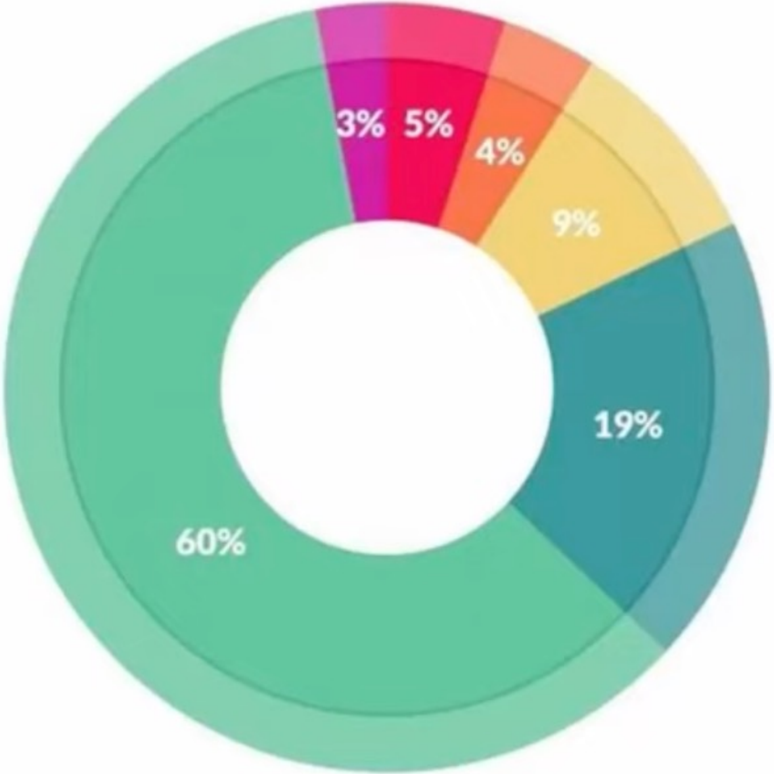
LECTURE 10

Introduction to Modeling, SLR

Understanding the usefulness of models and the simple linear regression model

Data Science, Spring 2024 @ Knowledge Stream

Sana Jabbar



What data scientists spend the most time doing

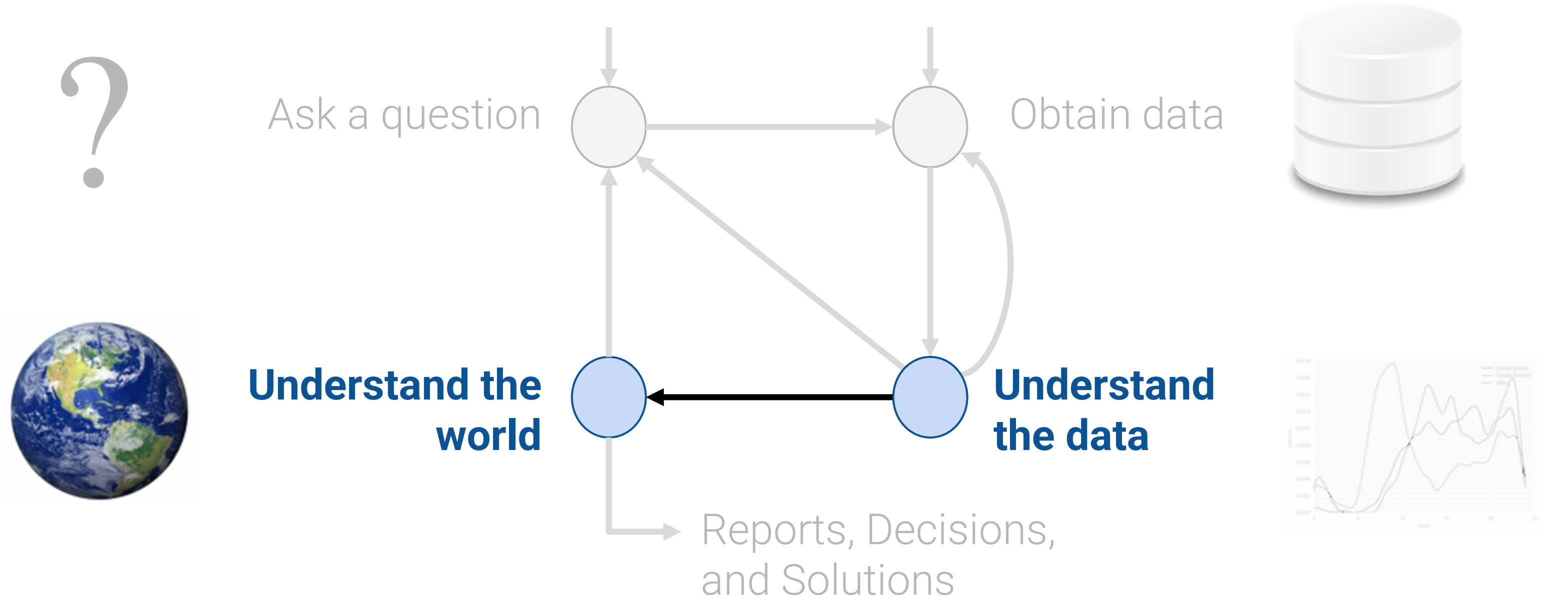
- *Building training sets: 3%*
- *Cleaning and organizing data: 60%*
- *Collecting data sets; 19%*
- *Mining data for patterns: 9%*
- *Refining algorithms: 4%*
- *Other: 5%*

