Lecture 14

Introduction to Modeling

EECS 398-003: Practical Data Science, Fall 2024

practicaldsc.org • github.com/practicaldsc/fa24

Announcements 📣

- Midterm Exam scores are available on Gradescope. Solutions are available at **study.practicaldsc.org/fa24-midterm**, and regrade requests are due tomorrow night.
    - If you want to meet with Suraj (or anyone else) to walk through your Midterm Exam and talk about study strategies moving forward, email us!
- Homework 6 is due **tonight**. See **#180 on Ed** for a clarification.

  If you get rate limited in Question 4, you can change your model from `llama-8b-8192` to another model listed here.

Agenda

- Course overview.
- Machine learning and models.
- The constant model.
- Minimizing mean squared error using calculus.
- Another loss function.

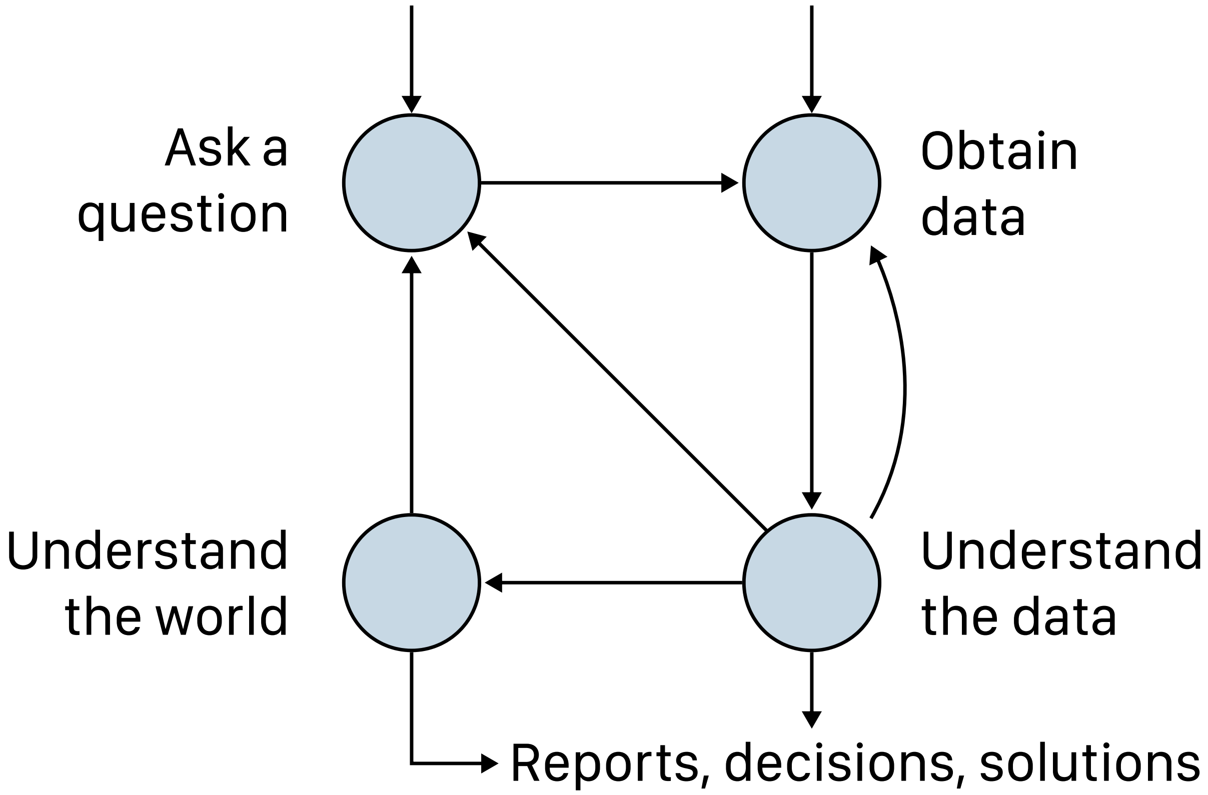
The next few lectures (and next homework!) will be primarily **math-based**.

- For these lectures, we'll post blank slides as a PDF before class, and annotated slides after class.
- If there are any code demos, we'll post those before class, too.
- **Come to discussion tomorrow for math review and practice!**

Course overview

EECS 398, Part 1

- In Lecture 1, we said the first half of this course would be about **data wrangling**.
  - Week 1: Python and Jupyter Notebooks.
  - Weeks 2-3: `numpy`, `pandas`, and Exploratory Data Analysis.
  - Weeks 4-5: Missing Data; Web Scraping and APIs.
  - Weeks 5-6: Text Processing.
  - Week 7: **Midterm Exam**.
- You're proficient in working with messy data using industry-standard tools.
- But, you've also developed an understanding of **how** processes work under the hood.
  - How many rows result from an inner join of these two DataFrames?
  - How do we quantify how important a term is to a document?
  - How do we describe a particular class of strings using mathematical notation?



The **data science lifecycle**.

EECS 398, Part 2

- The second half of this course is about **applied machine learning**.
  - Weeks 8-10: Linear Regression through Linear Algebra.
  - Weeks 11-12: Generalization, Regularization, and Cross-Validation.
  - Weeks 12-14: Gradient Descent and Logistic Regression.
  - Weeks 15-16: Unsupervised Learning, **Final Exam**.
- More generally, we'll learn how to practically build models that can make **predictions about future data** given some data from the past.
- To do so, we'll also learn the **mathematical underpinnings** of these models, so that you understand how they actually work.

  The tools may change in the future, but the ideas won't!

so we'll do math,
but with a purpose!

Machine learning and models

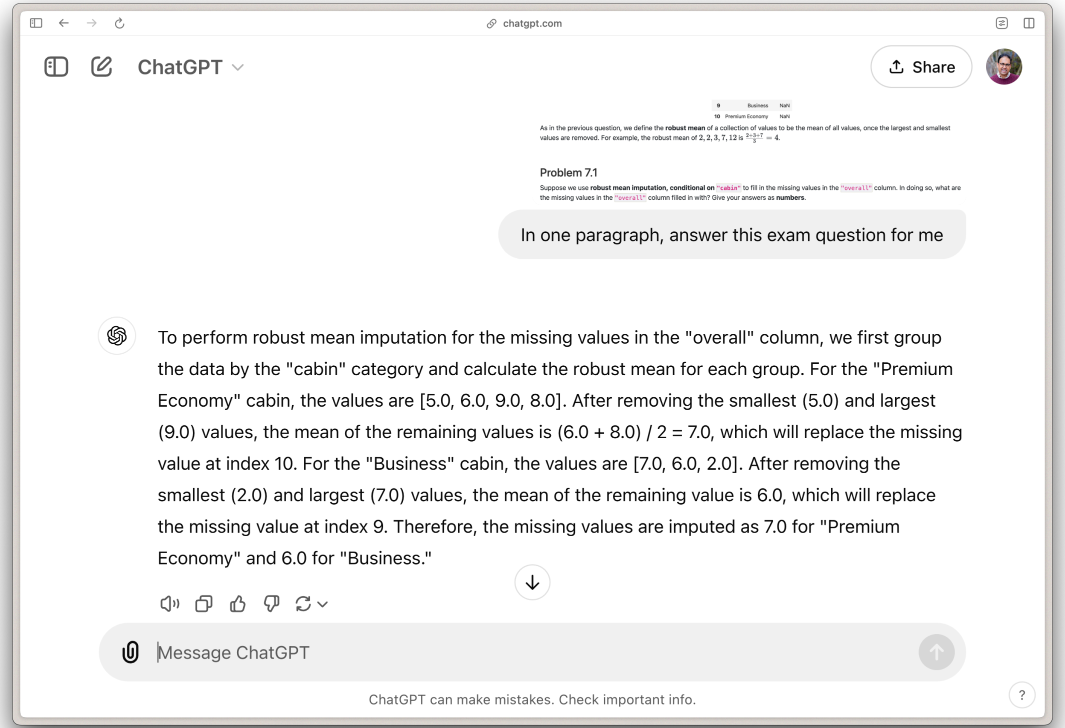
Machine learning is about $\underbrace{\textbf{automatically}}_{\text{without "hard-coding"}}$ learning patterns from data.

Example: Handwritten digit classification

Humans are good at understanding handwriting,

but how do we get computers to understand handwriting?

