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LECTURE 11

Constant Model, Loss, and Transformations

Adjusting the Modeling Process: different models, loss functions, and data transformations.

Data 100/Data 200, Spring 2023 @ UC Berkeley

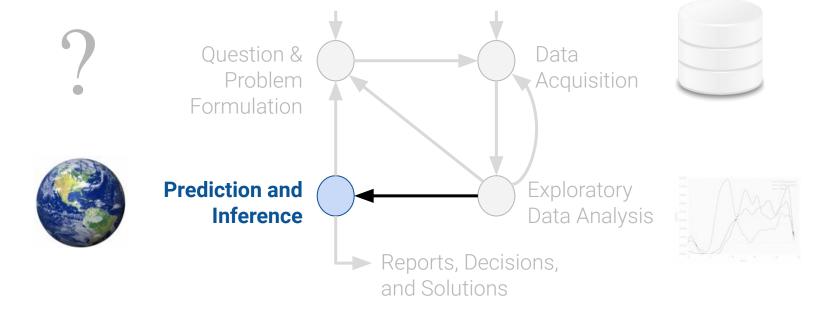
Narges Norouzi and Lisa Yan

Content credit: Acknowledgments



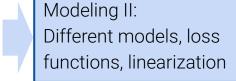
Plan for Next Few Lectures: Modeling







Modeling I: Intro to Modeling, Simple Linear Regression





Modeling III: Multiple Linear Regression





Today's Roadmap

Lecture 11, Data 100 Spring 2023

Modeling Process Review

Changing the Model: Constant Model + MSE

Changing the Loss: Constant Model + MAE

Revisiting SLR Evaluation

Transformations to Fit Linear Models

Introducing Notation for Multiple Linear

Regression



The Modeling Process (Simple Linear Regression)



1. Choose a model

How should we represent the world?

2. Choose a loss function

How do we quantify prediction error?

3. Fit the model

How do we choose the best parameters of our model given our data?

4. Evaluate model performance

How do we evaluate whether this process gave rise to a good model?



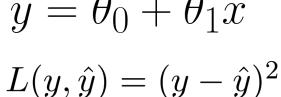
Review of the The Modeling Process (Simple Linear Regression)



2. Choose a loss

function

$$\hat{y} = \theta_0 + \theta_1 x$$



$$\hat{y_i}$$
 (SLR)

$$\hat{R}(\theta) = \frac{1}{n} \sum_{i=1}^{n} (y_i - (\theta_0 + \theta_1 x))^2$$

$$\hat{y} = \hat{\theta}_0 + \hat{\theta}_1 x \begin{cases} \hat{\theta}_0 = \bar{y} - \hat{\theta}_1 \bar{x} \\ \hat{\theta}_1 = r \frac{\sigma_y}{\sigma_x} \end{cases}$$



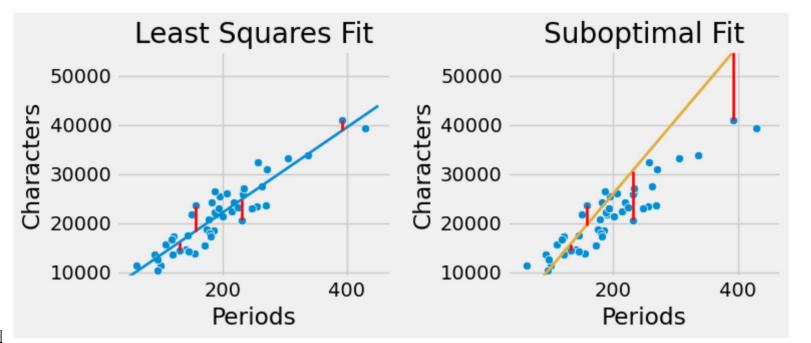
Minimizing MSE is Minimizing Squared Residuals



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

Lower residuals = better MSE fit!

Residual ("error") in prediction





Terminology: Prediction vs. Estimation



These terms are often used somewhat interchangeably, but there is a subtle difference between them.

Estimation is the task of using data to calculate model parameters.

Prediction is the task of using a model to predict outputs for unseen data.

We **estimate** parameters by minimizing average loss...

$$\hat{y} = \hat{\theta}_0 + \hat{\theta}_1 x$$

...then we **predict** using these estimates.

Least Squares Estimation is when we choose the

parameters that minimize MSE.





Changing the Model: Constant Model + MSE

Lecture 11, Data 100 Spring 2023

Modeling Process Review

Changing the Model: Constant Model + MSE

Changing the Loss: Constant Model + MAE

Revisiting SLR Evaluation

Transformations to Fit Linear Models

Introducing Notation for Multiple Linear Regression



The Modeling Process: Using a Different Model



1. Choose a model

SLR model Constant Model?
$$\hat{y} = ??$$
 $\hat{y} = \theta_0 + \theta_1 x$

2. Choose a loss function

- L2 Loss
- Mean Squared Error (MSE)

3. Fit the model

Minimize average loss with calculus

4. Evaluate model performance

Visualize, Root MSE

You work at a local boba tea store and want to estimate the sales each day.

Here's your data from 5 randomly selected previous days, arbitrarily sorted by number of drinks sold:

{20, 21, 22, 29, 33}

How many drinks will you sell tomorrow?

- **A.** 0
- **B.** 25
- **C.** 22
- **D.** 100
- E. Something else



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You work at a local boba tea store and want to estimate the sales each day. Here's your data from 5 randomly selected previous days, arbitrarily sorted by number of drinks sold: {20, 21, 22, 29, 33}

(i) Start presenting to display the poll results on this slide.



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You work at a local boba tea store and want to estimate the sales each day.

Here's your data from 5 randomly selected previous days, arbitrarily sorted by number of drinks sold:

{20, 21, 22, 29, 33}

How many drinks will you sell tomorrow?

