Lecture 11

Introduction to Machine Learning

EECS 398: Practical Data Science, Winter 2025

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Agenda 📆

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

The next few lectures (and Homework 6!) will be primarily **math-based**.

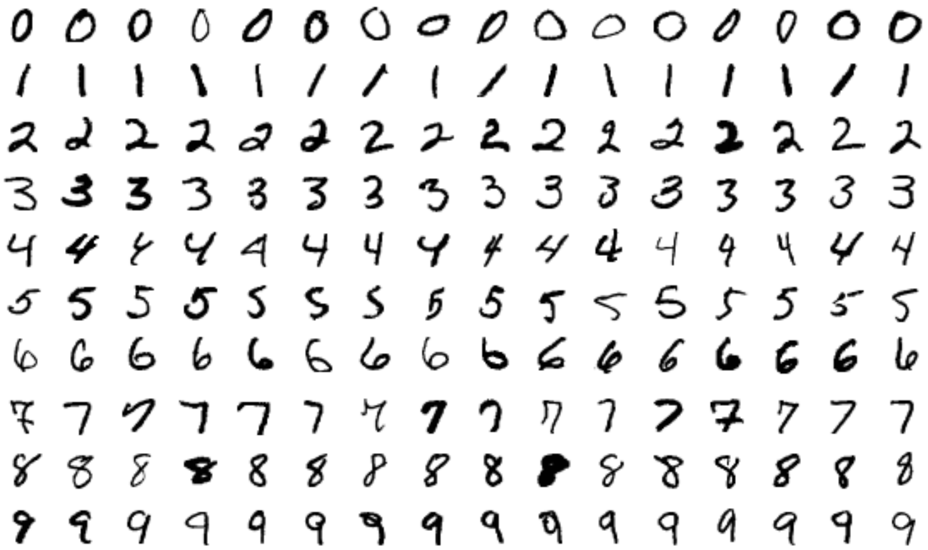
- For these lectures, we'll post blank slides as a PDF before class, and annotated slides after class.
- If there are any code demos, we'll post those before class, too.

Machine learning and models

Machine learning is about **automatically** learning patterns from data.

without hard-coding

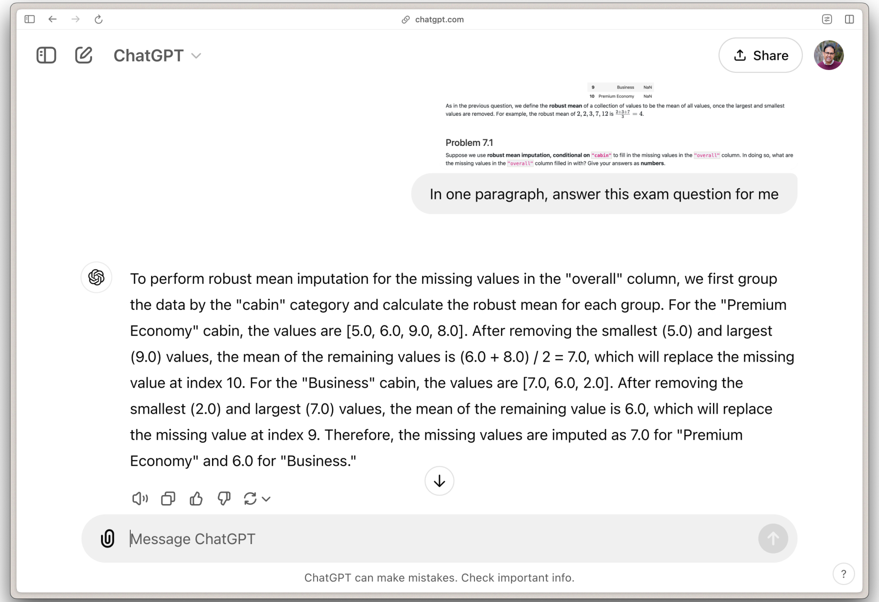
Example: Handwritten digit classification



Humans are good at understanding handwriting,

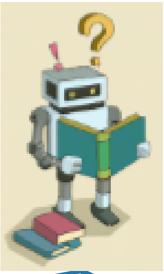
but how do we get computers to understand handwriting?

Example: ChatGPT



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

Taxonomy of machine learning



dataset contains an "answer" column that we try to predict

semi-supervised → ChatGPT

Labeled data → Supervised learning

Unlabeled data → Unsupervised learning

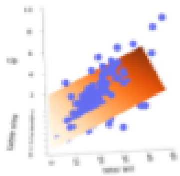
Reward → Reinforcement learning

Supervised learning:
- Quantitative prediction → Regression
- Categorical prediction → Classification

Unsupervised learning:
- Dimensionality reduction
- Clustering

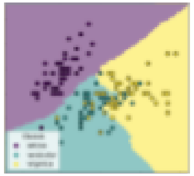
Reinforcement learning → AlphaGo

Regression



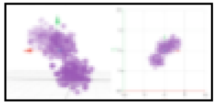
e.g. predict commute time, final exam grade

Classification

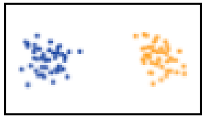


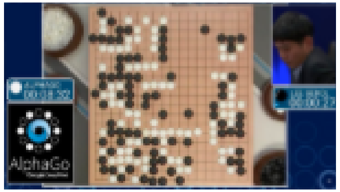
e.g. predicting COVID vs. not, or dog vs. cat vs. turkey