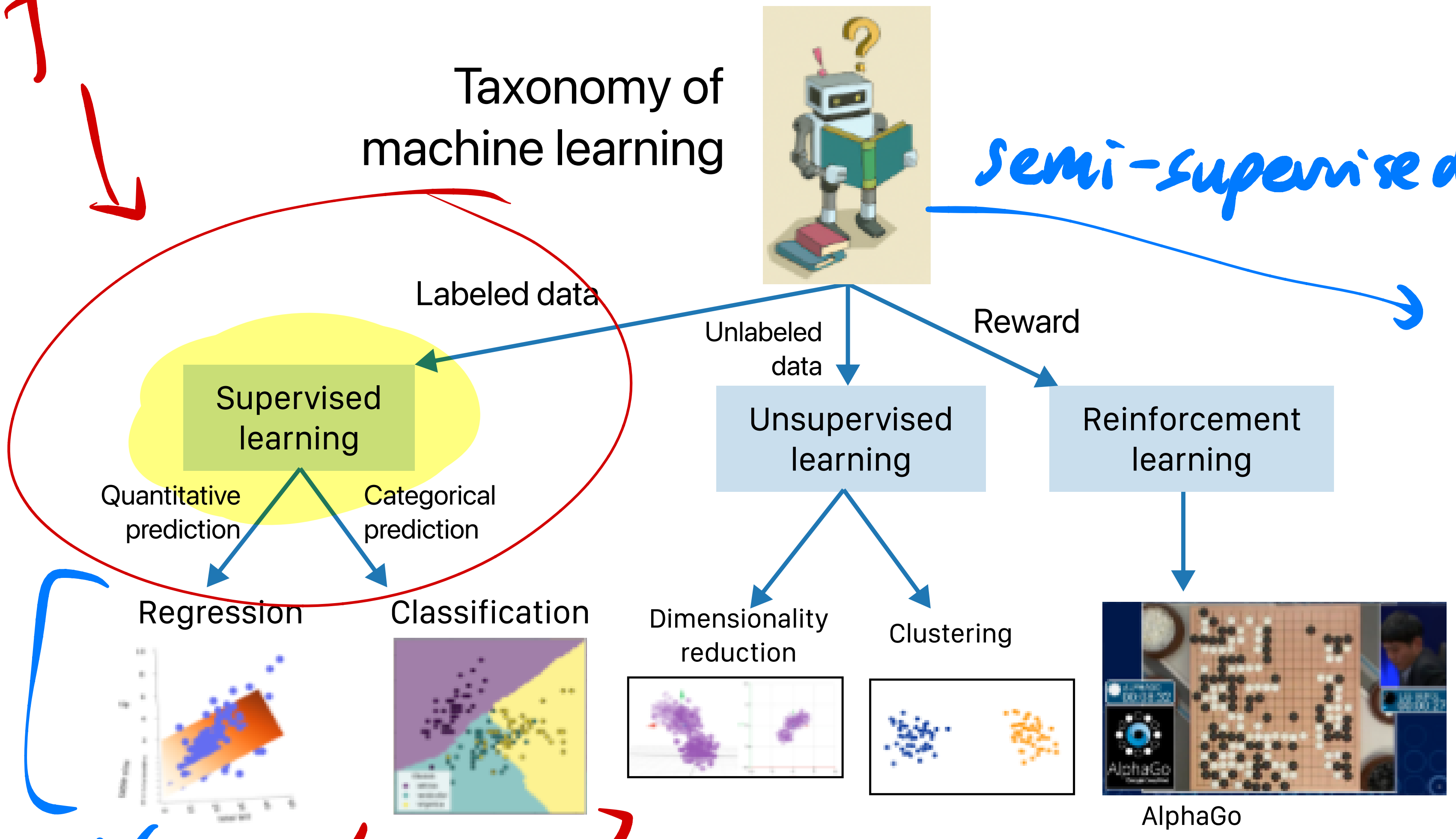
Example: ChatGPT



How did ChatGPT know how to answer Question 7 from the Fall 2024 Midterm?

our focus

Taxonomy of machine learning



semi-supervised → ChatGPT

e.g. predict salary, final exam %, child's height, etc.

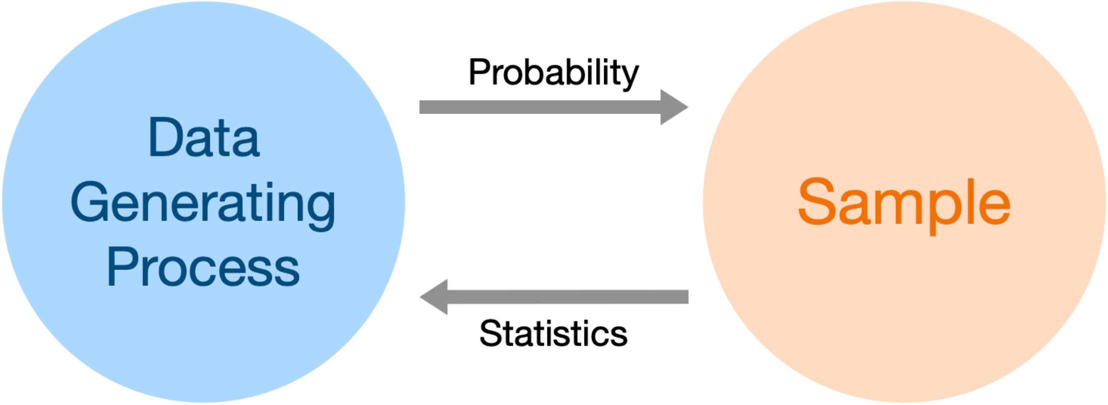
e.g. predict "dog", "cat", "hamster" from an image

EECS 203
binomial dist.

A biased coin flips heads with probability 0.8.

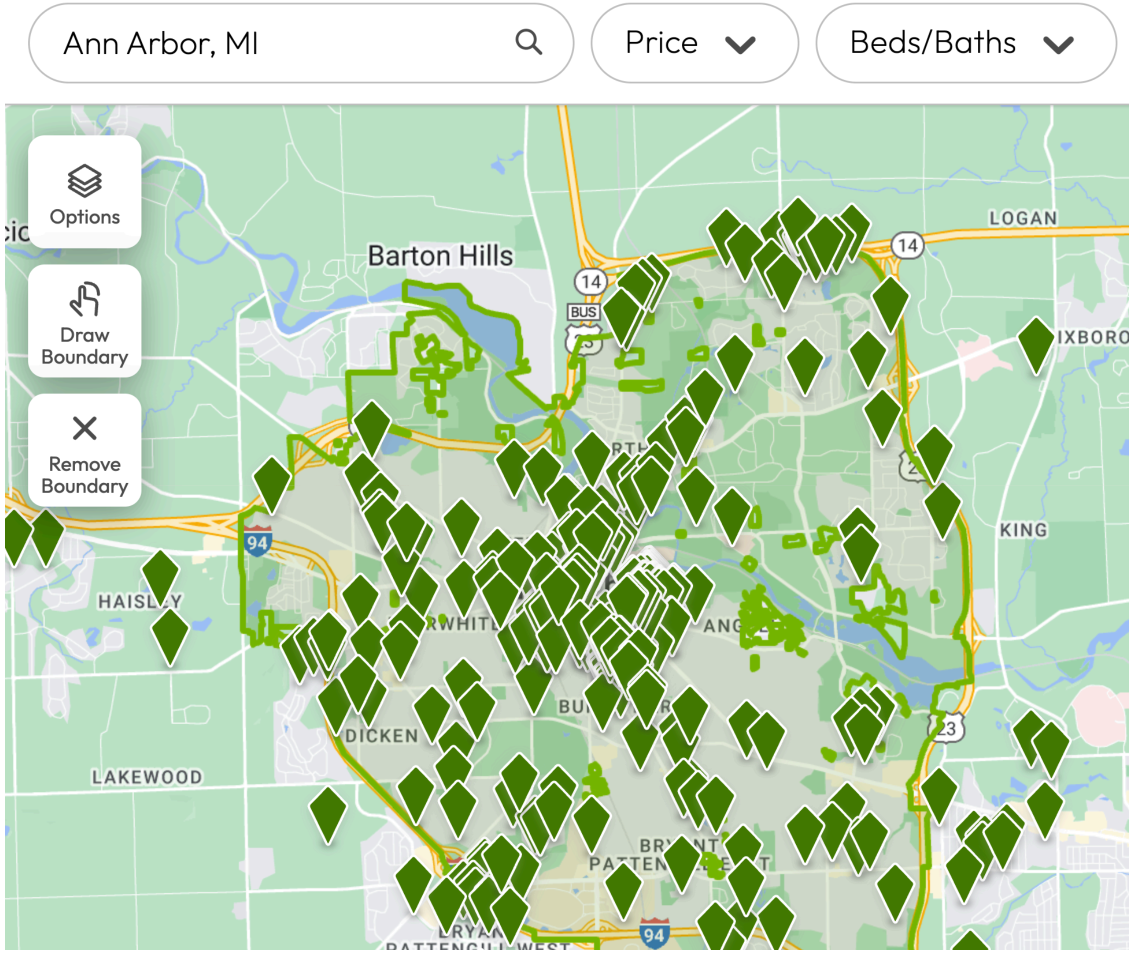
I flip it 100 times. What's the probability of seeing 65 heads?

statistics / ML



I found a coin on the ground, and don't know if it's fair.

I flip it 100 times and see 65 heads. What is the most likely bias of the coin?



You might be starting to look for off-campus apartments for next year, none of which are in your price range.

time of day

	date	day	departure_hour	minutes
0	5/22/2023	Mon	8.450000	63.0
1	9/18/2023	Mon	7.950000	75.0
2	10/17/2023	Tue	10.466667	59.0
3	11/28/2023	Tue	8.900000	89.0
4	2/15/2024	Thu	8.083333	69.0