- **A**. 0
- **B.** 25
- **C.** 22
- **D.** 100
- E. Something else

This is a constant model.





The **constant model**, also known as a **summary statistic**, summarizes the data by always "predicting" the same number—i.e., predicting a constant.

It ignores any relationships between variables:

- For instance, boba tea sales likely depend on the time of year, the weather, how the customers feel, whether school is in session, etc.
- Ignoring these factors is a simplifying assumption.

The constant model is also a parametric, statistical model:

$$\hat{y} = \theta_0$$





The **constant model**, also known as a **summary statistic**, summarizes the data by always "predicting" the same number—i.e., predicting a constant.

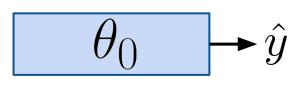
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- For instance, boba tea sales likely depend on the time of year, the weather, how the customers feel, whether school is in session, etc.
- Ignoring these factors is a **simplifying assumption**.

The constant model is also a parametric, statistical model:

$$\hat{y} = \theta_0$$

- Our parameter θ_0 is 1-dimensional. $\theta_0 \in \mathbb{R}$
- We now have no input into our model; we predict $\hat{y}=\theta_0$.
- Like before, we can still determine the best θ_0 that minimizes **average loss** on our data.





The Modeling Process: Using a Different Model





1. Choose a model

 $\frac{\text{SLR model}}{\hat{y} = \theta_0 + \theta_1 x}$

Constant Model

del $\hat{y}= heta_0$

2. Choose a loss function

L2 Loss

Mean Squared Error (MSE)

(Let's stick with MSE.)

3. Fit the model

Minimize average loss with calculus

4. Evaluate model Visualize, performance Root MSE



The Modeling Process: Using a Different Model



1. Choose a model

SLR model

Constant Model

 $\hat{y} = \theta_0$

2. Choose a loss

2 Loss

Mean Squared Error (MSE)

3. Fit the model

function

Minimize average loss with calculus

How does this step change?

4. Evaluate model performance

Visualize, Root MSE



Fit the Model: Rewrite MSE for the Constant Model



Recall that Mean Squared Error (MSE) is average squared loss (L2 loss) over the data $\mathcal{D} = \{y_1, y_2, \dots, y_n\}$:

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

L2 loss on a single datapoint

Given the **constant model** $\hat{y} = \theta_0$:

$$\hat{R}(\theta) = \frac{1}{n} \sum_{i=1}^{n} (y_i - \theta_0)^2$$

We **fit the model** by finding the optimal $\hat{\theta}_0$ that minimizes the MSE.



Fit the Model: Three Approaches



$$\hat{R}(\theta) = \frac{1}{n} \sum_{i=1}^{n} (y_i - \theta_0)^2$$

Approach 1 If you want to prove the general case for any data, you could directly minimize the objective. We can show that average loss is minimized by

$$\hat{\theta}_0 = mean(y) = \bar{y}$$

Approach 2 If you know your data $\mathcal{D}=\{20,21,22,29,33\}$, you could modify the objective by plugging in values first:

$$R(\theta) = \frac{1}{5}((20 - \theta_0)^2 + (21 - \theta_0)^2 + (22 - \theta_0)^2 + (29 - \theta_0)^2 + (33 - \theta_0)^2)$$

Approach 3 Algebraic trick.

We review Approach 1 on the next slide.

Approach 2 is left as practice; Approach 3 is in bonus slides.



Fit the Model: Calculus for the General Case



1. Differentiate with respect to θ_0 :

$$\frac{d}{d\theta_0}R(\theta) = \frac{d}{d\theta_0}(\frac{1}{n}\sum_{i=1}^n(y_i-\theta_0)^2)$$

$$= \frac{1}{n}\sum_{i=1}^n\frac{d}{d\theta_0}(y_i-\theta_0)^2 \quad \text{Derivative of sum is sum of derivatives}$$

$$= \frac{1}{n}\sum_{i=1}^n 2(y_i-\theta_0)(-1) \quad \text{Chain rule}$$

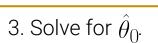
$$-2\sum_{i=1}^n (y_i-\theta_0)^2 \quad \text{Derivative of sum is sum of derivatives}$$

$$= \frac{-2}{n} \sum_{i=1}^{n} (y_i - \theta_0)$$

Simplify constants

2. Set equal to 0.

$$0 = \frac{-2}{n} \sum_{i=1}^{n} (y_i - \theta_0)$$





Fit the Model: Calculus for the General Case



1. Differentiate with respect to
$$\theta_0$$
:
$$\frac{d}{d\theta}R(\theta) = \frac{d}{d\theta}(\frac{1}{2}\sum_{i=1}^{n}(y_i - \theta_0)^2)$$

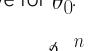
$$\frac{d}{d\theta_0}R(\theta) = \frac{d}{d\theta_0} \left(\frac{1}{n} \sum_{i=1}^n (y_i - \theta_0)^2\right)$$

$$=\frac{1}{n}\sum_{i=1}^{n}\frac{d}{d\theta_0}(y_i-\theta_0)^2$$
 Derivative of sum is sum of derivatives

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$$=\frac{1}{n}\sum_{i=1}^{n}\frac{2(y_i-\theta_0)(-1)}{2(y_i-\theta_0)(-1)}$$
 Chain rule

3. Solve for
$$\hat{\theta}_0$$
.



$$\sqrt{2}\sum_{n=1}^{\infty}(a_{n}-\theta_{n})=$$

 $0 = \frac{1}{n} \sum_{i=1}^{n} (y_i - \theta_0) = \sum_{i=1}^{n} (y_i - \theta_0)$

$$\stackrel{n}{\sum} \theta_0$$

Separate sums

$$=\sum_{i=1}^{n}y_i-\sum_{i=1}^{n}\theta_0 \qquad \text{Separate sums}$$

$$=(\sum_{i=1}^{n}y_i)-n\times\theta_0 \quad \text{c+c+...+c=nxc}$$



$$= \frac{-2}{n} \sum_{i=1}^{n} (y_i - \theta_0)$$
 Simplify constants

$$\sum_{i=1}^{l=1} y_i$$

2. Set equal to
$$0$$
.
$$n \times \theta_0 = (\sum_{i=1}^n y_i)$$

$$\hat{\theta}_0 = \frac{1}{n} (\sum_{i=1}^n y_i) \Longrightarrow \hat{\theta}_0 = \bar{y}$$





Interpreting $\theta_0 = \bar{u}$



This is the optimal parameter for constant model + MSE.

constant + MSE

- It holds true regardless of what data sample you have.
- It provides some formal reasoning as to why the mean is such a common summary statistic.

