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⚠️ Reminder to start the Zoom recording!

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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 2025 @ UC Berkeley

Narges Norouzi and Josh Grossman

Content credit: Acknowledgments

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Announcements

Lecture 11, Data 100 Spring 2025

Grad Students:

- Grad project released!
- Project proposal due **Monday, March 3**
- Use Ed thread #666 for group matching

Catch-up hour:

- Every Friday, 3-4pm in VLSB 2032
- Q&A session for **past content**

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Plan for Next Few Lectures: Modeling

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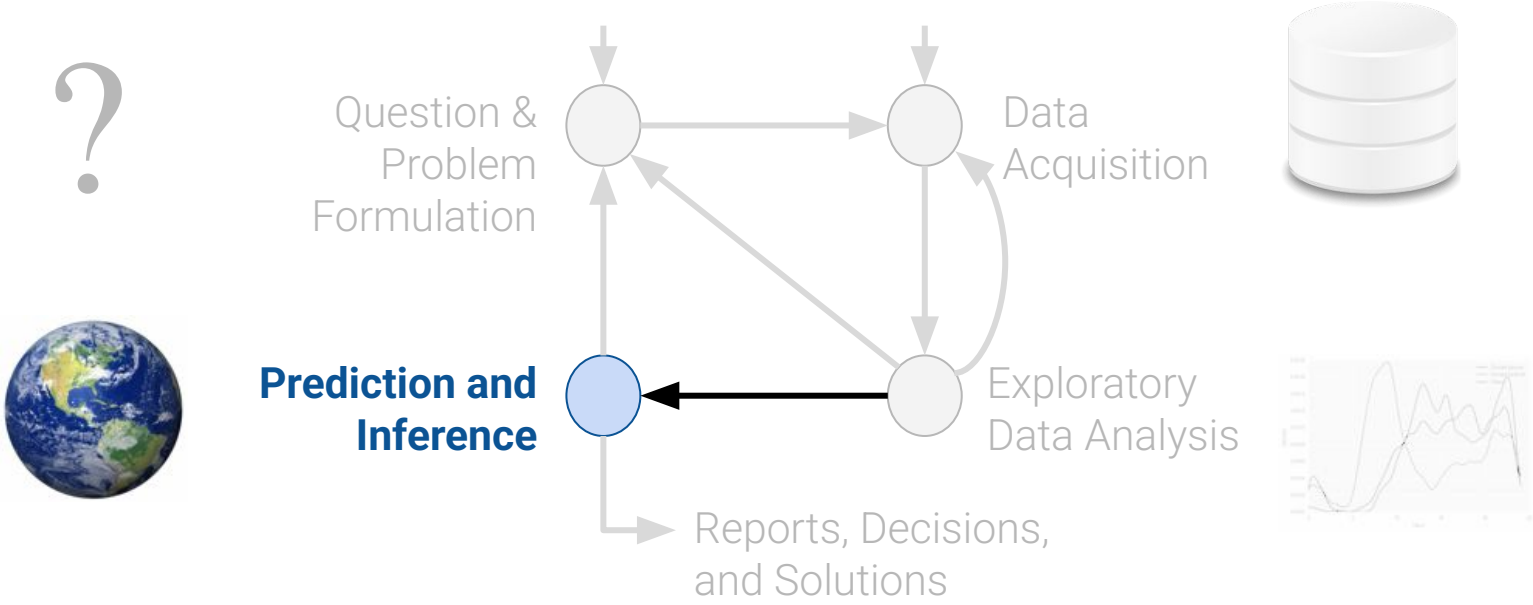

(today)

Modeling I: Intro to Modeling, Simple Linear Regression	→	**Modeling II: Different models, loss functions, linearization**	→	Modeling III: Multiple Linear Regression

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Today's Roadmap

Lecture 11, Data 100 Spring 2025

Modeling Process

- Iteration 1: SLR + MSE (last time!)
- Iteration 2: Constant Model + MSE
- Iteration 3: Constant Model + MAE

Transformations of Linear Models

Notation for Multiple Linear Regression

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Iteration 2: Constant Model + MSE

Lecture 11, Data 100 Spring 2025

Modeling Process

- Iteration 1: SLR + MSE (last time!)
- **Iteration 2: Constant Model + MSE**
- Iteration 3: Constant Model + MAE

Transformations of Linear Models

Notation for Multiple Linear Regression

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Visualizing the sum of squared error for simple linear regression (SLR)

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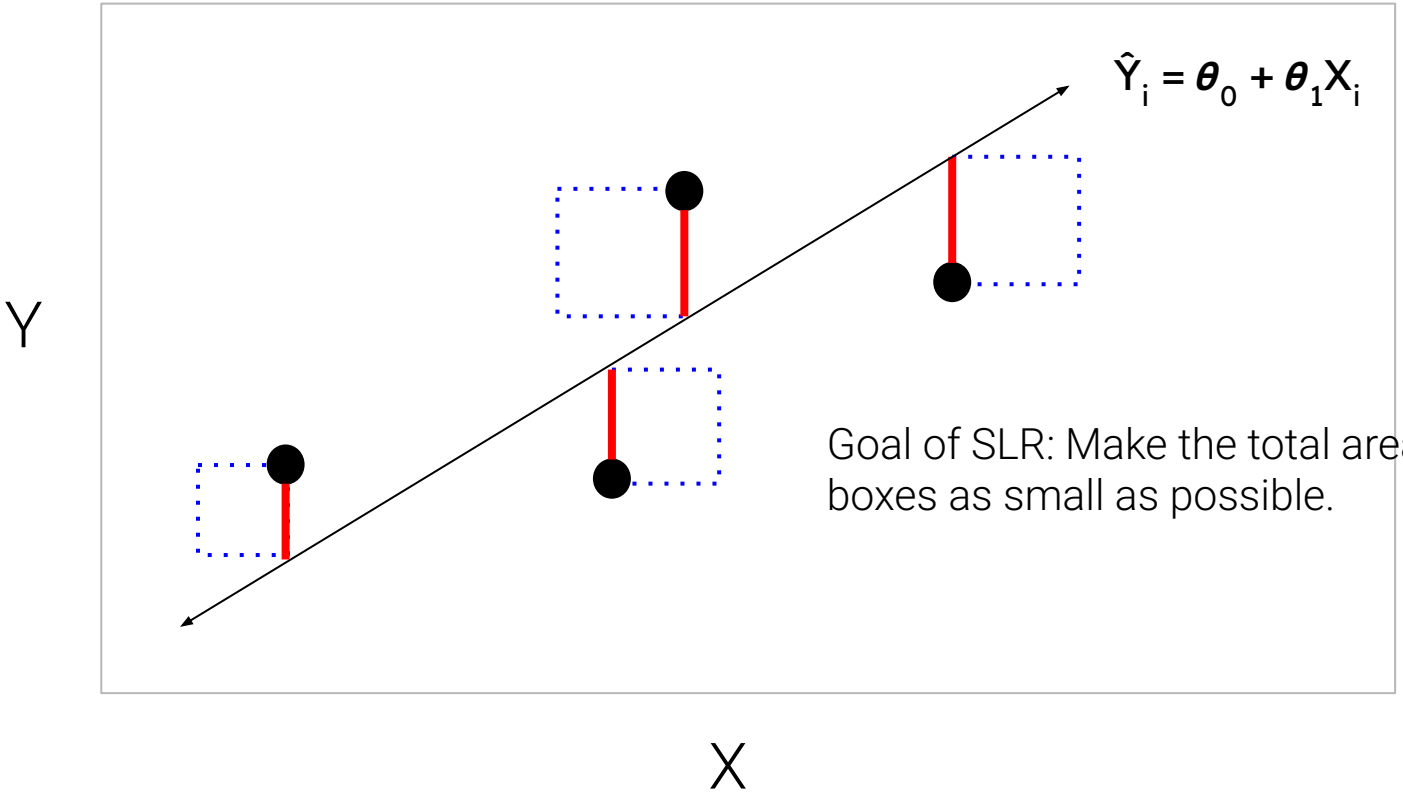

Goal of SLR: Make the total area of the boxes as small as possible.