Dimensionality reduction

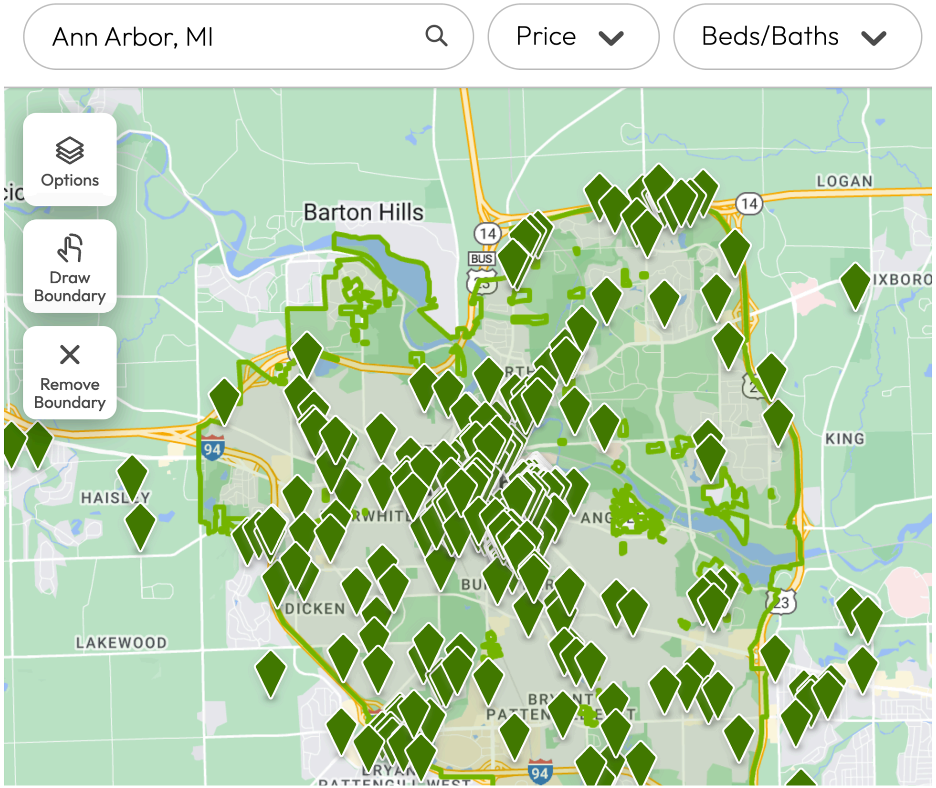


Clustering





AlphaGo



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

time of day, measured in hours

	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

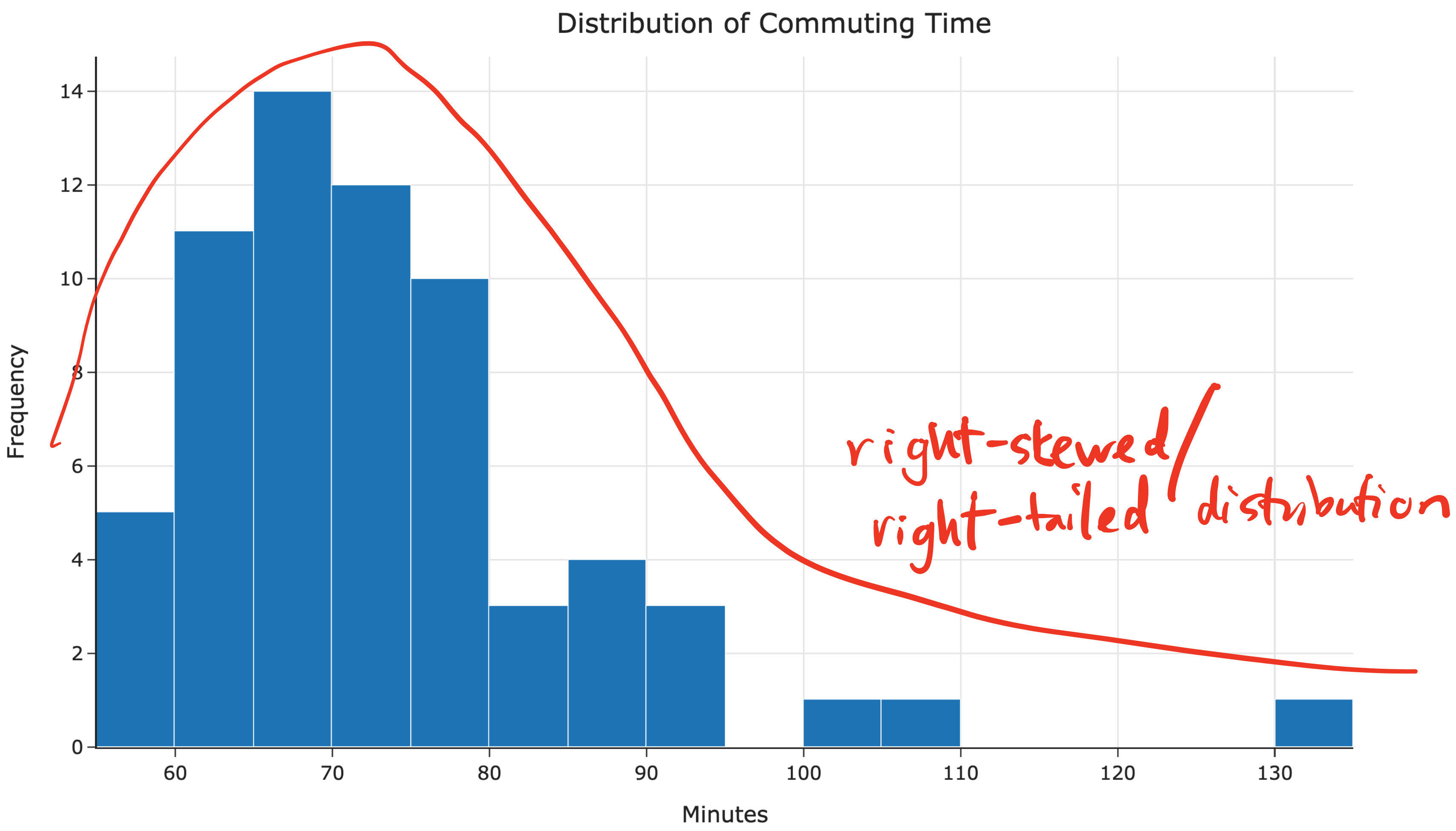
$\approx$ 8:26AM ish

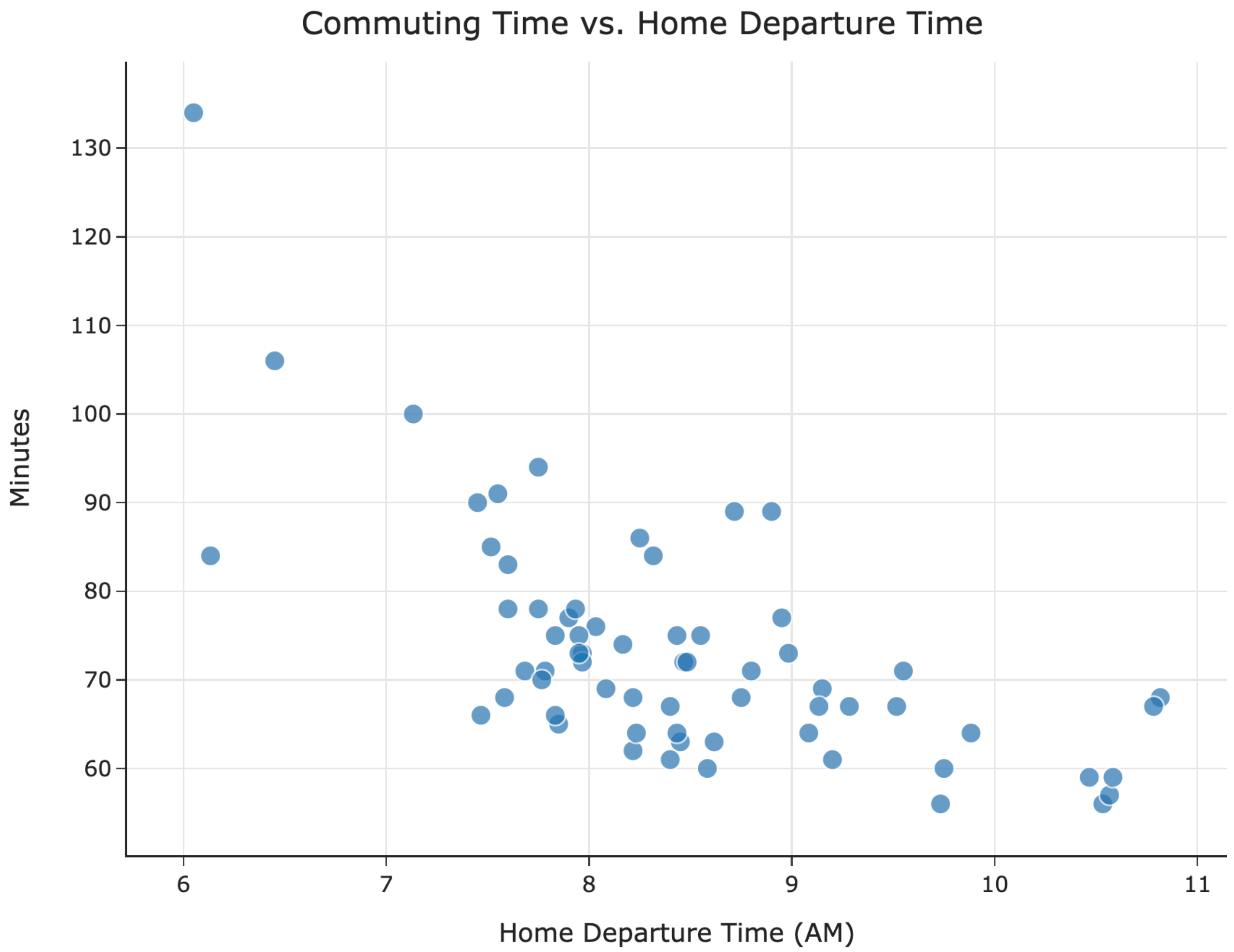
...

