Linear Regression

... and the modeling philosophy

GENERAL ASSEMBLY

Agenda

- What is ~~statistical modeling~~ machine learning?
- What is linear regression?
- The inner mechanics of linear regression
- Assumptions of linear regression, and how to check them
- What do we do if those assumptions aren't met?

What is Machine Learning?

Machine learning is the process of letting your **machine** use data to **learn** the relationship between some predictors (*x*-variables) and some response(s) (*y*-variables).

What is Machine Learning?

Machine learning is the process of letting your **machine** use data to **learn** the relationship between some predictors (*x*-variables) and some response(s) (*y*-variables).

This is a fancy way of saying **statistical modeling**.

Ok then, so what is statistical modeling?

Statistical modeling is the process of combining data with **statistical theory** to **model** the real-world relationship between predictors (*x*-variables) and some response(s) (*y*-variables).

Ok then, so what is statistical modeling?

Statistical modeling is the process of combining data with **statistical theory** to **model** the real-world relationship between predictors (*x*-variables) and some response(s) (*y*-variables).

This is a more down-to-earth way of saying **machine learning**.

Two* Kinds of ML

In essence, all machine learning models fall into one of two categories:

- **Supervised learning** - Given X, can we predict Y?
- **Unsupervised learning** - What does X look like, *really?* There is no Y.

*There are more. Kinda. The big third category is **reinforcement learning**, which is a field still in the process of being invented.

Two Kinds of Supervised Learning

Supervised learning models fall into two different buckets:

Regression - this is when our *y*-variable is numeric.

- *“Given the past values of the stock price of Apple, what will tomorrow’s closing price be?”*
- *“Given the annual precipitation, average temperature, and soil pH, what will this year’s harvest yield be?”*
- *“Given the square footage, number of bedrooms, number of bathrooms, and quality of school district, what will the price of this home be?”*

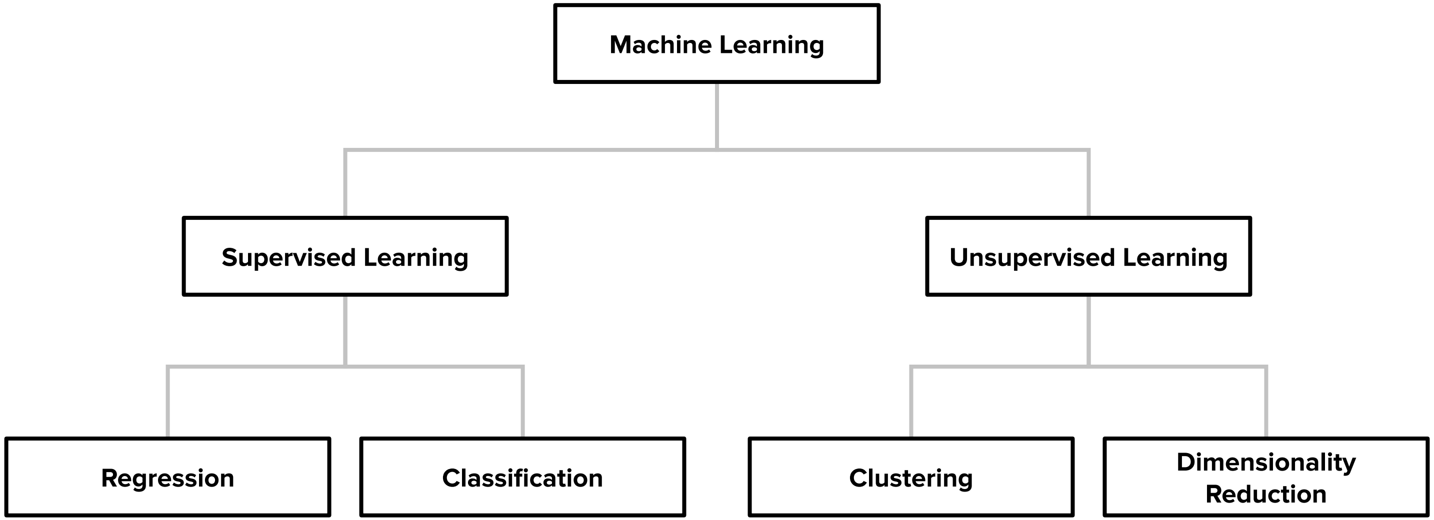
Two Kinds of Supervised Learning

Supervised learning models fall into two different buckets:

