Lecture 3 – Mean Squared Error and Empirical Risk Minimization

DSC 40A, Fall 2022 @ UC San Diego

Dr. Truong Son Hy, with help from **many others**

Announcements

- Look at the readings linked on the course website!
- First Discussion: Monday, October 3rd 2022
  First Homework Release: Friday September 30th 2022
  First Groupwork Release: Thursday September 29th 2022
  Groupwork Relsease Day: Thursday afternoon
  Groupwork Submission Day: Monday midnight
  Homework Release Day: Friday after lecture
  Homework Submission Day: Friday before
- See `dsc40a.com/calendar` for the Office Hours schedule.

Agenda

- Recap from Lecture 2 – minimizing mean absolute error and formulating mean squared error.
- Minimizing mean squared error.
- Comparing the median to the minimizer of mean squared error.
- Empirical risk minimization.

Recap from Lecture 2

The median minimizes mean absolute error

- Our problem was: find h^* which minimizes the mean absolute error, $R(h) = \frac{1}{n} \sum_{i=1}^{n} |y_i - h|$.
- **Regardless of if n is odd or even**, the answer is $h^* = \text{Median}(y_1, \ldots, y_n)$. The **best prediction**, in terms of mean absolute error, is the **median**.
  - When n is odd, this answer is unique.
  - When n is even, any number between the middle two data points also minimizes mean absolute error.
  - We define the median of an even number of data points to be the mean of the middle two data points.

The mean absolute error is not differentiable

- We can't compute $\frac{d}{dh}|y_i - h|$.
- Remember: $|y_i - h|$ measures how far h is from y_i.
- **Question:** Is there something besides $|y_i - h|$ which:
  1. Measures how far h is from y_i, *and*
  2. is **differentiable**?

The mean absolute error is not differentiable

- We can't compute $\frac{d}{dh}|y_i - h|$.

- Remember: $|y_i - h|$ measures how far h is from y_i.

- **Question:** Is there something besides $|y_i - h|$ which:
  1. Measures how far h is from y_i, *and*
  2. is **differentiable**?
- **Answer:** **Squared error**.

The squared error

- Let h be a prediction and y be the true value (i.e. the "right answer"). The **squared error** is:

$$|y - h|^2 = (y - h)^2$$

- Like absolute error, squared error measures how far h is from y.

- But unlike absolute error, the squared error is **differentiable**:

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

The squared error

- Let h be a prediction and y be the true value (i.e. the "right answer"). The **squared error** is:

$$|y - h|^2 = (y - h)^2$$

- Like absolute error, squared error measures how far h is from y.

- But unlike absolute error, the squared error is **differentiable**:

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

The new idea

- Find h^* by minimizing the **mean squared error**:

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

- Strategy: Take the derivative, set it equal to zero, and solve for the minimizer.

Minimizing mean squared error

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

Discussion Question

Which of these is dR_{sq}/dh?

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

b) 0

c) $\sum_{i=1}^{n} y_i$

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

Answer: D

Solution

We have:

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

Remember that $(c \cdot f)'(x) = c \cdot f'(x)$ where c is a constant wrt x:

Solution

We have:

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

Remember that $(c \cdot f)'(x) = c \cdot f'(x)$ where c is a constant wrt x:

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

Remember that $(\sum_i f_i)'(x) = \sum_i f_i'(x)$:

Solution

We have:

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

Remember that $(c \cdot f)'(x) = c \cdot f'(x)$ where c is a constant wrt x:

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

Remember that $(\sum_i f_i)'(x) = \sum_i f_i'(x)$:

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

Set to zero and solve for minimizer

Equation:

$$\frac{dR_{\text{sq}}}{dh} = 0$$

We need to solve this equation to find the criticial point**s**.

Set to zero and solve for minimizer

Equation:

$$\frac{dR_{\text{sq}}}{dh} = 0$$

We need to solve this equation to find the criticial points.

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

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

Set to zero and solve for minimizer

Equation:

$$\frac{dR_{\text{sq}}}{dh} = 0$$

We need to solve this equation to find the criticial point**s**.

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

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

Set to zero and solve for minimizer

Equation:

$$\frac{dR_{\text{sq}}}{dh} = 0$$

We need to solve this equation to find the criticial point**s**.

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

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

Set to zero and solve for minimizer

Equation:

$$\frac{dR_{\text{sq}}}{dh} = 0$$

We need to solve this equation to find the criticial point**s**.

