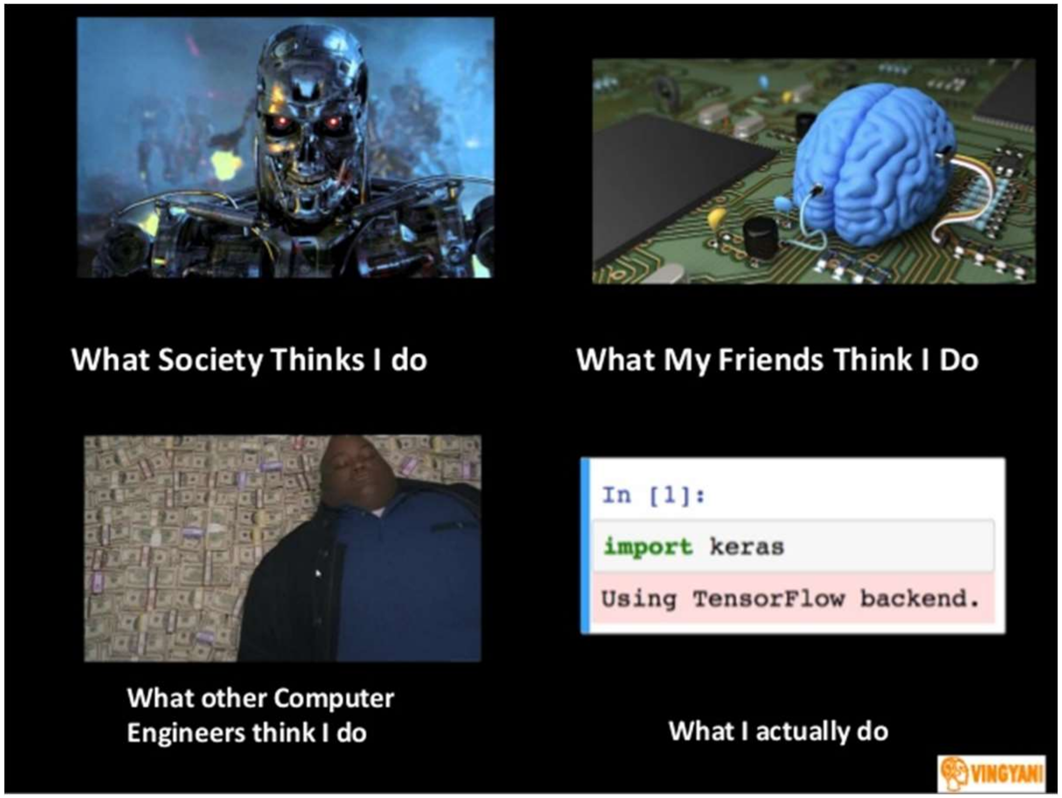
DATA SCIENCE 102:
INTRODUCTION TO MACHINE LEARNING

AGENDA

- What is Machine Learning?
- Types of Machine Learning
    - Applications of Machine Learning
- General Machine Learning Steps using Sci-Kit Learn
    - Fundamentals
        - Standard steps
        - Reading the library
    - Examples
        - Regression

WHAT IS MACHINE LEARNING

WHAT IS MACHINE LEARNING


What Society Thinks I do
What My Friends Think I Do
What other Computer Engineers think I do
What I actually do
VINGYANI

```
In [1]:
import keras
Using TensorFlow backend.
```

WHAT IS MACHINE LEARNING

A study of *algorithms and statistical models*

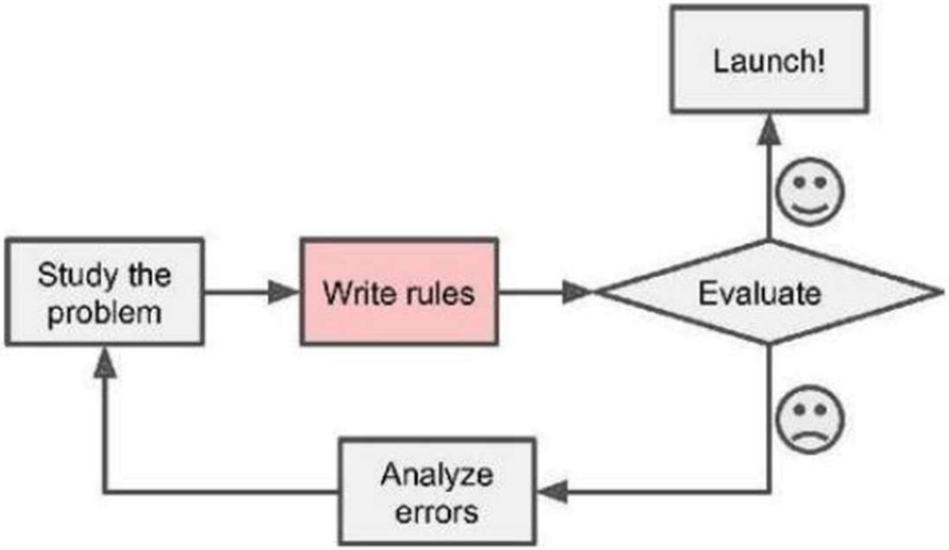
that computers use to perform a specific task effectively

without being explicitly programmed

EXAMPLE - SPAM EMAIL DETECTION

Without Machine Learning

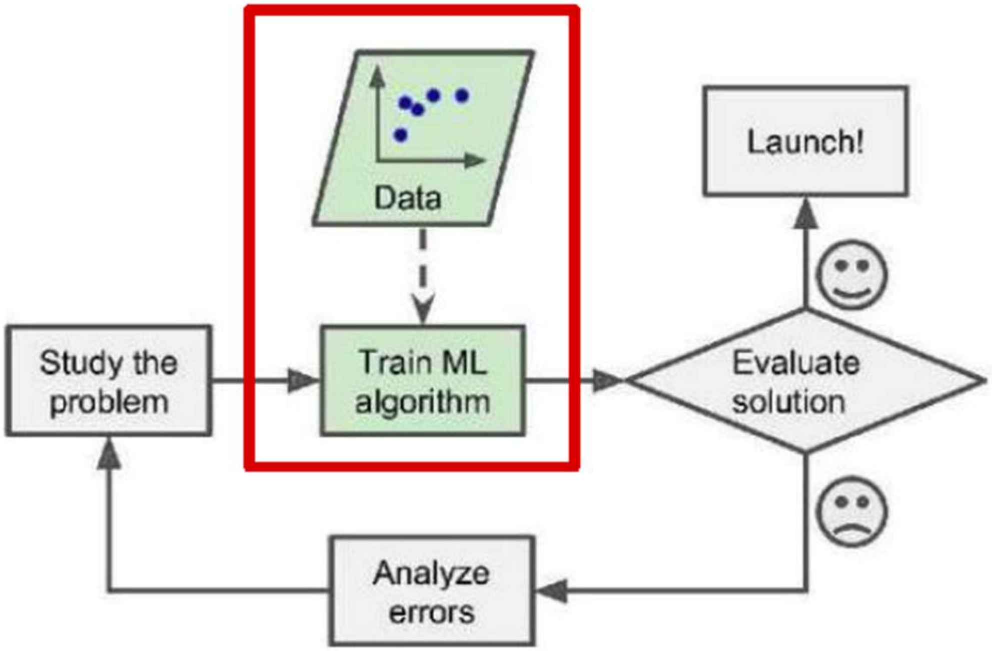
- You will write explicit rules to filter out emails containing words like:
    - *"4U", "Loan", "Prince", "Money Transfer", "Free"*
- Classify any email that contain these text as spam email



EXAMPLE - SPAM EMAIL DETECTION

With Machine Learning

- You train a model on some train data (spam & non-spam emails) with an algorithm that **infers** characteristics and patterns of spam emails
- The trained model can then apply learnt rules to detect signals of spam in an incoming email



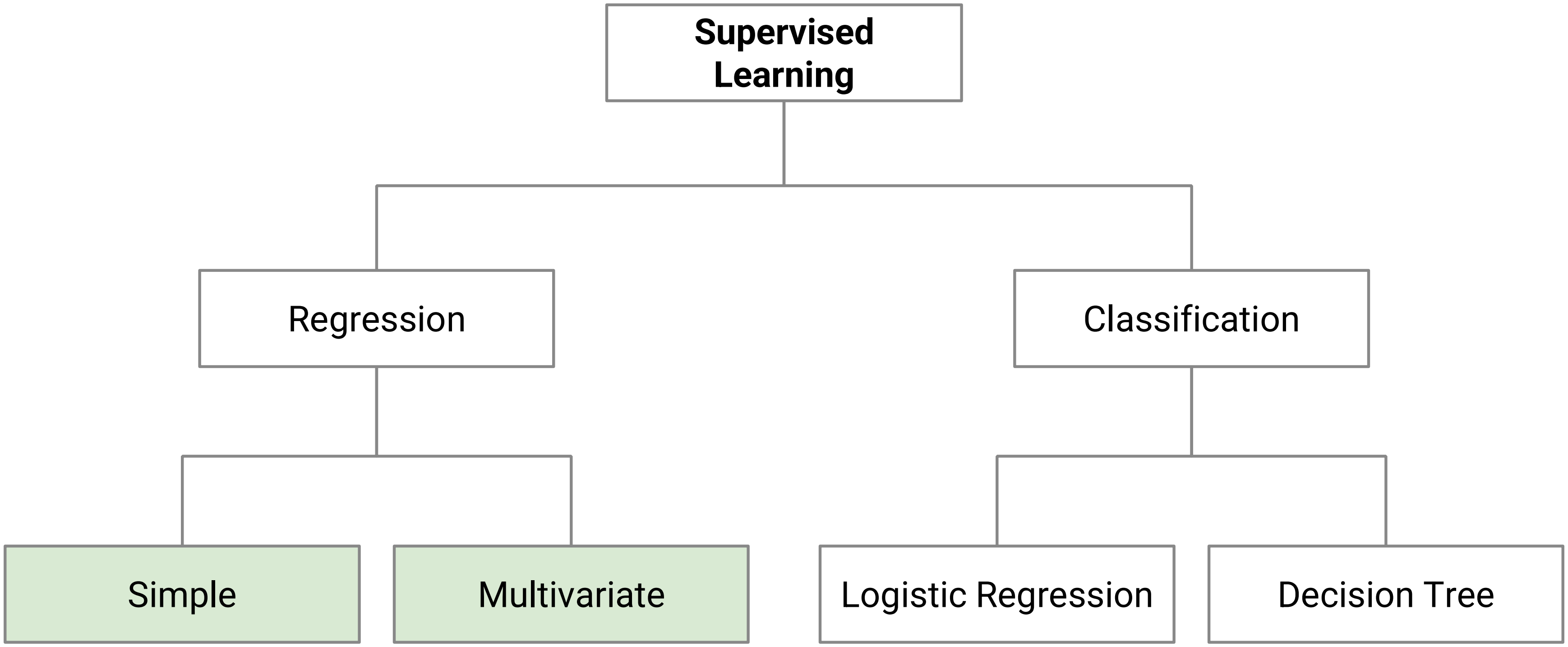
TYPES OF MACHINE LEARNING

- Types of Machine Learning
- Supervised Applications
- Unsupervised Applications

