Lecture 2

Empirical Risk Minimization

DSC 40A, Summer 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 is released, and is due on **Friday, August 9th**.
    - We will soon 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).

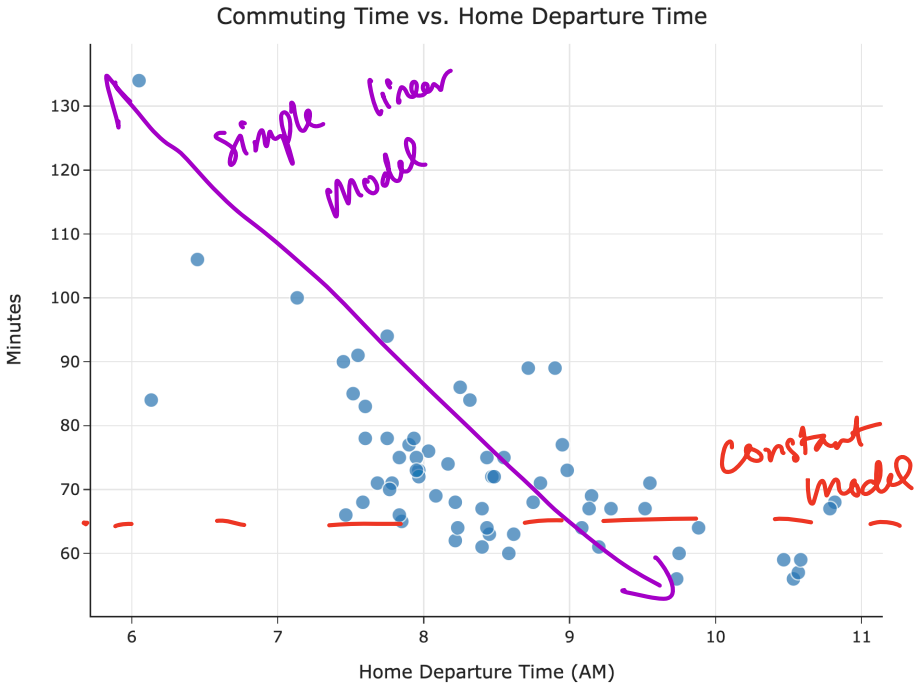
Question 🤔

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, $H(x) = h$.
  - The simple linear regression model, $H(x) = w_0 + w_1 x$.
- 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: $H(x) = h$

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

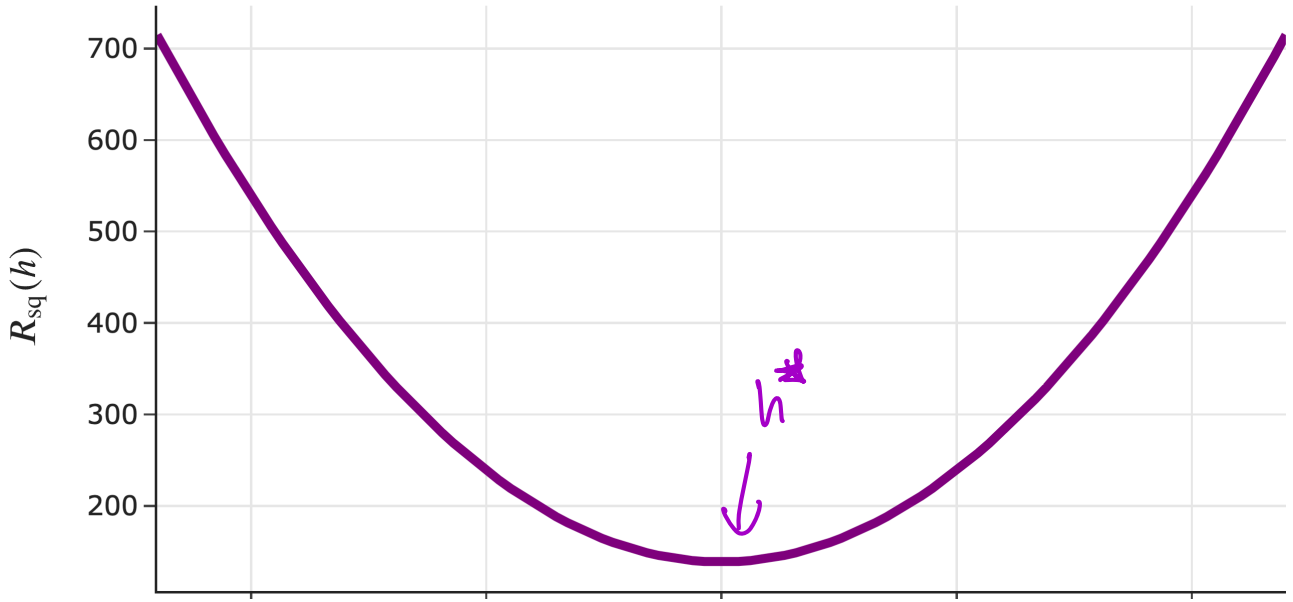
- For example, if we predict $h = 100$, then:

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

- **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:

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

↳ for i in range (1, n+1):

- 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
  - $\frac{d}{dx}c(x) = \frac{d}{dx}a(x) + \frac{d}{dx}b(x)$.

derivative of a sum is sum of the derivative

- 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 $(y_i - h)^2$.

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

Question 🤔

Answer at q.dsc40a.com

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

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

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

Fact: if $c(x) = k \cdot a(x)$ where k is a constant

then $\frac{\partial}{\partial x} c(x) = k \frac{\partial}{\partial x} a(x)$

⇒ we can pull the constant in front

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

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

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

Know from before

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

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

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

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

multiply both sides by $\frac{-n}{2}$

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

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

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

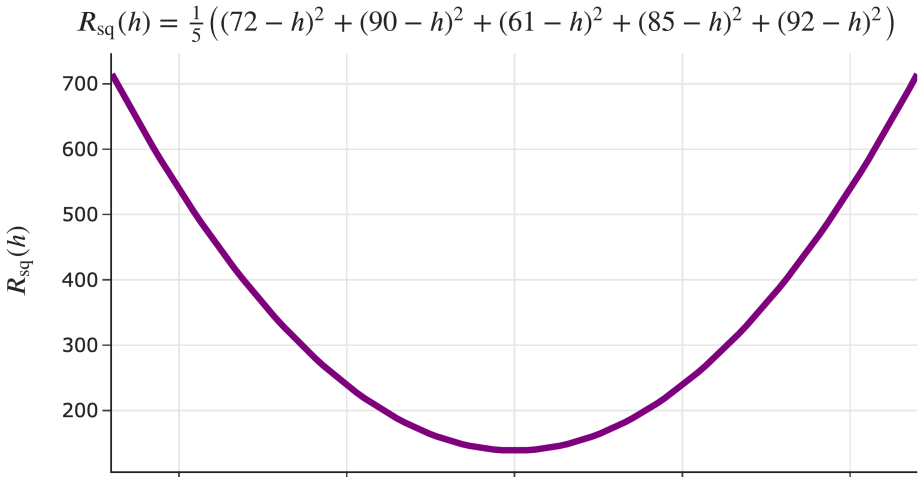
$$\sum_{i=1}^{n} y_i - n \cdot h = 0$$

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

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

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

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.

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

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

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

So $R_{sq}(h)$ opens up : 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:

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

"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

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

"the input argument that minimizes"

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

argmax

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:

$H(x) = w_0 + w_1 \cdot x$

2. Choose a loss function.

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

($H(x_i)$ for h; $H(x_i)$ for the squared term)

Another choice? Soon!

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.

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

actual

predicted

$H(x_i)$ ($w_0 + w_1 x$)

(w)

- 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**.

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

Squared loss vs. absolute loss

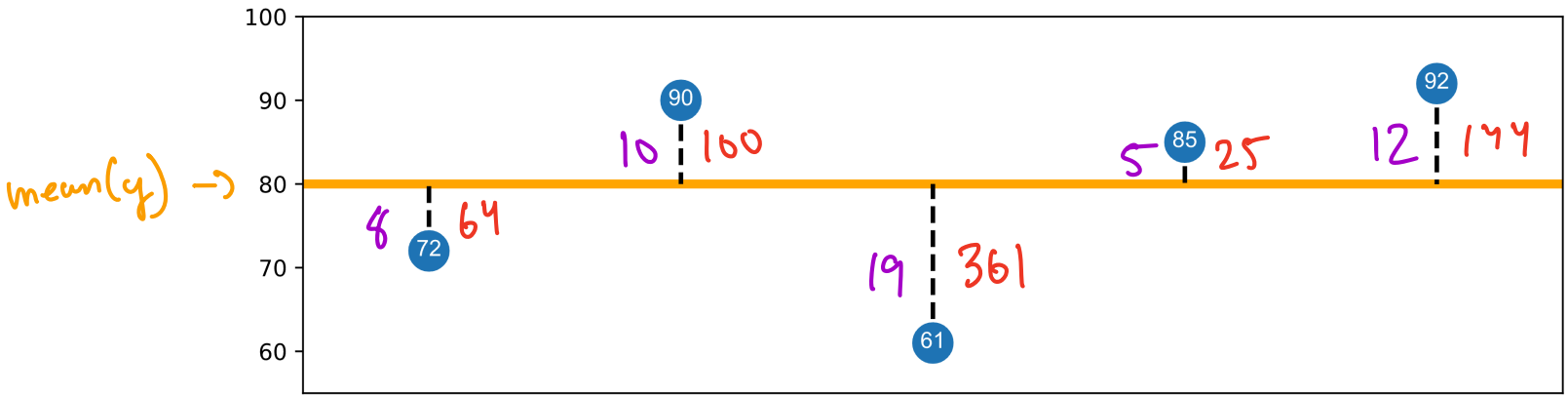
80 = $\bar{y}$, mean of the y_is
minimizes mean squared loss

