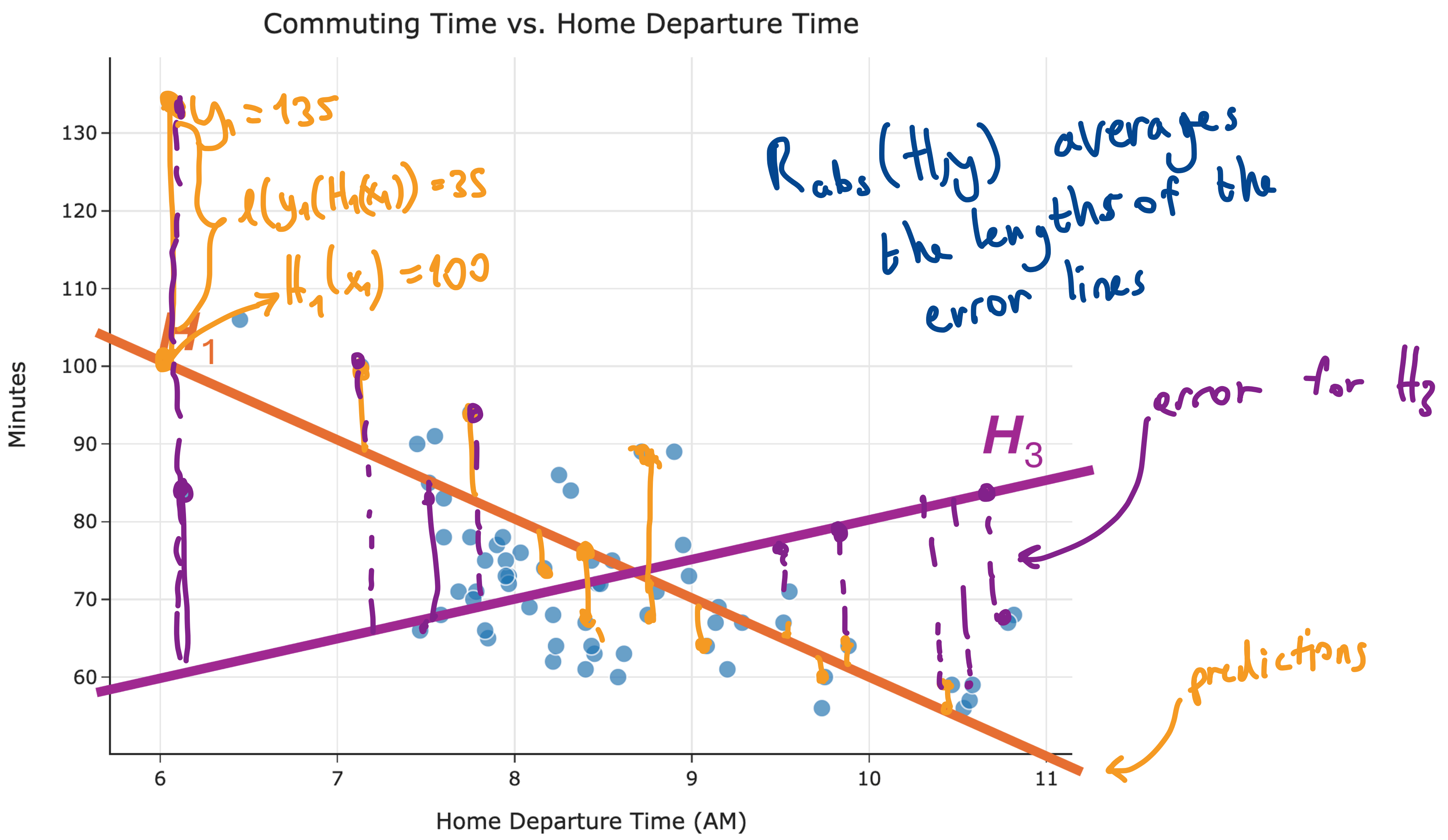
actual commute time

- We want the **best** prediction, $H^*(x)$.
- The smaller $R_{\text{abs}}(h)$ is, the better the hypothesis.

