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LECTURE 10

Introduction to Modeling, SLR

Understanding the usefulness of models and the simple linear regression model

Data 100/Data 200, Spring 2023 @ UC Berkeley

Narges Norouzi and Lisa Yan

Content credit: Narges Norouzi, Will Fithian, Lisa Yan, Suraj Rampure, Ani Adhikari, Deborah Nolan, Joseph Gonzalez

Plan for Next Few Lectures: Predictive modeling

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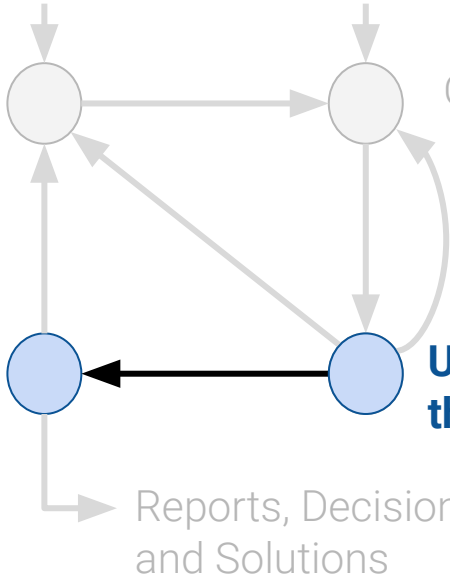

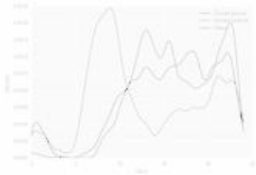

(today)

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 10, Data 100 Spring 2023

What Is A Model?

Data 8 Review: Regression Line, Correlation

The Modeling Process: Definitions

Loss Functions

Minimizing Average Loss (Empirical Risk)

Interpreting SLR: Slope, Anscombe's Quartet

Evaluating the Model: RMSE, Residual Plot

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Last time: Population vs. Sample

- The **population** is a set of individuals (people / bacteria / villages) in the **real world** that we are interested in learning about.
- The **sample** is a (usually smaller) subset of data we can actually collect & analyze.
- If we pick a good sampling scheme, the sample is **representative** of the population (in practice that is often hard to accomplish!).
- If so, we can hope that patterns we find in the data will reflect patterns in the wider world (but **how closely?** Question of **inference** which we will discuss later).

Next few lectures: predictive modeling

- General setting: we observe **pairs** $\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$
- Assume they are representative of some underlying population of interest.
- **Question (prediction):** If we see x, what is the best prediction for y?
- **Question (association):** if x changes, how much bigger or smaller is y (on avg)?
- **Question (causation):** if we make x one unit larger, how much larger will y get (on avg)?

What Is A Model?

Lecture 10, Data 100 Spring 2023

What Is A Model?

Data 8 Review: Simple Linear Regression and Correlation

The Modeling Process: Definitions

Loss Functions

Minimizing Average Loss on Data

Interpreting SLR: Slope

Evaluating the Model: RMSE, Residual Plot

What Is A Model?

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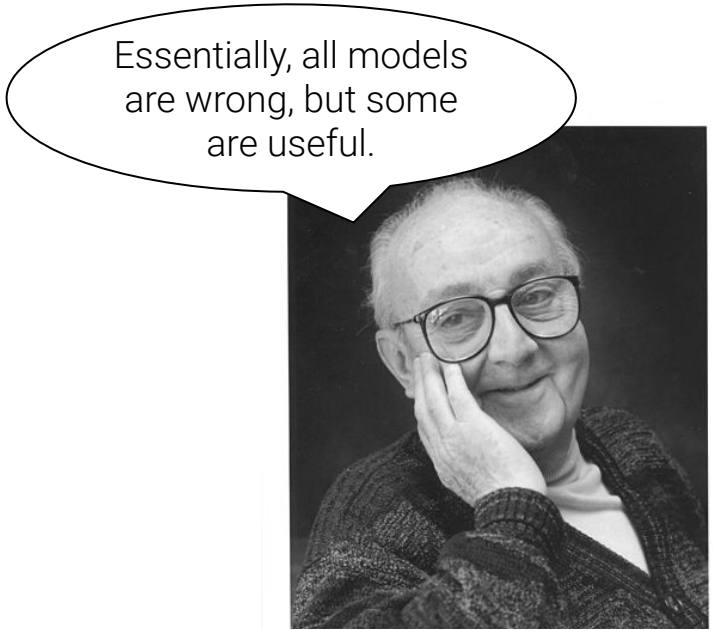
A model is an **idealized representation** of a system.

Example:
We model the fall of an object on Earth as subject to a constant acceleration of 9.81 m/s² due to gravity.

- While this describes the behavior of our system, it is merely an approximation.
- It doesn't account for the effects of air resistance, local variations in gravity, etc.
- But in practice, it's accurate enough to be useful!



George Box, Statistician (1919-2013)

Known for	"All models are wrong"
	Response-surface methodology
	EVOP
	q-exponential distribution
	Box–Jenkins method
	Box–Cox transformation

Two Reasons for Building Models

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Reason 1:

To understand **complex phenomena** occurring in the world we live in.

- What factors play a role in the growth of COVID-19?
- How do an object's velocity and acceleration impact how far it travels? (Physics: $d = d_0 + vt + \frac{1}{2}at^2$)

Often times, we care about creating models that are **simple and interpretable**, allowing us to understand what the relationships between our variables are.

Reason 2:

To make **accurate predictions** about unseen data.

- Can we predict if an email is spam or not?
- Can we generate a one-sentence summary of this 10-page long article?