Data Cleaning

Data Cleaning

ML Models

Plan for Next Few Lectures: Modeling



(today)

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

Today's Roadmap

Lecture 10

- What is a Model?
  - Regression Line, Correlation
- The Modeling Process
  - Choose a Model
  - Choose a Loss Function
  - Fit the Model
  - Evaluate the Model

What is a Model?

Lecture 10

- **What is a Model?**
  - Regression Line, Correlation
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  - Choose a Model
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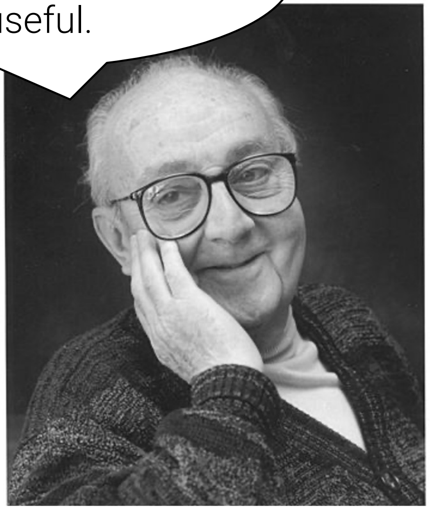
What is a Model?

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!

Essentially, all models are wrong, but some are 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

Three Reasons for Building Models

Reason 1:

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

- How are the parents' average heights related to the children's average heights?
- How do an object's velocity and acceleration impact how far it travels?

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.

Reason 3:

To make **causal inferences** about if one thing causes another thing.

- Can we conclude that smoking *causes* lung cancer?
- Does a job training program cause increases in employment and wage?

Much harder question because most statistical tools are designed to infer association not causation

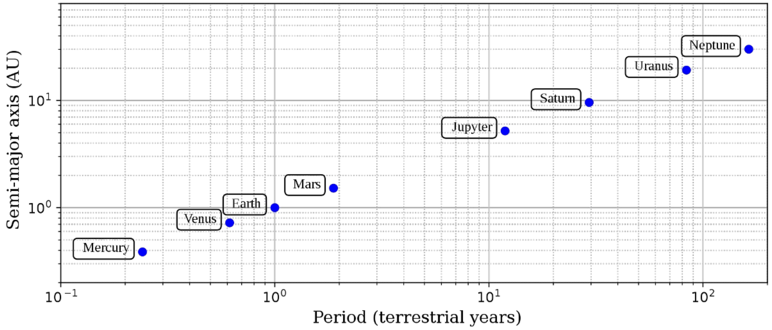
Most of the time, we want to strike a balance between **interpretability** and **accuracy**.

Common Types of Models

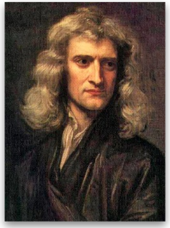
Deterministic physical (mechanistic) models: Laws that govern how the world works.