Fun fact: The minimum MSE is the **sample variance**. $R(\hat{\theta}_0) = R(\bar{y}) = \frac{1}{n}\sum_{i=1}^n (y_i - \bar{y})^2 = \sigma_y^2$

Note the difference:

$$R(\hat{\theta}_0) = \min_{\theta_0} R(\theta_0) = \sigma_y^2 \qquad \text{vs} \qquad \hat{\theta}_0 = \underset{\theta_0}{\operatorname{argmin}} \ R(\theta_0) = \bar{y}$$
 The **minimum value** of

In modeling, we care less about **minimum loss** $R(\hat{\theta}_0)$ and more about the **minimizer** of loss $\hat{\theta}_0$.



constant + MSE

The Modeling Process: Using a Different Model



1. Choose a model

Constant Model

 $\hat{y} = \theta_0$ Constant Model

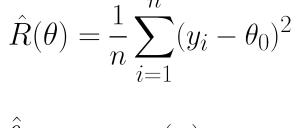
2. Choose a loss

function

Mean Squared Error (MSE)



Minimize average loss with calculus



4. Evaluate model performance

3. Fit the model

Visualize, Root MSE

$$\hat{\theta}_0 = mean(y) = \bar{y}$$



[Data] Comparing Two Different Models, Both Fit with MSE

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Suppose we wanted to predict dugong ages.



image source

Compare

Constant Model

$$\hat{y} = \theta_0$$

Data: Sample of ages.

$$\mathcal{D} = \{y_1, y_2, \dots, y_n\}$$

Simple Linear Regression

$$\hat{y} = \theta_0 + \theta_1 x$$

Data: Sample of (length, age)s.

$$\mathcal{D} = \{(x_1, y_1), (x_2, y_2),$$

$$\ldots, (x_n, y_n)$$



[Loss] Comparing Two Different Models, Both Fit with MSE



Constant Model

$$\hat{y} = \theta_0$$

$$\hat{ heta}_0$$
 is **1-D**.

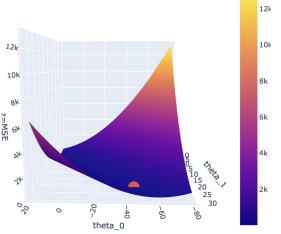
Loss surface is **2-D**.

|| |-|| ||

Simple Linear Regression
$$\hat{y} = \theta_0 + \theta_1 x$$

$$\hat{ heta} = [\hat{ heta_0}, \hat{ heta_1}]$$
 is **2-D**.

Loss surface is **3-D**.





[Fit] Comparing Two Different Models, Both Fit with MSE



Constant Model

$$\hat{y} = \theta_0$$

RMSE: **7.72**

Simple Linear Regression 328

$$\hat{y} = \theta_0 + \theta_1 x$$

RMSE **4.31**

Compare

See notebook for code

Interpret the RMSE (Root Mean Square Error):

- Constant error is HIGHER than linear error
- Constant model is **WORSE** than linear model (at least for this metric)

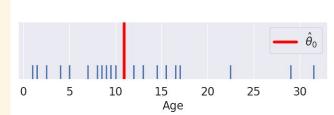


[Fit] Comparing Two Different Models, Both Fit with MSE

$$\hat{y} = \theta_0$$

RMSE:

Predictions on a rug plot.



Constant Model

$$\hat{y} = \theta_0$$

7.72

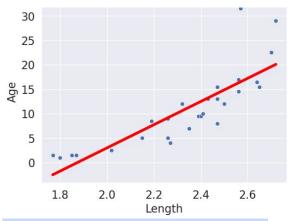
Simple Linear Regression 3280763

$$\hat{y} = \theta_0 + \theta_1 \hat{x}$$

RMSE

4.31

Predictions on a **scatter plot**.



Not a great linear fit visually? We'll come back to this...

Compare

See notebook for code



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The best estimator for a constant model with MSE loss is the mean of the y values

① Start presenting to display the poll results on this slide.





Changing the Loss: Constant Model + MAE

Lecture 11, Data 100 Spring 2023

Modeling Process Review

Changing the Model: Constant Model + MSE

Changing the Loss: Constant Model + MAE

Revisiting SLR Evaluation

Transformations to Fit Linear Models

Introducing Notation for Multiple Linear Regression



The Modeling Process: Using a Different Loss Function



1. Choose a model

Constant Model

 $\hat{y} = \theta_0$

2. Choose a loss

L2 Loss

Mean Squared Erro (MSE)

Suppose instead we use **L1 loss**. Average loss then becomes **Mean Absolute Error (MAE)**.

3. Fit the model

function

Minimize average loss with calculus

4. Evaluate model performance

Visualize, Root MSE



The Modeling Process: Using a Different Loss Function



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Constant Model

 $\hat{y} = \theta_0$

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Suppose instead we use **L1 loss**. Average loss then becomes **Mean Absolute Error (MAE)**.

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function

Minimize average loss with calculus

How does this step change?

