# What is Machine Learning?

Lab – 07

# Machine Learning

- Section Overview:
  - What is Machine Learning?
  - Difference between Supervised and Unsupervised Learning
  - Supervised Learning Process
  - Evaluating performance
  - Overfitting

# What is Machine Learning?

- Machine learning is a method of data analysis that automates analytical model building.
- Using algorithms that iteratively learn from data, machine learning allows computers to find hidden insights without being explicitly programmed where to look.

# What is it used for?

- Fraud detection.
- Web search results.
- Real-time ads on web pages
- Credit scoring.
- Prediction of equipment failures.
- New pricing models.
- Network intrusion detection.
- Recommendation Engines
- Customer Segmentation
- Text Sentiment Analysis
- Customer Churn
- Pattern and image recognition.
- Email spam filtering.

# Machine Learning

- There are different types of machine learning we will focus on during the next sections of the course:
  - Supervised Learning
  - Unsupervised Learning

# Machine Learning

- Machine Learning
  - Automated analytical models.
- Neural Networks
  - A type of machine learning architecture modeled after biological neurons.
- Deep Learning
  - A neural network with more than one hidden layer.

# Machine Learning

- Let's begin by learning about one of the most common machine learning tasks- Supervised Learning!

# SUPERVISED LEARNING

# Supervised Learning

- **Supervised learning** algorithms are trained using **labeled** examples, such as an input where the desired output is known.
- For example, a segment of text could have a category label, such as:
  - **Spam** vs. **Legitimate** Email
  - **Positive** vs. **Negative** Movie Review

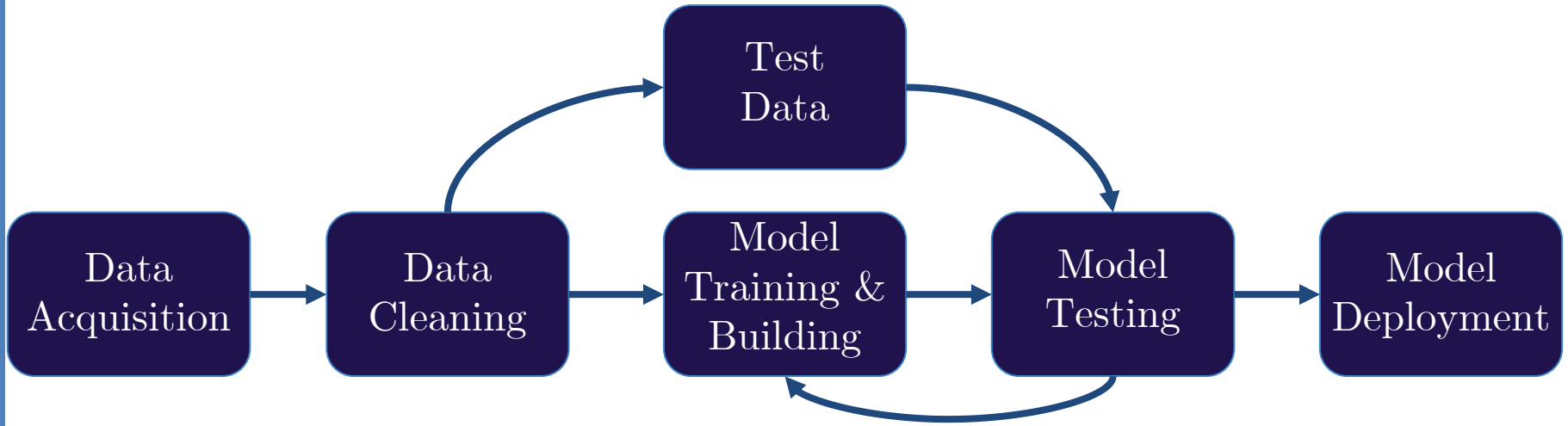
# Supervised Learning

- The network receives a set of inputs along with the corresponding correct outputs, and the algorithm learns by comparing its actual output with correct outputs to find errors.
- It then modifies the model accordingly.

# Supervised Learning

- Supervised learning is commonly used in applications where historical data predicts likely future events.

# Machine Learning Process



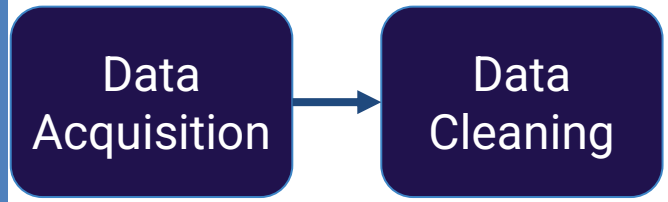
# Machine Learning Process

- Get your data! Customers, Sensors, etc...

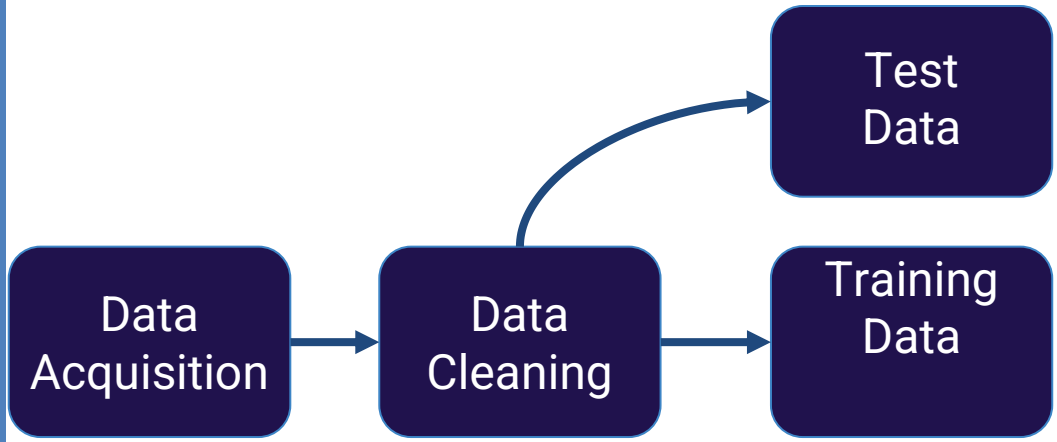
Data Acquisition

# Machine Learning Process

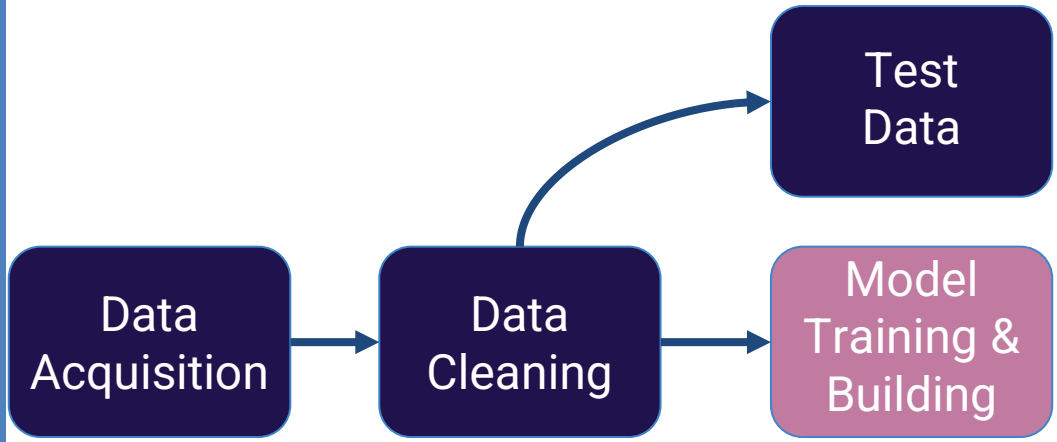
- Clean and format your data (using Pandas)