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

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

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

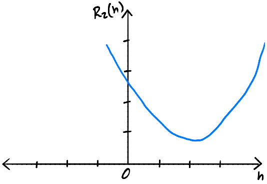
The equation only returns to us a single critical point that is the mean.

The mean minimizes mean squared error

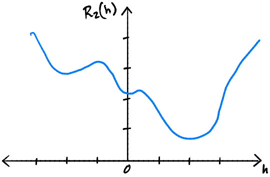
- Our new problem was: find h^* which minimizes the mean squared error, $R_{sq}(h) = \frac{1}{n}\sum_{i=1}^{n}(y_i - h)^2$.
  - The answer is: $\text{Mean}(y_1, \ldots, y_n)$.
    The equation returns to us a single critical point, but we still need to prove that this is indeed the global minimum.
  - The **best prediction**, in terms of mean squared error, is the **mean**.
  - This answer is always unique!
- **Note:** While we used calculus to minimize mean squared error here, there are other ways to do it!
  - Hint (next lectures): Solve by an iterative algorithm.

Discussion Question

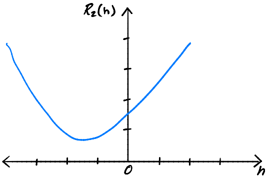
Suppose $y_1, \ldots, y_n$ are salaries. Which plot could be $R_{sq}(h)$?



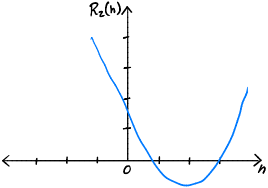
(a)



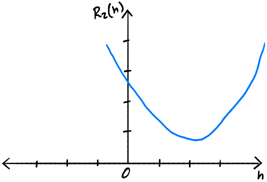
(b)



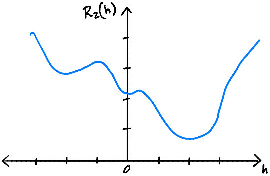
(c)



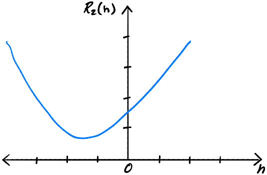
(d)



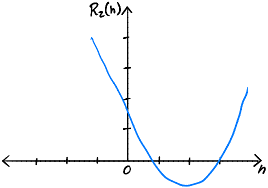
(a)



(b)



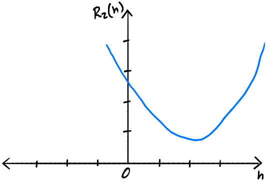
(c)



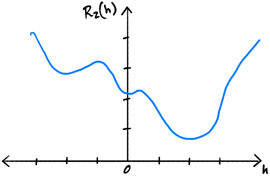
(d)

Because $R_{sq}(h) \geq 0$, so we eliminate D.

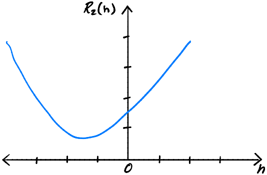
Because $y_i > 0$ so $\frac{1}{n}\sum_i y_i > 0$, thus we eliminate C.



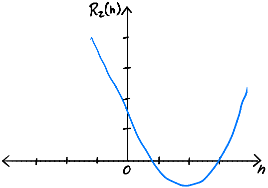
(a)



(b)



(c)



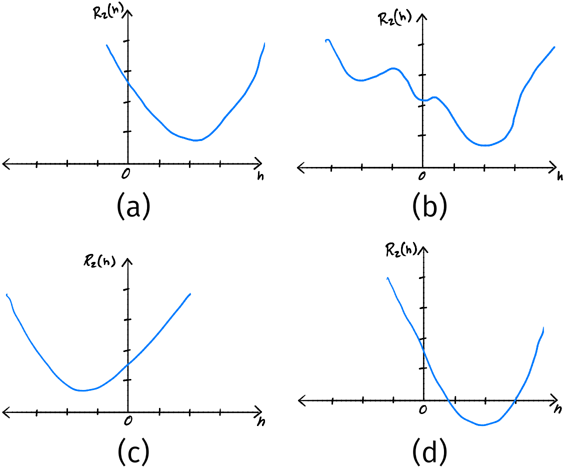
(d)

Because $R_{sq}(h) \geq 0$, so we eliminate D.