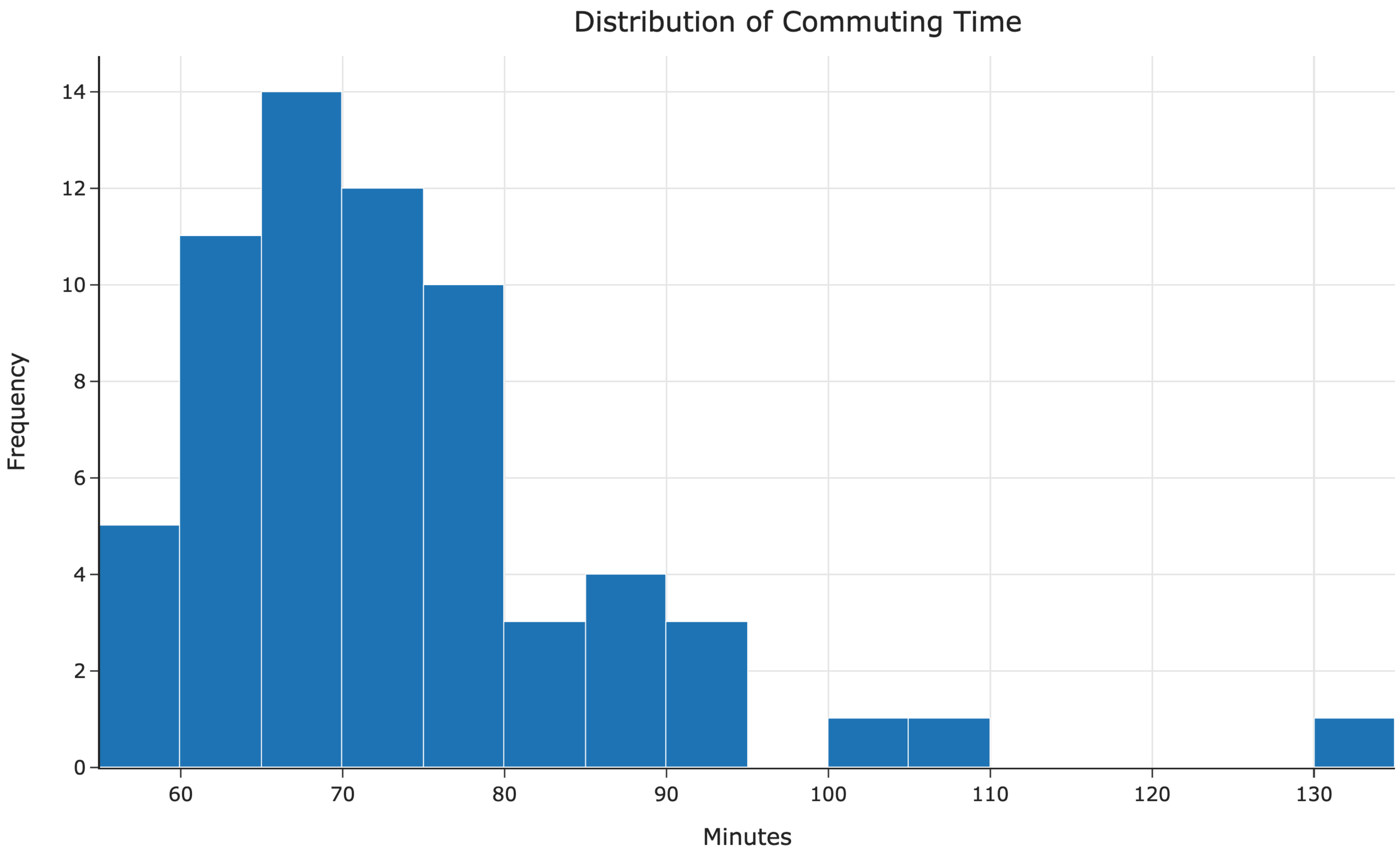
...

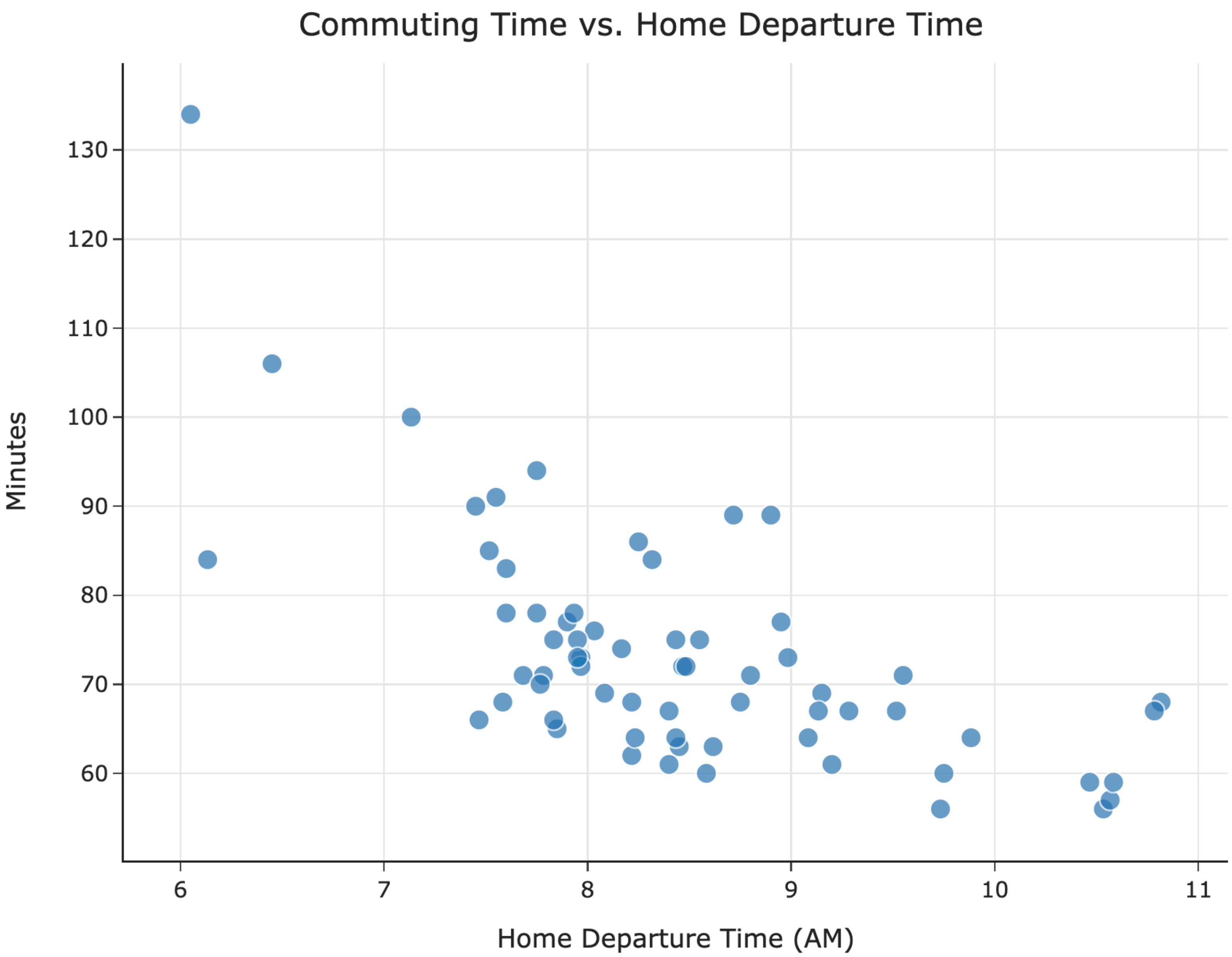
8AM + 45% of an hour
= 8:25 ish AM

You decide to live with your parents in Detroit and commute.

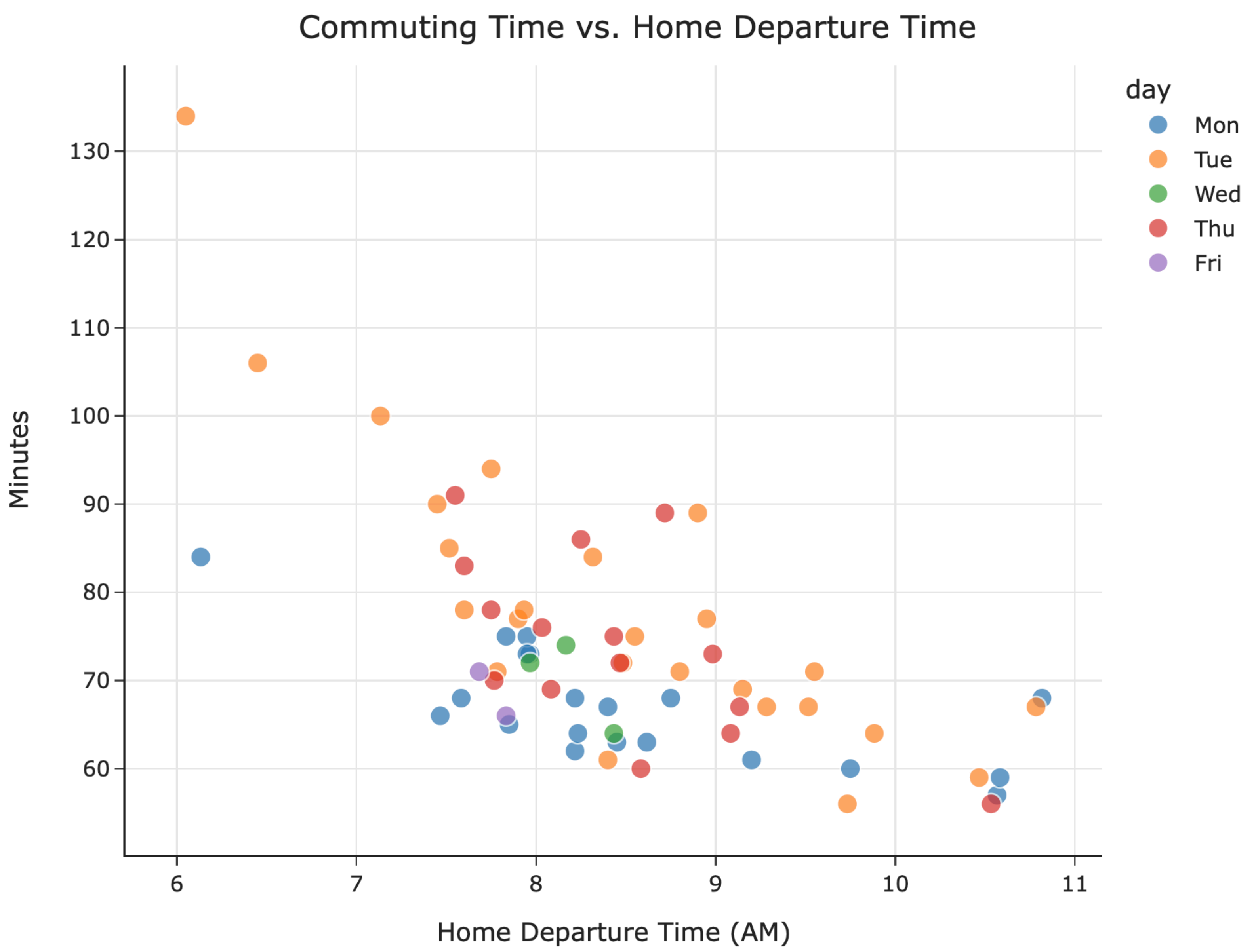
You keep track of how long it takes you to get to school each day.