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Visualizing the sum of squared error for a constant model

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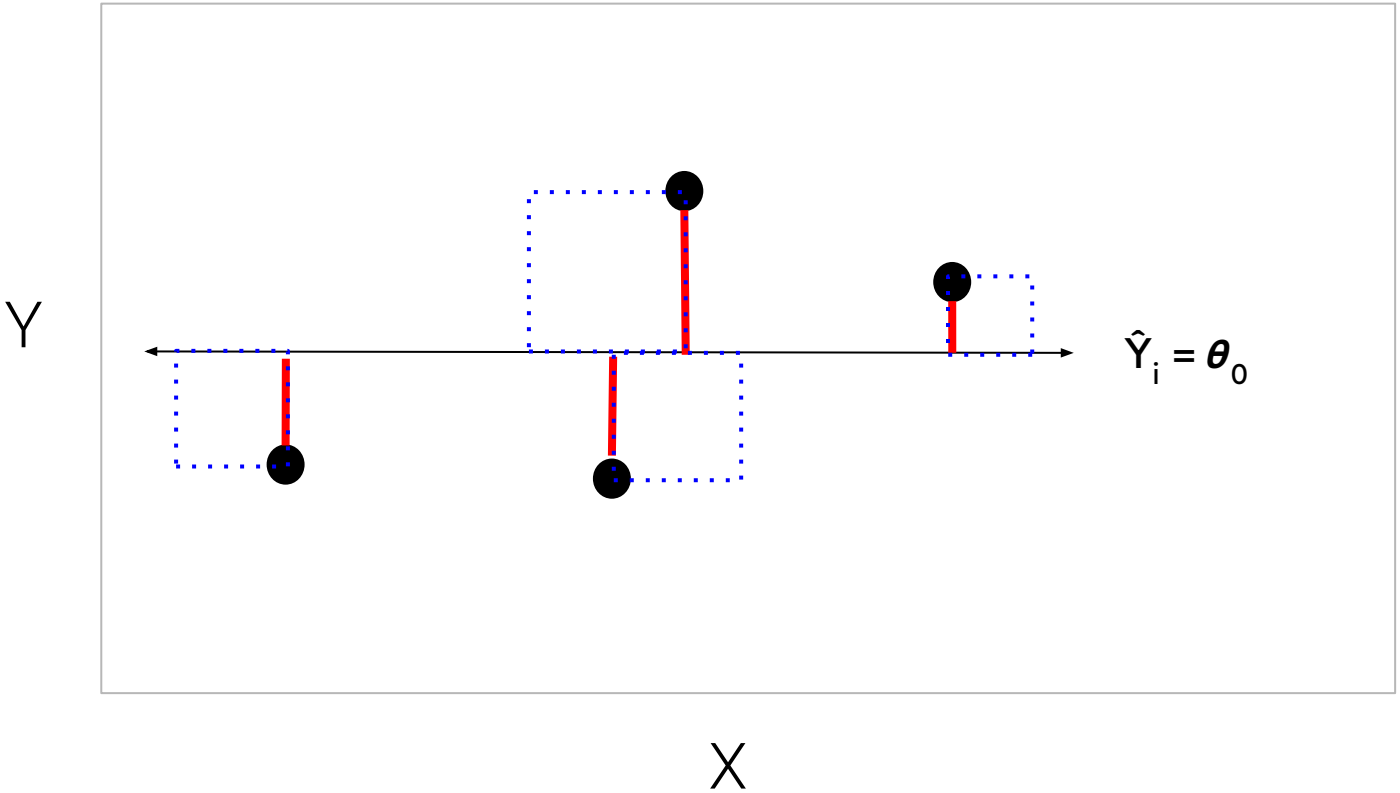

Also known as an intercept-only model.

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R^2 measures quality of linear model fit relative to constant model

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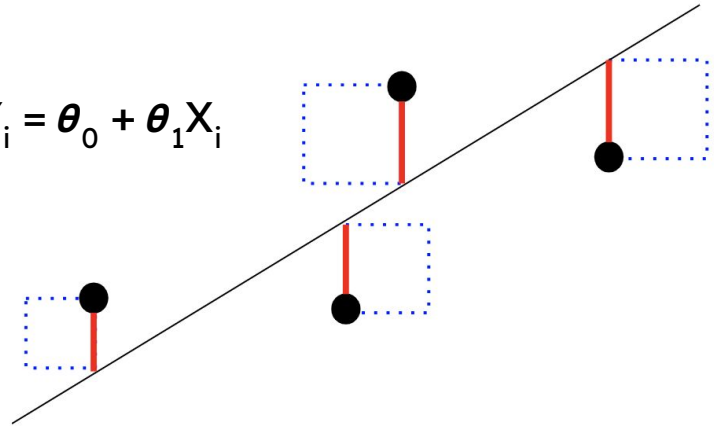
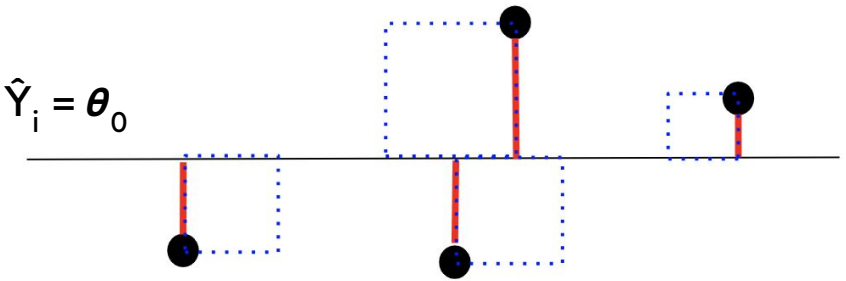
$\hat{Y}_i = \theta_0 + \theta_1 X_i$



$\hat{Y}_i = \theta_0$



$$R^2 = \frac{\Delta \text{ in area}}{\text{Constant model area}}$$

For SLR, $R^2 = r^2$. More on R^2 in a later lecture!

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The Modeling Process: Using a Different Model

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1. Choose a model

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

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

2. Choose a loss function

L2 Loss

Mean Squared Error (MSE)

3. Fit the model

Minimize average loss with calculus

4. Evaluate model performance

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The Constant Model

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You work at a local boba shop and want to predict the daily number of drinks sold.

Here's your data from 5 randomly selected previous days:

$$\{20, 29, 22, 21, 33\}$$

You have other info (e.g., the weather and day of week), but you *ignore everything except the historical # of drinks sold*.

Your model always predicts the same number.

This is a **constant model**.

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The Constant Model

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The **constant model** **always predicts the same number**—i.e., 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**.

Like SLR, the constant model is a parametric, statistical model:

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

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The Constant Model

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Our parameter $\boldsymbol{\theta}_0$ is 1-dimensional. $\theta_0 \in \mathbb{R}$

Unlike SLR, no input needed to generate a prediction; we always predict $\hat{y} = \theta_0$

Like before, we can still determine the best $\boldsymbol{\theta}_0$ that minimizes **average loss** on our data.

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

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The Modeling Process: Using a Different Model

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1. Choose a model ✅

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

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

2. Choose a loss function

L2 Loss

Mean Squared Error (MSE)

$$\hat{R}(\theta) = \underbrace{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}_{\text{"Average loss" "Objective function" "Mean squared error"}}$$

3. Fit the model

Minimize average loss with calculus

4. Evaluate model performance

Why is there a hat above R? We are *estimating* the average loss with a sample. Estimated values often have a hat. Technically, there is also a "true" loss for the entire population from which our sample is drawn. We would write the expression for this "true" loss without a hat. Don't worry about this for Data 100!

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The Modeling Process: Using a Different Model

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1. Choose a model ✅

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

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

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L2 Loss

Mean Squared Error (MSE)

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

3. Fit the model

Minimize average loss with calculus

How does this step change?

4. Evaluate model performance

Why is there a hat above R? We are *estimating* the average loss with a sample. Estimated values often have a hat. Technically, there is also a "true" loss for the entire population from which our sample is drawn. We would write the expression for this "true" loss without a hat. Don't worry about this for Data 100!

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Fit the Model: Rewrite MSE for the Constant Model

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

$$\hat{R}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \underbrace{(y_i - \hat{y}_i)^2}_{\text{L2 loss on a single datapoint}}$$

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

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

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

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Fit the Model: Where We Are Headed

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

With calculus, we can show that the average loss (i.e., our objective function) is minimized by

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

Given a dataset, we can also find the minimizing $\boldsymbol{\theta}_0$ with an iterative algorithm. More soon!

