What is Machine Learning?

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Machine Learning

- Before we jump into Neural Networks, Tensorflow, Keras API etc… its a good idea to understand a few fundamental ideas regarding machine learning.
- In this section we'll cover some important theory and concepts surrounding machine learning.

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Machine Learning

- Section Overview:
  - What is Machine Learning?
  - What is Deep 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.

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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.

What are Neural Networks?

- Neural Networks are a way of modeling biological neuron systems mathematically.
- These networks can then be used to solve tasks that many other types of algorithms can not (e.g. image classification)
- Deep Learning simply refers to neural networks with more than one hidden layer.

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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!

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Supervised Learning

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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.

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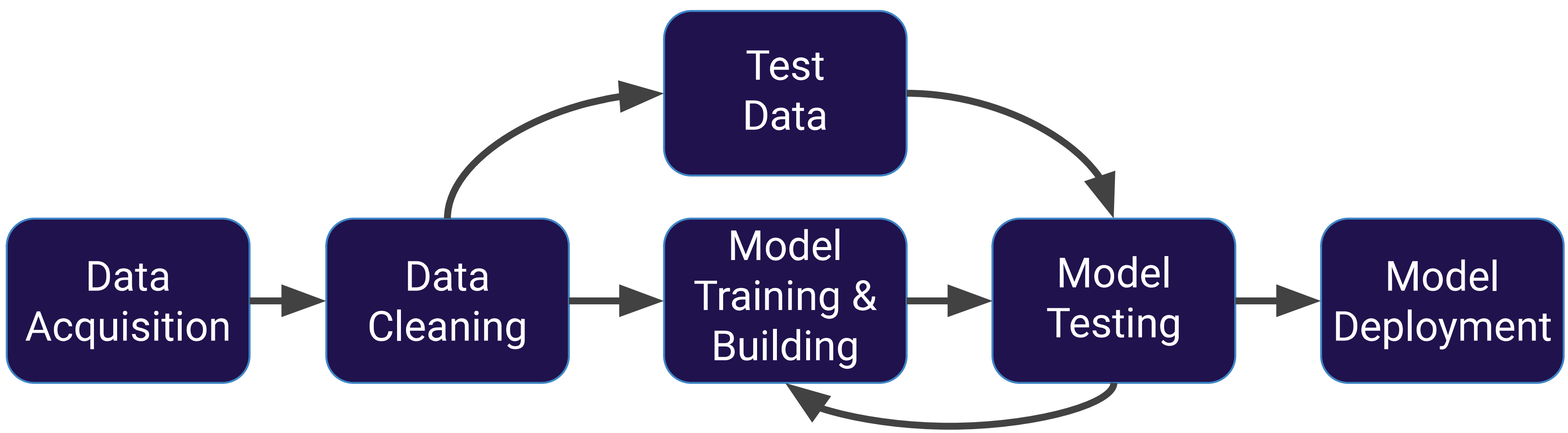
Supervised Learning

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

Machine Learning Process



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Machine Learning Process

- Get your data! Customers, Sensors, etc…

Data Acquisition

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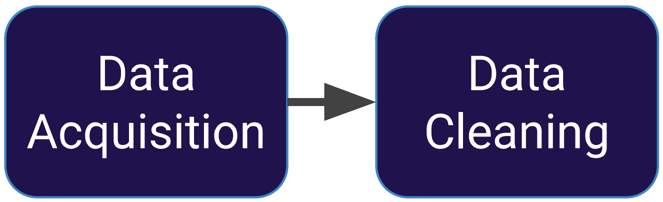
Machine Learning Process

- Clean and format your data (using Pandas)



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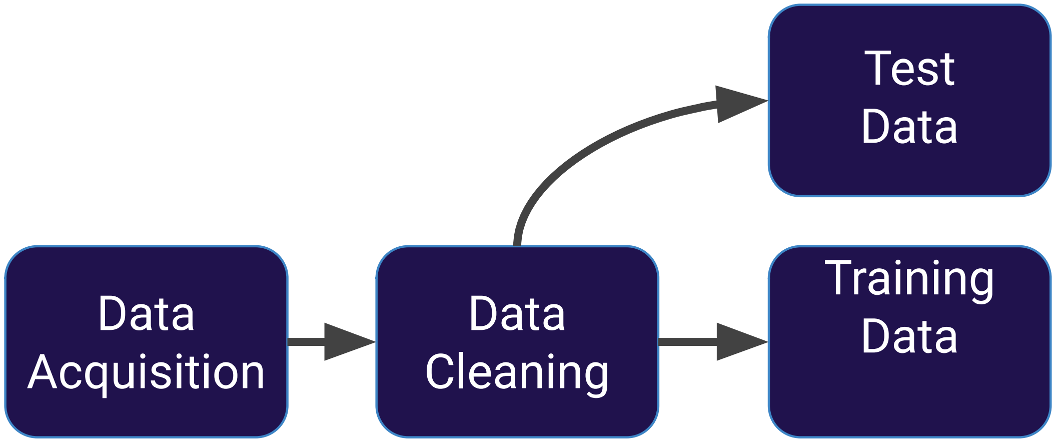
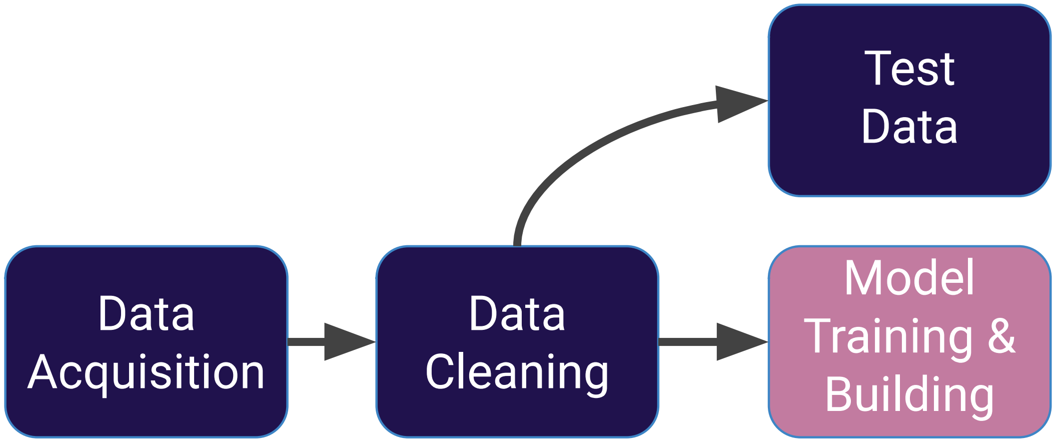
Machine Learning Process