TYPES OF MACHINE LEARNING

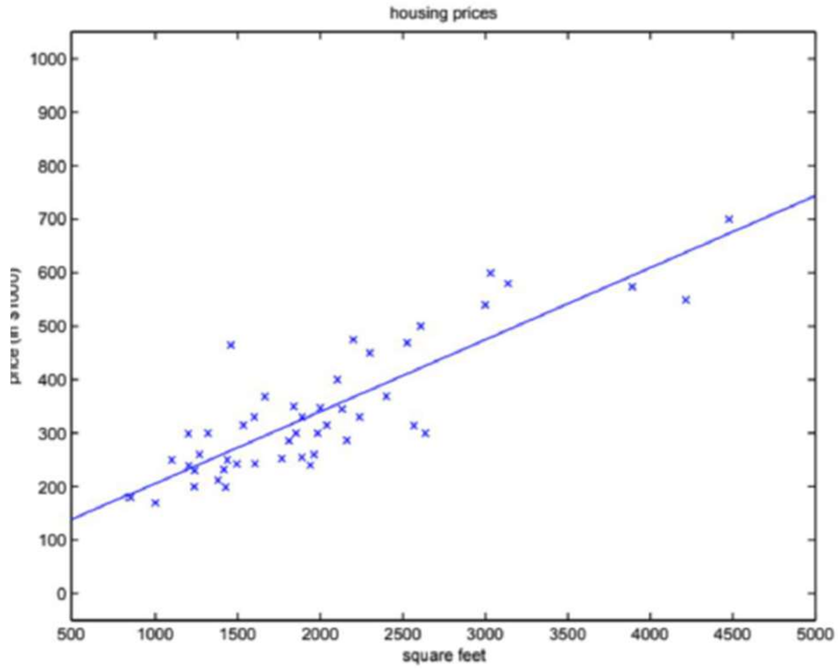
- Supervised Learning
  - Based on **labelled data,** makes **predictions** on a test set
- Unsupervised Learning
  - Based on **unlabelled data**, algorithm **discovers patterns** within the dataset

SUPERVISED LEARNING



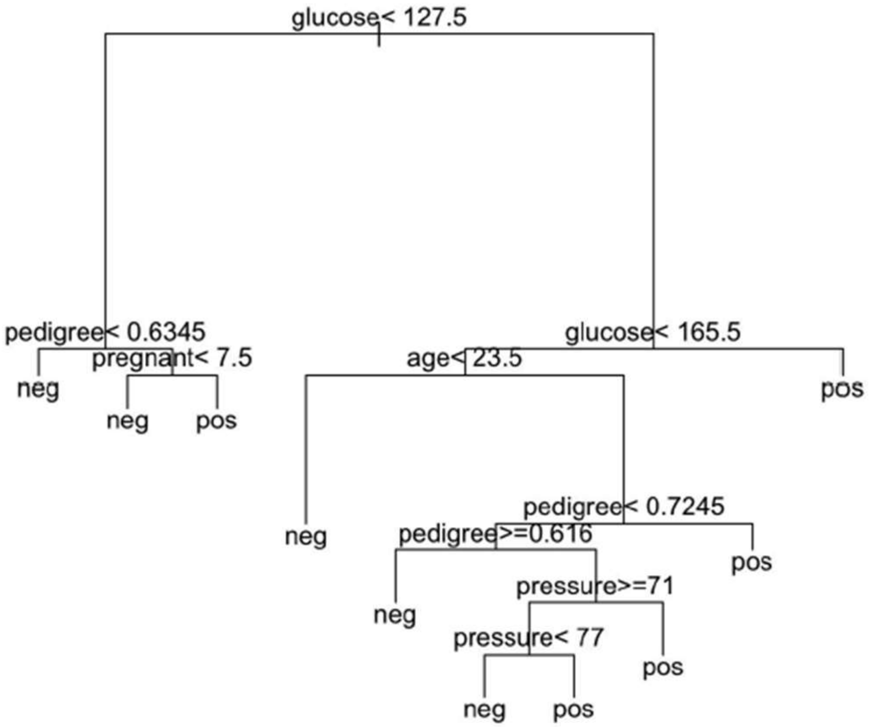
SUPERVISED APPLICATIONS

- Regression
  - Predict Housing Price (Target Variable) from Housing Floor Area (Input Feature)



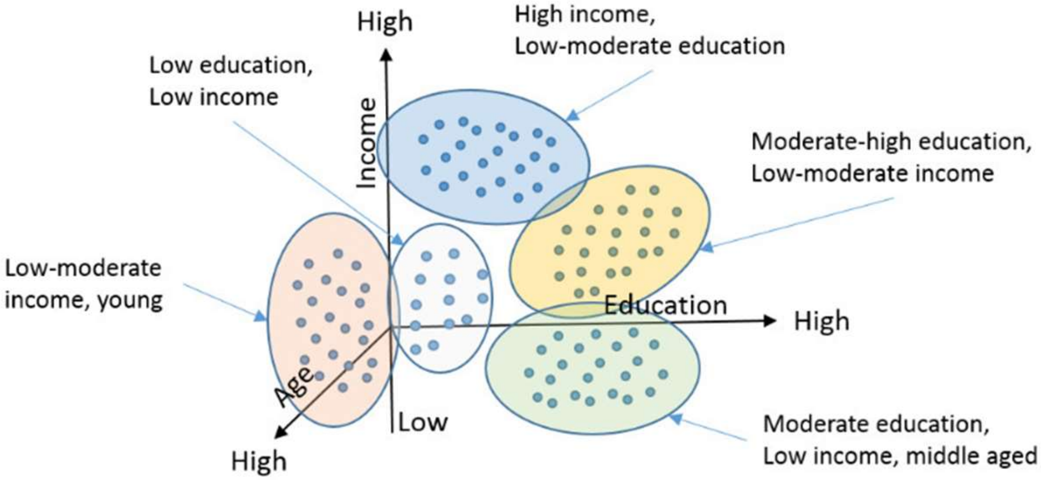
SUPERVISED APPLICATIONS

- Classification
  - Predict if a patient has diabetes (Yes/No)



UNSUPERVISED APPLICATIONS

- Clustering
    - Given a set of unlabelled data points, identify cluster each point belongs to



GENERAL MACHINE LEARNING STEPS USING SKLEARN

- Fundamentals
  - Standard Steps
  - Reading the library
- Examples
  - Regression

FUNDAMENTALS - STANDARD STEPS

When using any machine learning models with scikit learn, the following steps are usually applied in order:

Step 1: Choose a class of machine learning model from the library

Step 2: Choose the model’s hyperparameters by instantiating with desired values (tuning)

Step 3: Arrange data into features and target

Step 4: Fit model to your data by using the `fit()` method of the model

Step 5: Apply the model to new data:

- For supervised learning, using the `predict()` method
- For unsupervised learning, using the `predict()` or `transform()` method

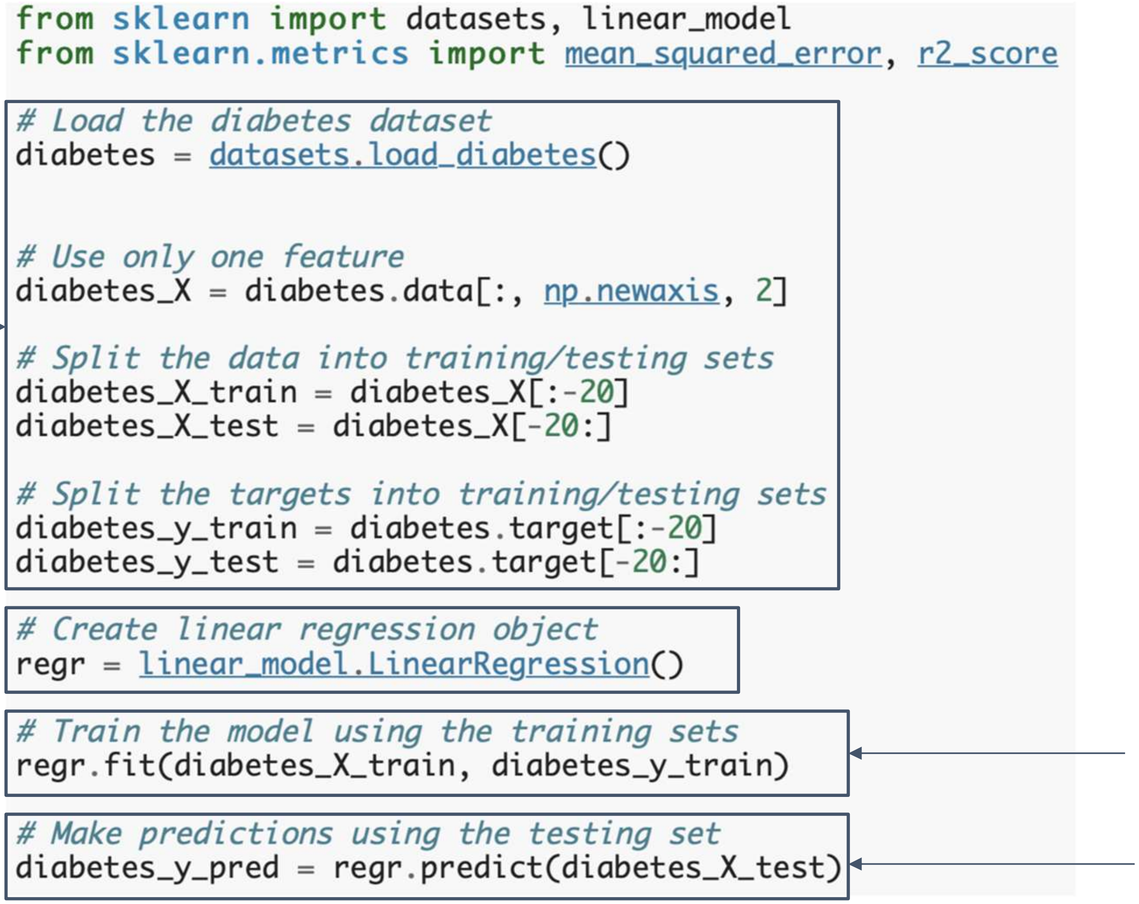
Python Data Science Handbook: Essential Tools for Working with Data by Jake VanderPlas (2016)