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Fit the Model: Calculus for the General Case

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1. Differentiate with respect to θ_0:

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

2. Set equal to 0.

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

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Fit the Model: Calculus for the General Case

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1. Differentiate with respect to θ_0:

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

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

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

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

2. Set equal to 0.

$$0 = \frac{-2}{n}\sum_{i=1}^{n}\left(y_i - \hat{\theta}_0\right)$$

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

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Fit the Model: Calculus for the General Case

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Fit the Model: Calculus for the General Case

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

$$0 = \frac{-2}{n}\sum_{i=1}^{n}\left(y_i - \hat{\theta}_0\right) = \sum_{i=1}^{n}\left(y_i - \hat{\theta}_0\right)$$

$$= \sum_{i=1}^{n} y_i - \sum_{i=1}^{n}\hat{\theta}_0$$ Separate sums

$$= \sum_{i=1}^{n} y_i - n \cdot \hat{\theta}_0$$ c + c + … + c = nxc

$$n \cdot \hat{\theta}_0 = \sum_{i=1}^{n} y_i$$

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

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Fit the Model: Calculus for the General Case

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1. Differentiate with respect to θ_0:

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

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

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$$0 = \frac{-2}{n}\sum_{i=1}^{n}\left(y_i - \hat{\theta}_0\right)$$

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

$$0 = \frac{\cancel{-2}}{\cancel{n}}\sum_{i=1}^{n}\left(y_i - \hat{\theta}_0\right) = \sum_{i=1}^{n}\left(y_i - \hat{\theta}_0\right)$$

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$$= \sum_{i=1}^{n} y_i - n \cdot \hat{\theta}_0$$ c + c + … + c = nxc

$$n \cdot \hat{\theta}_0 = \sum_{i=1}^{n} y_i$$

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

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Interpreting $\hat{\theta}_0 = \bar{y}$

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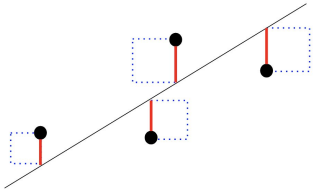
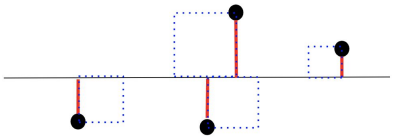
The **mean** of the outcomes achieves the minimum MSE of the constant model.

Minimum MSE is the **sample variance** of y → $$R(\hat{\theta}_0) = R(\bar{y}) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})^2 = \sigma_y^2$$

R^2 (from earlier) is interpreted as the fraction of **variance in y** "explained" by a linear model.

$$\mathrm{R}^2 = \frac{\Delta \text{ in area}}{\text{Constant model area}} = \frac{\mathrm{MSE}_{\text{constant model}} - \mathrm{MSE}_{\text{linear model}}}{\mathrm{MSE}_{\text{constant model}}}$$





Technical note: The area is the sum of squared errors, not the MSE. Area/n=MSE.
Also, the R in the average loss expression is unrelated to R^2.

Why "explained" is in quotes: There is no causality here!

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Interpreting $\hat{\theta}_0 = \bar{y}$

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$$R(\hat{\theta}_0) = \min_{\theta_0} R(\theta_0) = \sigma_y^2 \quad \text{vs} \quad \hat{\theta}_0 = \underset{\theta_0}{\operatorname{argmin}}\ R(\theta_0) = \bar{y}$$

The **minimum** MSE

The **arg**ument that **min**imizes MSE

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

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The Modeling Process: Using a Different Model

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1. Choose a model ✅

Constant Model

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

2. Choose a loss function ✅

L2 Loss

Mean Squared Error (MSE)

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

3. Fit the model ✅

Minimize average loss with calculus

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

4. Evaluate model performance

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

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Modeling the relationship of dugong age (y) and length (x).

A Dugong [image source]

Not a Dugong, a Dewgong [image source]

Constant Model

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

Data: Sample of ages.

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

Simple Linear Regression

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

Data: Sample of (length, age)s.

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

Demo

lec10.ipynb

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

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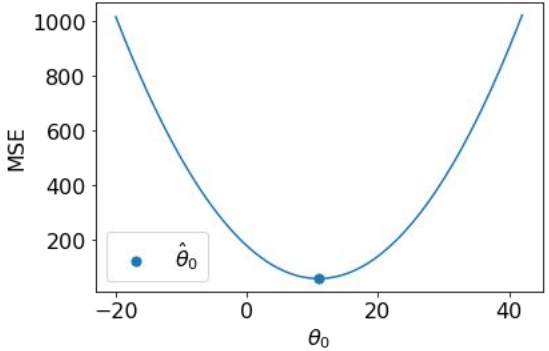
Constant Model

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

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

Loss surface is **2-D**.



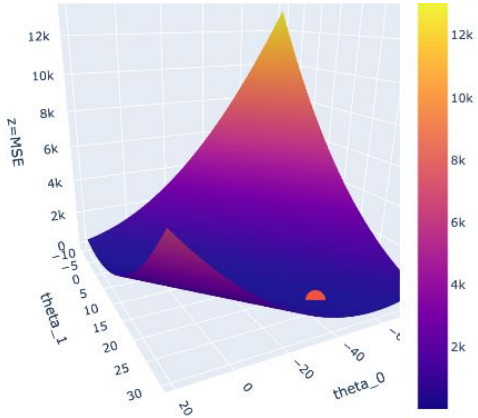
$$\hat{R}(\theta_0) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \theta_0)^2$$

Simple Linear Regression

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

$\hat{\theta} = [\hat{\theta}_0, \hat{\theta}_1]$ is **2-D**.

Loss surface is **3-D**.



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

Demo

lec10.ipynb

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

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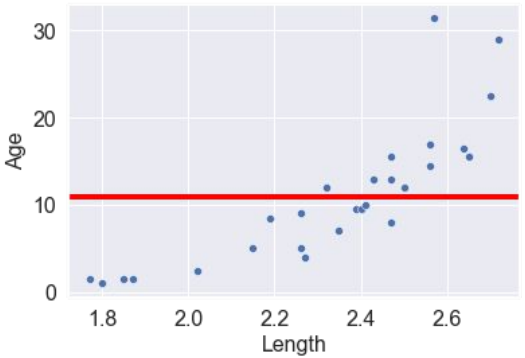
Constant Model

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

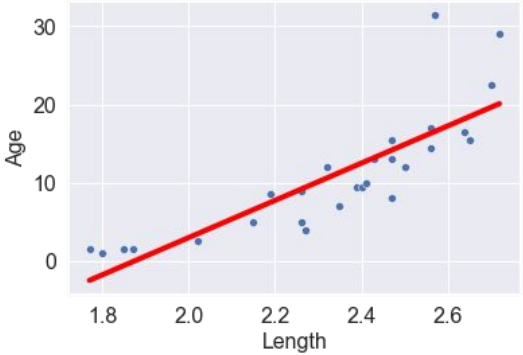
Root MSE (RMSE): **7.72**



Simple Linear Regression

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

Root MSE (RMSE): **4.31**



Interpretation of RMSE:

- Constant model RMSE is **higher** than linear model RMSE
- Constant model has a **poorer fit** than linear model, using RMSE as our metric.

Demo

lec10.ipynb

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

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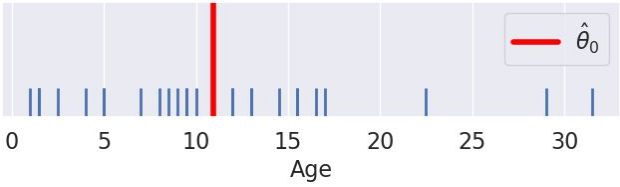
Constant Model

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

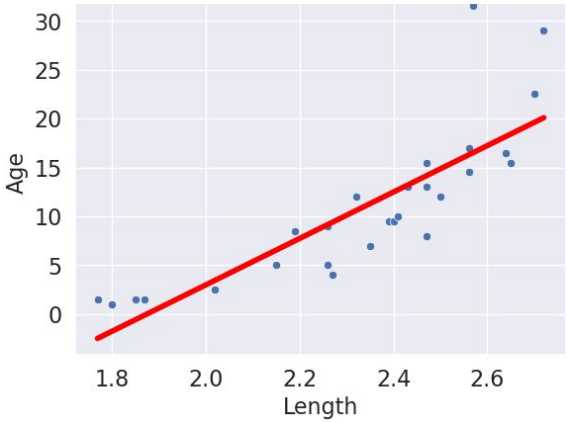
Predictions on a **rug plot**.



Simple Linear Regression

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

Predictions on a **scatter plot**.



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

Demo

lec10.ipynb

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Iteration 3: Constant Model + MAE

Lecture 11, Data 100 Spring 2025

Modeling Process

- Iteration 1: SLR + MSE (last time!)
- Iteration 2: Constant Model + MSE
- **Iteration 3: Constant Model + MAE**

Transformations of Linear Models

Notation for Multiple Linear Regression

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The Modeling Process: Using a Different Loss Function

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1. Choose a model

Constant Model

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

2. Choose a loss function

L1 Loss

Mean Absolute Error (MAE)

Let's repeat, but with **Mean Absolute Error (MAE)** as our average loss.

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

3. Fit the model

Minimize average loss with calculus

4. Evaluate model performance

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The Modeling Process: Using a Different Loss Function

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1. Choose a model ✅

Constant Model

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

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L1 Loss

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

3. Fit the model

Minimize average loss with calculus

How does this step change?