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Visualize, Root MSE



Fit the Model: Rewrite MAE for the Constant Model



Recall that Mean **Absolute** Error (MAE) is average **absolute** loss (L1 loss)

Recall that Mean **Absolute** Error (MAE) is average **absolute** loss (LT is over the data
$$\mathcal{D}=\{y_1,y_2,\dots,y_n\}$$
:
$$\hat{R}(\theta_0)=\frac{1}{n}\sum_{i=1}^n \frac{|y_i-\hat{y}_i|}{\sum_{\text{L1 loss on a single datapoint}} y_i$$

Given the constant model $\hat{y}= heta_0$:

$$\hat{R}(\theta_0) = \frac{1}{n} \sum_{i=1}^{n} |y_i - \theta_0|$$

We **fit the model** by finding the optimal $\,\, heta_{\Omega}$ that minimizes the MAE.



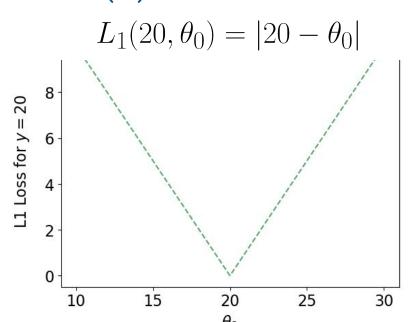
Exploring MAE: A Piecewise function

For the boba tea dataset {20, 21, 22, 29, 33}:

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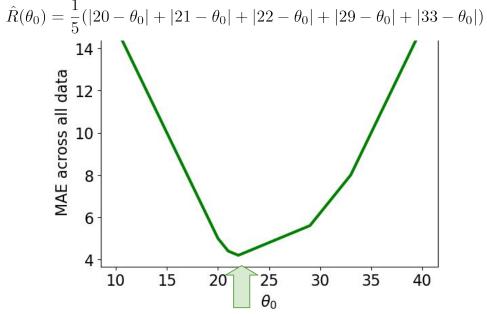
$$\hat{R}(\theta_0) = \frac{1}{n} \sum_{i=1}^{n} |y_i - \theta_0|$$

Absolute (L1) Loss on one observation:



An absolute value curve, centered at $\hat{\theta}_0$ = 20.

MAE (Mean Absolute Error) across all data:



Fit the Model: Calculus

1. Differentiate with respect to $\hat{\theta}_0$.

$$\frac{1}{d\theta_0}R(\theta_0) = \frac{d}{d\theta_0} \left(\frac{1}{n} \sum_{i=1}^n |y_i - \theta_0|\right)$$
$$= \frac{1}{n} \sum_{i=1}^n \frac{d}{d\theta_0} |y_i - \theta_0|$$

Absolute value!

The following derivation is beyond what we expect you to generate on your own. But you should understand it.





Fit the Model: Calculus



1. Differentiate with respect to θ_0 .

$$\frac{1}{d\theta_0}R(\theta_0) = \frac{d}{d\theta_0}\left(\frac{1}{n}\sum_{i=1}^n |y_i - \theta_0|\right)$$

Note: The derivative of the absolute value when the argument is 0 (i.e. when $\hat{y}= heta_0$) is technically undefined. We ignore this case in our derivation, since thankfully, it doesn't change our result (proof left to you).

$$=\frac{1}{n}\sum_{i=1}^{n}\frac{a}{d\theta_0}|y_i-\theta_0|$$

$$= \frac{1}{n} \sum_{i=1}^{n} \frac{\frac{d}{d\theta_0} |y_i - \theta_0|}{|y_i - \theta_0|}$$

$$|y_i - \theta_0| = \begin{cases} y_i - \theta_0 & \text{if } \theta_0 \le y_i \\ \theta_0 - y_i & \text{if } \theta_0 > y_i \end{cases}$$

$$\frac{d}{d\theta_0} |y_i - \theta_0| = \begin{cases} -1 & \text{if } \theta_0 < y_i \\ 1 & \text{if } \theta_0 > y_i \end{cases}$$



Take some time to process this math!

$$= \frac{1}{n} \left[\sum_{\theta_0 < y_i} (-1) + \sum_{\theta_0 > y_i} (+1) \right]$$



Fit the Model: Calculus



1. Differentiate with respect to θ_0 .

$$\frac{1}{d\theta_0}R(\theta_0) = \frac{d}{d\theta_0} \left(\frac{1}{n} \sum_{i=1}^n |y_i - \theta_0|\right)$$

$$= \frac{1}{n} \sum_{i=1}^n \frac{d}{d\theta_0} |y_i - \theta_0|$$

$$|y_i - \theta_0| = \begin{cases} \frac{1}{n} & \text{for } |y_i - \theta_0| \\ \text{for } |y_i - \theta_0| \end{cases}$$

$$= \frac{1}{n} \sum_{i=1}^{n} \frac{d}{d\theta_0} |y_i - \theta_0|$$

$$|y_i - \theta_0| = \begin{cases} y_i - \theta_0 & \text{if } \theta_0 \le y_i \\ \theta_0 - y_i & \text{if } \theta_0 > y_i \end{cases}$$

$$\frac{d}{d\theta_0} |y_i - \theta_0| = \begin{cases} -1 & \text{if } \theta_0 < y_i \\ 1 & \text{if } \theta_0 > y_i \end{cases}$$

$$= \frac{1}{n} \left[\sum_{\theta_0 < y_i} (-1) + \sum_{\theta_0 > y_i} (+1) \right]$$

Sum up for $i = 1, \ldots, n$: -1 if observation y_i > our prediction θ_0 ; +1 if observation y_i < our prediction θ_0 .