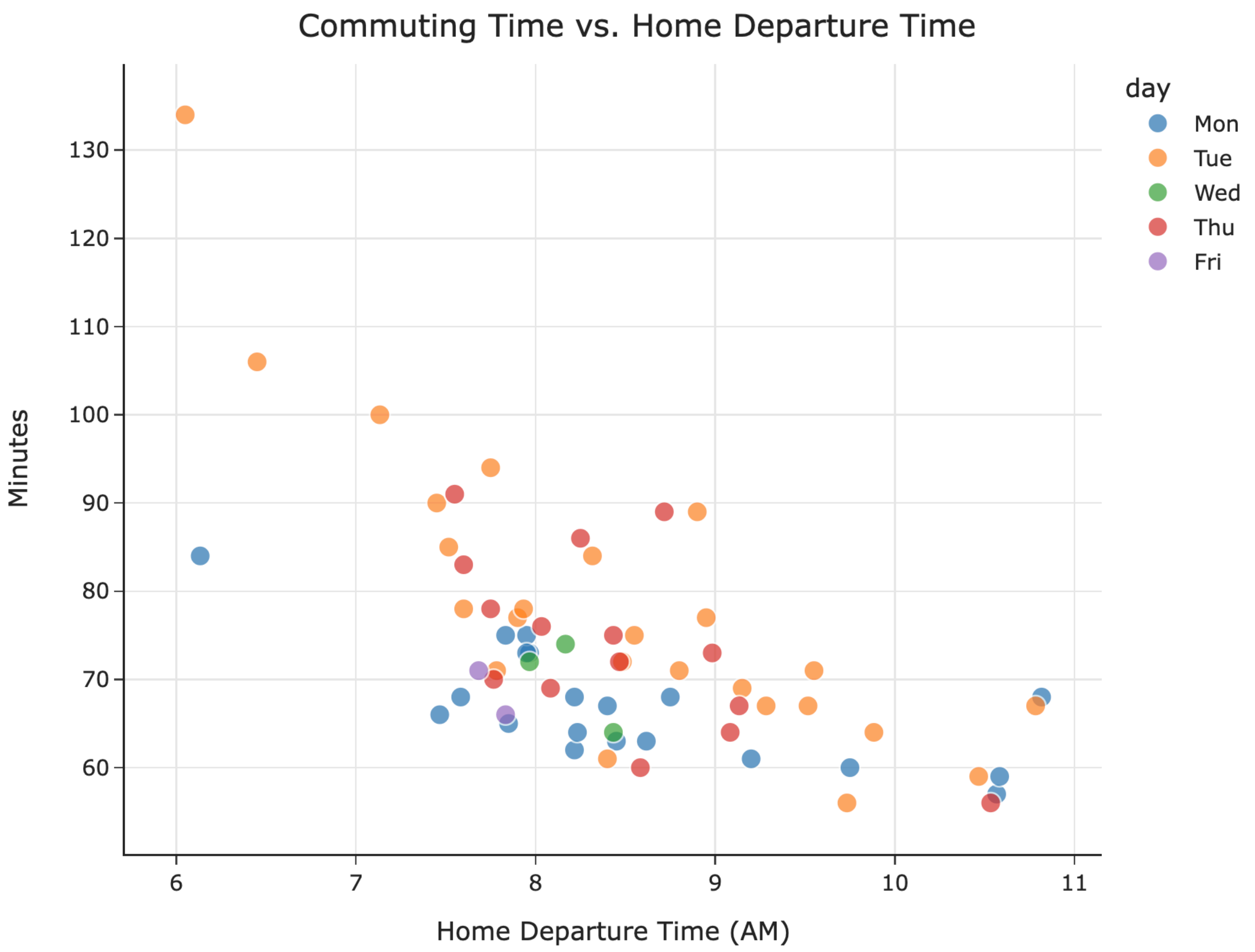
You decide to live with your parents in Detroit and commute.

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
Minutes
0
2
4
6
8
10
12
14
60
70
80
90
100
110
120
130
right-skewed/
right-tailed distribution


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

data from past

≈

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

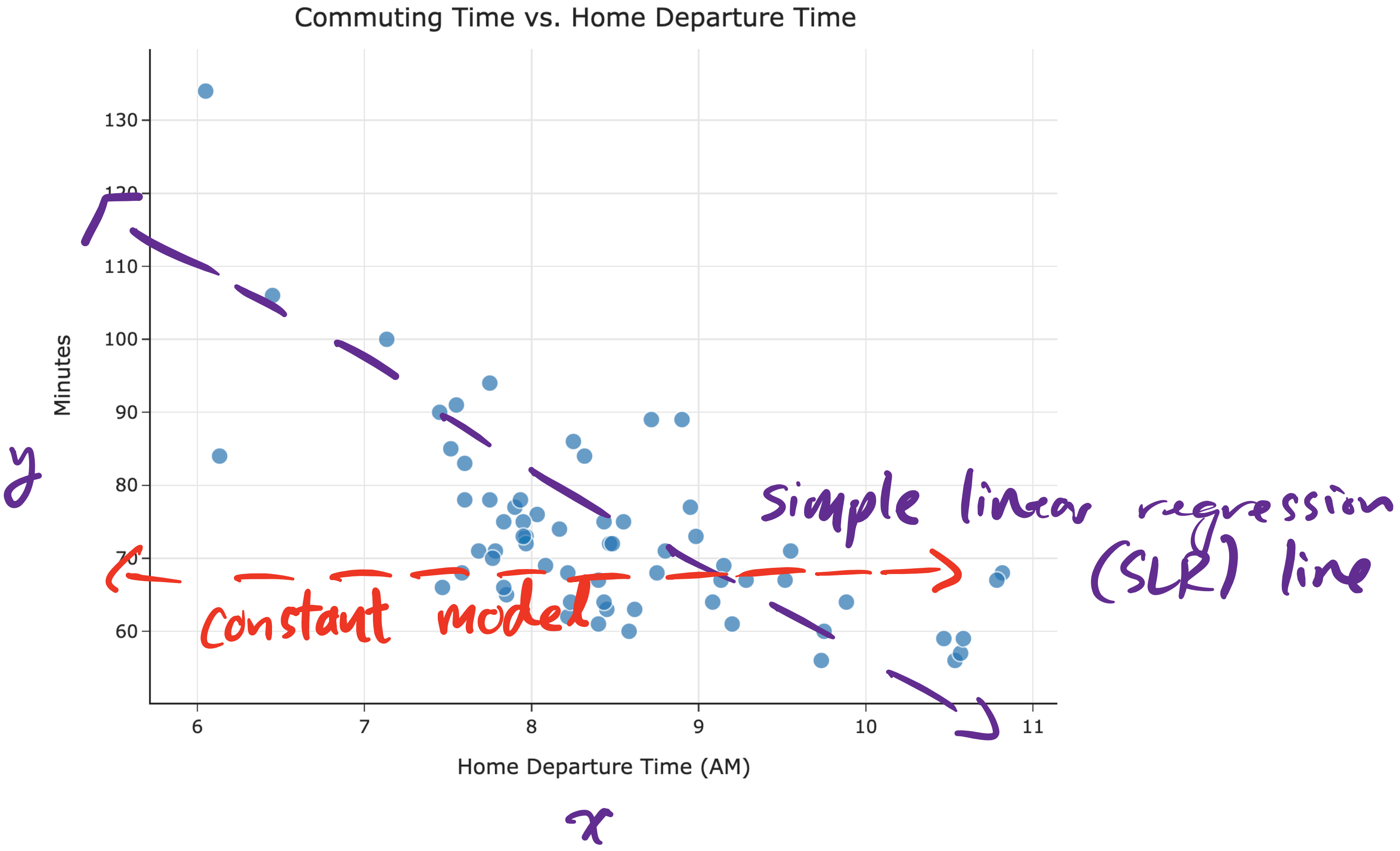
data from future!

