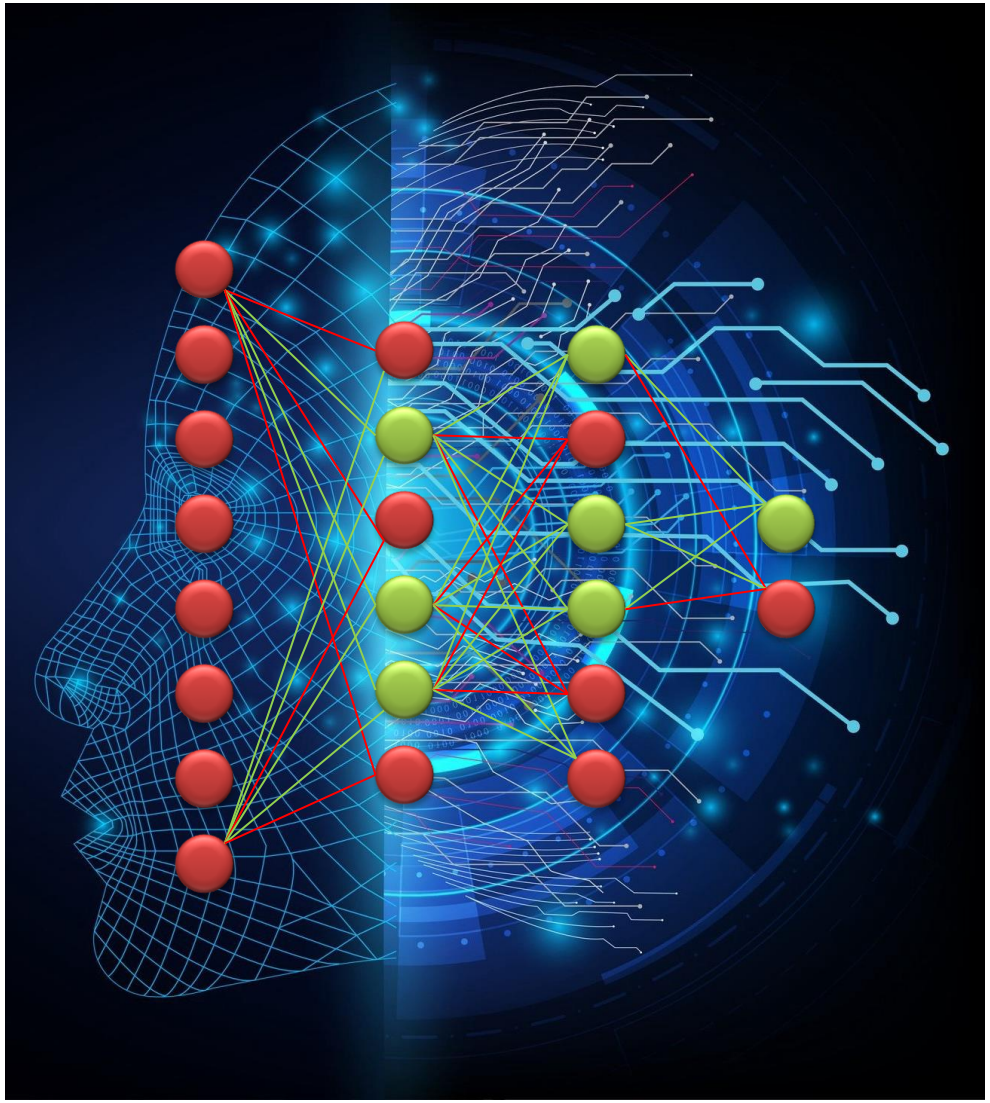
Introduction to Machine Learning for Geoscientists

Amr. Moslim



Today's Agenda

- What is Machine Learning?
- Machine Learning Vs Coding ?
- Machine Learning Algorithm Classes
- Machine Learning Algorithm
- Machine Learning Classifications
- Machine Learning Workflow
- Machine Learning technique
- How does ML work?
- Data Preparation
- Machine Learning Models Evaluation
- Machine Learning Algorithms

What's Machine Learning?

Machine learning is the field of AI that allows systems to learn from past data and make intelligent decisions on their own using algorithms without explicitly programed and improve its experience

Machine Learning vs Coding

Characteristics	Machine Learning Algorithms	Common coding
Objective	To teach the machine to create models to solve the problem without hard coding using data patterns	To use programming language to explicitly code the solution to the problem
Example: v = d/t	Data = (mass, height, width, velocity) Lm = linearregression() Lm.fit() Lm.predict()	Data = (d, t) def velocity(d,t): v = d/t return (v)
Tools	Python, R, Scikit learn, Tensorflow, etc…	Python, R, Visual Basic, Java, Go, Excel
Running time	Most of time in data wrangling and model evaluation	Most of the time in coding the problem and solution
Output	ML model and forecast	Data table, graphs, dashboards
Reproducibility	Yes with the same data formats	Yes with the same data formats
Domain knowledge	It is very important and highly recommended	a must

Machine Learning Algorithm Classes

Supervised Learning

Labeled data

- *Data has labels (reference) model should learn.*
- *Model should be continuously test based on the label prediction or classification.*

Unsupervised Learning

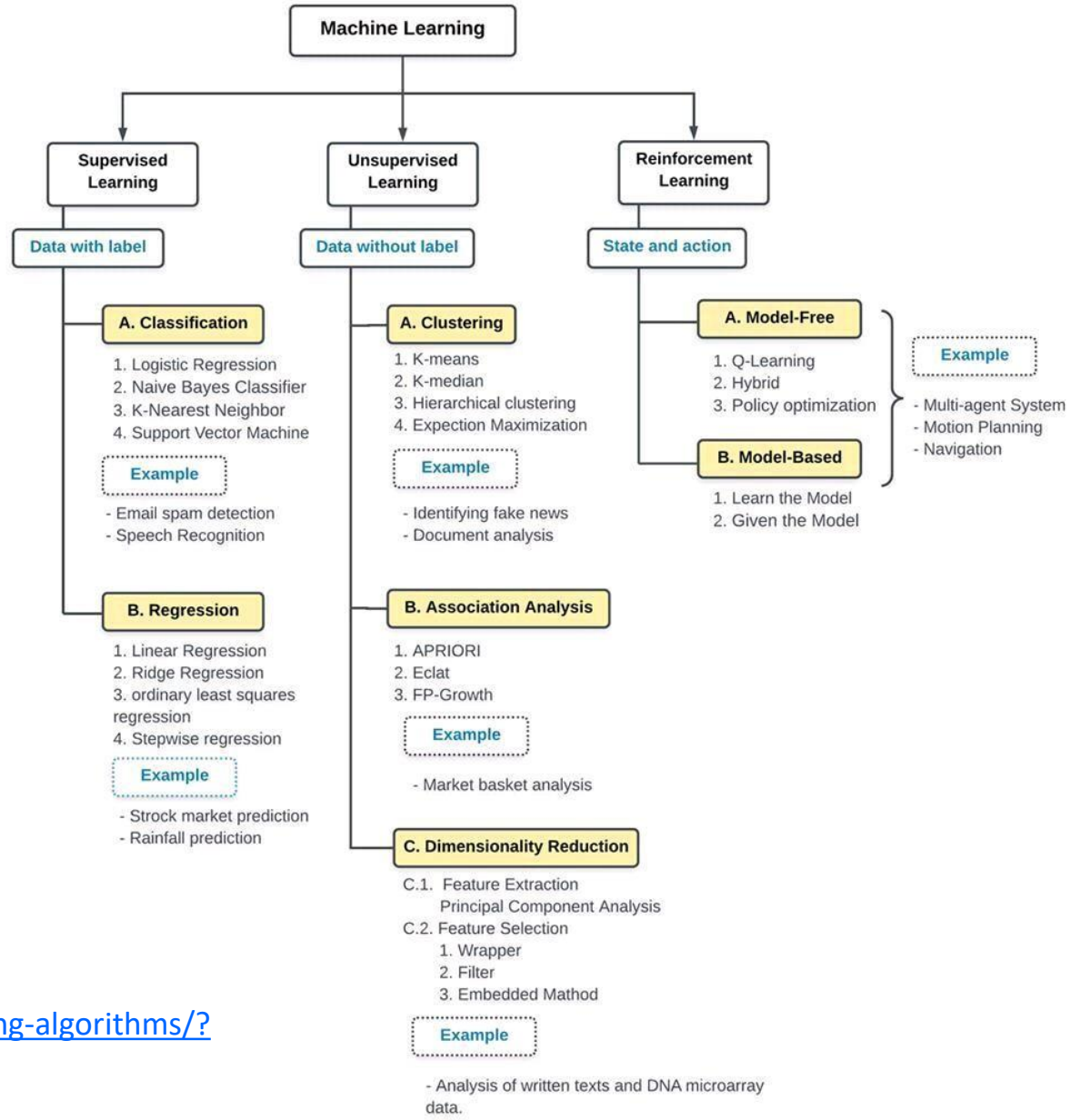
unlabeled data

- *Data has NO labels. Data learn from itself.*
- *Model should be judged based on certain criteria.*

Machine Learning Algorithms

Most commonly used Machine learning algorithms:

1. Linear Regression
2. Logistic Regression
3. Decision Tree
4. SVM
5. Naive Bayes
6. kNN
7. K-Means
8. Random Forest
9. Dimensionality Reduction Algorithms PCA
10. Gradient Boosting algorithms
    1. GBM
    2. XGBoost
    3. LightGBM
    4. CatBoost



https://www.analyticsvidhya.com/blog/2017/09/common-machine-learning-algorithms/?

Machine Learning Algorithm Classification

Supervised Learning

Labeled data prediction

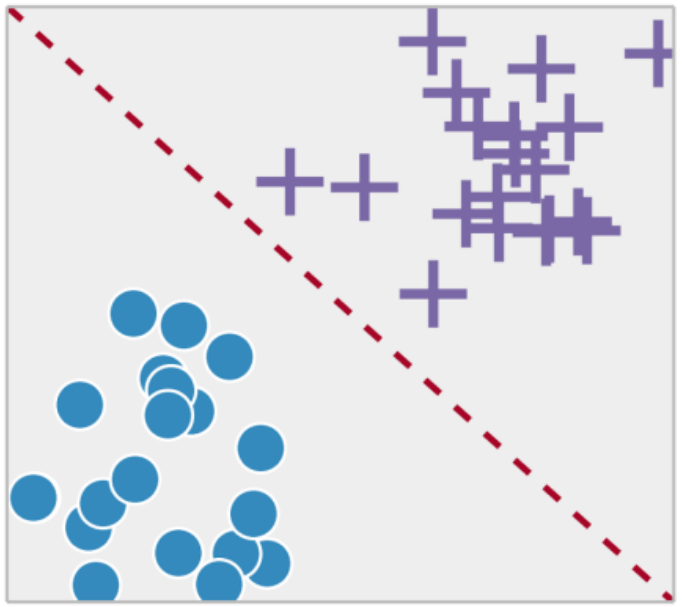
- Regression
- Classification

Unsupervised Learning

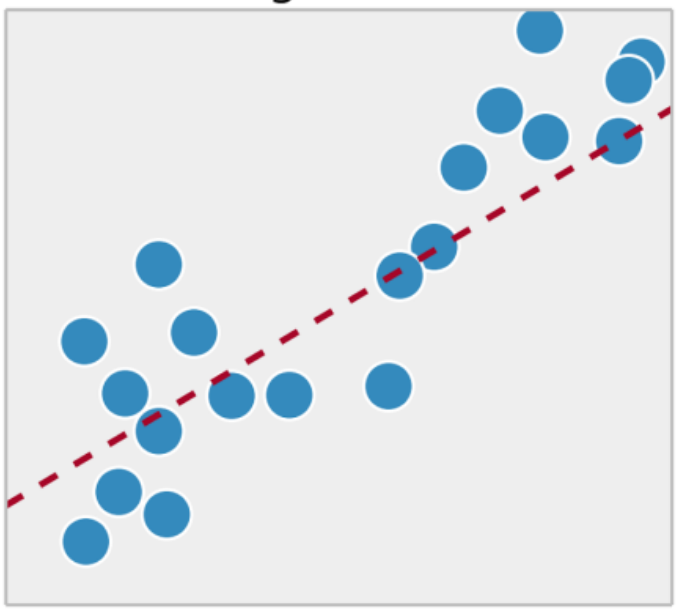
unlabeled data

- Dimensionality reduction
- Clustering

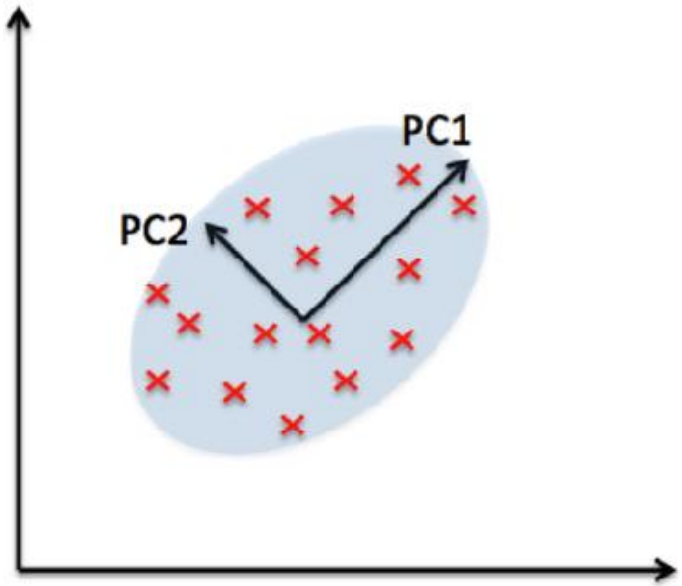
Classification



Regression



Dimensionality reduction



Machine Learning Algorithm Classification

Supervised Learning

Labeled data prediction

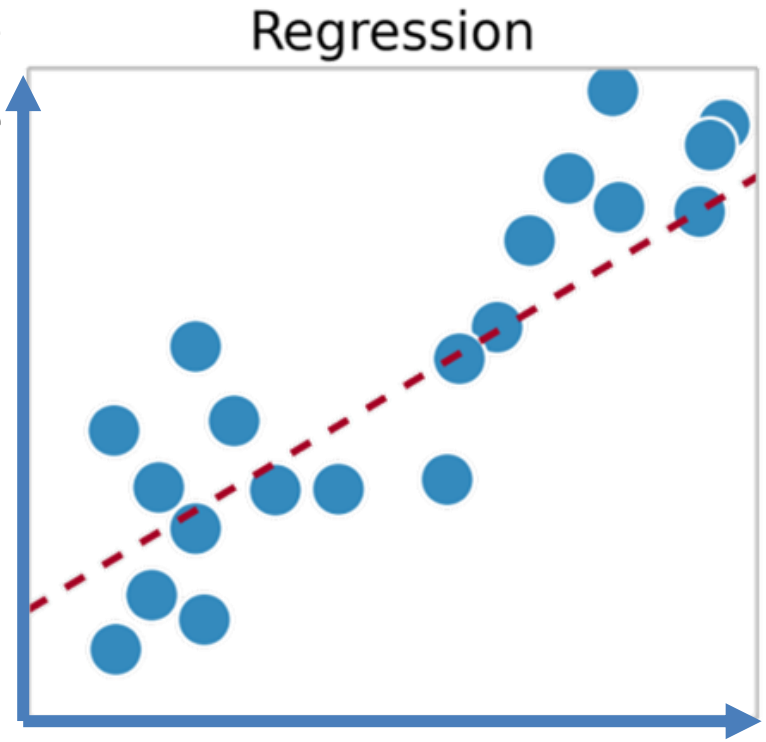
- Regression
- Classification

Regression:

is a set of statistical processes for estimating the relationships between a dependent variable and one or more independent variables.