Because $y_i > 0$ so $\frac{1}{n} \sum_i y_i > 0$, thus we eliminate C.

Because we only have a single critical point, we eliminate B.

Is there another mathematical reason to reject B?



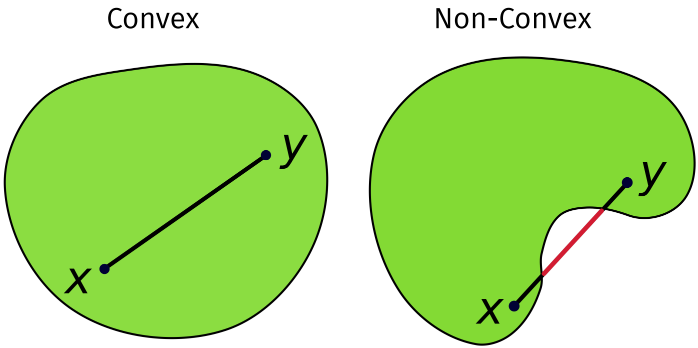
Because $R_{\text{sq}}(h) \geq 0$, so we eliminate D.

Because $y_i > 0$ so $\frac{1}{n} \sum_i y_i > 0$, thus we eliminate C.

Because we only have a single critical point, we eliminate B.

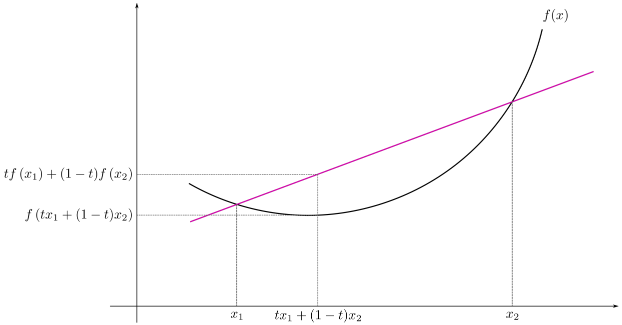
Is there another mathematical reason to reject B? **Convexity!**

Convex set



A subset of the Euclidean space is **convex** if, given any two points in the subset, the subset contains the whole line segment that joins them.

Convex function



Jensen's inequality:

$$f(tx_1 + (1-t)x_2) \leq tf(x_1) + (1-t)f(x_2)$$

for all $t \in [0, 1]$.

Properties of convex functions

- $|x|$ is a convex function.

Properties of convex functions

- $|x|$ is a convex function.
- x^2 is a convex function.

Properties of convex functions

- $|x|$ is a convex function.
- x^2 is a convex function.
- Sum of convex functions is a convex function.

Properties of convex functions

- $|x|$ is a convex function.
- x^2 is a convex function.
- Sum of convex functions is a convex function.
- MAE $\frac{1}{n}\sum_{i=1}^{n}|y_i - h|$ is a convex function.

Properties of convex functions

- $|x|$ is a convex function.
- x^2 is a convex function.
- Sum of convex functions is a convex function.
- MAE $\frac{1}{n}\sum_{i=1}^{n} |y_i - h|$ is a convex function.
- MSE $\frac{1}{n}\sum_{i=1}^{n} (y_i - h)^2$ is a convex function.

Properties of convex functions

- $|x|$ is a convex function.
- x^2 is a convex function.
- Sum of convex functions is a convex function.
- MAE $\frac{1}{n}\sum_{i=1}^{n}|y_i - h|$ is a convex function.
- MSE $\frac{1}{n}\sum_{i=1}^{n}(y_i - h)^2$ is a convex function.
- **If a convex function has a minimum, then that minimum is global.**
  Therefore, $h^* = \text{Mean}(y_1, .., y_n)$ for MSE.

Comparing the median and mean

Outliers

- Consider our original dataset of 5 salaries.

  90,000 94,000 96,000 120,000 160,000

- As it stands, the **median is 96,000** and the **mean is 112,000**.

- What if we add 300,000 to the largest salary?

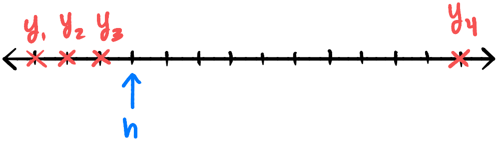
  90,000 94,000 96,000 120,000 460,000

- Now, the **median is still 96,000** but the **mean is 172,000**!

- **Key Idea:** The mean is quite **sensitive** to outliers.