FUNDAMENTALS - READING THE LIBRARY

- Determine what model is used, then delve into details of that model in the library, and the other required parts of the library
- Here are some of the common classes you would use:
  - `sklearn.`<a name of a model> (i.e `sklearn.linear_model)`
    - Access to all functionalities of that model
  - `sklearn.metrics`
    - Functionalities of assessing the performance of your models
  - `sklearn.model_selection`
    - Performs cross validation and tuning of parameters
  - `sklearn.feature_selection`
    - Reduce dimension of dataset to boost performance

Python Data Science Handbook: Essential Tools for Working with Data by Jake VanderPlas (2016)

EXAMPLE - REGRESSION



```
from sklearn import datasets, linear_model
from sklearn.metrics import mean_squared_error, r2_score
```

Step 3

```
# Load the diabetes dataset
diabetes = datasets.load_diabetes()


# Use only one feature
diabetes_X = diabetes.data[:, np.newaxis, 2]

# Split the data into training/testing sets
diabetes_X_train = diabetes_X[:-20]
diabetes_X_test = diabetes_X[-20:]

# Split the targets into training/testing sets
diabetes_y_train = diabetes.target[:-20]
diabetes_y_test = diabetes.target[-20:]
```

Step 1 & 2

```
# Create linear regression object
regr = linear_model.LinearRegression()
```

Step 4

```
# Train the model using the training sets
regr.fit(diabetes_X_train, diabetes_y_train)
```

Step 5

```
# Make predictions using the testing set
diabetes_y_pred = regr.predict(diabetes_X_test)
```

DATA SCIENCE 102: CLASSIFICATION

AGENDA

- What is Classification
- Logistic Regression
- Confusion Matrix

LEARNING OBJECTIVES

- Build an intuition for Logistic Regression
- Able to interpret results and performance from Logistic Regression
- Apply Confusion Matrix to evaluate classification model

LOGISTIC REGRESSION

- Intuition
- Confusion Matrix

Logistic Regression

- Logistic Regression is one of the basic and popular algorithms to solve a binary classification problems
- For each input, logistic regression outputs a probability that this input belongs to the 2 classes
  - Set a probability threshold boundary and that determines which class the input belongs to
- Binary classification problems (2 classes):
  - Emails (Spam / Not Spam)
  - Transactions (Fraudulent / Not Fraudulent)
  - Loan Default (Yes / No)

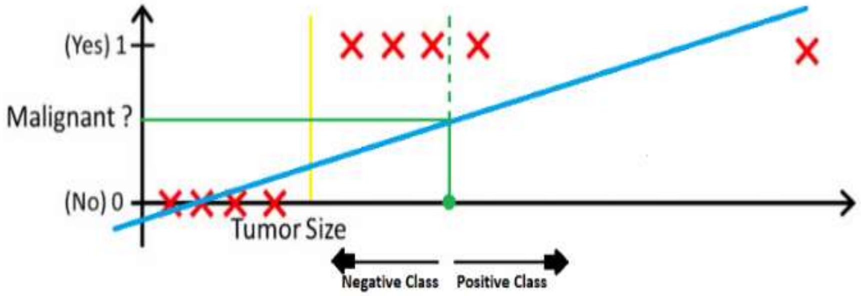
Why Not Use Linear Regression for Classification?

- Linear Regression is used to solve regression problems with continuous values
- Logistic Regression is used to solve classification problems with discrete categories
  - Binary classification (Classes 0 and 1)

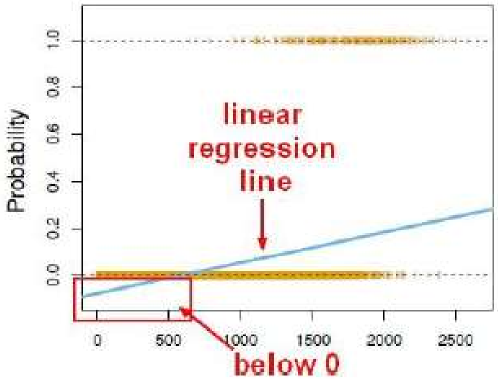
Why Not Use Linear Regression for Classification?

- Let’s say we want to predict the malignancy of a tumour based on its size
- We then plot a simple linear regression line and set the threshold as 0.5
  - Negative class – Tumour size on the left size
  - Positive class – Tumour size on the right size

Linear regression line is not a good fit

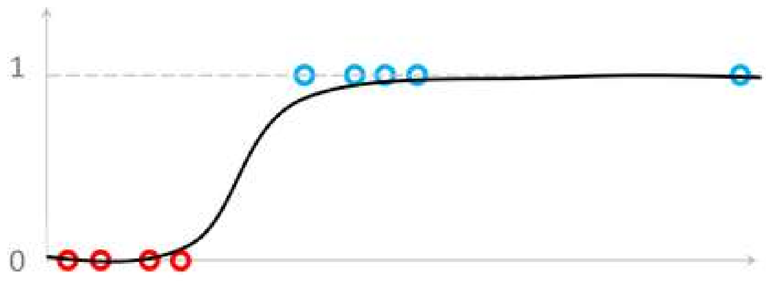


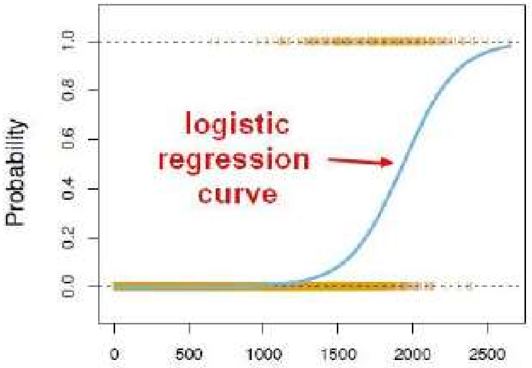
Another example: Negative probability



Why Not Use Linear Regression for Classification?

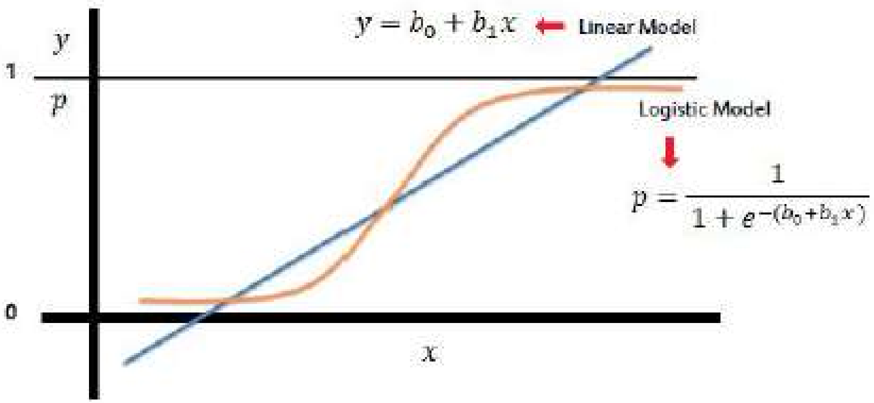
- Solution – Transform linear regression to a logistic regression curve
- Logistic regression is a Sigmoid function
  - Sigmoid function takes in any real value
  - Output probability between 0 and 1





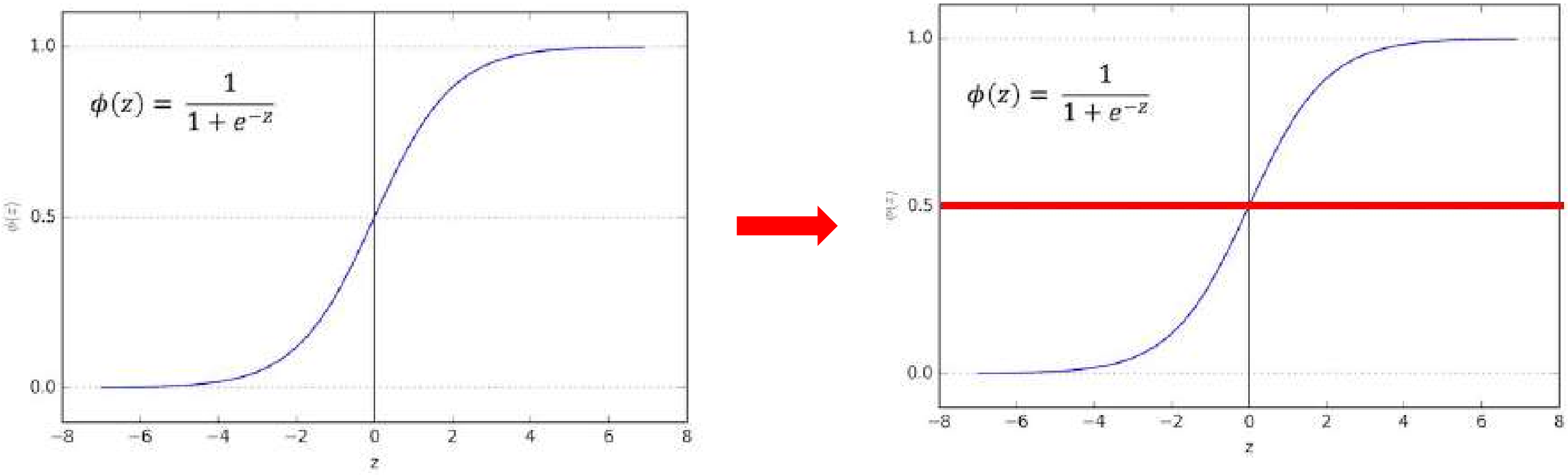
Sigmoid Function (Logistic Function)

- Take linear regression and put in into the Sigmoid function
- Sigmoid function outputs probability between 0 and 1