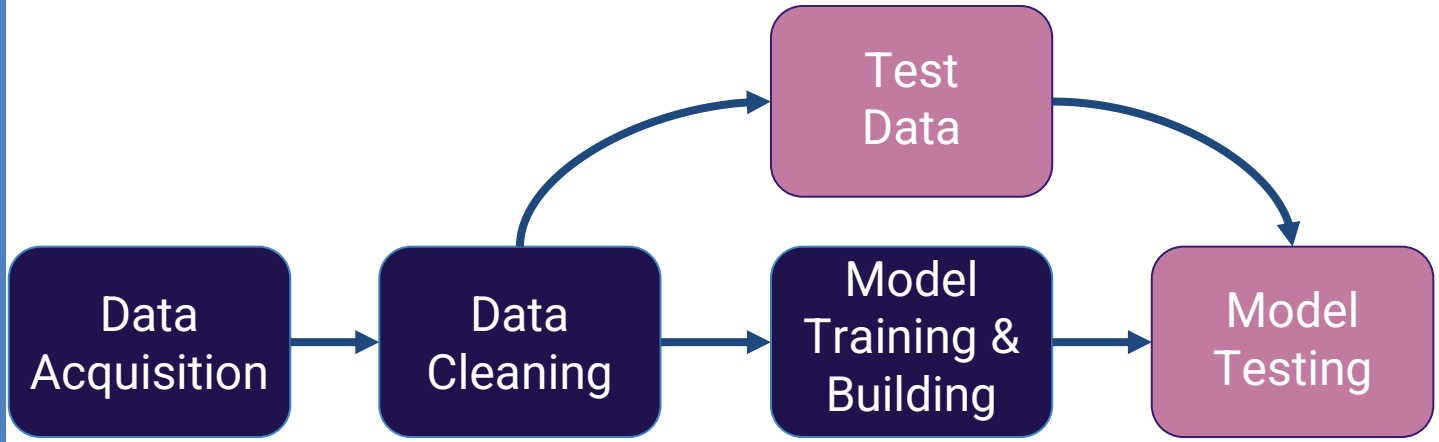
# Machine Learning Process



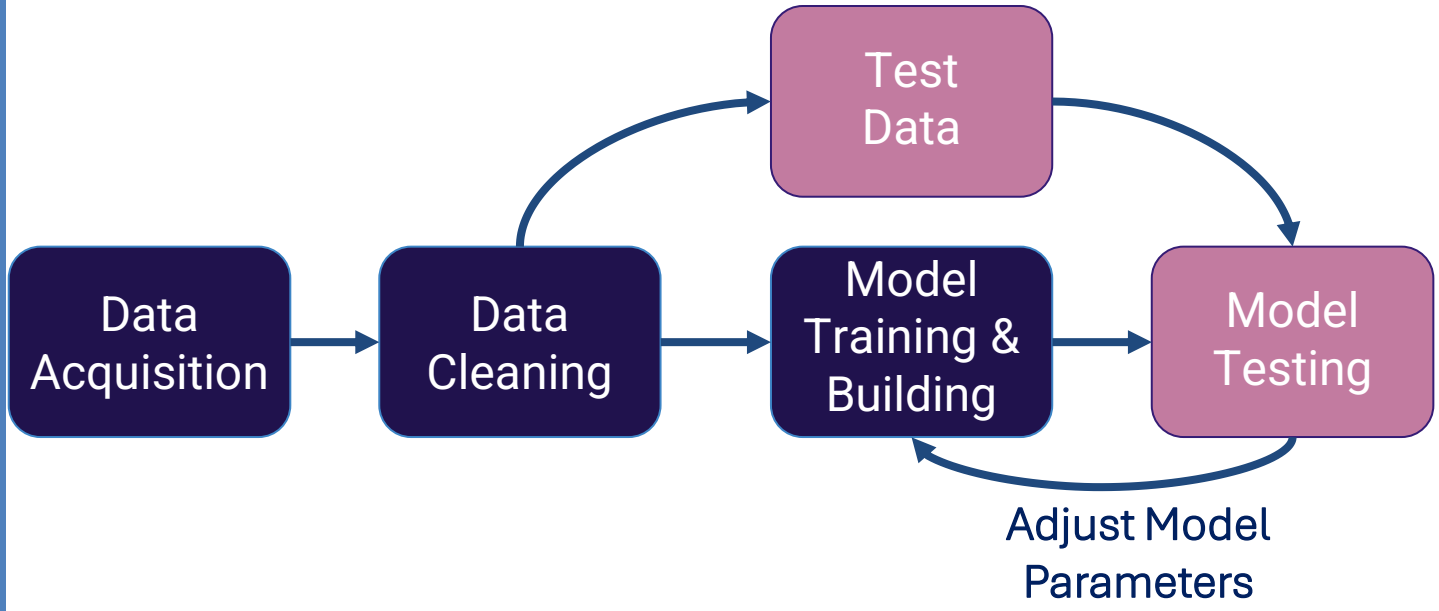
# Machine Learning Process



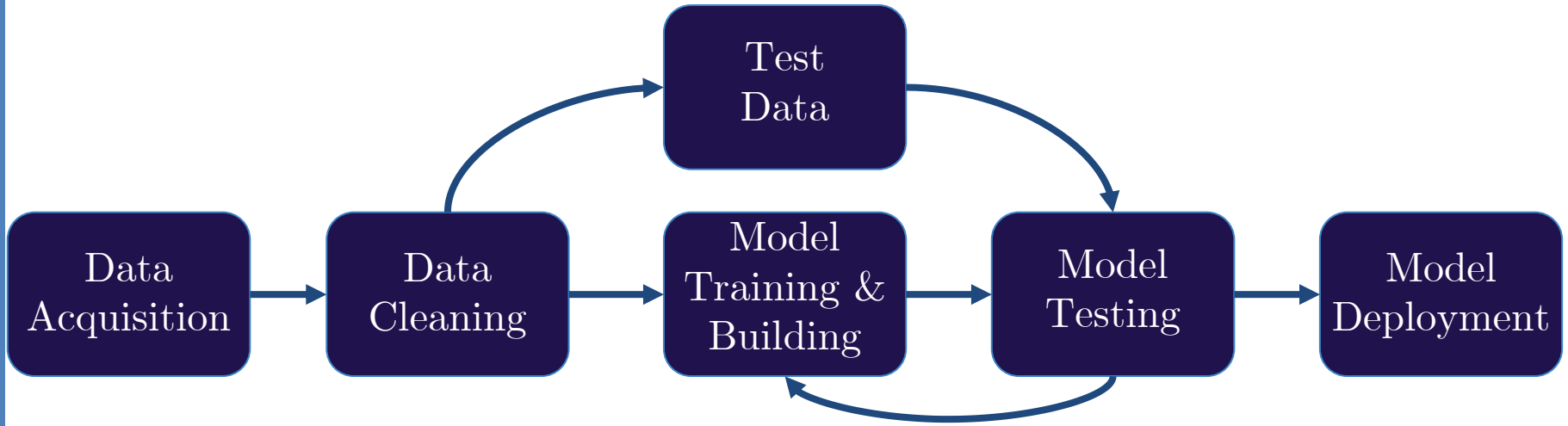
# Machine Learning Process



# Machine Learning Process



# Machine Learning Process



# Supervised Learning

- What we just showed is a simplified approach to supervised learning, it contains an issue!
- Is it fair to use our single split of the data to evaluate our models performance?
- After all, we were given the chance to update the model parameters again and again.