Machine Learning Process



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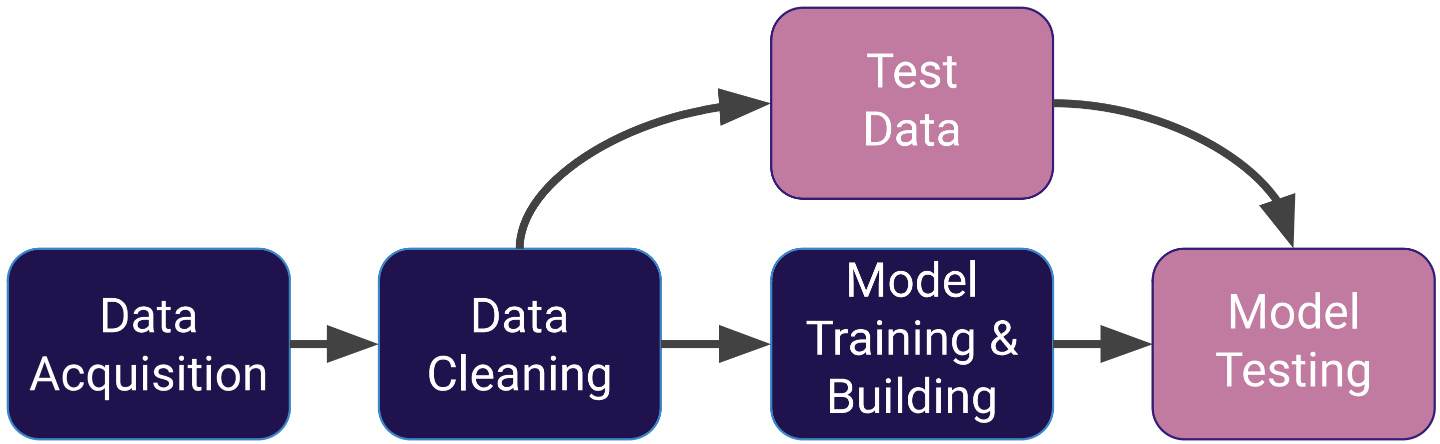
Machine Learning Process



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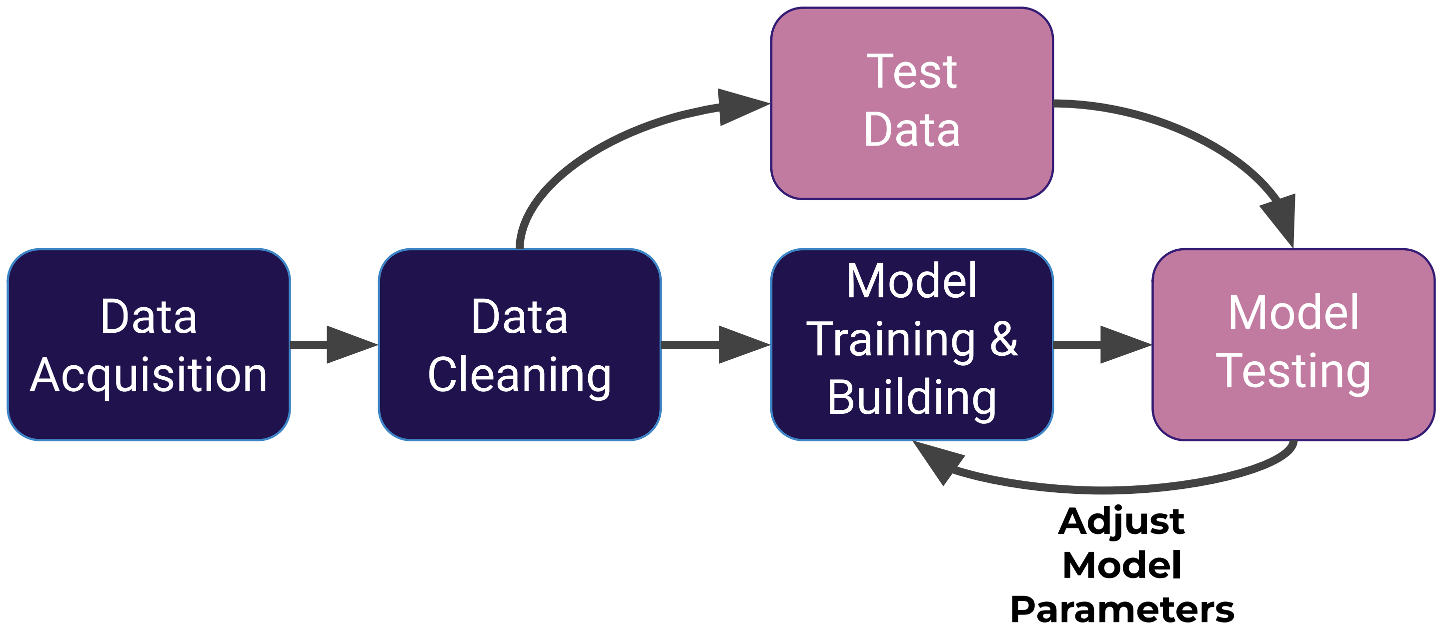
Machine Learning Process



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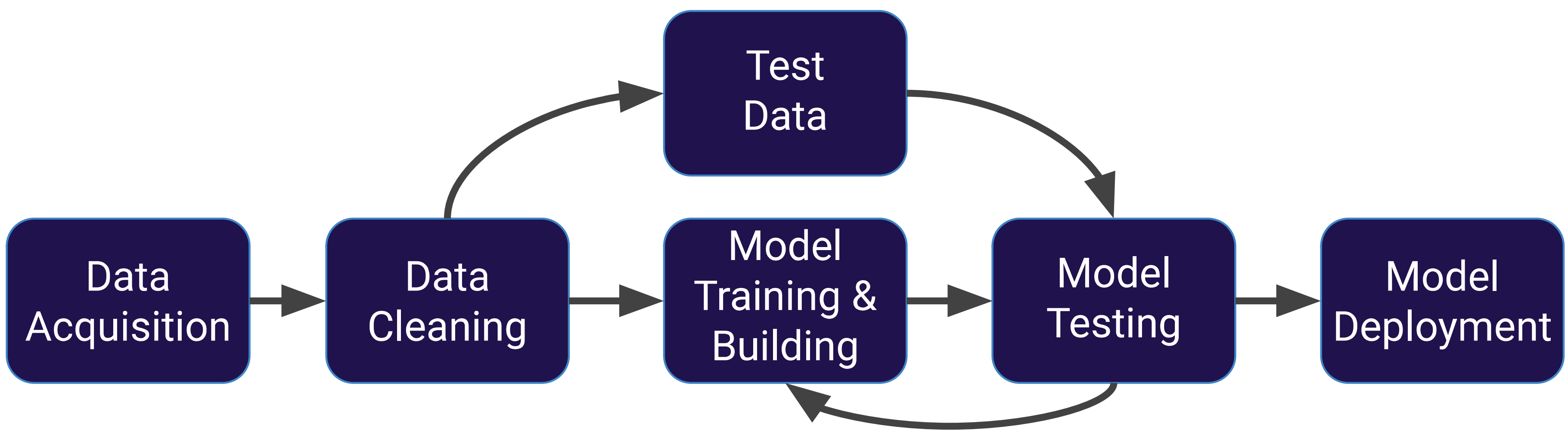
Machine Learning Process



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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).
- After going through the course, you will be able to easily perform another split to get **3 data sets** if you desire.