- Statistical Modeling Technique
- Types (Linear, Logistic, Polynomial, …)
- Data is numerical values (Not Categorical)

Example : missing logs predication



Machine Learning Algorithm Classification

Supervised Learning

Labeled data prediction

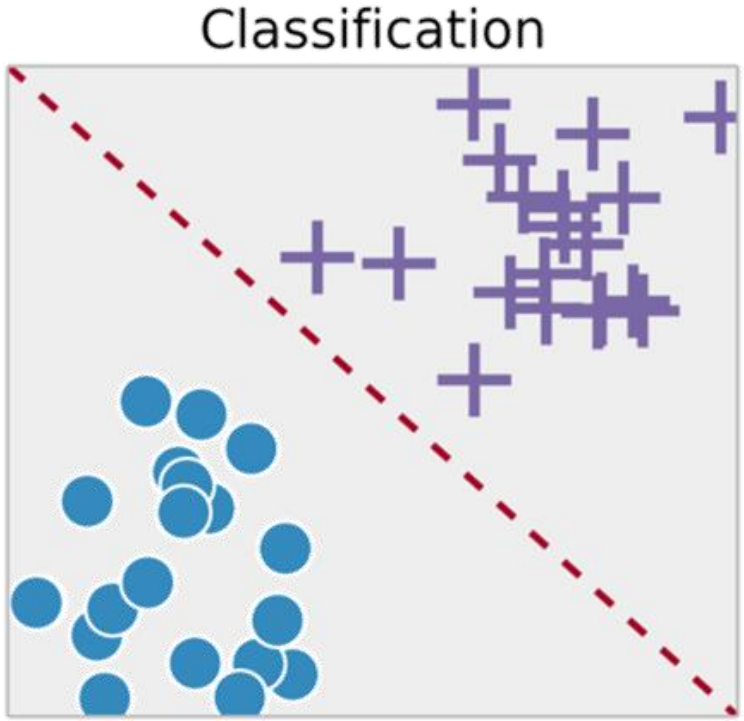
- Regression
- Classification

Classification: (Categorization)

systematic arrangement in groups or categories according to established criteria

- Uses predefined classes
- Belongs to which class

Example : Fraud Detection (Spam / No Spam)
Facies Classification



Machine Learning Algorithm Classification

Unsupervised Learning

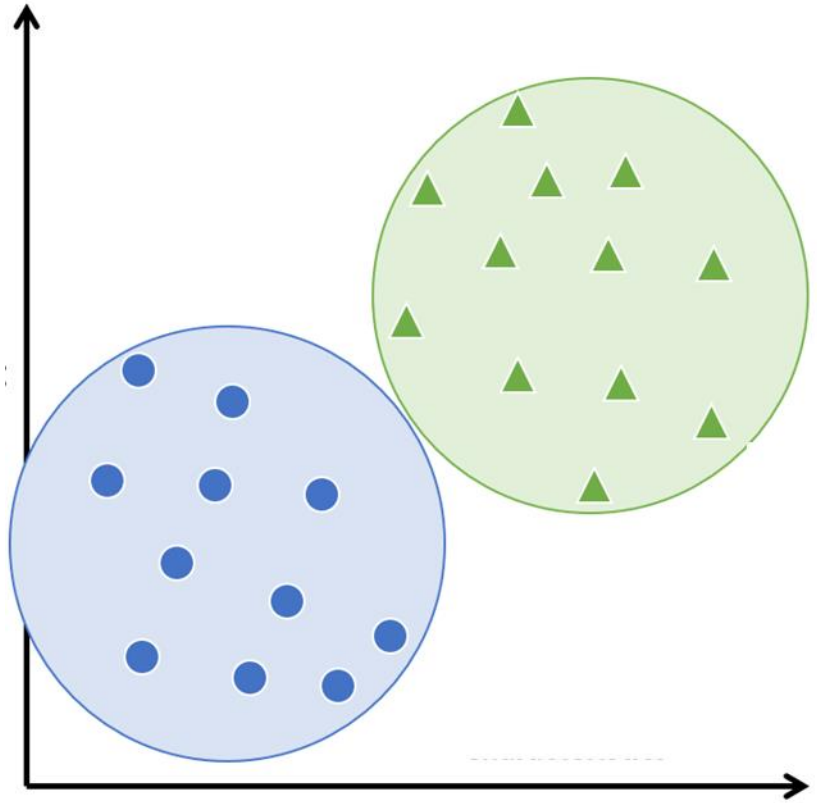
unlabeled data

- Dimensionality reduction
- Clustering

Clustering:

identifies similarities between objects, which it groups according to those characteristics in common and which differentiate them from other groups of objects. These groups are known as "clusters".

- NO predefined classes
- Similar data points properties clusters together



Example : Customer Segmentation

Facies Classification (first time ☺)

Machine Learning Algorithm Classification

Unsupervised Learning

unlabeled data

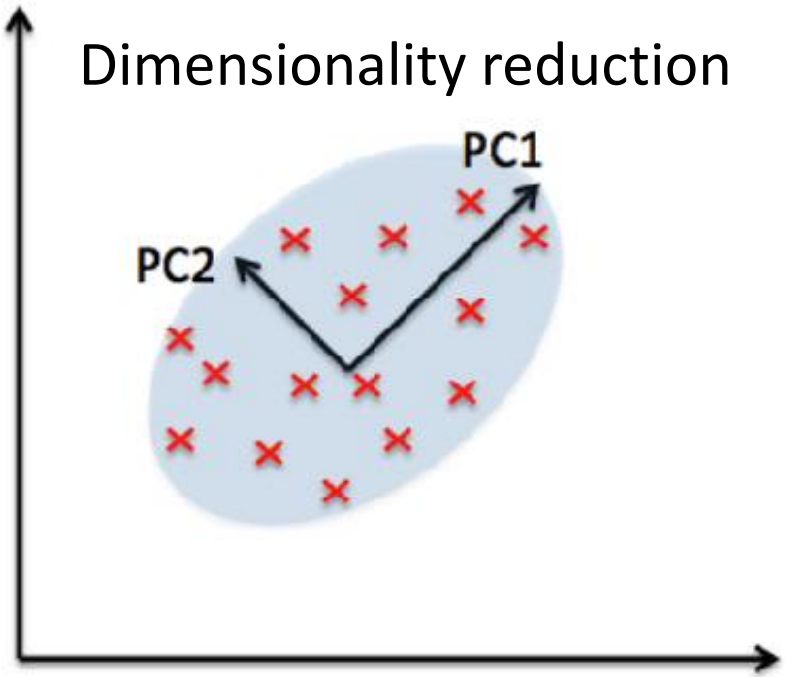
- Dimensionality reduction
- Clustering

Dimensionality Reduction:

Analyzing the datasets with an extremely high number of features
is often performed to obtain better input features for machine learning algorithms.

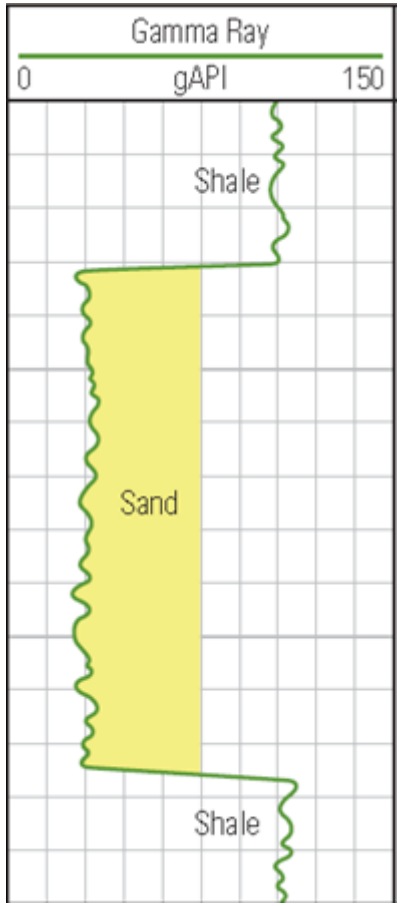
- It improves computational efficiency without sacrificing much on the prediction capability
- removes the collinearity