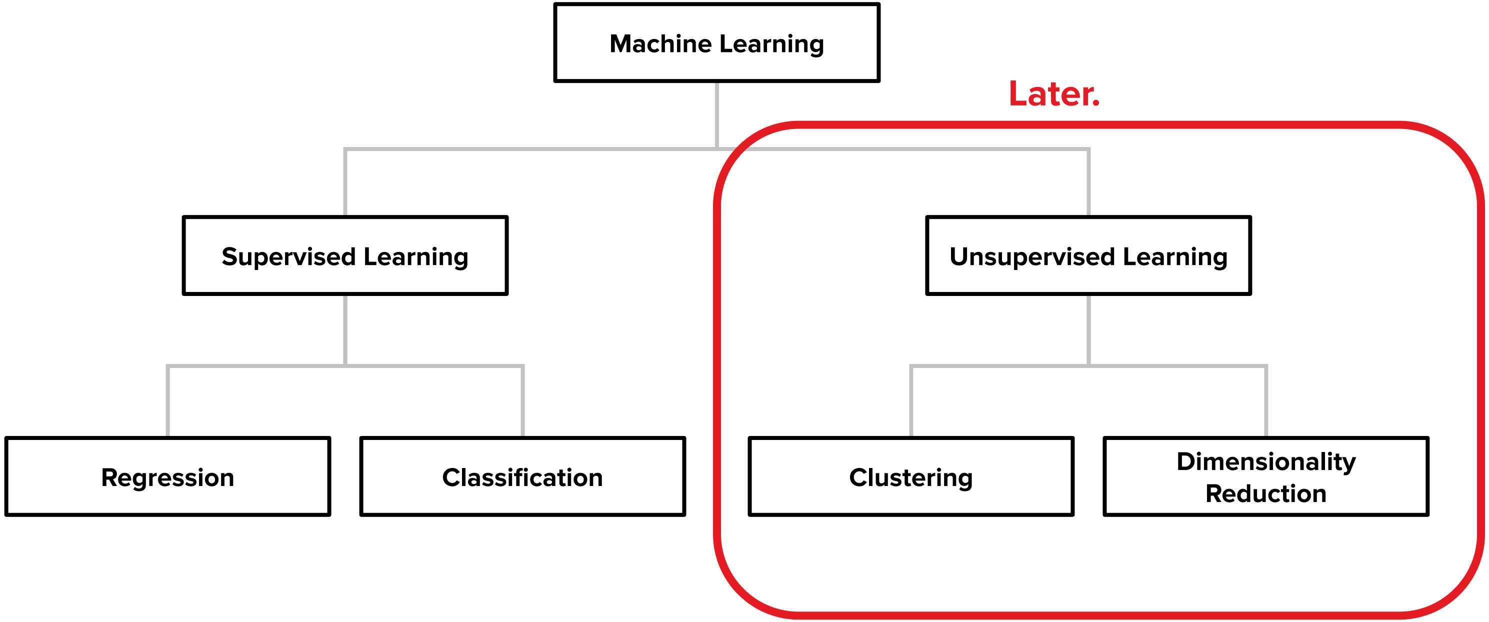
Classification - this is when our *y*-variable is a category. If it's a 0/1 yes/no kind of variable, we often call it **binary classification**. Otherwise, **multiclass classification**.

- *"Given this person's demographic information, how many tabs they have open, and where they live, will they make a purchase on my site?"*
- *"Given radar readouts, past weather, and almanac data, will it rain tomorrow?"*
- *"Given how many hours you study, how many hours you sleep, and your course load, will you pass the final exam?"*