This is a real dataset, collected by Joseph Hearn! However, he lived in the Seattle area, not Metro Detroit.


Distribution of Commuting Time
Frequency
0
2
4
6
8
10
12
14
60
70
80
90
100
110
120
130
Minutes



Commuting Time vs. Home Departure Time
Minutes
130
120
110
100
90
80
70
60
6
7
8
9
10
11
Home Departure Time (AM)


Commuting Time vs. Home Departure Time
Minutes
130
120
110
100
90
80
70
60
6
7
8
9
10
11
Home Departure Time (AM)
day
Mon
Tue
Wed
Thu
Fri

Goal: Predict your **commute time**, i.e. how long it will take to get to school.

This is a **regression** problem.

supervised learning

How can we do this? What will we need to assume?

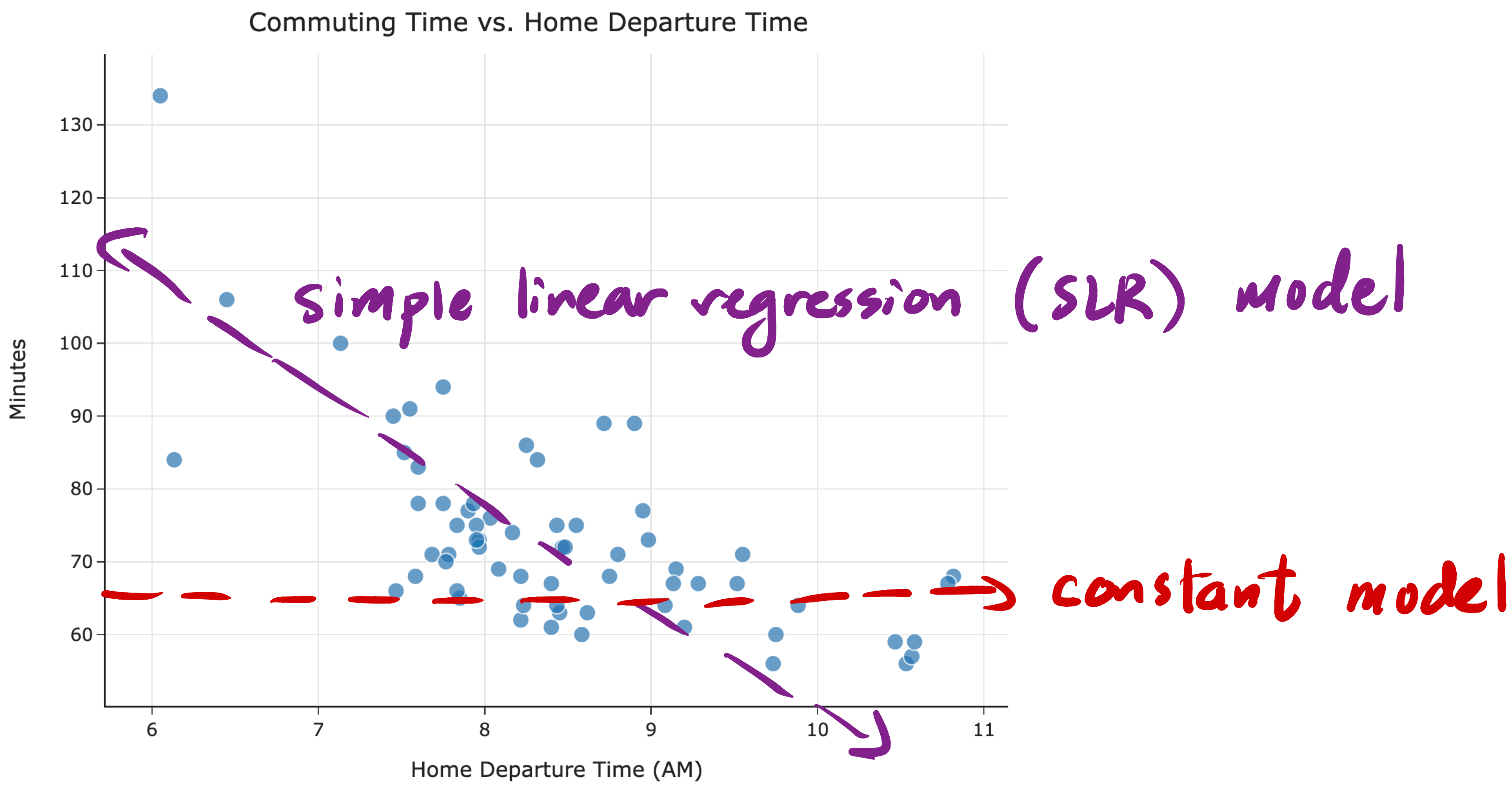
data in the future
≈
data from the past!

learning patterns from data!

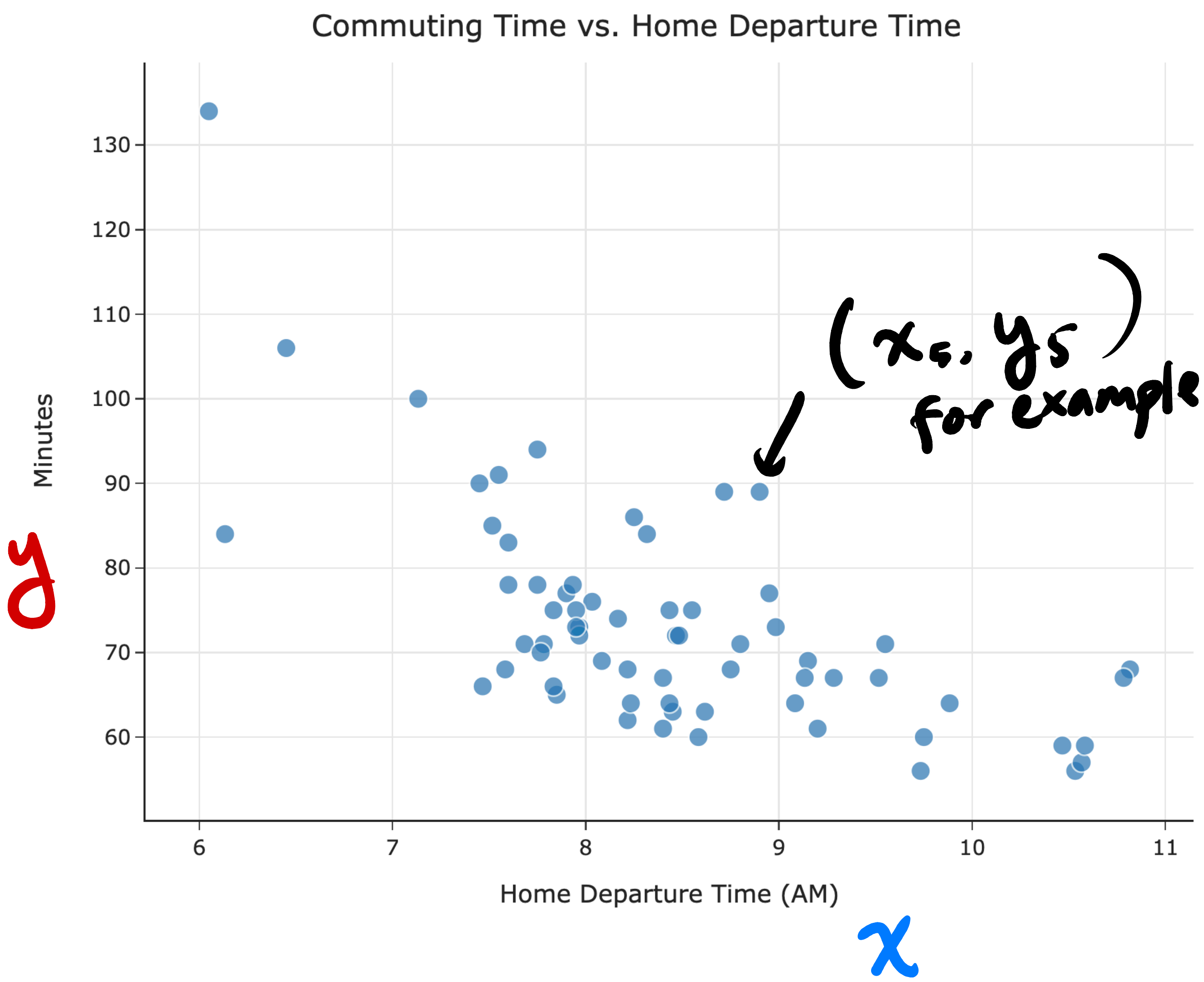
singular : "datum"

A **model** is a set of assumptions about how data were generated.