Dimensionality reduction

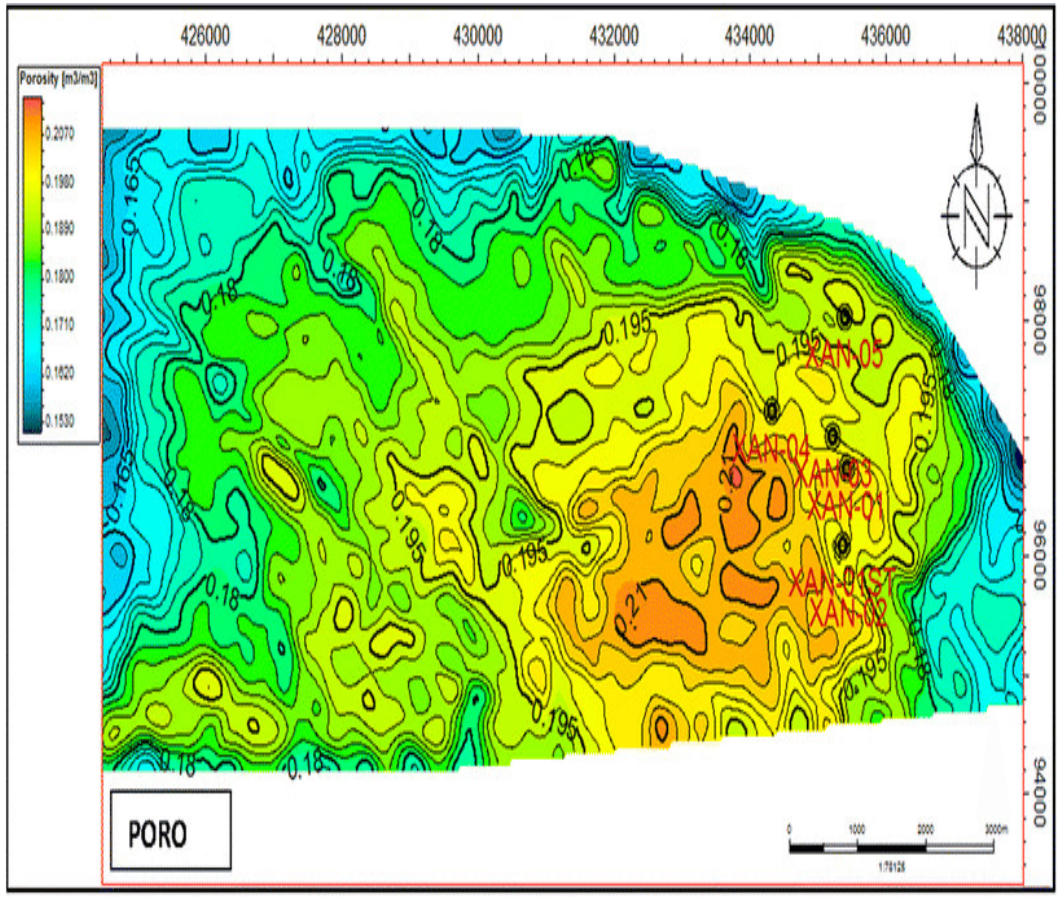


Machine Learning Algorithm Classification

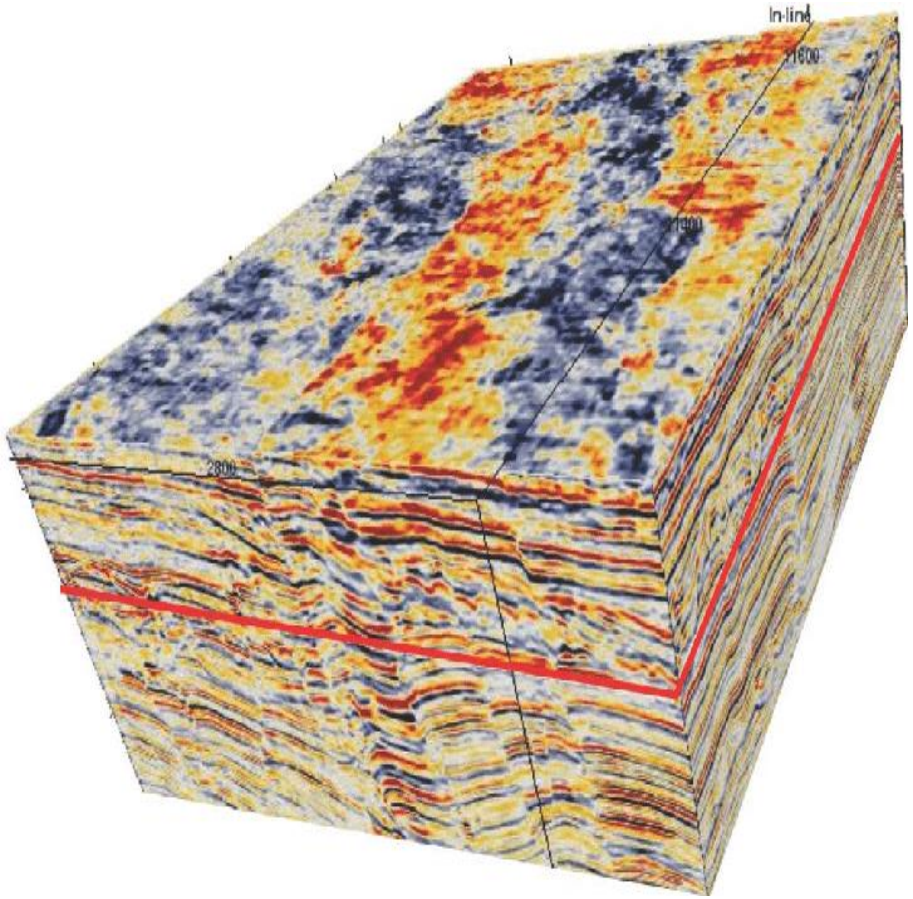
1D Graph



2D Maps



3D Cubes



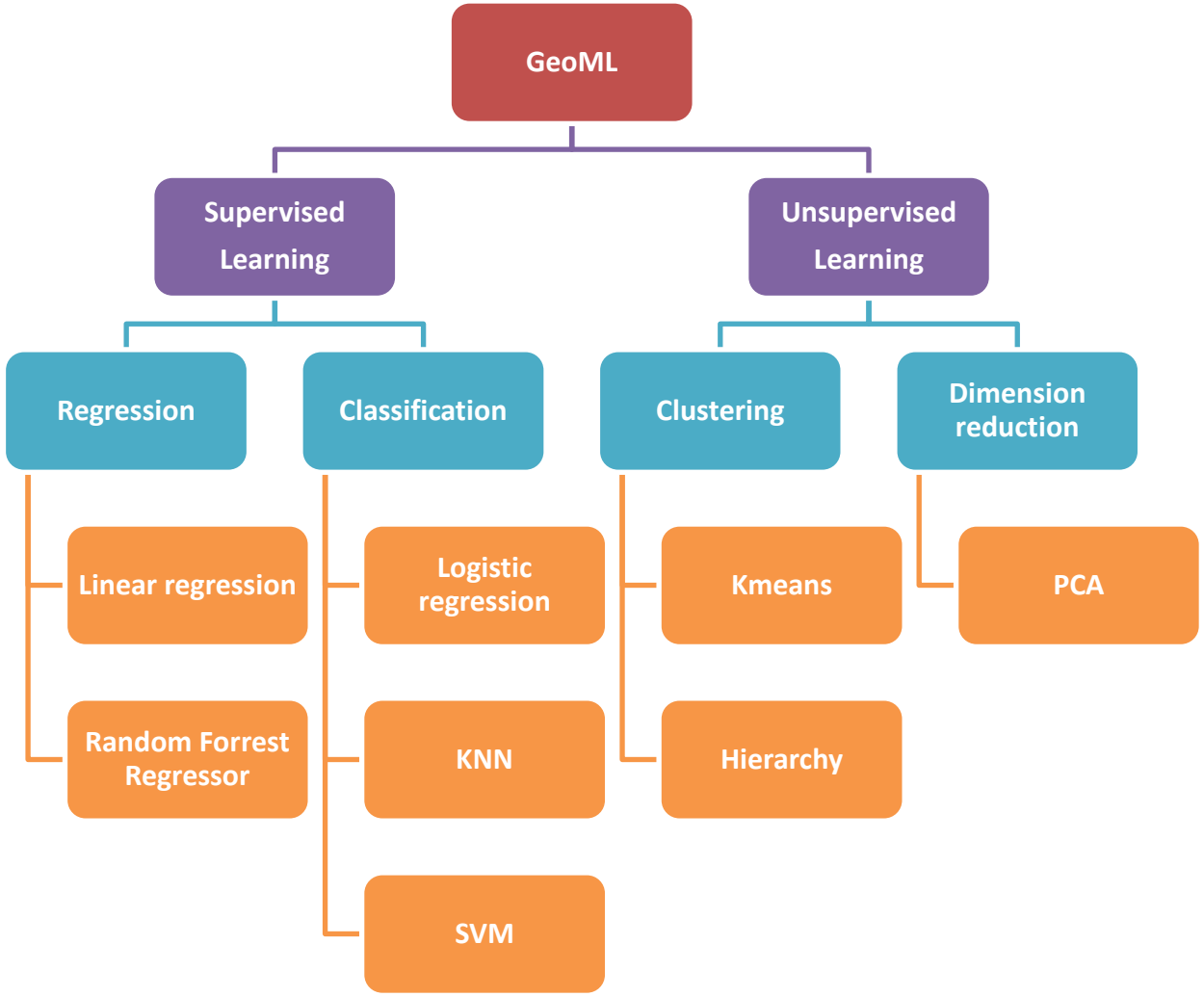
The curse of dimensionality

[Richard E. Bellman]

Machine Learning Algorithms

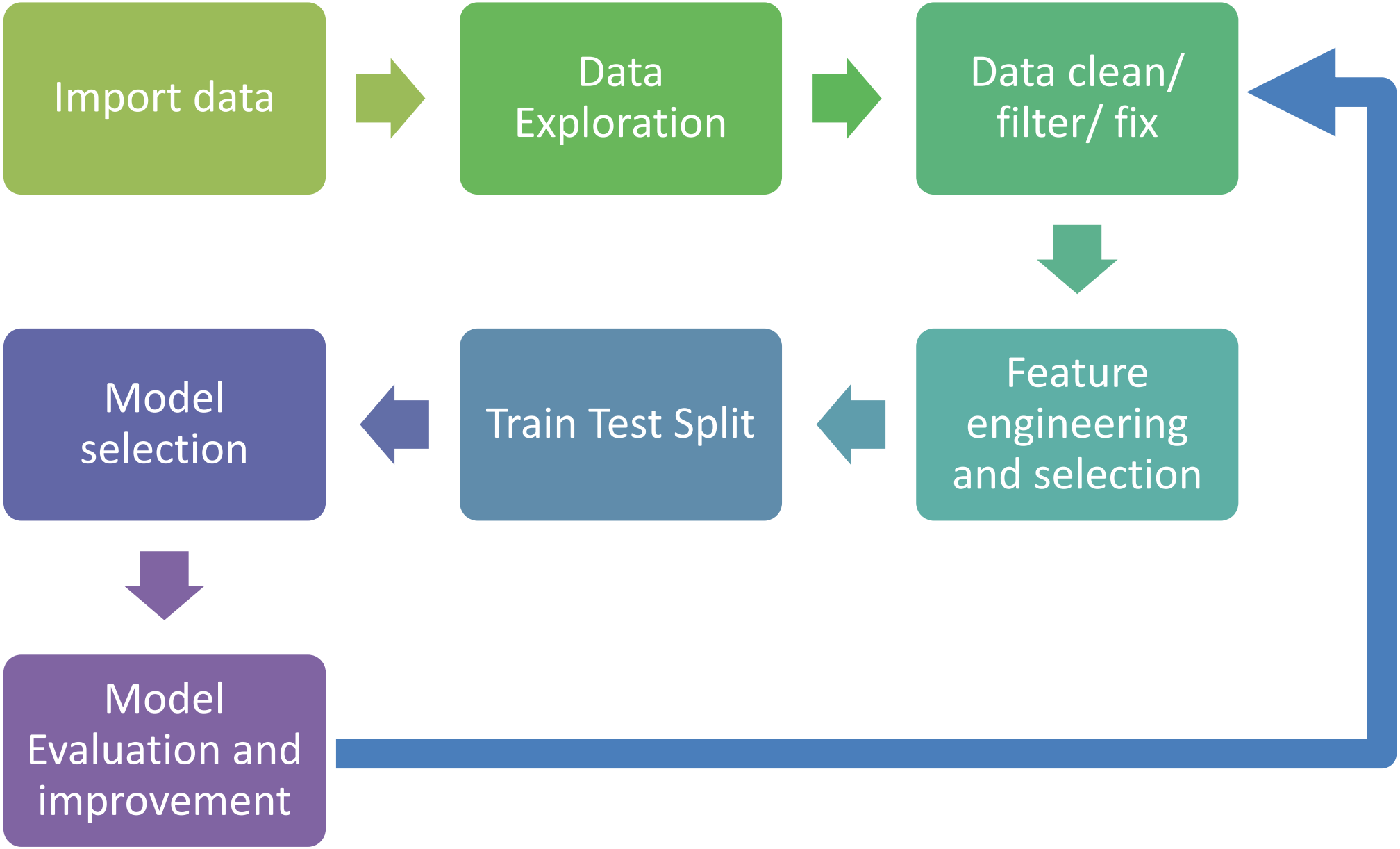
Most commonly used Machine learning algorithms:

1.Linear Regression
2.Logistic Regression
3.Decision Tree
4.SVM
5.Naive Bayes
6.kNN
7.K-Means
8.Random Forest
9.Dimensionality Reduction Algorithms (PCA)
10.Gradient Boosting algorithms
    1. GBM
    2. XGBoost
    3. LightGBM
    4. CatBoost

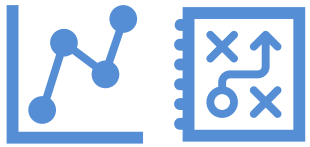


MACHINE LEARNING WORKFLOW

Machine Learning Work flow



Data Conditioning



Data Conditioning

- **Normalization:**

  usually means to scale a variable to have a values between 0 and 1

$$X_{norm} = \frac{X - Xmin}{Xmax - Xmin}$$

- **Standardization:**

  transforms data to have a mean of zero and a standard deviation of 1. not necessary to be between (0,1)

$$z = \frac{x - \mu}{\sigma}$$

x is a data point (x1, x2…xn).

μ is the sample mean.

σ is the sample standard deviation.

Data Conditioning

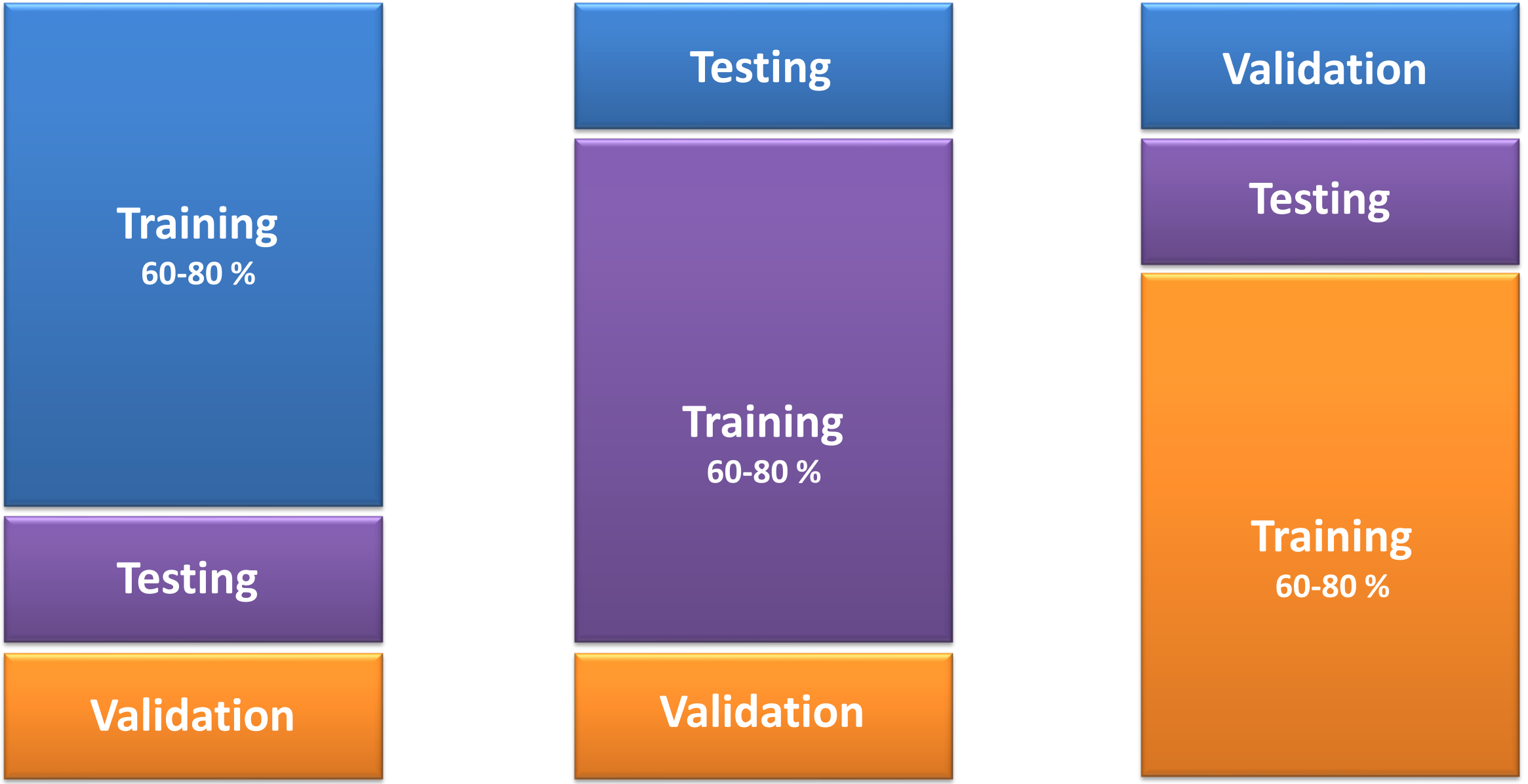
- ## One Hot Encoding :

GR	DT	Rho	Facies
57	105	2.2	Sand
110	53	2.11	Shale
40	59	2.7	Lime

GR	DT	Rho	Sand	Shale	Lime
57	105	2.2	1	0	0
110	53	2.11	0	1	0
40	59	2.7	0	0	1

- ## Missing Values Handling :
  - Remove data observation
  - Replace Missing data with mean value
  - Replace Missing data with value in-between previous and next value

Train – Test - Split



ML MODELS EVALUATION

Model Evaluation – Loss Function

Cost Function:

“It is a function that measures the performance of a model for any given data. Cost Function quantifies the error between predicted values and expected values and presents it in the form of a single real number”

Types of Cost functions:

- **MSE**

$$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2$$

- **RMSE**

$$\mathrm{RMSD} = \sqrt{\frac{\sum_{i=1}^{N}(x_i - \hat{x}_i)^2}{N}}$$

- **R2**

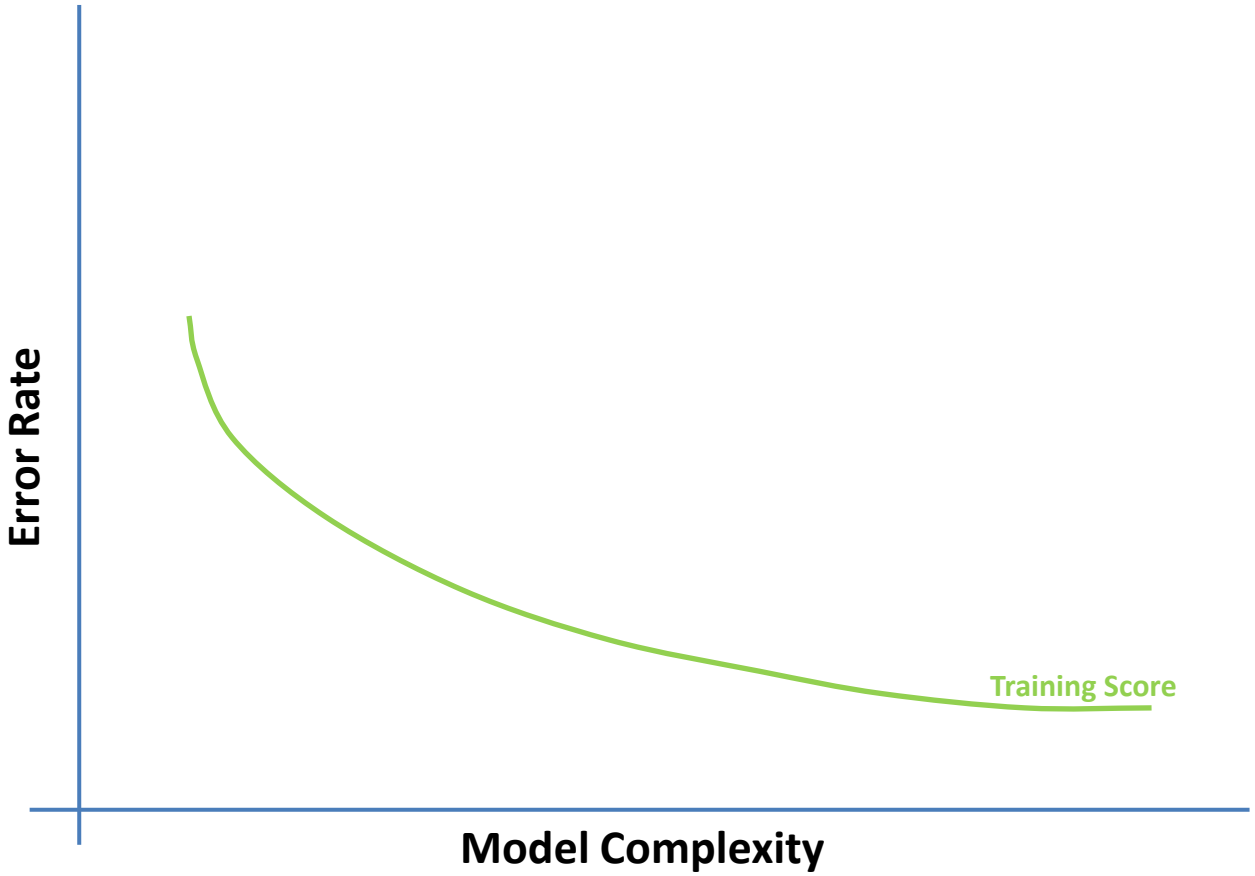
$$R^2 = 1 - \frac{RSS}{TSS}$$

R^2 = coefficient of determination

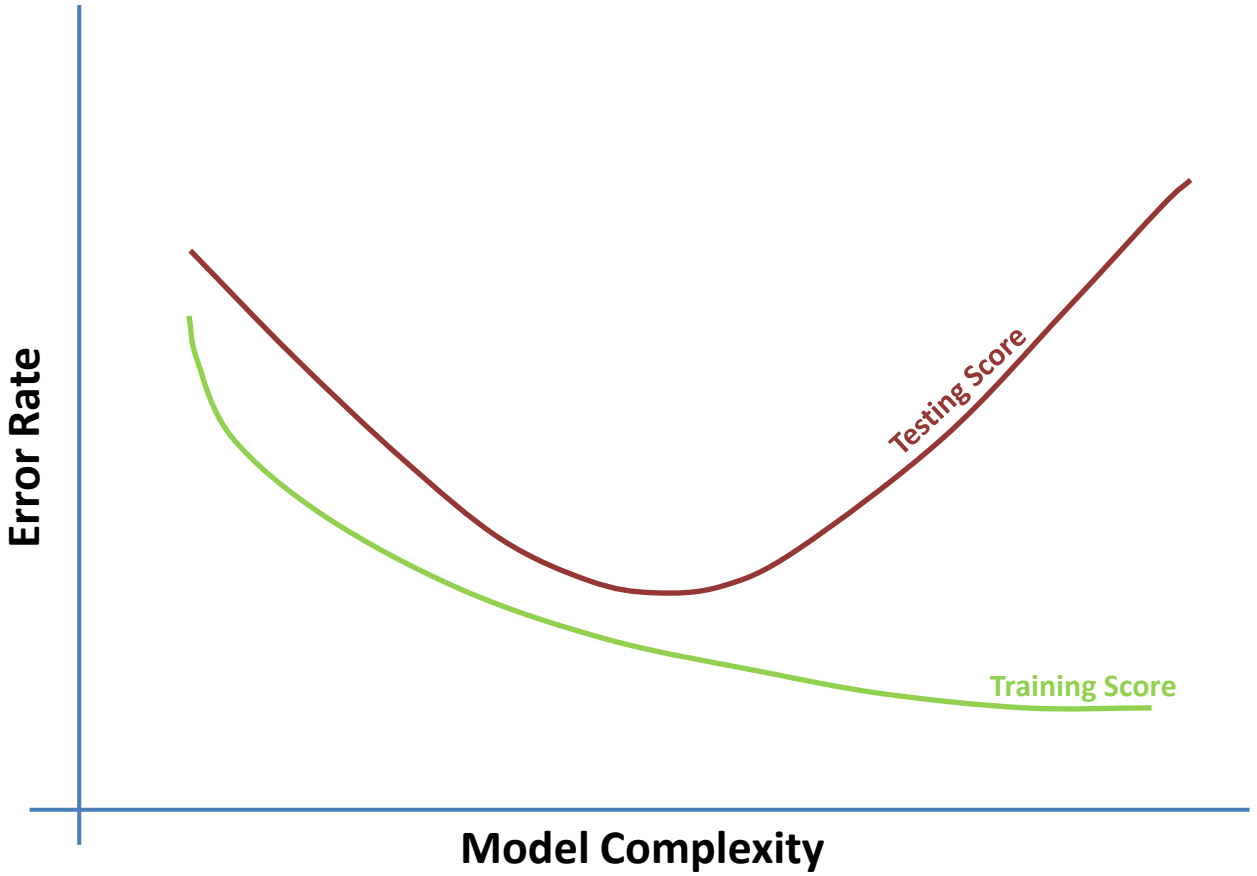
RSS = sum of squares of residuals

TSS = total sum of squares

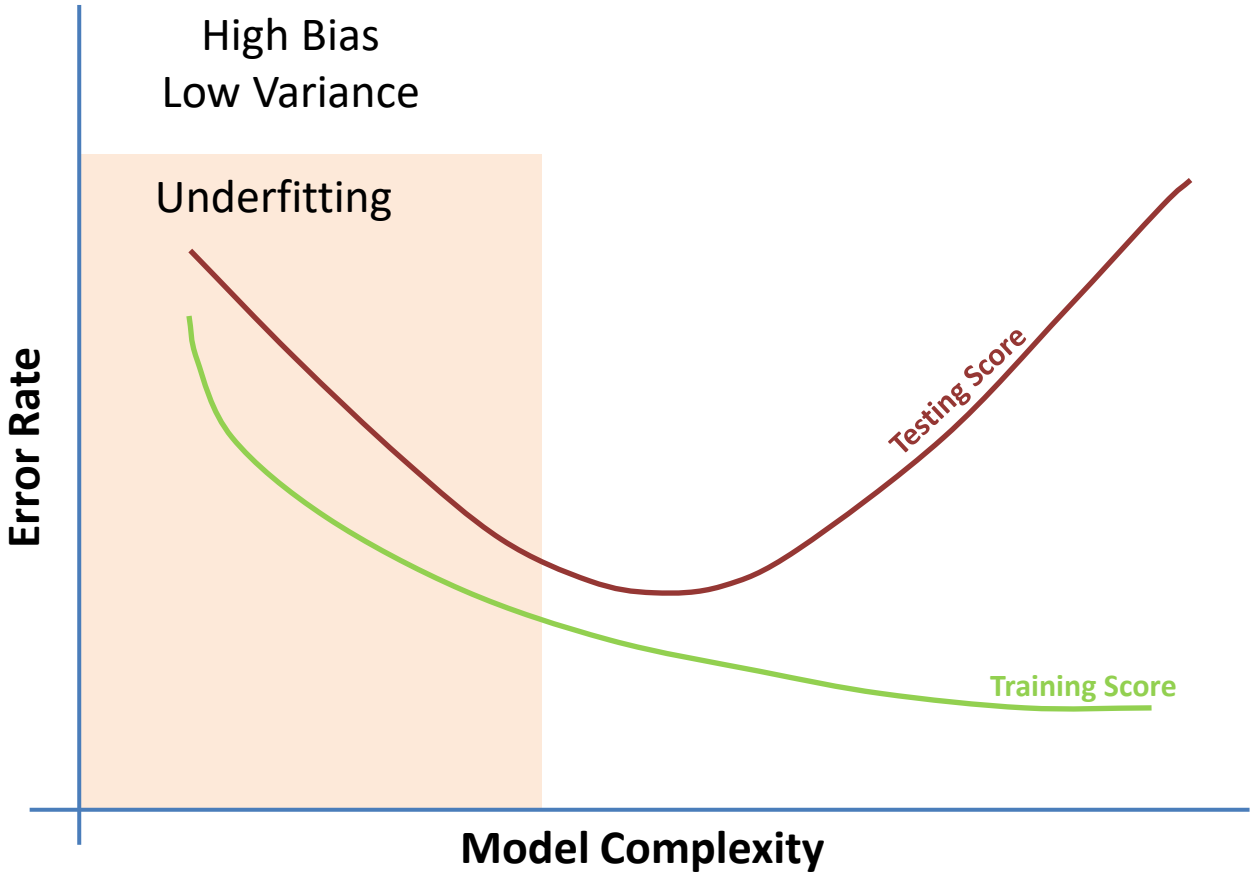
Model Evaluation - Error vs Model Complexity