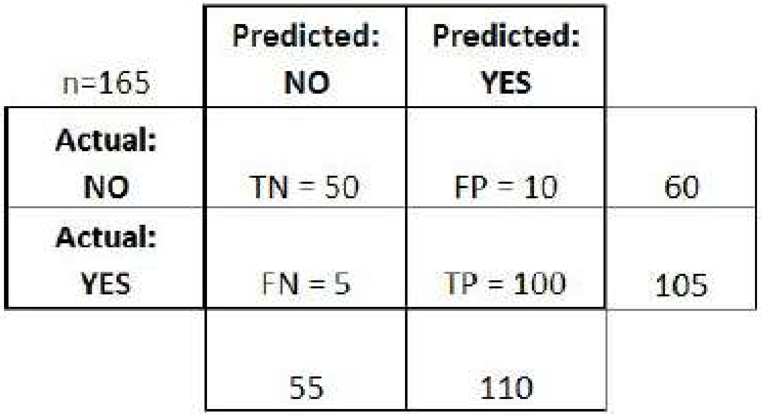
Sigmoid Function (Logistic Function)

- Sigmoid function outputs probability between 0 and 1
- Default probability threshold is set as 0.5 typically
    - Class 0 – Below 0.5
    - Class 1 – Above 0.5



Model Evaluation – Confusion Matrix

- To evaluate logistic regression model, confusion matrix is typically used for model evaluation
- Imagine now a doctor wants to use a logistic regression model to predict if patients have (or don't have) disease



n=165	Predicted: NO	Predicted: YES	
Actual: NO	TN = 50	FP = 10	60
Actual: YES	FN = 5	TP = 100	105
	55	110	

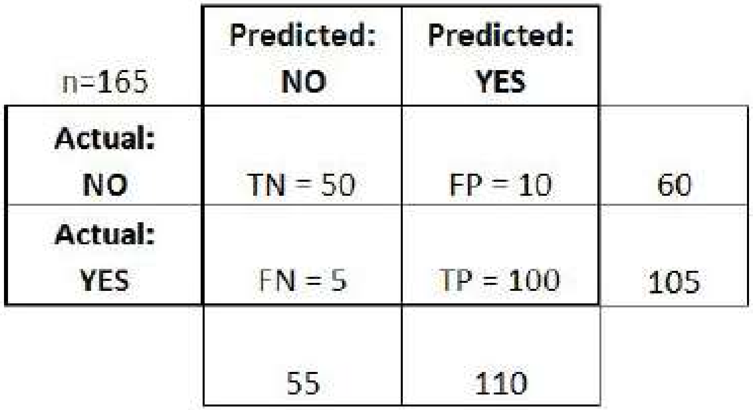
- True Positives (TP)
- True Negative (TN)
- False Positives (FP)
- False Negatives (FN)

Metrics for Model Evaluation is Classification

- Accuracy
  ➢ $\frac{TP+}{Total}$

- Precision
  ➢ $\frac{TP}{TP+}$

- Recall
  ➢ $\frac{TP}{TP+FN}$



n=165	Predicted: NO	Predicted: YES	
Actual: NO	TN = 50	FP = 10	60
Actual: YES	FN = 5	TP = 100	105
	55	110	

Precision: 100/110 → 90.9%

Recall: 100/105 → 95.2%

Example - Disease Detection

- We want to focus on Recall as the main metric
- Reduce FN and increases Recall
- Because if an infected patient goes through the test undetected, the risk is very high if the disease is contagious

DATA SCIENCE 102: REGRESSION

AGENDA

- What Is Regression
  - Applications of Regression
- Simple Linear Regression
  - Intuition
  - Interpretation
  - Ordinary Least Squares
  - Measure of Fit
  - Model Validation - Train Test Split
  - Performance Measures
  - Scikit Learn Example and Practice
- Multivariate Linear Regression
  - Interpretation
  - Feature Selection
  - Scikit Learn Example and Practice

LEARNING OBJECTIVES

- Build an intuition for Linear Regression
- Able to interpret results and performance from Linear Regression
- Discern difference between Single and Multivariate Linear Regression
- Importance of Feature Selection in Multivariate Linear Regression

WHAT IS REGRESSION

- Applications of regression

WHAT IS REGRESSION

- Regression Analysis is a model to develop an equation that shows how variables are related
- In regression terminology, the variable being predicted is the **dependent variable** and the variables being used to predict the dependent variable are called **independent variables** (predictor variables)
- Regression can be used in the following cases:
  - Predicting continuous labels
  - Classification (logistic regression)

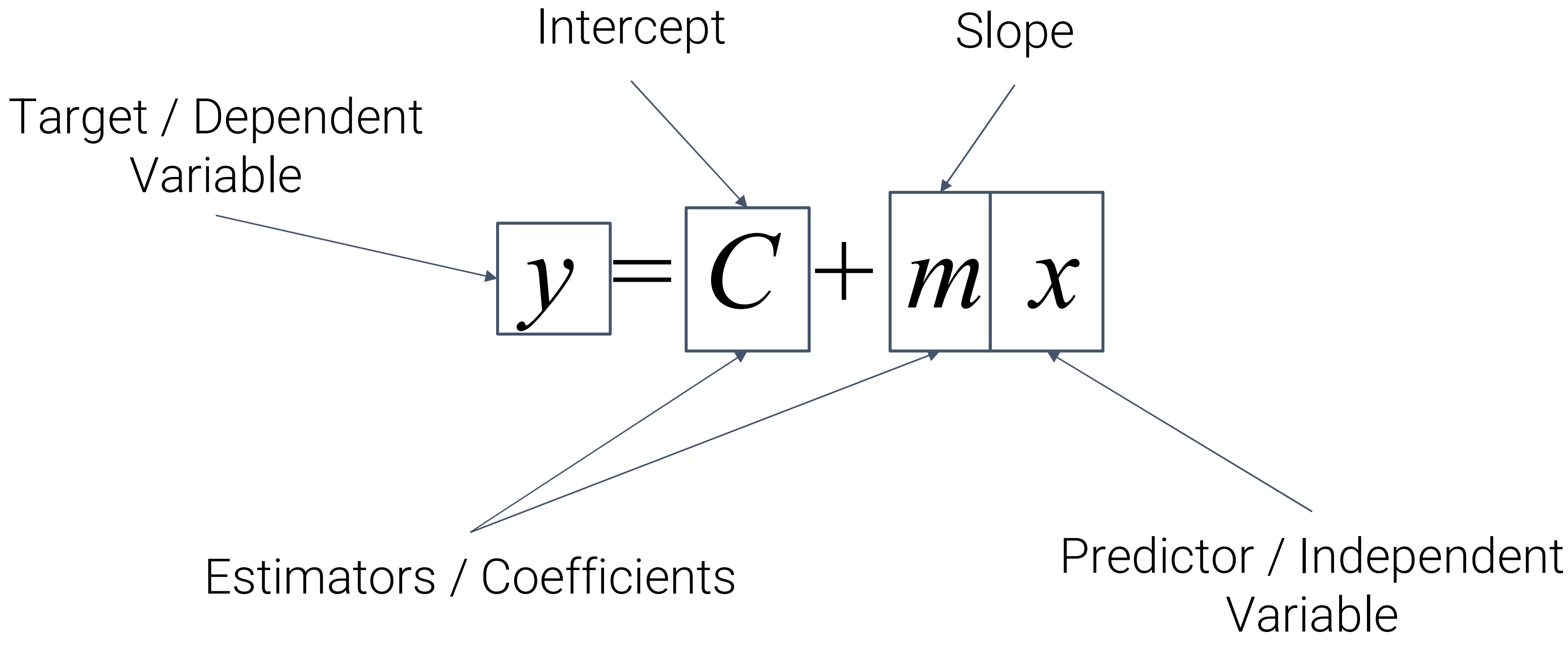
An Introduction to Statistical Learning (with applications in R) by Gareth James, Daniela Witten, Trevor Hastie and Robert Tibshirani (2013)

SIMPLE LINEAR REGRESSION

- Intuition
- Single vs Double variable
- Interpretation
- Ordinary Least Squares
- R Squared and Adjusted R Squared
- Performance Measures
- Train-Test-Split

INTUITION - THE REGRESSION EQUATION

Remember the y = mx + c you learnt in secondary school? That is essentially regression!



Intercept

Slope

Target / Dependent Variable

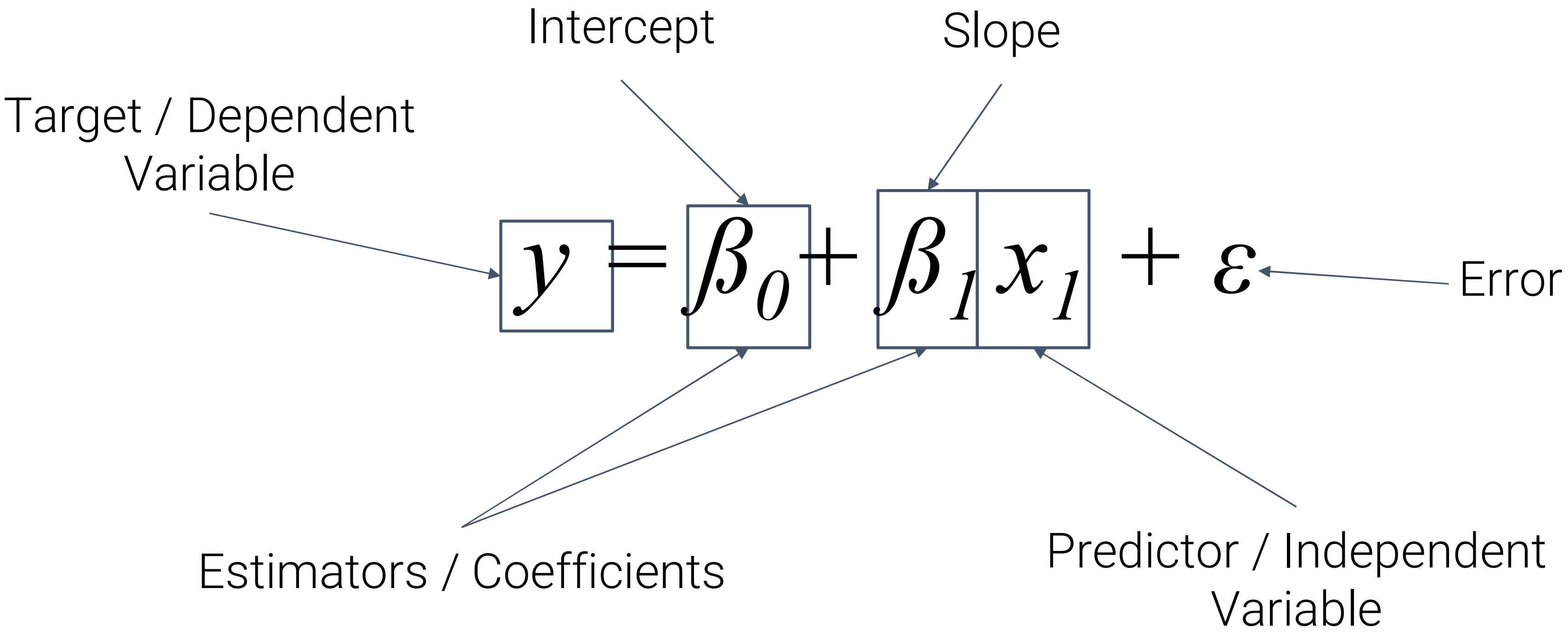
$$\boxed{y} = \boxed{C} + \boxed{m}\boxed{x}$$

