Lecture 15

Simple Linear Regression

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EECS 398-003: Practical Data Science, Fall 2024

practicaldsc.org • github.com/practicaldsc/fa24

Announcements 🤜

- Homework 7 is due on **Thursday**.
- We've released a Grade Report on Gradescope that has your current overall score in the class, scores on all assignments, and slip day usage so far.
 See #232 on Ed for more details.
- Some updates to the **Syllabus**:
 - You now have 8 slip days instead of 6!
 - The final homework, called the Portfolio Homework, will be an open-ended investigation using the tools from both halves of the semester. Details to come.
 - You'll end up making a website!
 - You can work with a partner, but can't drop it or use slip days on it.
- The IA application is out for next semester! Please consider applying, and let me know if you're interested.

Agenda

- Recap: Models and loss functions.
- Towards simple linear regression.
- Minimizing mean squared error for the simple linear model.
- Correlation.
- Interpreting the formulas.
- Connections to related models.

Recap: Models and loss functions

Overview



- We started by introducing the idea of a hypothesis function, H(x).
- We looked at two possible models:
 - $_{\circ}$ The constant model, H(x)=h.

 \circ The simple linear regression model, $H(x) \neq w_0 + w_1 x.$

 We decided to find the best constant prediction to use for predicting commute times, in minutes.

(actual - predicted)²

Recap: 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:

$$R_{
m sq}(h) = rac{1}{5}ig((72-h)^2+(90-h)^2+(61-h)^2+(85-h)^2+(92-h)^2ig)$$

• For example, if we predict h = 100, then:

$$egin{aligned} R_{
m sq}(100) &= rac{1}{5}ig((72-100)^2+(90-100)^2+(61-100)^2+(85-100)^2+(92-100)^2ig)\ &= \boxed{538.8} \end{aligned}$$

• We can pick any h as a prediction, but the smaller $R_{
m sq}(h)$ is, the better h is!

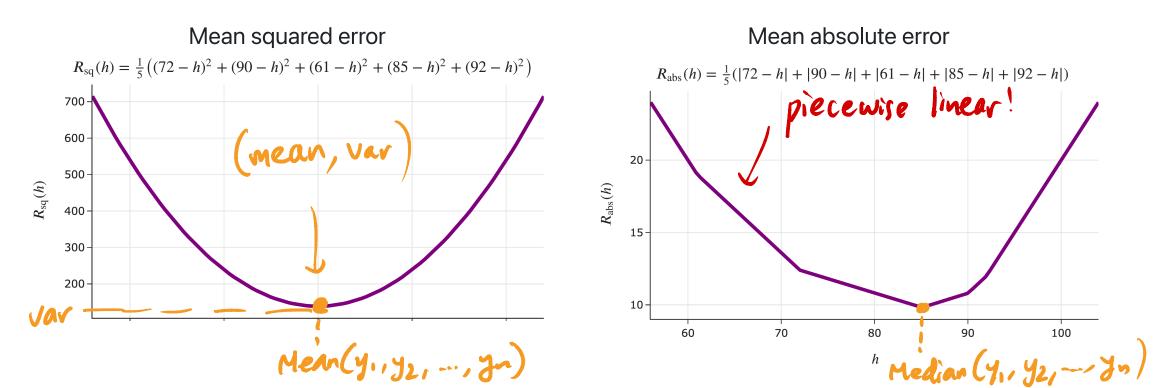
The modeling recipe

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

H(x) = h "constant model" 1. Choose a model. 2. Shouse a loss function. $L_{sq}(y_i, h) = (y_i - h)^2 L_{abs}(y_i, h) = (y_i - h)^2$ 3. Minimize average loss to find optimal model parameters. Rates $(h) = \frac{1}{h} = \frac{1}{h} \left[\frac{y_i - h}{y_i} \right]$ $R_{sq}(h) = \prod_{n \neq i} \frac{\hat{z}(y_i - h)^{i}}{\hat{z}(y_i - h)^{i}}$ \Rightarrow h^{*} = Median (y₁, y₂, -, y_n) =) h = Mean (y, y2, -... yn) proved using calculus!!!

Visualizing average loss

- Let's use the same example dataset, 72, 90, 61, 85, 92.
- Below are the graphs of:
 - Mean squared error, the average of squared loss across our dataset.
 - Mean absolute error, the average of absolute loss across our dataset.



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Empirical risk minimization

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

$$R_{\mathrm{sq}}(h) = rac{1}{n} \sum_{i=1}^{n} (y_i - h)^2 \implies h^* = \mathrm{Mean}(y_1, y_2, \dots, y_n)$$

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

$$egin{aligned} R_{ ext{abs}}(h) = rac{1}{n} \sum_{i=1}^n |y_i - h| \implies h^* = ext{Median}(y_1, y_2, \dots, y_n) \end{aligned}$$

Empirical risk minimization, in general

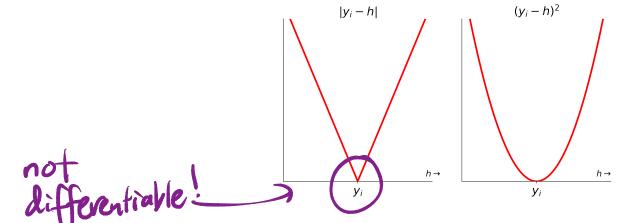
• Key idea: If L is any loss function, and H is any hypothesis function, the corresponding empirical risk is:

$$R(H)=rac{1}{n}\sum_{i=1}^n L(y_i,H(x_i))$$

- In Homework 7 (and last week's discussion), you saw several examples in which:
 - \circ You were given a new loss function L.
 - $\circ~$ You had to find the optimal parameter h^* for the constant model $H(x_i)=h.$

Choosing a loss function

- For the constant model H(x) = h, the **mean** minimizes mean **squared** error.
- For the constant model H(x) = h, the **median** minimizes mean **absolute** error.
- In practice, squared loss is the more common choice, as it's 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.

