Lecture 2

Empirical Risk Minimization

DSC 40A, Spring 2024

Announcements

- Remember, there is no Canvas: all information is at dsc40a.com.
- Please fill out the Welcome Survey if you haven't already.
- Homework 1 will be released tomorrow, and is due on **Thursday, April 11th**.
    - With it, we will release an Overleaf template, where you can *type* your solutions using $\LaTeX$.
    - This is optional for most homeworks, but **required** for Homework 2, because it's a good skill to have.
- Look at the office hours schedule here and plan to start regularly attending!
- There are now readings linked on the course website for the next few weeks – read them for supplementary explanations.
    - They cover the same ideas, but in a different order and with different examples.

Agenda

- Recap: Mean squared error.
- Minimizing mean squared error.
- Another loss function.
- Minimizing mean absolute error.
- A practice exam problem (time permitting).

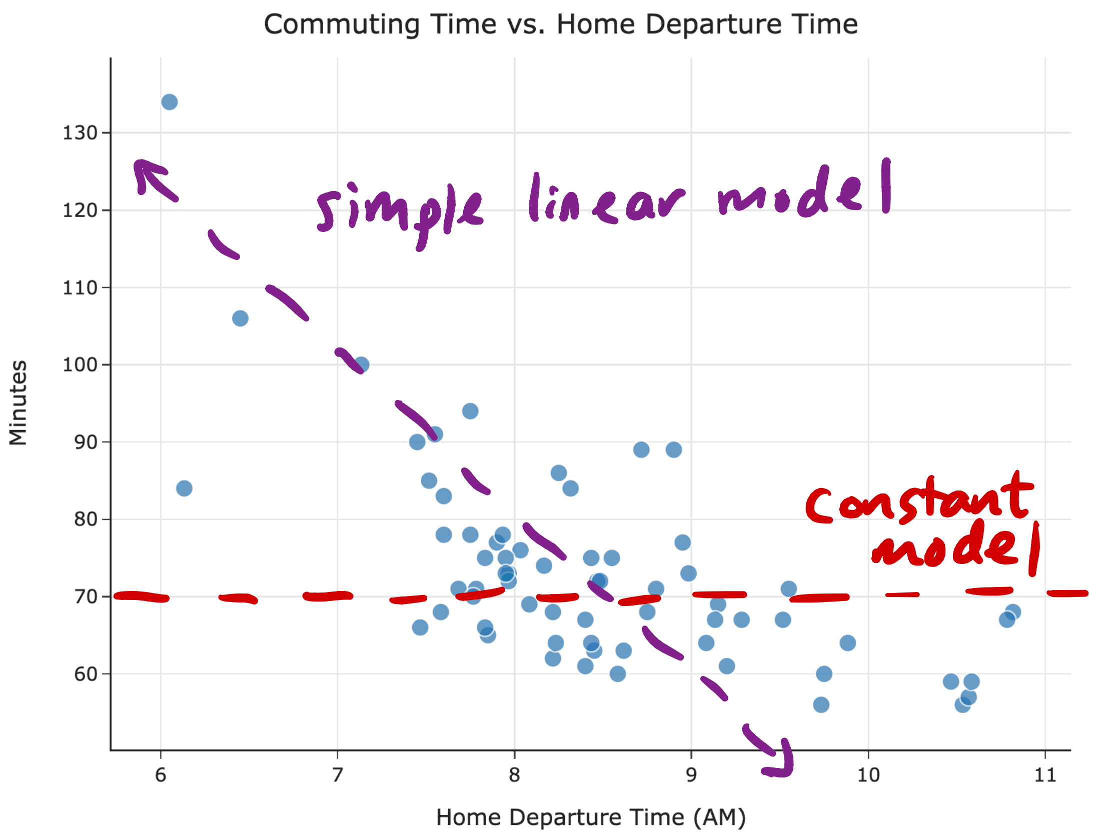
Question 🤔

Answer at q.dsc40a.com

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

Recap: Mean squared error

Overview



- We started by introducing the idea of a hypothesis function, $H(x)$.
- We looked at two possible models:
  - The constant model, $\underbrace{H(x) = h}$.
  - The simple linear regressionm model, $\underbrace{H(x) = w_0 + w_1 x}$.
- We decided to find the **best constant prediction** to use for predicting commute times, in minutes.