# Supervised Learning

- To fix this issue, data is often split into 3 sets
  - **Training Data**
    - Used to train model parameters
  - **Validation Data**
    - Used to determine what model hyperparameters to adjust
  - **Test Data**
    - Used to get some final performance metric

# Supervised Learning

- This means after we see the results on the **final test set** we don't get to go back and adjust any model parameters!
- This final measure is what we label the true performance of the model to be.

# Supervised Learning

- In this course, in general we will simplify our data by using a simple **train/test split.**
- We will simply train and then evaluate on a test set (leaving the option to students to go back and adjust parameters).

# OVERFITTING AND UNDERFITTING

# Machine Learning

- Now that we understand the full process for supervised learning, let's touch upon the important topics of **overfitting** and **underfitting.**

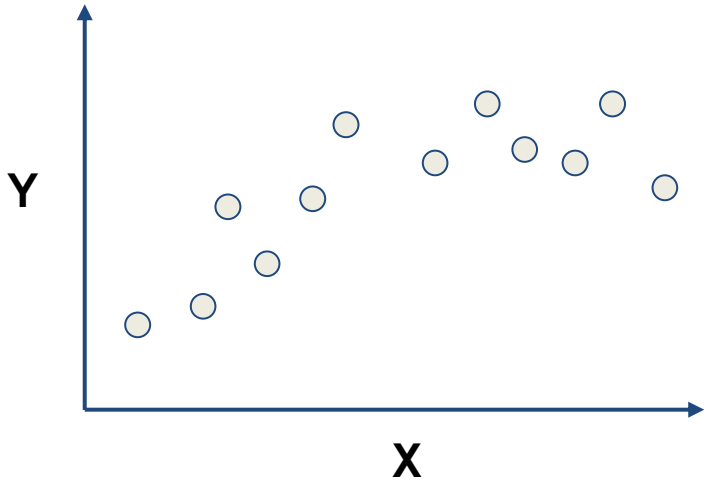
'

# Machine Learning

- **Overfitting**
  - The model fits too much to the noise from the data.
  - This often results in **low error on training sets but high error on test/validation sets.**