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

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

 $y_1=72$ $y_2=90$ $y_3=61$ $y_4=85$ $y_5=292$ • Now, the median is 5 but the mean is 20!

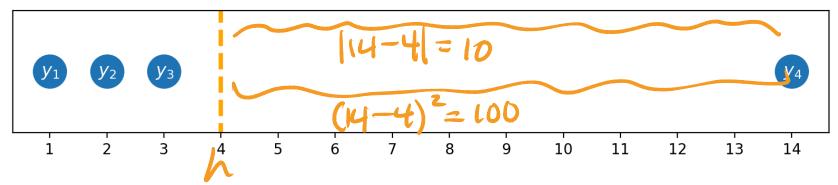
• Key idea: The mean is quite sensitive to outliers. But why?

$$\frac{80 \times 5 + 200}{5} = 80 + \frac{200}{5}$$
$$= 80 + 40 = 120$$

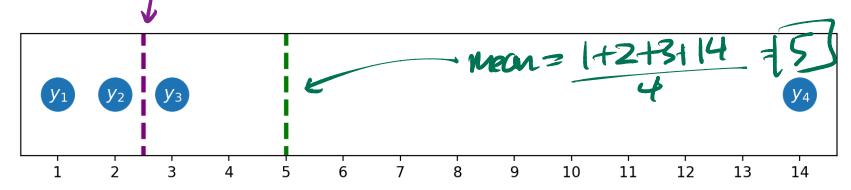
61 72 85 90 292

Outliers

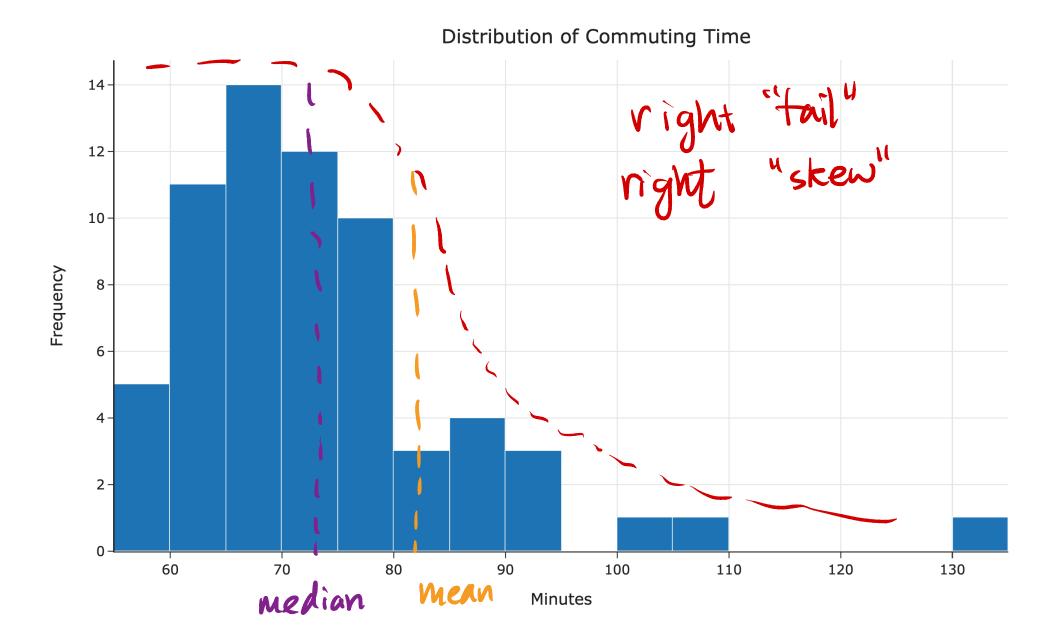
• Below, $|y_4-h|$ is 10 times as big as $|y_3-h|$, but $(y_4-h)^2$ is 100 times $(y_3-h)^2$.



• The result is that the mean is "pulled" in the direction of outliers, relative to the median. median = 2.5



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

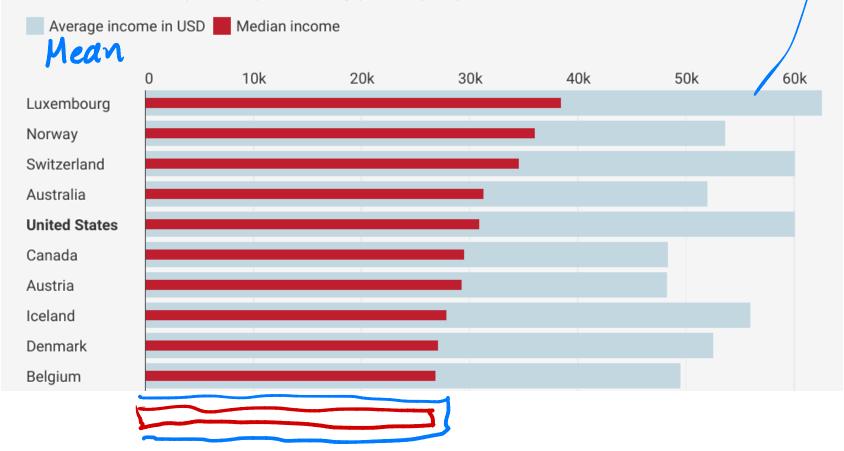


mean is dragged <u>up</u> by large outliers

Example: Income inequality

Average vs median income

Median and mean income between 2012 and 2014 in selected OECD countries, in USD; weighted by the currencies' respective <u>purchasing power</u> (PPP).