Mean squared error

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

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

- The **mean squared error** of the constant prediction h is:

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

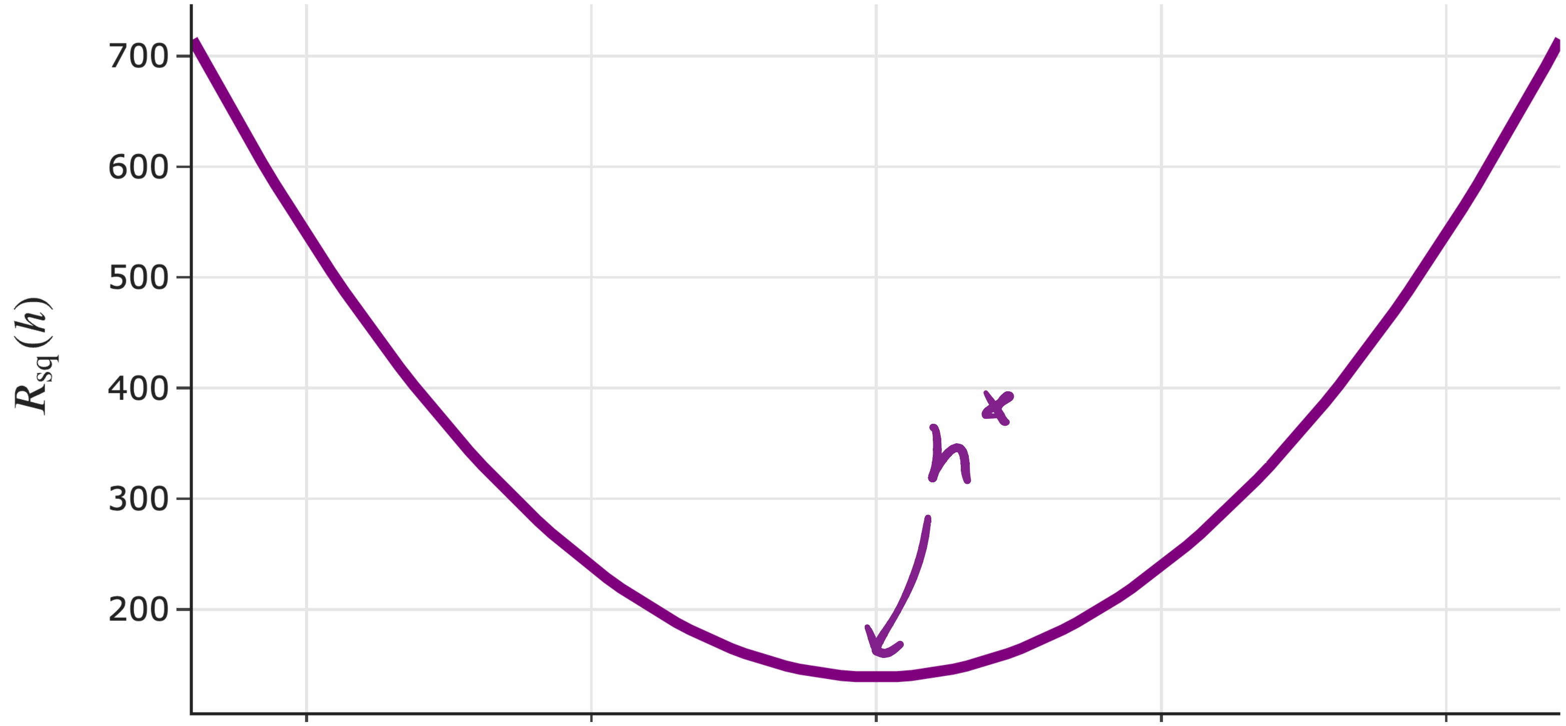
- For example, if we predict $h = 100$, then:

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

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

Visualizing mean squared error

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



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

The best prediction

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

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

- We want the **best** prediction, 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^*?**

using calculus!

Minimizing mean squared error

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 oof 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 $(y_i - h)^2$.

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

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

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

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

Question 🤔

Answer at q.dsc40a.com

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

Fact:

If $c(x) = k \cdot a(x)$, where k is some constant, then

$$\frac{d}{dx} c(x) = k \cdot \frac{d}{dx} a(x)$$

$\Rightarrow$ we can pull the constant in front!

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 $R_{\text{sq}}(h)$

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

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

← from two slides ago!