Fit the Model: Calculus

1. Differentiate with respect to $\hat{\theta}_0$.

The Differentiate with respect to
$$\theta_0$$
.
$$\frac{1}{d\theta_0}R(\theta_0) = \frac{d}{d\theta_0}(\frac{1}{n}\sum_{i=1}^n|y_i-\theta_0|)$$

$$= \frac{1}{n}\sum_{i=1}^n\frac{d}{d\theta_0}|y_i-\theta_0|$$

$$|y_i-\theta_0| = \begin{cases} y_i-\theta_0 & \text{if } \theta_0 \leq y_i \\ \theta_0-y_i & \text{if } \theta_0 > y_i \end{cases}$$

$$0 := \frac{1}{n} \left[\sum_{\theta_0 < y_i} (-1) + \sum_{\theta_0 > y_i} (+1) \right]$$

$$0 := -1$$

3. Solve for θ_0 .

$$0 = -\sum_{\theta_0 < y_i} 1 + \sum_{\theta_0 > y_i} 1$$
$$\sum_{i=1}^{\infty} 1 = \sum_{i=1}^{\infty} 1$$

$$=\frac{1}{n}[\sum_{\theta_0 < y_i} (-1) + \sum_{\theta_0 > y_i} (+1)]$$
 Where do we go from here?

 $\left| \frac{d}{d\theta_0} |y_i - \theta_0| = \begin{cases} -1 & if \ \theta_0 < y_i \\ 1 & if \ \theta_0 > y_i \end{cases} \right|$

Median Minimizes MAE for the Constant Model

The constant model parameter $\theta = \theta_0$ that minimizes MAE must satisfy:

$$\sum_{\theta_0 < y_i} 1 = \sum_{\theta_0 > y_i} 1$$
 # observations # observations greater than $\hat{\theta}_0$ less than $\hat{\theta}_0$

In other words, theta needs to be such that there are an equal # of points to the left and right.

This is the definition of the **median!**
$$\hat{\theta}_0 = median(y)$$

For example, in our bubble tea dataset {20, 21, 22, 29, 33}, the point in green (22) is the median.

It is the value in the "middle."





Summary: Loss Optimization, Calculus, and...Critical Points?



First, define the **objective function** as average loss.

- Plug in L1 or L2 loss.
- Plug in model so that resulting expression is a function of §.

Then, find the **minimum** of the objective function:

- 1. Differentiate with respect to %.
- 2. Set equal to 0.
- 3. Solve for $\hat{\theta}$.

Repeat w/partial derivatives if multiple parameters

Recall **critical points** from calculus: $R(\hat{\theta})$ could be a minimum, maximum, or saddle point!

- We should technically also perform the second derivative test, i.e., show $R''(\hat{ heta})>0$.
- You will prove on homework that MSE has a property—convexity—that guarantees that $R(\hat{\theta})$ is a global minimum.
- The proof of convexity for MAE is beyond this course.

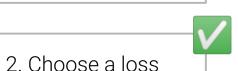


The Modeling Process: Using a Different Loss Function



Constant Model

$$\hat{y} = \theta_0$$



Mean Absolute Error (MAE)



function

Minimize average loss with calculus

$$\hat{R}(\theta_0) = \frac{1}{n} \sum_{i=1}^{n} |y_i - \theta_0|$$

$$\hat{\theta}_0 = median(y)$$



Visualize, Root MSE



[Estimator] Two Constant Models, Fit to Different Losses

MSE (Mean Squared Loss)

$$\hat{R}(\theta) = \frac{1}{n} \sum_{i=1}^{n} (y_i - \theta_0)^2 \qquad \hat{R}(\theta_0) = \frac{1}{n} \sum_{i=1}^{n} |y_i - \theta_0|$$

Minimized with **sample mean**:

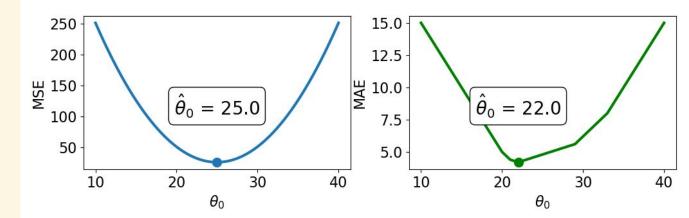
$$\hat{\theta}_0 = mean(y) = \bar{y}$$
 $\hat{\theta}_0 = median(y)$

MAE (Mean Absolute Loss) 3280763

$$\hat{R}(\theta_0) = \frac{1}{n} \sum_{i=1}^{n} |y_i - \theta_0|$$

Minimized with sample median:

$$\hat{\theta}_0 = median(y)$$



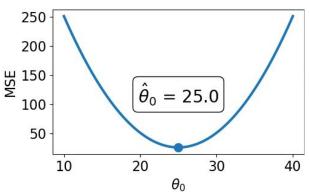
Compare



[Loss] Two Constant Models, Fit to Different Losses

MSE (Mean Squared Loss)

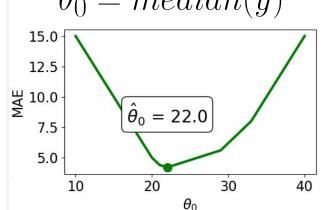
$$\hat{\theta}_0 = mean(y) = \bar{y}$$



Smooth. Easy to minimize using numerical methods (in a few weeks).

MAE (Mean Absolute Loss) 3280763





Piecewise. at each of the "kinks," it's not differentiable. Harder to minimize.





[Outlier] Two Constant Models, Fit to Different Losses

data = {20, 21, 22, 29, 33, **1033**}

MSE (Mean Squared Loss)

Minimized with **sample mean**:

$$\hat{\theta}_0 = mean(y) = \bar{y}$$

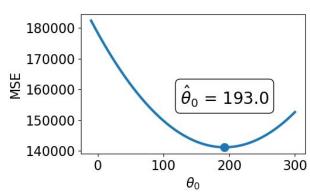
Sensitive to outliers (since they change mean substantially).
Sensitivity also depends on the dataset size.