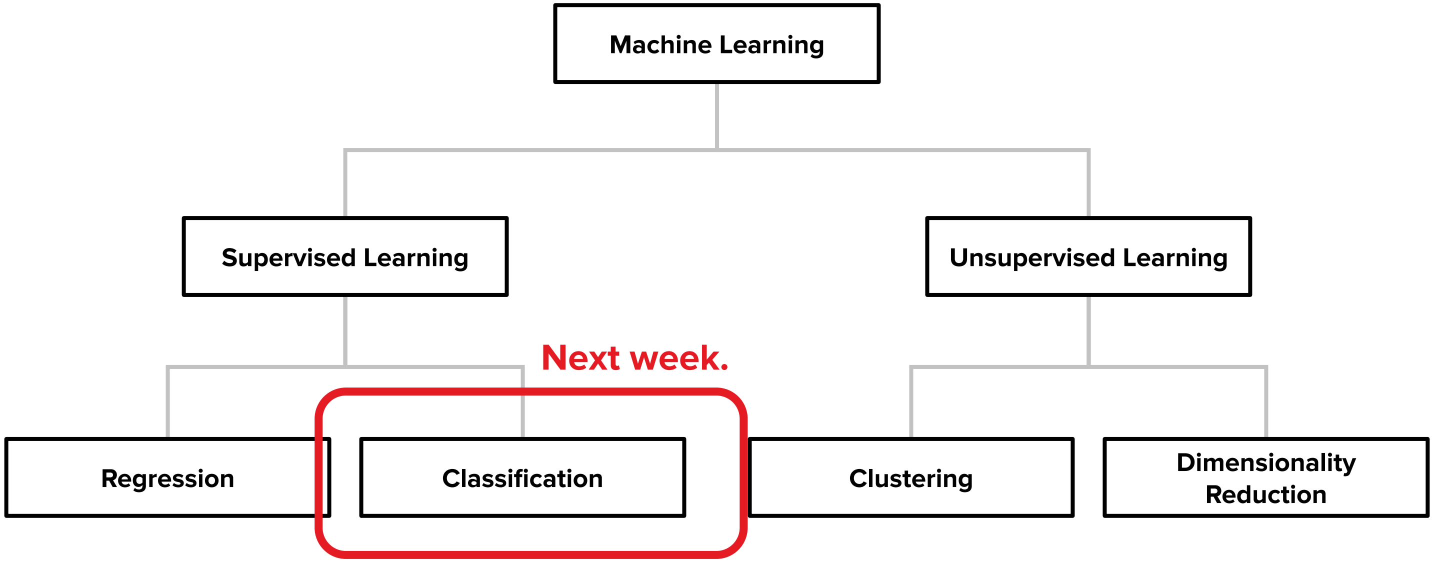
Roadmap of ML



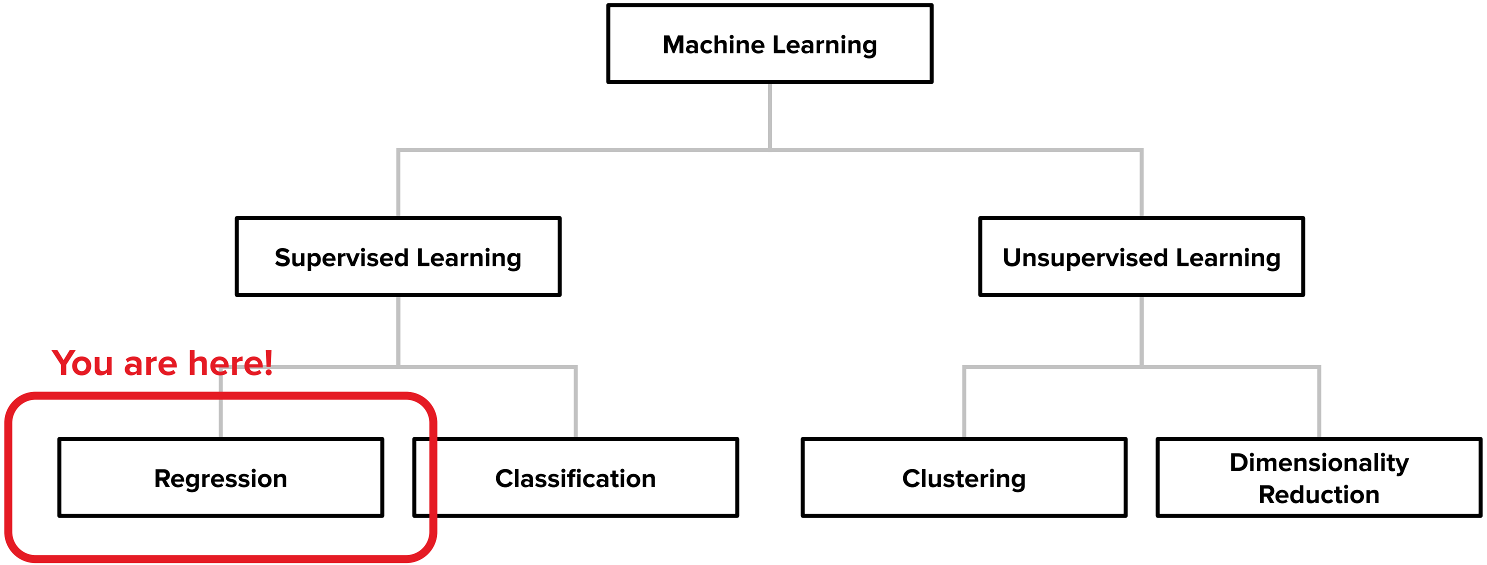
Roadmap of ML



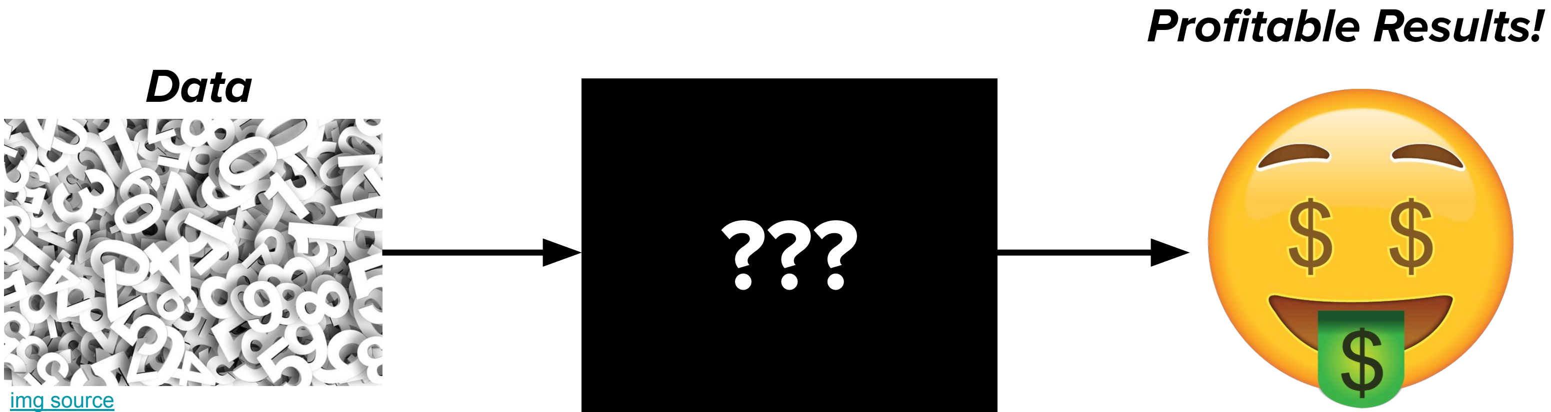
Roadmap of ML



Roadmap of ML

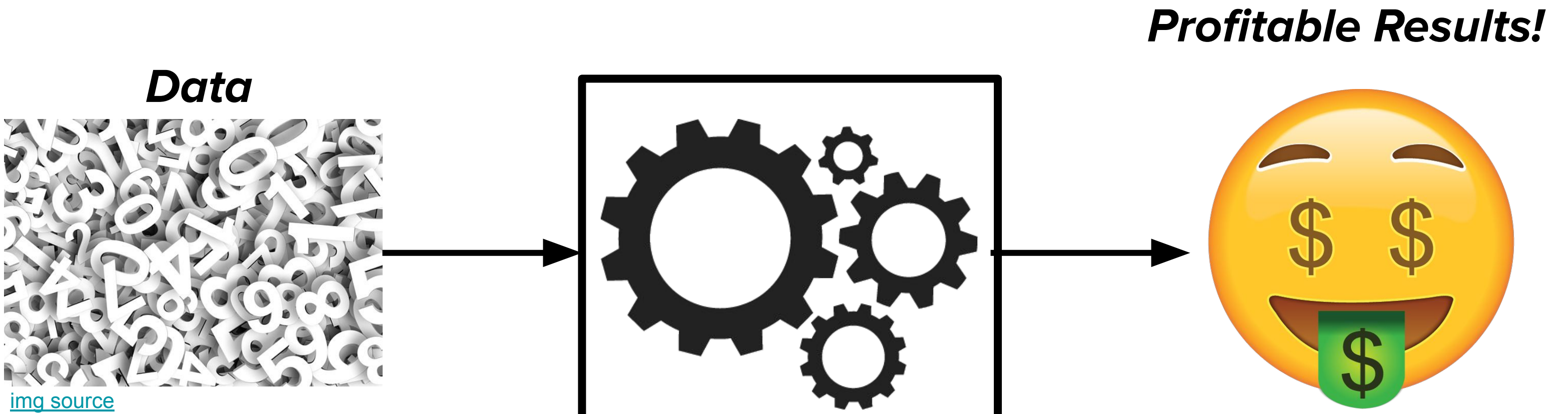


Supervised Learning Transparency



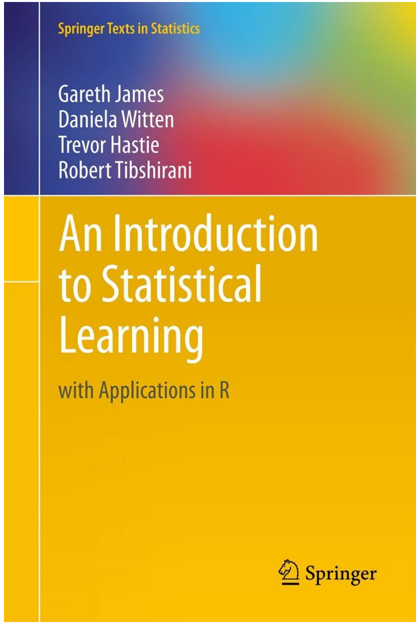
img source

Supervised Learning Transparency