Summary: Choosing a loss function

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

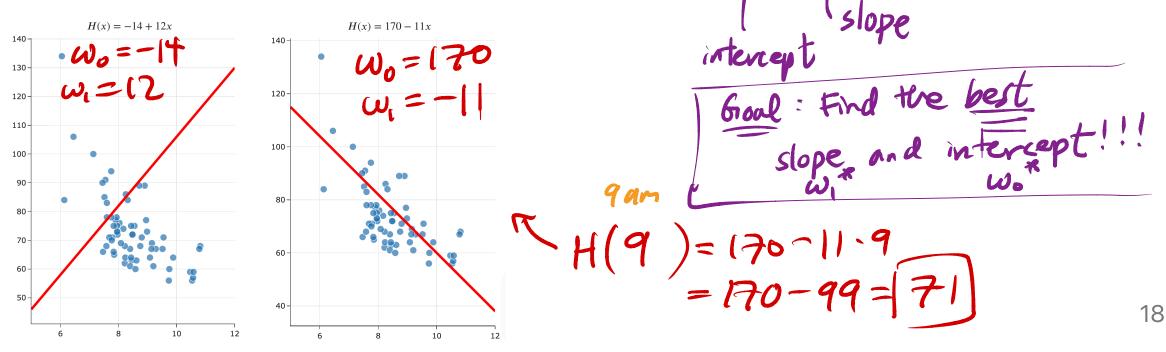
Loss	Minimizer	Always Unique?	Robust to Outliers?	Differentiable?
$L_{ m sq}(y_i,h)=(y_i-h)^2$	mean	yes 🗸	no 🗙	yes 🗸
$L_{ m abs}(y_i,h) = y_i-h $	median	no 🗙	yes 🗸	no 🗙
$L_{0,1}(y_i,h)=egin{cases} 0 & y_i=h\ 1 & y_i eq h \end{cases}$	mode	no 🗙	yes 🗸	no 🗙
$L_\infty(y_i,h)$ See HW 7, Question 5.	???	yes 🗸	no 🗙	no 🗙

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

Towards simple linear regression

Recap: Hypothesis functions and parameters

- A hypothesis function, H, takes in an x as input and returns a predicted y.
- Parameters define the relationship between the input and output of a hypothesis function.
- Example: The simple linear regression model, $H(x) = w_0 + w_1 x$, has two parameters: w_0 and w_1 .



The modeling recipe

1. Choose a model. Before: H(x) = h

NOW: $H(x) = W_0 + W_1 X$

2. Choose a loss function.

$$L_{\mathcal{R}}(y_{i}, H(\pi_{i})) = (y_{i} - H(\pi_{i})) = (y_{i} - (\omega_{0} + \omega_{1} \pi_{i}))$$
$$= (y_{i} - (\omega_{0} + \omega_{1} \pi_{i}))$$

3. Minimize average loss to find optimal model parameters.

=)
$$K_{sq}(H) = \frac{1}{n} \sum_{i=1}^{n} (y_i - (w_0 + w_i \times i))$$

definition $H(x_i)$

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Minimizing mean squared error for the simple linear model

- We'll choose squared loss, since it's the easiest to minimize.
- Our goal, then, is to find the linear hypothesis function $H^*(x)$ that minimizes empirical risk:

$$R_{ ext{sq}}(H) = rac{1}{n}\sum_{i=1}^n \left(y_i - H(x_i)
ight)^2$$

• Since linear hypothesis functions are of the form $H(x) = w_0 + w_1 x$, we can re-write $R_{
m sq}$ as a function of w_0 and w_1 :

$$R_{\rm sq}(w_0,w_1) = \frac{1}{n} \sum_{i=1}^n \left(y_i - (w_0 + w_1 x_i)\right)^2$$

$$R_{\rm sq}(w_0,w_1) = \frac{1}{n} \sum_{i=1}^n \left(y_i - (w_0 + w_1 x_i)\right)^2$$

$$R_{\rm sq}(w_0,w_1) = \frac{1}{n} \sum_{i=1}^n \left(y_i - (w_0 + w_1 x_i)\right)^2$$

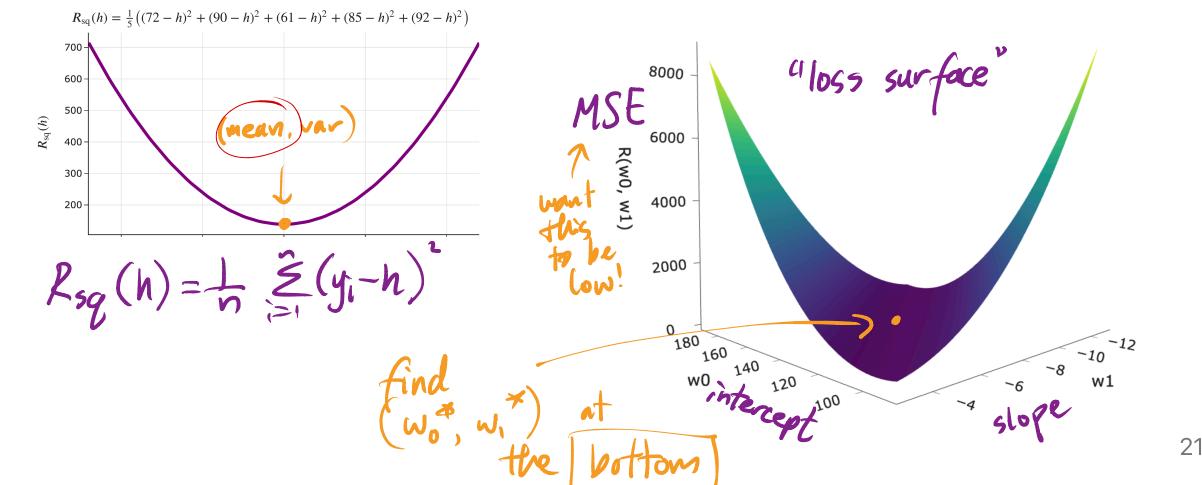
- How do we find the parameters w_0^* and w_1^* that minimize $R_{
m sq}(w_0,w_1)$?

$$F_{sq}(\omega_0, \omega_1) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - (\omega_0 + \omega_i x_i) \right)^2$$

Loss surface

For the constant model, the graph of $R_{ m sq}(h)$ looked like a parabola.

What does the graph of $R_{
m sq}(w_0,w_1)$ look like for the simple linear regression model?