learn a pattern from our data

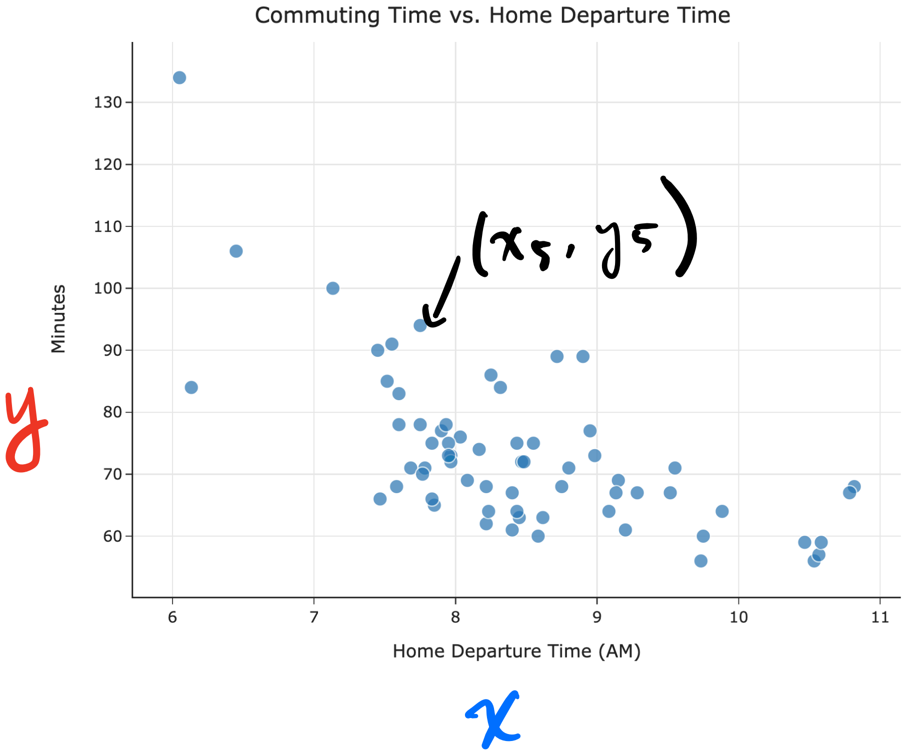
"Occam's razor": simplest explanation is most likely

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

Possible models



Notation

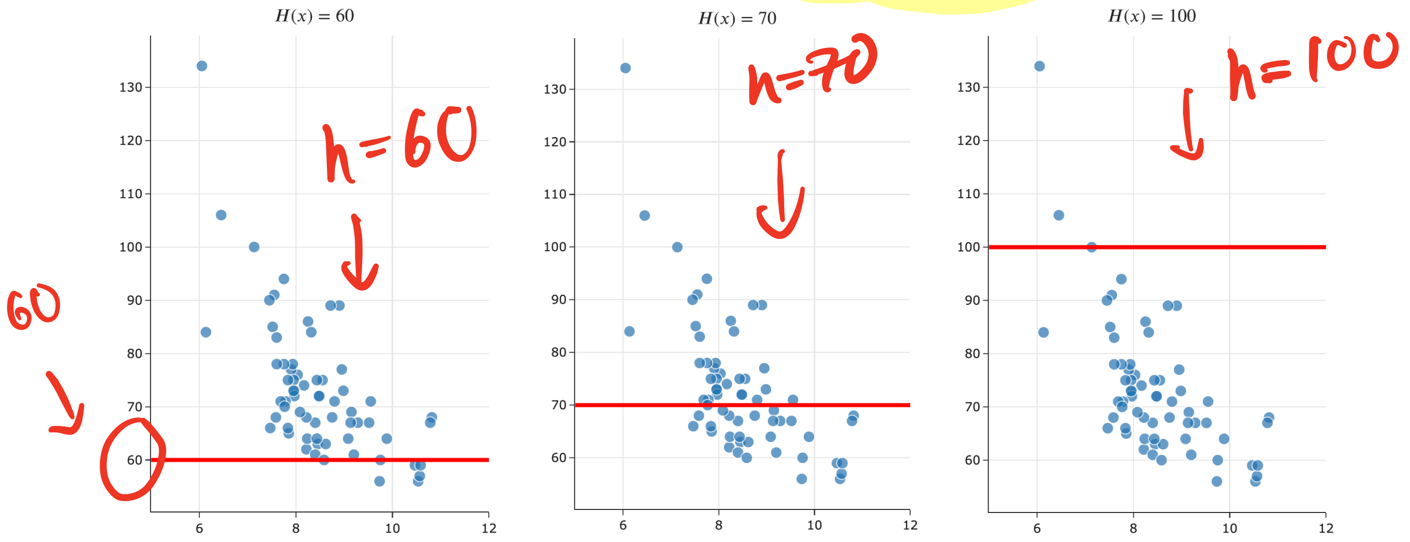


- x: "input", "independent variable", or "feature".
- y: "response", "dependent variable", or "target". the thing we are predicting
- The ith observation is denoted (x_i, y_i).
- **We use x_is to predict y_is.**

Hypothesis functions and parameters

used for making predictions!

- A hypothesis function, H, takes in an x_i as input and returns a predicted y_i.
- **Parameters** define the relationship between the input and output of a hypothesis function.
- **Example**: The constant model, $H(x_i) = h$, has one parameter: h.

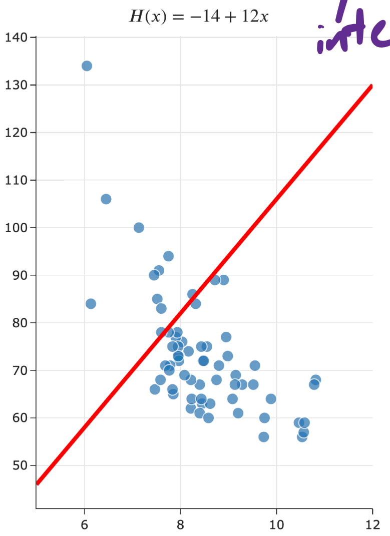


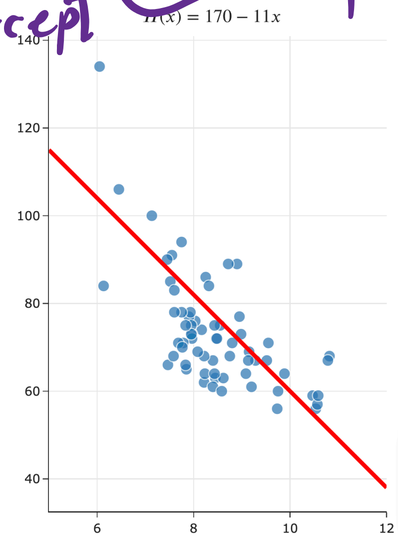
Hypothesis functions and parameters

- A hypothesis function, H, takes in an x_i as input and returns a predicted y_i.
- **Parameters** define the relationship between the input and output of a hypothesis function.
- **Example**: The simple linear regression model, $\underbrace{H(x_i) = w_0 + w_1 x_i}_{y = mx + b\text{, just fancier!}}$, has two parameters: w_0 and w_1.