Other times, we care more about making extremely accurate predictions, at the cost of having an uninterpretable model. These are sometimes called **black-box models**, and are common in fields like deep learning.

Most of the time, we want to strike a balance between interpretability and accuracy.

Common Types of Models

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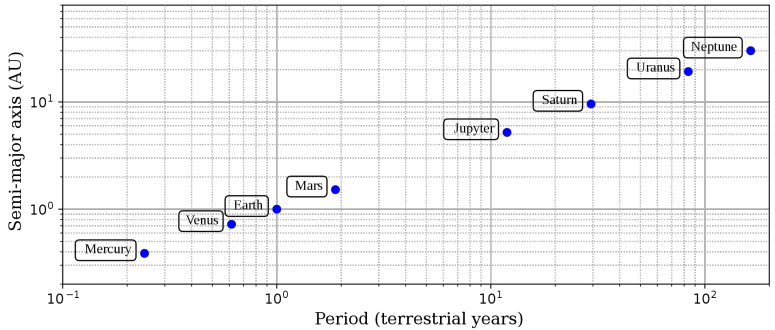
Deterministic physical (mechanistic) models: Laws that govern how the world works.

Kepler's Third Law of Planetary Motion (1619)

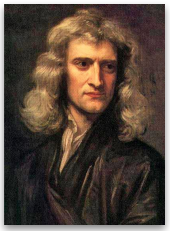
The ratio of the square of an object's orbital period with the cube of the semi-major axis of its orbit is the same for all objects orbiting the same primary.

$$T^2 \propto R^3$$



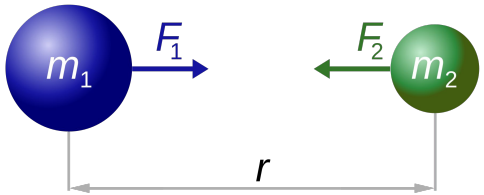
Newton's Laws: motion and gravitation (1687)

Newton's second law of motion models the relationship between the mass of an object and the force required to accelerate it.



$$\mathbf{F} = m\mathbf{a}$$

$$F = G\frac{m_1 m_2}{r^2}$$



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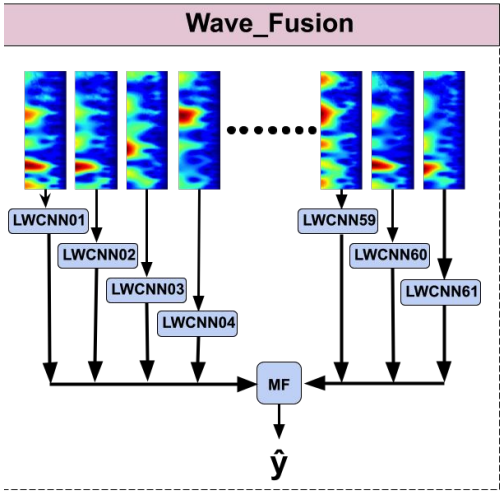
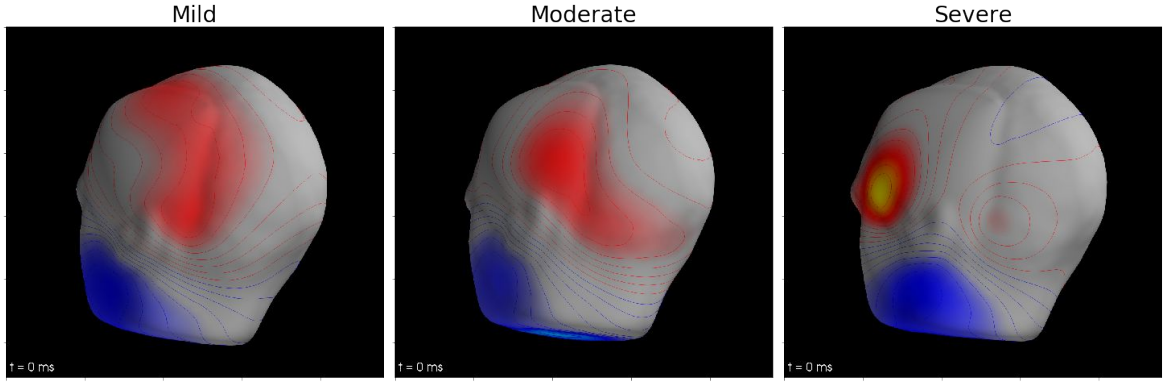
Probabilistic models

- Models of how random processes evolve.
- Often motivated by understanding of an unpredictable system.





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Data 8 Review: Simple Linear Regression & Correlation