Possible models



Notation

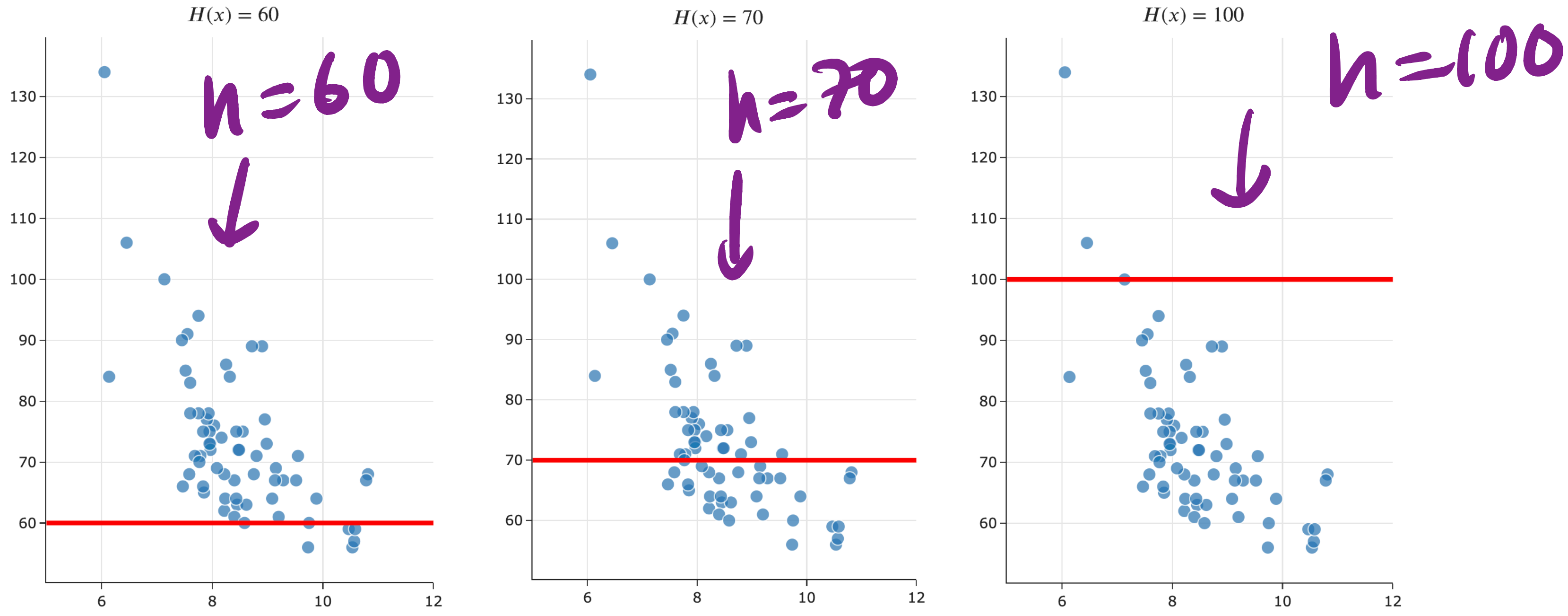


- x: "input", "independent variable", or "feature".
- y: "response", "dependent variable", or "target".
- **We use x to predict y.**
- The ith observation is denoted (x_i, y_i).

Hypothesis functions and parameters

used for making predictions!

- 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.
- **Example**: The constant model, $H(x) = h$, has one parameter: h.

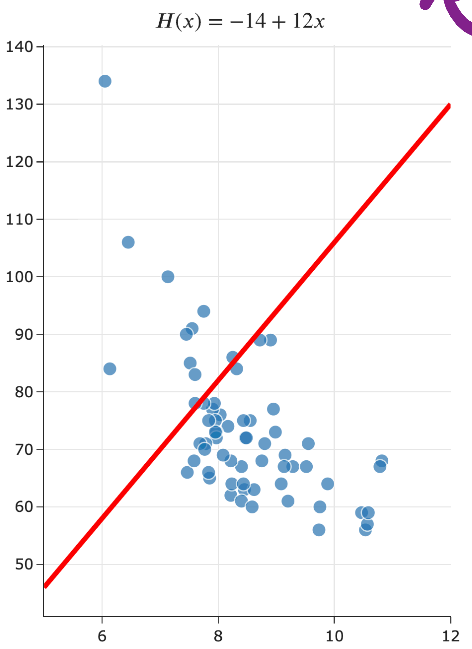


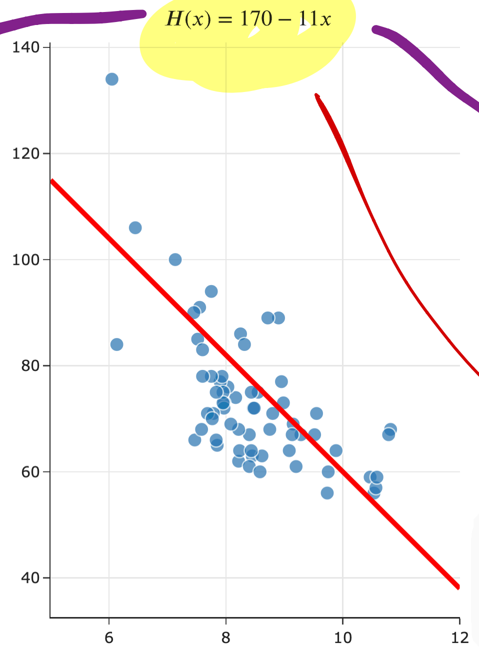
Hypothesis functions and parameters

- 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.
- **Example**: The simple linear regression model, $H(x) = \underbrace{w_0 + w_1 x}_{\text{fancy } y=mx+b}$, has two parameters: w_0 and w_1.

slope

intercept





e.g. leave at 10AM
predicted commute
$= H(10) = 170 - 11 \cdot 10 = \boxed{60}$

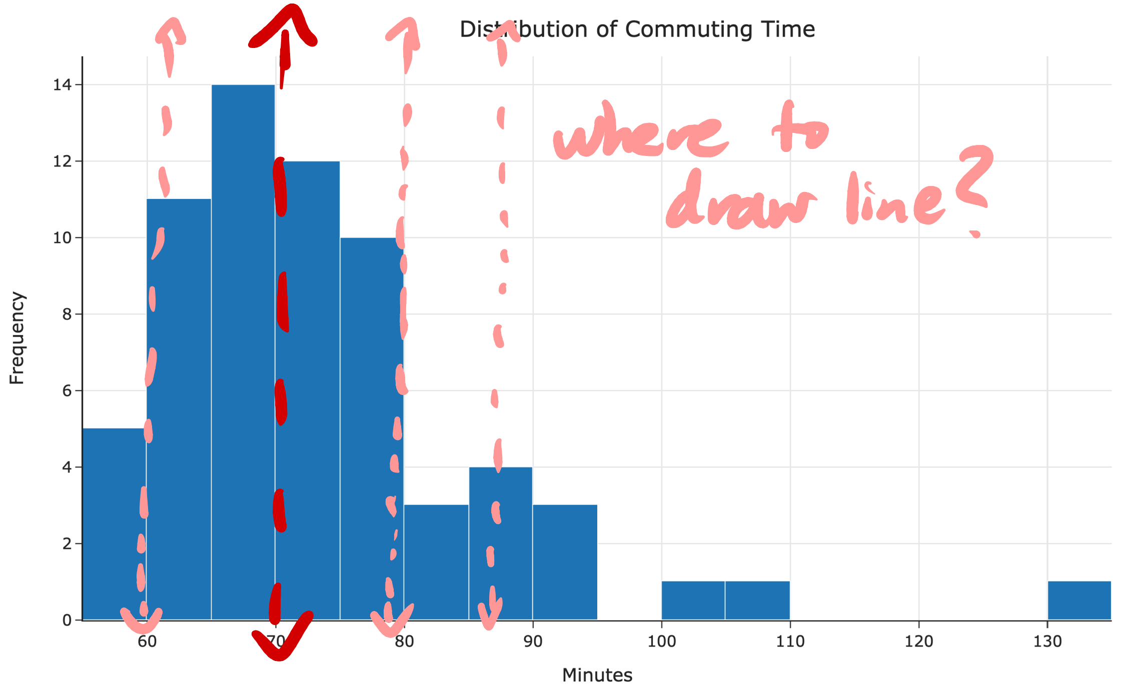
Question 🤔

Answer at practicaldsc.org/q

What questions do you have?

The constant model

The constant model



which of these constant predictions is "the best"?

A concrete example

- Let's suppose we have just a smaller dataset of just five historical commute times in minutes.

$$
\begin{aligned}
y_1 &= 72 \\
y_2 &= 90 \\
y_3 &= 61 \\
y_4 &= 85 \\
y_5 &= 92
\end{aligned}
$$

- Given this data, can you come up with a prediction for your future commute time? How?

ideas mentioned in lecture:

mean, median, most recent, $\frac{\text{min} + \text{max}}{2}$

Some common approaches

- The **mean**:

$$\frac{1}{5}(72 + 90 + 61 + 85 + 92) = \boxed{80}$$

- The **median**:

$$61 \qquad 72 \qquad \boxed{85} \qquad 90 \qquad 92$$

- Both of these are familiar **summary statistics**.

  Summary statistics summarize a collection of numbers with a single number, i.e. they result from an **aggregation**.

- But which one is better? Is there a "best" prediction we can make?

The cost of making predictions

- A **loss function** quantifies how bad a prediction is for a single data point.
  - If our prediction is **close** to the actual value, we should have **low** loss.
  - If our prediction is **far** from the actual value, we should have **high** loss.
- A good starting point is error, which is the difference between actual and predicted values.

actual commute time

$$e_i = y_i - H(x_i)$$

predicted commute time

- Suppose my commute **actually** takes 80 minutes.
  - If I predict 75 minutes: 80 − 75 = 5
  - If I predict 72 minutes: 80 − 72 = 8 ← worse prediction, more loss!
  - If I predict 100 minutes: 80 − 100 = −20

issue! some ⊕, some ⊖

Squared loss

- One loss function is squared loss, L_{sq}, which computes $(\text{actual} - \text{predicted})^2$.