intercept

slope





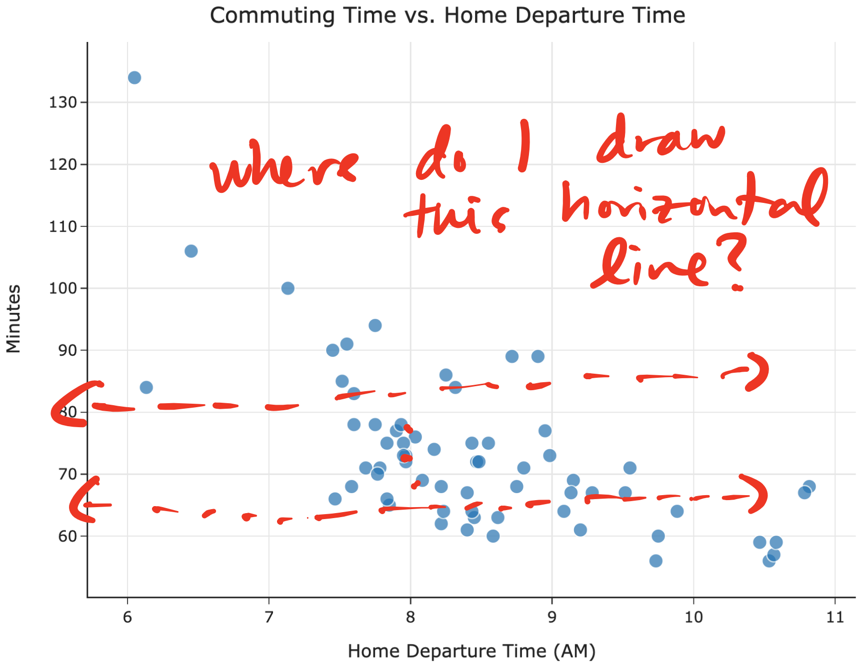
Question 🤔

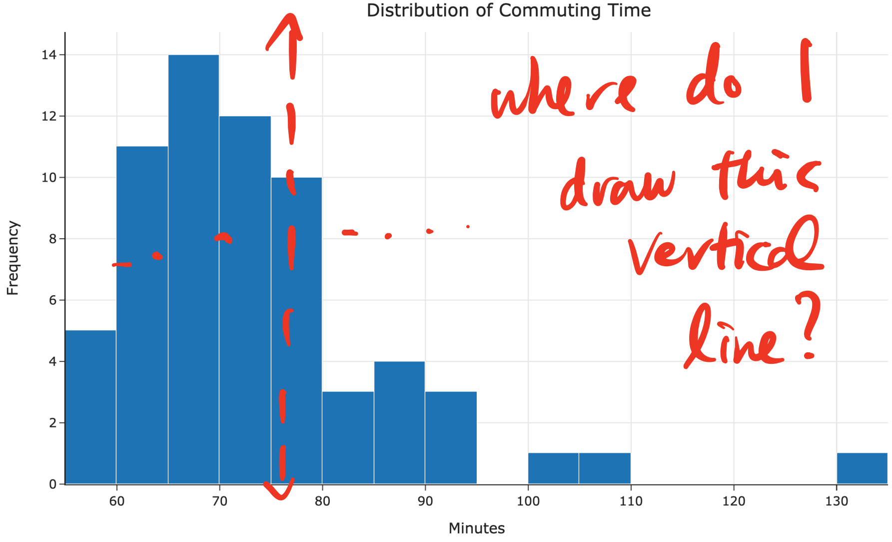
Answer at practicaldsc.org/q

What questions do you have?

The constant model

The constant model





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?

mean of y's : 80

median : 85

a random one

most common (mode)

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

low loss = good!

- 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.

$$e_i = \overbrace{y_i}^{\text{actual commute time}} - \underbrace{H(x_i)}_{\text{predicted commute time}}$$

- Suppose my commute **actually** takes 80 minutes.

  $y_i = 80$
  - If I predict 75 minutes: $80 - 75 = \boxed{5}$
  - If I predict 72 minutes: $80 - 72 = \boxed{8}$
  - If I predict 100 minutes: $80 - 100 = \boxed{-20}$

$-20 < 5$, but 100 is a worse prediction!

Squared loss

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

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

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

- 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.

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

$\vdots$

Goal: Come up with a single number that describes how good/bad $h=85$ is.

- 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, $h = 80$:

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

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

L: loss for one data point

R: average loss across all data

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 "**r**isk", as in "empirical risk." We'll see this term again soon.

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

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

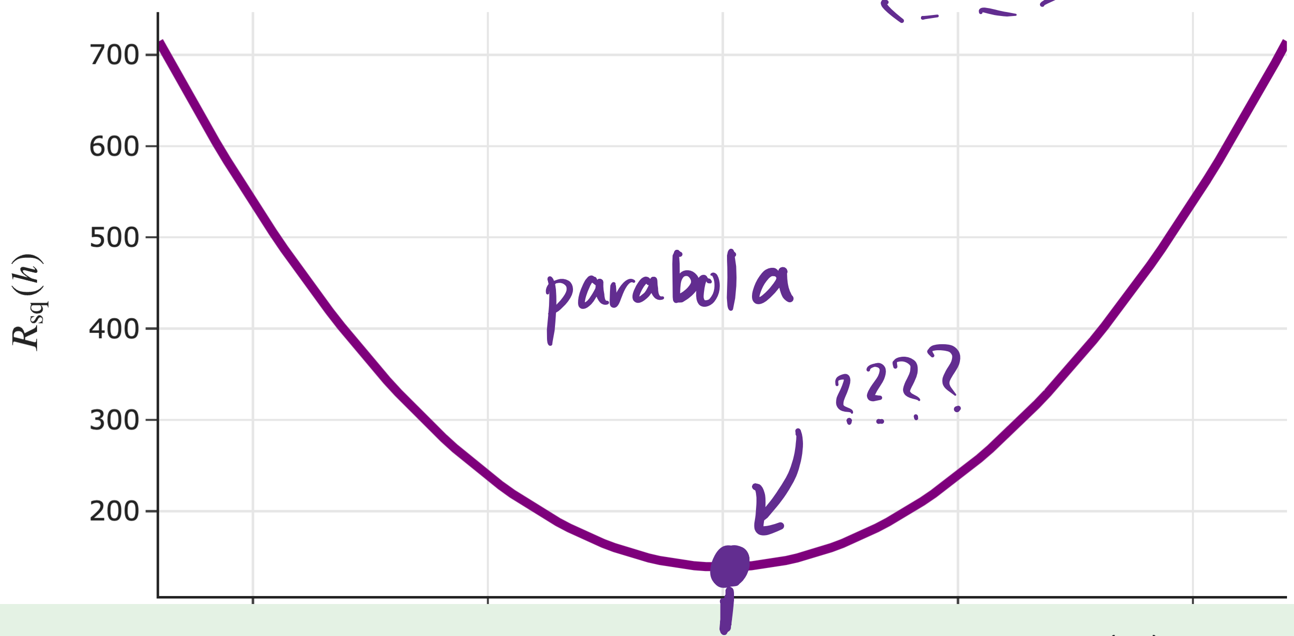
- **We can pick any h as a prediction, but the smaller $R_{\text{sq}}(h)$ is, the better h is!**

Activity

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

each individual loss function is quadratic; sum of quadratics is quadratic

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



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:

$$R_{sq}(h) = \frac{1}{n}\left[(y_1 - h)^2 + (y_2 - h)^2 + \cdots + (y_n - h)^2 \right]$$

squared

- Or, using **summation notation**:

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

The best prediction

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

h is the only unknown; the y_i's are my data

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

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

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.
- $R_{\text{sq}}(h)$ is an example of an **objective function**, a function that needs to be minimized.

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 $(y_i - h)^2$.