Lecture 10, Data 100 Spring 2023

[Data 8 Review] The Regression Line

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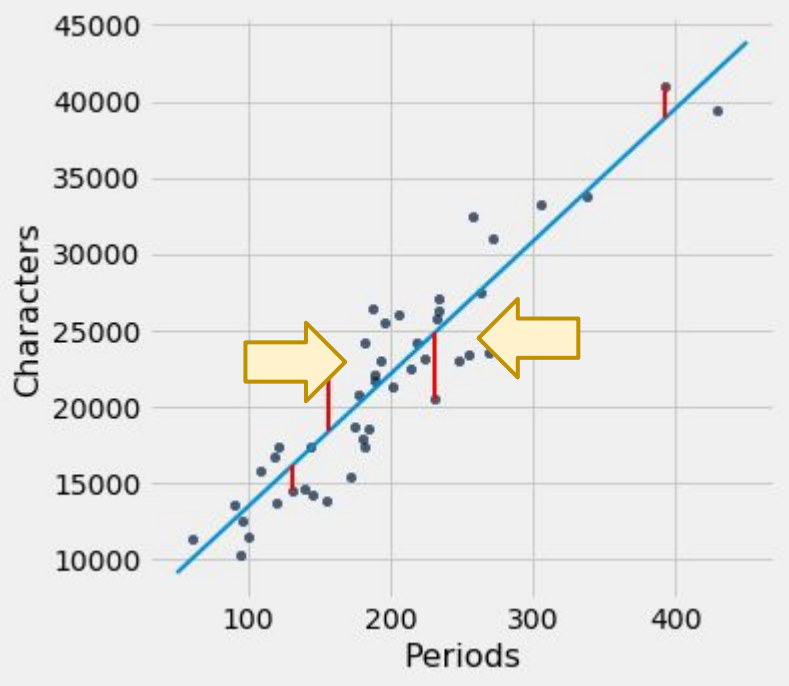
From Data 8 (textbook):

> The **regression line** is the unique straight line that minimizes the **mean squared error** of estimation among all straight lines.

$$\text{slope} = r \cdot \frac{\text{SD of } y}{\text{SD of } x}$$

$$\text{intercept} = \text{average of } y - \text{slope} \cdot \text{average of } x$$

$$\textbf{residual} = \text{observed value} - \text{regression estimate}$$



For every chapter of the novel *Little Women*, Estimate the **# of characters** $\hat{y}$ based on the **# of periods** x in that chapter.

[Data 8 Review] The Regression Line

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correlation

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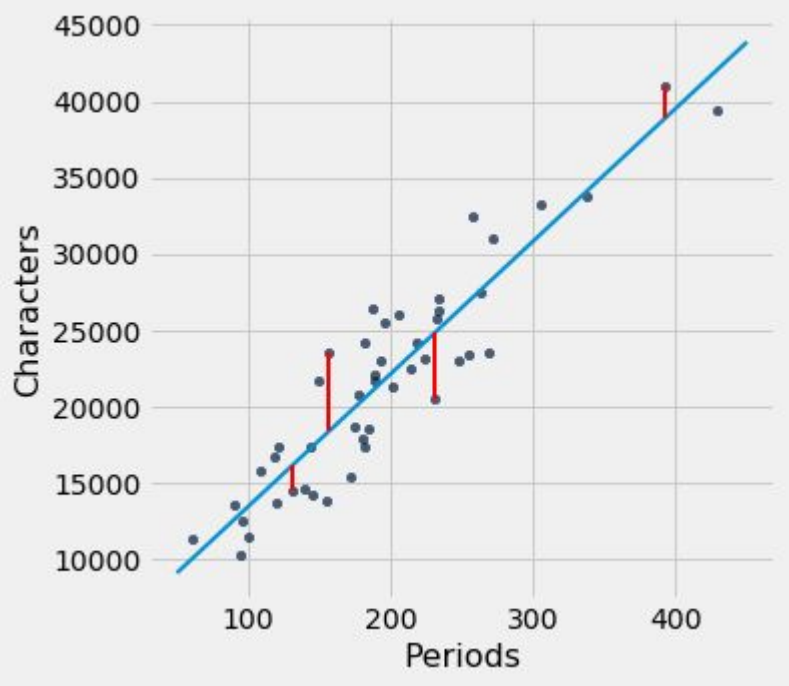

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[Data 8 Review] Correlation

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From Data 8 (textbook):

> The **correlation** r is the average of the product of x and y, both measured in standard units.

$$r = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{x_i - \bar{x}}{\sigma_x}\right)\left(\frac{y_i - \bar{y}}{\sigma_y}\right)$$

Define the following:

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

$\bar{x}, \bar{y}$ means; σ_x, σ_y standard deviations

- x_i in standard units: $\frac{x_i - \bar{x}}{\sigma_x}$
- r is also known as Pearson's correlation coefficient.
- Side note: **covariance** is $\frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y}) = r\sigma_x\sigma_y$

[Data 8 Review] Correlation

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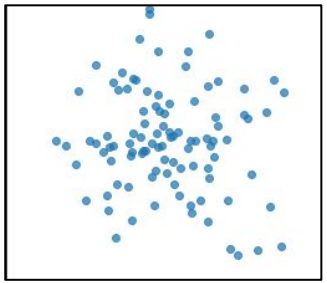
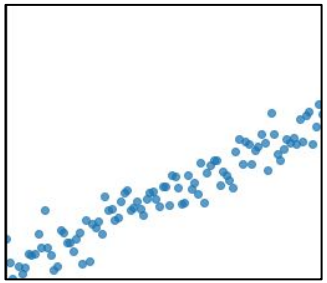
Correlation measures the strength of a **linear association** between two variables.