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

$$= \underbrace{(\text{predicted} - \text{actual})^2}_{\text{symmetric}}$$

- Note that for the constant model, $H(x_i) = h$, so we can simplify this to:

$$L_{\text{sq}}(y_i, h) = (y_i - h)^2$$

- Squared loss is not the only loss function that exists!

  Soon, we'll learn about absolute loss. Different loss functions have different pros and cons.

A concrete example, revisited

- Consider again our smaller dataset of just five historical commute times in minutes.

$$y_1 = 72 \rightarrow (72-85)^2 = 169$$
$$y_2 = 90 \rightarrow (90-85)^2 = 25$$
$$y_3 = 61$$
$$y_4 = 85$$
$$y_5 = 92$$

Goal: Find a single number that describes the quality of $h=85$ across my entire dataset.

- Suppose we predict the median, $h = 85$. What is the squared loss of 85 for each data point?

Averaging squared losses

- We'd like a single number that describes the quality of our predictions across our entire dataset. One way to compute this is as the **average of the squared losses**.

- For the median, $h = 85$:

$$\frac{1}{5}\left((72 - 85)^2 + (90 - 85)^2 + (61 - 85)^2 + (85 - 85)^2 + (92 - 85)^2\right) = \boxed{163.8}$$

- For the mean, $h = 80$:

$$\frac{1}{5}\left((72 - 80)^2 + (90 - 80)^2 + (61 - 80)^2 + (85 - 80)^2 + (92 - 80)^2\right) = \boxed{138.8}$$

low loss = good!

- Which prediction is better? Could there be an even better prediction?

80 is better, because its average squared loss is lower!

low loss = good!

- L: loss for a single point
- R: average loss across whole dataset

Mean squared error

- Another term for **average squared loss** is **mean squared error (MSE)**.
- The mean squared error on our smaller dataset for any prediction h is of the form:

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

R stands for "risk", as in "empirical risk." We'll see this term again soon.

- For example, if we predict $h = 100$, then:

$$\begin{aligned} R_{\text{sq}}(100) &= \frac{1}{5}\left((72-100)^2 + (90-100)^2 + (61-100)^2 + (85-100)^2 + (92-100)^2\right) \\ &= \boxed{538.8} \end{aligned}$$

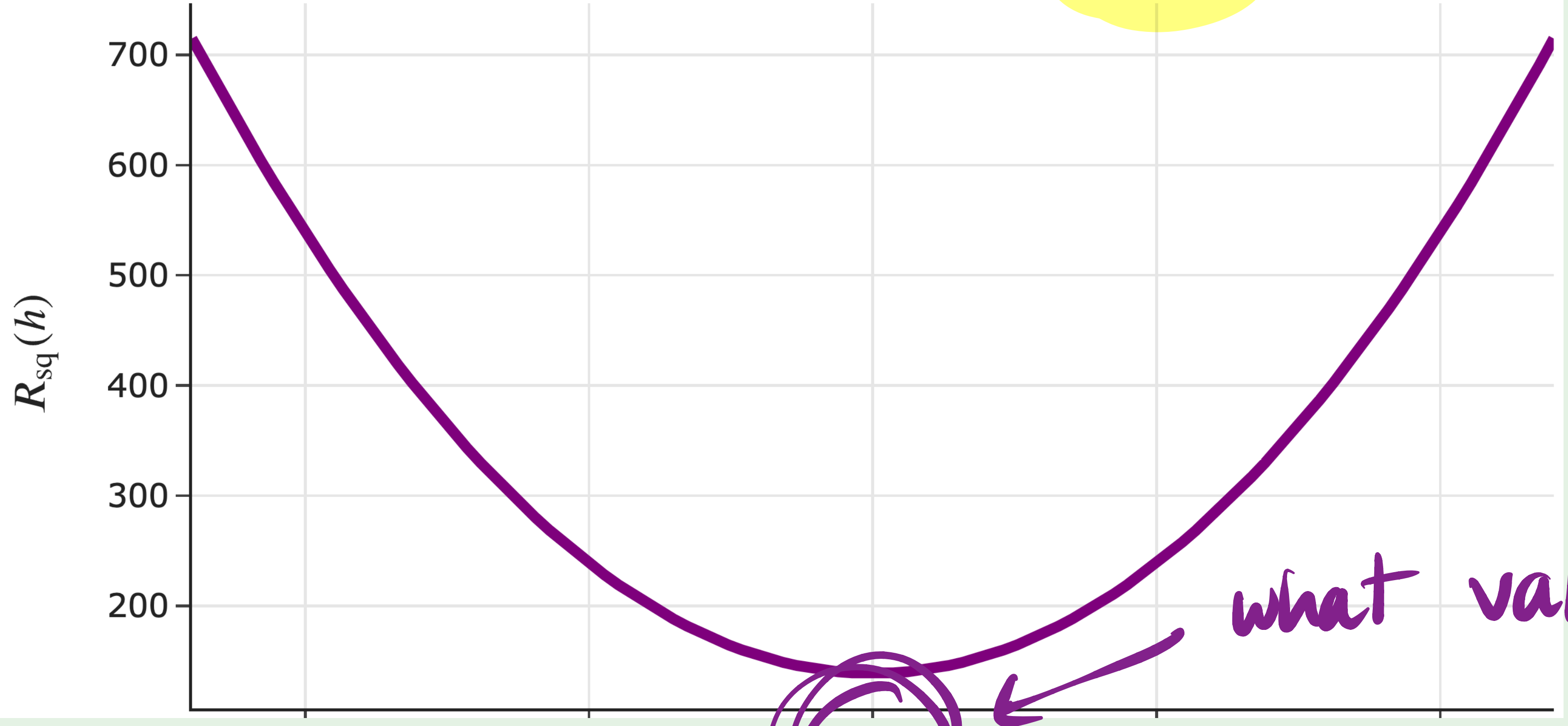
- **We can pick any h as a prediction, but the smaller $R_{\text{sq}}(h)$ is, the better h is!**

$(85-h)^2$ is a parabola centered @ $h=85$

Activity

Answer at practicaldsc.org/q (use the free response box!)

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



what value is here?

Which h corresponds to the vertex of $R_{\text{sq}}(h)$?

Mean squared error, in general

- Suppose we collect n commute times, $y_1, y_2, \ldots, y_n$.
- The mean squared error of the prediction h is:

$$R_{sq}(h) = \frac{1}{n}\left[(y_1-h)^2 + \underbrace{(y_2-h)^2}_{\text{squared loss for point 2}} + \ldots + (y_n-h)^2\right]$$

- Or, using **summation notation**:

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

As a for-loop:

```
total = 0
for i in range(1, n+1):
    total += y[i]
total = total / n
```

The best prediction

only unknown is h!

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

$y_1, \ldots, y_n$ are known (they're my data!)

- We want the **best** constant prediction, among all constant predictions h.
- The smaller $R_{sq}(h)$ is, the better h is.
- **Goal**: Find the h that minimizes $R_{sq}(h)$.

  The resulting h will be called h^*.
- **How do we find h^*?**

special → best → smallest MSE

Minimizing mean squared error using calculus

Minimizing using calculus

- We'd like to minimize:

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

- In order to minimize $R_{\text{sq}}(h)$, we:
    1. take its derivative with respect to h,
    2. set it equal to 0,
    3. solve for the resulting h^*, and
    4. perform a second derivative test to ensure we found a minimum.

Step 0: The derivative of $(y_i - h)^2$

- Remember from calculus that:
  - if $c(x) = a(x) + b(x)$, then
  - $\frac{d}{dx}c(x) = \frac{d}{dx}a(x) + \frac{d}{dx}b(x)$.
- This is relevant because $R_{\text{sq}}(h) = \frac{1}{n}\sum_{i=1}^{n}(y_i - h)^2$ involves the sum of n individual terms, each of which involve h.
- So, to take the derivative of $R_{\text{sq}}(h)$, we'll first need to find the derivative of $(y_i - h)^2$.

① power rule
② chain rule

$$\frac{d}{dh}(y_i - h)^2 = \underbrace{2(y_i - h)}_{①} \underbrace{\frac{d}{dh}(y_i - h)}_{②}$$

$$= 2(y_i - h)(-1) = -2(y_i - h) = 2(h - y_i)$$

Question 🤔

Answer at practicaldsc.org/q

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

Which of the following is $\frac{d}{dh} R_{\text{sq}}(h)$?