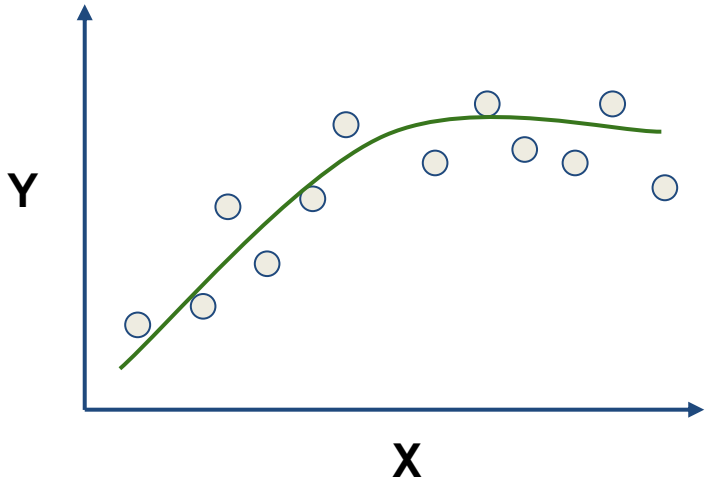
# Machine Learning

## Data



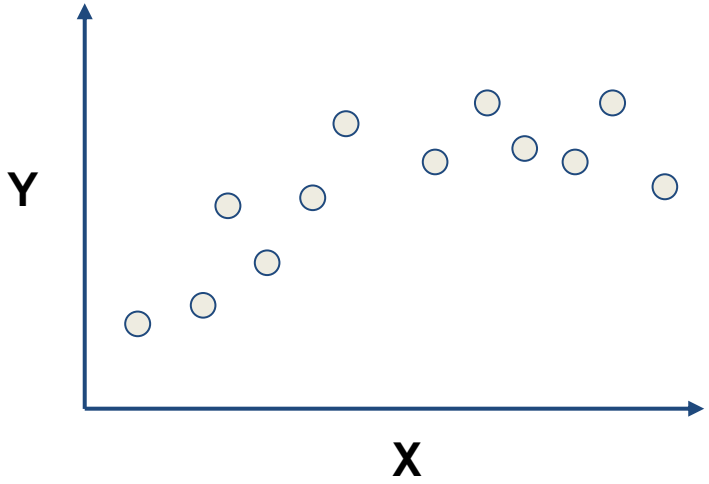
# Machine Learning

## Good Model



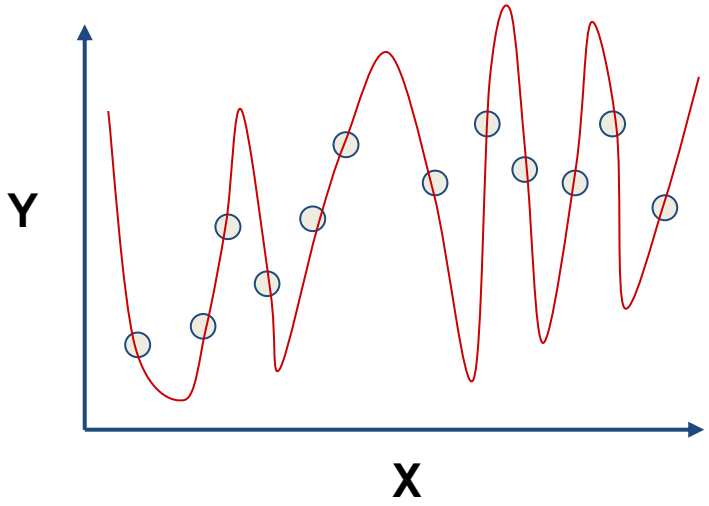
# Machine Learning

- **Overfitting**



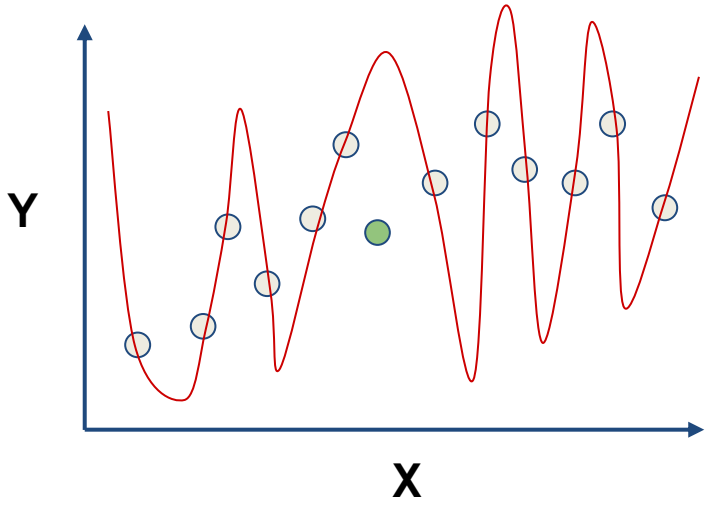
# Machine Learning

- **Overfitting**



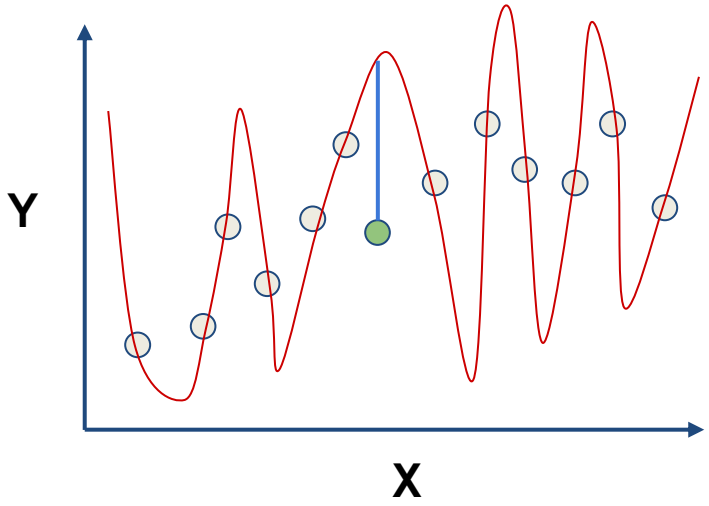
# Machine Learning

- **Overfitting**



# Machine Learning

- **Overfitting**



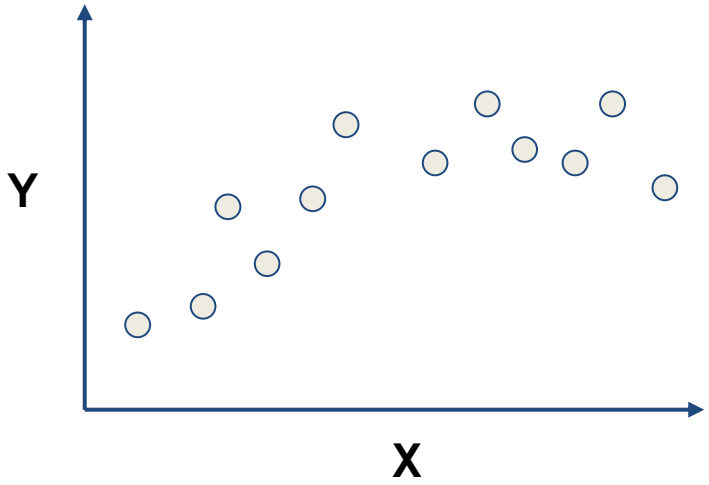
# Machine Learning

- Underfitting
  - Model does not capture the underlying trend of the data and does not fit the data well enough.
  - Low variance but high bias.
  - Underfitting is often a result of an excessively simple model.

- High variance indicates that the model is highly sensitive to the training data and might be overfitting, resulting in predictions that can widely vary based on the specific data used for training.
- High bias means that the model is overly simplistic and cannot capture the complexity of the underlying data, leading to systematic errors.

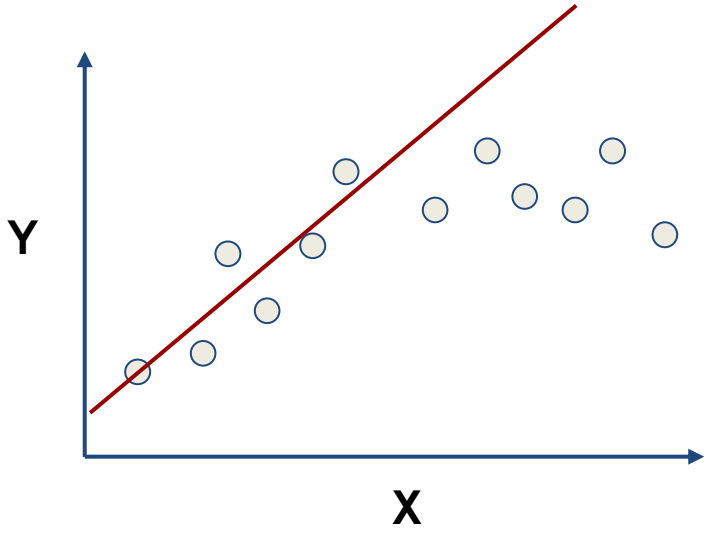
# Machine Learning

## Data



# Machine Learning

## Underfitting

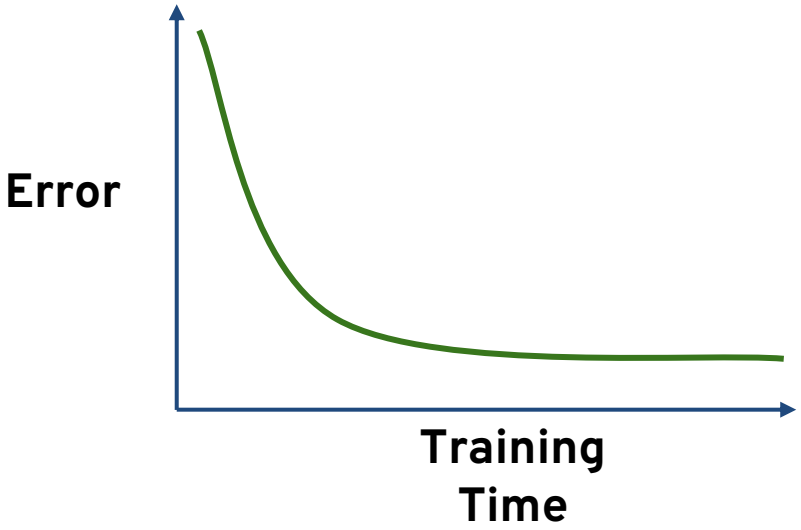


# Machine Learning

- This data was easy to visualize, but how can we see underfitting and overfitting when dealing with multi dimensional data sets?
- First let's imagine we trained a model and then measured its error over training time.