Overfitting and Underfitting

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Machine Learning

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

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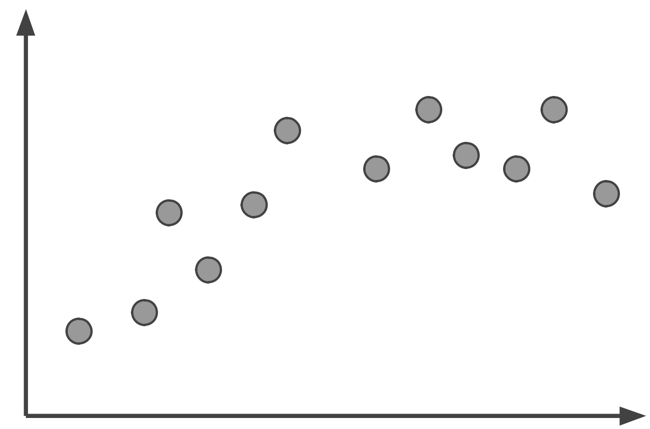
Machine Learning

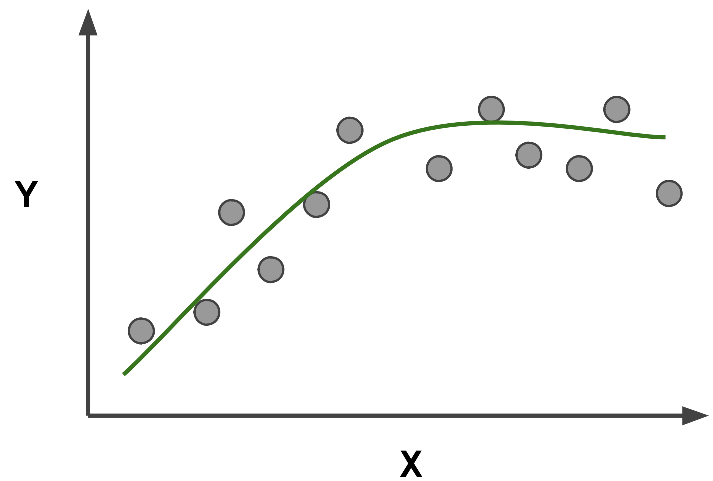
- **Overfitting**
  - The model fits too much to the noise from the data.
  - This often results in **low error on training sets but high error on test/validation sets.**

Data



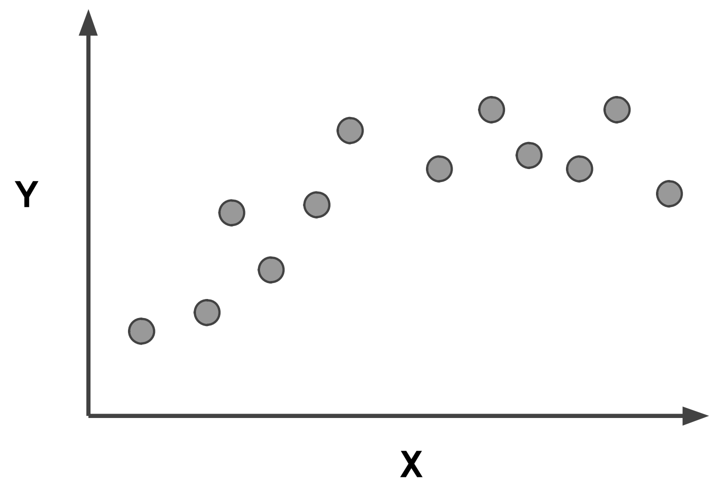
Machine Learning

Good Model



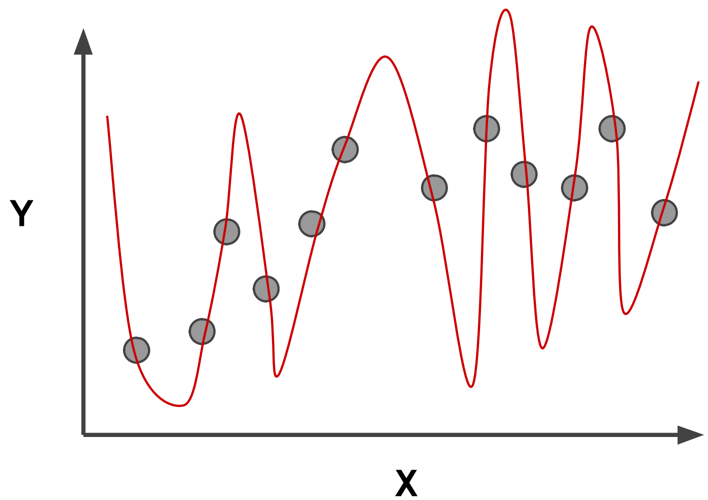
Machine Learning

- **Overfitting**



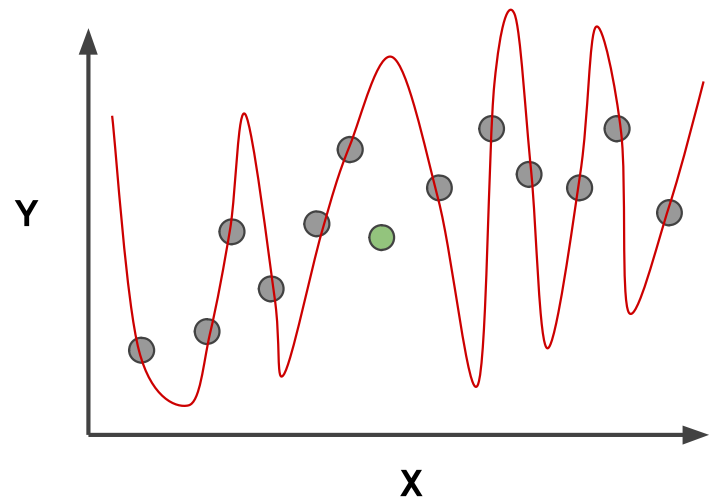
Machine Learning

- **Overfitting**



Machine Learning

- **Overfitting**



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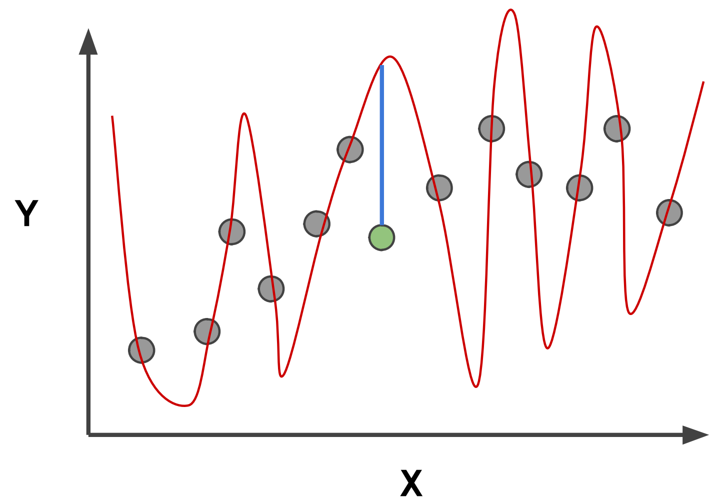
Machine Learning