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

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

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

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

multiply both sides by $\left(-\frac{n}{2}\right)$

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

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

$$= nh$$

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

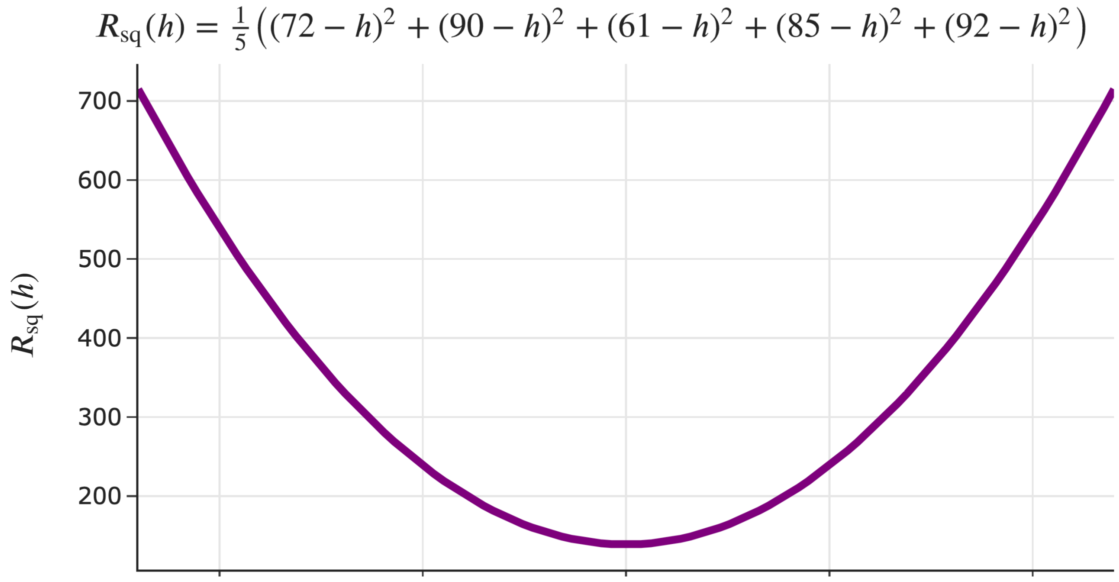
$$\sum_{i=1}^{n} y_i - nh = 0$$

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

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

$$= \text{Mean}(y_1, y_2, \dots, y_n)$$

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.

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

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

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

So, $R_{sq}(h)$ opens upwards, so 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:

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

"y bar"

- 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

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

is

"the argument 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**.

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.

$H(x) = h$

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

2. Choose a loss function.

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

Another choice?

3. Minimize average loss to find optimal model parameters.

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

Another optimal model parameter, h^*?

Question 🤔

Answer at q.dsc40a.com

What questions do you have?

Another loss function

Another loss function

- Last lecture, 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.

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

- 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**.

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

80, the mean of the ys, minimizes the average squared loss

⇒ but not necessarily the average absolute loss!