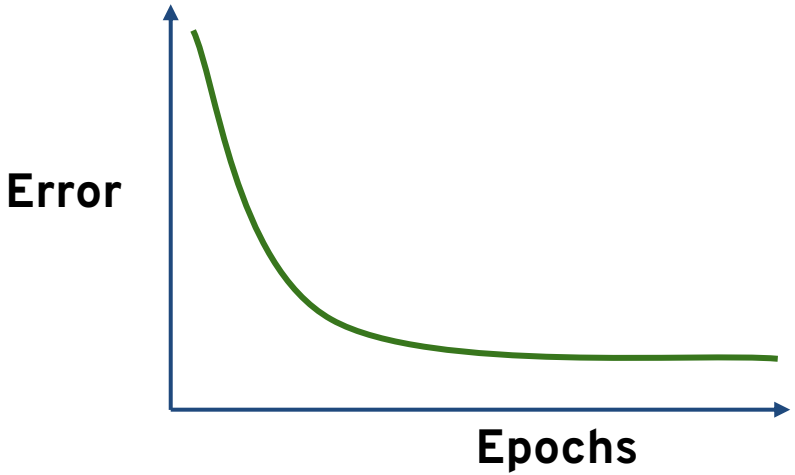
# Machine Learning

- Good Model



# Machine Learning

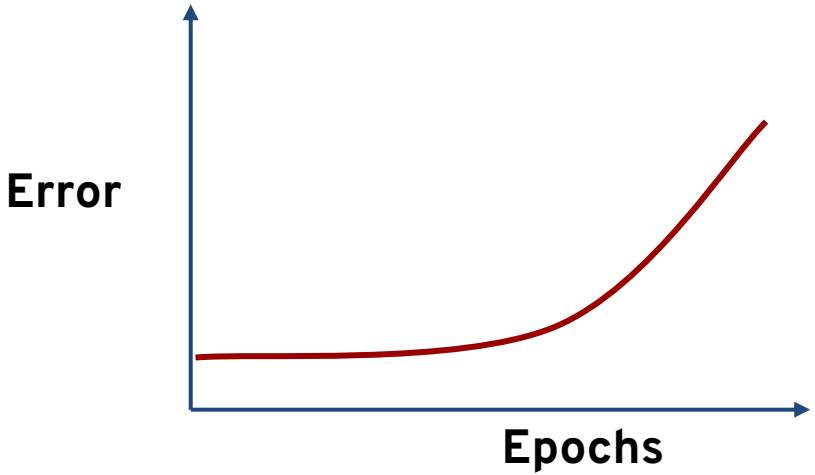
- Good Model




"epochs" refers to the number of times a learning algorithm iteratively processes the entire training dataset during the training phase. In each epoch, the model goes through the entire dataset, updates its parameters based on the training data, and tries to minimize the difference between its predicted outputs and the actual targets (labels)

# Machine Learning

- Bad Model



# Machine Learning

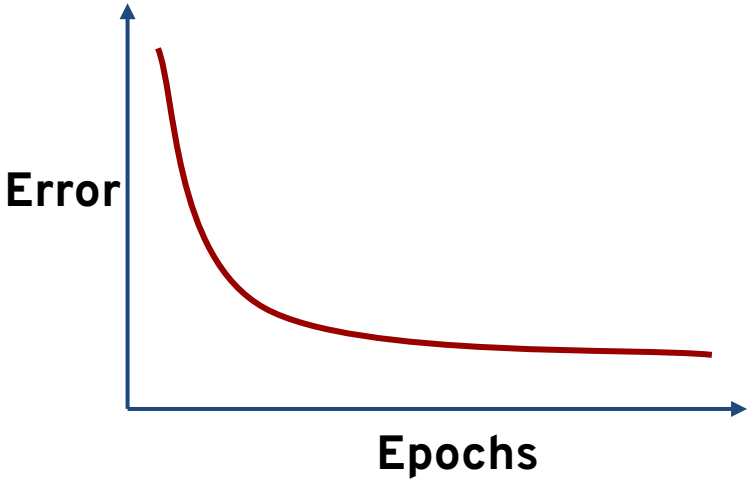
- When thinking about overfitting and underfitting we want to keep in mind the relationship of model performance on the training set versus the test/validation set.

# Machine Learning

- Let's imagine we split our data into a **training set** and a **test set**

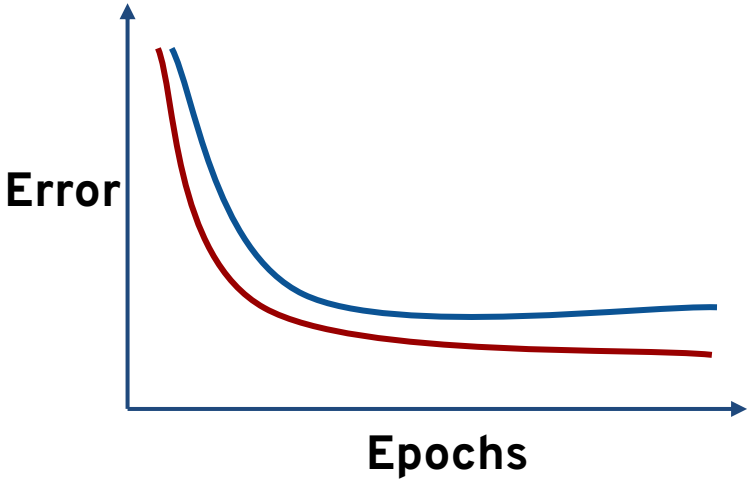
# Machine Learning

- We first see performance on the **training set**



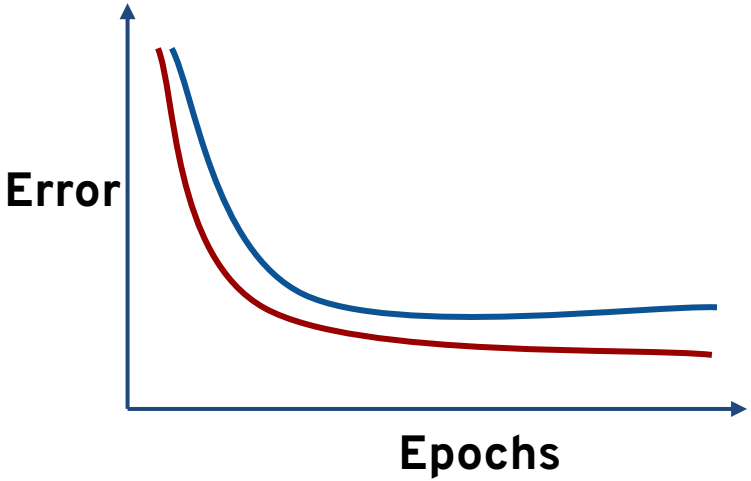
# Machine Learning

- Next we check performance on the **test set**



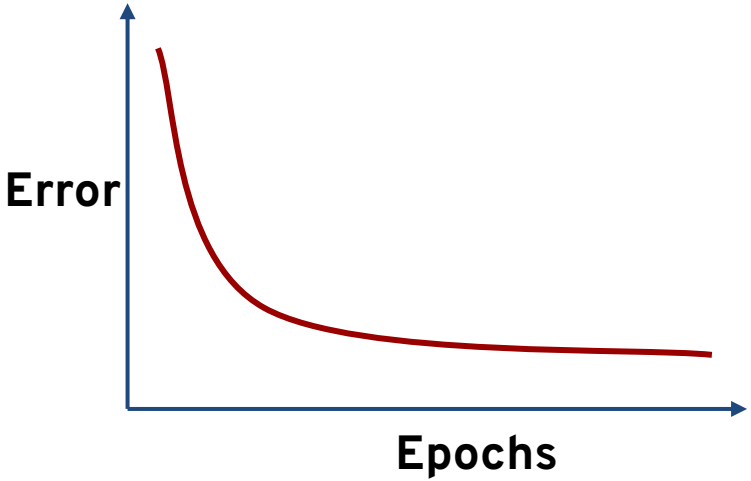
# Machine Learning

- Ideally the model would perform well on both, with similar behavior.