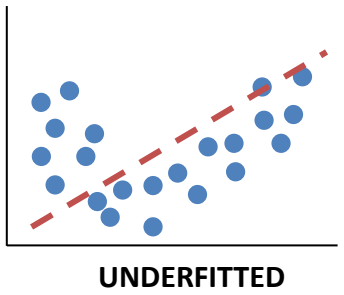


Model Evaluation - Error vs Model Complexity

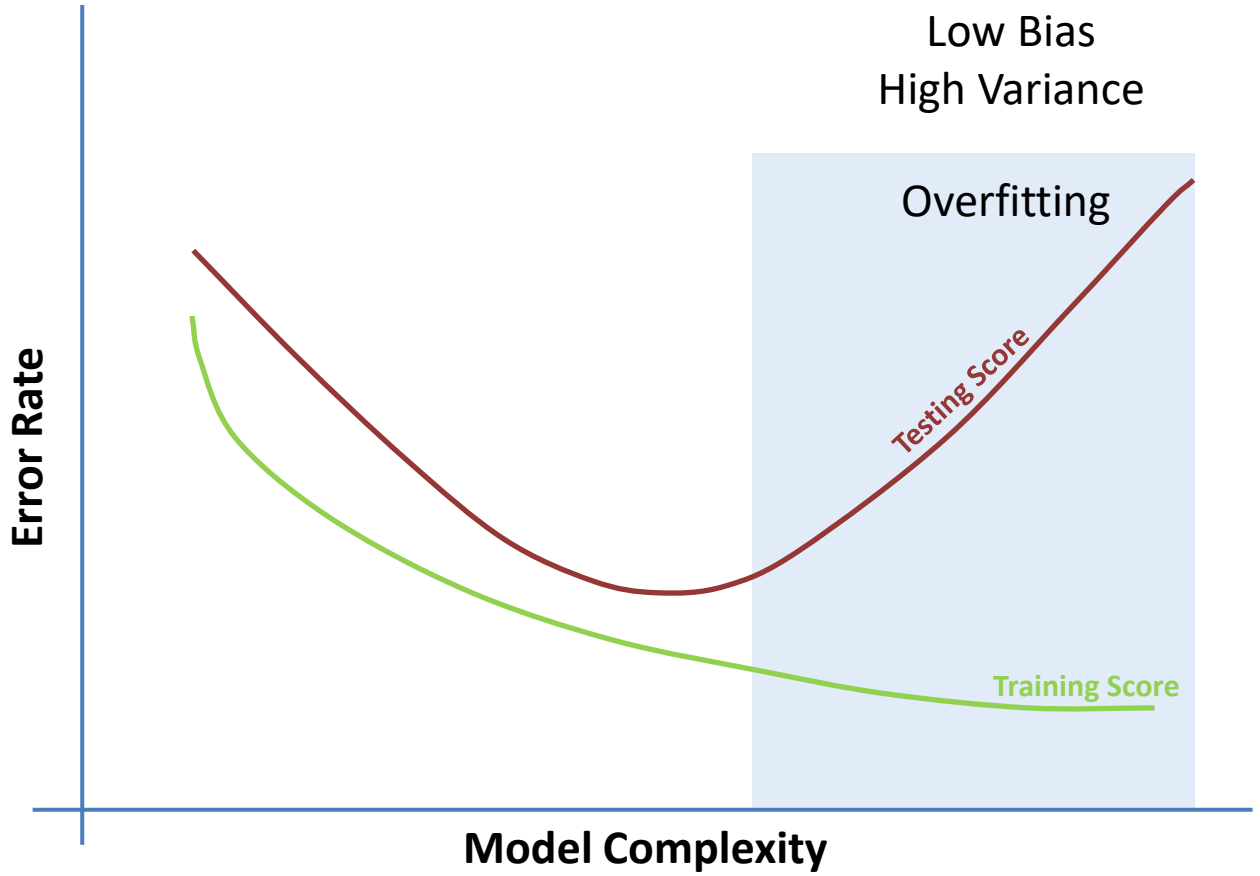


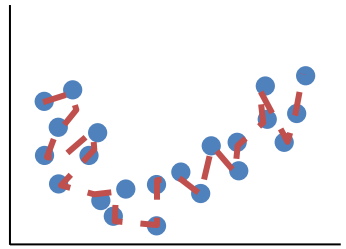
Model Evaluation – Underfitting



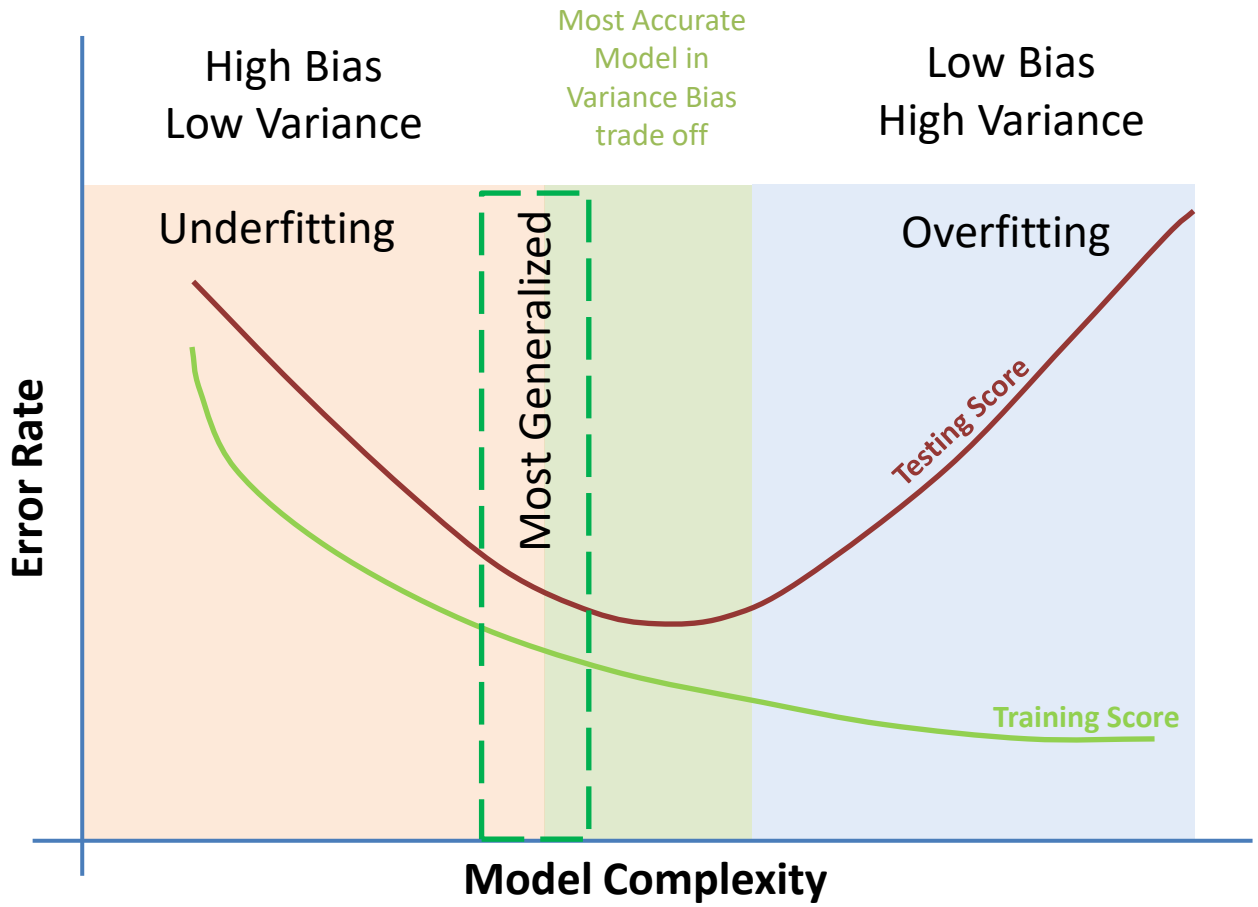


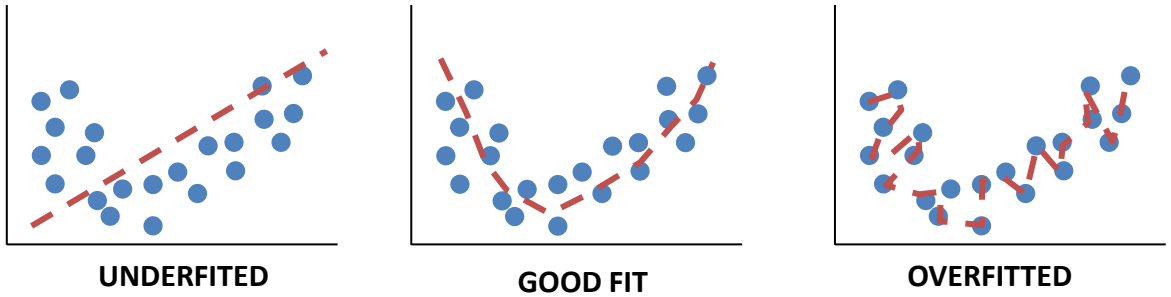
Model Evaluation - Overfitting



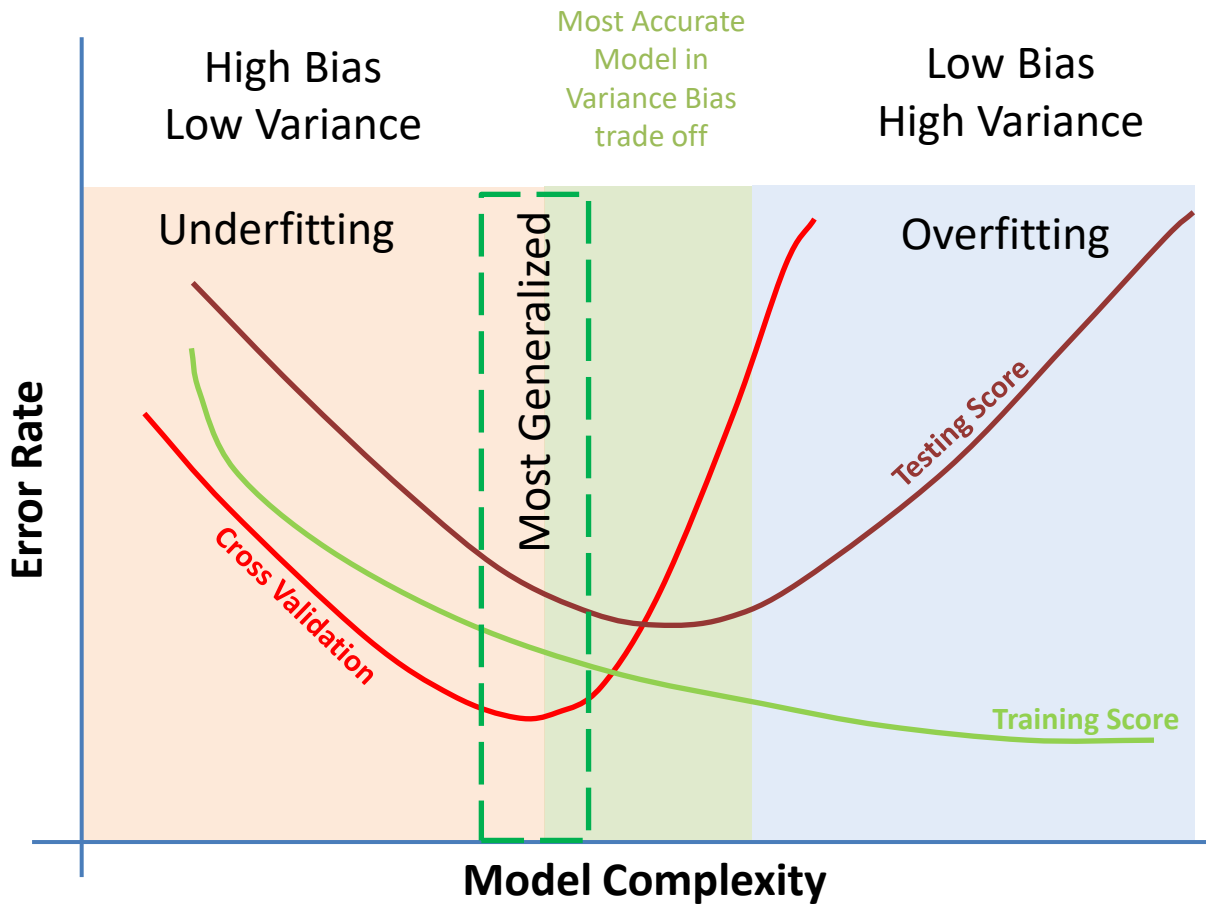


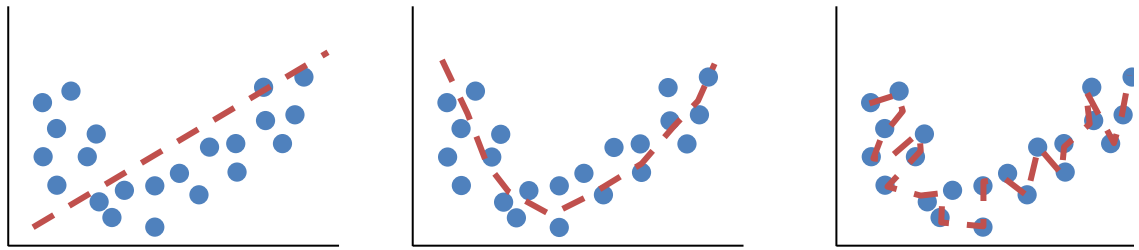
Model Evaluation - Good Fit



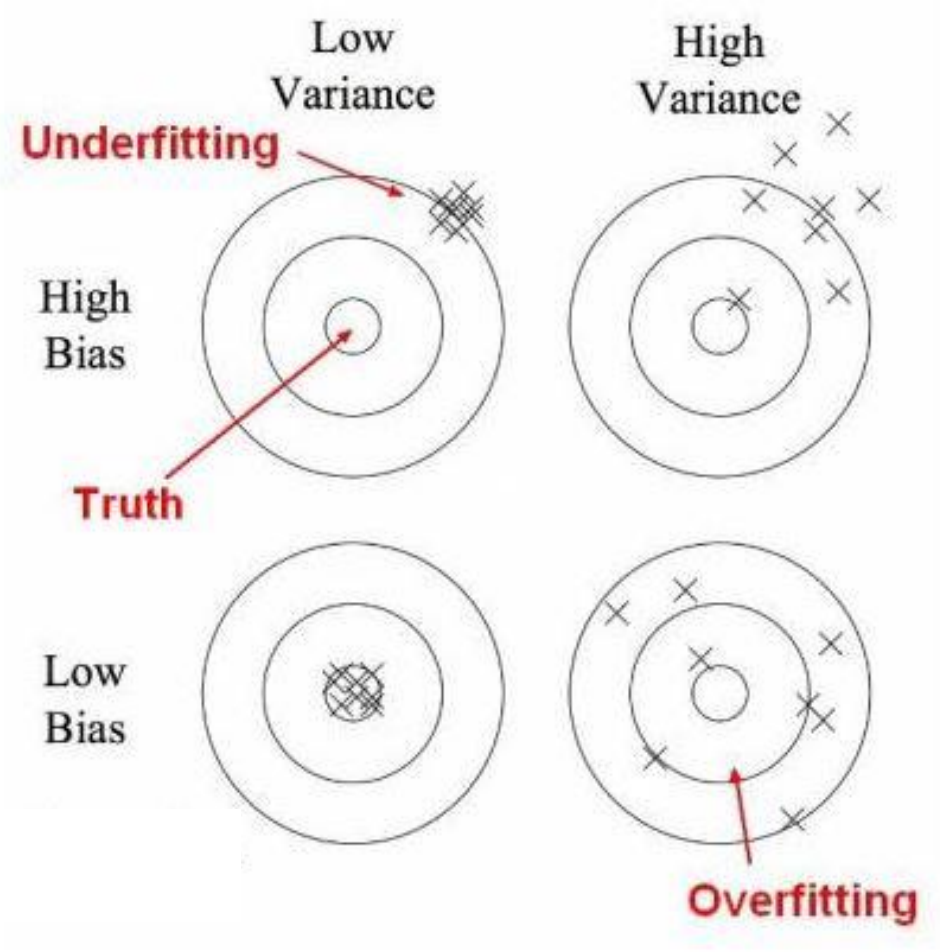


Model Evaluation



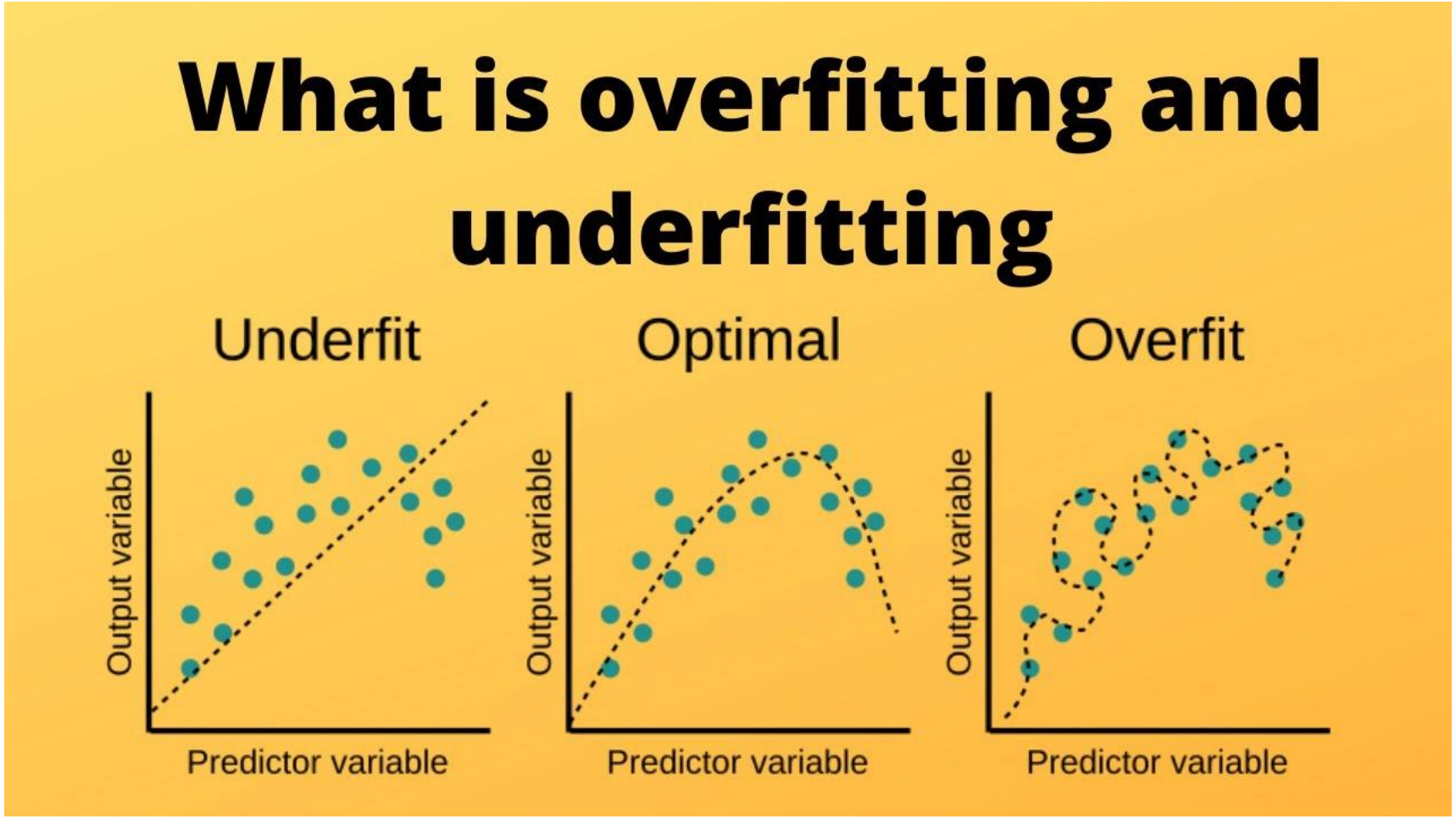


Most Accurate



UNDERFITED GOOD FIT OVERFITTED

Model Evaluation



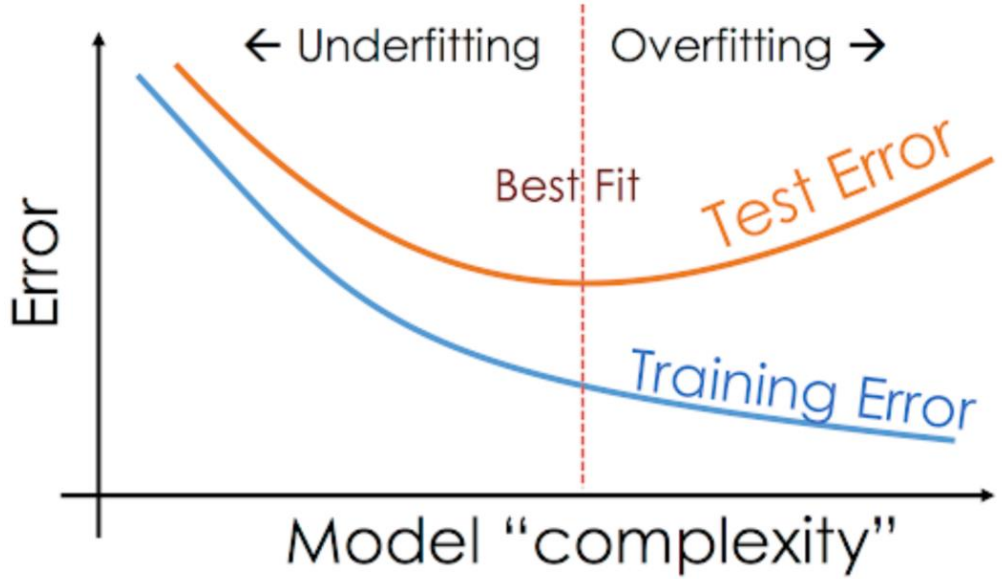
Model Evaluation

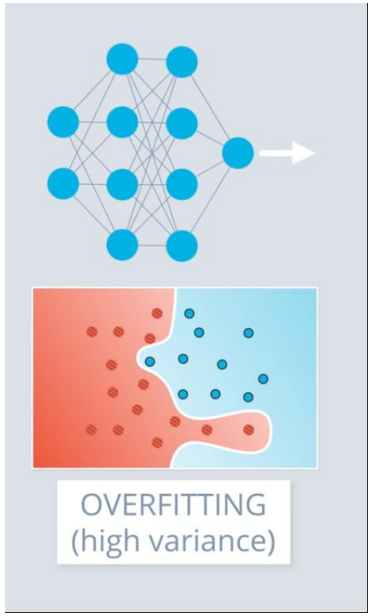
Overfitting means the model has been trained too well