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

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

← used both the power rule ① and chain rule ②

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

last slide: $\frac{d}{dh}(y_i-h)^2=-2(y_i-h)$

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

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

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

from 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 $-\frac{n}{2}$

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

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

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

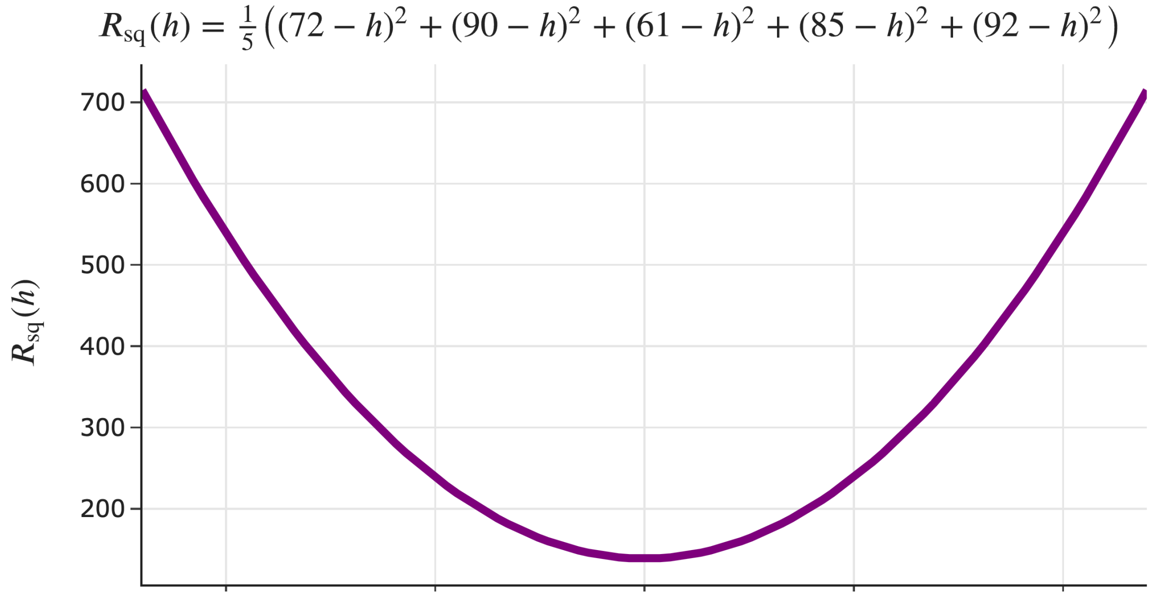
$$\sum_{i=1}^{n} y_i - nh = 0$$

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

$$\boxed{h^* = \frac{\sum_{i=1}^{n} y_i}{n} = \text{Mean}(y_1, y_2, \dots, y_n)}$$

Watch the derivation video here: https://youtu.be/NSIEP74ifyg

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.

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, $H(x_i) = h$, and
  - the squared loss function, $L_{\text{sq}}(y_i, h) = (y_i - h)^2$.

Aside: Terminology

- Another way of writing:

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

is:

"the input that minimizes"

$$h^* = \underset{h}{\operatorname{argmin}} \left(\frac{1}{n}\sum_{i=1}^{n}(y_i - h)^2 \right)$$

- h^* is the solution to an **optimization problem**, where the objective function is $R_{\text{sq}}(h) = \frac{1}{n}\sum_{i=1}^{n}(y_i - h)^2$.

next class →

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.

    2. Choose a loss function.

    3. Minimize average loss to find optimal model parameters.

- 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.

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

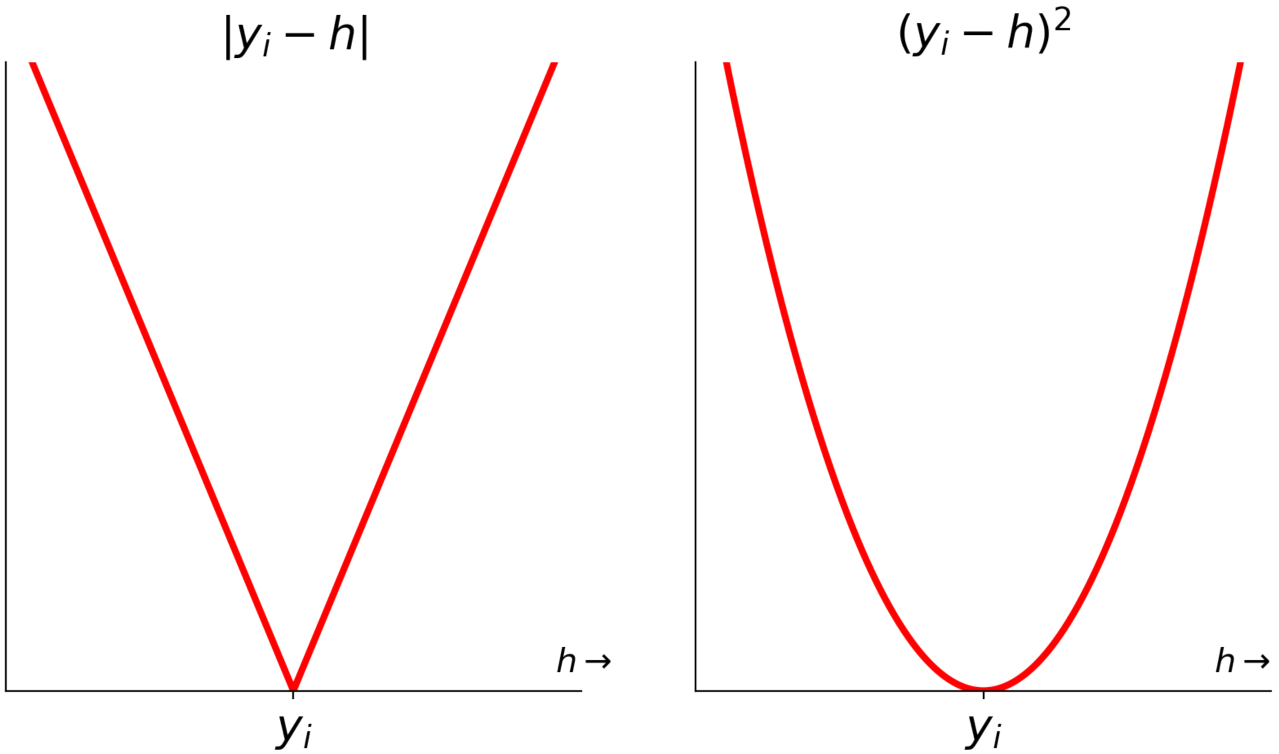
- The solution was to **square** the errors, so that all are non-negative. The resulting loss function is called **squared loss**.

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

- 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 **average absolute loss**, or **mean 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** (a new objective function).
- 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:

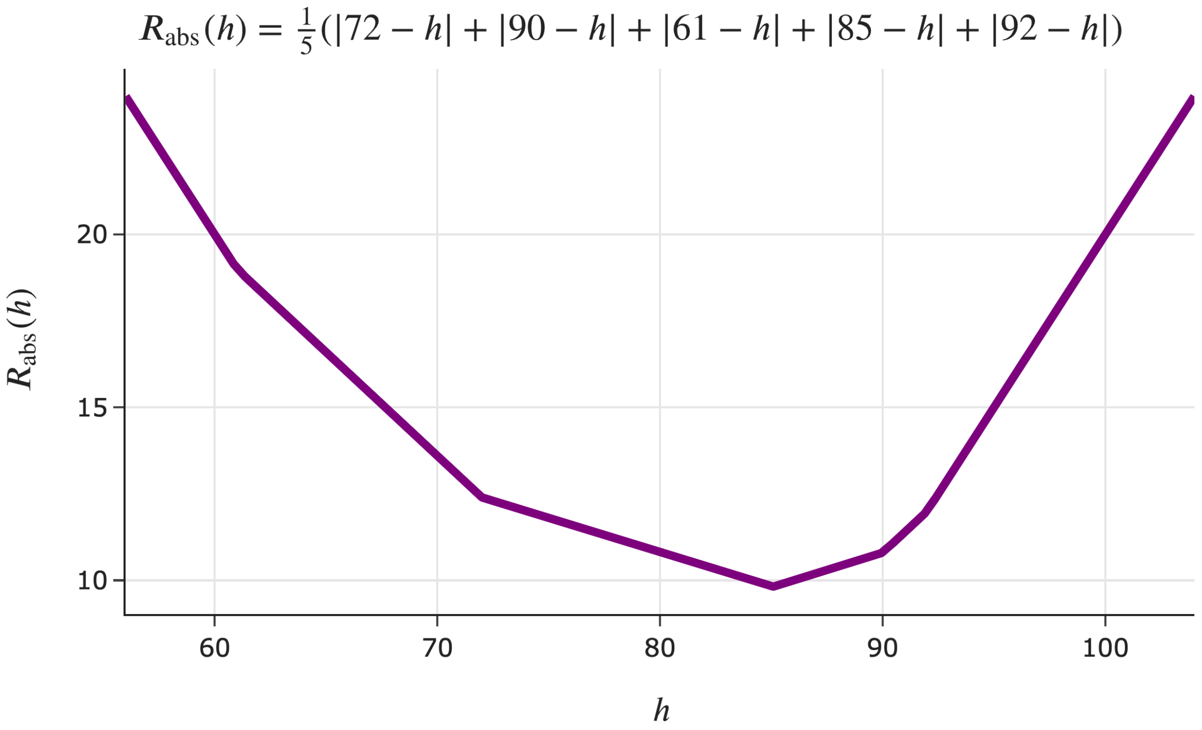
$$h^* = \text{Median}(y_1, y_2, \dots, y_n)$$