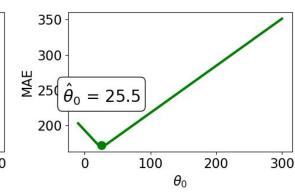
MAE (Mean Absolute Loss) 3280763 Minimized with sample median:

$$\hat{\theta}_0 = median(y)$$

More robust to outliers.

Compare



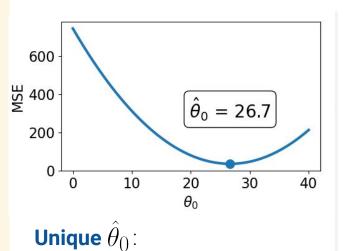


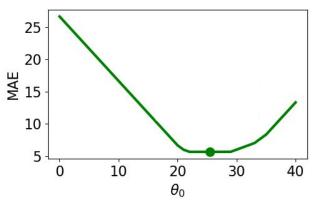
Uniqueness under Different Loss Functions

MSE (Mean Squared Error)

MAE (Mean Absolute Error)

Suppose we add a 6th observation to our bubble tea dataset: {20, 21, 22, 29, 33, **35**}





Compare

$$\hat{\theta}_0 = \frac{1}{n} \left(\sum_{i=1}^n y_i \right)$$

Infinitely many $\hat{\theta}_0$ s. Any $\hat{\theta}_0$ in range (22, 29) minimizes MAE.

(In practice: With an even # of datapoints, set median to mean of two middle points, e.g., 25.5).



slido



The best estimator for a constant model with MAE loss is the ----- of the y values.

① Start presenting to display the poll results on this slide.





Revisiting SLR Evaluation (from Lecture 10)

Lecture 11, Data 100 Spring 2023

Modeling Process Review

Changing the Model: Constant Model + MSE

Changing the Loss: Constant Model + MAE

Revisiting SLR Evaluation

Transformations to Fit Linear Models
Introducing Notation for Multiple Linear
Regression



Four Mysterious Datasets (Anscombe) + Least Squares



Ideal model evaluation steps, in order:

- Visualize original data, Compute Statistics
- Performance Metrics
 For our simple linear least square model, use RMSE (we'll see more metrics later)
- 3. Residual Visualization

4 datasets could have similar aggregate statistics but still be wildly different:

```
x_mean : 9.00, y_mean : 7.50
x_stdev: 3.16, y_stdev: 1.94
r = Correlation(x, y): 0.816
ahat: 3.00, bhat: 0.50
RMSE: 1.119
```



Visualize, Then Quantify!

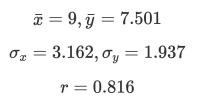


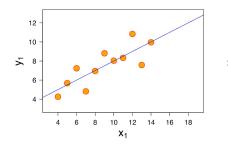
Anscombe's quartet refers to the following four sets of points on the right.

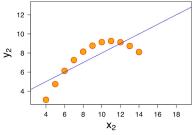
- They each have the same mean of x, mean of y, SD of x, SD of y, and r value.
- Since our optimal Least Squares SLR model only depends on those quantities, they all have the same regression line.

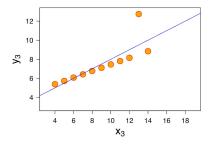
However, only one of these four sets of data makes sense to model using SLR.

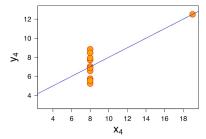
Before modeling, you should always visualize your data first!













Four Mysterious Datasets + Least Squares

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Ideal model evaluation steps, in order:

- Visualize original data, Compute Statistics
- 2. Performance Metrics
 For our simple linear least square model,
 use RMSE (we'll see more metrics later)

3. Residual Visualization

From Data 8 (textbook):

The residual plot of a good regression shows no pattern.

4 datasets could have similar aggregate statistics but still be wildly different: x_mean : 9.00, y_mean : 7.50

x_stdev: 3.16, y_stdev: 1.94 r = Correlation(x, y): 0.816 ahat: 3.00, bhat: 0.50

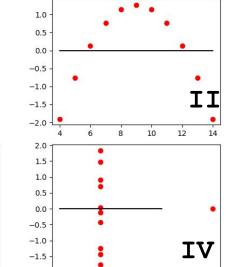
RMSE: 1.119

 $\langle \mathcal{D} \rangle$

 \supset

 $\hat{\mathcal{L}}$

Diat: 6



7.5 10.0 12.5 15.0 17.5





Transformations to Fit Linear Models

Lecture 11, Data 100 Spring 2023

Modeling Process Review

Changing the Model: Constant Model + MSE

Changing the Loss: Constant Model + MAE

Revisiting SLR Evaluation

Transformations to Fit Linear Models

Introducing Notation for Multiple Linear Regression



Tukey-Mosteller Bulge Diagram (From Lecture 08)

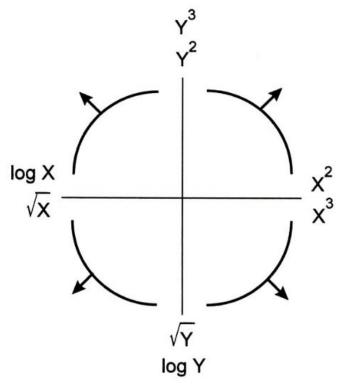


The **Tukey-Mosteller Bulge Diagram** is a guide to possible transforms to try to get linearity.

- There are multiple solutions. Some will fit better than others.
- sqrt and log make a value "smaller".
- Raising to a value to a power makes it "bigger".
- Each of these transformations equates to increasing or decreasing the scale of an axis.