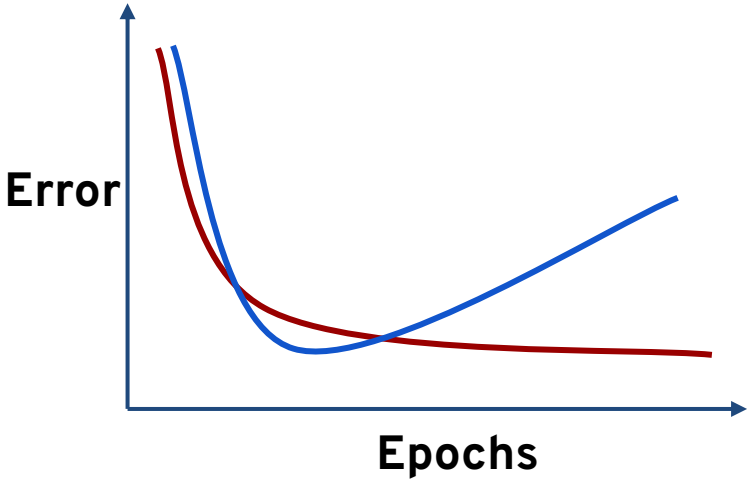
# Machine Learning

- But what happens if we overfit on the training data? That means we would perform poorly on new test data!



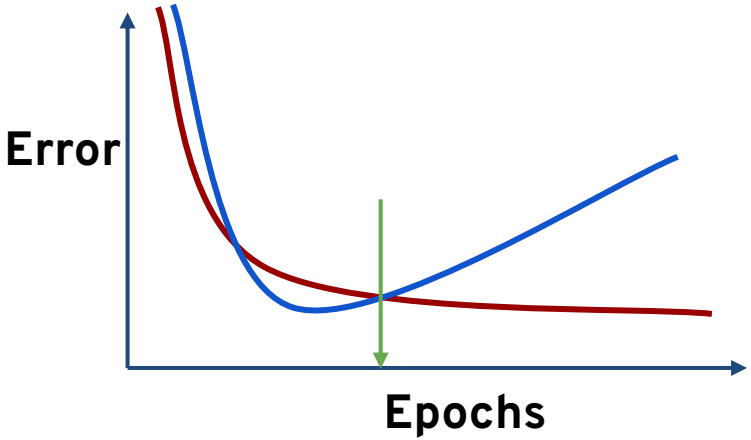
# Machine Learning

- But what happens if we overfit on the training data? That means we would perform poorly on new test data!



# Machine Learning

- This is a good indication of training too much on the training data, you should look for the point to cut off training time!



# Machine Learning

- We'll check on this idea again when we actually begin creating models!
- For now just be aware of this possible issue!

# EVALUATING PERFORMANCE

## CLASSIFICATION

# Model Evaluation

- We just learned that after our machine learning process is complete, we will use performance metrics to evaluate how our model did.
- Let's discuss classification metrics in more detail!

# Model Evaluation

- The key classification metrics we need to understand are:
  - Accuracy
  - Recall
  - Precision
  - F1-Score

# Model Evaluation

- But first, we should understand the reasoning behind these metrics and how they will actually work in the real world!

# Model Evaluation

- Typically in any classification task your model can only achieve two results:
  - Either your model was correct in its prediction.
  - Or your model was incorrect in its prediction.

# Model Evaluation

- Fortunately incorrect vs correct expands to situations where you have multiple classes.
- For the purposes of explaining the metrics, let's imagine a binary classification situation, where we only have two available classes.

# Model Evaluation

- In our example, we will attempt to predict if an image is a dog or a cat.
- Since this is supervised learning, we will first **fit/train** a model on **training data**, then **test** the model on **testing data**.
- Once we have the model's predictions from the **X_test** data, we compare it to the **true y values** (the correct labels).

# Model Evaluation

# Model Evaluation

**Test Image from X_test**

TRAINED MODEL

# Model Evaluation

**Test Image from X_test**

TRAINED MODEL

DOG

**Correct Label from y_test**

# Model Evaluation

**Test Image from X_test**

DOG

**Correct Label from y_test**

TRAINED MODEL

DOG

**Prediction on Test Image**

# Model Evaluation

**Test Image from X_test**

TRAINED MODEL

DOG

**Prediction on Test Image**

DOG

**Correct Label from y_test**

DOG == DOG ?

**Compare Prediction to Correct Label**

# Model Evaluation

**Test Image from X_test**

TRAINED MODEL

CAT

**Prediction on Test Image**

DOG

**Correct Label from y_test**

DOG == CAT ?

**Compare Prediction to Correct Label**

# Model Evaluation

- We repeat this process for all the images in our X test data.
- At the end we will have a count of correct matches and a count of incorrect matches.
- The key realization we need to make, is that **in the real world**, **not all incorrect or correct matches hold equal value!**

# Model Evaluation

- Also in the real world, a single metric won't tell the complete story!
- To understand all of this, let's bring back the 4 metrics we mentioned and see how they are calculated.
- We could organize our predicted values compared to the real values in a **confusion matrix.**

# Model Evaluation

- **Accuracy**
  - Accuracy in classification problems is the **number of correct predictions** made by the model divided by the **total number of predictions.**

# Model Evaluation

- **Accuracy**
  - For example, if the **X_test** set was 100 images and our model **correctly** predicted 80 images, then we have **80/100.**
  - **0.8** or **80% accuracy.**

# Model Evaluation

- **Accuracy**
  - Accuracy is useful when target classes are well balanced
  - In our example, we would have roughly the same amount of cat images as we have dog images.

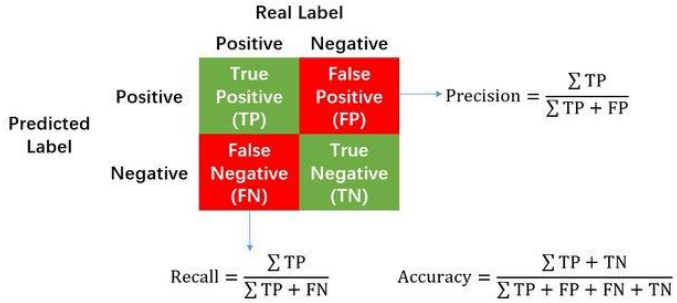
# Model Evaluation

- **Accuracy**
  - Accuracy is **not** a good choice with **unbalanced** classes!
  - Imagine we had 99 images of dogs and 1 image of a cat.
  - If our model was simply a line that always predicted **dog** we would get 99% accuracy!