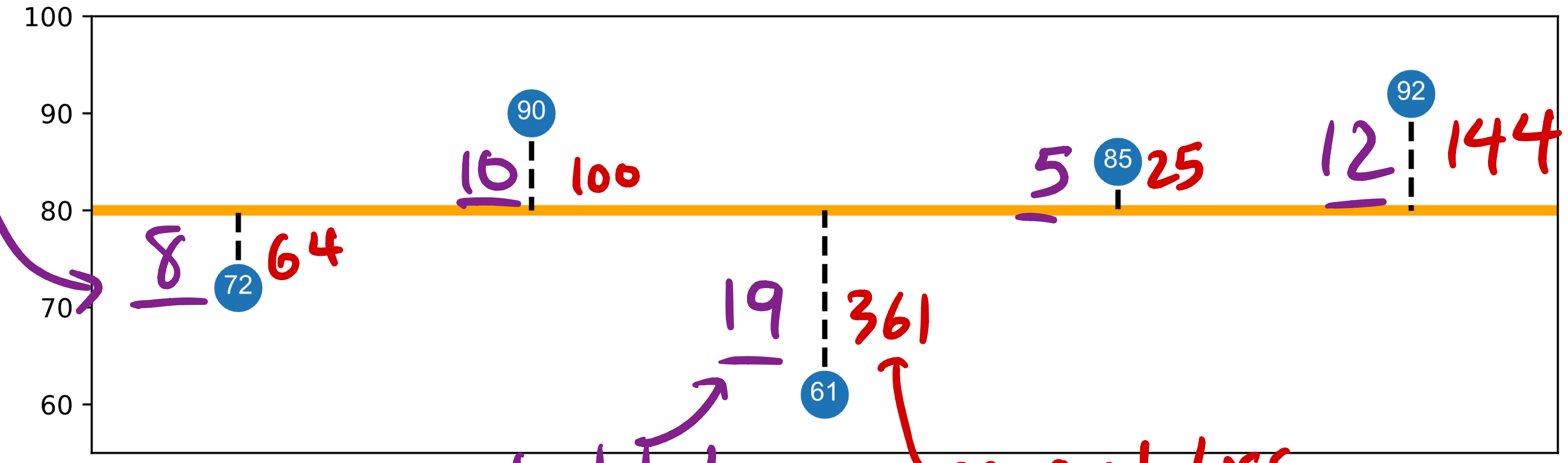
Squared loss vs. absolute loss

For the constant model, $H(x_i) = h$, so we can simplify our loss functions as follows:

- Squared loss: $L_{\text{sq}}(y_i, h) = (y_i - h)^2$.
- Absolute loss: $L_{\text{abs}}(y_i, h) = |y_i - h|$.

Consider, again, our example dataset of five commute times and the prediction $h = 80$.

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



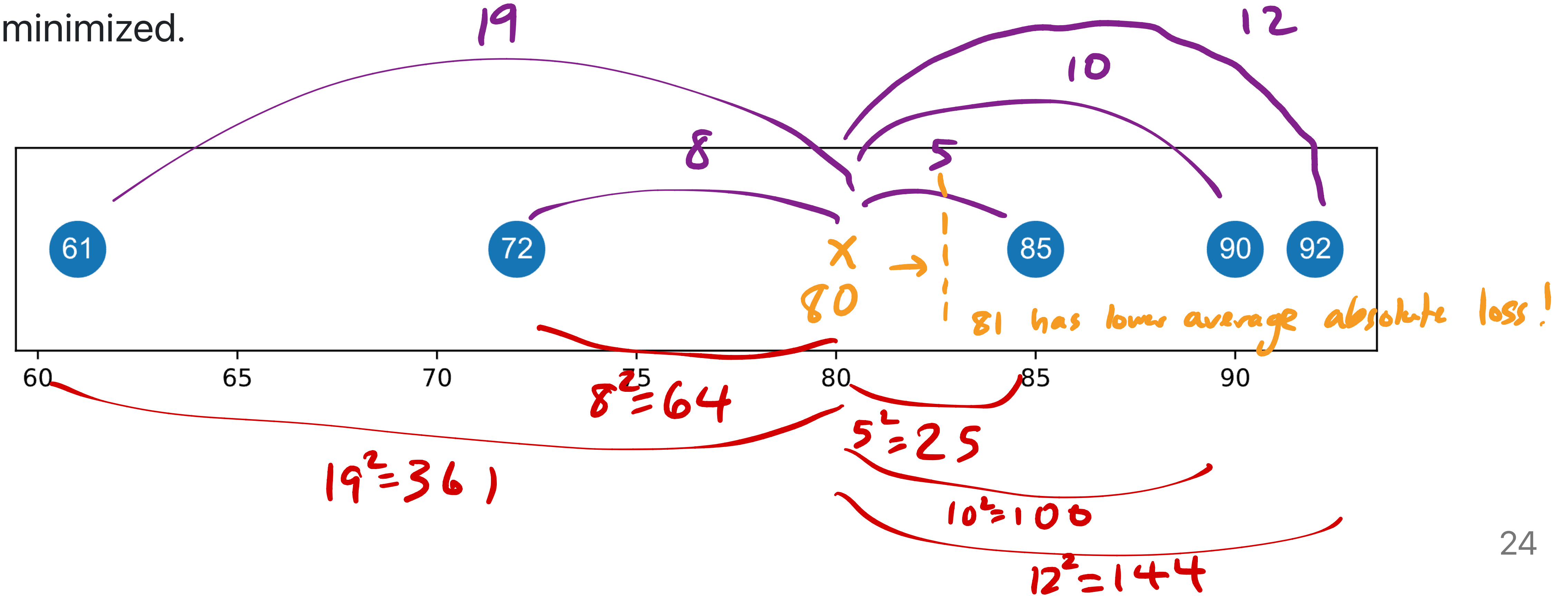
← mean(y)

absolute loss

squared loss

Squared loss vs. absolute loss

- When we use squared loss, h^* is the point at which the average squared loss is minimized.
- When we use absolute loss, h^* is the point at which the average absolute loss is minimized.