Other goals other than linearity are possible

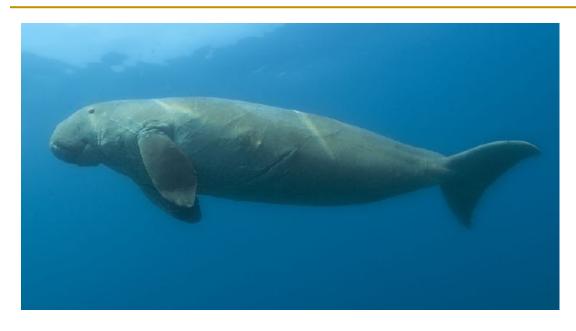
- E.g. make data appear more symmetric.
- Linearity allows us to fit lines to the transformed data





Back to Least Squares Regression with Dugongs





From Data 8 (<u>textbook</u>):

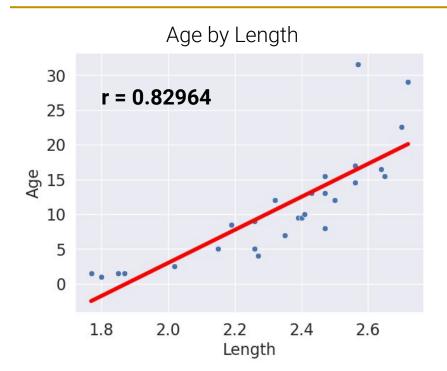
The residual plot of a good regression shows no pattern.

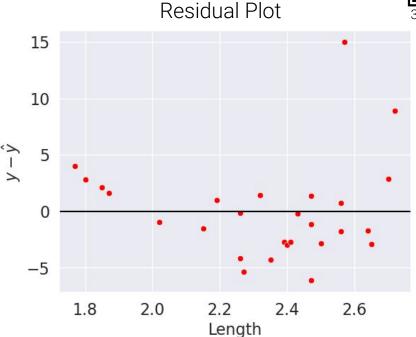
https://inferentialthinking.com/chapters/15 /5/Visual_Diagnostics.html 52



Back to Least Squares Regression with Dugongs







Residual plot shows a clear pattern! On closer inspection, the scatter plot **curves upward**.

Q: How can we fit a curve to this data with the tools we have?

A: Transform the Data.



Transforming Dugongs

Suppose we do a log(y) transformation (we'll explain why soon).

Notice that the resulting model is

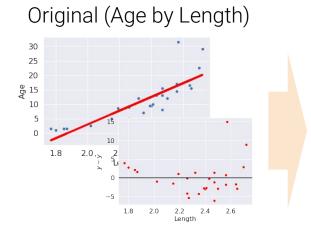
still linear in the parameters $\theta = [\theta_0, \theta_1]$: $log(y) = \theta_0 + \theta_1 x$

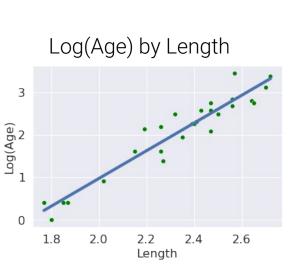
In other words, if we apply the variable transform $z = \log(y)$:

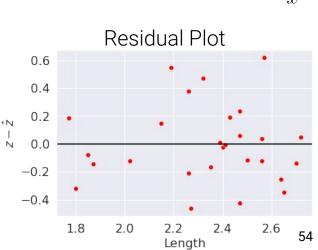
$$\begin{aligned}
\log(y) &= \theta_0 + \theta_1 x \\
\hat{z} &= \theta_0 + \theta_1 x
\end{aligned}$$

$$1x R(\theta) = \frac{1}{n} \sum_{i=1}^{n} (z_i - \hat{z}_i)^2$$

$$\hat{\theta}_0 = \bar{z} - \hat{\theta}_1 \bar{x} \hat{\theta}_1 = r \frac{\sigma_z}{2}$$







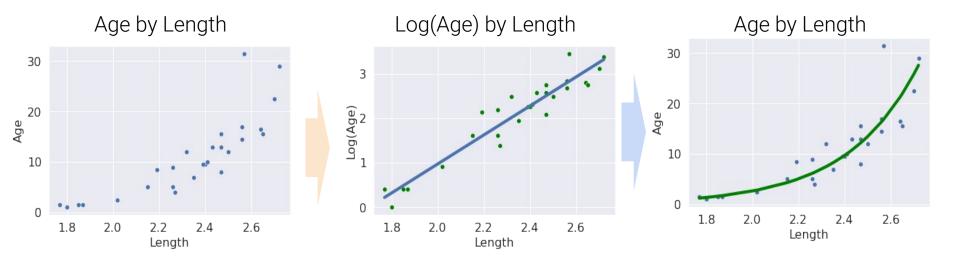


Fit a Curve using Least Squares Regression



$$z = \log(y)$$







Tukey-Mosteller Bulge Diagram

If your data "bulges" in a direction, transform x and/or y in that direction.

Each of these transformations equates to increasing or decreasing the scale of an axis.

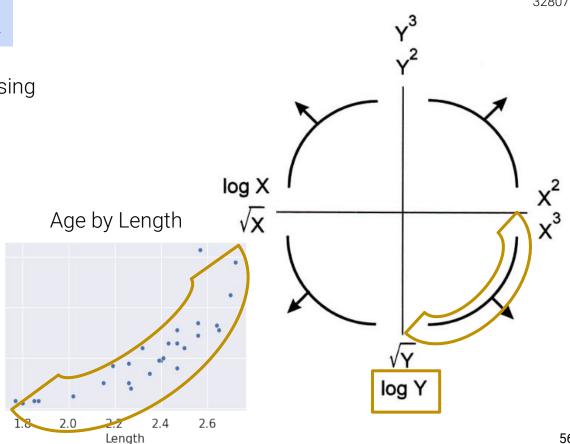
30

20 Age

10

- Roots and logs make a value "smaller".
- Raising to a power makes a value "bigger".

There are multiple solutions! Some will fit better than others.