Minimizing mean squared error for the simple linear model

Minimizing multivariate functions

• Our goal is to find the parameters w_0^* and w_1^* that minimize mean squared error:

$$R_{ ext{sq}}(w_0,w_1) = rac{1}{n}\sum_{i=1}^n \left(y_i - (w_0 + w_1 x_i)
ight)^2$$

- $R_{
 m sq}$ is a function of two variables: w_0 and w_1 .
- To minimize a function of multiple variables:
 - Take partial derivatives with respect to each variable.
 - Set all partial derivatives to 0 and solve the resulting system of equations.
 - Ensure that you've found a minimum, rather than a maximum or saddle point (using the second derivative test for multivariate functions).
- To save time, we won't do the derivation live in class, but you are responsible for it!
 Here's a video of me walking through it.

Example

Find the point (x, y, z) at which the following function is minimized.

$$f(x,y) = x^{2} - 8x + y^{2} + 6y - 7$$

$$f(x,y) = 2x - 8$$

$$f(x,y) = 2x - 8 = 0$$

$$f(x,y) = 2x - 8$$

Minimizing mean squared error

$$R_{ ext{sq}}(w_0,w_1) = rac{1}{n}\sum_{i=1}^n \left(y_i - (w_0 + w_1 x_i)
ight)^2$$

To find the w_0^* and w_1^* that minimize $R_{
m sq}(w_0,w_1)$, we'll:

1. Find
$$\frac{\partial R_{sq}}{\partial w_0}$$
 and set it equal to 0.
2. Find $\frac{\partial R_{sq}}{\partial w_1}$ and set it equal to 0.

3. Solve the resulting system of equations.

$$R_{sq}(w_{0},w_{1}) = \frac{1}{n} \sum_{i=1}^{n} (y_{i} - (w_{0} + w_{1}x_{i}))^{2}$$

$$\frac{\partial R_{sq}}{\partial w_{0}} = \frac{1}{n} \sum_{i=1}^{n} 2(y_{i} - (w_{0} + \omega_{1}x_{i}))(-1)$$

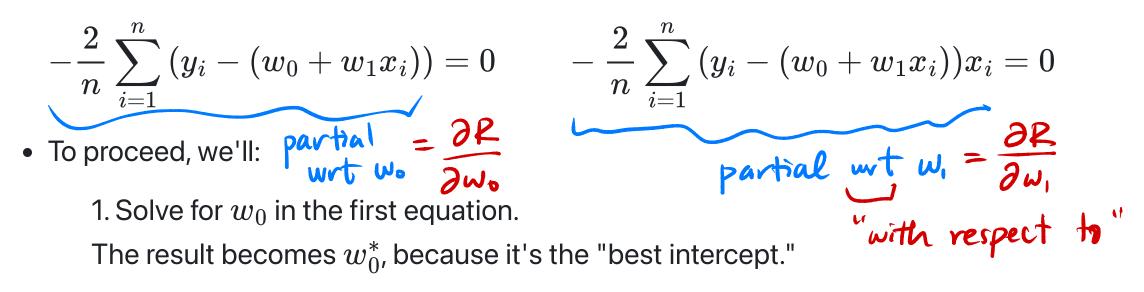
$$= \left[-\frac{2}{n} \sum_{i=1}^{n} (y_{i} - (w_{0} + \omega_{1}x_{i}))\right]$$
the coefficient on we define the work of the coefficient of the coefficient

$$\begin{aligned} R_{\rm sq}(w_0,w_1) &= \frac{1}{n} \sum_{i=1}^n \left(y_i - (w_0 + w_1 x_i) \right)^2 \\ \frac{\partial R_{\rm sq}}{\partial w_1} &= \frac{1}{n} \sum_{i=1}^n 2\left(y_i^* - (\omega_0 + \omega_1 x_i) \right) (-x_i^*) & \text{the coefficient} \\ &= -\frac{2}{n} \sum_{i=1}^n \left(y_i^* - (\omega_0 + \omega_1 x_i) \right) x_i & \text{we expand} \\ &= i - \frac{2}{n} \sum_{i=1}^n \left(y_i^* - (\omega_0 + \omega_1 x_i) \right) x_i & \text{we expand} \\ &= i - x_i \end{aligned}$$

Strategy

system of 2 equations, 2 unknowns!

• We have a system of two equations and two unknowns (w_0 and w_1):



2. Plug w_0^* into the second equation and solve for w_1 . The result becomes w_1^* , because it's the "best slope."

Groal: Isolate Wo. Solving for w_0^* $\sum_{i=1}^{2} w_{o} = w_{o} + w_{o} + \cdots + w_{o}$ $-rac{2}{n}\sum_{i=1}^{n}\left(y_{i}-(w_{0}+w_{1}x_{i})
ight)=0$ Meon -Witn $\overset{\tilde{z}}{\underset{i=1}{\overset{\tilde{z}}{=}}} (y_i - \omega_o - \omega_i x_i)$ Ju ω_{p} = () $\frac{2}{1-1}y_i - \frac{2}{1-1}w_0 - \frac{2}{1-1}w_1 \tau_i$ X LEYi where 1 $\eta w_0 - w_1 \neq \chi_1 = 0$ $\overline{x} = \frac{1}{n} \sum_{i=1}^{n} \overline{x}_i$ $\sum_{i=1}^{n} y_i - w_i \sum_{i=1}^{n} x_i = n w_0$ 29