- **The model knows too much details for every data point**
- **The model includes noise as well as the data**
- **Negatively impact the models ability to generalize**
- **More likely to happen in nonlinear / nonparametric data**

Characteristics of Overfitting:

- High Variance
- Low Bias
- Low standard deviation
- No generalization





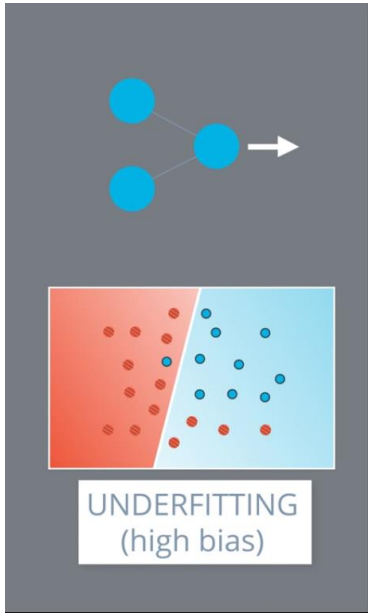
Model Evaluation

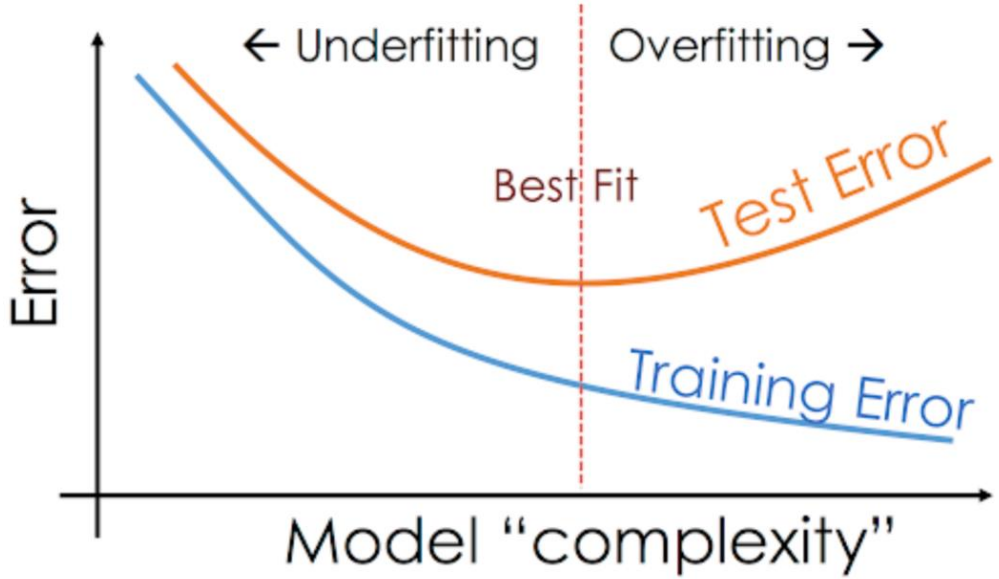
under-fitting means the model is too simple for the training data and test data

- The model knows so little for the whole data set
- It will have poor performance on the training data
- Negatively impact the models ability to generalize
- It is easy to detect given a good performance metric

Characteristics of Overfitting:

- Low Variance
- High Bias
- High standard deviation
- Low generalization





Model Evaluation - How to Overcome Overfitting / Underfitting

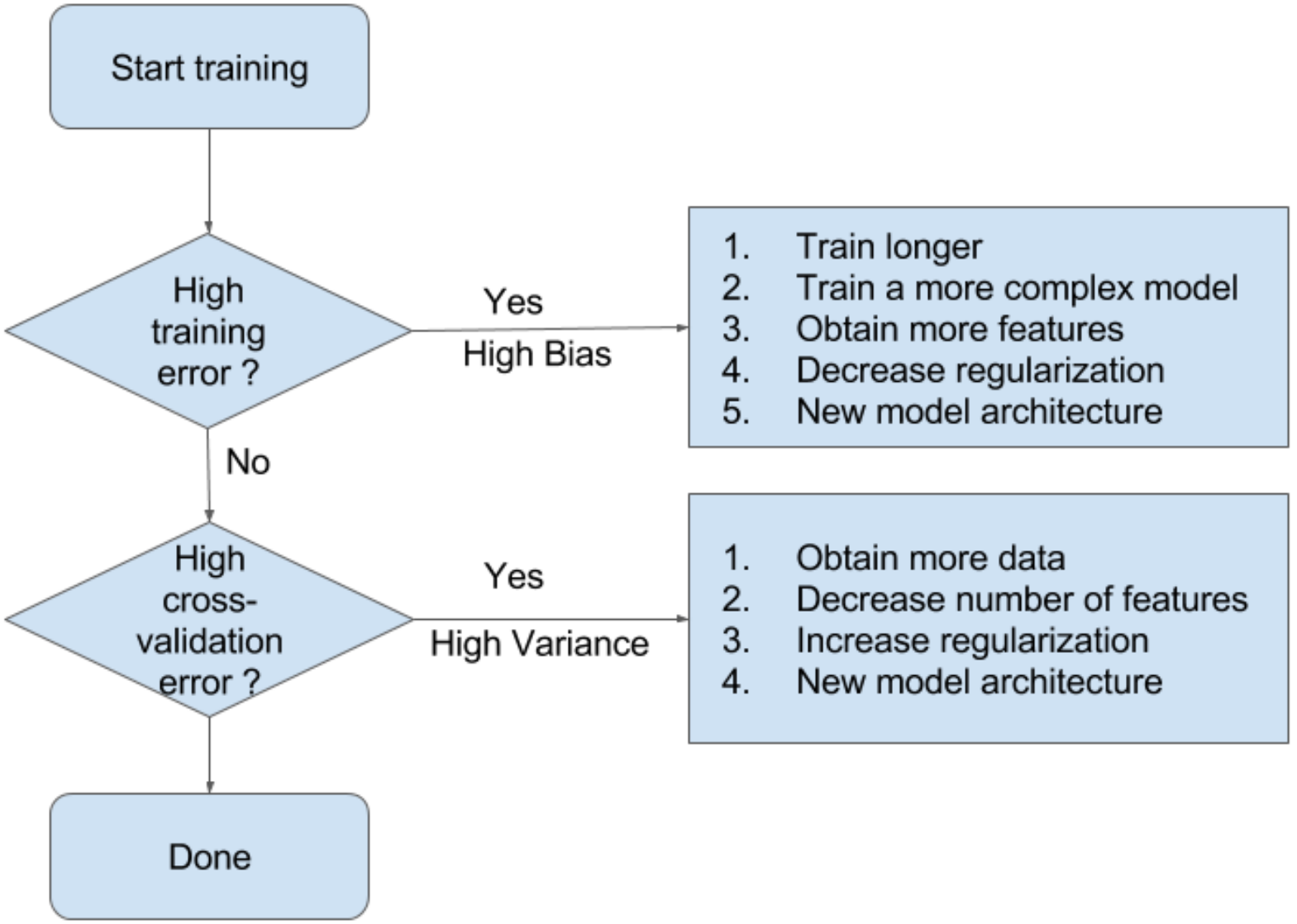
- **Create a validation set:**
  - a subset of your training data that you hold back from your machine learning algorithms until the very end of your project to ground check the model performance.

- **Feature engineering :**
  - You try tune the features matrix, specially with collinearity and dependencies that might incline the model to over fit.

- **Use cross validation:**
  - Using cross validation is a gold standard in applied machine learning for estimating model accuracy on unseen data. If you have the data, using a validation dataset is also an excellent practice

- **Use algorithms hyper-parameters :**
  - Each algorithm has a set of parameters that can be used to handle the fitting problems

Model Evaluation - How to Overcome Overfitting / Underfitting



HOW DOES ML WORK?

Linear Regression

- ***Objective:***

  model the expected value of a continuous variable, ***Y***, as a linear function of the continuous predictor, ***X***

- ***Model structure:***

  $Y = Ax + B$

- ***Model assumptions:***

  Y is normally distributed, errors are normally distributed, and independent

- ***Parameter estimates and interpretation:***

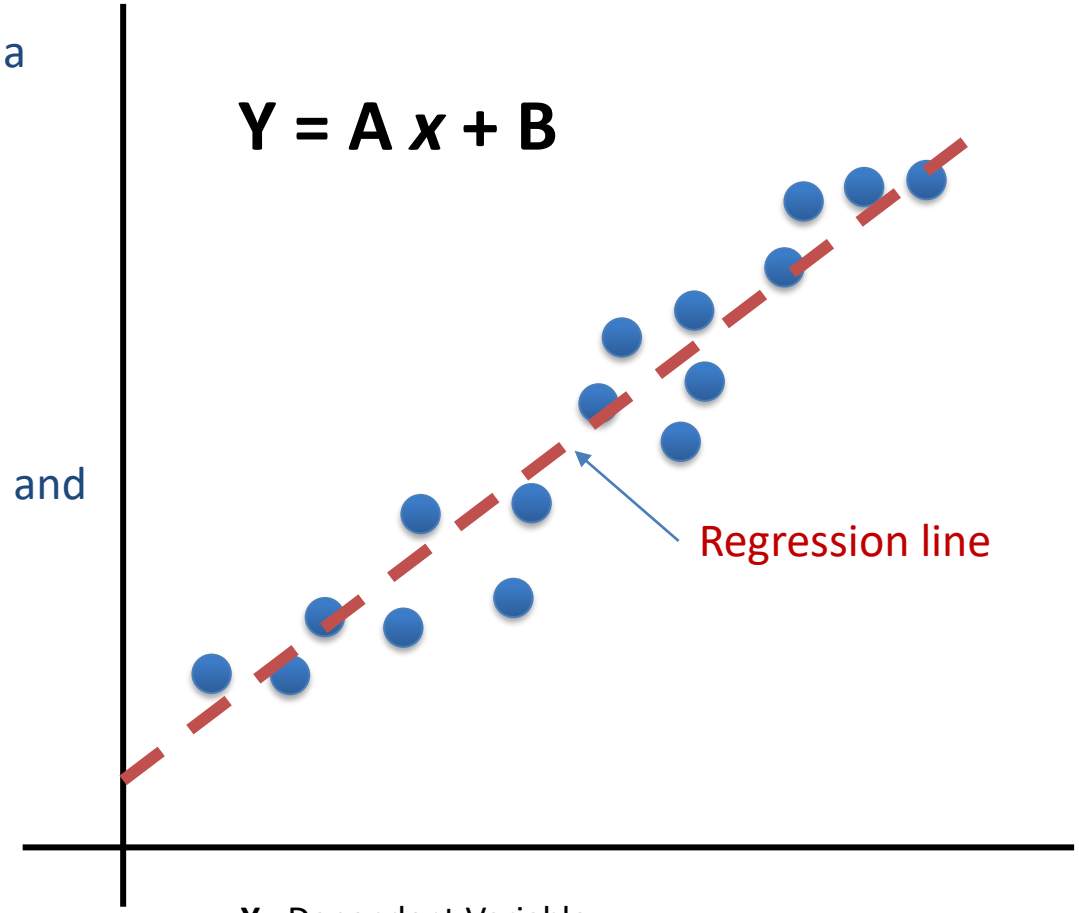
  B the intercept, and **A** is estimate of the slope

- ***Model fit:***

  R^2, residual analysis

- ***Model selection:***

  possible predictors, which variables to include?



Y : Dependent Variable
A : Slope
***x* :** Independent variable
B : Intercept

Linear Regression - Gradient Descent

- ***Objective:***

  To minimize the error function to close to zero (Cost Function) If possible.

- ***Function structure:***

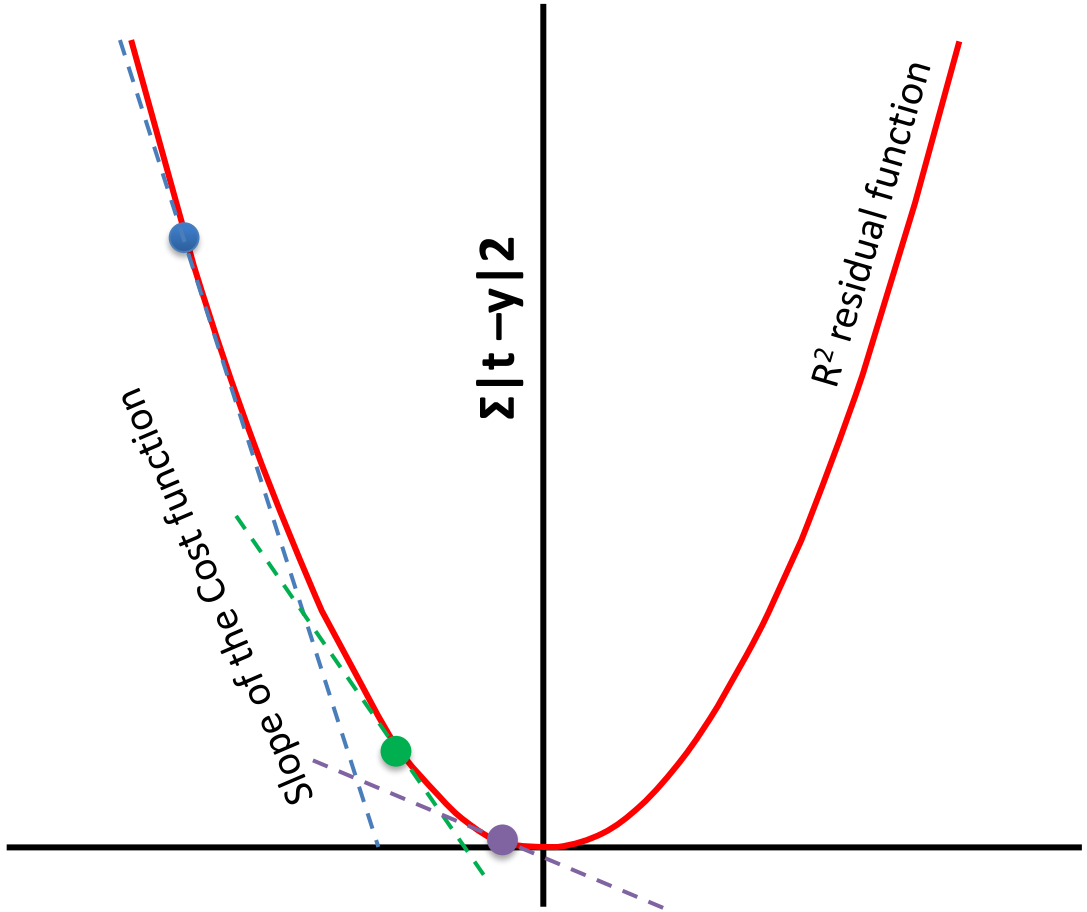
  Cost function : $\Sigma \left| t - y \right|^2$