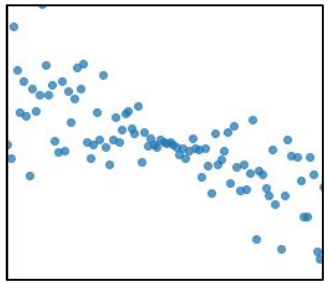
$|r| < 1$



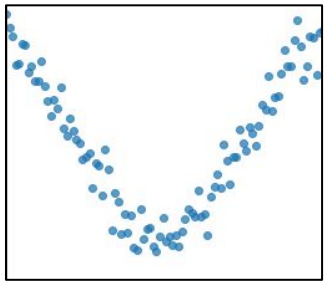
r = −0.121



r = 0.951



r = −0.723



⚠ **r = 0.056**

[Data 8 Review] The Regression Line

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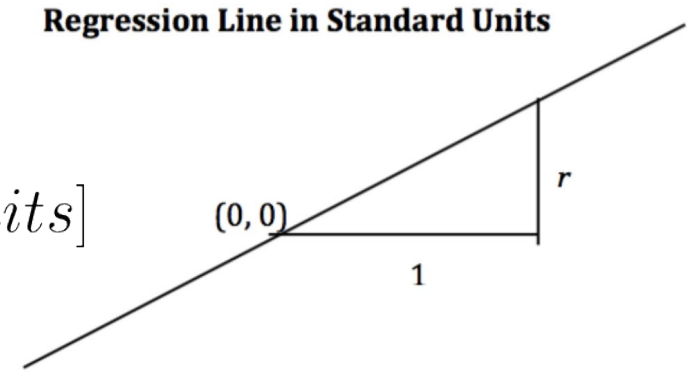
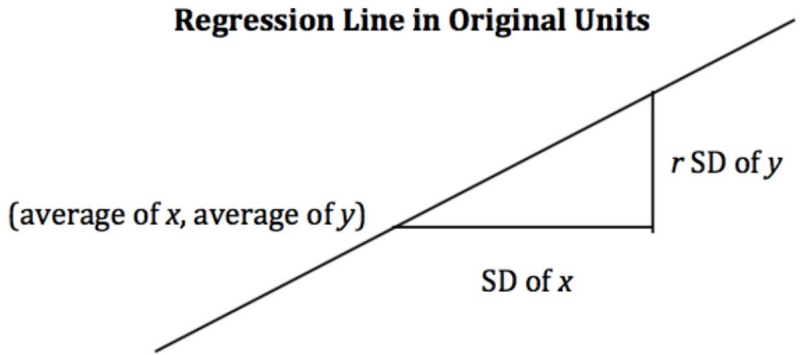
- When the variables x and y are measured in standard units, the regression line for predicting y based on x has slope r passes through the origin and the equation will be:

$$\hat{y} = r \times x \; [both \; measured \; in \; standard \; units]$$



- In the original units of the data, this becomes:

$$\frac{\hat{y} - \bar{y}}{\sigma_y} = r \times \frac{x - \bar{x}}{\sigma_x}$$



[Data 8 Review] The Regression Line

$$\frac{\hat{y} - \bar{y}}{\sigma_y} = r \times \frac{x - \bar{x}}{\sigma_x}$$

$$\hat{y} = \sigma_y \times r \times \frac{x - \bar{x}}{\sigma_x} + \bar{y}$$

$$\hat{y} = \left(\frac{r\sigma_y}{\sigma_x}\right) \times x + \left(\bar{y} - \frac{r\sigma_y}{\sigma_x}\bar{x}\right)$$

Recall regression line equation is defined as:

$$\hat{y} = \hat{a} + \hat{b}x$$

Goal: Derive and define everything on this slide!

slope: $r\frac{SD\ of\ y}{SD\ of\ x} = r\frac{\sigma_y}{\sigma_x}$

intercept: $\bar{y} - slope \times \bar{x}$

Error for the i-th data point: $e_i = y_i - \hat{y}_i$

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The Modeling Process: Definitions

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Simple Linear Regression Model (SLR)

Data 8 notation: $\hat{y} = a + bx$ → Data 100 notation: $\hat{y} = \theta_0 + \theta_1 x$

SLR is a **parametric model**: it is described by a few **parameters** (in this case θ_0, θ_1)

- No one tells us the parameters: the data informs us about them.
- The x values are **not** parameters because we directly observe them.
- Sample-based **estimate** of θ_0, θ_1 written as $\hat{\theta}_0, \hat{\theta}_1$.

Usually, we pick the parameters that appear "best" according to some criterion we choose

- Usually standing in as a proxy for fit to new data.

Parametric Model Notation

y True outputs

$\hat{y}$ Predicted outputs

For data:

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

The i-th datapoint is an **observation**:

- y_i is the i-th **output** (aka dependent variable)
- x_i is the i-th **feature** (aka independent variable)
- $\hat{y}_i$ is the i-th **prediction** (aka estimation).

Model parameter(s)

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

Any linear model with parameters $\theta = [\theta_0, \theta_1]$

Estimated parameter(s), “best” fit to data in some sense

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

The "best" fitting linear model with parameters $\hat{\theta} = [\hat{\theta}_0, \hat{\theta}_1]$

Which is best?

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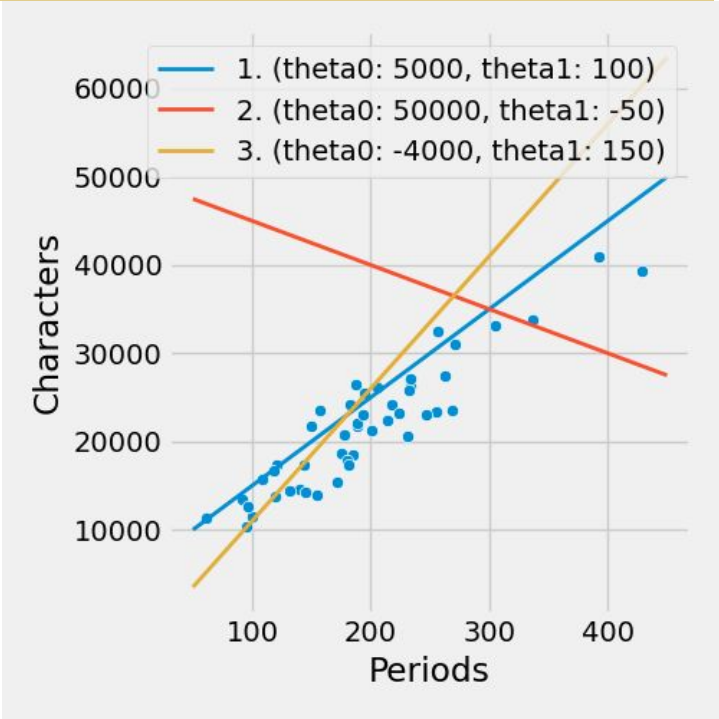
Based on your interpretation of the data, which are the "optimal parameters" for this linear model?

