Lecture 3 – Mean Squared Error and Empirical Risk Minimization

DSC 40A, Fall 2022 @ UC San Diego

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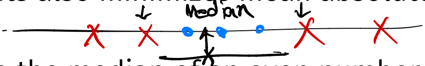
Agenda

- 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**?

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- 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**.

$$(y_i - h)^2$$

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**:

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

w.r.t h

$$= 2(h-y)$$

The mean squared error

- Suppose we predicted a future salary of $h_1 = 150{,}000$ *before* collecting data.

salary	absolute error of h_1	squared error of h_1
90,000	60,000	$(60{,}000)^2$
94,000	56,000	$(56{,}000)^2$
96,000	54,000	$(54{,}000)^2$
120,000	30,000	$(30{,}000)^2$
160,000	10,000	$(10{,}000)^2$

total squared error: 1.0652×10^{10}

mean squared error: 2.13×10^9

- A good prediction is one with small **mean squared error**.

The mean squared error

- Now suppose we had predicted $h_2 = 115{,}000$.

salary	absolute error of h_2	squared error of h_2
90,000	25,000	$(25{,}000)^2$
94,000	21,000	$(21{,}000)^2$
96,000	19,000	$(19{,}000)^2$
120,000	5,000	$(5{,}000)^2$
160,000	45,000	$(45{,}000)^2$

total squared error: 3.47×10^9

mean squared error: 6.95×10^8

h_2 is better than h_1

- A good prediction is one with small **mean squared error**.

The new idea

- Make prediction by minimizing the **mean squared error**:

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

- Strategy: Take derivative, set to zero, solve for minimizer.

Minimizing mean squared error

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

$$\frac{dR_{sq}}{dh} = \frac{1}{n}\frac{d}{dh}\left(\sum (y_i-h)^2\right)$$

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

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

$$= \frac{1}{n}\sum 2(h-y_i)$$

Discussion Question

Which of these is dR_{sq}/dh?

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

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

b) 0

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

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

Solution

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

$$\frac{dR_{sq}}{dh} = 0 \implies \text{solve for } h^*$$

Set to zero and solve for minimizer

find h^* such that $\frac{d R_{sq}(h)}{dh} = 0$

$f(h)$

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

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

const

$$\underbrace{h + h + \cdots + h}_{n \text{ times}}$$

$$y_1 + y_2 + \cdots + y_n$$

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

Mean

The mean minimizes mean squared error

- Our new problem was: find h^* which minimizes the mean squared error, $R_{sq}(h) = \frac{1}{n}\sum_{i=1}^{n}(y_i - h)^2$. $\leftarrow$ new error function
  - The answer is: $\text{Mean}(y_1, \ldots, y_n)$.
  - 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!
  - See Homework 2.

Discussion Question

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

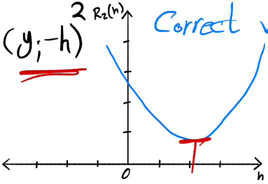
$y_i \geq 0$

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

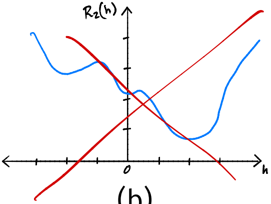
$a_i h^2 + b_i h + c_i$

$\deg R_{sq} \leq 2$

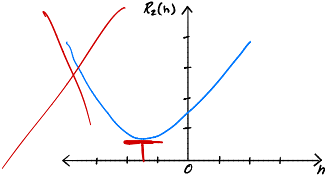
Correct ✓



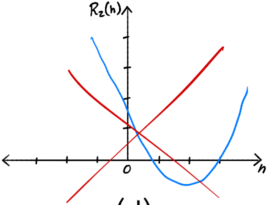
(a) pos



(b)



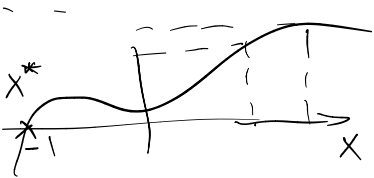
neg (c)



(d)

$f(x) = 0 \implies$

$x^* = -1$



Comparing the median and mean

Outliers

- Consider our original dataset of 5 salaries.

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

  Med 300,000

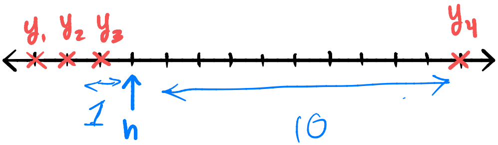
- As it stands, the **median is 96,000** and the **mean is 112,000**.
- What if we add 300,000 to the largest salary?

  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 $|y_3 - h|$.