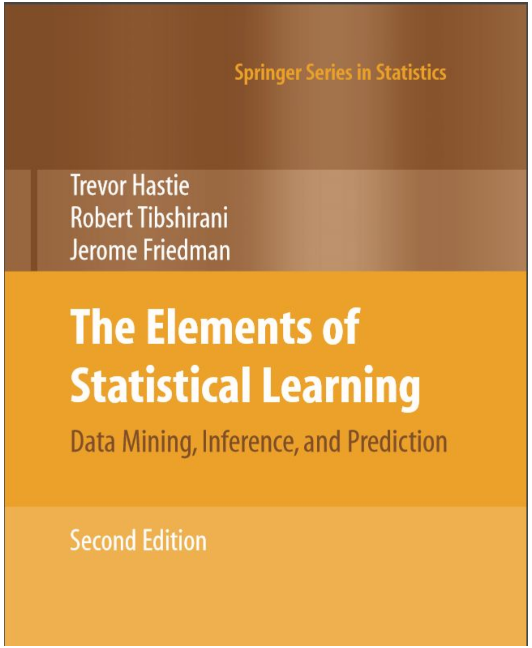


img source

The Tim Book Book Club



Undergraduate math level, very readable



All topics ISL has but at the graduate math level. A few additional chapters.

Linear Regression

Supervised, white-box, regression

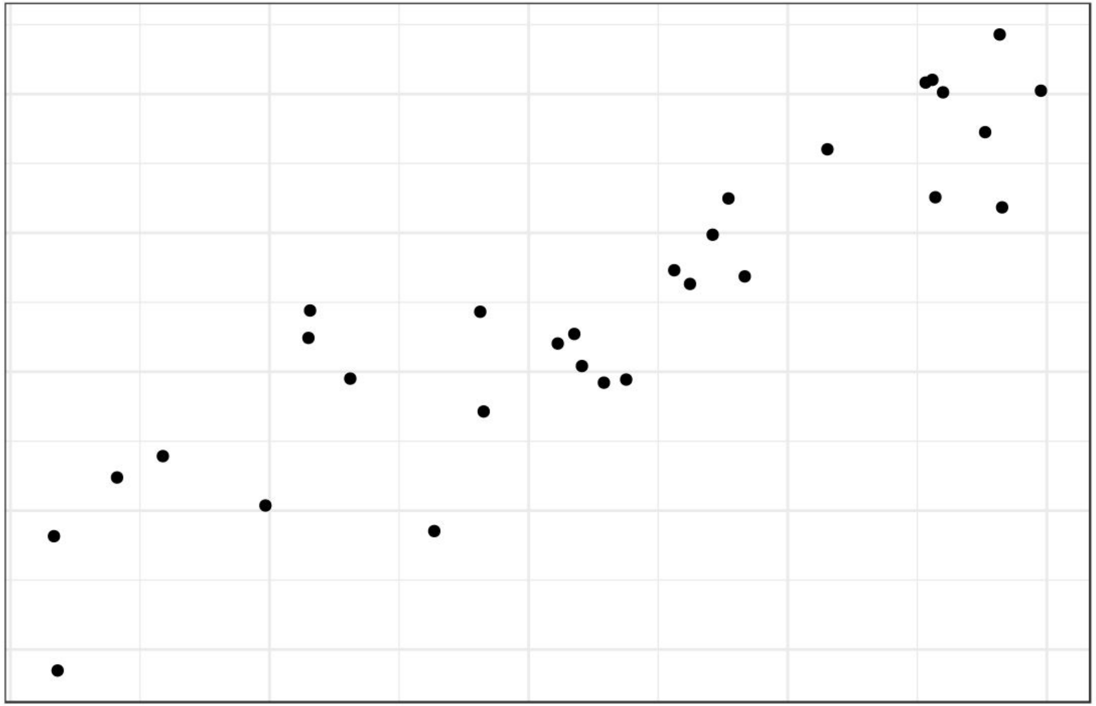
What is linear regression?