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

$$\hat{\theta}_0 =? \quad \hat{\theta}_1 =?$$



We only had 3 values to choose from to find the optimal parameter. In practice, our parameter domain is all reals, i.e., $\theta = [\theta_0, \theta_1] \in \mathbb{R}^2$

For every chapter of the novel *Little Women*, Estimate the **# of characters** $\hat{y}$ based on the **# of periods** x in that chapter.

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Which of the lines matches the data better?

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Simple Linear Regression: Our First Model

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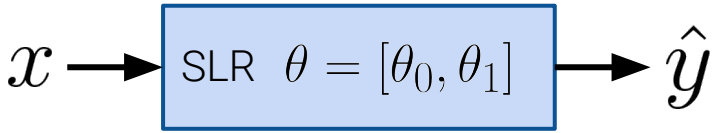
Simple Linear Regression Model (SLR)

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

SLR is a **parametric model**, meaning
we choose the "best" **parameters**
for slope and intercept based on data.

- We often express θ as a single parameter vector.
- x is **not** a parameter! It is input to our model.



- Note that the true relationship between x and y is usually non-linear.
  This is why $\hat{y}$ (and not y) appears in our **estimated linear model** expression.

- Other parametric models we'll see soon: $\hat{y} = \theta$ $\hat{y} = x^T\theta$ $\hat{y} = \frac{1}{1+\exp(-x^T\vec{\theta})}$
- Note: Not all statistical models have parameters! KDEs are non-parametric models.

The Modeling Process

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1. Choose a model ✅

How should we represent the world?

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

SLR model

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?

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

4. Evaluate model performance

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

Reflect

Loss Functions

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The Modeling Process

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1. Choose a model ✅

How should we represent the world?

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

SLR model

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

Loss Functions

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We need some metric of how "good" or "bad" our predictions are.

A **loss function** characterizes the **cost**, error, or fit resulting from a particular choice of model or model parameters.

- Loss quantifies how bad a prediction is for a **single** observation.
- If our prediction $\hat{y}$ is **close** to the actual value y, we want **low loss**.
- If our prediction $\hat{y}$ is **far** from the actual value y, we want **high loss**.

$$L(y, \hat{y})$$

There are many definitions of loss functions!

The choice of loss function:

- Affects the accuracy and computational cost of estimation.
- Depends on the estimation task:
  - Are outputs quantitative or qualitative?
  - Do we care about outliers?
  - Are all errors equally costly? (e.g., false negative on cancer test)

L2 and L1 Loss

L2 Loss or Squared Loss

$$L(y, \hat{y}) = (y - \hat{y})^2$$

- Widely used.
- Also called "L2 loss".
- Reasonable:
  - $\hat{y} = y$ → good prediction → good fit → no loss
  - $\hat{y}$ far from y → bad prediction → bad fit → *lots of loss*

L1 Loss or Absolute Loss

$$L(y, \hat{y}) = |y - \hat{y}|$$

- Sounds worse than it is.
- Also called "L1 loss".
- Reasonable:
  - $\hat{y} = y$ → good prediction → good fit → no loss
  - $\hat{y}$ far from y → bad prediction → bad fit → *some loss*

L2 and L1 Loss for SLR

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Squared Loss (L2 Loss)

$$L(y, \hat{y}) = (y - \hat{y})^2$$

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

$$L(y, \hat{y}) = (y - (\theta_0 + \theta_1 x))^2$$

Absolute Loss (L1 Loss)

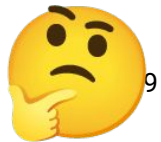
$$L(y, \hat{y}) = |y - \hat{y}|$$

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

1. What is the SLR L1 Loss?

2. Why don't we directly use residual error as the loss function? $(y - \hat{y})$

3. Which loss function is better: L1 or L2?



L2 and L1 Loss for SLR

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Squared Loss (L2 Loss)

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

$$L(y, \hat{y}) = (y - (\theta_0 + \theta_1 x))^2$$

Absolute Loss (L1 Loss)

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

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L2 and L1 Loss for SLR

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

1 $L(y, \hat{y}) = |y - (\theta_0 + \theta_1 x)|$

Why don't we directly use residual error as the loss function? $e = (y - \hat{y})$ 2

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Why don't we use residual error directly and instead we use absolute loss or squared loss?

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L2 and L1 Loss for SLR

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Squared Loss (L2 Loss)

$$L(y, \hat{y}) = (y - \hat{y})^2$$

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

$$L(y, \hat{y}) = (y - (\theta_0 + \theta_1 x))^2$$

Absolute Loss (L1 Loss)

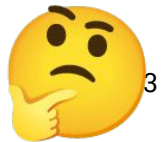
$$L(y, \hat{y}) = |y - \hat{y}|$$

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

1 $L(y, \hat{y}) = |y - (\theta_0 + \theta_1 x)|$

Why don't we directly use residual error as the loss function? $e = (y - \hat{y})$ 2

- Doesn't work: big negative residuals shouldn't cancel out big positive residuals!