- **Overfitting**

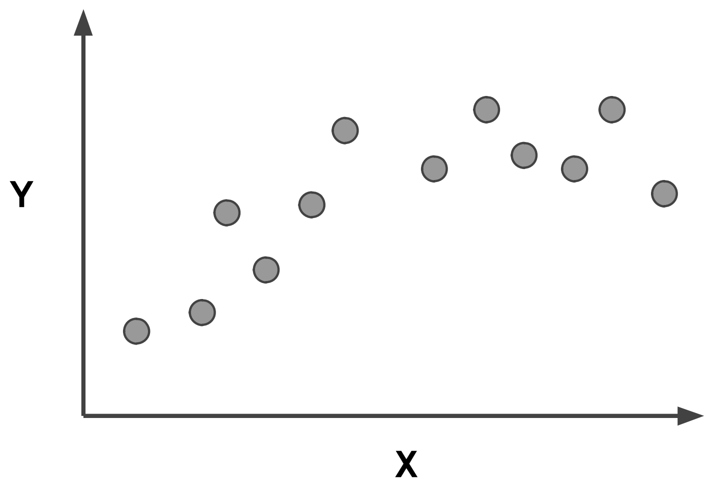


Machine Learning

- **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.

Machine Learning

Data



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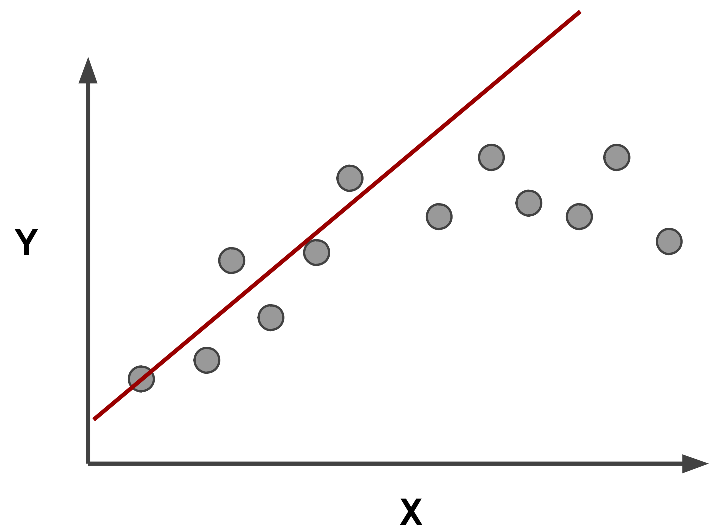
Underfitting

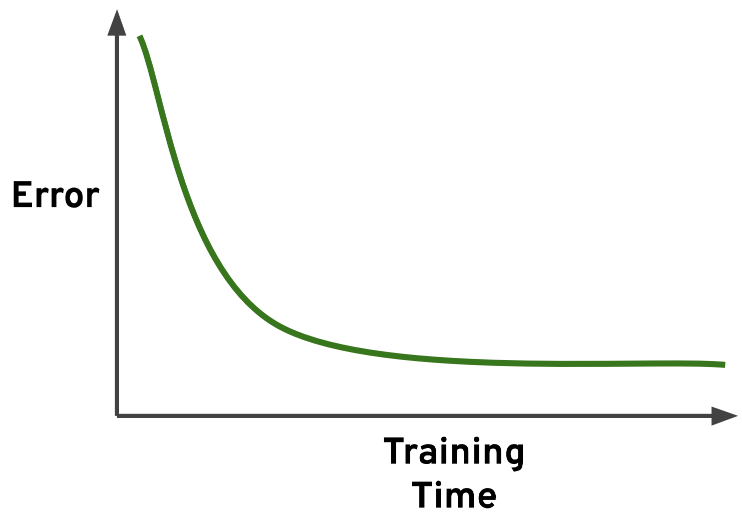


Machine Learning

- 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



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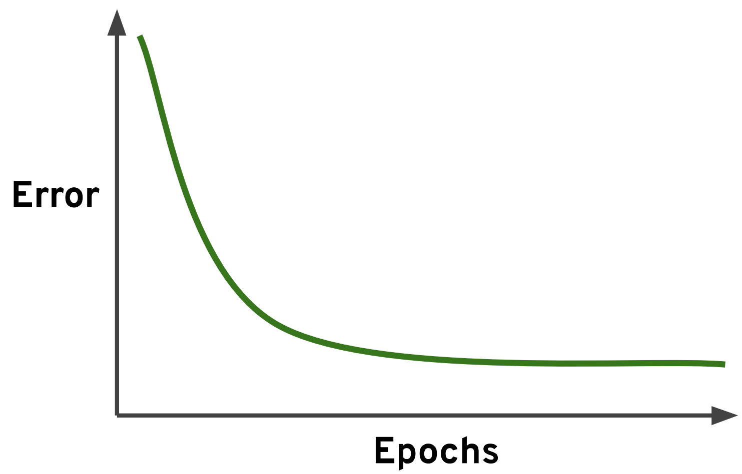
Machine Learning

- Good Model



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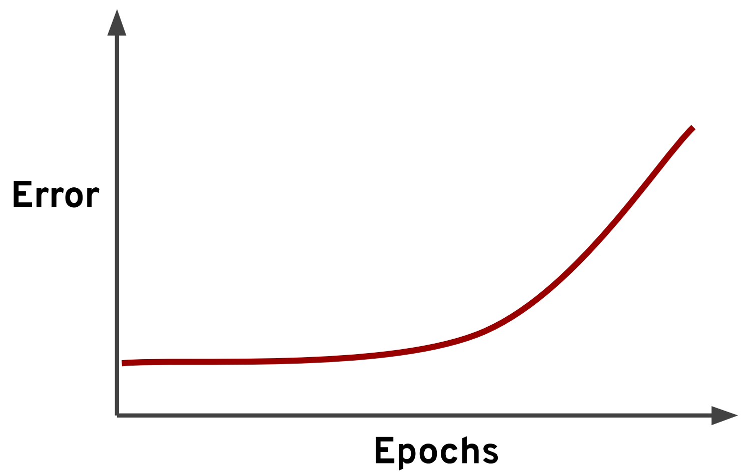
Machine Learning

- Bad Model



Machine Learning

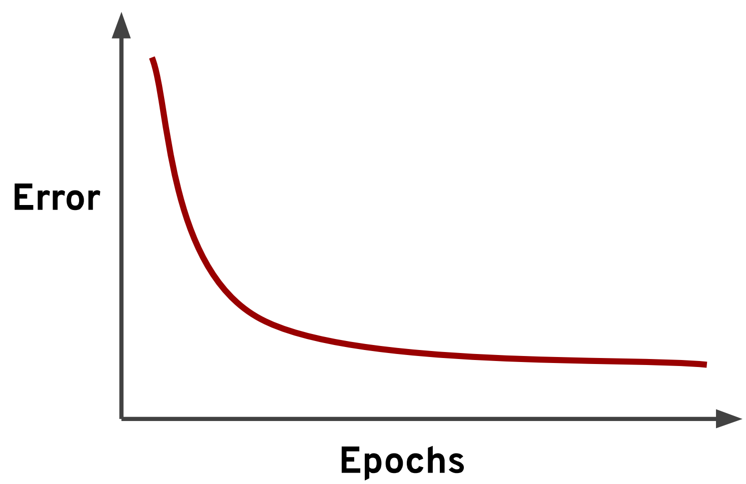
- When thinking about **overfitting** and **underfitting** we want to keep in mind the relationship of model performance on the training set versus the test/validation set.