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.

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

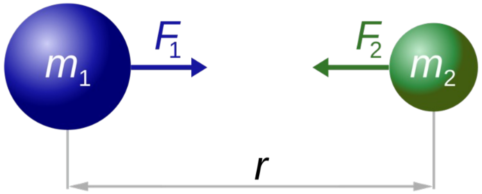


Newton's Laws: motion and gravitation (1687)
Newton's second law of motion models the relationship between the mass of an object and the force required to accelerate it.



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

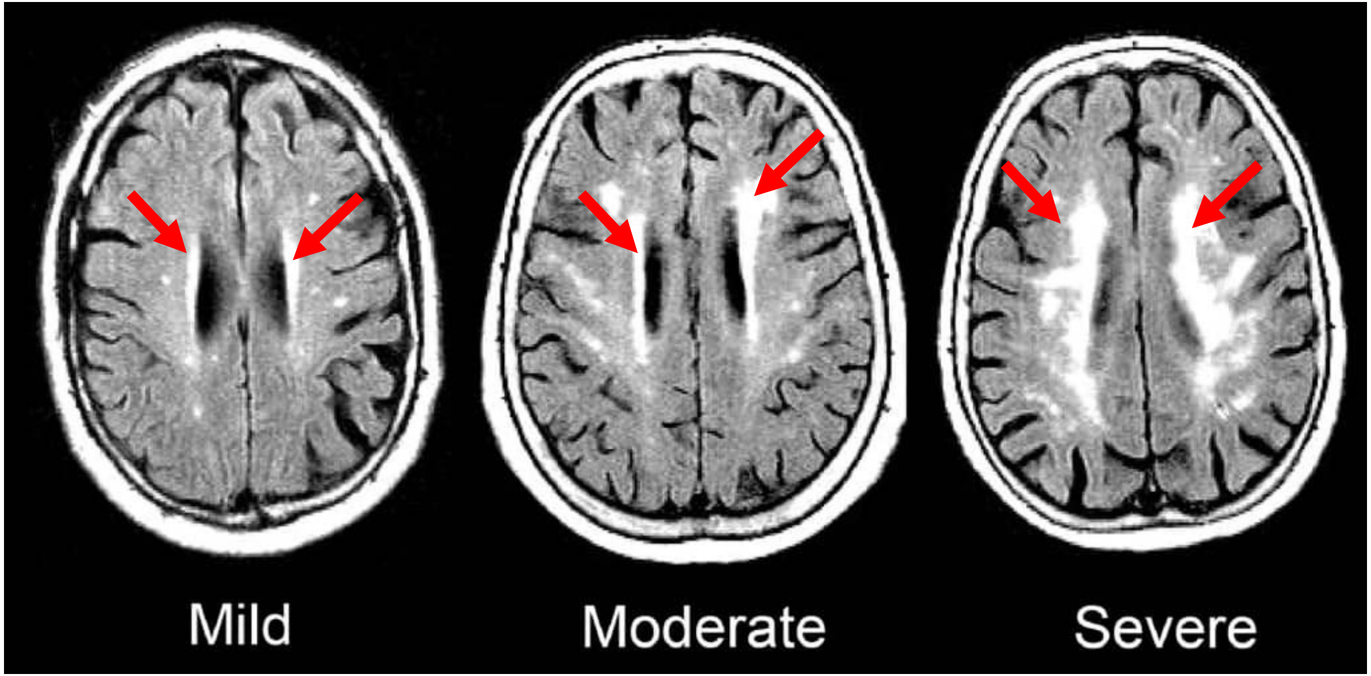
$$F = G\frac{m_1 m_2}{r^2}$$



Common Types of Models

Probabilistic models

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



Regression Line & Correlation

Lecture 10

- What is a Model?
- **Regression Line, Correlation**
- The Modeling Process
  - Choose a Model
  - Choose a Loss Function
  - Fit the Model
  - Evaluate the Model