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 prediction, h^*.
- Previously, we used calculus to find the optimal model parameter h^* that minimized R_{sq} – that is, when using squared loss.
- Can we use calculus to minimize $R_{\text{abs}}(h)$, too?

Minimizing mean absolute error

Minimizing using calculus, again

We'd like to minimize:

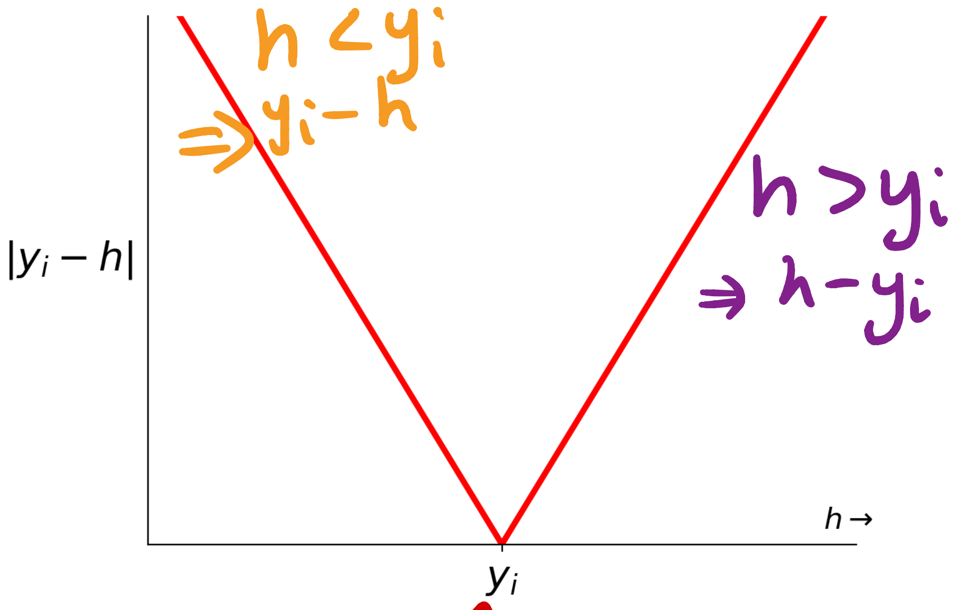
$$R_{\text{abs}}(h) = \frac{1}{n} \sum_{i=1}^{n} \underbrace{|y_i - h|}$$

first, find the derivative of the individual loss!

In order to minimize $R_{\text{abs}}(h)$, 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 $|y_i - h|$



when $h = y_i$,

$|y_i - h| = |0| = 0$

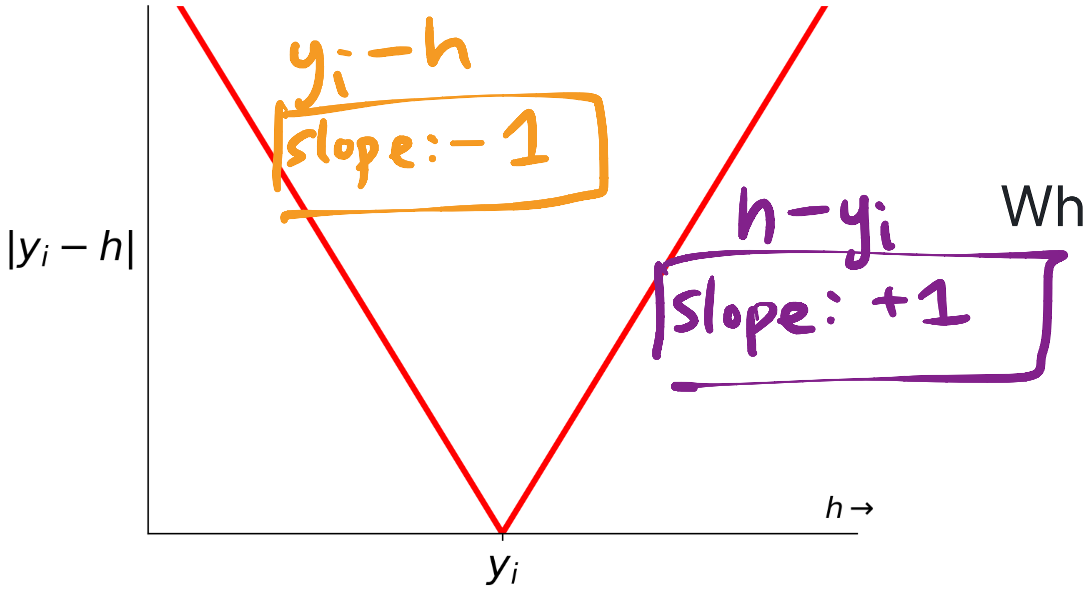
Remember that $|x|$ is a **piecewise linear** function of x:

$$|x| = \begin{cases} x & x > 0 \\ 0 & x = 0 \\ -x & x < 0 \end{cases}$$

So, $|y_i - h|$ is also a piecewise linear function of h:

$$|y_i - h| = \begin{cases} y_i - h & h < y_i \\ 0 & y_i = h \\ h - y_i & h > y_i \end{cases}$$

Step 0: The "derivative" of $|y_i - h|$



$$|y_i - h| = \begin{cases} y_i - h & h < y_i \\ 0 & y_i = h \\ h - y_i & h > y_i \end{cases}$$

What is $\frac{d}{dh}|y_i - h|$?

$$\frac{d}{dh}|y_i - h| = \begin{cases} -1 & h < y_i \\ \text{undefined!!!} & y_i = h \\ +1 & h > y_i \end{cases}$$

ignore for now!

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

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

$$\frac{d}{dh}|y_i - h| = \begin{cases} -1 & h < y_i \\ \text{undefined!!!} & y_i = h \\ +1 & h > y_i \end{cases}$$

ignore for now!

$$= \frac{1}{n}\underbrace{\sum_{i=1}^{n}\frac{d}{dh}|y_i - h|}$$

a sum of a bunch of +1s and −1s!

we +1 whenever $h > y_i$, and −1 whenever $h < y_i$.

$$= \frac{1}{n}\left[\#(h > y_i) - \#(h < y_i)\right]$$

slope of mean absolute error

IMPORTANT!

Example $h = 79$

61	72	85	90	92

$$\frac{d}{dh}R(79) = \frac{2-3}{5} = -\frac{1}{5}$$

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

$$\frac{d}{dh} R_{abs}(h) = \frac{1}{n}\left[\#(h > y_i) - \#(h < y_i)\right] = 0$$

multiply both sides by n

$$\Rightarrow \boxed{\#(h > y_i)} = \boxed{\#(h < y_i)}$$

The h^* that minimizes mean absolute error is the one where

\# points to the left of h

=

\# points to the right of h

$\Rightarrow$ $\boxed{\text{median!}}$

The median minimizes mean absolute error!