- A. 0
- B. $\sum_{i=1}^{n} y_i$
- C. $\frac{1}{n} \sum_{i=1}^{n} (y_i - h)$
- D. $\frac{2}{n} \sum_{i=1}^{n} (y_i - h)$
- E. $-\frac{2}{n} \sum_{i=1}^{n} (y_i - h)$

Step 1: The derivative of $R_{\text{sq}}(h)$

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

$$= \frac{1}{n}\sum_{i=1}^{n} \frac{d}{dh}(y_i - h)^2$$

two slides ago!

$$= \frac{1}{n}\sum_{i=1}^{n}(-2)(y_i - h)$$

$$\boxed{\frac{d}{dh} R_{sq}(h) = -\frac{2}{n}\sum_{i=1}^{n}(y_i - h)}$$

Steps 2 and 3: Set to 0 and solve for the minimizer, h^*

$$-\frac{2}{n}\sum_{i=1}^{n}(y_i - h) = 0$$

← multiply BS by $-\frac{n}{2}$

$$\sum_{i=1}^{n}(y_i - h) = 0$$

$$\sum_{i=1}^{n} y_i - \sum_{i=1}^{n} h = 0$$

$$\sum_{i=1}^{n} y_i - h\sum_{i=1}^{n} 1 = 0$$

n

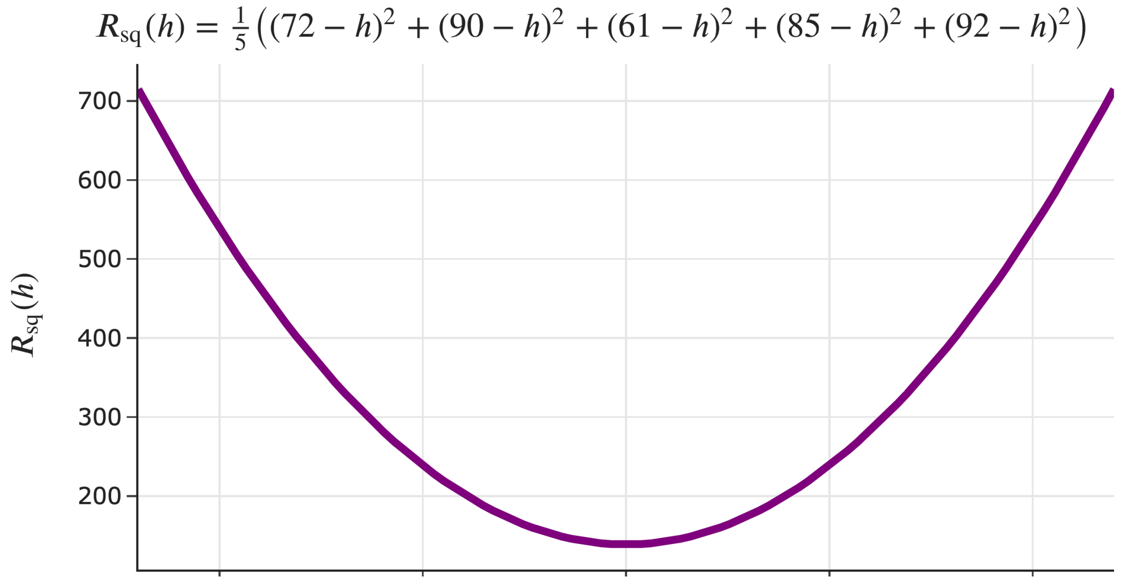
$$\sum_{i=1}^{n} y_i - nh = 0$$

$$\sum_{i=1}^{n} y_i = nh$$

$$h = \frac{\sum_{i=1}^{n} y_i}{n}$$

$$= \text{Mean}(y_1, \ldots, y_n)$$

Step 4: Second derivative test



We already saw that $R_{\text{sq}}(h)$ is **convex**, i.e. that it opens upwards, so the h^* we found must be a minimum, not a maximum.

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

$$\frac{dR_{sq}(h)}{dh} = -\frac{2}{n}\sum_{i=1}^{n}(y_i - h)$$

$$\frac{d^2}{dh^2}R_{sq}(h) = -\frac{2}{n}\underbrace{\sum_{i=1}^{n}(-1)}_{(-1)+(-1)+\dots+(-1) = -n} = -\frac{2}{\cancel{n}}(-\cancel{n}) = 2 \cdot 1 = \boxed{2} > 0$$

positive

$\Rightarrow R_{sq}(h)$ opens up $\cup$

$\Rightarrow h^*$ is a minimizer!

The mean minimizes mean squared error!

- The problem we set out to solve was, find the h^* that minimizes:

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

- The answer is:

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

- The **best constant prediction**, in terms of mean squared error, is always the **mean**.
- We call h^* our **optimal model parameter**, for when we use:
  - the constant model, $H(x) = h$, and
  - the squared loss function, $L_{\text{sq}}(y_i, h) = (y_i - h)^2$.

Aside: Notation

- Another way of writing:

$$h^* \text{ is the value of } h \text{ that minimizes } \underbrace{\frac{1}{n}\sum_{i=1}^{n}(y_i - h)^2}_{R_{sq}(h)}$$

is: //

$$h^* = \underbrace{\underset{h}{\operatorname{argmin}}}_{\text{"the argument that minimizes"}} \left(\frac{1}{n}\sum_{i=1}^{n}(y_i - h)^2 \right)$$

- h^* is the solution to an **optimization problem**.

The modeling recipe

- We've implicitly introduced a three-step process for finding optimal model parameters (like h^*) that we can use for making predictions:

    1. Choose a model.

    $H(x) = h$ constant

    Another choice: $H(x) = w_0 + w_1 x$

    2. Choose a loss function.

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

    a different loss f'n?

    3. Minimize average loss to find optimal model parameters.

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

    different optimal model parameter?

- Most modern machine learning methods today, including neural networks, follow this recipe, and we'll see it repeatedly this semester!

Question 🤔

Answer at practicaldsc.org/q

What questions do you have?

Another loss function

Another loss function

- We started by computing the **error** for each of our predictions, but ran into the issue that some errors were positive and some were negative.

predicted

$$e_i = y_i - H(x_i)$$

actual

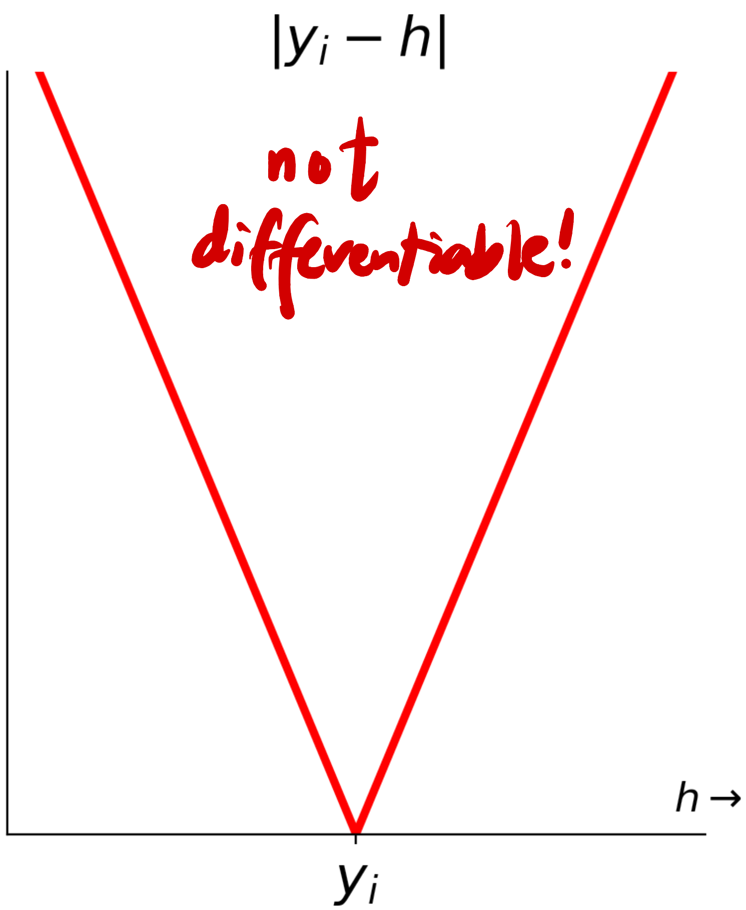
- The solution was to **square** the errors, so that all are non-negative. The resulting loss function is called **squared loss**.

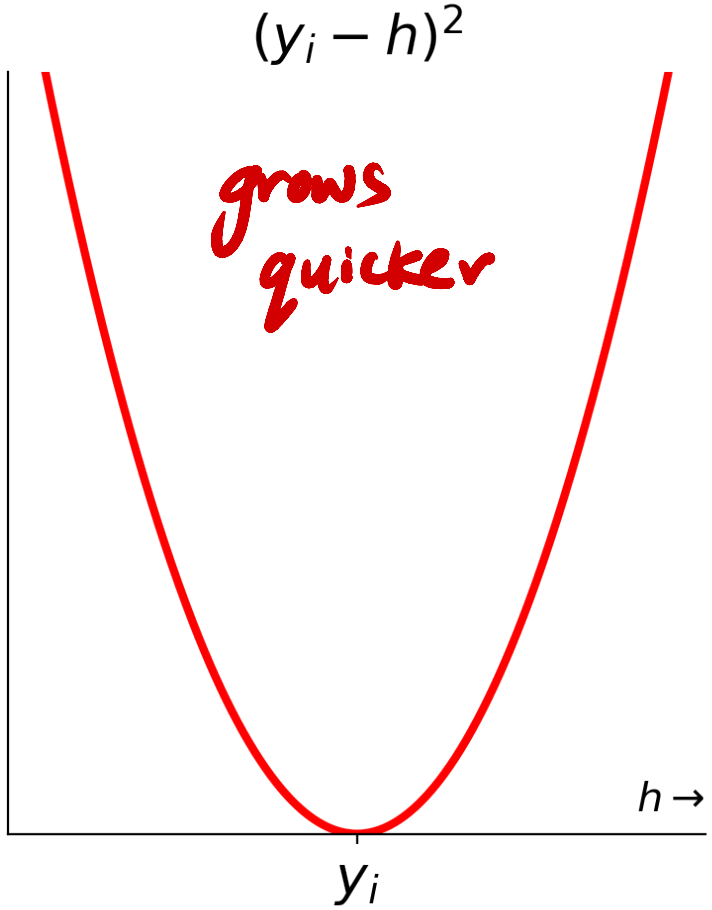
$$L_{\text{sq}}(y_i, H(x_i)) = (y_i - H(x_i))^2$$

- Another loss function, which also measures how far $H(x_i)$ is from y_i, is **absolute loss**.