- 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

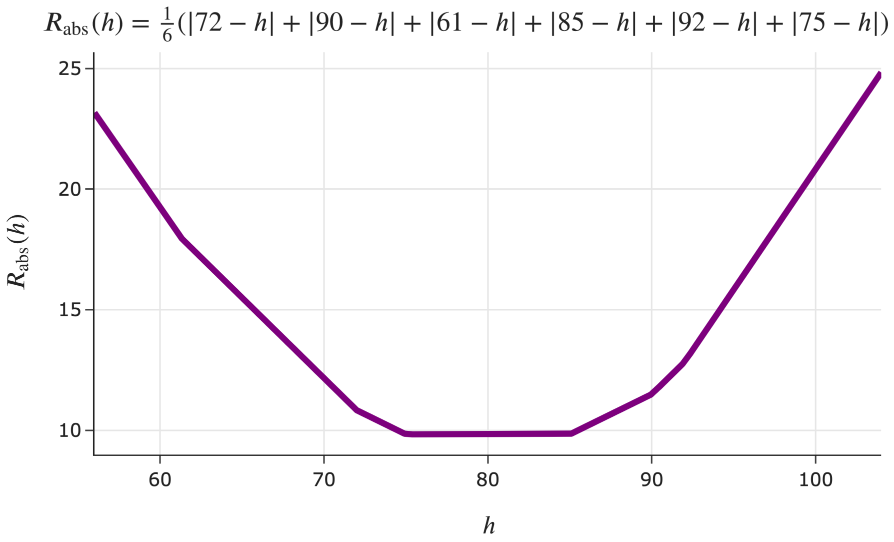


- Consider, again, our example dataset of five commute times.

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

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

Visualizing mean absolute error, with an even number of points



- What if we add a sixth data point?

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

- Is there a unique h^*?

The median minimizes mean absolute error!

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

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

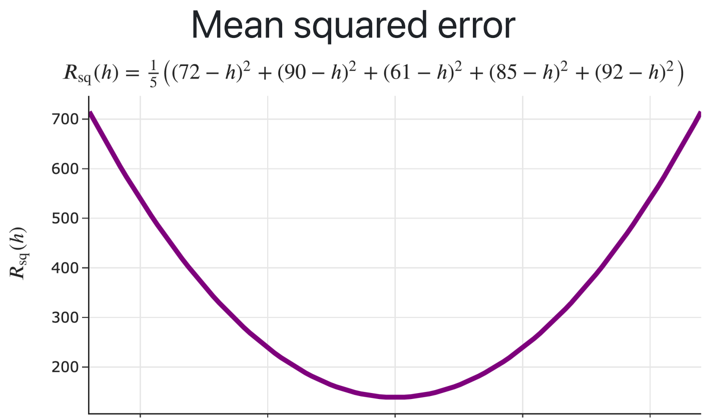
- The answer is:

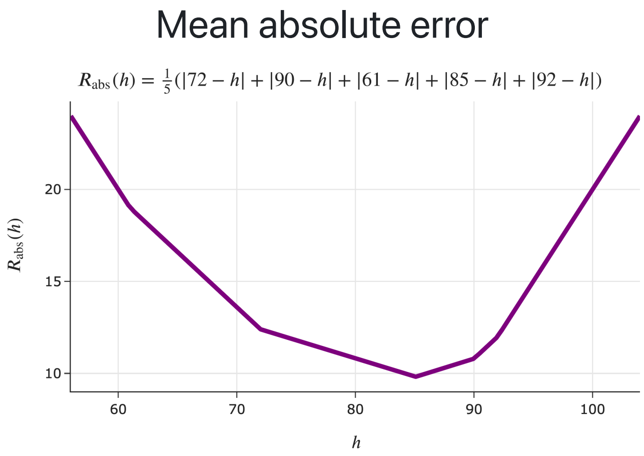
$$h^* = \text{Median}(y_1, y_2, \dots, y_n)$$

- 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 $H(x_i) = h$, the **mean** minimizes mean **squared** error.
- For the constant model $H(x_i) = h$, the **median** minimizes mean **absolute** error.
- In practice, squared loss is the more common choice, as the resulting objective function is more easily **differentiable**.





- But how does our choice of loss function impact the resulting optimal prediction?

Comparing the mean and median

- Consider our example dataset of 5 commute times.

$$y_1 = 72 \qquad y_2 = 90 \qquad y_3 = 61 \qquad y_4 = 85 \qquad y_5 = 92$$

- As of now, the **median is 85** and the **mean is 80**.
- What if we add 200 to the largest commute time, 92?

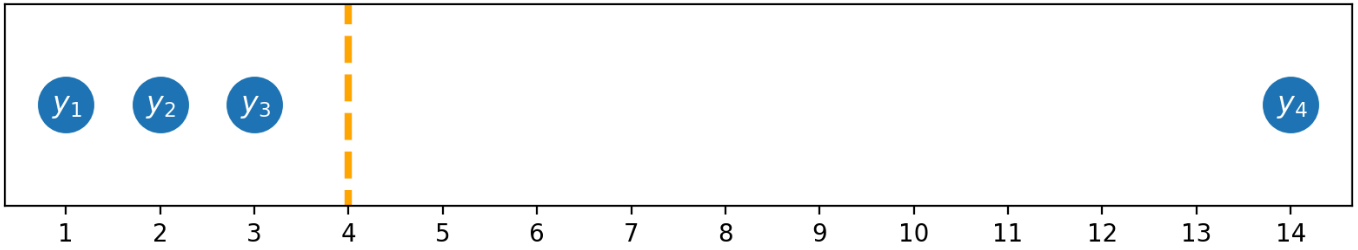
$$y_1 = 72 \qquad y_2 = 90 \qquad y_3 = 61 \qquad y_4 = 85 \qquad y_5 = 292$$

- Now, the median is but the mean is !
- **Key idea**: The mean is quite **sensitive** to outliers.

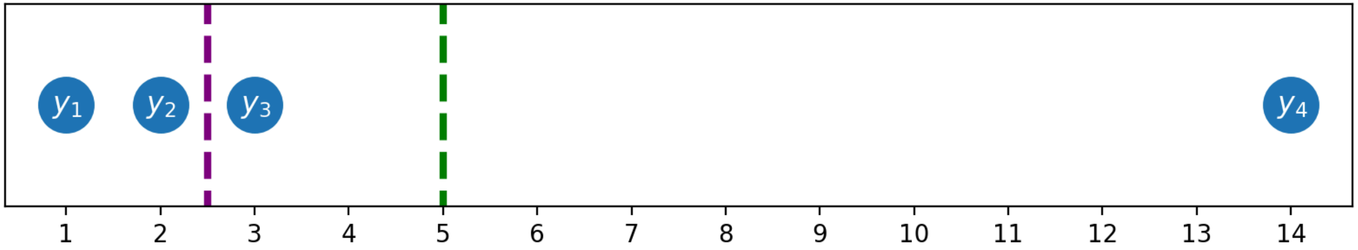
  But why?