4. Evaluate model performance

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Fit the Model: Rewrite MAE for the Constant Model

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Recall that Mean **Absolute** Error (MAE) is average **absolute** loss (L1 loss) over the data $\mathcal{D} = \{y_1, y_2, \ldots, y_n\}$:

$$\hat{R}(\theta_0) = \frac{1}{n} \sum_{i=1}^{n} \underbrace{|y_i - \hat{y}_i|}_{\text{L1 loss on a single datapoint}}$$

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

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

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

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Exploring MAE: A Piecewise function

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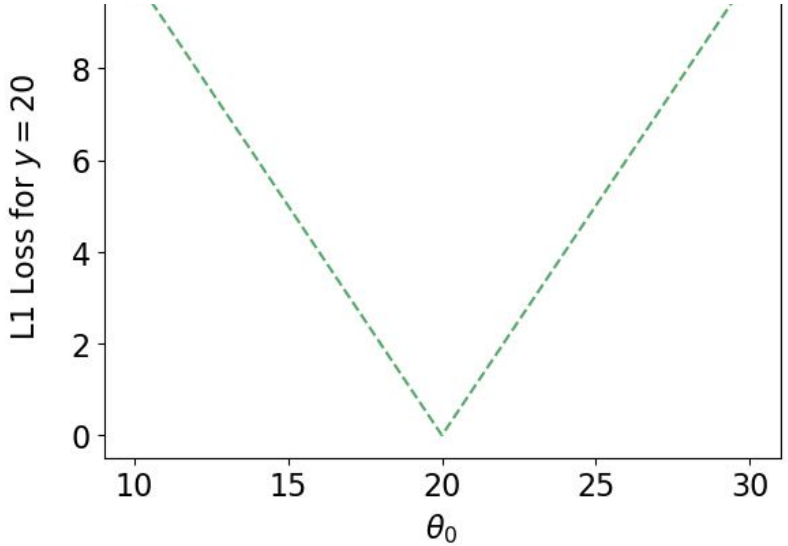
Boba dataset {20, 21, 22, 29, 33} (Mean=25)

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

Absolute (L1) Loss on one observation:

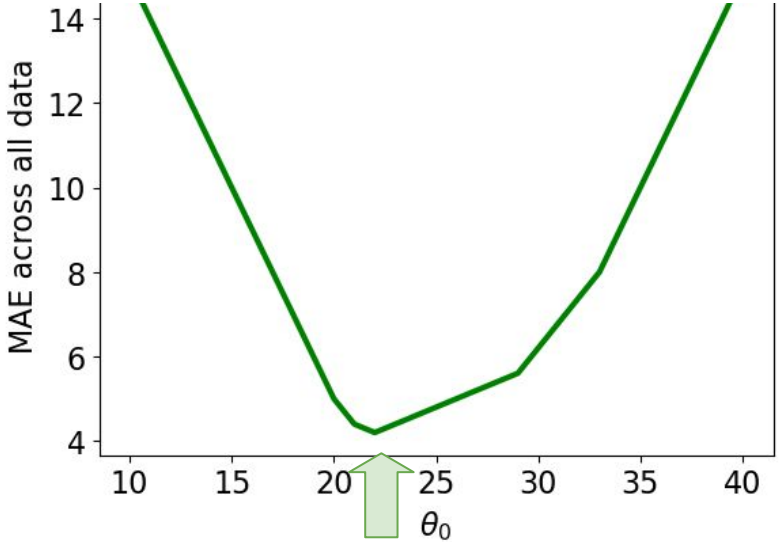
$$L_1(20, \theta_0) = |20 - \theta_0|$$



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

MAE (Mean Absolute Error) across all data:

$$\hat{R}(\theta_0) = \frac{1}{5}(|20-\theta_0| + |21-\theta_0| + |22-\theta_0| + |29-\theta_0| + |33-\theta_0|)$$



Piecewise linear function… minimized at… $\hat{\theta}_0$ = 22?

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Fit the Model: Calculus

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

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

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

⚠️ Absolute value!

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

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Fit the Model: Calculus

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

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

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

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

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Fit the Model: Calculus

2341552

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

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

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

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

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

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

Note: The derivative of the absolute value when the argument is 0 (i.e. when $\hat{y} = \theta_0$) is technically undefined. We ignore this case in our derivation, since thankfully, it doesn't change our result (proof left to you).

Sum up for $i = 1, \ldots, n$:

−1 if observation y_i > our prediction $\hat{\theta}_0$;

+1 if observation y_i < our prediction $\hat{\theta}_0$.

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Fit the Model: Calculus

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

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

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

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Sum up for $i = 1, \ldots, n$:

−1 if observation y_i > our prediction $\hat{\theta}_0$;

+1 if observation y_i < our prediction $\hat{\theta}_0$.

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Fit the Model: Calculus

2341552

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

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

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

2. Set equal to 0.

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

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Fit the Model: Calculus

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

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

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

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

2. Set equal to 0.

$$0 = \frac{1}{n} \sum_{\hat{\theta}_0 < y_i} (-1) + \frac{1}{n} \sum_{\hat{\theta}_0 > y_i} (1)$$

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

$$0 = -\frac{1}{n} \sum_{\hat{\theta}_0 < y_i} (1) + \frac{1}{n} \sum_{\hat{\theta}_0 > y_i} (1)$$

$$\sum_{\hat{\theta}_0 < y_i} (1) = \sum_{\hat{\theta}_0 > y_i} (1)$$

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Fit the Model: Calculus

2341552

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

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2. Set equal to 0.

$$0 = \frac{1}{n} \sum_{\hat{\theta}_0 < y_i} (-1) + \frac{1}{n} \sum_{\hat{\theta}_0 > y_i} (1)$$

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

$$0 = -\frac{1}{n} \sum_{\hat{\theta}_0 < y_i} (1) + \frac{1}{n} \sum_{\hat{\theta}_0 > y_i} (1)$$

$$\sum_{\hat{\theta}_0 < y_i} (1) = \sum_{\hat{\theta}_0 > y_i} (1)$$

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Median Minimizes MAE for the Constant Model

2341552

The constant model parameter $\theta = \hat{\theta}_0$ that minimizes MAE must satisfy:

$$\underbrace{\sum_{\hat{\theta}_0 < y_i} (1)}_{\substack{\text{\# observations} \\ \textbf{greater than } \hat{\theta}_0}} = \underbrace{\sum_{\hat{\theta}_0 > y_i} (1)}_{\substack{\text{\# observations} \\ \textbf{less than } \hat{\theta}_0}}$$

$\hat{\theta}_0$ needs to be located where there are **an equal number of y_i's to the left and right**.

This is the definition of the **median!**

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

For example, in our boba tea dataset {20, 21, 22, 29, 33}, the value **22** is the median.

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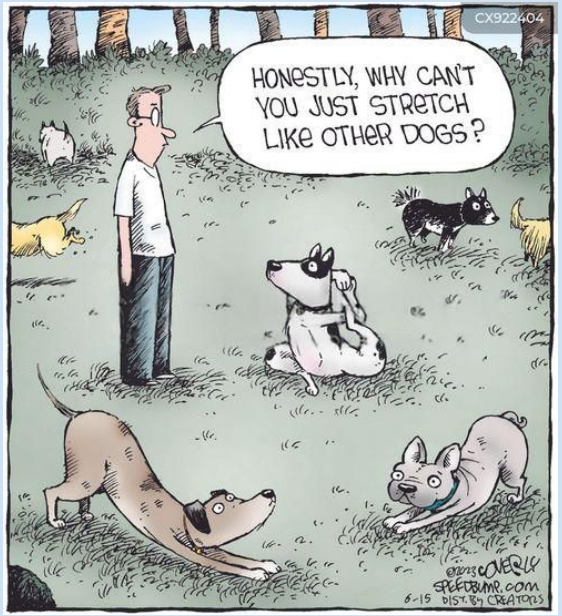

2-minute stretch break!

The next lecture relies on the geometric interpretation of linear algebra.

We recommend watching [this 3Blue1Brown video](#) (or better, the entire series) to get a solid understanding of the geometry of linear algebra.

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

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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 $\hat{\theta}$.

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

1. Differentiate with respect to $\hat{\theta}$.
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 $R''(\hat{\theta}) > 0$.
- 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.