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

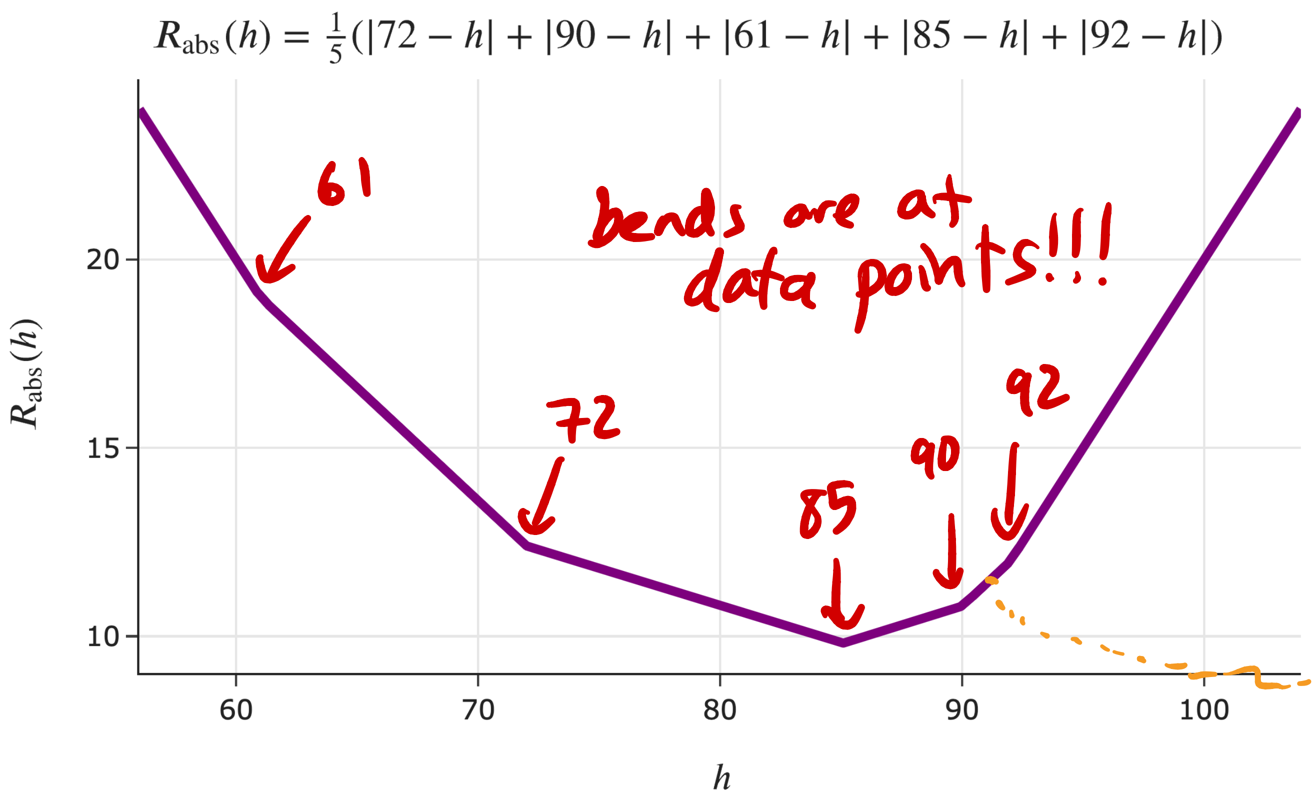
$$R_{\text{abs}}(h) = \frac{1}{n} \sum_{i=1}^{n} |y_i - h|$$

- The answer is:

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

- This is because the median has an equal number of data points to the left of it and to the right of 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.

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

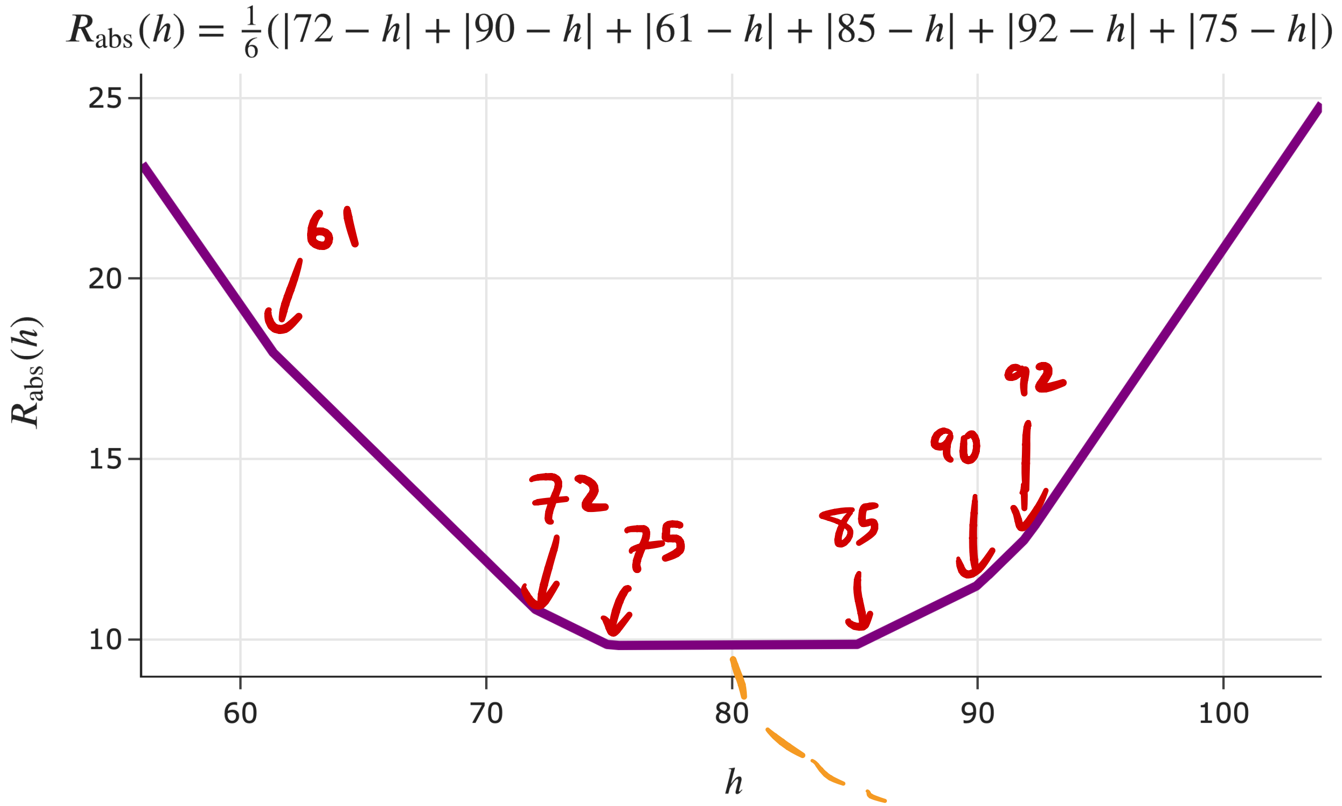
Where are the "bends" in the graph of $R_{\text{abs}}(h)$ – that is, where does its slope change?