The Regression Line

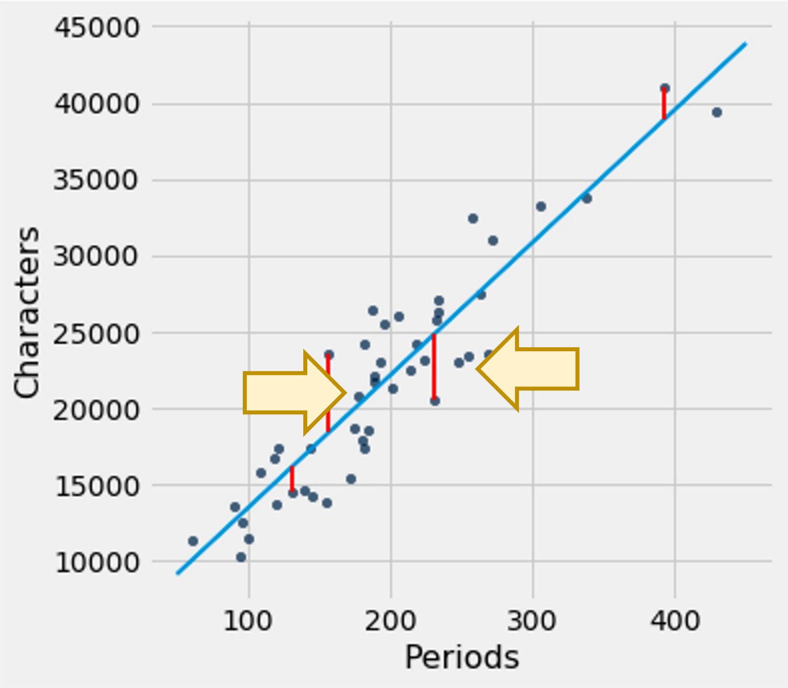
The **regression line** is the unique straight line that minimizes the **mean squared error** of estimation among all straight lines.

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

$$\begin{aligned}\text{intercept} = \ & \text{average of } y \\ & - \text{slope} \times \text{average of } x\end{aligned}$$

$$\text{regression estimate} = \text{intercept} + \text{slope} \times x$$

$$\boxed{\text{residual}} = \begin{aligned}&\text{observed } y \\ &-\text{regression estimate}\end{aligned}$$



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

The Regression Line

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correlation

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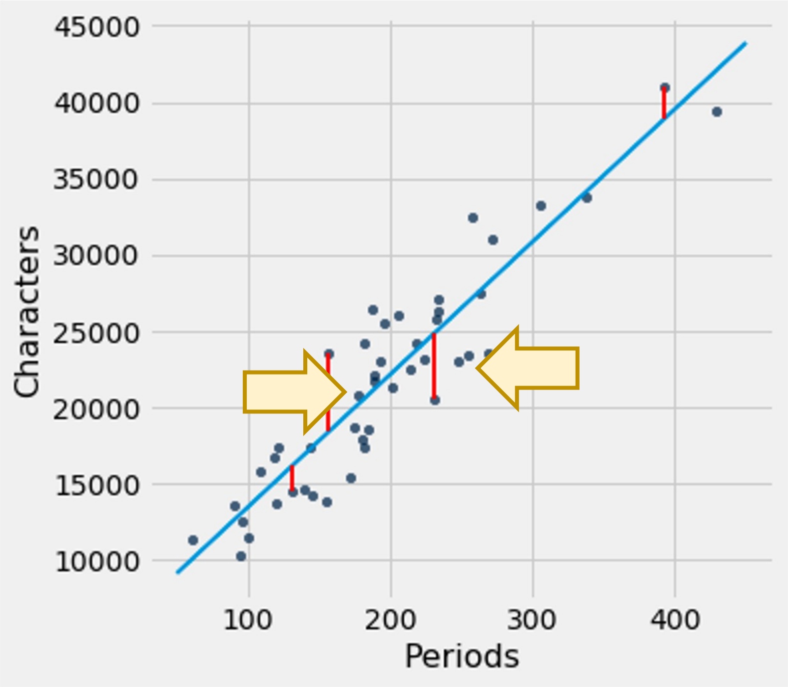

For every chapter of the novel *Little Women*, Estimate the **# of characters** $\hat{y}$ based on the **number of periods** x in that chapter.