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**



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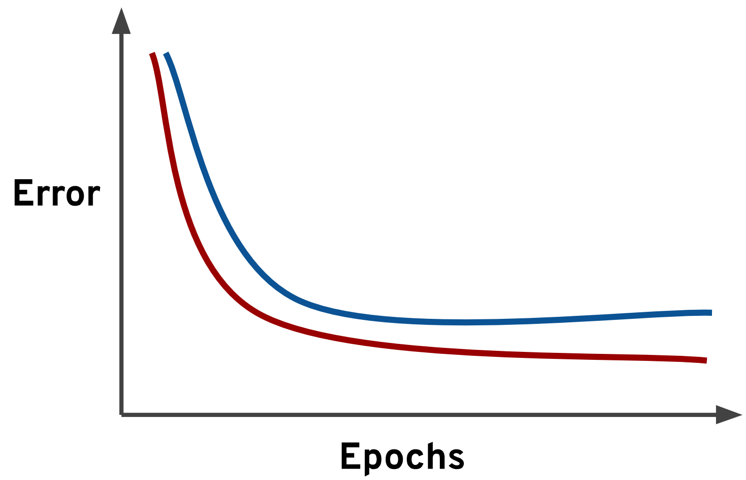
Machine Learning

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



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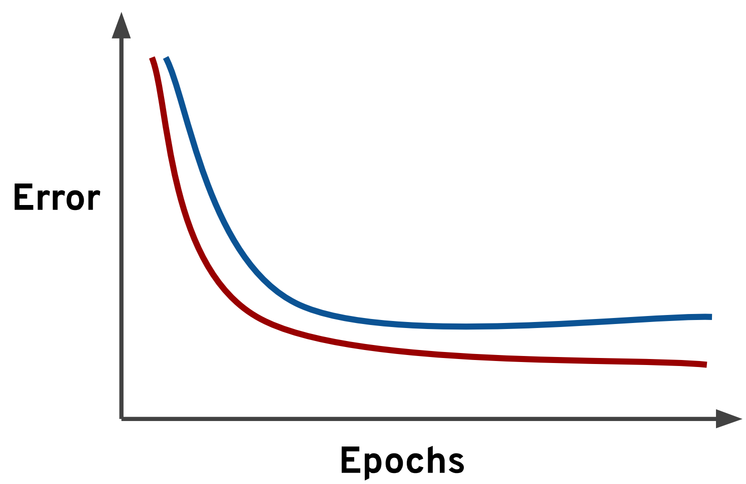
Machine Learning

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



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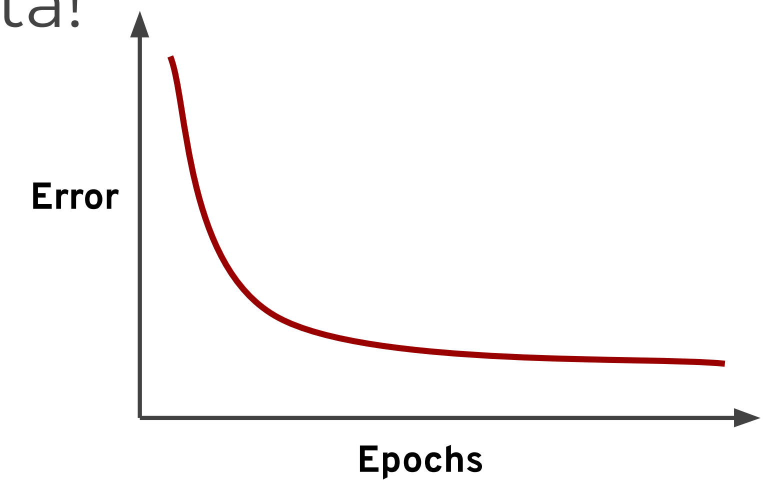
Machine Learning

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



Machine Learning

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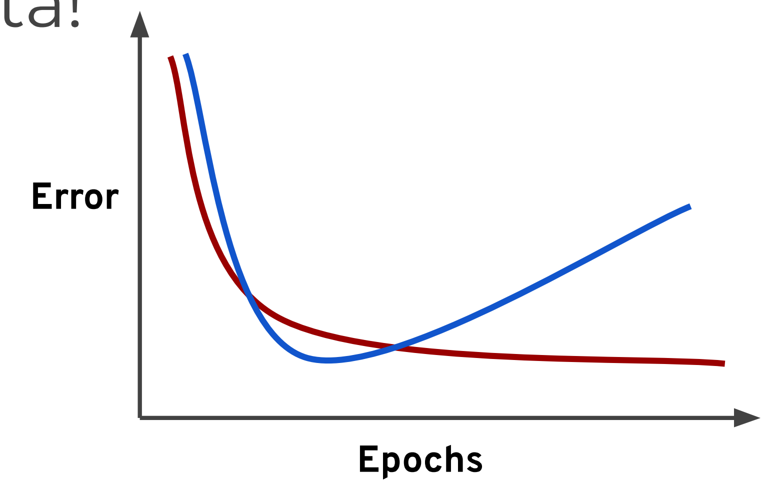

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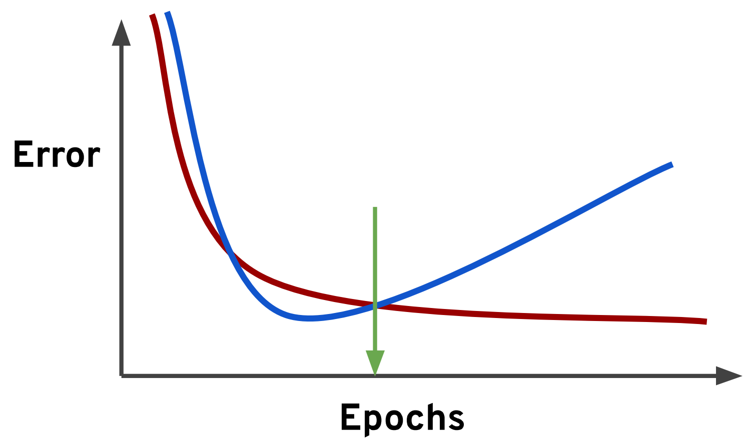
Machine Learning

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



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Machine Learning

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

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Evaluating Performance

CLASSIFICATION

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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!

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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.