Estimators / Coefficients

Predictor / Independent Variable

INTUITION - THE REGRESSION EQUATION

This is the adult, and machine-learning way of representing regression:



$$\boxed{y} = \boxed{\beta_0} + \boxed{\beta_1}\boxed{x_1} + \varepsilon$$

Intercept

Slope

Target / Dependent Variable

Error

Estimators / Coefficients

Predictor / Independent Variable

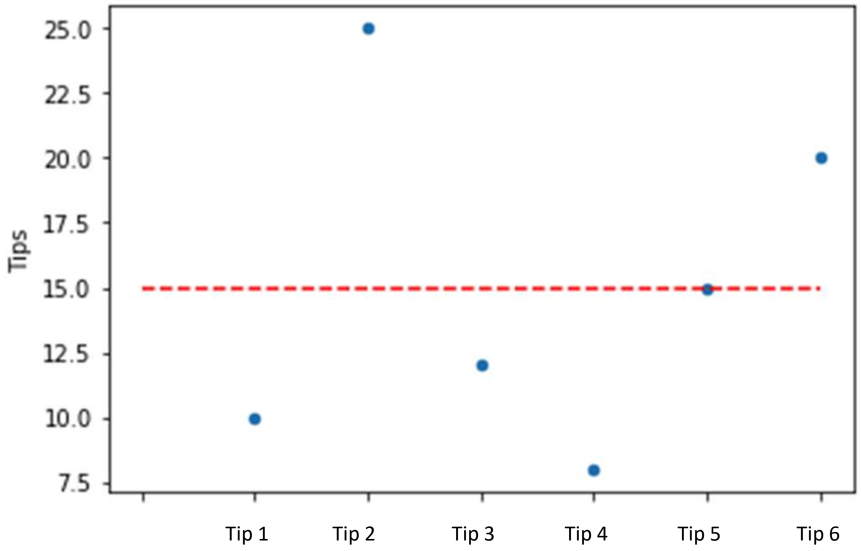
STUDY OF SINGLE VARIABLE - NO VALUE ON ITS OWN

- Predict future tips given the following dataset:
    - To “predict” future tips, use <u>average</u>

$$Tip = 0\ (No\ Predictor) + 15$$

$$Tip = 15$$

Tip #	Amount ($)
Tip 1	10
Tip 2	25
Tip 3	12
Tip 4	8
Tip 5	15
Tip 6	20

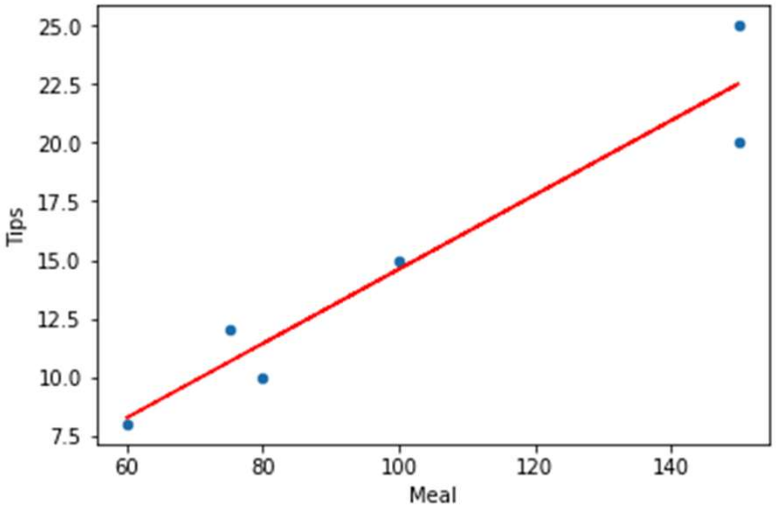


STUDY OF TWO VARIABLES - SIMPLE LINEAR REGRESSION

- Predict future tips given the following dataset
  - To “predict” future tips using linear regression

Tip #	Amount ($)	Meals ($)
Tip 1	10	80
Tip 2	25	150
Tip 3	12	75
Tip 4	8	60
Tip 5	15	100
Tip 6	20	150

$$Tip = -1.27 + 0.158\ (Meal)$$



INTERPRETATION

- After fitting the model, you can extract the coefficients (estimators) of the model by using `<variablenameofmodel>.coeff_`. To get the intercept, use, `<variablenameofmodel>.intercept_`
- Let's say given the following regression equation:

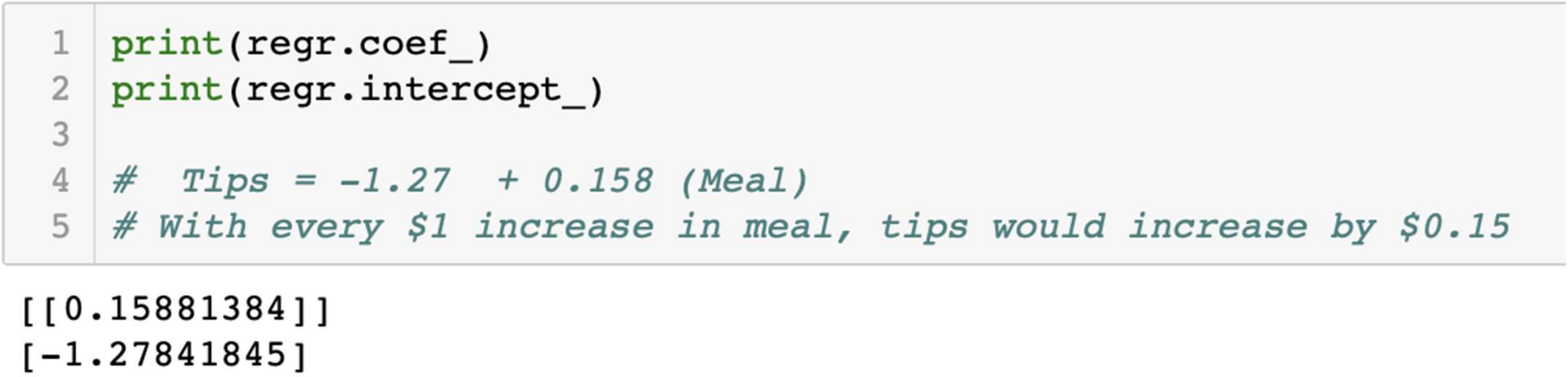
$$Tip = -1.27 + 0.158\ (Meal)$$

- We can interpret it as, given ***1 dollar increase*** in the cost of a meal, there will be an **increase** of tips by ***0.158 dollars***

INTERPRETATION - CODED EXAMPLE

- Let’s say given the following regression equation:

$$Tip = -1.27 + 0.158\ (Meal)$$



```python
print(regr.coef_)
print(regr.intercept_)

#  Tips = -1.27  + 0.158 (Meal)
# With every $1 increase in meal, tips would increase by $0.15
```

```
[[0.15881384]]
[-1.27841845]
```

- So what happens behind `.fit()` == OLS

HOW LINEAR REGRESSION EQN IS CONSTRUCTED - OLS

- Now we understand Linear regression is about creating an equation that shows how variables are related. In code form your “`.fit()`” will create this equation.

- This equation is useful in helping us (1) interpret relationship, and (2) predict output based on unseen input data

Means we can sub in any X-Value (meal) to predict tips

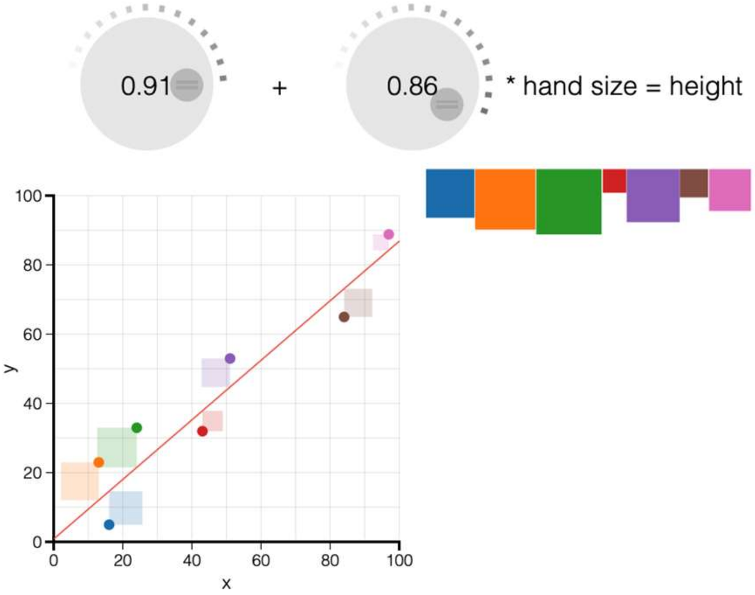
$$Tip = -1.27 + 0.158\,(Meal)$$

- Then the question is, how do we derive the y-intercept (β_0) and gradient (β_1)? Answer is: Ordinary Least Squares (OLS).