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The Modeling Process: Using a Different Loss Function

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1. Choose a model ✅

Constant Model

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

2. Choose a loss function ✅

L1 Loss

Mean Absolute Error (MAE)

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

3. Fit the model ✅

Minimize average loss with calculus

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

4. Evaluate model performance

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MSE and MAE: Comparing Optimal Parameters

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MSE (Mean Squared Error)

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

Minimized with **sample mean**:

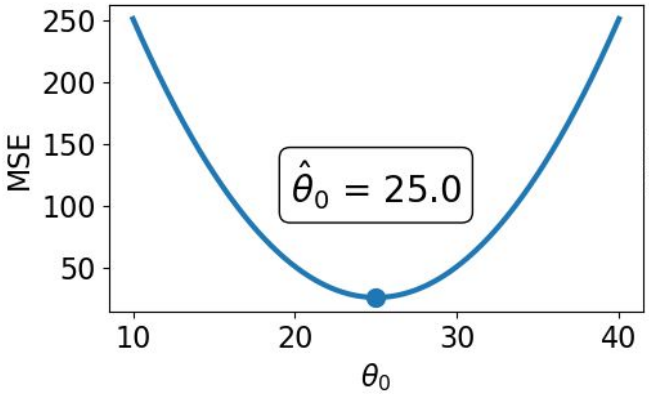
$$\hat{\theta}_0 = \text{mean}(y) = \bar{y}$$

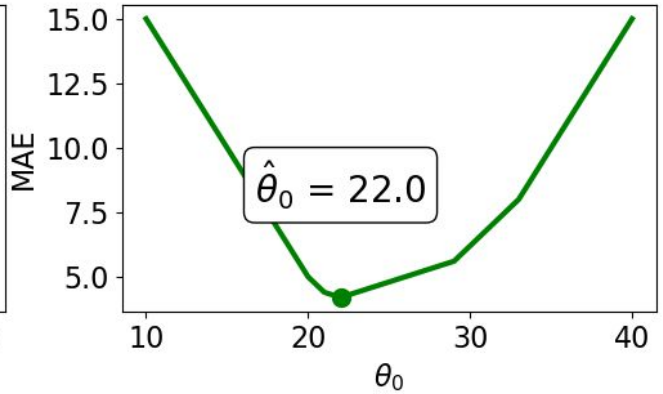
MAE (Mean Absolute Error)

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

Minimized with **sample median**:

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





Demo

lec10.ipynb

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MSE and MAE: Finding Minimizing Values

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MSE (Mean Squared Error)

Minimized with **sample mean**:

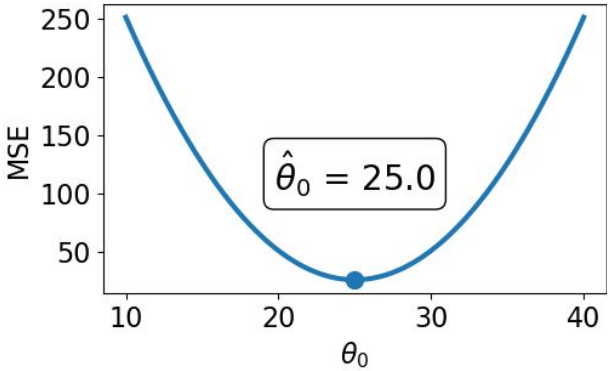
$$\hat{\theta}_0 = \text{mean}(y) = \bar{y}$$

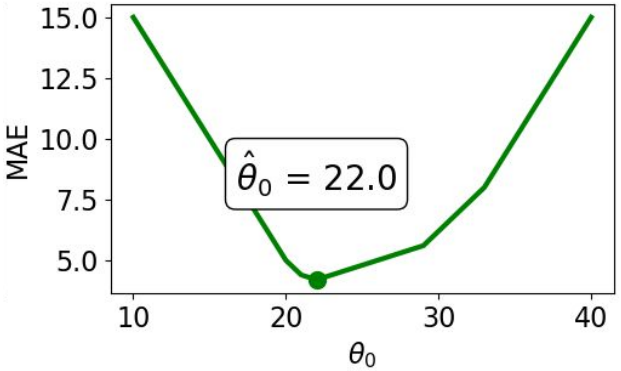
MAE (Mean Absolute Error)

Minimized with **sample median**:

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

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





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

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

Demo

lec10.ipynb

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MSE and MAE: Comparing Uniqueness of Solutions

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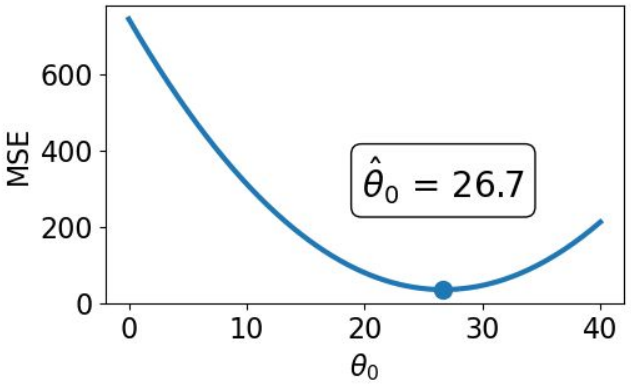
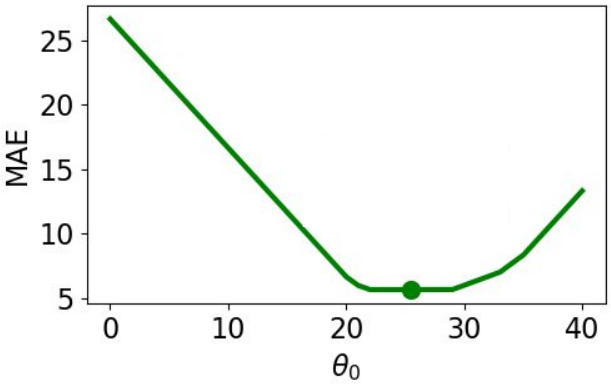
MSE (Mean Squared Error)

MAE (Mean Absolute Error)

Suppose we add a 6th observation to our bubble tea dataset:

{20, 21, 22, 29, 33, **35**}





Unique $\hat{\theta}_0$:

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

⚠️ **Infinitely many $\hat{\theta}_0$ s.** Any $\hat{\theta}_0$ in range (22, 29) minimizes MAE. Equal # of y_i's to left and right.

We typically choose the average of the boundary values (25.5).

Demo

lec10.ipynb

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MSE and MAE: Comparing Sensitivity to Outliers

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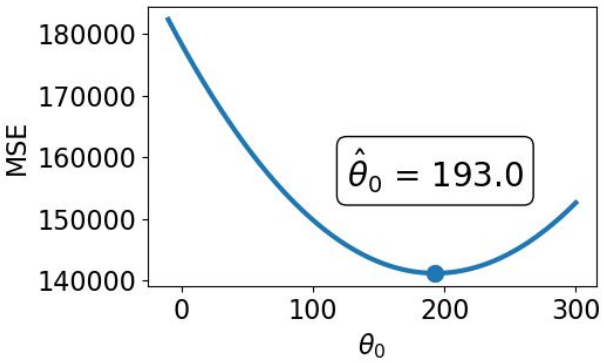
MSE (Mean Squared Error)
Minimized with **sample mean**:

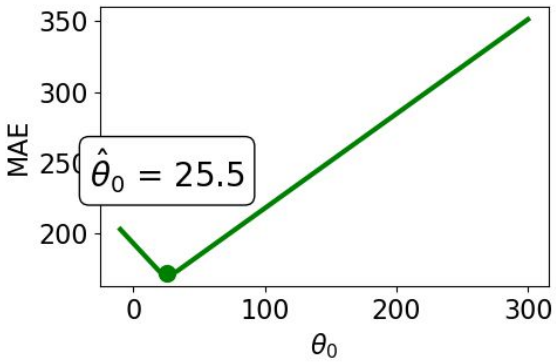
$$\hat{\theta}_0 = \text{mean}(y) = \bar{y}$$

MAE (Mean Absolute Error)
Minimized with **sample median**:

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

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





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

More robust to outliers.

Demo

lec10.ipynb

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Which of the following loss functions for the constant model are minimized when $\theta_0 = \bar{y}$?

Presenting with animations, GIFs or speaker notes? Enable our Chrome extension

slido

Which loss functions for the constant model are minimized when $\theta_0 = \bar{Y}$?

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✅ MSE: We saw earlier in lecture that $\bar{Y}$ minimizes MSE.

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

✅ SSE (Sum of squared error): The 1/n constant does not impact the minimizing θ_0.

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

❌ MAE: We saw earlier that the median of Y minimizes the MAE.

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

❌ SAE (Sum of absolute error): Like above, the 1/n constant does not impact the minimizing θ_0. So, the median of Y also minimizes the SAE.

$$\text{SAE} = \sum_{i=1}^{n}|y_i - \theta_0|$$

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Transformations of Linear Models

Lecture 11, Data 100 Spring 2025

Modeling Process

- Iteration 1: SLR + MSE (last time!)
- Iteration 2: Constant Model + MSE
- Iteration 3: Constant Model + MAE

Transformations of Linear Models

Notation for Multiple Linear Regression

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Back to Least Squares Regression with Dugongs

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From Data 8 (textbook): The residual plot of a good regression shows **no pattern**.