Mean absolute error

$R_{abs}(H_1, y) < R_{abs}(H_3, y)$

is worse than H_1



Finding the best hypothesis $H(x)$

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

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

Finding the best hypothesis $H(x)$

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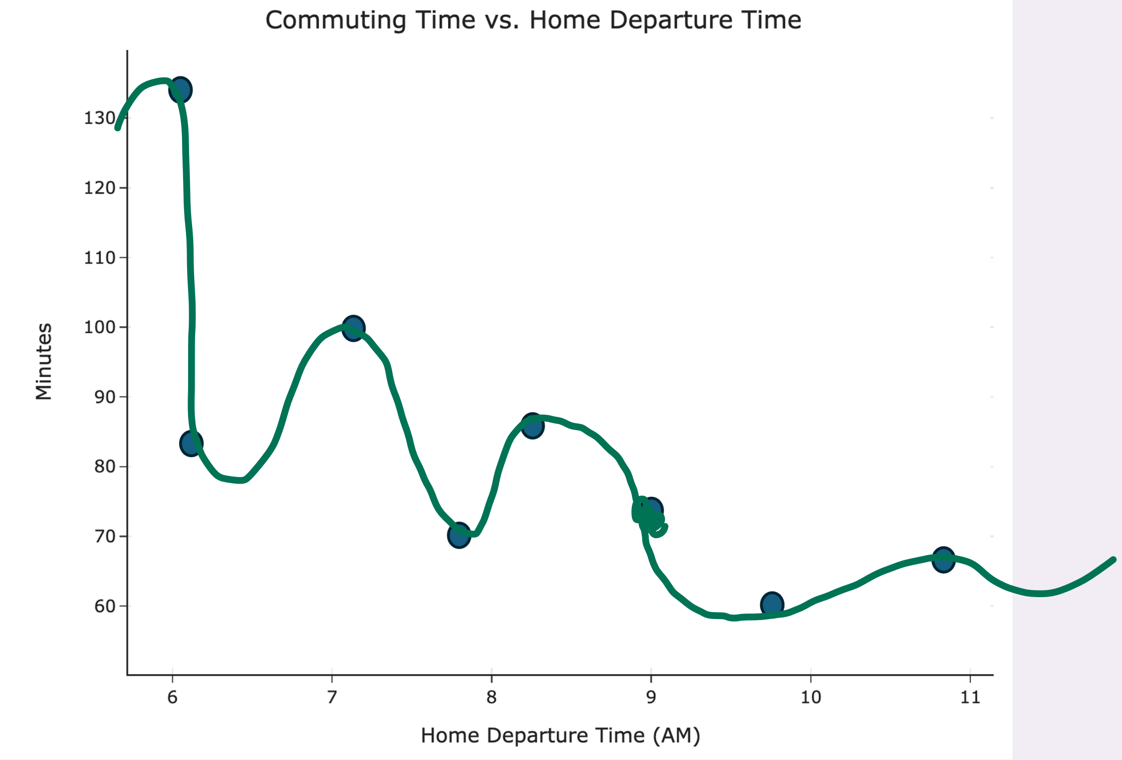
- **There are two problems with this.**

Question 🤔 Answer at q.dsc40a.com

Given the data below, is there a prediction rule H which has zero mean absolute error?