Solving for
$$w_1^*$$

$$-\frac{2}{n}\sum_{i=1}^n (y_i - (w_0 + w_1x_i))x_i = 0$$

$$\sum_{i=1}^n (y_i - \omega_0 - \omega_i x_i)x_i = 0$$

$$\int_{i=1}^\infty (y_i - (y_i - \omega_i x_i) - \omega_i x_i)x_i = 0$$

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

$$\int_{i=1}^\infty (y_i - y_i + \omega_i x_i - \omega_i x_i)x_i = 0$$

$$\hat{z} \left(y_{i} - \overline{y} - w_{i}^{T} \left(\pi_{i} - \overline{\pi} \right) \right) \pi_{i} = 0$$

$$\hat{z} \left(y_{i} - \overline{y} \right) \pi_{i} = \hat{z} w_{i}^{T} \left(\pi_{i} - \overline{\pi} \right) \pi_{i}$$

$$\hat{z} \left(y_{i} - \overline{y} \right) \pi_{i} = \hat{z} w_{i}^{T} \left(\pi_{i} - \overline{\pi} \right) \pi_{i}$$

$$\hat{z} \left(y_{i} - \overline{y} \right) \pi_{i} = w_{i}^{T} \hat{z} \left(\pi_{i} - \overline{\pi} \right) \pi_{i}$$

$$\hat{z} \left(y_{i} - \overline{y} \right) \pi_{i} = w_{i}^{T} \hat{z} \left(\pi_{i} - \overline{\pi} \right) \pi_{i}$$

$$\hat{z} \left(\pi_{i} - \overline{\chi} \right) \pi_{i}$$

$$\hat{z} \left(\pi_{i} - \overline{\chi} \right) \pi_{i}$$

Least squares solutions

• We've found that the values w_0^* and w_1^* that minimize $R_{
m sq}$ are:

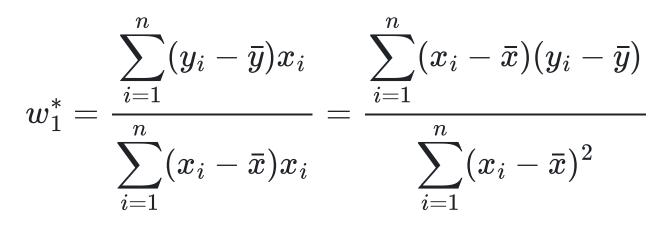
$$w_1^* = rac{\displaystyle\sum_{i=1}^n (y_i - ar{y}) x_i}{\displaystyle\sum_{i=1}^n (x_i - ar{x}) x_i} \qquad \qquad w_0^* = ar{y} - w_1^* ar{x}$$

where:

$$ar{x}=rac{1}{n}\sum_{i=1}^n x_i \qquad \qquad ar{y}=rac{1}{n}\sum_{i=1}^n y_i$$

• These formulas work, but let's re-write w_1^* to be a little more symmetric.

• Claim: Fact from Homework 7, Q.3.1: Fact from Homework 7, Q.3.1: $f(x_i - \overline{x}) = f(y_i - \overline{y}) = 0.$



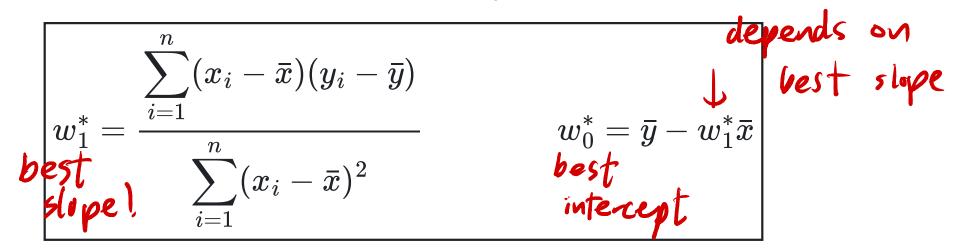
· Proof: First, consider the numerator:

$$(\overline{z} + \overline{s}) = \underbrace{\widehat{z}}_{i=1} (\overline{x}_i - \overline{x}) (y_i - \overline{y}) = \underbrace{\widehat{z}}_{i=1} (\overline{x}_i (y_i - \overline{y}) - \overline{x} (y_i - \overline{y})) = \underbrace{\widehat{z}}_{i=1} (y_i - \overline{y}) \times \underbrace{\widehat{z}}_{i=1} (y_i - \overline{y}) = \underbrace{\widehat{z}}_{i=1} (y_i - \overline{y}) \times \underbrace{\widehat{z}}_{i=1} (y_i - \overline{y}) = \underbrace{\widehat{z}}_{i=1} (y_i - \overline{y}) \times \underbrace{\widehat{z}}_{i=1} (y_i - \overline{y}) = \underbrace{\widehat{z}}_{i=1} (y_i - \overline{y}) \times \underbrace{\widehat{z}}_{i=1} (y_i - \overline{y}) = \underbrace{\widehat{z}}_{i=1} (y_i - \overline{y}) \times \underbrace{\widehat{z}}_{i=$$

Denominator follows similar logic: $F^{\text{RMS}} = \hat{Z}(\overline{x_i} - \overline{x}) = \hat{Z}(\overline{x_i} - \overline{x})(\overline{x_i} - \overline{x})$ $= \underbrace{\underbrace{\underbrace{\underbrace{\underbrace{x_{i}}}}_{i}}_{i} \underbrace{\underbrace{x_{i}}}_{i} - \underbrace{\underbrace{\underbrace{x_{i}}}_{i}}_{i} \underbrace{\underbrace{x_{i}}}_{i} \underbrace{x_{i}}_{i} \underbrace{x_{i}}_{i} \underbrace{x_{i}}_{i} \underbrace{x_{i}}}_{i} \underbrace{x_{i}}_{i} \underbrace{x_{i}} \underbrace{x_{i}}_{i} \underbrace{x_{i$ $= \sum_{i=1}^{2} (x_i - \overline{x}) x_i$

Least squares solutions

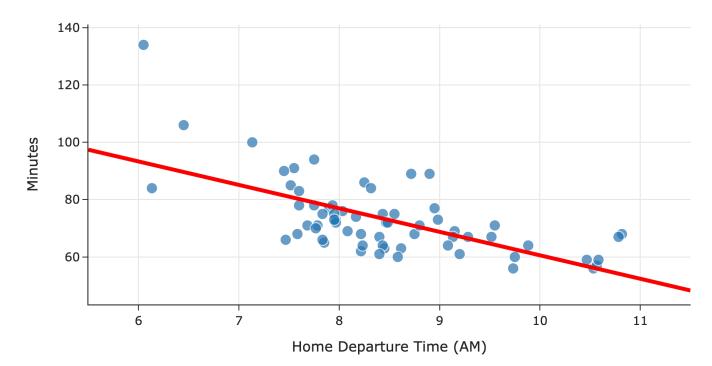
• The least squares solutions for the intercept w_0 and slope w_1 are:



- We say w_0^* and w_1^* are **optimal parameters**, and the resulting line is called the **regression line**.
- The process of minimizing empirical risk to find optimal parameters is also called "fitting to the data."
- To make predictions about the future, we use $ig| H^*(x) = w_0^* + w_1^* x ig|$

Code demo

• Let's test these formulas out in code!