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

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Back to Least Squares Regression with Dugongs

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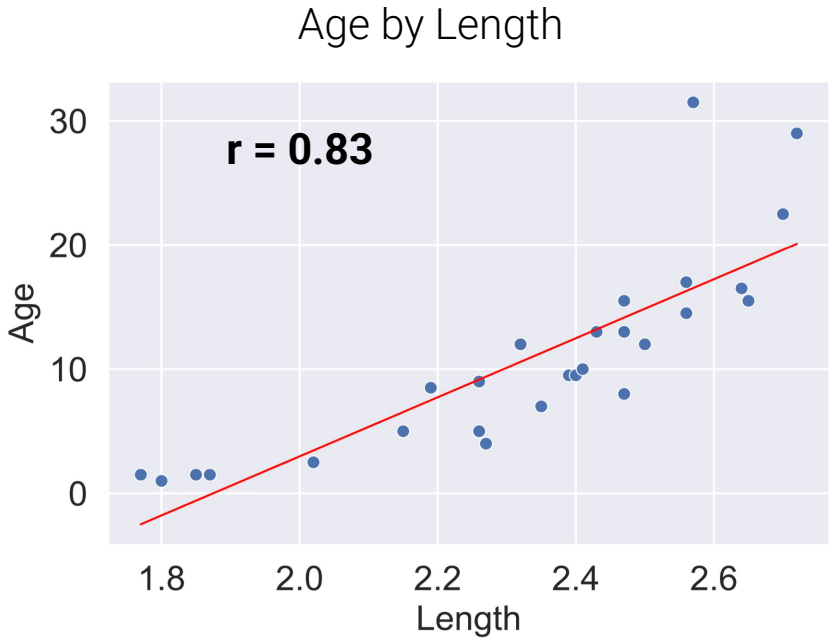

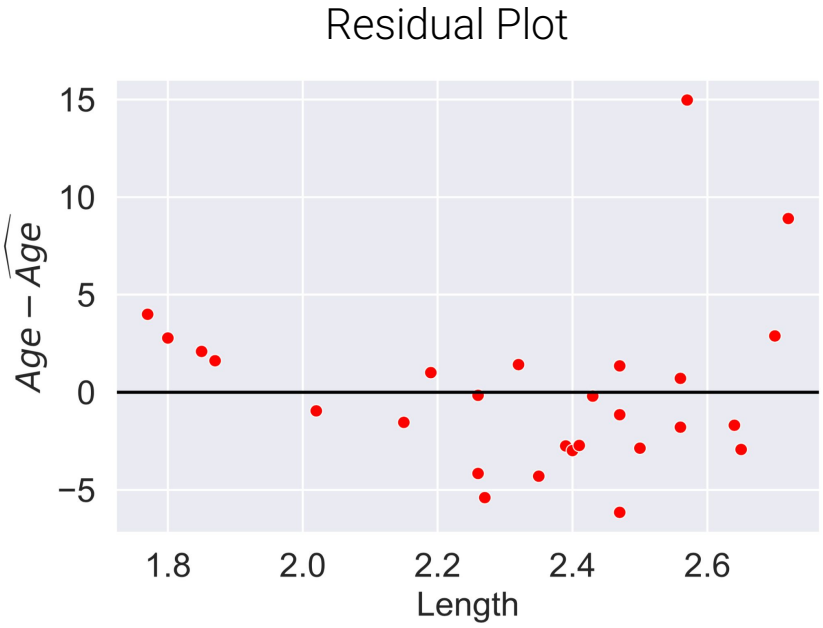

The scatter plot is **non-linear**, so the SLR **residual plot** shows a pattern indicative of a bad fit.

To improve the fit, we can **linearize** the data with a transformation.

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Possible Transformations

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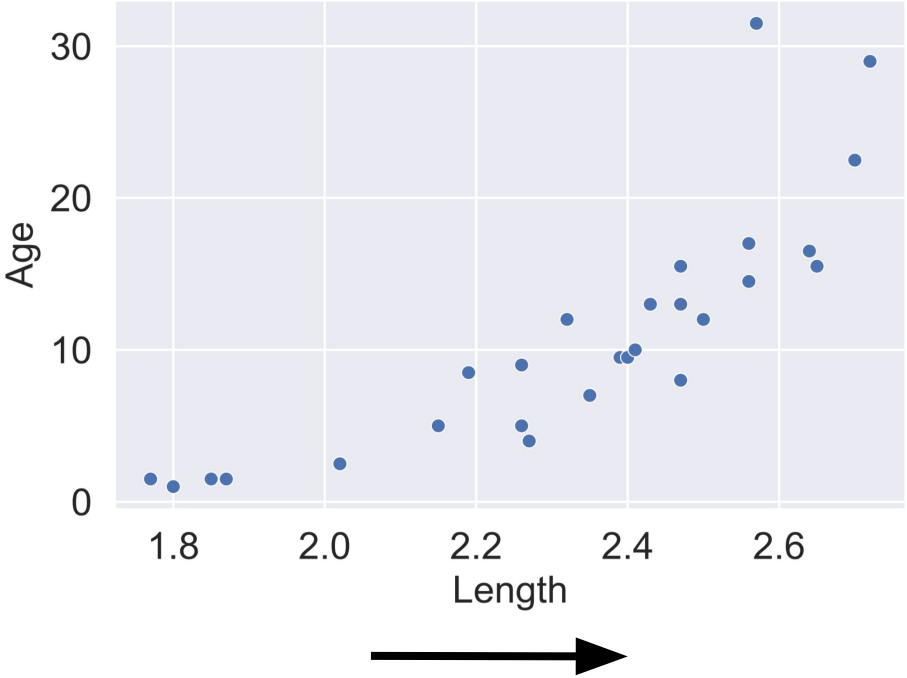
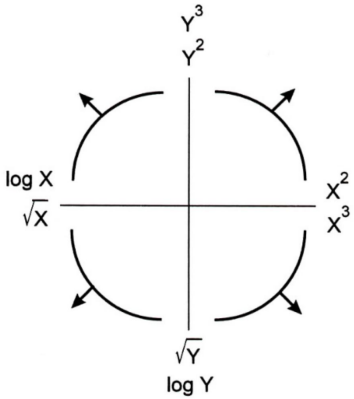
Large age values appear **unconstrained.**

Squish differences with **log(Age)** transform.





Large length values appear **compressed**.

Magnify differences with **(Length)^2** transform.

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Effect of log and squaring transformations

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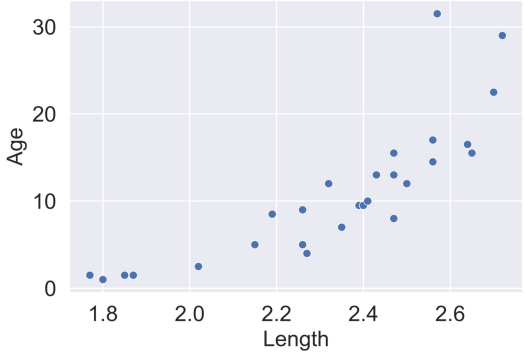
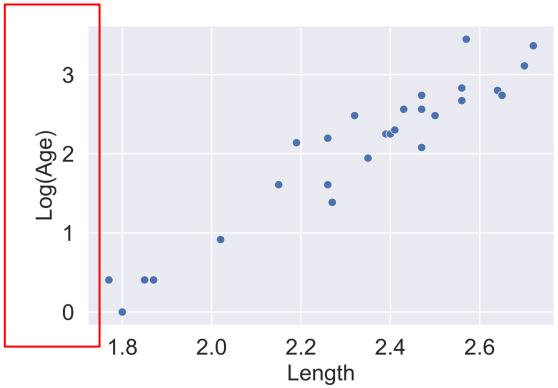
No transformation

[Raw; natural scale]

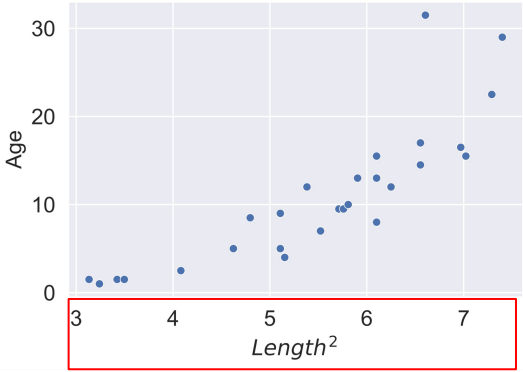


Log transformation



Big improvement in linearity.

Squaring transformation



Very subtle improvement in linearity.
Hard to see here—wait a few slides!