- A. yes
- B. no



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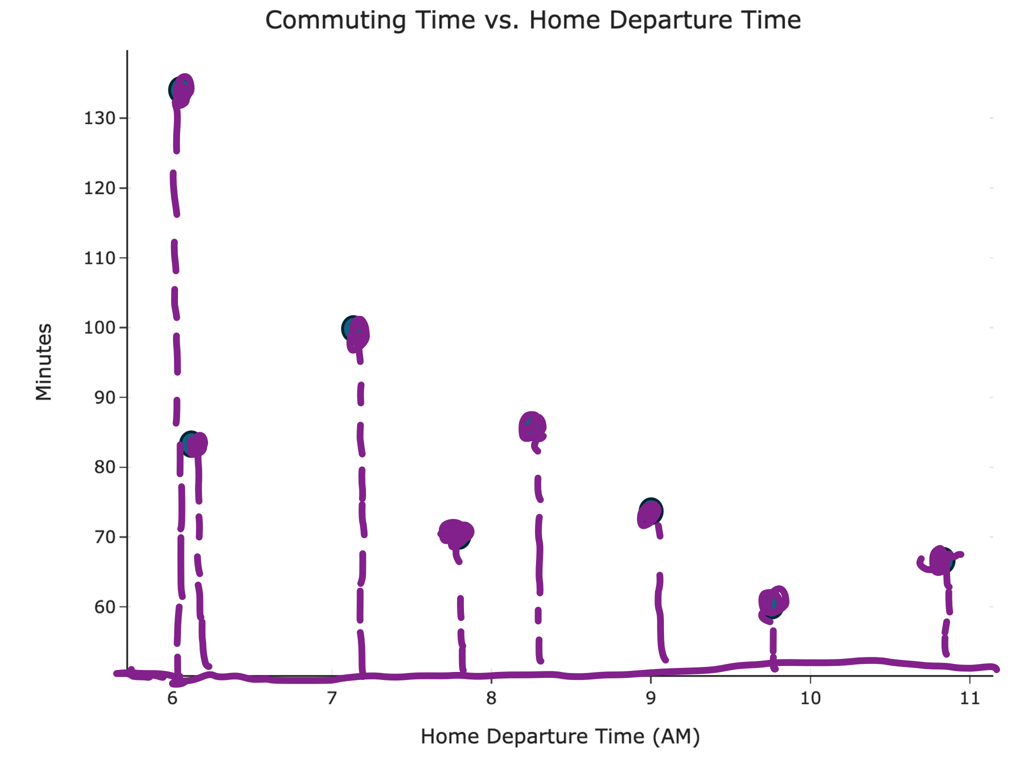

Problem

- 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: $H(x) = w_0 + w_1 x$. ← this week
  - Quadratic: $H(x) = w_0 + w_1 x_1 + w_2 x^2$. ← In a few weeks
  - Exponential: $H(x) = w_0 e^{w_1 x}$.
  - Constant: $H(x) = w_0$. ← last week

non linear

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

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

Finding the best linear model

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-
    - There is still a problem with this.

Problem #2

It is hard to minimize the mean absolute error:

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

- Not differentiable! we can't use calculus
- What can we do?

Minimizing mean squared error for the simple linear model

- We'll choose squared loss, since it's the easiest to minimize.
- Our goal, then, is to find the linear hypothesis function $H^*(x)$ that minimizes empirical risk:

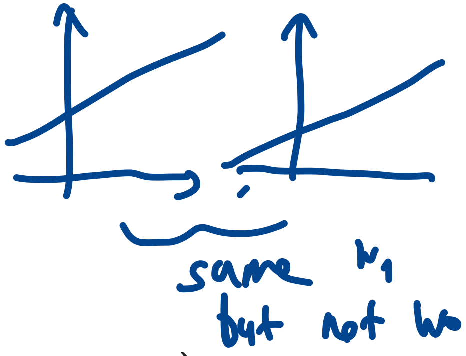
MSE

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

$\hookrightarrow H(x_i) = w_0 + w_1 x_i$

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

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

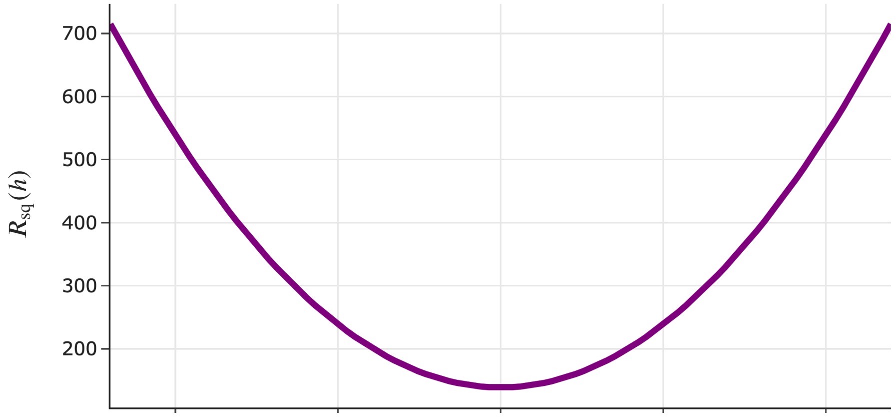


- **How do we find the parameters w_0^* and w_1^* that minimize $R_{\text{sq}}(w_0, w_1)$?**

Loss surface

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

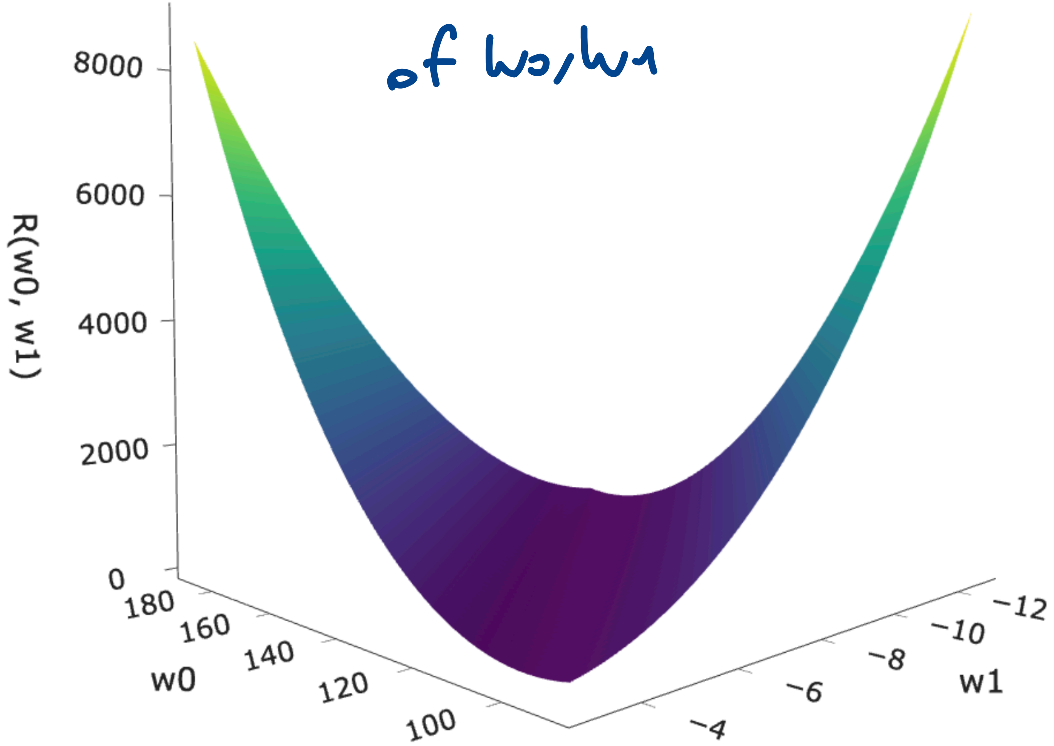
$$R_{\text{sq}}(h) = \frac{1}{5}\left((72-h)^2 + (90-h)^2 + (61-h)^2 + (85-h)^2 + (92-h)^2\right)$$



single parameter h

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

2d surface as func of w_0, w_1



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:

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

- 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. $\frac{\partial R_{sq}}{\partial w_0}, \frac{\partial R_{sq}}{\partial w_1}$
  - Set all partial derivatives to 0.
  - Solve the resulting system of equations. w_0^*, w_1^*
  - Ensure that you've found a minimum, rather than a maximum or saddle point (using the second derivative test for multivariate functions).

