Introduction to Modeling, SLR

Understanding the usefulness of models and the simple linear regression model

Content credit: <u>Acknowledgments</u>

Predictive Modeling

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).

What Is A Model?

What Is A Model?

: 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?

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!

Two Reasons for Building Models

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.

Common Types of Models

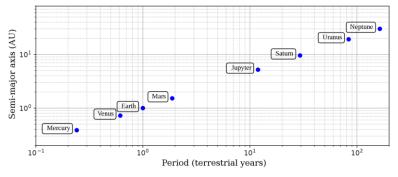
Deterministic physical (mechanistic) models: Laws that govern how the world works.

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.



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



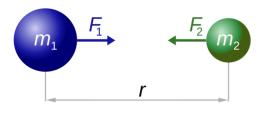
Newton's Laws: motion and gravitation (1687) Newton's second law of motion models the relationship between the mass of an object and

the force required to accelerate it.



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

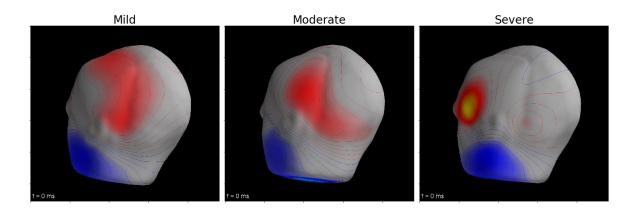
$$F = G\frac{m_1 m_2}{r^2}$$



Common Types of Models

Probabilistic models

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



Simple Linear Regression & Correlation

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The Regression Line

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

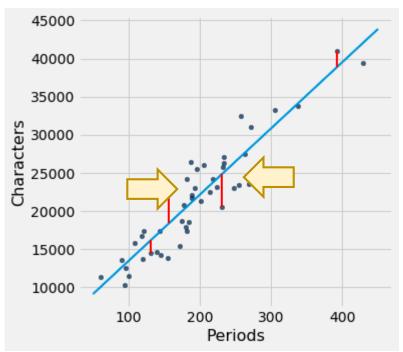
slope =
$$r \cdot \frac{\text{SD of } y}{\text{SD of } x}$$

$$intercept = average of y \\ - slope \cdot average of x$$

residual

= observed value

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.

The Regression Line

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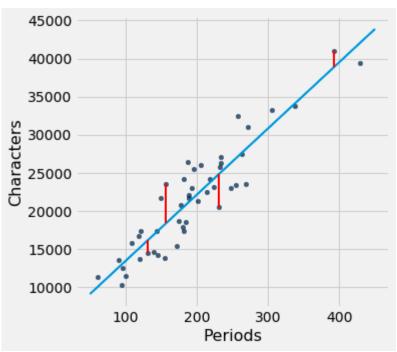
correlation

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

intercept = average of
$$y$$

- slope · average of x

residual = observed value - 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.

Correlation

The **correlation** is the average of the product of x_{γ} and y, both measured in standard units.

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

Define the following:

$$\mathcal{D}=\{(x_1,y_1),(x_2,y_2),\dots,(x_n,y_n)\}$$
 data $ar{x},ar{y}$ means; σ_x,σ_y standard deviations

Correlation

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

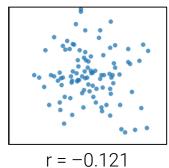
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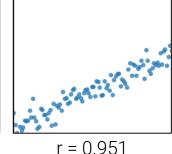
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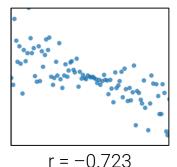
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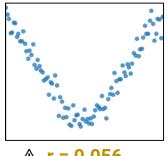
- ullet x_i in standard units: $rac{x_i ar{x}}{\sigma_x}$
- $oldsymbol{r}$ is also known as Pearson's correlation coefficient.

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









 \triangle r = 0.056

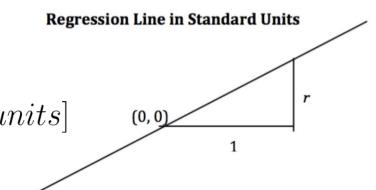
[The Regression Line

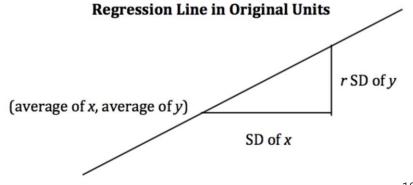
• When the variables x and y are measured in standard units, the regression line for predicting y based on x has slope r passes through the origin and the equation will be:

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

In the original units of the data, this becomes:

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





The Regression Line

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

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

Recall regression line equation is defined as:

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

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

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)

notation

$$\hat{y} = a + bx \qquad \longrightarrow \text{Another notation:} \ \hat{y} = \theta_0 + \theta_1 x$$

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

True outputs

Predicted outputs

For data:

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

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)
- $ullet \hat{y}_i$ is the i-th **prediction** (aka estimation).

Model parameter(s)

 $\hat{y} = \theta_0 + \theta_1 x \quad \text{Any linear model with parameters} \quad \theta = [\theta_0, \theta_1]$

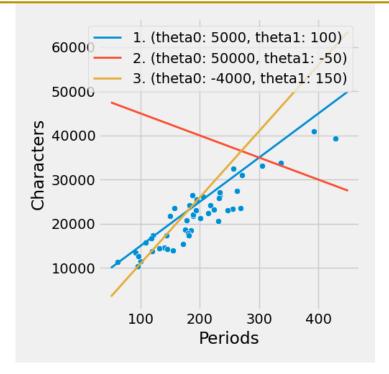
Estimated parameter(s), "best" fit to data in some sense $\hat{y} = \hat{\theta_0} + \hat{\theta_1} x \quad \text{The "best" fitting linear model with parameters } \hat{\theta} = [\hat{\theta_0}, \hat{\theta_1}]$

Which θ is best?