Correlation

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

Define the following:

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

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

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

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

Correlation

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- Correlation measures the strength of a **linear association** between two variables.
- It ranges **between -1 and 1.**
  - r = 1 indicates perfect linear association; r = -1 perfect negative association.
  - The closer r is to 0, the weaker the linear association is.
- It says nothing about **causation** or **non-linear association.**
  - Correlation does not imply causation.
  - When r = 0, the two variables are **uncorrelated**. However, they could still be related through some non-linear relationship.

Correlation

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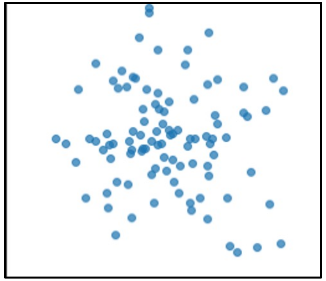
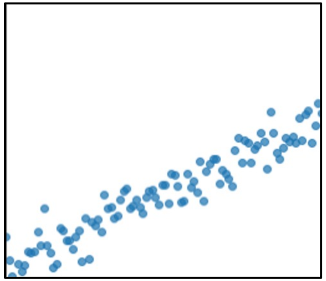
Correlation measures the strength of a **linear association** between two variables.

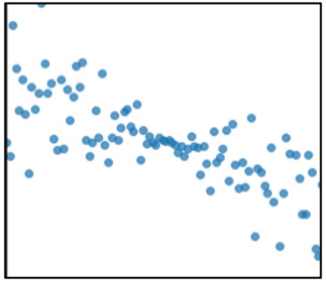
$$|r| \le 1$$



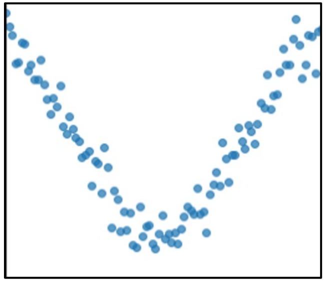
r = −0.121



r = 0.951



r = −0.723



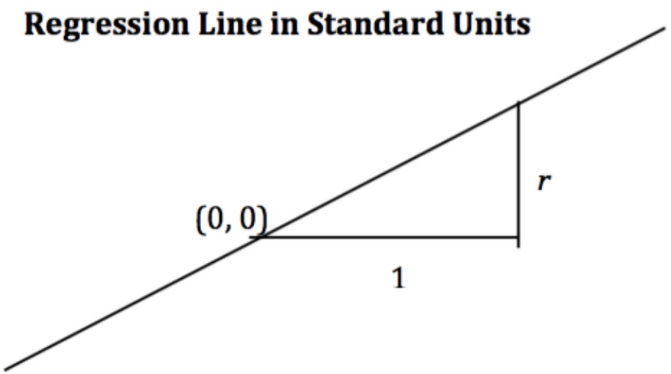
⚠️ **r = 0.056**

The Regression Line

- 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:

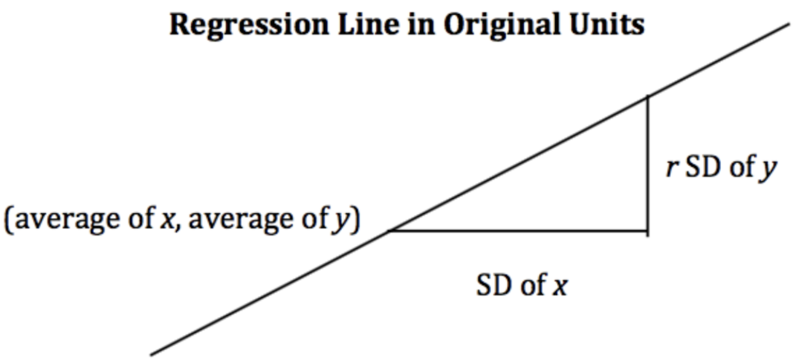
$$\hat{y} = r \times x$$

(both measured in standard units)



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

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



The Regression Line

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

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

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

Recall regression line equation is defined as:

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

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: $e_i = y_i - \hat{y}_i$

The Modeling Process

Lecture 10

Models in Data Science

We’ll treat a model as some mathematical rule to describe the relationships between variables.