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SLR outcomes always linear in the provided feature

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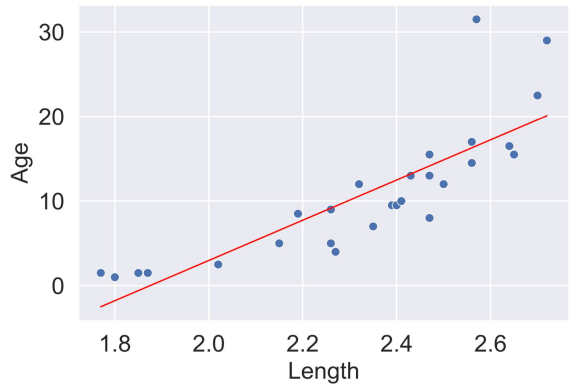
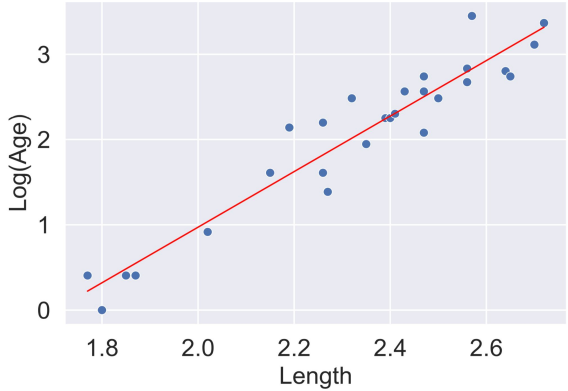
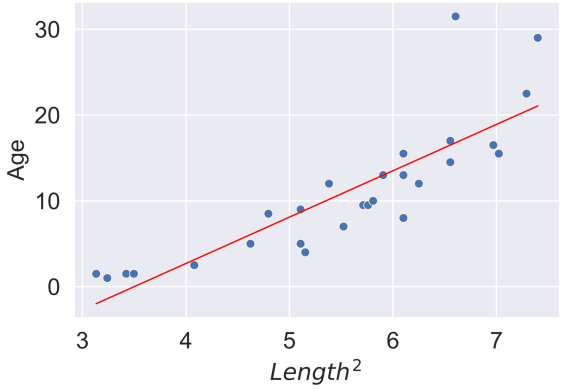
$$\widehat{\text{Age}} = \theta_0 + \theta_1 \text{Length}$$



$$\widehat{\log(\text{Age})} = \theta_0 + \theta_1 \text{Length}$$



$$\widehat{\text{Age}} = \theta_0 + \theta_1 \text{Length}^2$$



SLR doesn't "know" that the output is logged Age or the input is squared Length.

- To SLR, log(Age) and Length^2 are just vectors of values!
- The outcome provided to SLR is always modeled as linear in the provided feature.

Note: When squaring a feature, we usually include the linear feature for extra flexibility (e.g., $\hat{Y} = \theta_0 + \theta_1 X + \theta_2 X^2$). Next lecture!

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SLR outcomes always linear in the provided feature

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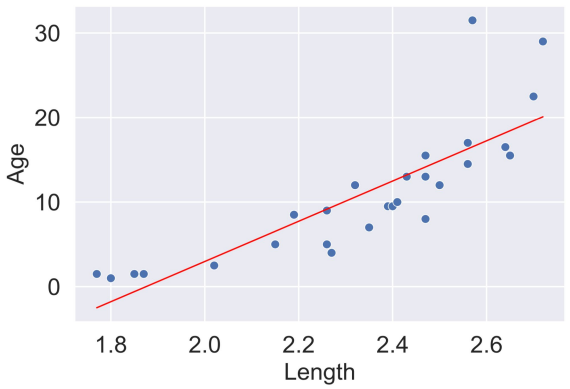
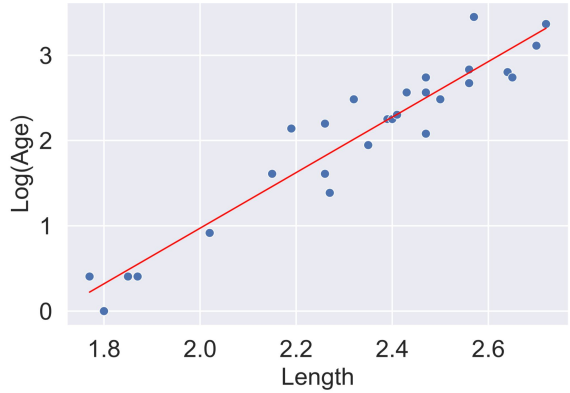
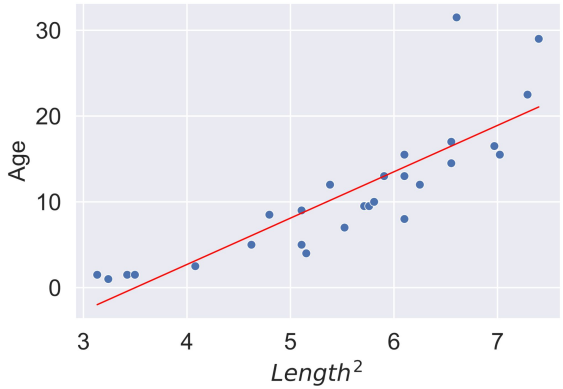
$$\widehat{\text{Age}} = \theta_0 + \theta_1 \text{Length}$$

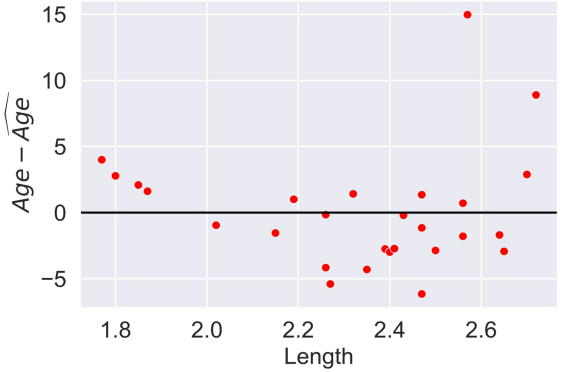


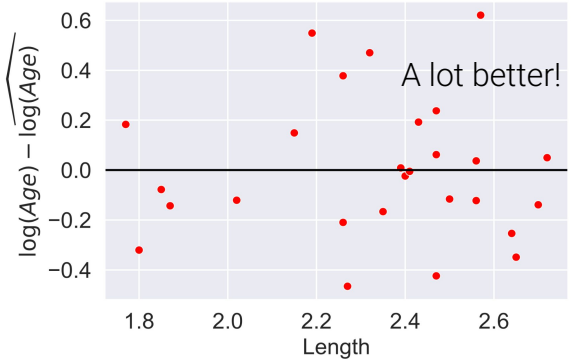
$$\widehat{\log(\text{Age})} = \theta_0 + \theta_1 \text{Length}$$

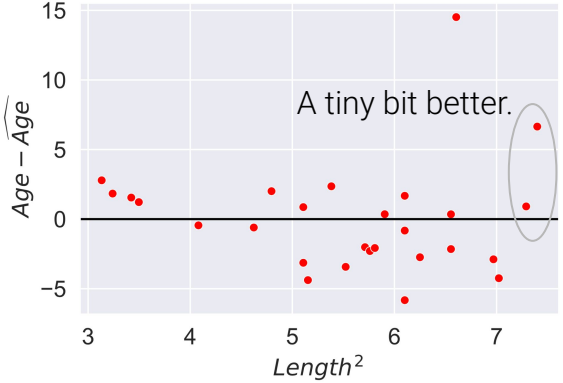


$$\widehat{\text{Age}} = \theta_0 + \theta_1 \text{Length}^2$$









Note: When squaring a feature, we usually include the linear feature for extra flexibility (e.g., $\hat{Y} = \theta_0 + \theta_1 X + \theta_2 X^2$). Next lecture!