Outliers

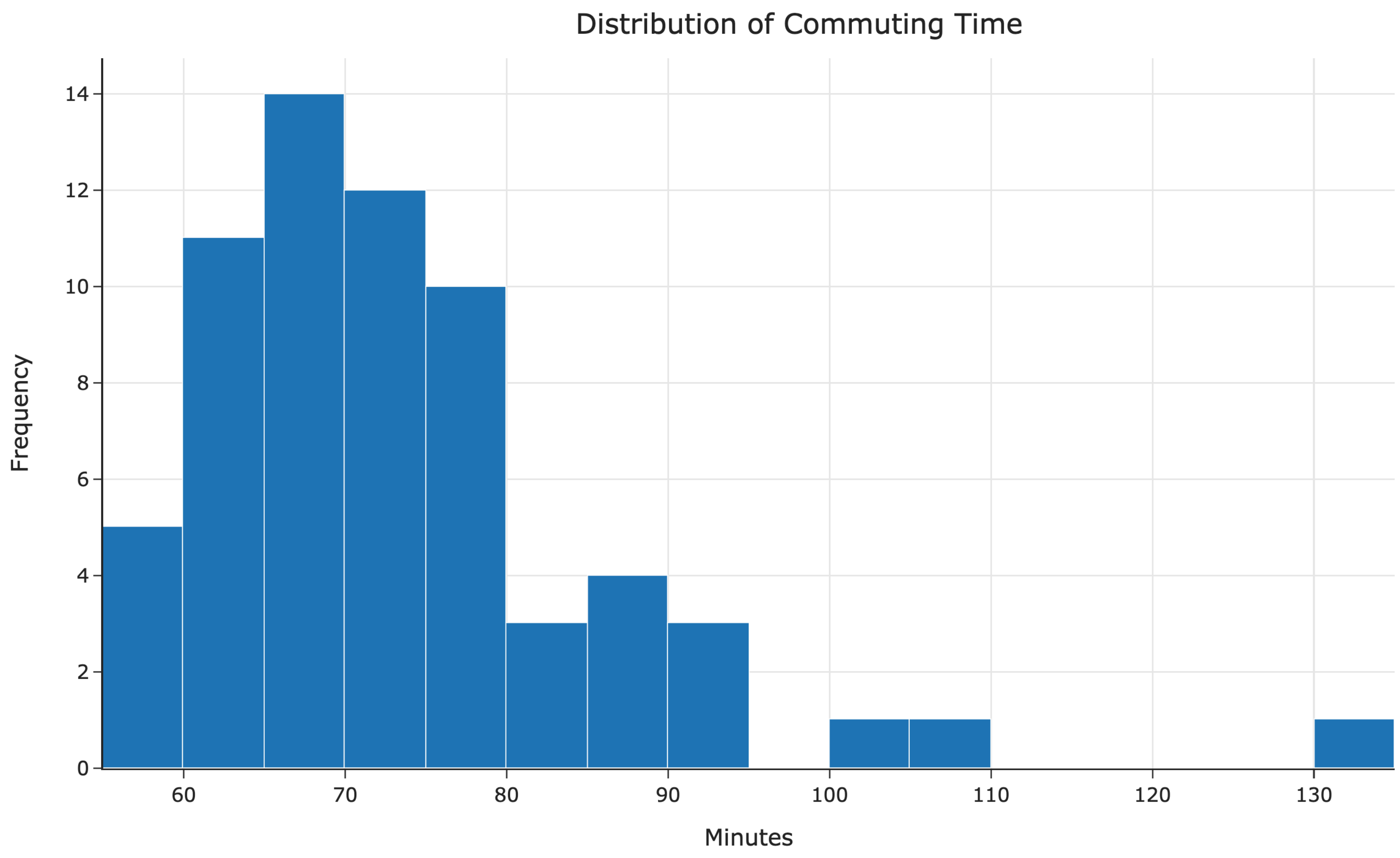
- Below, $|y_4 - h|$ is 10 times as big as $|y_3 - h|$, but $(y_4 - h)^2$ is 100 times $(y_3 - h)^2$.



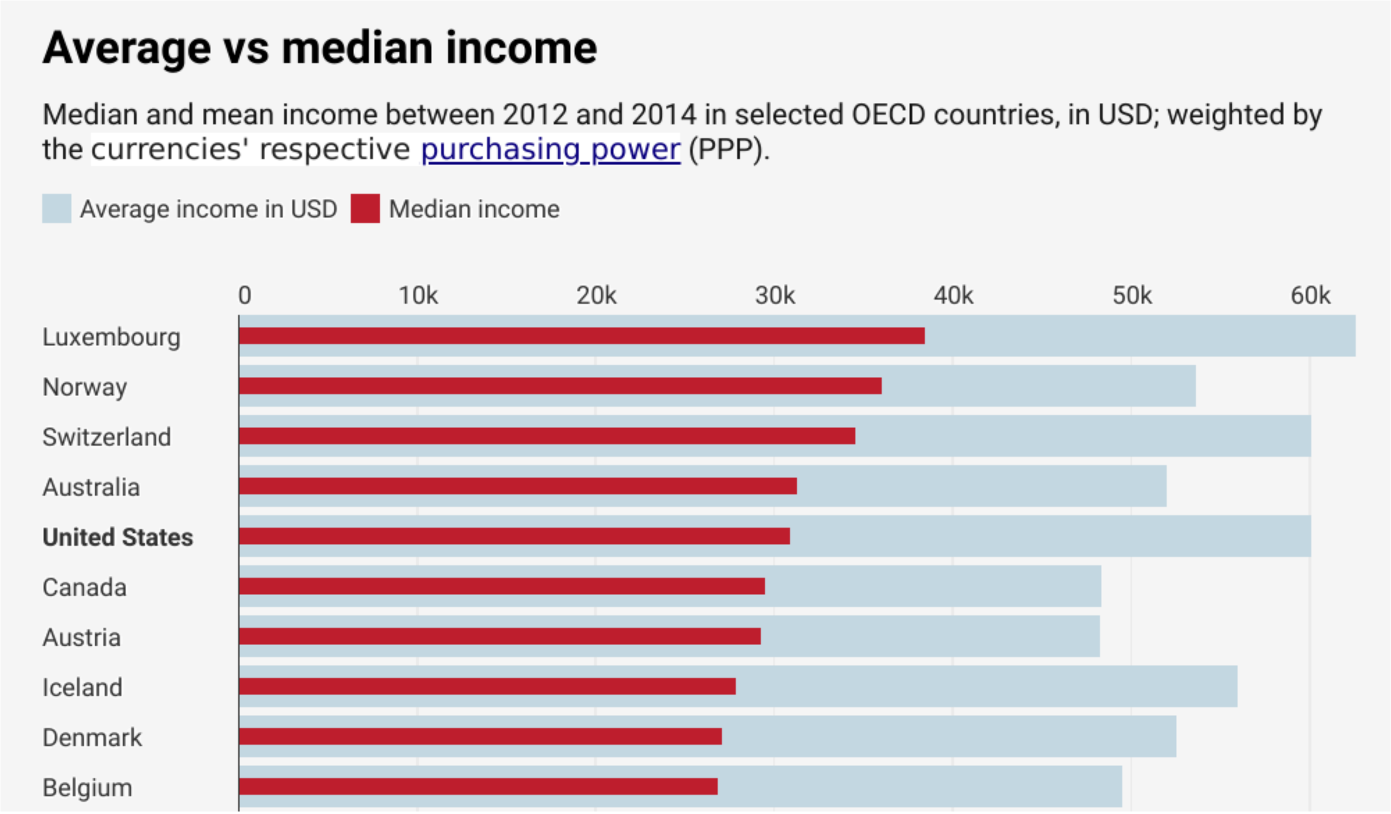
- The result is that the **mean** is "pulled" in the direction of outliers, relative to the **median**.



- As a result, we say the **median** – and absolute loss more generally – is **robust**.


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

Example: Income inequality



Summary: Choosing a loss function

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

Loss	Minimizer	Always Unique?	Robust to Outliers?	Differentiable?
$L_{\text{sq}}(y_i, h) = (y_i - h)^2$	mean	yes ✅	no ❌	yes ✅
$L_{\text{abs}}(y_i, h) = \lvert y_i - h \rvert$	median	no ❌	yes ✅	no ❌
$L_{0,1}(y_i, h) = \begin{cases} 0 & y_i = h \\ 1 & y_i \neq h \end{cases}$	mode	no ❌	yes ✅	no ❌
$L_\infty(y_i, h)$ See HW 6.	???	yes ✅	no ❌	no ❌

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

Question 🤔

Answer at practicaldsc.org/q

What questions do you have?