In ordinary least squares linear regression (often just referred to as **OLS**), we try to predict some response variable (*y*) from at least one independent variable (*x*). We believe there is a **linear** relationship between the two:

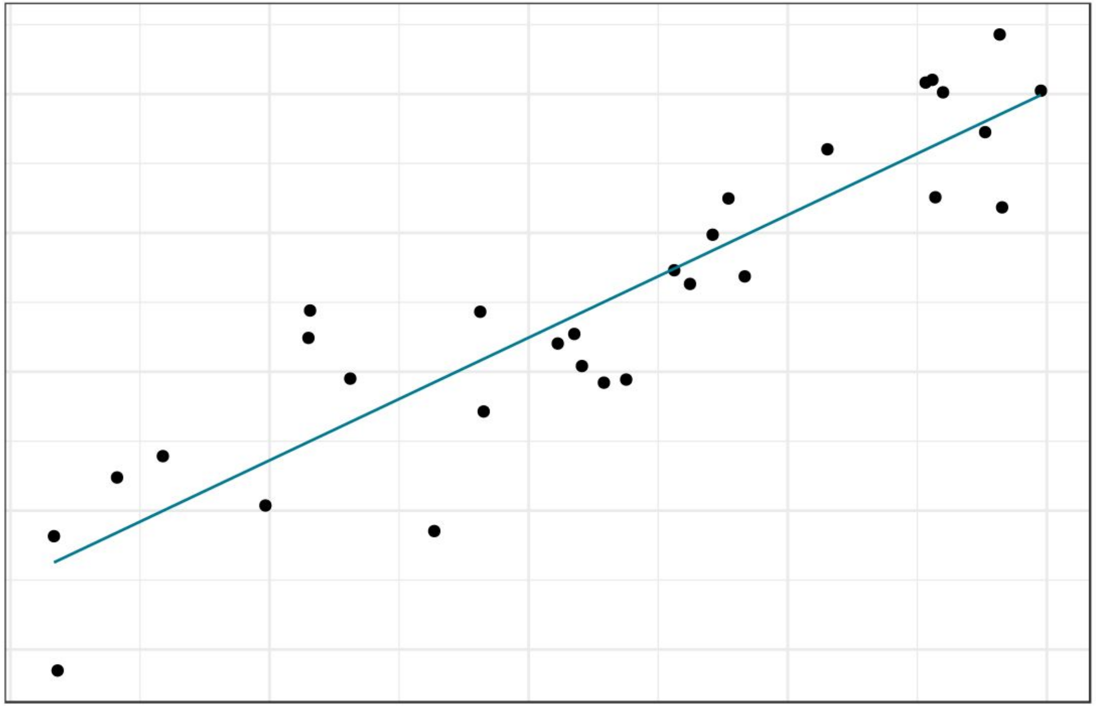
$$y = \beta_0 + \beta_1 x + \varepsilon$$

Where that funny looking “e” stands for “error” - it’s random noise inherent in our prediction because nothing will be perfect.

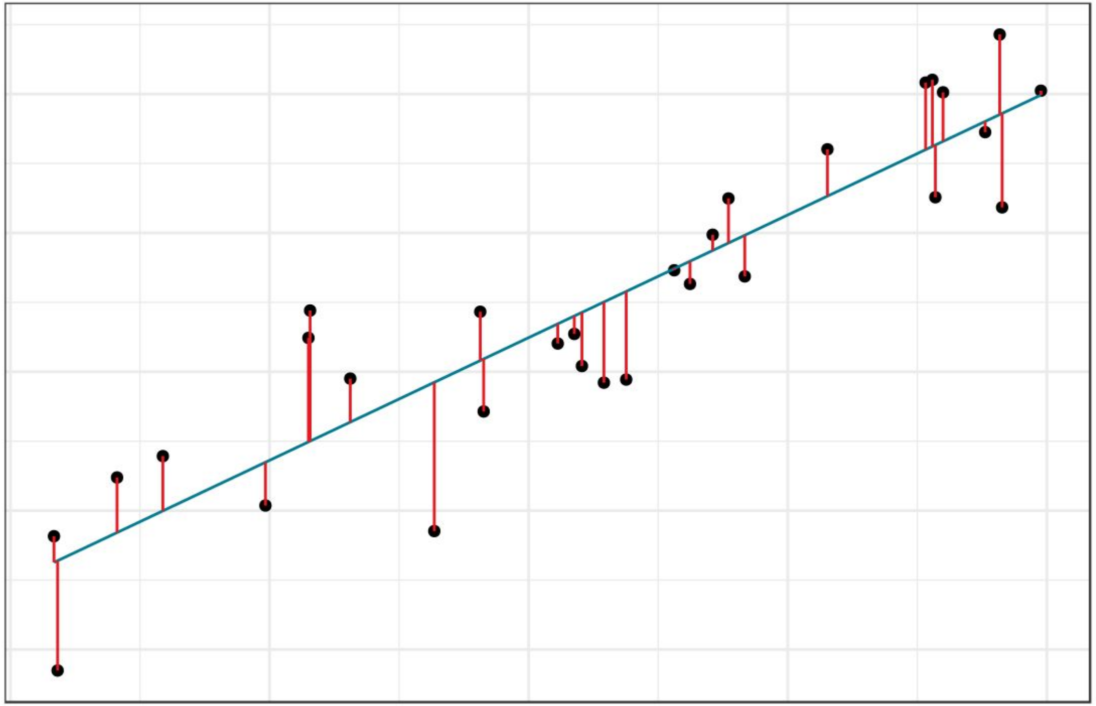
Graphically, this is:



Graphically, this is:



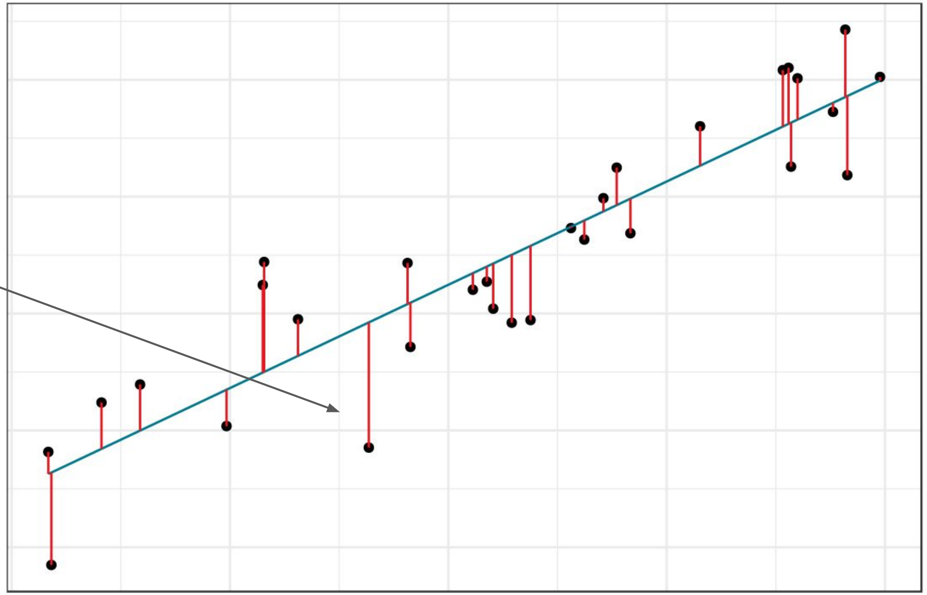
Graphically, this is:



Graphically, this is:

The difference between the actual and the predicted is called a **residual**, and the line of "best fit" minimizes all of these residuals.

Specifically, we minimize the **sum of the squared residuals**, hence the term "least squares".



Let’s fit one ourselves!

Notation

A boldface ***y*** denotes *all* of our response data. It's **bold because it's a vector**.
We typically reserve the letter *n* to be our **sample size**.

$$\mathbf{y} = (y_1,\ y_2,\ \ldots,\ y_n)$$

Notation

We put "hats" over variables to denote they are **predicted values**. That is, "y-hat" represents the predictions based on our original data.

$$\hat{\mathbf{y}} = (\hat{y}_1,\ \hat{y}_2,\ \ldots,\ \hat{y}_n)$$

Notation

Similarly, the betas are things we **estimate**, so they get hats too! Our y-hats are the results of using these estimated values to get predictions.

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$$

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$$

Notation

We often need to look at formulas is **summation notation**. Let's discuss these:

$$\sum_{i=1}^{4} i$$

$$\sum_{k=2}^{4} (k^2 - 1)$$

$$\frac{1}{n} \sum_{i=1}^{n} x_i$$

Notation

We often need to look at formulas is **summation notation**. Let's discuss these:

$$\sum_{i=1}^{4} i = 1 + 2 + 3 + 4 = 10$$

$$\sum_{k=2}^{4} (k^2 - 1)$$

$$\frac{1}{n} \sum_{i=1}^{n} x_i$$

Notation

We often need to look at formulas is **summation notation**. Let's discuss these:

$$\sum_{i=1}^{4} i = 1 + 2 + 3 + 4 = 10$$

$$\sum_{k=2}^{4} (k^2 - 1)$$

$$\frac{1}{n} \sum_{i=1}^{n} x_i$$

Notation

We often need to look at formulas is **summation notation**. Let's discuss these:

$$\sum_{i=1}^{4} i = 1 + 2 + 3 + 4 = 10$$

$$\sum_{k=2}^{4} (k^2 - 1) = 3 + 8 + 15 = 26$$

$$\frac{1}{n} \sum_{i=1}^{n} x_i$$

Notation

We often need to look at formulas is **summation notation**. Let's discuss these:

$$\sum_{i=1}^{4} i = 1 + 2 + 3 + 4 = 10$$

$$\sum_{k=2}^{4} (k^2 - 1) = 3 + 8 + 15 = 26$$

$$\frac{1}{n} \sum_{i=1}^{n} x_i = \bar{x}$$

The sample mean!

The Residual

Next, we define a **residual** as:

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

This measures how "off" our predictions were. It's either positive or negative depending on whether we overestimate or underestimate.

The Sum Squared Error

To get an aggregate measurement of the quality of our model, we often look at the **sum squared error**, or **SSE:**

$$SSE = \sum (y_i - \hat{y}_i)^2 = \sum e_i^2$$

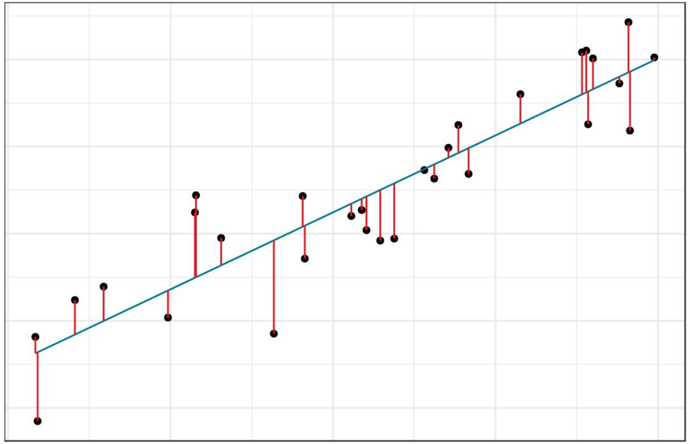
Or more commonly, the **mean squared error (MSE)**:

$$MSE = \frac{1}{n} \sum (y_i - \hat{y}_i)^2 = \frac{1}{n} \sum e_i^2$$

Fitting OLS models

Remember, this is the quantity we actually seek to **minimize** in order to find the best values of our betas!

$$MSE = \frac{1}{n}\sum(y_i - \hat{y}_i)^2 = \frac{1}{n}\sum(y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i))^2$$



Let’s check out the results!