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Visualizing log-transformed predictions on natural scale

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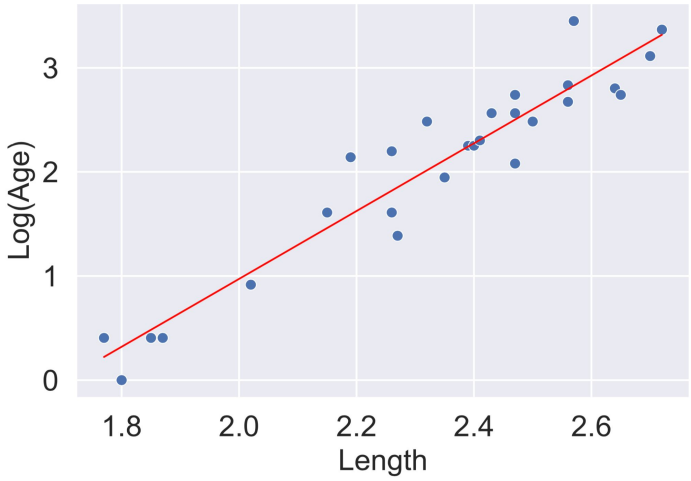
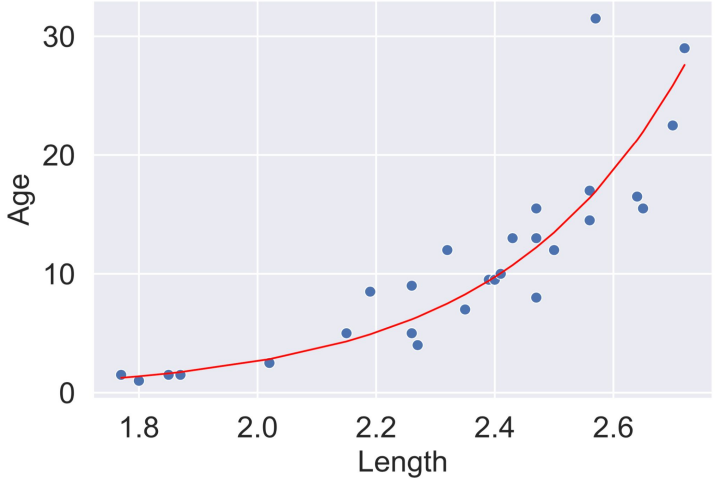
$$\widehat{\log(\text{Age})} = \theta_0 + \theta_1 \text{Length}$$



$$\widehat{\text{Age}} = e^{\theta_0 + \theta_1 \text{Length}}$$



Unlike SLR, <u>we</u> know that the y-variable is log(Age).

- To get Age predictions, we exponentiate the log(Age) predictions.

Log(Age) predictions are linear in Length. Age predictions are <u>not</u> linear in Length.

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Visualizing squared features on natural scale

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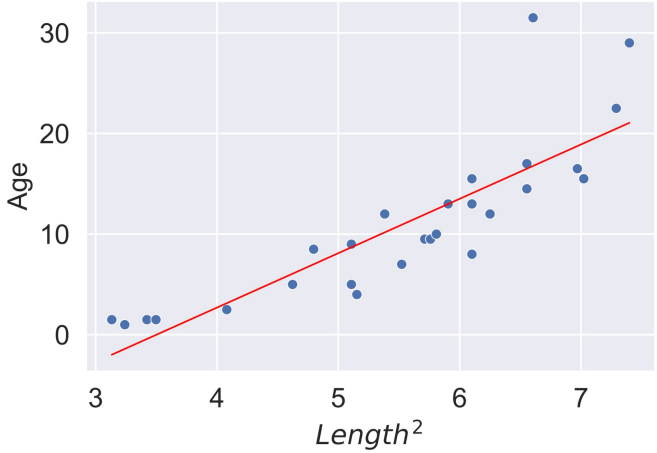
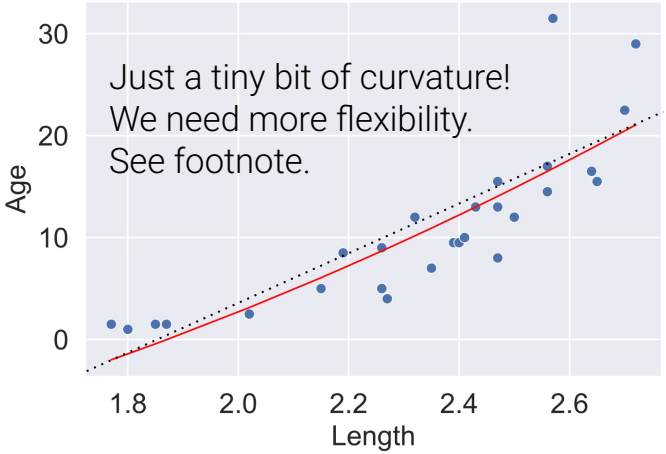
$$\widehat{\text{Age}} = \theta_0 + \theta_1 \text{Length}^2$$



$$\widehat{\text{Age}} = \theta_0 + \theta_1 \text{Length}^2$$



Black line is straight!

Unlike SLR, <u>we</u> know that the x-variable is Length^2!

- Predictions are already on the Age scale, so no need to change the y-axis.
- We can use the non-transformed feature (Length) on the x-axis to see non-linearities.

Age predictions are linear in Length^2, but not linear in Length.

Note: When squaring a feature, we usually include a linear term for extra flexibility (e.g., $\hat{Y} = \theta_0 + \theta_1 X + \theta_2 X^2$). Next lecture!

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Notation for Multiple Linear Regression

Lecture 11, Data 100 Spring 2025

Modeling Process

- Iteration 1: SLR + MSE (last time!)
- Iteration 2: Constant Model + MSE
- Iteration 3: Constant Model + MAE

Transformations of Linear Models

Notation for Multiple Linear Regression

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A Note on Terminology

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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)

1

Output

Outcome

Response

Dependent variable

2

Weight(s)

Parameter(s)

Coefficient(s)

4

Prediction

Predicted response

Estimated value

3

Estimator(s)

Optimal parameter(s)

5

Bolded terms are the most common in this course.

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

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Please rank the variables to match them with their appropriate terms (i.e., rank 2 should match "Outcome" / "Response" and rank 3 should match "Prediction"):

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slido

A Note on Terminology

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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)

x

Output

Outcome

Response

Dependent variable

y

Weight(s)

Parameter(s)

Coefficient(s)

θ

Prediction

Predicted response

Estimated value

$\hat{y}$

Estimator(s)

Optimal parameter(s)

$\hat{\theta}$

Bolded terms are the most common in this course.

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

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Extending SLR to more than one input

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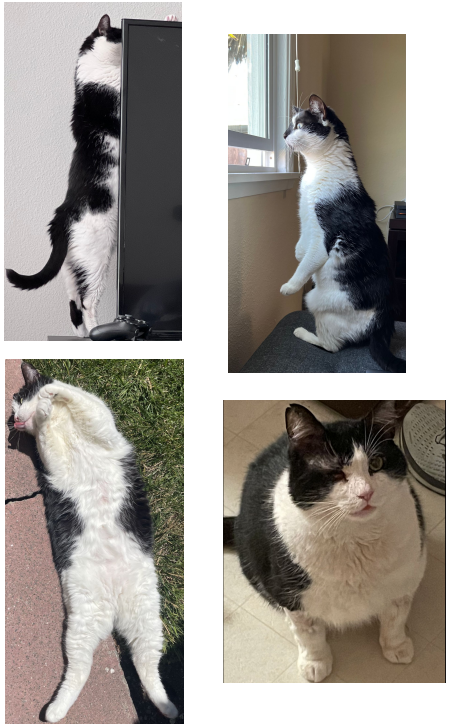
In SLR, we predict one output with one input.

In real prediction scenarios, we often want to account for more than one input.

Example: Predict cat's ages $\hat{y}$ as a linear model of 2 features: length x_1 **and** weight x_2.



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

intercept | parameter for length | parameter for weight

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Multiple Linear Regression (i.e., ordinary least squares, or OLS)

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Define the **multiple linear regression** model:

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

Parameter vector $\theta = [\theta_0, \theta_1, \ldots, \theta_p]$

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Multiple Linear Regression (i.e., ordinary least squares, or OLS)

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Define the **multiple linear regression** model:

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

Parameter vector $\theta = [\theta_0, \theta_1, \ldots, \theta_p]$

This is a **linear combination** of θ_j's, each scaled by x_j

In other words, $\hat{y}$ is linear in θ

$$(x_1, \ldots, x_p) \longrightarrow \boxed{\theta = [\theta_0, \theta_1, \ldots, \theta_p]} \longrightarrow \hat{y}$$

single input
(p features)

single
prediction

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Multiple Linear Regression (i.e., ordinary least squares, or OLS)

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

More on OLS in the next lecture!

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Lecture 11

Constant Model, Loss, and Transformations

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Bonus: Constant Model MSE, Algebraic Approach

Lecture 11, Data 100 Spring 2025

MSE Minimization Using an Algebraic Trick

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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 $\sum_{i=1}^{n}(y_i - \bar{y}) = 0$). We present that proof here:

$$\begin{aligned}\sum_{i=1}^{n}(y_i - \bar{y}) &= \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} \bar{y} \\ &= \sum_{i=1}^{n} y_i - n\bar{y} = \sum_{i=1}^{n} y_i - n \cdot \frac{1}{n}\sum_{i=1}^{n} y_i = \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} y_i \\ &= 0\end{aligned}$$

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:

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

Equal to the MSE of the sample mean!

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MSE Minimization Using an Algebraic Trick

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

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!

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Minimization Using an Algebraic Trick

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

- Since variance can't be negative, the first term is greater than or equal to 0.
  - 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.
  - This term does involve θ, and so picking the right value of θ will minimize our average loss.
  - We need to pick the θ that sets the second term to 0.
  - This is achieved when $\theta = \bar{y}$ In other words:

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

Looks familiar!

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