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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

TRAINED MODEL

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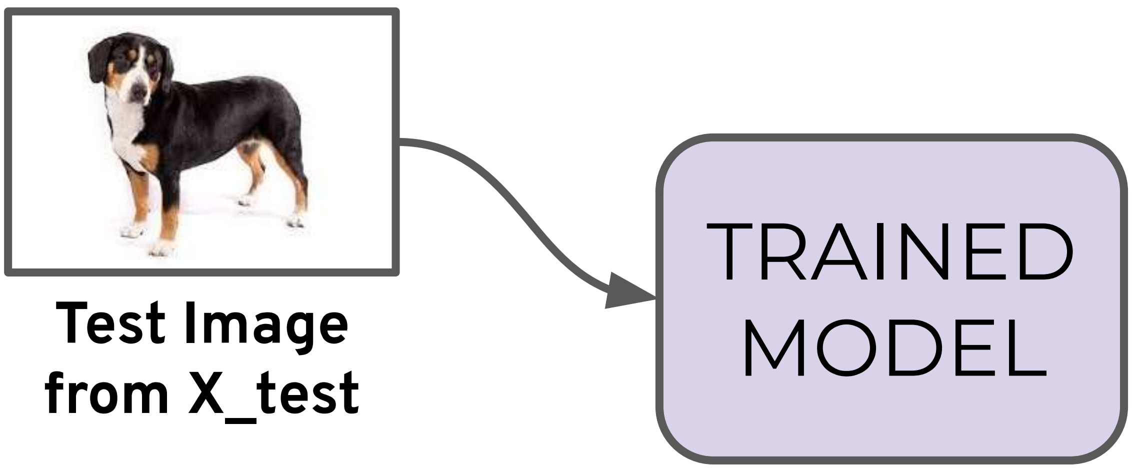
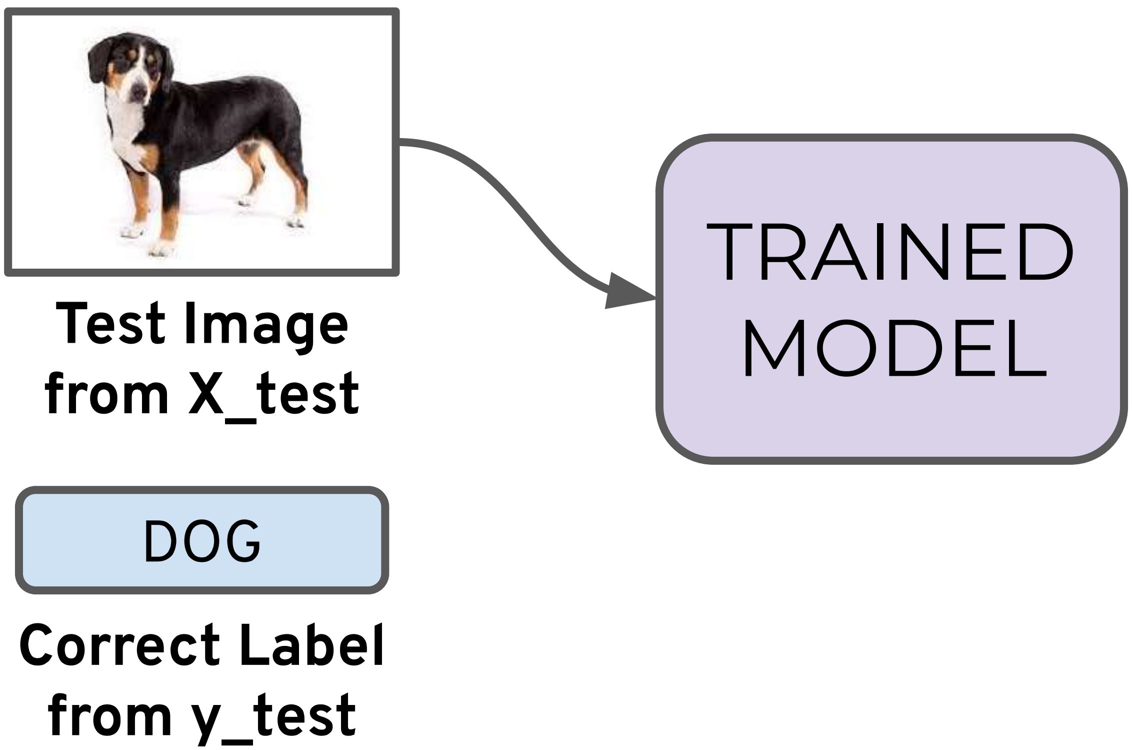
Model Evaluation



Model Evaluation



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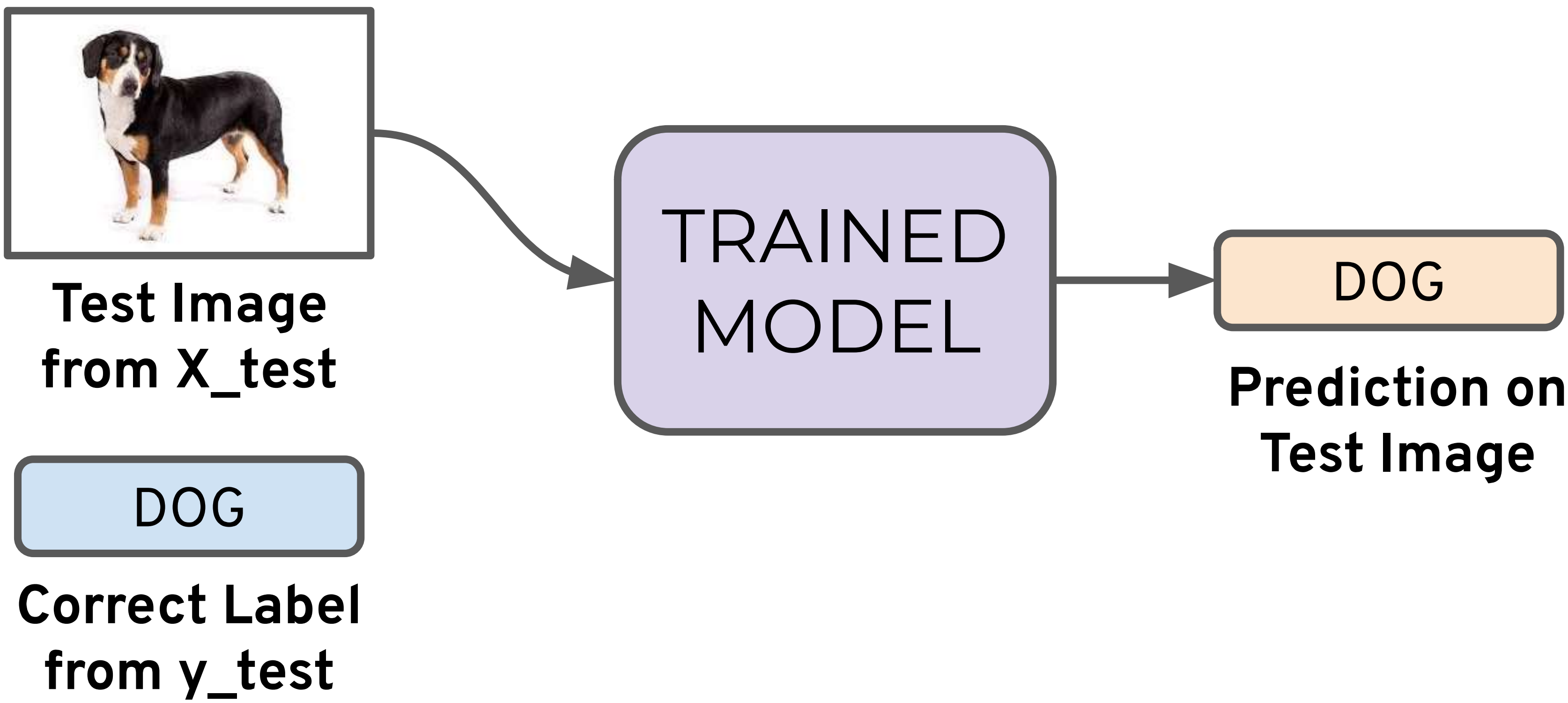
Model Evaluation