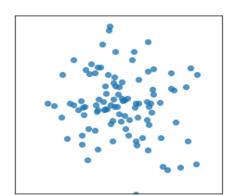
Predicted Commute Time = 142.25 - 8.19 * Departure Hour

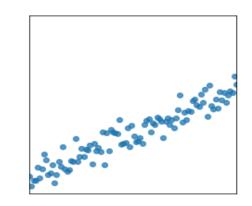
• The supplementary notebook is posted in the usual place on GitHub and the course website.

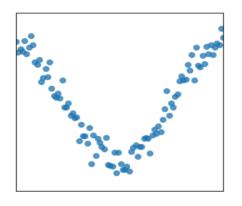
Correlation

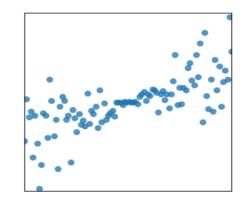
Quantifying patterns in scatter plots

- The correlation coefficient, *r*, is a measure of the strength of the linear
 association of two variables, *x* and *y*.
 Intuitively, it measures how tightly clustered a scatter plot is around a straight line.
 - It ranges between -1 and 1.





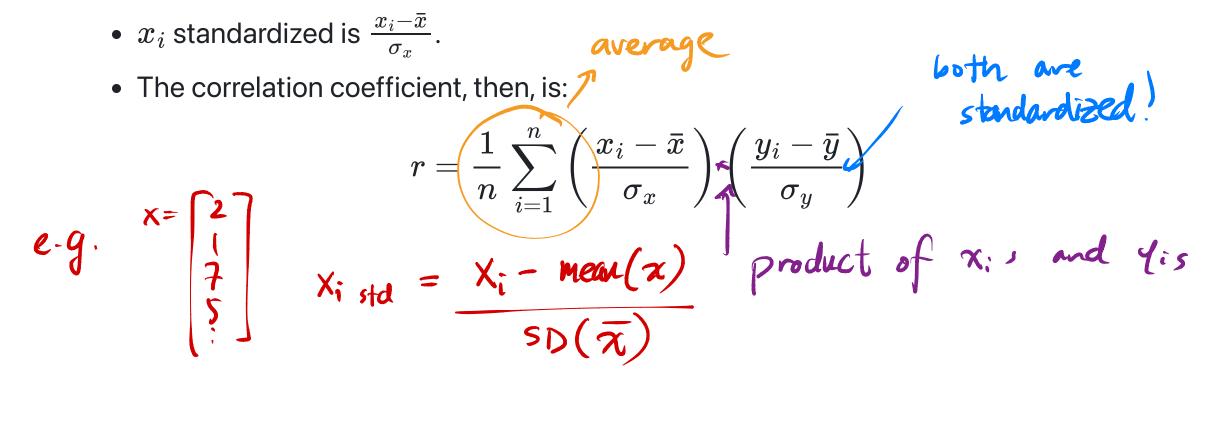


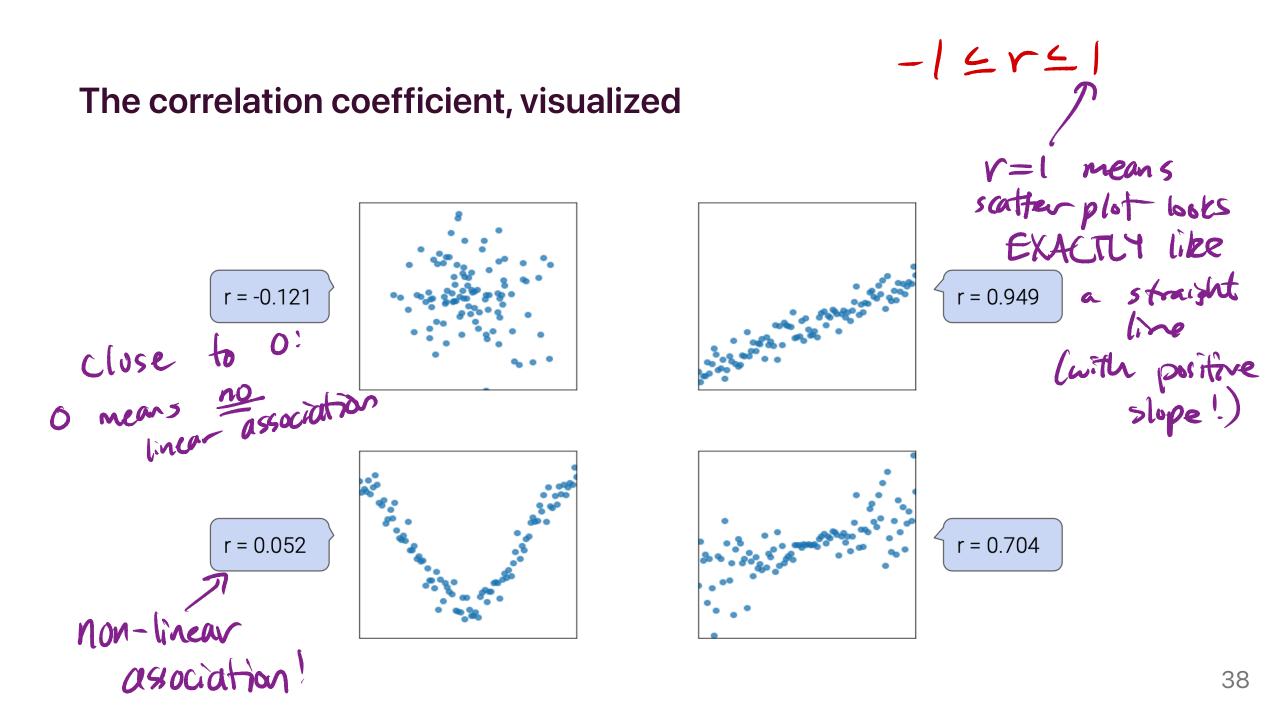


The correlation coefficient⁴

Pearson" correlation coefficient

- The correlation coefficient, r, is defined as the average of the product of x and y, when both are standardized.
- Let σ_x be the standard deviation of the x_i s, and \bar{x} be the mean of the x_i s.