Next time

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

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

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

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

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

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

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

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

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

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:

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

Proof:

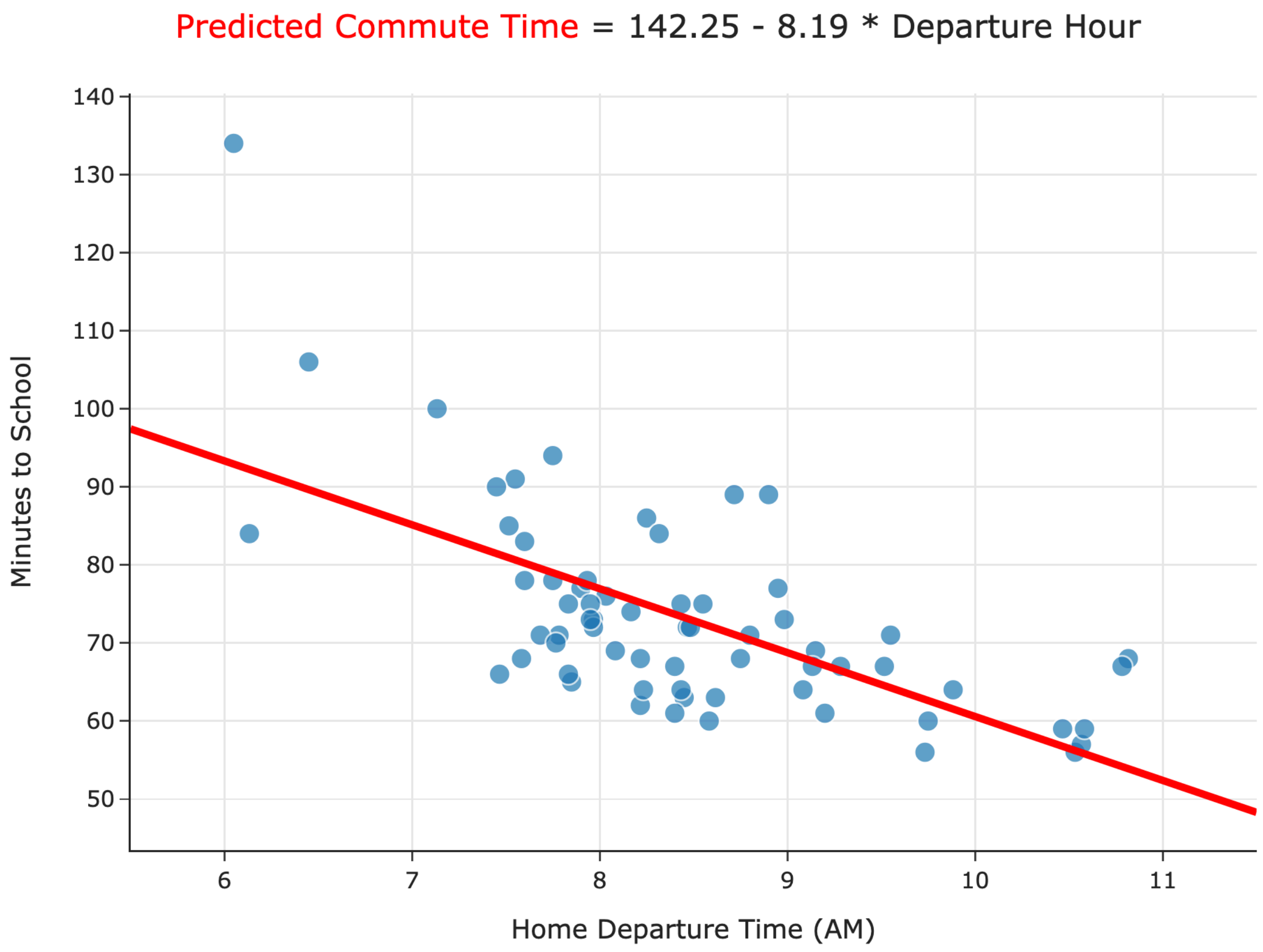
Least squares solutions

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

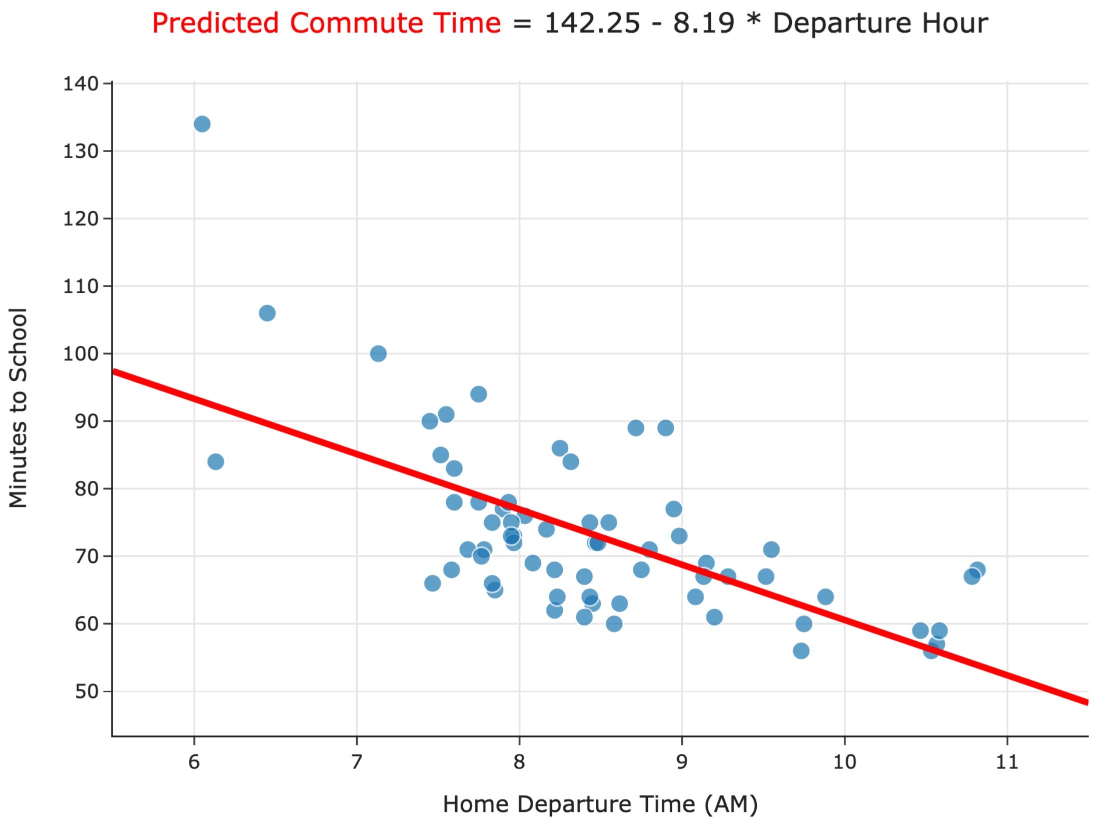
$$\boxed{w_1^* = \frac{\displaystyle\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\displaystyle\sum_{i=1}^{n}(x_i - \bar{x})^2} \qquad\qquad w_0^* = \bar{y} - w_1^*\bar{x}}$$

- 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!