Dataset

x	y
x_1	y_1
x_2	y_2
$\vdots$	$\vdots$
x_n	y_n

Observation

$$(x_i, y_i)$$

- Independent variable
- **Input**
- **Feature**
- **Attribute**

- Dependent variable
- **Output**
- **Outcome**
- **Response**

Prediction

If we use x to predict y, the predictions are denoted as $\hat{y} = \{\hat{y}_1, \hat{y}_2, \ldots, \hat{y}_n\}$

Models

Some models we will see in the next few lectures:

$$\hat{y}_i = \theta_0 + \theta_1 x_i$$

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

$$\hat{y}_i = x_i^\top \theta$$

Parametric models

Models in Data Science: Parametric Models

Parametric models are described by a few **parameters** $(\boldsymbol{\theta_0, \theta_1, \text{etc.}})$

- No one tells us the parameters: the data informs us about them.
- The x, y values are **not** parameters because we directly observe them.
- Sample-based **estimate** of parameter θ is written as $\hat{\theta}$.
- Usually, we pick the parameters that appear "**best**" according to some criterion we choose.

θ Model parameter(s)

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

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

$\hat{\theta}$ 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 $\hat{\theta} = [\hat{\theta}_0, \hat{\theta}_1]$

Models in Data Science: Parametric Models

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Note: Not all statistical models have parameters!

KDEs, k-Nearest Neighbor classifiers are non-parametric models.

θ Model paramet

inear model with

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$\hat{\theta}$ 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 $\hat{\theta} = [\hat{\theta}_0, \hat{\theta}_1]$

The Modeling Process

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?

Choose a Model

Lecture 10

- What is a Model?
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Simple Linear Regression: Our First Model

Simple Linear Regression Model (SLR)

$$\hat{y} = a + bx \quad \longrightarrow \quad \hat{y} = \theta_0 + \theta_1 x$$

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.

$$x \longrightarrow \boxed{\text{SLR} \quad \theta = [\theta_0, \theta_1]} \longrightarrow \hat{y}$$

- 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.

The Modeling Process

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

Lecture 10

The Modeling Process

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 quantify prediction error?

3. Fit the model

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

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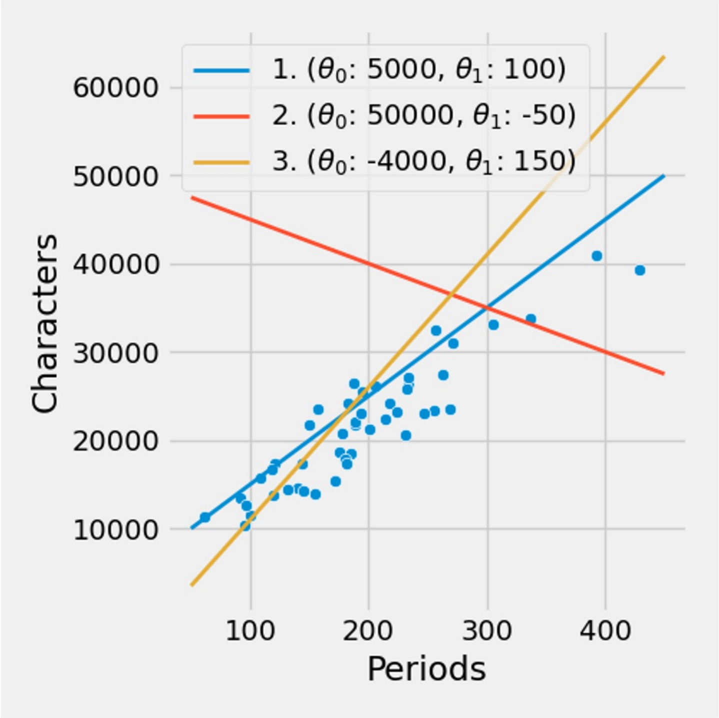
How do we evaluate whether this process gave rise to a good model?

Which θ is best?

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.

Loss Functions

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

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*

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

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    $\rightarrow$ bad fit
    $\rightarrow$ *lots of loss*

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

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

Absolute Loss

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

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

Residuals as loss function?