- ***Model assumptions:***

  Slope of the *cost function* ~= Zero, then it is the best prediction

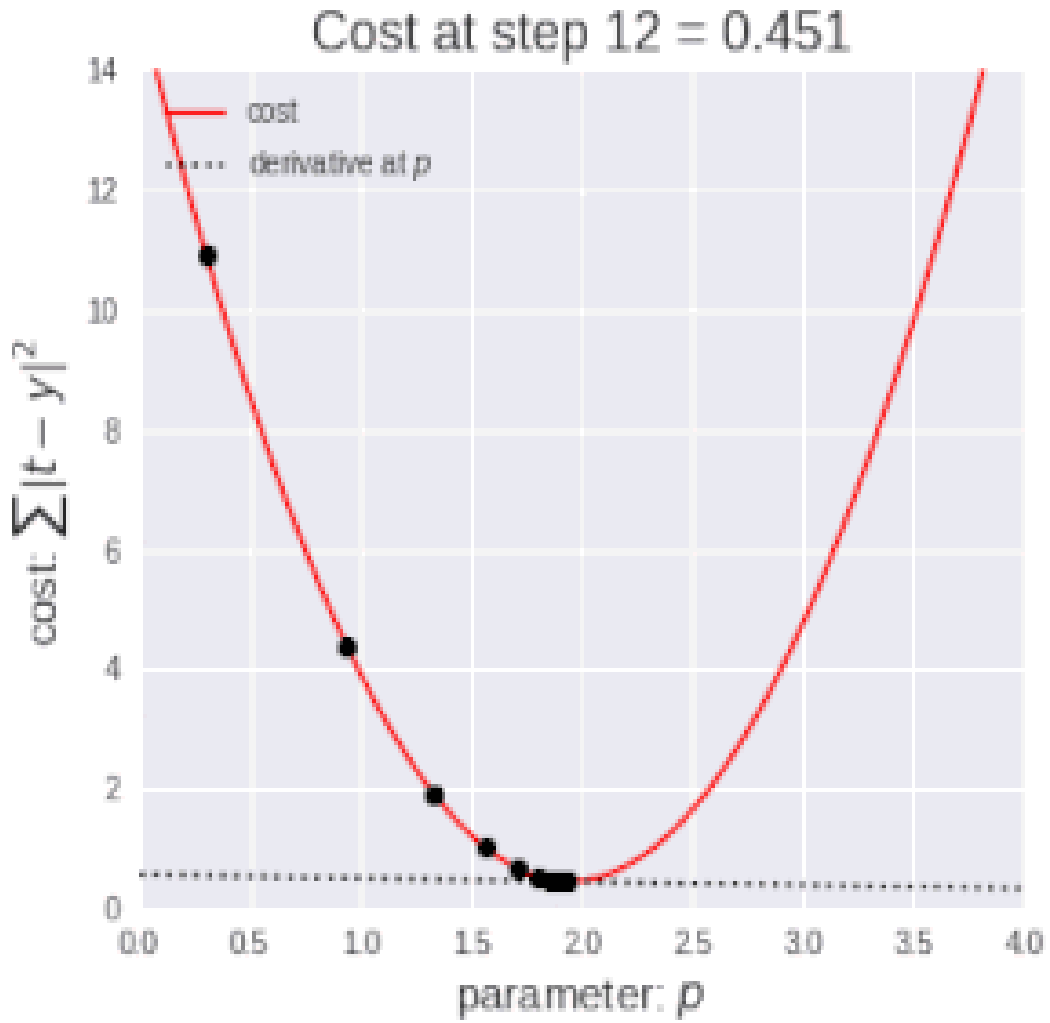
- ***Parameter estimates and interpretation:***

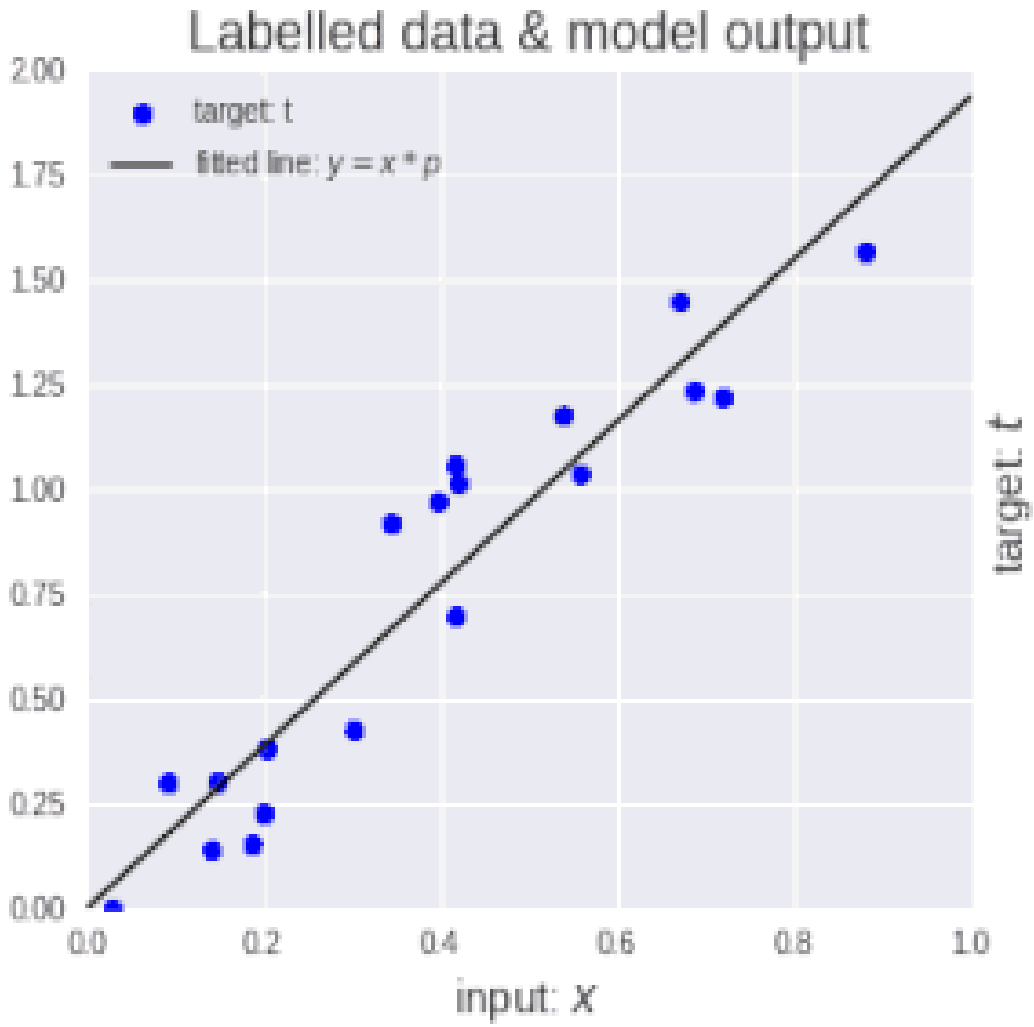
  - Slope first derivative over certain iterations,
  - Learning rate



Y : Cost Function (Loss function, Error)
A : Slope
x **:** N# of iterations

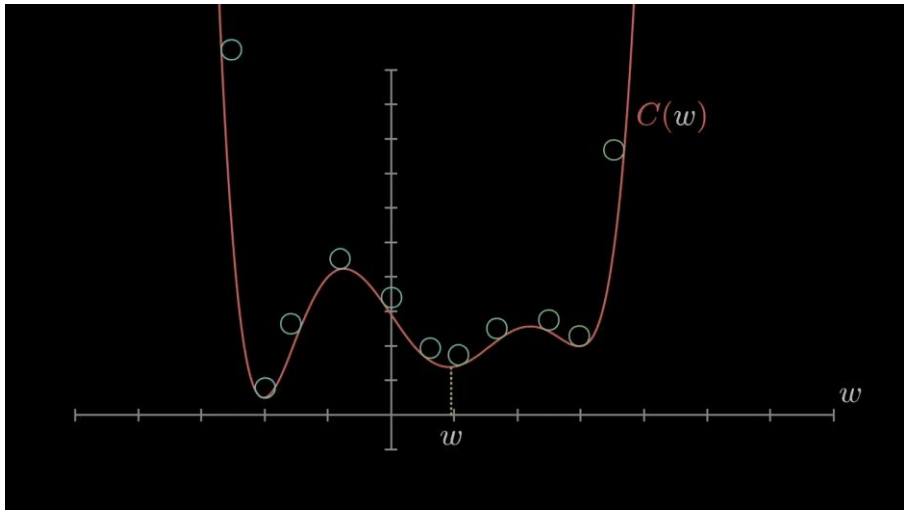
Linear Regression - Gradient Descent

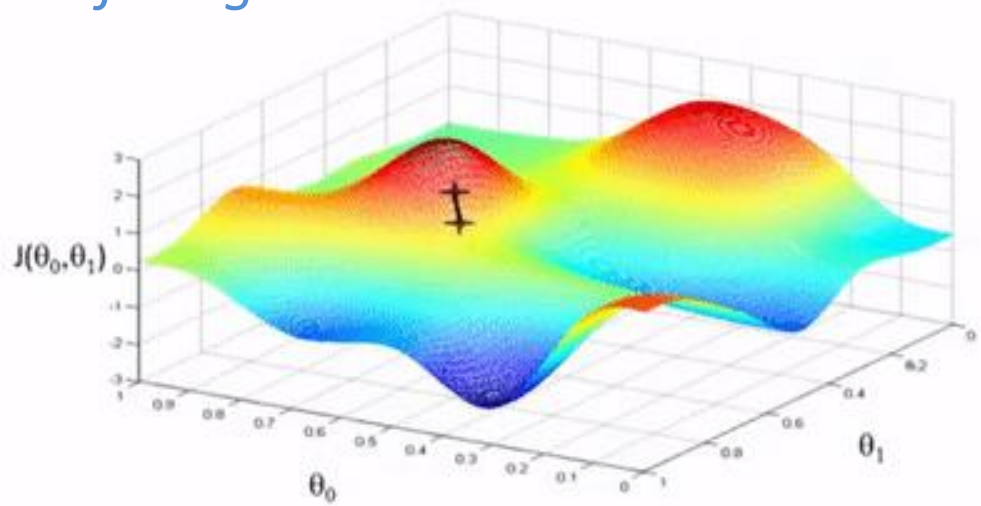




Gradient Descent

- *Gradient descent is based on calculus.*
- *Gradient descent is different from one algorithm to another based on the complexity of the algorithm and no# of variables (dimensions)*
- *It always has local minima.*
- *Learning rate is the essential step to reach a healthy GD*
- *Learning rate can be cause of overfitting or underfitting*





Machine Learning Algorithms

K-Means Classification

- ***Objective:***

  To be able to cluster the data based on the input variable or variables and find cluster centroids

- ***Model structure:***

  Euclidean distance = $\sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$

- ***Model assumptions:***

  - Cluster centroids are in the middle of each cluster
  - Each cluster has a centroid and data is scattered around it

- ***Parameter estimates and interpretation:***

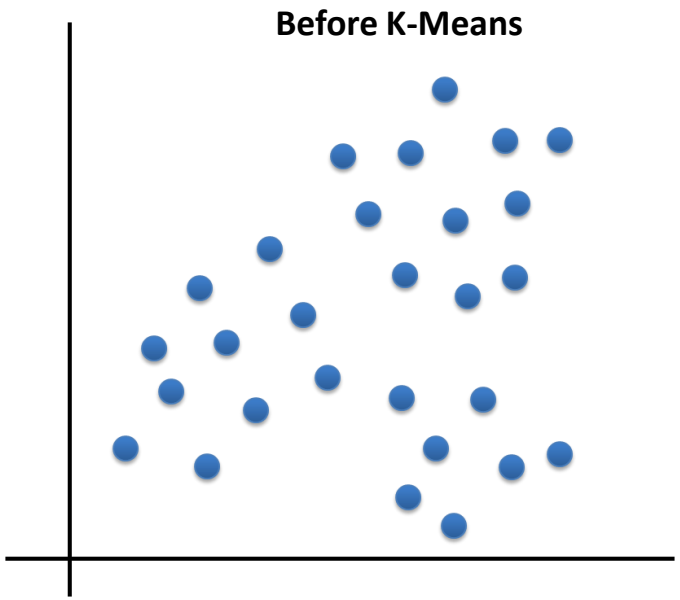
  Find Euclidian distance that correspond to each centroid

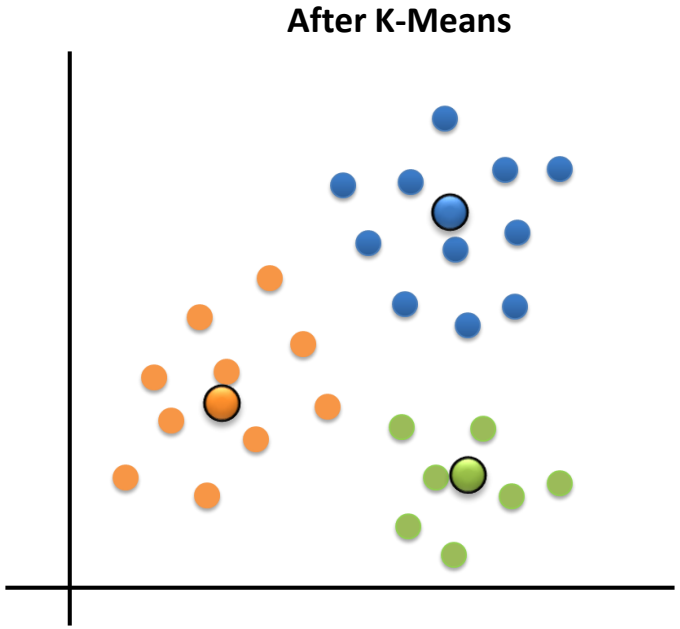
- ***Model fit:***

  R^2, residual analysis

- ***Model selection:***

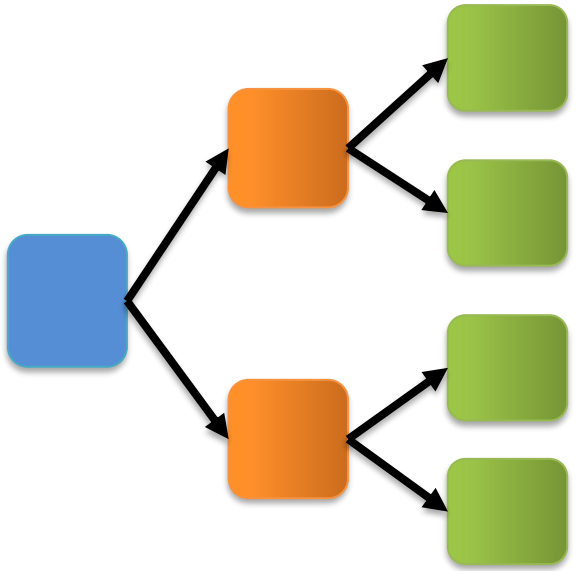
  How Many Centroids ?