LINE Assumptions

OLS Assumptions

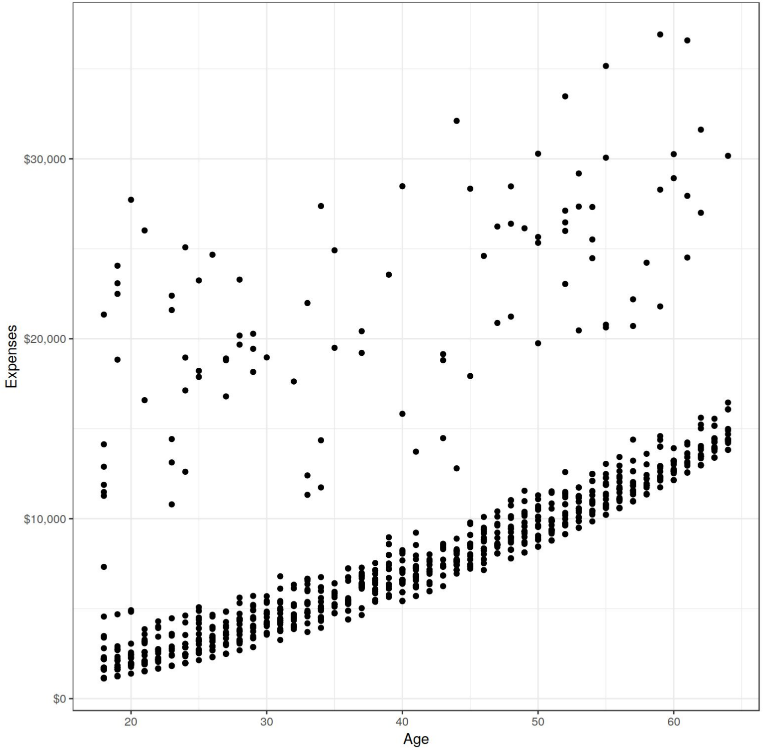
Conducting OLS comes with some pretty steep assumptions that should be satisfied before believing the results. Luckily, there's a nice acronym to remember them:

OLS Assumptions

Conducting OLS comes with some pretty steep assumptions that should be satisfied before believing the results. Luckily, there's a nice acronym to remember them:

- **L** - Linearity. Relationship between *x* and *y* should be approximately linear.
- **I** - Independence. Your observations should not affect one another.
- **N** - Normality. Our residuals should be approximately normally distributed.
- **E** - Equal variances, aka "**homoscedasticity**". Residuals should have approximately equal variances for each *x*.

L is for Linearity



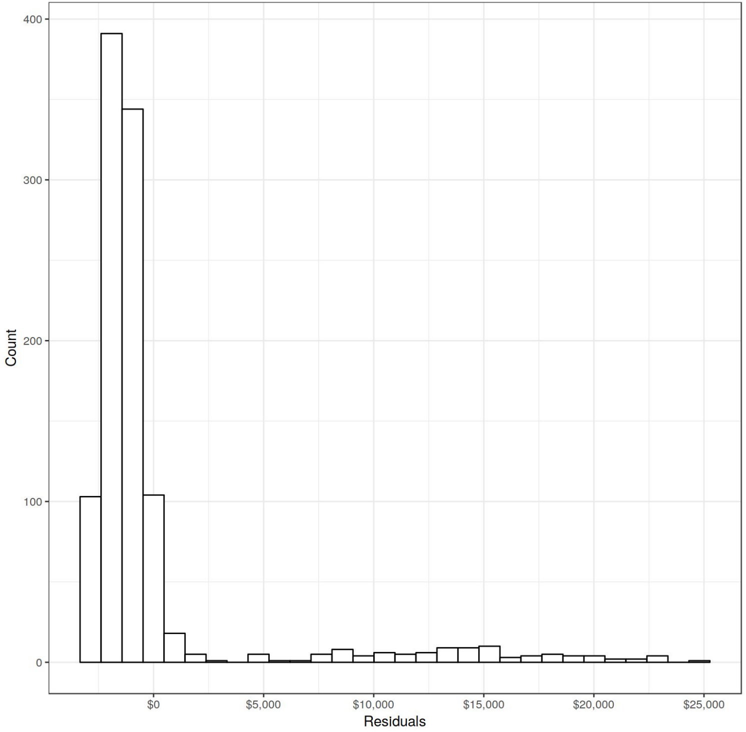
I is for Independence

Are our samples independent from one another?

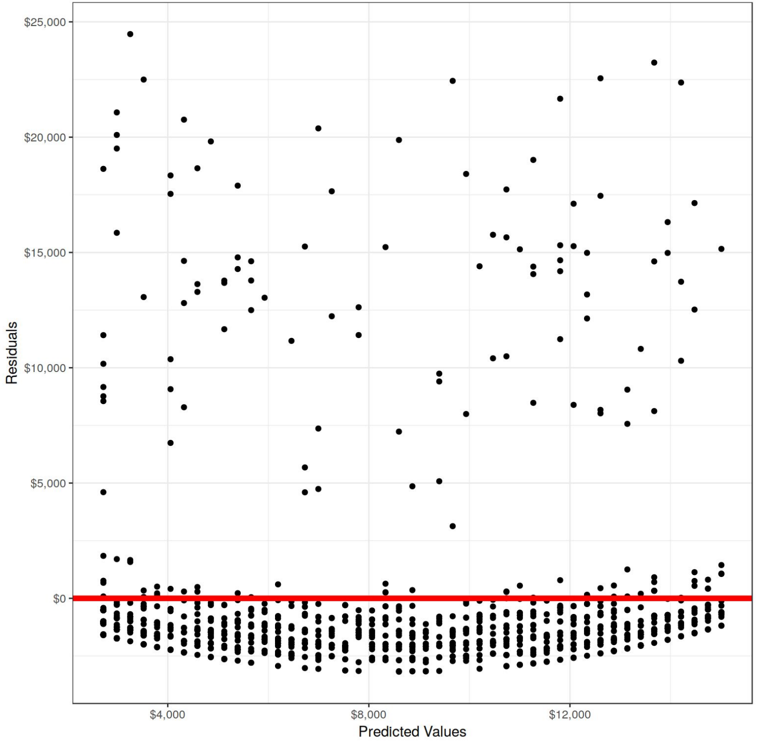
Yes, these samples were collected independently.