# Model Evaluation

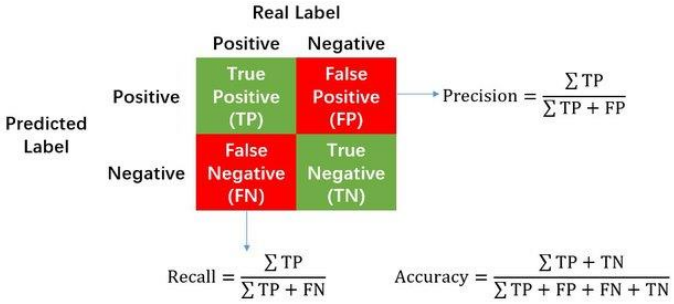
- Accuracy
  - Imagine we had 99 images of dogs and 1 image of a cat.
  - If our model was simply a line that always predicted **dog** we would get 99% accuracy!
  - In this situation we'll want to understand **recall** and **precision**

# Model Evaluation

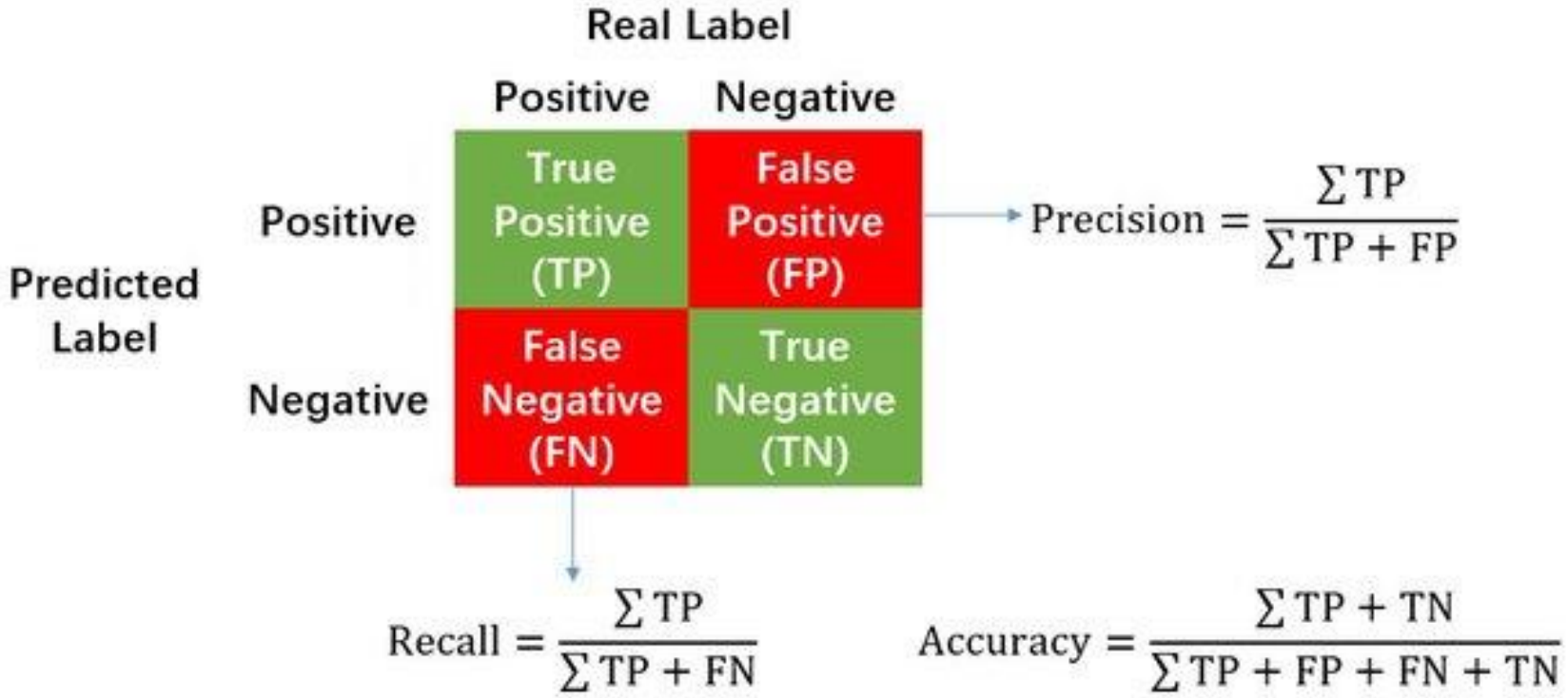



- **Recall / Sensitivity**
  - Ability of a model to find all the relevant cases within a dataset.
  - The precise definition of recall is the number of true positives **divided by** the number of **true positives** plus the number of **false negatives**.
  - Recall, also known as **sensitivity**, hit rate, or true positive rate (TPR), measures the ability of the model to identify positive instances correctly.

# Model Evaluation




- **Precision**
  - Ability of a classification model to identify only the relevant data points.
  - Precision is defined as the number of true positives **divided** by the number of true positives plus the number of false positives.
  - Precision, also known as positive predictive value (PPV), is a metric that measures the accuracy of positive predictions made by the model.


Real Label
Positive
Negative
Predicted Label
Positive
Negative
True Positive (TP)
False Positive (FP)
False Negative (FN)
True Negative (TN)
Precision = ∑TP / ∑TP + FP
Recall = ∑TP / ∑TP + FN
Accuracy = ∑TP + TN / ∑TP + FP + FN + TN

# Model Evaluation

- Recall and Precision
  - Often you have a trade-off between Recall and Precision.
  - While **recall** expresses the ability to find all relevant instances in a dataset, precision expresses the proportion of the data points our model says was relevant actually were relevant.

# Model Evaluation

- F1-Score
  - In cases where we want to find an optimal blend of precision and recall we can combine the two metrics using what is called the F1 score.

# Model Evaluation

- F1-Score
  - The F1 score is the harmonic mean of precision and recall taking both metrics into account in the following equation:

$$F_1 = 2 * \frac{precision * recall}{precision + recall}$$

# Model Evaluation

- F1-Score
  - We use the harmonic mean instead of a simple average because it punishes extreme values.
  - A classifier with a precision of 1.0 and a recall of 0.0 has a simple average of 0.5 but an F1 score of 0.

# Model Evaluation

- We can also view all correctly classified versus incorrectly classified images in the form of a confusion matrix.

# Confusion Matrix

| | | predicted condition | |
|---|---|---|---|
| | total population | prediction positive | prediction negative |
| **true condition** | condition positive | **True Positive (TP)** | **False Negative (FN)** (type II error) |
| | condition negative | **False Positive (FP)** (Type I error) | **True Negative (TN)** |

# Confusion Matrix

| | | **predicted condition** | | |
|---|---|---|---|---|
| | total population | prediction positive | prediction negative | Prevalence $= \frac{\Sigma \text{ condition positive}}{\Sigma \text{ total population}}$ |
| **true condition** | condition positive | **True Positive (TP)** | **False Negative (FN)** (type II error) | True Positive Rate (TPR), Sensitivity, Recall, Probability of Detection $= \frac{\Sigma \text{ TP}}{\Sigma \text{ condition positive}}$ |
| | condition negative | **False Positive (FP)** (Type I error) | **True Negative (TN)** | False Positive Rate (FPR), Fall-out, Probability of False Alarm $= \frac{\Sigma \text{ FP}}{\Sigma \text{ condition negative}}$ |
| | Accuracy $= \frac{\Sigma \text{ TP} + \Sigma \text{ TN}}{\Sigma \text{ total population}}$ | Positive Predictive Value (PPV), Precision $= \frac{\Sigma \text{ TP}}{\Sigma \text{ prediction positive}}$ | False Omission Rate (FOR) $= \frac{\Sigma \text{ FN}}{\Sigma \text{ prediction negative}}$ | Positive Likelihood Ratio (LR+) $= \frac{\text{TPR}}{\text{FPR}}$ |
| | | False Discovery Rate (FDR) $= \frac{\Sigma \text{ FP}}{\Sigma \text{ prediction positive}}$ | Negative Predictive Value (NPV) $= \frac{\Sigma \text{ TN}}{\Sigma \text{ prediction negative}}$ | Negative Likelihood Ratio (LR−) $= \frac{\text{FNR}}{\text{TNR}}$ |

# Model Evaluation

- The main point to remember with the confusion matrix and the various calculated metrics is that they are all fundamentally ways of comparing the predicted values versus the true values.
- What constitutes "**good**" metrics, will really depend on the specific situation!