Another way to express w_1^*

• It turns out that w_1^* , the optimal slope for the linear hypothesis function when using squared loss (i.e. the regression line), can be written in terms of r!

$$w_1^* = rac{\displaystyle\sum_{i=1}^n (x_i - ar{x})(y_i - ar{y})}{\displaystyle\sum_{i=1}^n (x_i - ar{x})^2} = r rac{\sigma_y}{\sigma_x}$$

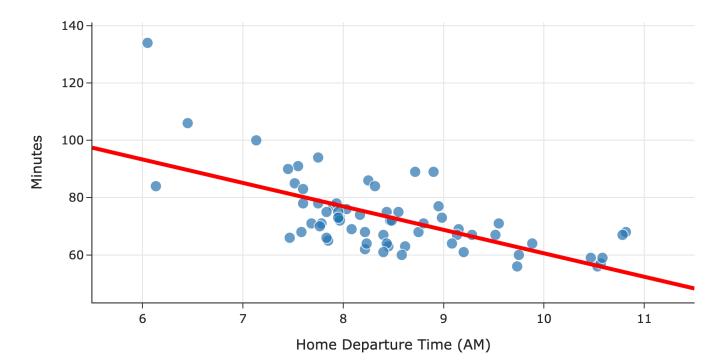
- It's not surprising that r is related to w_1^* , since r is a measure of linear association.
- Concise way of writing w_0^* and w_1^* :

$$w_1^* = r rac{\sigma_y}{\sigma_x}$$
 $w_0^* = ar{y} - w_1^* ar{x}$
 γ_{slipe} intercept

Proof that $w_1^* = r rac{\sigma_y}{\sigma_x}$ definition of $\frac{1}{n} \stackrel{\sim}{=} \left(\frac{x_i - \overline{x}}{\sigma_x} \right)$ r $\sigma_{\chi}^{2} = \frac{1}{n} \hat{\mathcal{E}}(\chi_{i} - \overline{\chi})$ $(x_i - \overline{x})(y_i - \overline{y})$ ì≍ MO. $(x_i - \overline{x})(y_i - \overline{y})$ constant, separate from outer sum 1=1 5(7:-7 = LHS $\hat{\boldsymbol{\varsigma}}(\boldsymbol{x},-\boldsymbol{\overline{x}})$ 40

Code demo

• Let's test these new formulas out in code and see if they match the earlier formulas!



Predicted Commute Time = 142.25 - 8.19 * Departure Hour

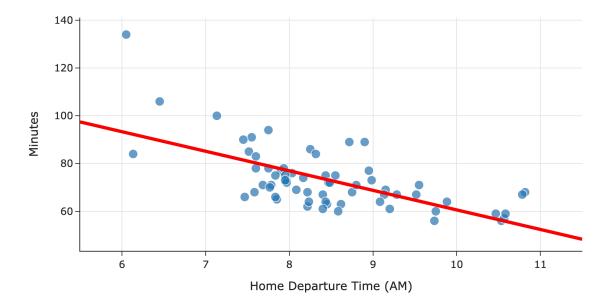
• The supplementary notebook is posted in the usual place on GitHub and the course website.

will cover the rest on Thursday in Lecture 16!

Interpreting the formulas

Causality

• Can we conclude that leaving later causes you to get to school quicker 2,



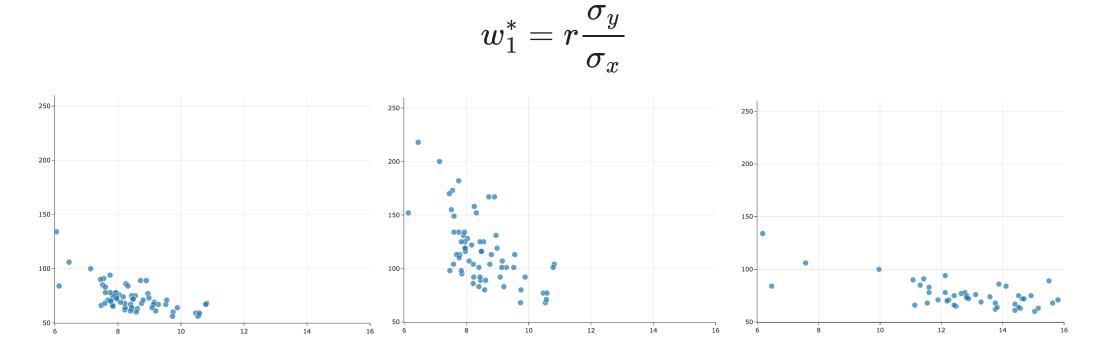
Predicted Commute Time = 142.25 - 8.19 * Departure Hour

Interpreting the slope

$$w_1^* = r rac{\sigma_y}{\sigma_x}$$

- The units of the slope are **units of** *y* **per units of** *x*.
- In our commute times example, in $H^*(x) = 142.25 8.19x$, our predicted commute time decreases by 8.19 minutes per hour.

Interpreting the slope



- Since $\sigma_x \geq 0$ and $\sigma_y \geq 0$, the slope's sign is r's sign.
- As the y values get more spread out, σ_y increases, so the slope gets steeper.
- As the x values get more spread out, σ_x increases, so the slope gets shallower.