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

Absolute loss vs. squared loss





Mean absolute error

- Suppose we collect n commute times, $y_1, y_2, \ldots, y_n$.
- The **<u>average</u> absolute loss**, or **<u>mean</u> absolute error (MAE)**, of the prediction h is:

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

- We'd like to find the best constant prediction, h^*, by finding the h that minimizes **mean absolute error**.
- Any guesses?

The median minimizes mean absolute error!

- It turns out that the constant prediction h^* that minimizes mean absolute error,

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

  is:

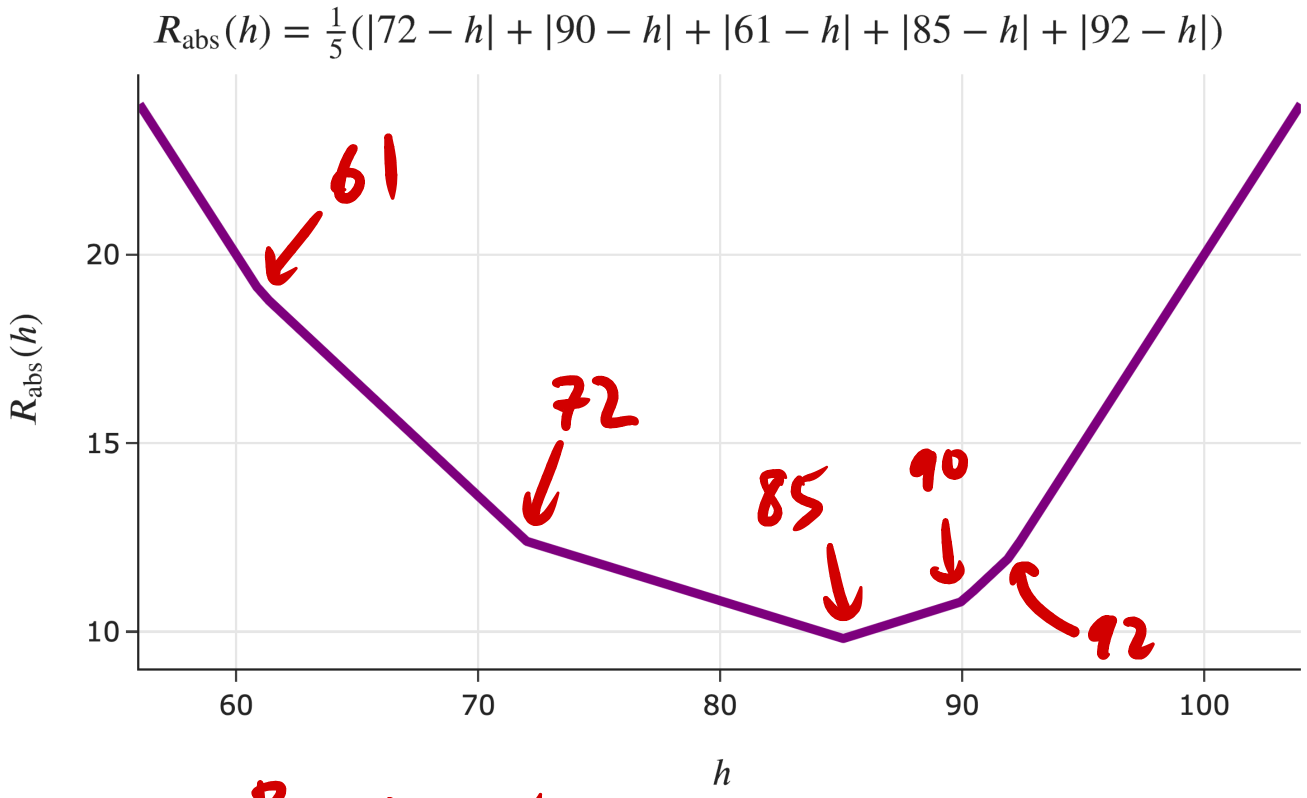
$$h^* = \text{Median}(y_1, y_2, \ldots, y_n)$$

- We won't prove this in lecture, but **this extra video** walks through it.

  Watch it!

- To make a bit more sense of this result, let's graph $R_{\text{abs}}(h)$.

Visualizing mean absolute error



Bends at the data points!

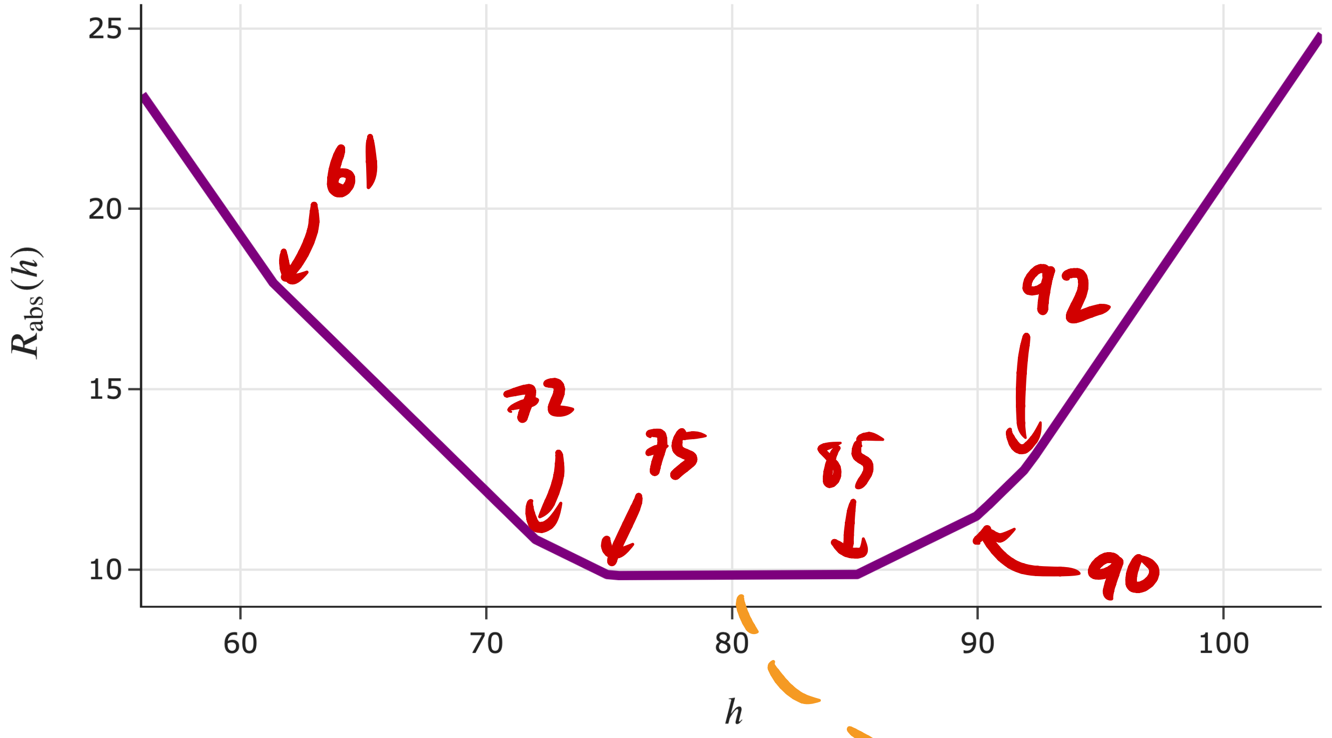
- Consider, again, our example dataset of five commute times.

$$72, 90, 61, 85, 92$$

- Where are the "bends" in the graph of $R_{\text{abs}}(h)$ – that is, where does its slope change?

Visualizing $\overbrace{\text{mean absolute error}}^{\text{MAE}}$, with an even number of points

$$R_{\text{abs}}(h) = \frac{1}{6}(|72 - h| + |90 - h| + |61 - h| + |85 - h| + |92 - h| + |75 - h|)$$



- What if we add a sixth data point?

$$72, 90, 61, 85, 92, 75$$

- Is there a unique h^*?

No, h^* is not unique!
Any value in the range
$75 \leq h^* \leq 85$
minimizes MAE!

The median minimizes mean absolute error!

- The new problem we set out to solve was, find the h^* that minimizes:

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

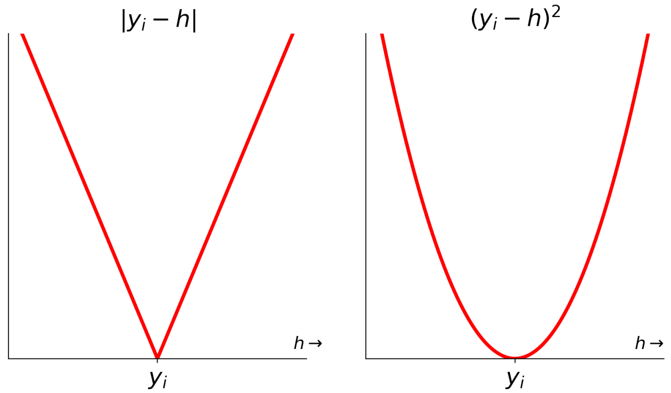
- The answer is:

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

- The **best constant prediction**, in terms of mean absolute error, is always the **median**.
    - When n is odd, this answer is unique.
    - When n is even, any number between the middle two data points (when sorted) also minimizes mean absolute error.
    - When n is even, define the median to be the mean of the middle two data points.

Choosing a loss function

- For the constant model $H(x) = h$, the **mean** minimizes mean **squared** error.
- For the constant model $H(x) = h$, the **median** minimizes mean **absolute** error.
- In practice, squared loss is the more common choice, as it's easily **differentiable**.



- But how does our choice of loss function impact the resulting optimal prediction?
- We'll discuss this more next class.

Question 🤔

Answer at practicaldsc.org/q

What questions do you have?