ORDINARY LEAST SQUARES - VISUALISATION OF PROCESS

- Ordinary Least Squares (Least Squares Method) is aimed at **minimizing** the sum of squared residuals (SSR), i.e keep the errors (ε) as low as possible

Annotation on betas



Click here to view a visualisation of OLS in action: http://setosa.io/ev/ordinary-least-squares-regression/

ORDINARY LEAST SQUARES - KEY CONCEPT

- Intuitively, OLS is fitting a line through the sample points such that the sum of squared errors (SSR) is as small as possible, hence the term least squares
- The OLS regression line always goes through the mean of the sample (y)
- The residual, e, is an estimate of the error term, ε, and is the difference between the fitted line (sample regression function) and the sample point
- The sum of the OLS residuals is zero

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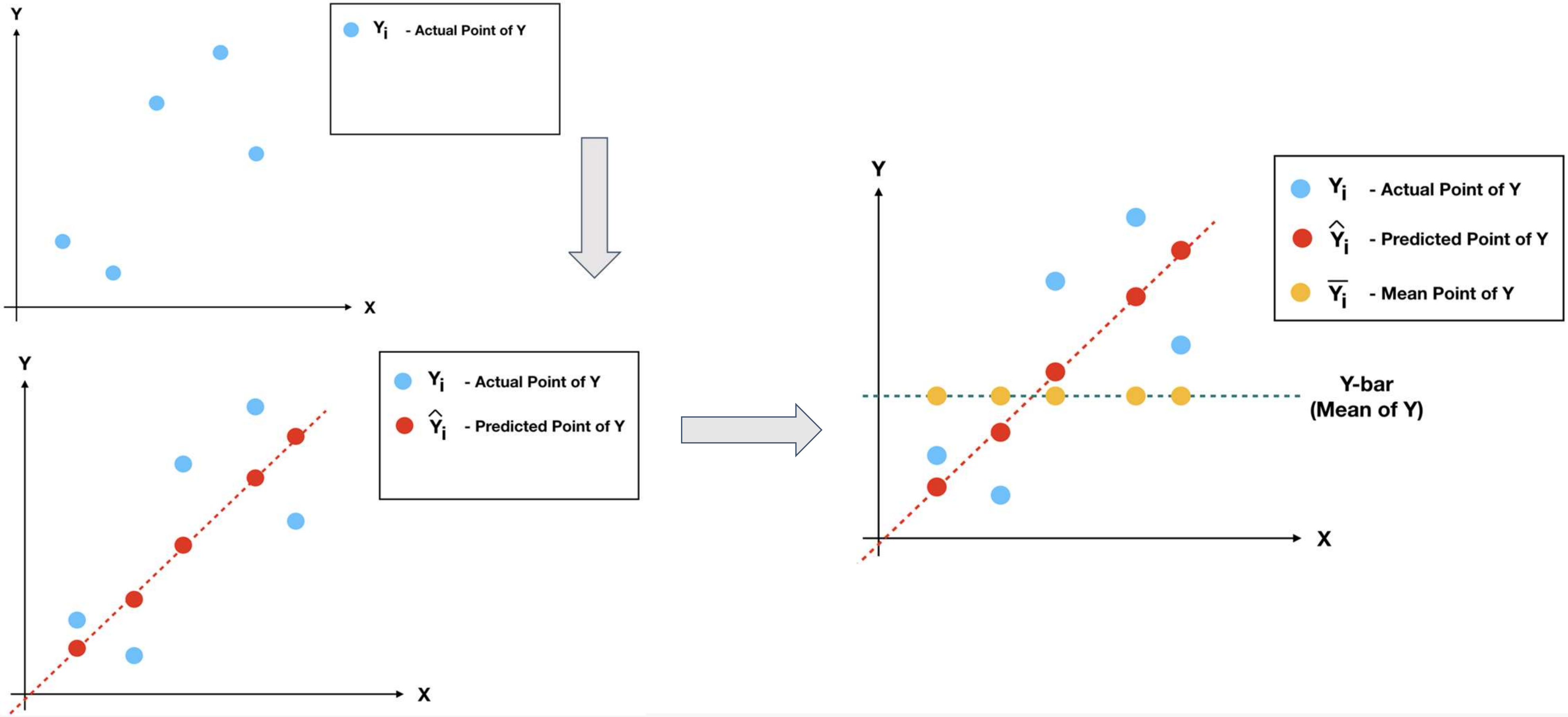
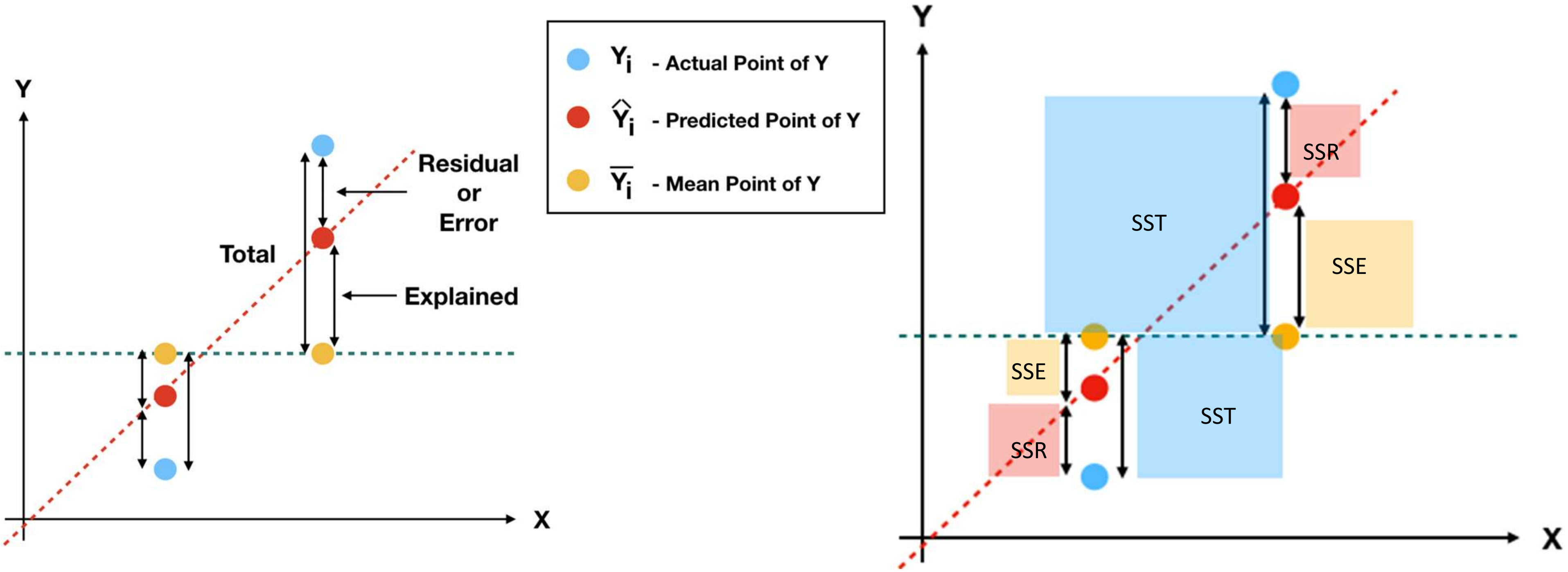
ORDINARY LEAST SQUARES - BUILDING BLOCKS EXPLAINED


Y
X
● Y_i - Actual Point of Y
Y
X
● Y_i - Actual Point of Y
● $\hat{Y}_i$ - Predicted Point of Y
Y
X
● Y_i - Actual Point of Y
● $\hat{Y}_i$ - Predicted Point of Y
● $\overline{Y}_i$ - Mean Point of Y
Y-bar
(Mean of Y)

ORDINARY LEAST SQUARES - BUILDING BLOCKS EXPLAINED


Y
X
Residual
or
Error
Total
Explained
● Y_i - Actual Point of Y
● $\hat{Y}_i$ - Predicted Point of Y
● $\overline{Y}_i$ - Mean Point of Y
Y
X
SST
SSR
SSE
SSE
SSR
SST

MEASURING FIT BETWEEN VALUES AND PREDICTED LINE - R^2

- A measure of how well the sample values fit the predicted regression line is **goodness of fit**

- R (also known as Pearson's R) is the sample correlation coefficient; ranges from -1 to 1; >0 = positive correlation, <0 = negative correlation

- R^2 (R-squared) is known as the coefficient of determination; range from 0 to 1

$$\frac{\text{SSE}}{\text{SSR} + \text{SSE}} = \frac{\text{SSE}}{\text{SST}} = \text{R}^2$$

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CALCULATION OF R^2

- Each observation (y_i) on the linear regression as made up of an explained part ($\hat{y}_i$) and an unexplained part (e_i):

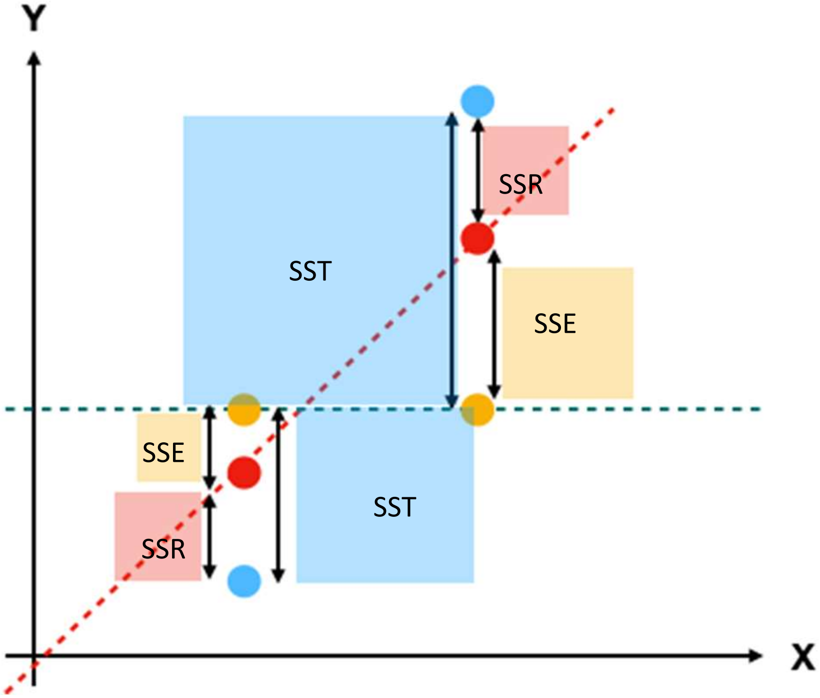
$$y_i = \hat{y}_i + e_i$$

Total sum of squares (SST) = $\sum (y_i - \bar{y}_i)^2$

Explained sum of squares (SSE) = $\sum (\hat{y}_i - \bar{y}_i)^2$

Residual sum of squares (SSR) = $\sum (y_i - \hat{y}_i)^2$

SST = SSE + SSR



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AN ALTERNATIVE OF MEASURING FIT - ADJUSTED R^2

- Adjusted R^2 modifies the original R^2 by incorporating the sample size and the number of explanatory variables in the model