Outliers

- The mean is quite **sensitive** to outliers.



- $|y_4 - h|$ is 10 times as big as $|y_3 - h|$.

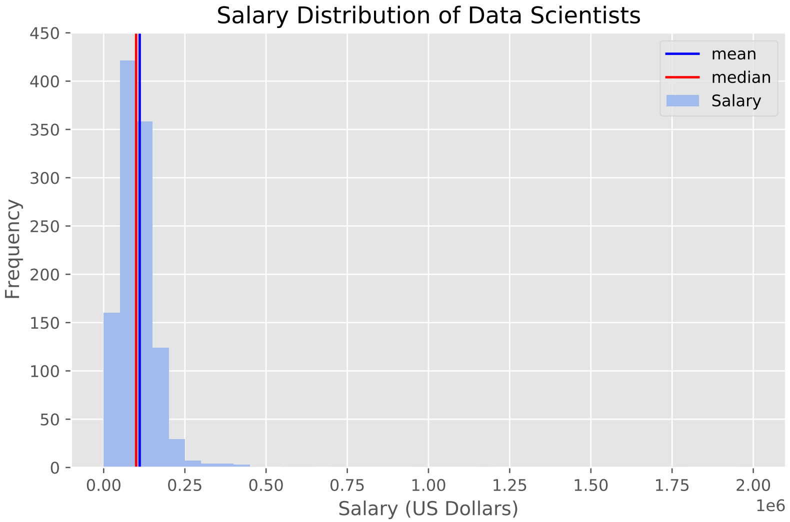
- But $(y_4 - h)^2$ is 100 times as big as $(y_3 - h)^2$.
  - This "pulls" h^* towards y_4.

- Squared error can be dominated by outliers.

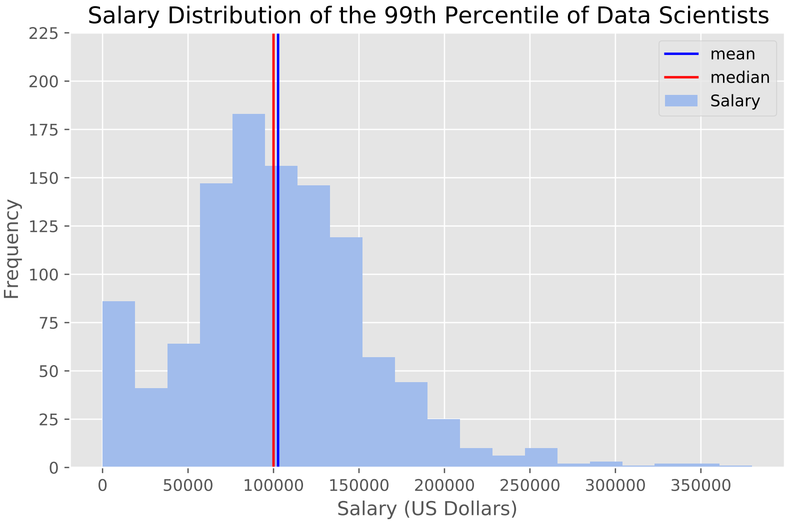
Example: Data Scientist Salaries

- Dataset of 1121 self-reported data science salaries in the United States from the 2018 StackOverflow survey.
- Median = $100,000.
- Mean = $110,933.
- Max = $2,000,000.
- Min = $6.31.
- 95th Percentile: $200,000.