Interpreting the intercept

Predicted Commute Time = 142.25 - 8.19 * Departure Hour

- $w_0^*=ar{y}-w_1^*ar{x}$
- What are the units of the intercept?

• What is the value of $H^*(ar x)$?



Answer at practicaldsc.org/q

We fit a regression line to predict commute times given departure hour. Then, we add 75 minutes to all commute times in our dataset. What happens to the resulting regression line?

- A. Slope increases, intercept increases.
- B. Slope decreases, intercept increases.
- C. Slope stays the same, intercept increases.
- D. Slope stays the same, intercept stays the same.



Answer at practicaldsc.org/q

Consider a dataset with just two points, (2, 5) and (4, 15). Suppose we want to fit a linear hypothesis function to this dataset using squared loss. What are the values of w_0^* and w_1^* that minimize empirical risk?

- A. $w_0^*=2$, $w_1^*=5$
- B. $w_0^*=3$, $w_1^*=10$
- + C. $w_0^*=-2$, $w_1^*=5$
- + D. $w_0^*=-5$, $w_1^*=5$

Connections to related models



Answer at practicaldsc.org/q

Suppose we chose the model $H(x) = w_1 x$ and squared loss. What is the optimal model parameter, w_1^* ?

• A.
$$rac{\sum_{i=1}^n (x_i - ar{x})(y_i - ar{y})}{\sum_{i=1}^n (x_i - ar{x})^2}$$

• B. $rac{\sum_{i=1}^n x_i y_i}{\sum_{i=1}^n x_i^2}$

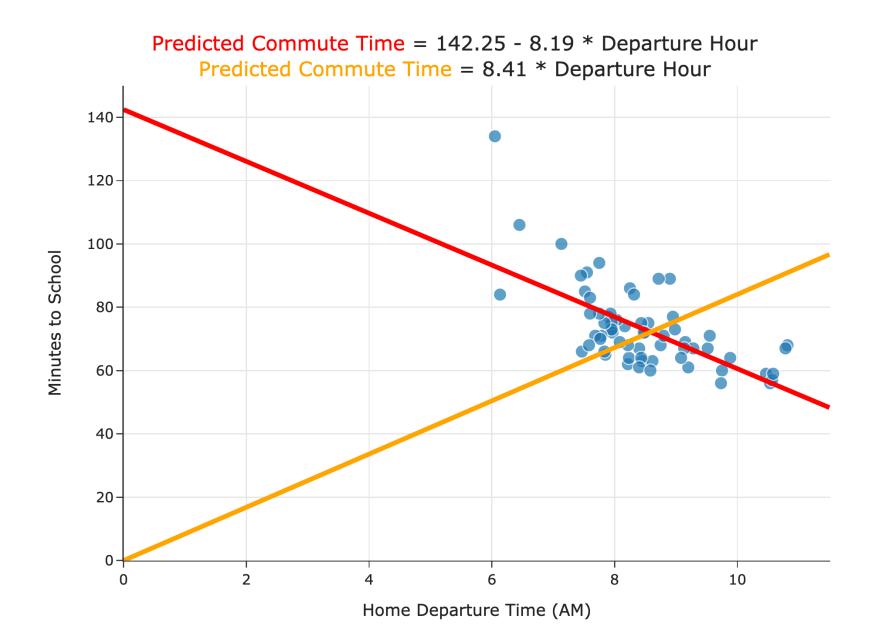
• C.
$$rac{\sum_{i=1}^n x_i y_i}{\sum_{i=1}^n x_i^2}$$

• D. $rac{\sum_{i=1}^n y_i}{\sum_{i=1}^n x_i}$

Exercise

Suppose we chose the model $H(x) = w_1 x$ and squared loss.

What is the optimal model parameter, w_1^st ?



Exercise

Suppose we choose the model $H(x) = w_0$ and squared loss.

What is the optimal model parameter, w_0^st ?

Comparing mean squared errors

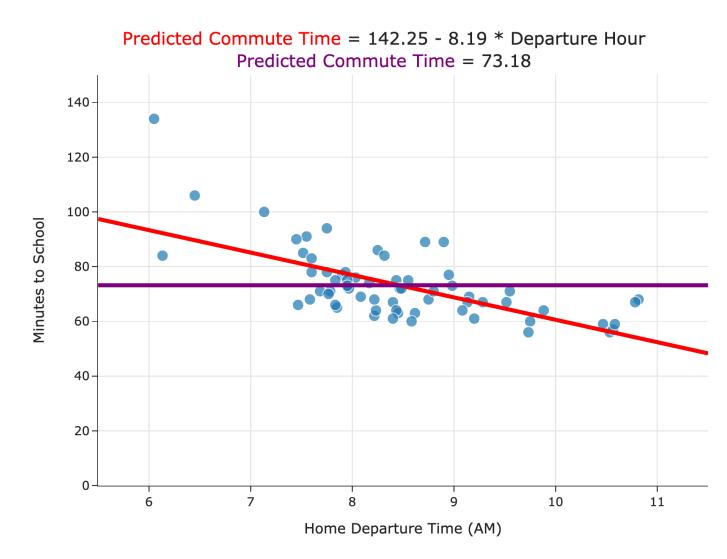
- With both:
 - $\circ\,$ the constant model, H(x)=h, and
 - $\circ\,$ the simple linear regression model, $H(x)=w_0+w_1x$,

when we chose squared loss, we minimized mean squared error to find optimal parameters:

$$R_{ ext{sq}}(H) = rac{1}{n}\sum_{i=1}^n \left(y_i - H(x_i)
ight)^2$$

• Which model minimizes mean squared error more?

Comparing mean squared errors



$$ext{MSE} = rac{1}{n}\sum_{i=1}^n \left(y_i - H(x_i)
ight)^2$$

- The MSE of the best simple linear regression model is ≈ 97 .
- The MSE of the best constant model is ≈ 167 .
- The simple linear regression model is a more flexible version of the constant model.