L2 and L1 Loss for SLR

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Squared Loss (L2 Loss)

$$L(y, \hat{y}) = (y - \hat{y})^2$$

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

$$L(y, \hat{y}) = (y - (\theta_0 + \theta_1 x))^2$$

Absolute Loss (L1 Loss)

$$L(y, \hat{y}) = |y - \hat{y}|$$

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

1 $L(y, \hat{y}) = |y - (\theta_0 + \theta_1 x)|$

Why don't we directly use residual error as the loss function? $e = (y - \hat{y})$ 2

- Doesn't work: big negative residuals shouldn't cancel out big positive residuals!

Which loss function is better: L1 or L2? 3

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If we want to penalize large residuals more than small residuals, which loss function is more ideal?

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

L2 and L1 Loss for SLR

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Squared Loss (L2 Loss)

$$L(y, \hat{y}) = (y - \hat{y})^2$$

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

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Why don't we directly use residual error as the loss function? $e = (y - \hat{y})$ 2

- Doesn't work: big negative residuals shouldn't cancel out big positive residuals!

Which loss function is better: L1 or L2? L2 penalizes larger residuals more. 3

Empirical Risk is Average Loss over Data

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We care about how bad our model's predictions are for our entire data set, not just for one point. A natural measure, then, is of the **average loss** (aka **empirical risk**) across all points.

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

$$\hat{R}(\theta) = \frac{1}{n} \sum_i L(y_i, \hat{y}_i)$$

Function of the parameter θ (holding the data fixed) because θ determines $\hat{y}$.

The average loss on the sample tells us how well it fits the data (not the population).

But hopefully these are close.

Empirical Risk is Average Loss over Data

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$$\hat{R}(\theta) = \frac{1}{n} \sum_i L(y_i, \hat{y}_i)$$

The colloquial term for average loss depends on which loss function we choose.

L2 loss → **Mean Squared Error (MSE)**

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

L1 loss → **Mean Absolute Error (MAE)**

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

The Modeling Process

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1. Choose a model ✅

How should we represent the world?

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

SLR model

2. Choose a loss function ✅

How do we quantify prediction error?

$$L(y, \hat{y}) = (y - \hat{y})^2$$

Squared loss

3. Fit the model

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

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

MSE for SLR

4. Evaluate model performance

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

The combination of model + loss that we focus on today is known as **least squares regression**.

The Modeling Process

1357201

1. Choose a model ✅

How should we represent the world?

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

2. Choose a loss function ✅

How do we quantify prediction error?

$$L(y, \hat{y}) = (y - \hat{y})^2$$ Squared loss

3. Fit the model

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

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

We want to find $\hat{\theta}_0, \hat{\theta}_1$ that minimize this **objective function**.

4. Evaluate model performance

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

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Minimizing Average Loss on Data

Lecture 10, Data 100 Spring 2023

Minimizing MSE for the SLR Model

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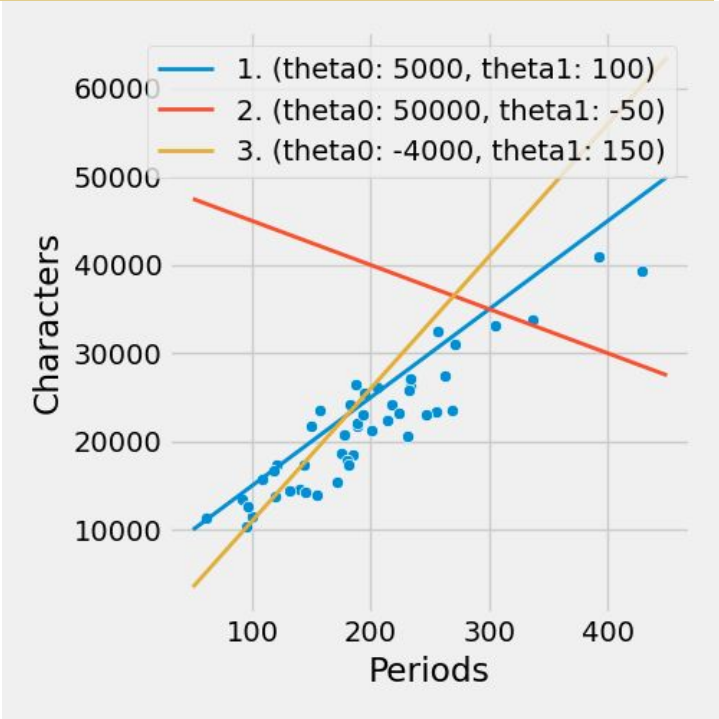
Recall: we wanted to pick the **regression line**

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

To minimize the (sample) **Mean Squared Error**:

$$\begin{aligned}\hat{R}(\theta) &= \frac{1}{n}\sum_i L(y_i, \hat{y}_i) \\ &= \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \\ &= \frac{1}{n}\sum_{i=1}^{n}(y_i - (\theta_0 + \theta_1 x_i))^2\end{aligned}$$

To find the best values, we **take derivatives** with respect to the choice variables θ_0, θ_1



For every chapter of the novel *Little Women*, Estimate the **# of characters** $\hat{y}$ based on the **# of periods** in that chapter.