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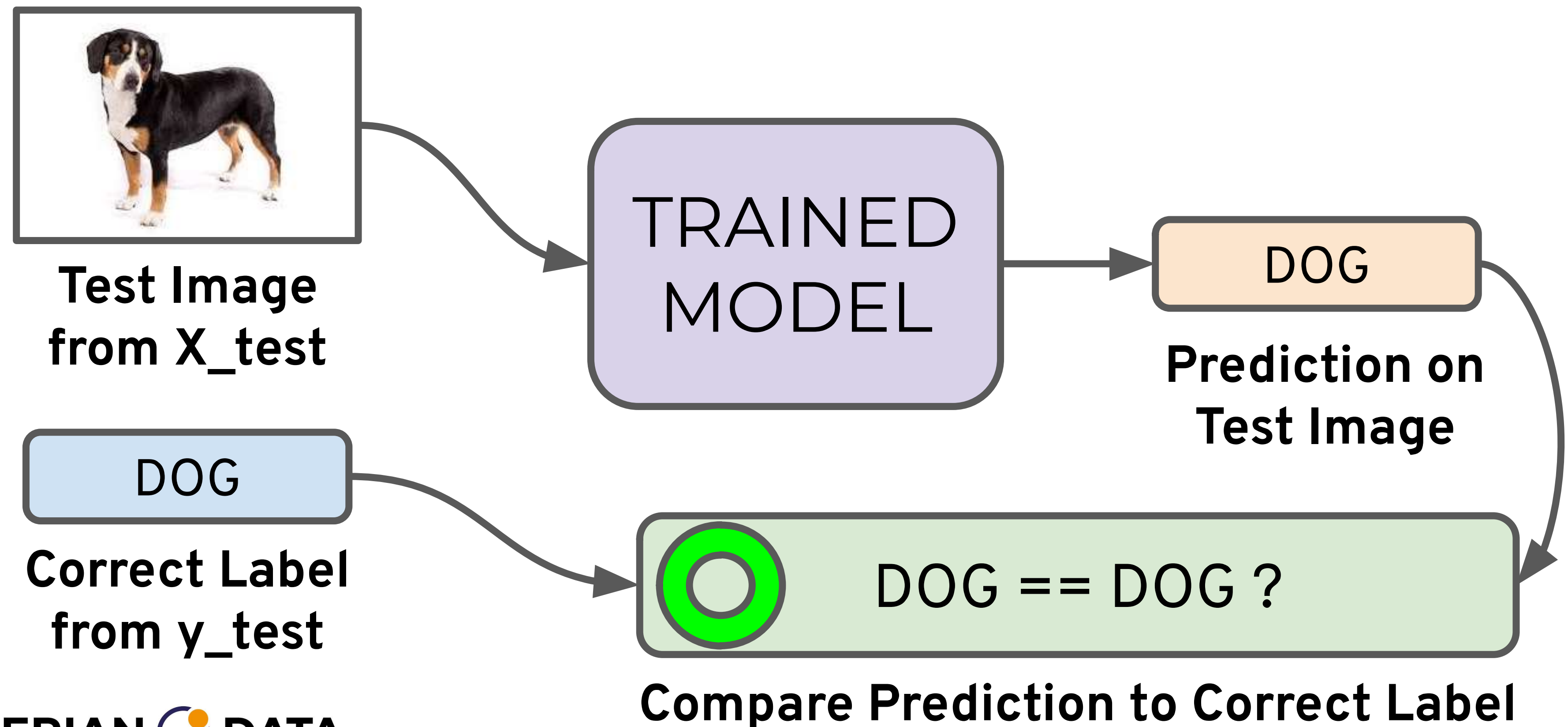
Model Evaluation



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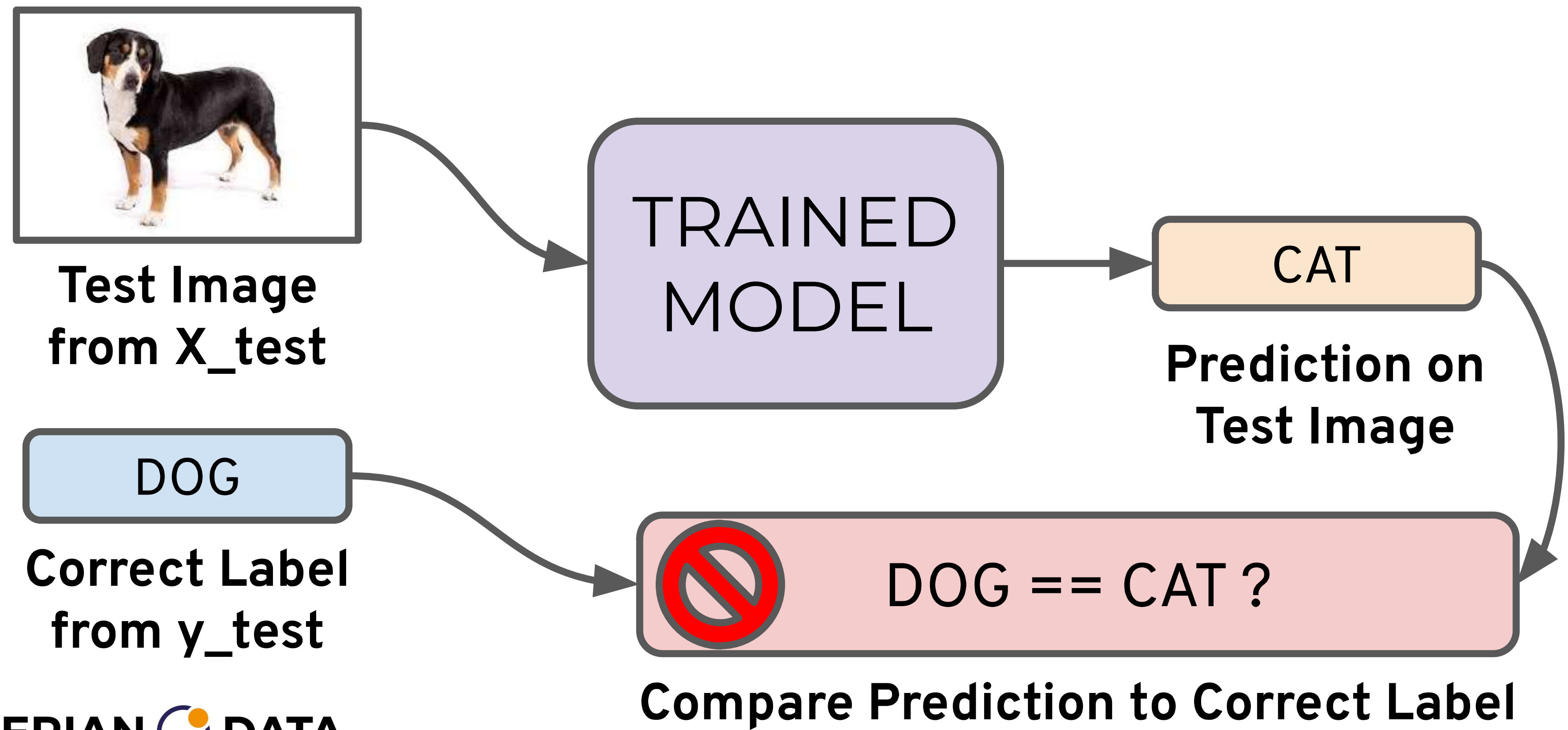
Model Evaluation