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

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

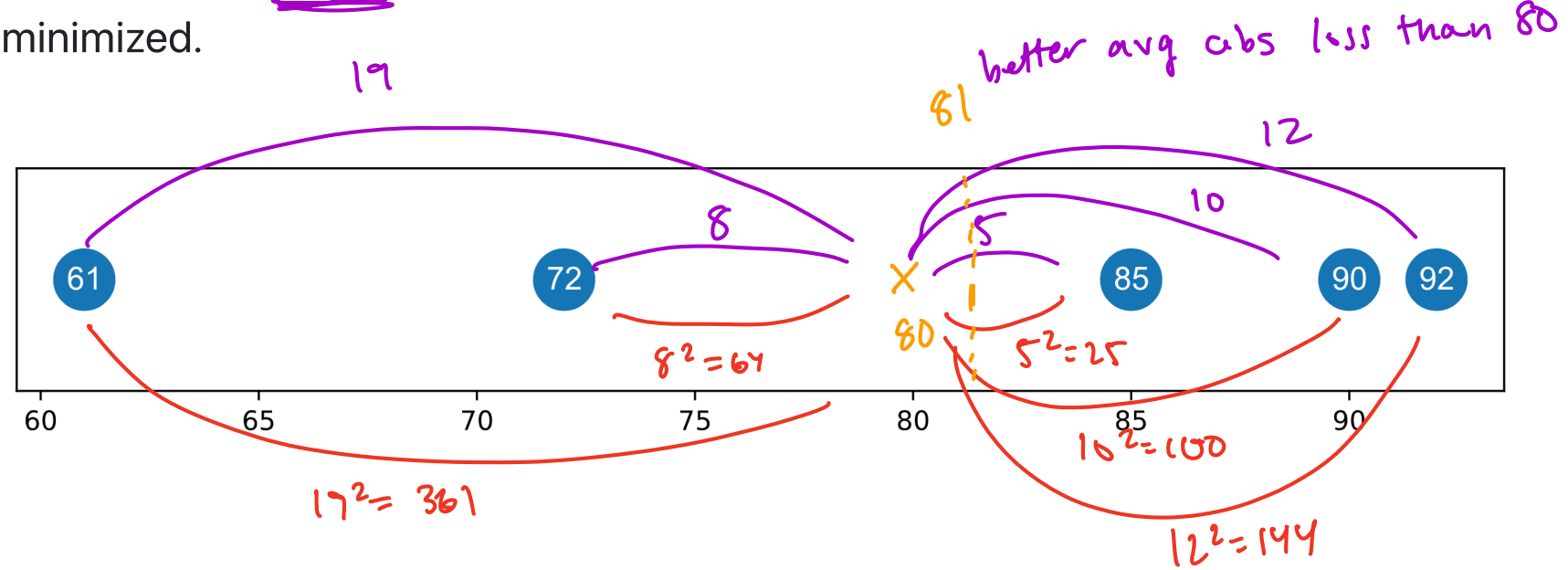
Consider, again, our example dataset of five commute times and the prediction $h = 80$.

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



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 **<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 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:

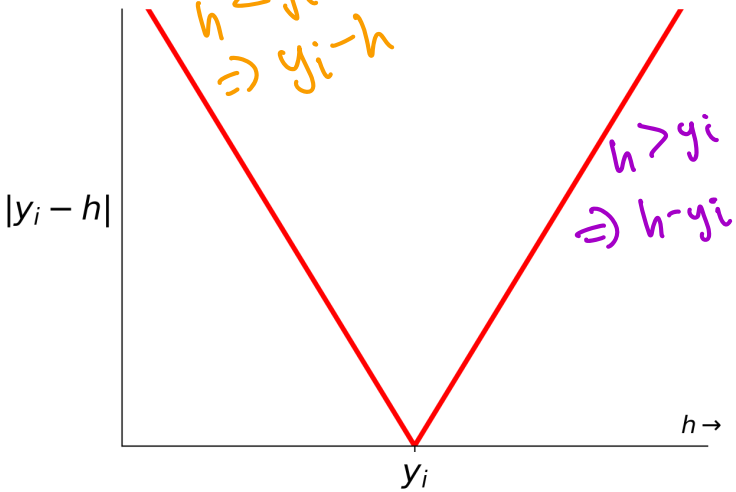
$$R_{\text{abs}}(h) = \frac{1}{n}\sum_{i=1}^{n}|y_i - h|$$

find 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 $|y_i - h|$



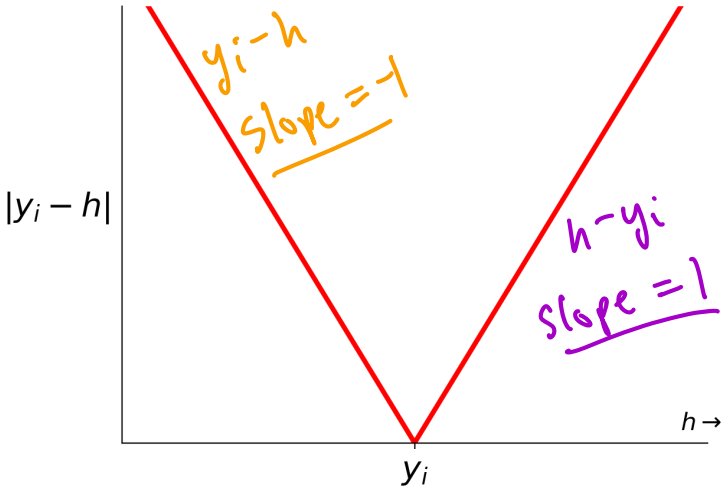
Remember that $|x|$ is a **piecewise linear** function of x:

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

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

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

- -1 : $h < y_i$
- ?? : $y_i = h$
- 1 : $h > y_i$

undefined, ignore for now

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

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

$\frac{d}{dh}|y_i - h| = \begin{cases} -1 & h < y_i \\ ?? & y_i = h \\ 1 & h > y_i \end{cases}$

undefined, ignore for now

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

Sum of a bunch of +1s and −1s

+1 when $h > y_i$

−1 when $h < y_i$

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

"slope of mean absolute error"

Important!

Ex

79 = h

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^*

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

$$\Rightarrow \#(h > y_i) = \#(h < y_i)$$

The h^* that minimizes mean absolute error for $H(x) = h$ is the value where

points left of h = # points right of h $\Rightarrow$ median!

The median minimizes mean absolute error!

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

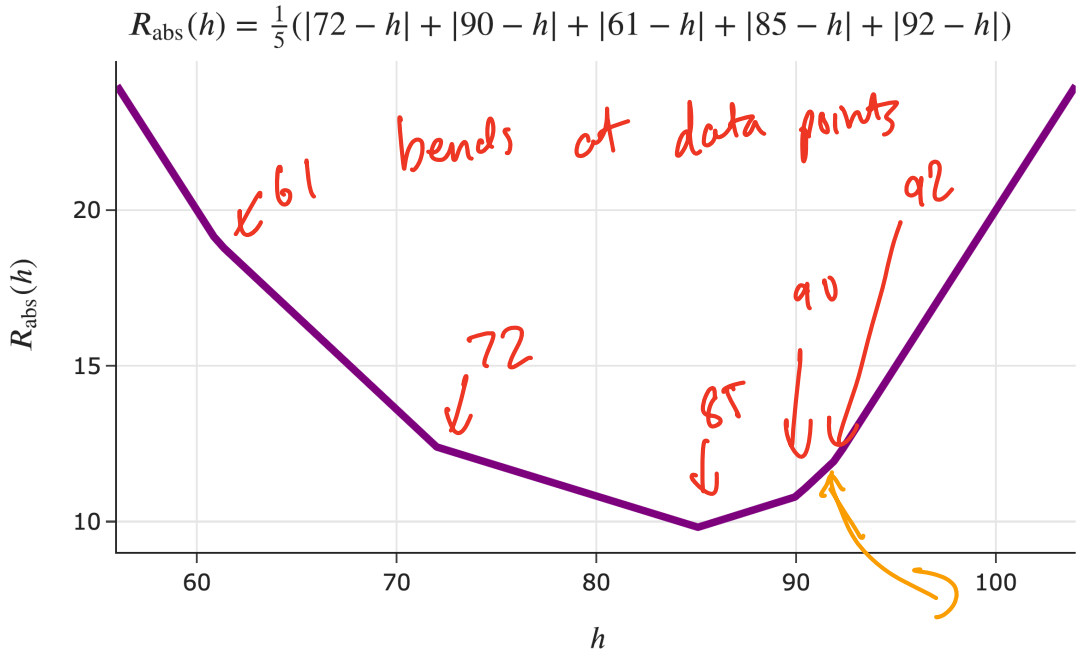
$$R_{\text{abs}}(h) = \frac{1}{n} \sum_{i=1}^{n} |y_i - h|$$

- 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.