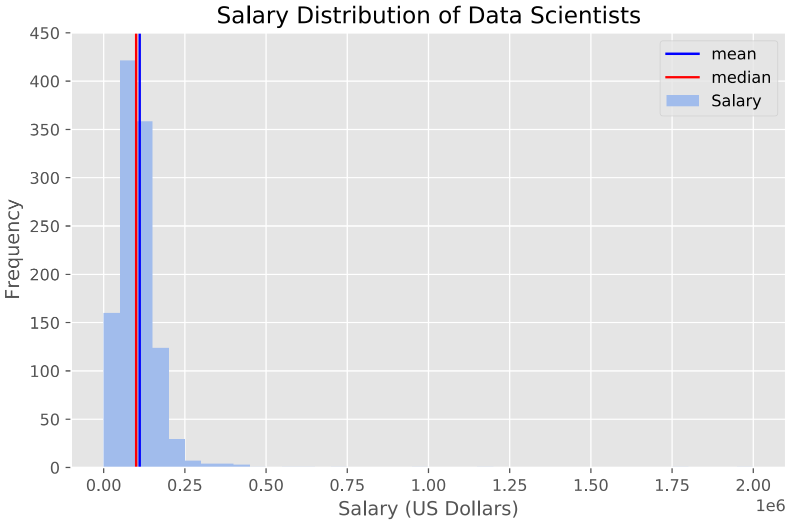
- But $(y_4 - h)^2$ is 100 times as big as $(y_3 - h)^2$.
  - This "pulls" h^* towards y_4.

- Squared error can be dominated by outliers.

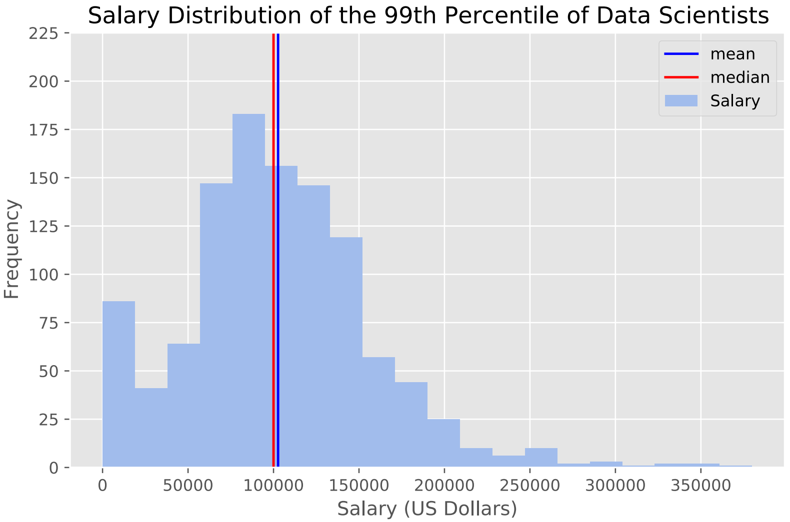
Example: Data Scientist Salaries

- 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.

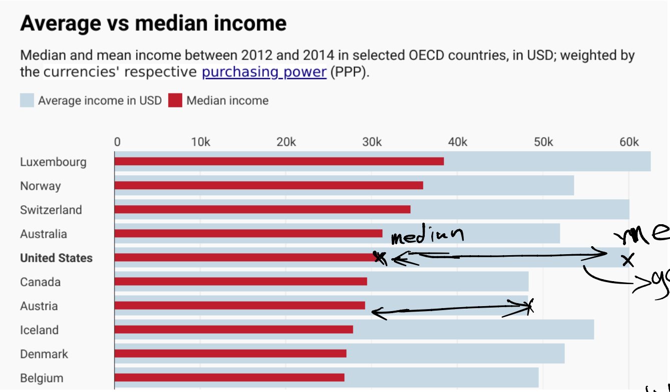
Example: Data Scientist Salaries



Example: Data Scientist Salaries



Example: Income Inequality



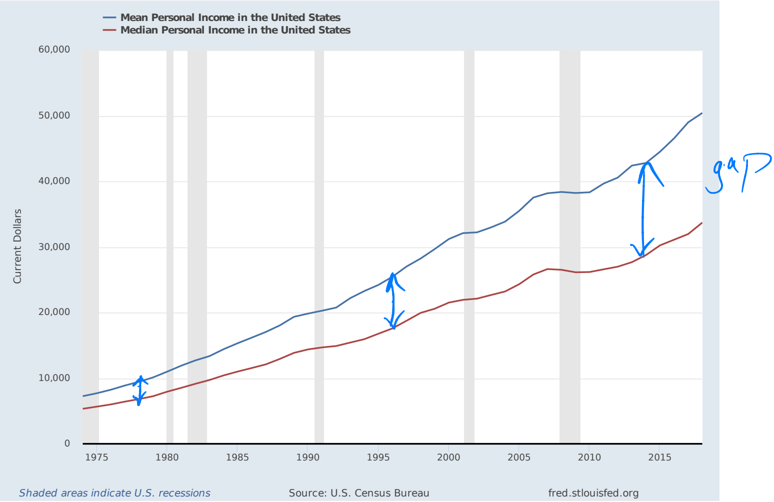
mean

gap is large

& equality

Chart: Lisa Charlotte Rost, Datawrapper

Example: Income Inequality



MAE (Mean Absolute Error) → is not sesitive to outliers

but MSE is!

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**:

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

loss functions

- 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**:

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

- The **squared loss**:

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

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)**.

h^*

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:

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

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Discussion Question

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

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

To answer, go to `menti.com` and enter the code 7933 4859.

Minimizing empirical risk

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

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.