The most common time we'd have to worry about this assumption is when we have **time series data**, when multiple measurements are made on a subject over time.

N is for Normality



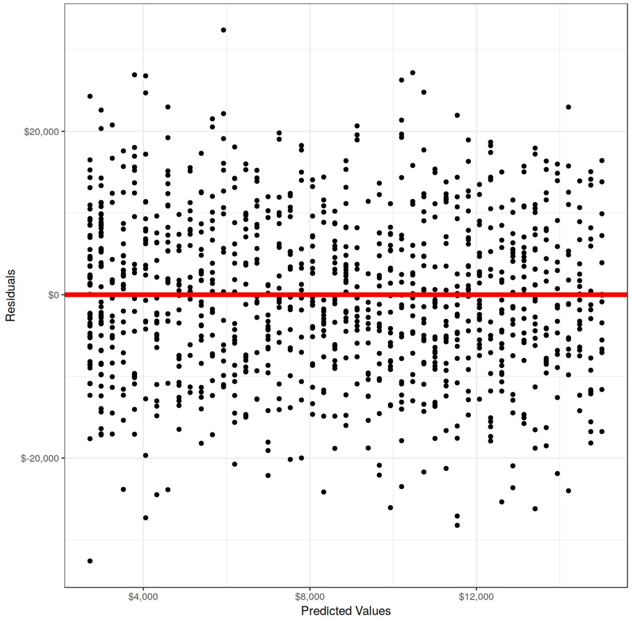
E is for Equal Variances



E is for Equal Variance

Yuck! We want to see **absolute randomness** in our residual plots. That is, no pattern whatsoever. We can clearly see a parabolic pattern in our residual plot.

Here's an example of an ideal residual plot.



What to do if our LINE assumptions are violated?!

A common scenario in linear model is when you have:

- A slightly **curvilinear** relationship between *x* and *y*
- Very right-skew residuals
- Residuals that tend to spread out from right to left (a “fan shape”)

One quick fix that should improve all of these issues is doing **log regression**.
That is, simply take the natural log of *y* before modeling!

Let’s see if our model passes!

Categorical Features

Categorical Features

How do we work with categorical variables in our model? In the first half of this lesson, you saw that we can simply use **binary categorical features** as 0/1 variables.

But what if our variable has more than two **levels**?

First some more notation!

Notation: Design Matrix

Mathematically speaking, every time we fit a model, we need a data matrix, sometimes called a **design matrix**:

$$X = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1p} \\ 1 & x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix}$$

Notation: Design Matrix

Mathematically speaking, every time we fit a model, we need a data matrix, sometimes called a **design matrix**:

$$X = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1p} \\ \boxed{1 & x_{21} & x_{22} & \cdots & x_{2p}} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix}$$

Each **row** is an **observation.**

Notation: Design Matrix

Mathematically speaking, every time we fit a model, we need a data matrix, sometimes called a **design matrix**:

$$X = \begin{bmatrix} 1 & x_{11} & \boxed{x_{12}} & \cdots & x_{1p} \\ 1 & x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix}$$

Each **column** is a variable.

Notation: Design Matrix

Mathematically speaking, every time we fit a model, we need a data matrix, sometimes called a **design matrix**:

$$X = \begin{bmatrix} \boxed{\begin{matrix} 1 \\ 1 \\ \vdots \\ 1 \end{matrix}} & \begin{matrix} x_{11} \\ x_{21} \\ \vdots \\ x_{n1} \end{matrix} & \begin{matrix} x_{12} \\ x_{22} \\ \vdots \\ x_{n2} \end{matrix} & \begin{matrix} \cdots \\ \cdots \\ \vdots \\ \cdots \end{matrix} & \begin{matrix} x_{1p} \\ x_{2p} \\ \vdots \\ x_{np} \end{matrix} \end{bmatrix}$$

The first column is all 1s and corresponds to the **intercept**. (sklearn handles this automatically)

Dummy Columns

For a categorical variable with *k* levels, we need to make one **dummy column** for each:

Season
Summer
Spring
Spring
Fall
Fall
Summer
Winter

$$X = \begin{array}{ccccc} & \text{W} & \text{Sp} & \text{Su} & \text{F} \end{array}$$

$$X = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 \end{bmatrix}$$

Dummy Columns

But wait! This is actually not ok - the intercept term is simply the sum of all of these four columns! In linear algebra terms, this is called being **rank-deficient**, and will make our model impossible to fit.

$$X = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 \end{bmatrix}$$

Dummy Columns

So, we next have to **drop any column**. The default in pandas is to drop the first. This means our first column (in this case, Winter) corresponds to the **baseline category**. When interpreting, everything is **relative to this column.**

$$X = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 \end{bmatrix}$$

Dummy Columns

So, we next have to **drop any column**. The default in pandas is to drop the first. This means our first column (in this case, Winter) corresponds to the **baseline category**. When interpreting, everything is **relative to this column.**

$$X = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

Let’s see it for ourselves!