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

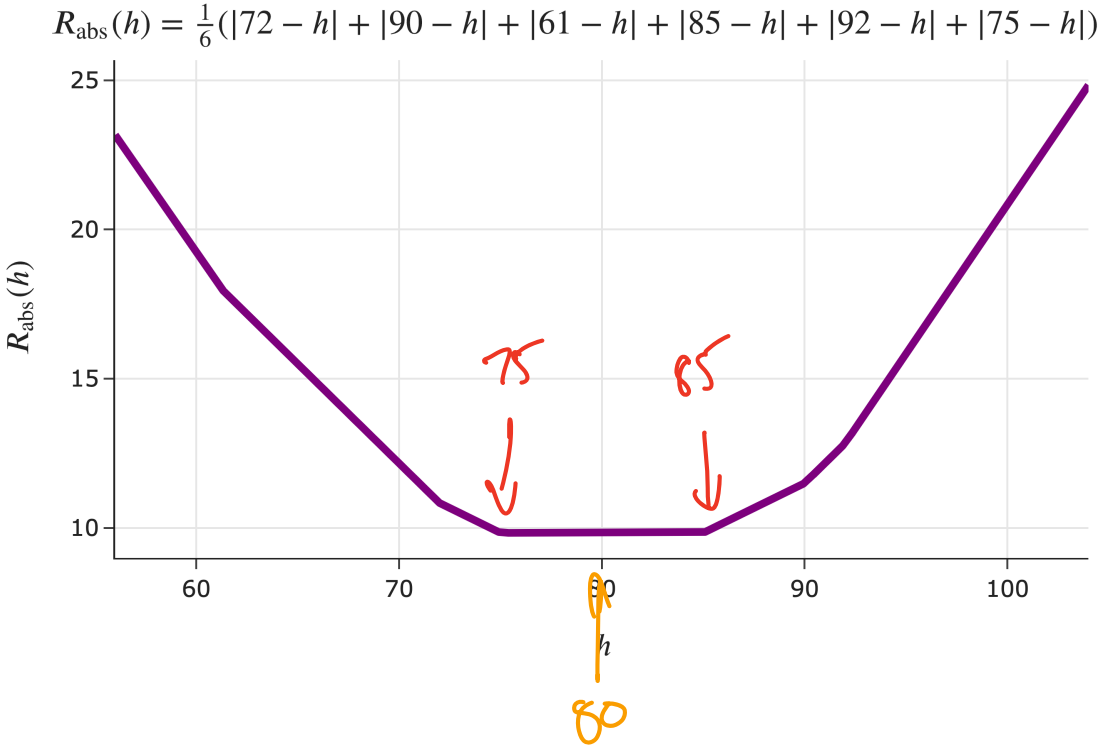
Where are the "bends" in the graph of $R_{\text{abs}}(h)$ – that is, where does its slope change?

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

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

$= \frac{3}{5}$

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 unique h^*

Any h^* in range

80 ✓

$75 \leq h^* \leq 85$

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:

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

- 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.

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:

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

single datum

all data

Question 🤔

Answer at q.dsc40a.com

What questions do you have?

RMSE = root mean squared error $\Rightarrow \sqrt{\text{MSE}}$

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

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

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.~~ released.
- 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 $x_1 \leq x_2 \leq \ldots \leq x_n$,

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

$f(x) = -3x + 4$

$\text{EM}(\{x_i\}) = \frac{x_1 + x_n}{2}$

$f\left(\frac{x_1 + x_n}{2}\right)$

$-3\left(\frac{x_1 + x_n}{2}\right) + 4$

$\text{EM}(-3x_1 + 4, -3x_2 + 4, \ldots, -3x_n + 4)$

largest smallest

$\Downarrow$

$\frac{(-3x_1 + 4) + (-3x_n + 4)}{2} = \frac{-3x_1 - 3x_n}{2} + 4 = -3\left(\frac{x_1 + x_n}{2}\right) + 4$