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

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

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



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.

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. $\mathcal{X} \longrightarrow \mathtt{SLR} \; \theta = [\theta_0, \theta_1] \longrightarrow \hat{\mathcal{Y}}$

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

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

What is a model?

Data 8 Review: Simple Linear Regression

and Correlation

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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?
 - o Do we care about outliers?
 - Are all errors equally costly? (e.g., false negative on cancer test)

L2 Loss or Squared Loss

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

- Widely used.
- Also called "L2 loss".
- Reasonable:
 - $\begin{array}{ccc} \circ & \hat{y} = y \xrightarrow{\hspace{0.1cm} \to} \operatorname{good} \operatorname{prediction} \\ & \hat{y} & \xrightarrow{\hspace{0.1cm} \to} \operatorname{good} \operatorname{fit} \xrightarrow{\hspace{0.1cm} \to} \operatorname{no} \\ \operatorname{loss} & y \end{array}$
 - o far from \rightarrow bad prediction \rightarrow bad fit \rightarrow *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:

$$\begin{array}{ccc} \circ & \hat{y} = y \to \operatorname{good\ prediction} \\ & & \to \operatorname{good\ fit} \to \operatorname{no} \\ & & \\ \hat{\mathcal{Y}} \mathrm{ss} & & y \end{array}$$

o far from → bad prediction
 → bad fit → some loss

Squared Loss (L2 Loss)

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

For an SLR model $\hat{y}= heta_0+ heta_1x$:

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

Absolute Loss (L1 Loss)

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

For an SLR model $\,\hat{y}=\theta_0+\theta_1x$:

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?

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

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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!

Doesitt work. Dig flegative residuals shouldn't cancer out Dig positive residuals:

L2 penalizes larger residuals more.

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

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

Function of the parameter heta (holding the data fixed) because heta 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.

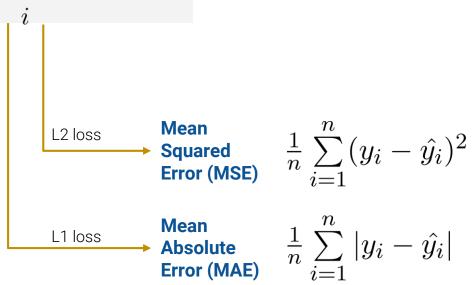
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The colloquial term for average loss depends on which loss function we choose.



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

How do we quantify prediction error?

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Squared loss

How do we choose the 3. Fit the model 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.

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

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

Minimizing Average Loss on Data

What is a model?

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

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

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

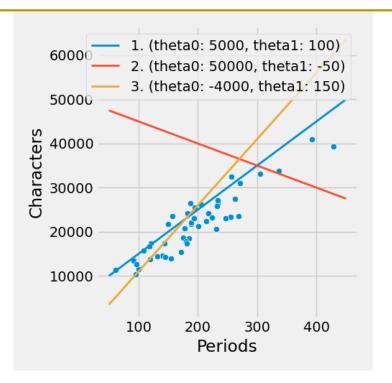
To minimize the (sample) **Mean Squared Error**:

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

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

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

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.

Recall: we wanted to pick the regression line $\hat{y} = \hat{\theta_0} + \hat{\theta_1} x$

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

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**:

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

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

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:**

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

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

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

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

$$\frac{1}{n}\sum_{i}y_{i}-\hat{y}_{i}=0 \quad \boxed{1} \quad \text{and} \quad \frac{1}{n}\sum_{i}(y_{i}-\hat{y}_{i})x_{i}=0 \quad \boxed{2}$$

$$\frac{1}{n}\sum_{i}(y_{i}-\theta_{0}-\theta_{1}x_{i})=0 \Longleftrightarrow (\frac{1}{n}\sum_{i}y_{i})-\theta_{0}-\theta_{1}(\frac{1}{n}\sum_{i}x_{i})=0$$

$$\iff \bar{y}-\theta_{0}-\theta_{1}\bar{x}=0$$

$$\iff \theta_{0}=\bar{y}-\theta_{1}\bar{x}$$

From Estimating Equations to Estimators

Goal: Choose $heta_0, heta_1$ to solve two estimating equations:

$$rac{1}{n}\sum_i y_i - \hat{y}_i = 0$$
 and $rac{1}{n}\sum_i (y_i - \hat{y}_i)x_i = 0$ 2

Now, let's try:
$$f 2$$
 - $f 1$ * $ar{x}$

$$\frac{1}{n} \sum_{i} (y_i - \hat{y}_i) x_i - \frac{1}{n} \sum_{i} (y_i - \hat{y}_i) \bar{x} = 0 \iff \frac{1}{n} \sum_{i} (y_i - \hat{y}_i) (x_i - \bar{x}) = 0$$
(a) $\hat{x}_i = \hat{x}_i + \hat{x}_i = 0$ (b) $\hat{x}_i = 0$ (c) $\hat{x}_i = 0$

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

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

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Squared loss

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

4. Evaluate model performance

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

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

Interpreting SLR: Slope

What is a model?

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

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).

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

predicted weight = 2 + 0.5 * length





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?

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.

Evaluating the Model: RMSE, Residual Plot

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Evaluating Models

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

1. Performance metrics:

Root Mean Square Error (RMSE)

- $ext{RMSE} \qquad = \sqrt{rac{1}{n} \sum_{i=1}^n (y_i \hat{y_i})^2}$
- 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)

1. Visualization:

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