- Can be found in `sklearn.metrics.r2_score` or `LinearRegression.score()`

$$R^2_{adj} = 1 - \left[\frac{(1 - R^2)(n - 1)}{n - k - 1}\right]$$

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R-SQUARED VS. ADJUSTED R-SQUARED

- Both R^2 and the adjusted R^2 (Adj-R^2) gives an idea of how many data points fall within the line of the regression equation
- The main difference is:
  - R^2 tells you every single variable explains the *variation* in the depend variable (y)
  - Adj-R^2 tells you the **percentage of variation** explained only by the independent variables that actually affect the dependent variable

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R-SQUARED VS. ADJUSTED R-SQUARED

- Formula for Adj-R^2 :

$$\text{Adjusted } R^2 \ (R^2_{adj}) = 1 - \left[\frac{(1-R^2)(n-1)}{n-k-1}\right]$$

  - n is the number of points in your data sample
  - k is the number of independent variables (predictors) excluding constants

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R-SQUARED VS. ADJUSTED R-SQUARED

- The adjusted R^2 (Adj-R^2) penalizes for adding more independent variables that do not fit the model.
- As R^2 increases with every predictor added to a model, it can appear to be a **better fit** with more terms added to the model, but this can be misleading
- Adding too many variables and polynomials may run into the trouble of **overfitting**, thus a misleading high R^2 value can lead to misleading projections
- In short, adjusted R^2 is preferred over R^2 in multivariate linear regression.

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MEASURING FIT VS MEASURING PERFORMANCE

- Measuring Fit - Quantified via R^2 / Adjusted $R^{2,}$ is a measure of how well the seen / known values fit the predicted regression line

- Measuring Performance - is a measure of how well the predicted regression line can predict unseen/unknown values (Quantified RMSE or MAE)

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PERFORMANCE MEASURES - LINEAR REGRESSION

- For linear regression there are several measures to assess the performance of the model:
  - **MAE** (`sklearn.metrics.mean_absolute_error`)
    - Mean Absolute Error
    - Whether predictions are, on average, over/under predicting the outcome
  - **RMSE** - (`sklearn.metrics.mean_squared_error` then use ** 0.5)
    - Root Mean Squared Error
    - Differences between predicted vs observed/actual values
    - Similar to standard error
    - Lower is better
    - 0 means perfect fit to data *(not the best, could be overfitting)*
- Can be found in the `sklearn.metrics` part of `sklearn`

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PERFORMANCE MEASURES - LINEAR REGRESSION

- How are RMSE and MAE derived?
- Answer: Via Model-Validation (Train-Test-Split)

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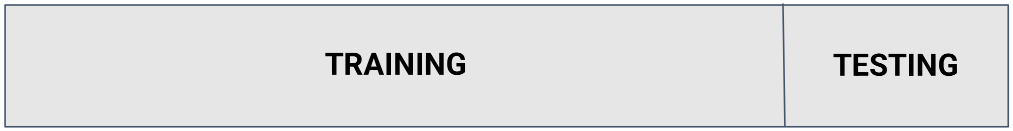
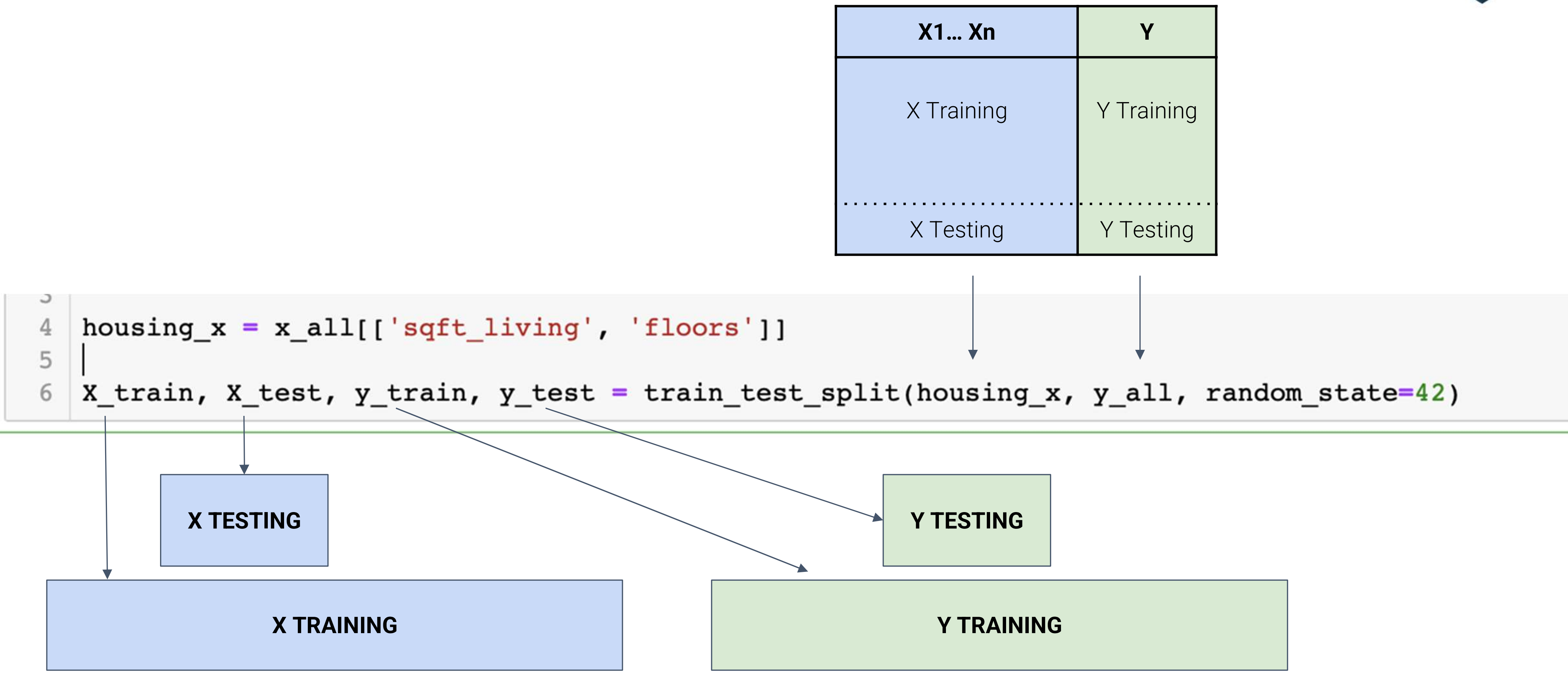
MODEL VALIDATION - TRAIN TEST SPLIT

- *After selecting and fitting* a machine learning model, like Linear Regression for example, we need to ensure that we validate our model **by comparing some of the training data and comparing the prediction against its known value**
- One of the ways to validate the model would be to use *Holdout Sets*, basically splitting the given datasets for training and testing
- We can use Scikit learn's `train_test_split` to split our datasets
- By default, it is an 80-20 split (80% training, 20% testing)



An Introduction to Statistical Learning (with applications in R) by Gareth James, Daniela Witten, Trevor Hastie and Robert Tibshirani (2013)

MODEL VALIDATION - TRAIN TEST SPLIT - CODED EXAMPLE



X1… Xn	Y
X Training	Y Training
X Testing	Y Testing

```
housing_x = x_all[['sqft_living', 'floors']]

X_train, X_test, y_train, y_test = train_test_split(housing_x, y_all, random_state=42)
```

SCIKIT LEARN EXAMPLE AND PRACTICE*

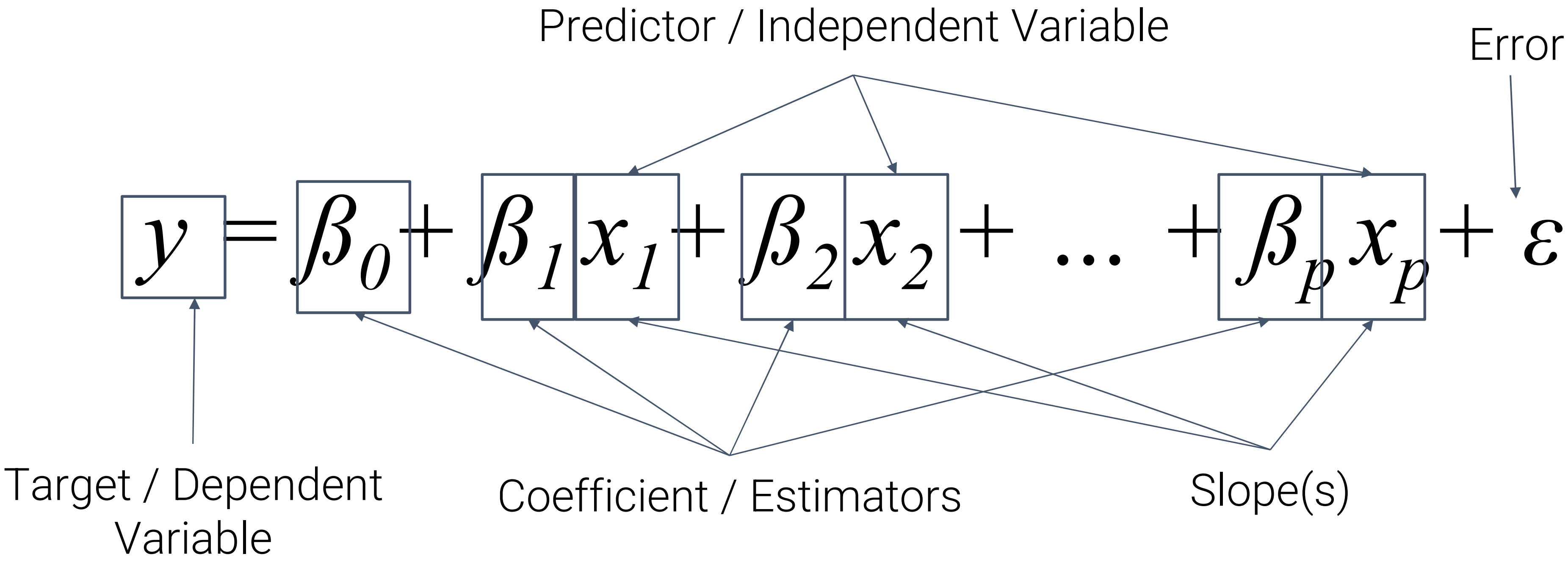
- Try out the practice in your in-class notebook 5
- Remember the 5 common steps for using SKLearn