Introducing Notation for Multiple Linear Regression

Lecture 11, Data 100 Spring 2023

Modeling Process Review

Changing the Model: Constant Model + MSE

Changing the Loss: Constant Model + MAE

Revisiting SLR Evaluation

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A Note on Terminology



There are several equivalent terms in the context of regression.

Feature(s)

Covariate(s)

Independent variable(s)

Explanatory variable(s)

Predictor(s)

Input(s)

Regressor(s)

Output

Outcome

Response

Dependent variable

Weight(s)

Parameter(s)

Coefficient(s)

Prediction

Predicted response

Estimated value

Estimator(s)

Optimal parameter(s)

Bolded terms are the most common in this course.

Match each column with the appropriate term: $x,y,\hat{y},\theta,\hat{\theta}$

A Note on Terminology



There are several equivalent terms in the context of regression.

Feature(s)

Covariate(s)

Independent variable(s)

Explanatory variable(s)

Predictor(s)

Input(s)

Regressor(s)

 ${\mathcal X}$

Bolded terms are the most common in this course.

Output

Outcome

Response

Dependent variable

0

Weight(s)

Parameter(s)

Coefficient(s)

 θ

Prediction

Predicted response

Estimated value

Ź

Estimator(s)

Optimal parameter(s)



A datapoint (x, y) is also called an **observation**.



Multiple Linear Regression



Define the **multiple linear regression** model:

$$\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_p x_p$$

Parameters are
$$\theta=[\theta_0,\theta_1,\dots,\theta_p]$$
 Is this linear in θ ? A. no B. yes C. maybe



Multiple Linear Regression

■# ... ■ ■ Fr & ... 3280763

Define the **multiple linear regression** model:

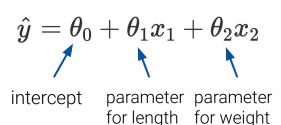
$$\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_p x_p$$

Parameters are
$$heta = [heta_0, heta_1, \dots, heta_p]$$

Yes! This is a linear combination of θ_j 'S, each scaled by x_j .

$$(x_1,\ldots,x_p) \longrightarrow \theta = [\theta_0,\theta_1,\ldots,\theta_p] \longrightarrow \hat{\mathcal{Y}}$$
 single input (p features) single prediction

Example: Predict dugong ages \hat{y} as a linear model of 2 features: length x_1 and weight x_2 .







$$\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_p x_p$$

More on Multiple Linear Regression on Thursday





Bonus: Constant Model MSE, Approach 3



MSE minimization using an algebraic trick



It turns out that in this case, there's another rather elegant way of performing the same minimization algebraically, but without using calculus.

- We present this derivation in the next few slides.
- In this proof, you will need to use the fact that the **sum of deviations from the mean is 0** (in other words, that $\sum_{i=0}^{n} (y_i \bar{y}) = 0$). We present that proof here:

$$egin{aligned} \sum_{i=1}^n (y_i - ar{y}) &= \sum_{i=1}^n y_i - \sum_{i=1}^n ar{y} \ &= \sum_{i=1}^n y_i - nar{y} = \sum_{i=1}^n y_i - n\cdotrac{1}{n} \sum_{i=1}^n y_i = \sum_{i=1}^n y_i - \sum_{i=1}^n y_i \ &= 0 \end{aligned}$$

For example, this mini-proof shows 1+2+3+4+5 is the same as 3+3+3+3+3.

• Our proof will also use the definition of the variance of a sample. As a refresher:

$$\sigma_y^2 = rac{1}{n} \sum_{i=1}^n (y_i - ar{y})^2$$

Equal to the MSE of the sample mean!



MSE minimization using an algebraic trick



$$\begin{split} R(\theta) &= \frac{1}{n} \sum_{i=1}^{n} (y_i - \theta)^2 \\ &= \frac{1}{n} \sum_{i=1}^{n} \left[(y_i - \bar{y}) + (\bar{y} - \theta) \right]^2 \\ &= \frac{1}{n} \sum_{i=1}^{n} \left[(y_i - \bar{y})^2 + 2(y_i - \bar{y})(\bar{y} - \theta) + (\bar{y} - \theta)^2 \right] \\ &= \frac{1}{n} \left[\sum_{i=1}^{n} (y_i - \bar{y})^2 + 2(\bar{y} - \theta) \sum_{i=1}^{n} (y_i - \bar{y}) + n(\bar{y} - \theta)^2 \right] \\ &= \frac{1}{n} \sum_{i=1}^{n} (y_i - \bar{y})^2 + \frac{2}{n} (\bar{y} - \theta) \cdot 0 + (\bar{y} - \theta)^2 \\ &= \sigma_y^2 + (\bar{y} - \theta)^2 \end{split}$$
 from the previous slide

variance of sample!

This proof relies on an algebraic trick. We can write the difference **a - b** as **(a - c) + (c - b)**, where a, b, and c are any numbers.

Using that fact, we can write $y_i - \theta = (y_i - \bar{y}) + (\bar{y} - \theta)$, where $\bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i$, our sample mean.

Also note: going from line 3 to 4, we distribute the sum to the individual terms. This is a property of sums you should become familiar with!



Minimization using an algebraic trick



In the previous slide, we showed that $R(heta) = \sigma_y^2 + (ar{y} - heta)^2$

- Since variance can't be negative, the first term is greater than or equal to 0.
 - o Of note, the first term doesn't involve θ at all. Changing our model won't change this value, so for the purposes of determining $\hat{\theta}$, we can ignore it.
- The second term is being squared, and so also must be greater than or equal to 0.
 - \circ This term does involve $\, heta\,$, and so picking the right value of $\, heta\,$ will minimize our average loss.
 - \circ We need to pick the heta that sets the second term to 0.
 - \circ This is achieved when $heta=ar{y}$. In other words:

$$\hat{ heta} = ar{y} = \mathbf{mean}(y)$$

Looks familiar!