Minimizing MSE for the SLR Model

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Recall: we wanted to pick the **regression line** $\hat{y} = \hat{\theta}_0 + \hat{\theta}_1 x$

To minimize the (sample) **Mean Squared Error**: $MSE(\theta_0, \theta_1) = \frac{1}{n}\sum_{i=1}^{n}(y_i - (\theta_0 + \theta_1 x_i))^2$

To find the best values, we set derivatives equal to zero to **obtain the optimality conditions:**

$$\frac{\partial}{\partial \theta_0} MSE = 0$$

$$\frac{\partial}{\partial \theta_1} MSE = 0$$

Partial Derivative of MSE with Respect to θ_0, θ_1

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$$\frac{\partial}{\partial \theta_0} MSE = \frac{\partial}{\partial \theta_0} \frac{1}{n} \sum_{i=1}^{n} (y_i - \theta_0 - \theta_1 x_i)^2$$

Derivative of sum is sum of derivatives

$$= \frac{1}{n} \sum_{i=1}^{n} \frac{\partial}{\partial \theta_0} (y_i - \theta_0 - \theta_1 x_i)^2$$

Chain rule

$$= \frac{1}{n} \sum_{i=1}^{n} 2(y_i - \theta_0 - \theta_1 x_i)(-1)$$

Simplify constants

$$= \boxed{-\frac{2}{n} \sum_{i=1}^{n} (y_i - \theta_0 - \theta_1 x_i)}$$

$$\frac{\partial}{\partial \theta_1} MSE = \frac{\partial}{\partial \theta_1} \frac{1}{n} \sum_{i=1}^{n} (y_i - \theta_0 - \theta_1 x_i)^2$$

Derivative of sum is sum of derivatives

$$= \frac{1}{n} \sum_{i=1}^{n} \frac{\partial}{\partial \theta_1} (y_i - \theta_0 - \theta_1 x_i)^2$$

Chain rule

$$= \frac{1}{n} \sum_{i=1}^{n} 2(y_i - \theta_0 - \theta_1 x_i)(-x_i)$$

Simplify constants

$$= \boxed{-\frac{2}{n} \sum_{i=1}^{n} (y_i - \theta_0 - \theta_1 x_i) x_i}$$

Minimizing MSE for the SLR Model

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Recall: we wanted to pick the **regression line** $\hat{y} = \hat{\theta}_0 + \hat{\theta}_1 x$

To minimize the (sample) **Mean Squared Error**: $MSE(\theta_0, \theta_1) = \frac{1}{n}\sum_{i=1}^{n}(y_i - (\theta_0 + \theta_1 x_i))^2$

To find the best values, we set derivatives equal to zero to **obtain the optimality conditions:**

$$0 = \frac{\partial}{\partial \theta_0} MSE = -\frac{2}{n}\sum_{i=1}^{n} y_i - \theta_0 - \theta_1 x_i \iff \frac{1}{n}\sum_i y_i - \hat{y}_i = 0$$ **1**

"Equivalent"

$$0 = \frac{\partial}{\partial \theta_1} MSE = -\frac{2}{n}\sum_{i=1}^{n}(y_i - \theta_0 - \theta_1 x_i)x_i \iff \frac{1}{n}\sum_i (y_i - \hat{y}_i)x_i = 0$$ **2**

To find the best θ_0, θ_1, we need to solve the **estimating equations** on the right.

From Estimating Equations to Estimators

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Goal: Choose θ_0, θ_1 to solve two estimating equations:

$$\frac{1}{n}\sum_i y_i - \hat{y}_i = 0 \quad \boxed{1} \qquad \text{and} \qquad \frac{1}{n}\sum_i (y_i - \hat{y}_i)x_i = 0 \quad \boxed{2}$$

1

$$\frac{1}{n}\sum_i (y_i - \theta_0 - \theta_1 x_i) = 0 \iff (\frac{1}{n}\sum_i y_i) - \theta_0 - \theta_1(\frac{1}{n}\sum_i x_i) = 0$$

$$\iff \bar{y} - \theta_0 - \theta_1 \bar{x} = 0$$

$$\iff \theta_0 = \bar{y} - \theta_1 \bar{x}$$

From Estimating Equations to Estimators

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Goal: Choose θ_0, θ_1 to solve two estimating equations:

$$\frac{1}{n}\sum_i y_i - \hat{y}_i = 0 \quad \boxed{1} \qquad \text{and} \qquad \frac{1}{n}\sum_i (y_i - \hat{y}_i)x_i = 0 \quad \boxed{2}$$

Now, let's try: $\boxed{2}$ - $\boxed{1}$ * $\bar{x}$

$$\frac{1}{n}\sum_i (y_i - \hat{y}_i)x_i - \frac{1}{n}\sum_i (y_i - \hat{y}_i)\bar{x} = 0 \iff \frac{1}{n}\sum_i (y_i - \hat{y}_i)(x_i - \bar{x}) = 0$$

$$(using\ \hat{y}_i = \theta_0 + \theta_1 x_i) \Rightarrow \frac{1}{n}\sum_i (y_i - \theta_0 - \theta_1 x_i)(x_i - \bar{x}) = 0$$

$$(using\ \theta_0 = \bar{y} - \theta_1 \bar{x}) \Rightarrow \frac{1}{n}\sum_i (y_i - \bar{y} + \theta_1\bar{x} - \theta_1 x_i)(x_i - \bar{x}) = 0$$

$$\Rightarrow \frac{1}{n}\sum_i (y_i - \bar{y} - \theta_1(x_i - \bar{x}))(x_i - \bar{x}) = 0$$

From Estimating Equations to Estimators

$$\Rightarrow \frac{1}{n}\sum_i (y_i - \bar{y} - \theta_1(x_i - \bar{x}))(x_i - \bar{x}) = 0$$

$$\Rightarrow \frac{1}{n}\sum_i (y_i - \bar{y})(x_i - \bar{x}) = \theta_1 \frac{1}{n}\sum_i (x_i - \bar{x})^2$$