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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.**

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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!

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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
  - 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.

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.

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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.

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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 $= \frac{\Sigma \text{ TP}}{\Sigma \text{ condition positive}}$
true condition	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).

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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!)

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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

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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.

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Evaluating Regression

- Let’s discuss some of the most common evaluation metrics for regression:
  - Mean Absolute Error
  - Mean Squared Error
  - Root Mean Square Error

Evaluating Regression

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

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

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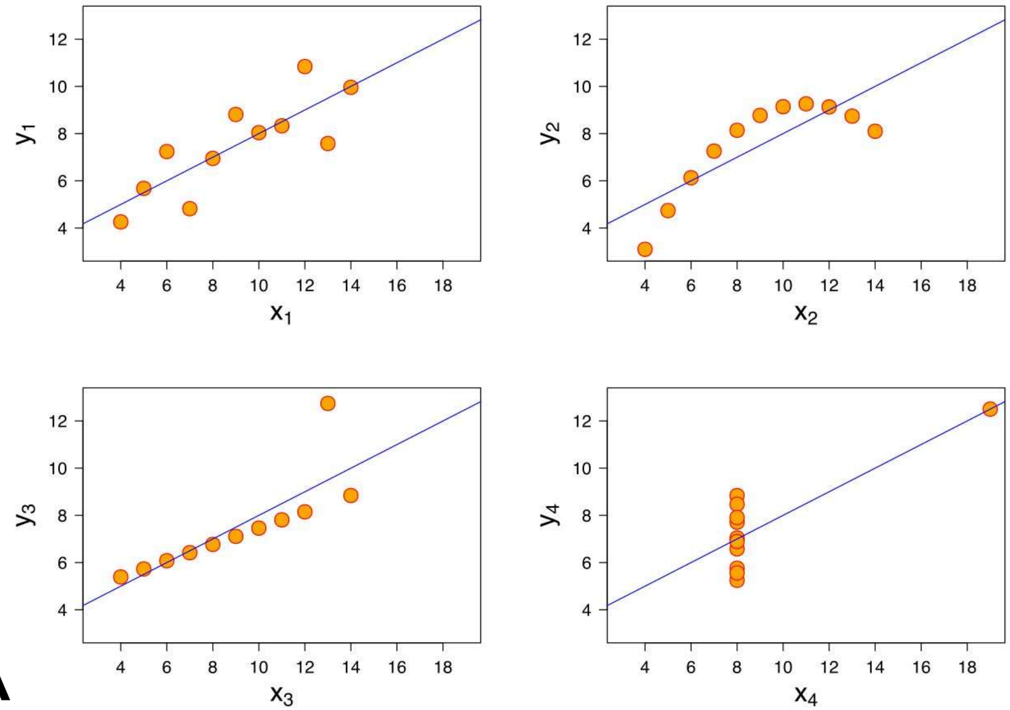
Evaluating Regression

- MAE won’t punish large errors however.



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Evaluating Regression

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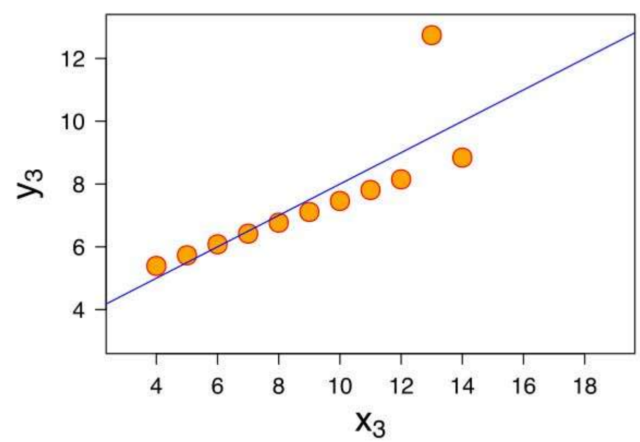
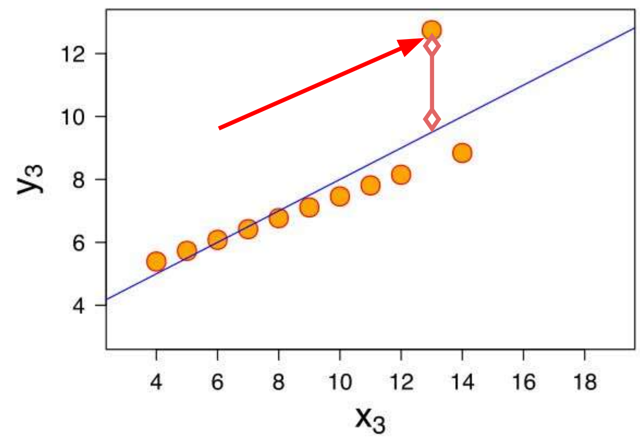


Evaluating Regression

- We want our error metrics to account for these!



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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.

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

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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.

Unsupervised Learning

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Machine Learning

- We've covered supervised learning, where the **label was known** due to **historical labeled data.**
- But what happens when we don't have historical labels?

Machine Learning

- There are certain tasks that fall under unsupervised learning:
  - Clustering
  - Anomaly Detection
  - Dimensionality Reduction

Machine Learning

- Clustering
  - Grouping together **unlabeled** data points into categories/clusters
  - Data points are assigned to a cluster based on similarity

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Machine Learning

- Anomaly Detection
  - Attempts to detect outliers in a dataset
  - For example, fraudulent transactions on a credit card.

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Machine Learning

- Dimensionality Reduction
    - Data processing techniques that reduces the number of features in a data set, either for compression, or to better understand underlying trends within a data set.

Machine Learning

- Unsupervised Learning
    - It’s important to note, these are situations where we **don’t** have the correct answer for historical data!
    - Which means evaluation is much harder and more nuanced!

Unsupervised Process

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Machine Learning

- Later on in the course, we'll explore unsupervised learning processes with specialized neural network structures, such as autoencoders.