MULTIVARIATE LINEAR REGRESSION

- Intuition and Interpretation
- R-Squared vs. Adjusted R-Squared
- Feature Selection

INTUITION

- Multivariate linear regression incorporates **more than one predictors** into the equation



Predictor / Independent Variable

Error

$$\boxed{y} = \boxed{\beta_0} + \boxed{\beta_1}\boxed{x_1} + \boxed{\beta_2}\boxed{x_2} + \ldots + \boxed{\beta_p}\boxed{x_p} + \varepsilon$$

Target / Dependent Variable

Coefficient / Estimators

Slope(s)

INTERPRETATION

- Let’s say given the following regression equation:

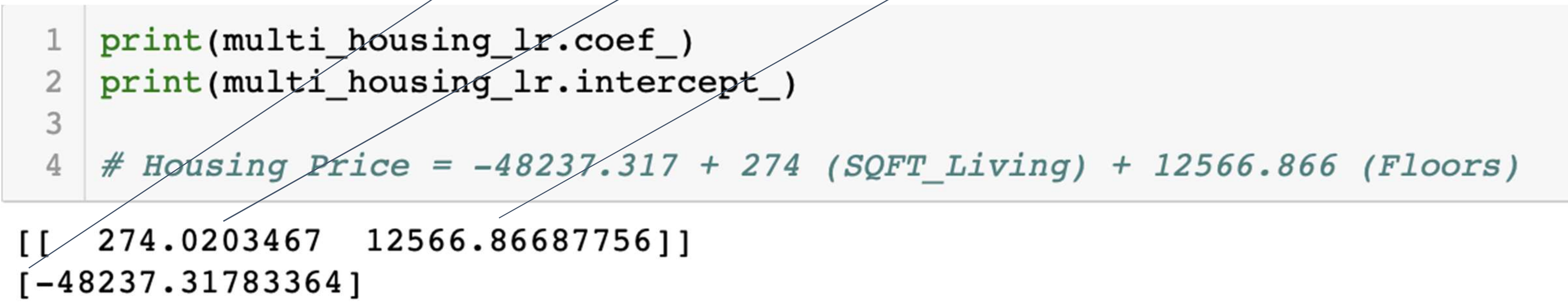
$$HousingPrice\ (\$) = -\ 48237.317 + 274\ SQFT + 12566.866\ Floor + \varepsilon$$

- We can interpret it as, given 1 SQFT increase, Housing Price increases by $274; given 1 floor increase, Housing Price increase by $12566.866

INTERPRETATION - CODED EXAMPLE

- Let’s say given the following regression equation:

$$\textit{HousingPrice}\ (\$) = -\ 48237.317 + 274\ \textit{SQFT} + 12566.866\ \textit{Floor} + \varepsilon$$



```
print(multi_housing_lr.coef_)
print(multi_housing_lr.intercept_)

# Housing Price = -48237.317 + 274 (SQFT_Living) + 12566.866 (Floors)
```

```
[[  274.0203467   12566.86687756]]
[-48237.31783364]
```

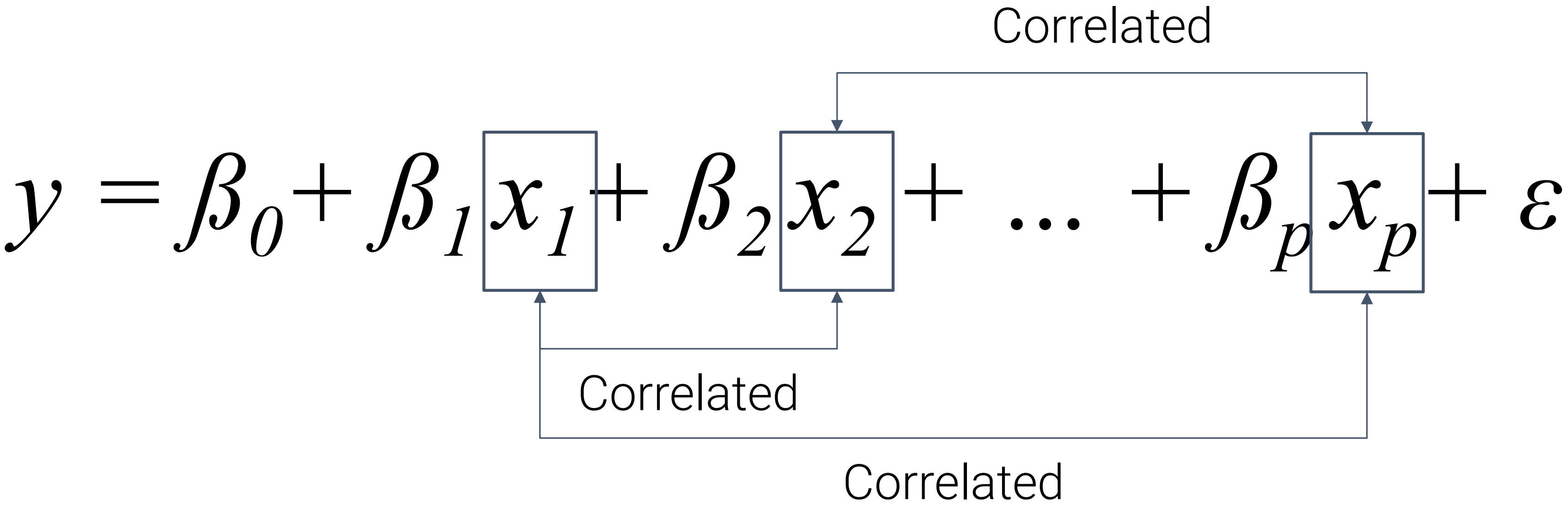
FEATURE SELECTION

- Why don’t we just use all the variables in the world and just apply it to our model?
  - Expensive or not feasible
  - Sometimes fewer predictors are better
  - More predictors could lead to possibly more missing data
  - Lesser predictors allow for greater insight into “influence”
  - Unstable regression coefficient due to multicollinearity
- Approach to reducing / selecting predictors:
  - Domain expert eliminate irrelevant predictors
  - Summary statistics - Frequency and correlation plots

Data Mining for Business Analytics: Concepts, Techniques, and Applications in R by GalitShmueli, Peter C. Bruce, InbalYahav, Nitin R. Patel, Kenneth C. LichtendahlJr. (2018)

FEATURE SELECTION - MULTICOLLINEARITY

- Multicollinearity occurs when **one predictor variable** in a model can be linearly predicted with other **predictor variables**.



$$y = \beta_0 + \beta_1 \boxed{x_1} + \beta_2 \boxed{x_2} + \ \dots \ + \beta_p \boxed{x_p} + \varepsilon$$

FEATURE SELECTION - MULTICOLLINEARITY

- Consequences of this issue includes:
  - Loss of precision
  - R^2 value takes on a high value despite not being statistically significant
  - Some of the signs of the coefficient might change
- Remedies to this problem includes:
  - Dropping problem variables *(selecting which feature to drop)*
  - Remedy using domain expertise
  - Get more data

FEATURE SELECTION - MULTICOLLINEARITY INTUITION

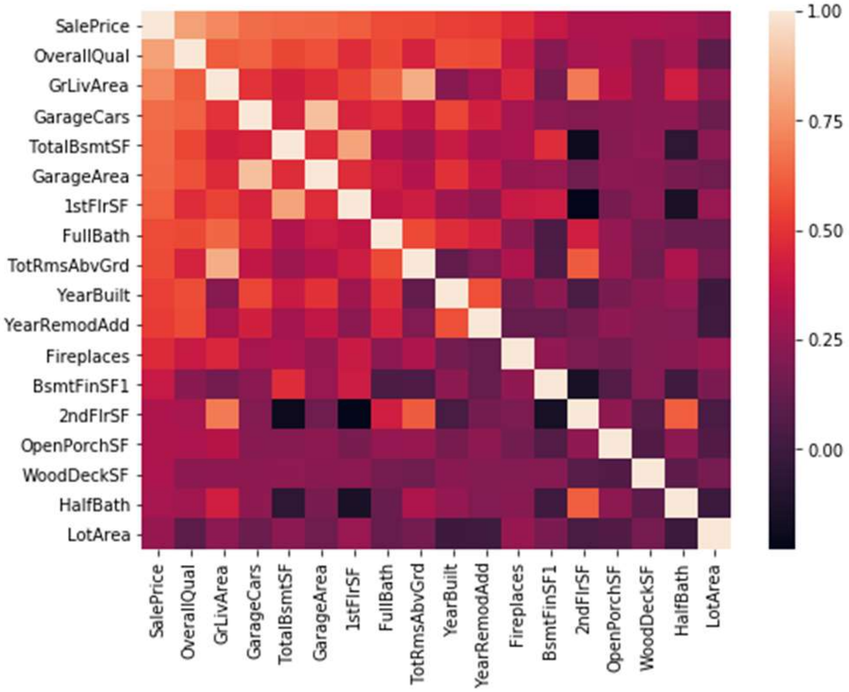
- Given the following dataset, there is a clear multicollinearity between the two predictor variables

House (#)	Price ($)	Price per square **foot** ($)	Price per square **metre** ($)
1	10000	80	240
2	25000	150	450
3	12000	75	225
4	8000	60	180
5	1500	100	300
6	2000	150	450

$$Price = \beta_0 + \beta_1 \, SQFT + \beta_2 \, SQM + \varepsilon$$

FEATURE SELECTION - DETECTING MULTICOLLINEARITY

- You can detect the correlation between variables using a correlation matrix (Rule of thumb: correlation coefficients > 0.8 signals multicollinearity)



FEATURE SELECTION - DETECTING MULTICOLLINEARITY

- Other ways of detecting multicollinearity include:
  - Variance Inflation Factor
  - Low Variance
  - `sklearn.feature_selection.f_regression`

SCIKIT LEARN EXAMPLE AND PRACTICE*

- Try out practice 2 in your in-class notebook
- Make sure you are able to identify the features which are correlated

THANK YOU!

HACKWAGON

• ACADEMY •