Why don't we directly use residual error as the loss function?

$$e = (y - \hat{y})$$

- Doesn't work: big negative residuals shouldn't cancel out big positive residuals!
    - Our predictions can be very off, but we can still get a zero residual.

Empirical Risk is Average Loss over Data

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 the model fits the data (not the population).

But hopefully these are close.

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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

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

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

MSE for SLR

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?

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

The Modeling Process

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How should we represent the world?

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

SLR model

2. Choose a loss function ✅

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Squared loss

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

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

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?

Fit the Model

Lecture 10, Data 100 Fall 2023

Minimizing MSE for the SLR Model

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

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

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

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

Estimating Equations

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

$$0 = \frac{\partial}{\partial \theta_0} MSE = -\frac{2}{n}\sum_{i=1}^{n}\left(y_i - \hat{\theta}_0 - \hat{\theta}_1 x_i\right) \iff \boxed{\frac{1}{n}\sum_i y_i - \hat{y}_i = 0}$$

"Equivalent"

$$0 = \frac{\partial}{\partial \theta_1} MSE = -\frac{2}{n}\sum_{i=1}^{n}\left(y_i - \hat{\theta}_0 - \hat{\theta}_1 x_i\right)x_i \iff \boxed{\frac{1}{n}\sum_i (y_i - \hat{y}_i)x_i = 0}$$

Estimating equations

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

From Estimating Equations to Estimators

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

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

and

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

$\boxed{1}$

Separating terms

$$\frac{1}{n}\sum_{i=1}^{n}\left(y_i - \hat{\theta}_0 - \hat{\theta}_1 x_i\right) = 0 \Longleftrightarrow \overbrace{\left(\frac{1}{n}\sum_{i=1}^{n} y_i\right)}^{\bar{y}} - \hat{\theta}_0 - \hat{\theta}_1 \overbrace{\left(\frac{1}{n}\sum_{i=1}^{n} x_i\right)}^{\bar{x}} = 0$$

$$\Longleftrightarrow \bar{y} - \hat{\theta}_0 - \hat{\theta}_1 \bar{x} = 0$$

$$\Longleftrightarrow \hat{\theta}_0 = \bar{y} - \hat{\theta}_1 \bar{x}$$

From Estimating Equations to Estimators

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

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

and

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

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

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

$$\left(\text{using } \hat{y_i} = \hat{\theta}_0 + \hat{\theta}_1 x_i\right) \Rightarrow \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \hat{\theta}_0 - \hat{\theta}_1 x_i\right)(x_i - \bar{x}) = 0$$

$$\left(\text{using } \hat{\theta}_0 = \bar{y} - \hat{\theta}_1\bar{x}\right) \Rightarrow \frac{1}{n}\sum_i \left(y_i - \bar{y} + \hat{\theta}_1\bar{x} - \hat{\theta}_1 x_i\right)(x_i - \bar{x}) = 0$$

$$\Rightarrow \frac{1}{n}\sum_i \left((y_i - \bar{y}) - \hat{\theta}_1(x_i - \bar{x})\right)(x_i - \bar{x}) = 0$$

From Estimating Equations to Estimators

$$\Rightarrow \frac{1}{n}\sum_i \left[(y_i - \bar{y})(x_i - \bar{x}) - \hat{\theta}_1 (x_i - \bar{x})^2\right] = 0$$

$$\Rightarrow \frac{1}{n}\sum_i (y_i - \bar{y})(x_i - \bar{x}) = \hat{\theta}_1 \frac{1}{n}\sum_i (x_i - \bar{x})^2$$

Reminder

$$\sigma_x^2 = \frac{1}{n}\sum_{i=1}^{n} (x_i - \bar{x})^2$$

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

Plug in definitions of correlation and SD:

$$r\sigma_y\sigma_x = \hat{\theta}_1 \sigma_x^2$$

Solve for $\hat{\theta}_1$:

$$\hat{\theta}_1 = r\frac{\sigma_y}{\sigma_x}$$

Estimating Equations

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.

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

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!)

The Modeling Process

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

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

4. Evaluate model performance

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

Lecture 10

Introduction to Modeling, SLR