Plug in definitions of correlation and SD:

$$r = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{x_i - \bar{x}}{\sigma_x}\right)\left(\frac{y_i - \bar{y}}{\sigma_y}\right)$$

$$r\sigma_x\sigma_y = \theta_1\sigma_x^2$$

Solve for θ_1:

$$\theta_1 = r\frac{\sigma_y}{\sigma_x}$$

Estimating Equations

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Estimating equations are the equations that the model fit has to solve. They help us:

- Derive the estimates
- Understand what our model is paying attention to

$$\frac{1}{n}\sum_i y_i - \hat{y}_i = 0$$

$$\frac{1}{n}\sum_i (y_i - \hat{y}_i)x_i = 0$$

For SLR:

- The residuals should **average to zero** (otherwise we should fix the intercept!)
- The residuals should be **orthogonal to the predictor variable** (or we should fix the slope!)

Very important for HW 5

The Modeling Process

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How should we represent the world?

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SLR model

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MSE for SLR

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

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

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Interpreting SLR: Slope

Lecture 10, Data 100 Spring 2023

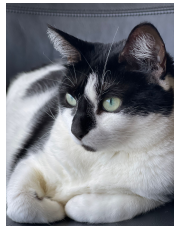
Interpreting the Least Squares Linear Regression Model

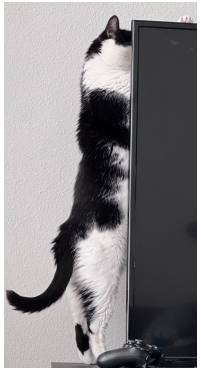
You may sometimes hear the prediction task defined as: "**regressing** y on x."

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

Suppose we fit a model that predicts a cat's weight (in pounds) given its length (in inches).

```
predicted weight = 2 + 0.5 * length
```





Interpreting the Least Squares Linear Regression Model

You may sometimes hear the prediction task defined as: "**regressing** y on x."

Suppose we fit a model that predicts a Chihuahua's weight (in pounds) given its length (in inches).

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

```
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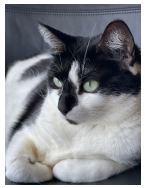

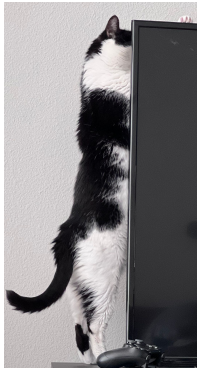

Interpreting the slope?

By definition, the slope measures the increase in y (pounds) for a 1 unit increase in x (1 inch).

1. Does this mean that if a cat in the dataset grows 1 inch, we estimate that they will get 0.5 pounds heavier? What does it actually mean?

Interpreting the Least Squares Linear Regression Model

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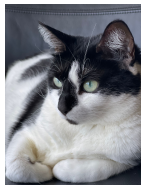

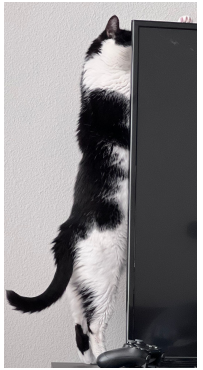

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By definition, the slope measures the increase in y (pounds) for a 1 unit increase in x (1 inch).

1. Does this mean that if a cat in the dataset grows 1 inch, we estimate that they will get 0.5 pounds heavier? What does it actually mean? **No!**

- The model we created shows **association**, not causation.
- The data we collected is a snapshot of several cats at one instance of time (**cross-sectional**), not snapshots of cats over time (**longitudinal**).

Slope interpretation: If two cats have a 1 inch height difference, their estimated weight difference is 0.5 lbs.

Interpreting the Least Squares Linear Regression Model

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

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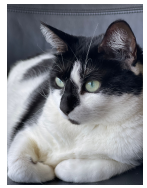

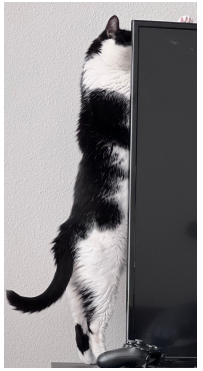

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By definition, the slope measures the increase in y (pounds) for a 1 unit increase in x (1 inch).

1. Does this mean that if a cat in the dataset grows 1 inch, we estimate that they will get 0.5 pounds heavier? What does it actually mean? **No!**

Predicting on wildly different data?

Domestic shorthair range from 8-10 pounds, and 13-16 inches in length.
Maine Coon range from 10-25 pounds, and 19-40 inches in length.

2. Should we use this model to predict the weight of all cat breeds? **No!**

Evaluating the Model: RMSE, Residual Plot

Lecture 10, Data 100 Spring 2023

Evaluating Models

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What are some ways to determine if our model was a good fit to our data?

1. **Visualize data, compute statistics:**

   Plot original data.
   Compute column means, standard deviation.
   If we want to fit a linear model, compute correlation r.

2. **Performance metrics:**

   Root Mean Square Error (RMSE)

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

   - It is the square root of MSE, which is the average loss that we've been minimizing to determine optimal model parameters.
   - RMSE is in the same units as y.
   - A lower RMSE indicates more "accurate" predictions (lower "average loss" across data)

3. **Visualization:**

   Look at a residual plot of $e_i = y_i - \hat{y}_i$ visualize the difference between actual and predicted y values.

Demo Slides

Four Mysterious Datasets + Least Squares

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Ideal model evaluation steps, in order:

1. **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**

It is tempting to only look at step 2.
But you need to always visualize!!!!