# Model Evaluation

- Still confused on the confusion matrix?
- No problem! Check out the Wikipedia page for it, it has a really good diagram with all the formulas for all the metrics.
- Throughout the training, we'll usually just print out metrics (e.g. accuracy).

# Model Evaluation

- Let's think back on this idea of:
  - What is a good enough accuracy?
- This all depends on the context of the situation!
- Did you create a model to predict presence of a disease?
- Is the disease presence well balanced in the general population? (Probably not!)

# Model Evaluation

- Often models are used as quick diagnostic tests to have **before** having a more invasive test (e.g. getting urine test before getting a biopsy)
- We also need to consider what is at stake!

# Model Evaluation

- Often we have a precision/recall trade off, We need to decide if the model will should focus on fixing False Positives vs. False Negatives.
- In disease diagnosis, it is probably better to go in the direction of False positives, so we make sure we correctly classify as many cases of disease as possible!

# Model Evaluation

- All of this is to say, machine learning is not performed in a “vacuum”, but instead a collaborative process where we should consult with experts in the domain (e.g. medical doctors)

# EVALUATING PERFORMANCE

## REGRESSION

# Evaluating Regression

- Let's take a moment now to discuss evaluating Regression Models
- Regression is a task when a model attempts to predict continuous values (unlike categorical values, which is classification)

# Evaluating Regression

- You may have heard of some evaluation metrics like accuracy or recall.
- These sort of metrics aren't useful for regression problems, we need metrics designed for continuous values!

# Evaluating Regression

- For example, attempting to predict the price of a house given its features is a regression task.
- Attempting to predict the country a house is in given its features would be a classification task.

# Evaluating Regression

- Let's discuss some of the most common evaluation metrics for regression:
  - Mean Absolute Error (MAE)
  - Mean Squared Error (MSE)
  - Root Mean Square Error (RMSE)

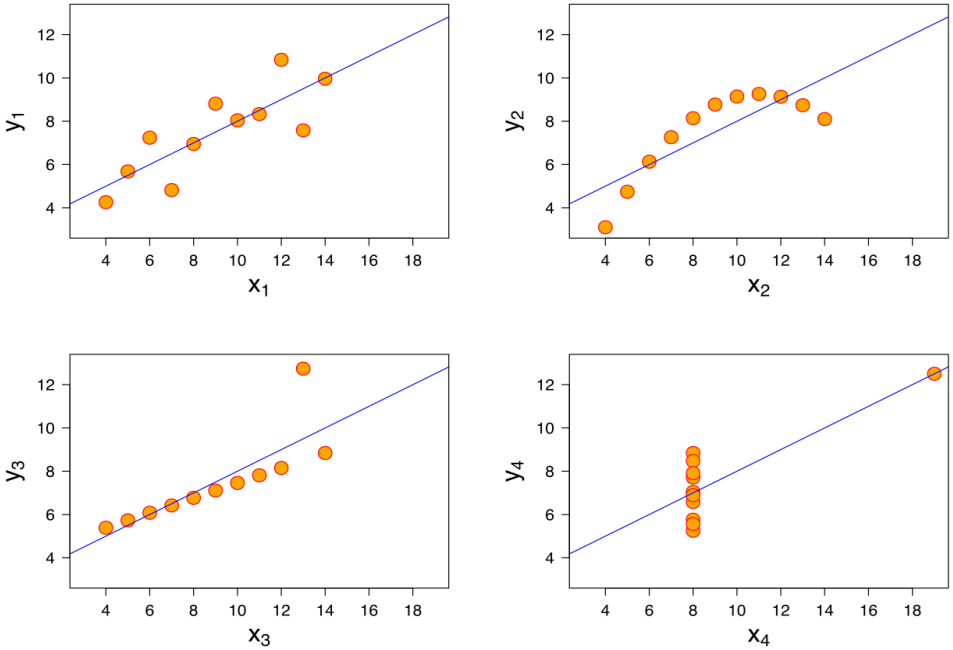
# Evaluating Regression

- Mean Absolute Error (MAE)
  - This is the mean of the absolute value of errors.
  - Easy to understand

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

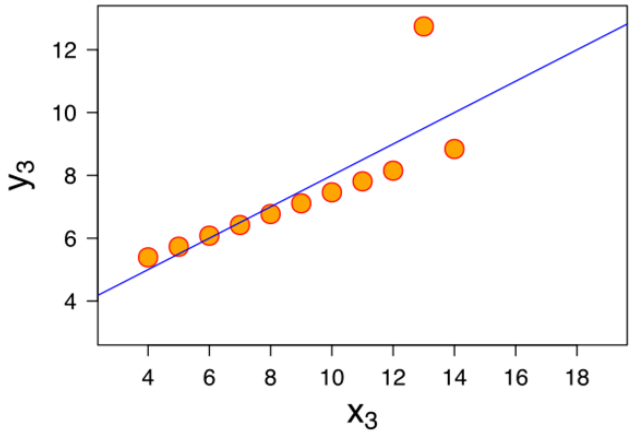
# Evaluating Regression

- MAE won't punish large errors however.



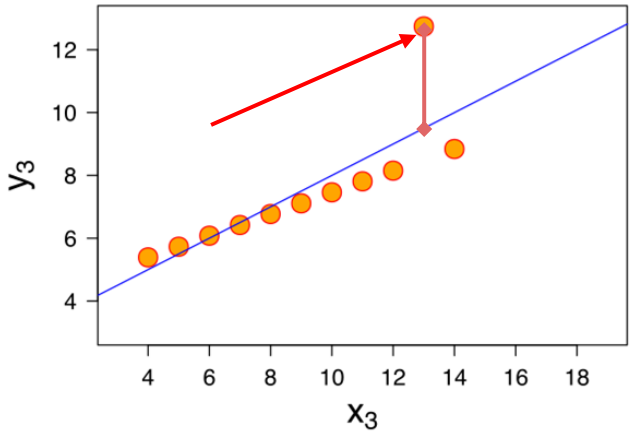
# Evaluating Regression

- MAE won't punish large errors however.



# Evaluating Regression

- We want our error metrics to account for these!



# Evaluating Regression

- **Mean Squared Error (MSE)**
  - This is the mean of the squared errors.
  - Larger errors are noted more than with MAE, making MSE more popular.

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

# Evaluating Regression

- **Root Mean Square Error (RMSE)**
  - This is the root of the  mean of the squared errors.
  - Most popular (has same units as y)

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

# Machine Learning

- Most common question from students:
  - “Is this value of RMSE good?”
  - Context is everything!
  - A RMSE of $10 is fantastic for predicting the price of a house, but horrible for predicting the price of a candy bar!

# Machine Learning

- Compare your error metric to the average value of the label in your data set to try to get an intuition of its overall performance.
- Domain knowledge also plays an important role here!

# Machine Learning

- Context of importance is also necessary to consider.
- We may create a model to predict how much medication to give, in which case small fluctuations in RMSE may actually be very significant.

# Evaluating Regression

- You should now feel comfortable with the various methods of evaluating a regression task.

# Thank You