$$\frac{d}{dh} R_{\text{abs}}(h) = \frac{1}{n}\left[\#\text{left} - \#\text{right}\right]$$

$$\frac{d}{dh} R_{\text{abs}}(91) = \frac{1}{5}\left[4 - 1\right]$$

$$= \frac{3}{5}$$

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^*?

No, h^* is not unique!

Any value in the range

$75 \leq h^* \leq 85$

minimizes mean absolute error!

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.

The modeling recipe, again

We've now made two full passes through our "modeling recipe."

1. Choose a model.

   $H(x) = h$

2. Choose a loss function.

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

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

3. Minimize average loss to find optimal model parameters.

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

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

Empirical risk minimization

- The formal name for the process of minimizing average loss is **empirical risk minimization**.
- Another name for "average loss" is **empirical risk**.
- When we use the squared loss function, $L_{\text{sq}}(y_i, h) = (y_i - h)^2$, the corresponding empirical risk is mean squared error:

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

- When we use the absolute loss function, $L_{\text{abs}}(y_i, h) = |y_i - h|$, the corresponding empirical risk is mean absolute error:

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

Empirical risk minimization, in general

Key idea: If $L(y_i, h)$ is **any** loss function, the corresponding empirical risk is:

$$R(h) = \frac{1}{n} \sum_{i=1}^{n} L(y_i, h)$$

Question 🤔

Answer at q.dsc40a.com

What questions do you have?

Summary, next time

- $h^* = \text{Mean}(y_1, y_2, \ldots, y_n)$ minimizes mean squared error, $R_\text{sq}(h) = \frac{1}{n} \sum_{i=1}^n (y_i - h)^2$.
- $h^* = \text{Median}(y_1, y_2, \ldots, y_n)$ minimizes mean absolute error, $R_\text{abs}(h) = \frac{1}{n} \sum_{i=1}^n |y_i - h|$.
- $R_\text{sq}(h)$ and $R_\text{abs}(h)$ are examples of **empirical risk** – that is, average loss.
- **Next time**: What's the relationship between the mean and median? What is the significance of $R_\text{sq}(h^*)$ and $R_\text{abs}(h^*)$?

A practice exam problem

An exam problem? Already?

- Homework 1 is going to be released tomorrow.
- In it, you'll be asked to *show* or *prove* that various facts hold true – but you may have never done this before!
- To help you practice, we'll walk through an old exam problem together.
- We'll be releasing another problem walkthrough video sometime over the weekend, that also shows you how to use the Overleaf template and type up your solutions.

Define the extreme mean (EM) of a dataset to be the average of its largest and smallest values. Let $f(x) = -3x + 4$.

Show that for any dataset $x_1 \leq x_2 \leq \ldots \leq x_n$,

$$\mathrm{EM}(f(x_1), f(x_2), \ldots, f(x_n)) = f(\mathrm{EM}(x_1, x_2, \ldots, x_n))$$