Example: Data Scientist Salaries



Example: Data Scientist Salaries



Example: Income Inequality

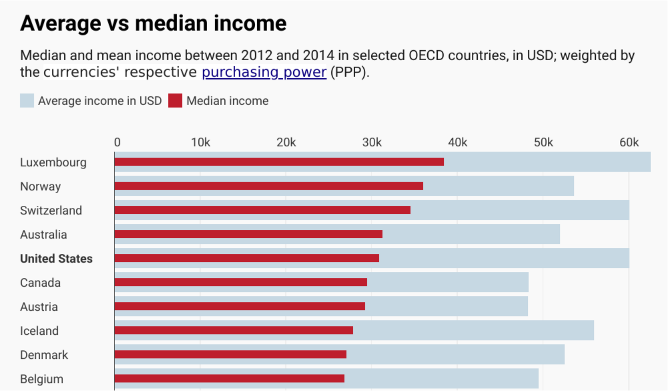
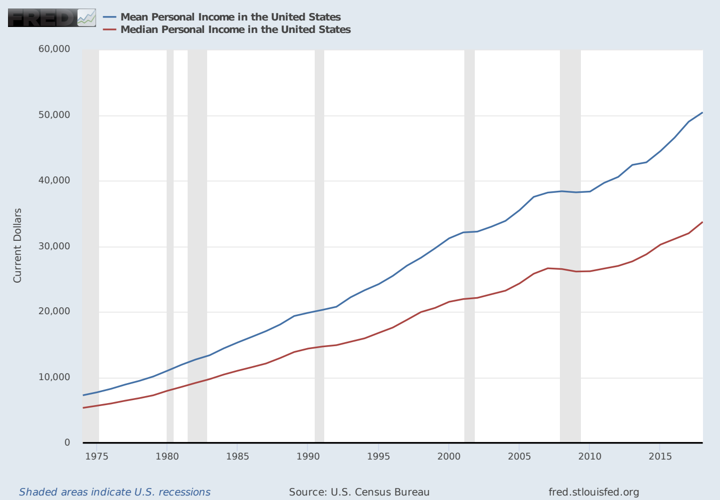


Chart: Lisa Charlotte Rost, Datawrapper

Example: Income Inequality



Empirical risk minimization

A general framework

- We started with the **mean absolute error**:

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

- Then we introduced the **mean squared error**:

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

- They have the same form: both are averages of some measurement that represents how different h is from the data.

A general framework

- Definition: A **loss function** $L(h, y)$ takes in a prediction h and a true value (i.e. a "right answer"), y, and outputs a number measuring how far h is from y (bigger = further).

- The **absolute loss**:

$$L_{\text{abs}}(h, y) = |y - h|$$

- The **squared loss**:

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

A general framework

- Suppose that $y_1, \ldots, y_n$ are some data points, h is a prediction, and L is a loss function. The **empirical risk** is the average loss on the data set:

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

- The goal of learning: find h that minimizes R_L. This is called **empirical risk minimization (ERM)**.

The learning recipe

1. Pick a loss function.

2. Pick a way to minimize the average loss (i.e. empirical risk) on the data.

- **Key Idea**: The choice of loss function determines the properties of the result. **Different loss function = different minimizer = different predictions!**
  - Absolute loss yields the median.
  - Squared loss yields the mean.
  - The mean is easier to calculate but is more sensitive to outliers.

Example: 0-1 Loss

1. Pick as our loss function the **0-1 loss**:

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

2. Minimize empirical risk:

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

Example: 0-1 Loss

1. Pick as our loss function the **0-1 loss**:

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

2. Minimize empirical risk:

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

Discussion Question

Suppose $y_1, \dots, y_n$ are all distinct. Find $R_{0,1}(y_1)$.

a) 0 b) $\frac{1}{n}$ c) $\frac{n-1}{n}$ d) 1

Answer: C.

Minimizing empirical risk

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

Notice that:

$$R_{0,1}(h) = \frac{n - \#(h = y_i)}{n}$$

We select h^* as the value appearing the highest number of times in $\{y_1, y_2, .., y_n\}$, that is called the **mode**.

Different loss functions lead to different predictions

Loss	Minimizer	Outliers	Differentiable
L_{abs}	median	**insensitive**	**no**
L_{sq}	mean	**sensitive**	**yes**
$L_{0,1}$	mode	**insensitive**	**no**

- The optimal predictions are all **summary statistics** that measure the **center** of the data set in different ways.

Summary

Summary

- $h^* = \text{Mean}(y_1, \dots, y_n)$ minimizes $R_{sq}(h) = \frac{1}{n}\sum_{i=1}^{n}(y_i - h)^2$, i.e. the mean minimizes mean squared error.

- The mean absolute error and the mean squared error fit into a general framework called **empirical risk minimization**.
  - Pick a loss function. We've seen absolute loss, $|y - h|^2$, squared loss, $(y - h)^2$, and 0-1 loss.

  - Pick a way to minimize the average loss (i.e. empirical risk) on the data.

- By changing the loss function, we change which prediction is considered the best.

Next time

- **Spread** – what is the meaning of the value of $R_{abs}(h^*)$? $R_{sq}(h^*)$?
- Creating a new loss function and trying to minimize the corresponding empirical risk.
  - We'll get stuck and have to look for a new way to minimize.