K-Means Classification

Decision Tree



- ***Objective:***

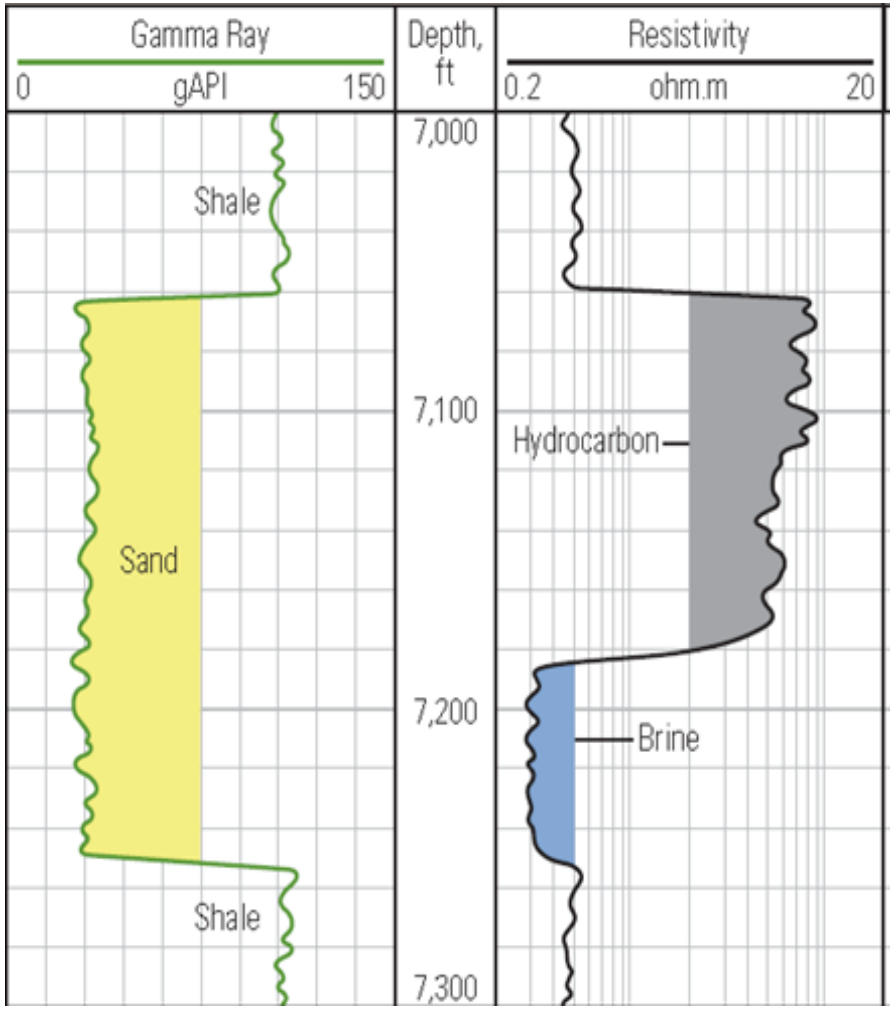
  To be able to build decision boundaries based on the maximum variance between variables

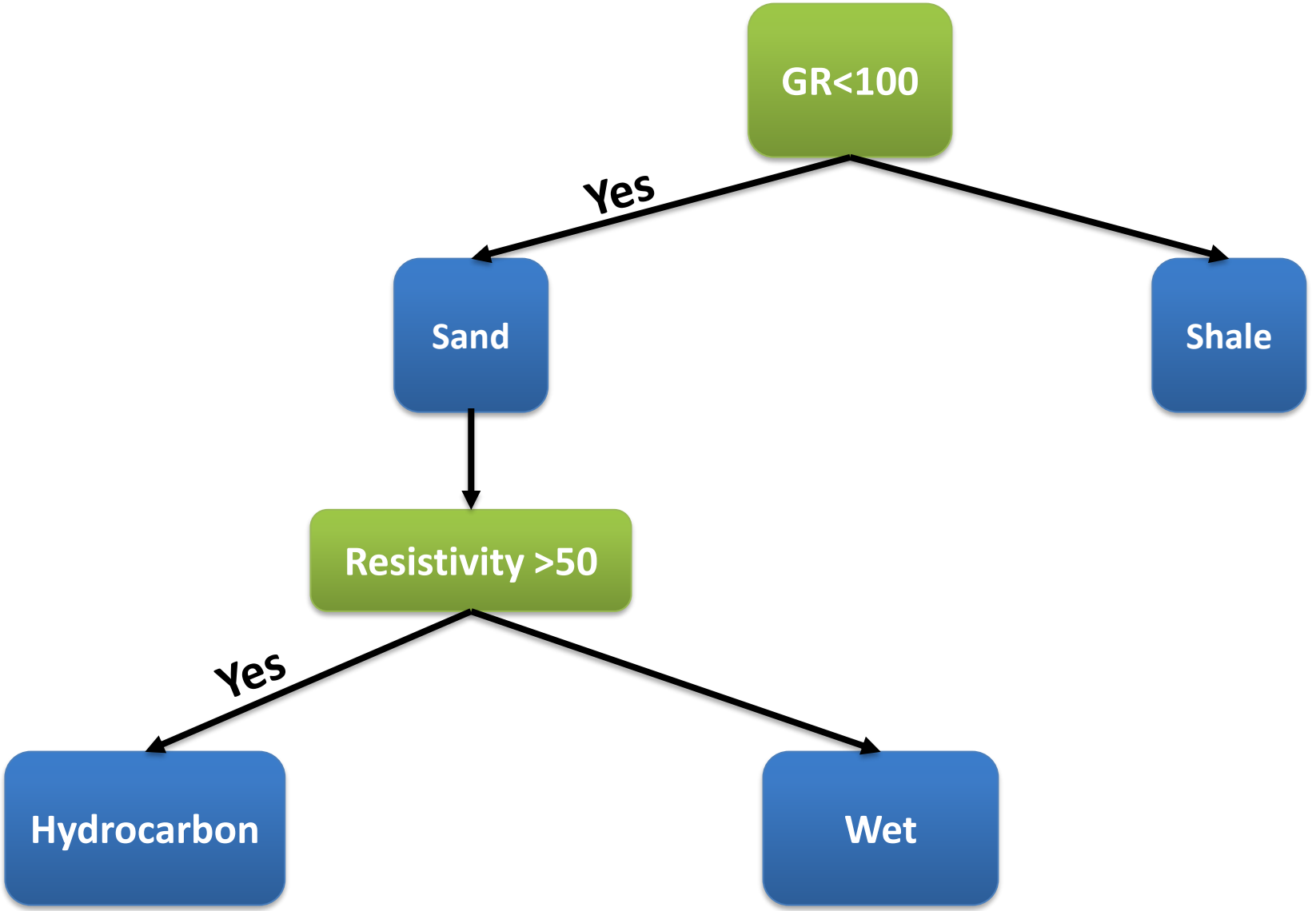
- ***Model structure:***
  - Pick the best attribute/feature. The best attribute is one which best splits or separates the data.
  - Ask the relevant question.
  - Follow the answer path.
  - Go to step 1 with different attribute until you arrive to the answer.

- ***Model fit:***

  R^2, Confusion Matrix

Decision Tree





Random Forest

- ***Objective:***

  To be able to build decision boundaries based on the maximum variance between variables

- ***Model structure:***

  Step 1 : *Select random samples from a given dataset.*

  Step 2 : *Construct a decision tree for every sample.*

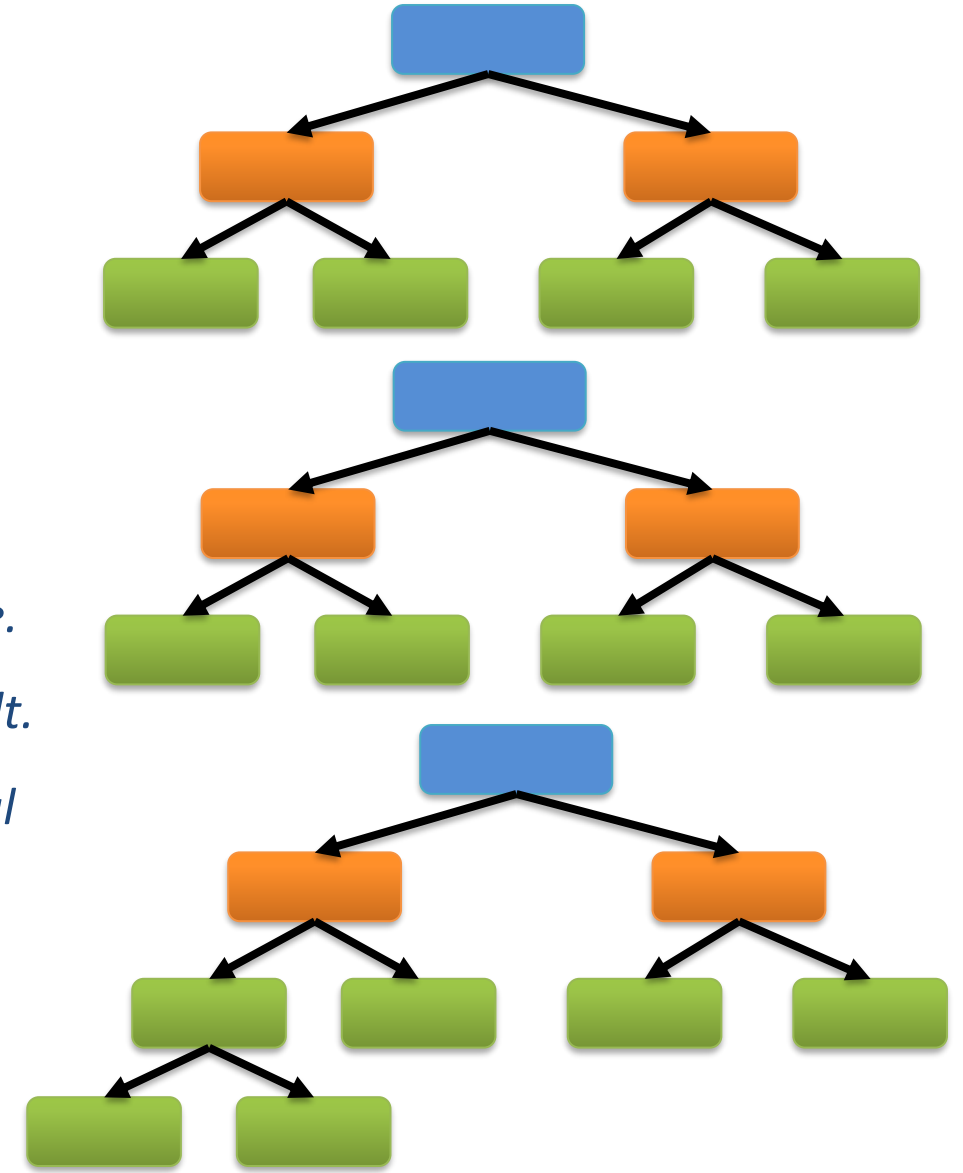
  Step 3 : *Get the prediction result from every decision tree.*

  Step 4 : *Voting will be performed for every predicted result.*

  Step 5 : *Select the most voted prediction result as the final prediction result.*

- ***Model fit:***

  R^2, Confusion Matrix



Principle Component Analysis

- ***Objective:***

  to reduce the dimensionality of large data sets, by transforming a large set of variables into a smaller one that still contains most of the information in the large set

- ***Model structure:***

$$\begin{bmatrix} Cov(x,x) & Cov(x,y) & Cov(x,z) \\ Cov(y,x) & Cov(y,y) & Cov(y,z) \\ Cov(z,x) & Cov(z,y) & Cov(z,z) \end{bmatrix}$$

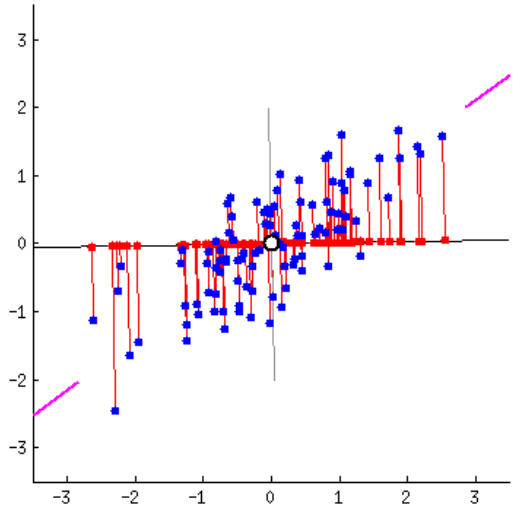
  Step 1 : *Standardization – $Z = x\text{-}\mu/\sigma$*

  Step 2 : *Construct a Covariance Matrix.*

  Step 3 : *Compute Eigenvectors and Eigenvalues.*

  Step 4 : *Feature Vector: Matrix of important Principal components.*

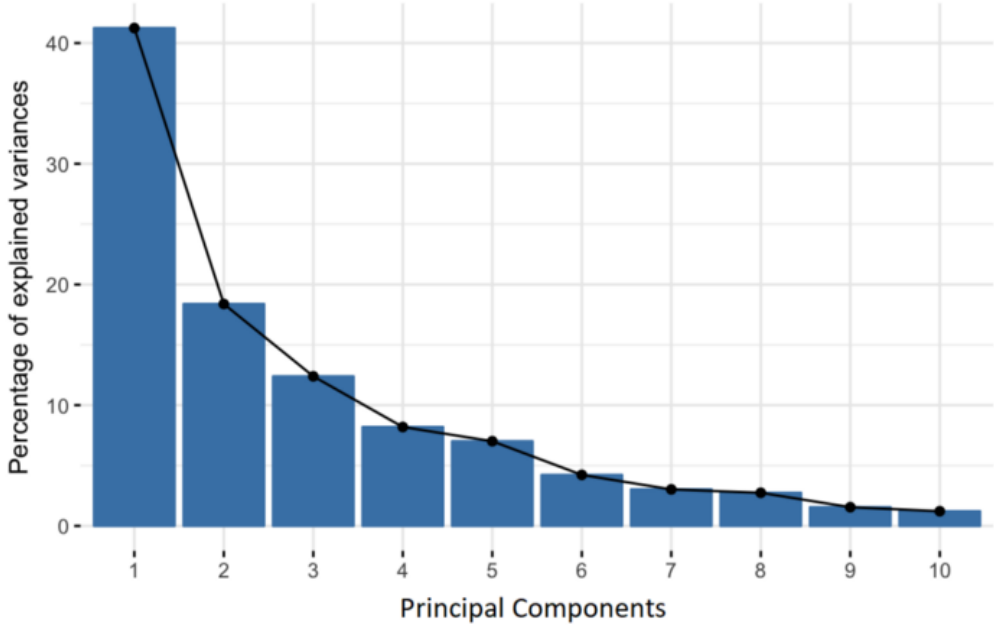
  Step 5 : *Final Dataset = Final Vector ^{T} * Standardized Original Dataset ^{T}*



Principle Component Analysis

Key points on PCA:

- PCA is considered the variance of mixtures.
- PCA is the directions of Maximal amount of variance.
- 1st PC holds the largest possible Variance.
- Numbers of PC = Number of the dimensions (variables).
- Eigenvectors = direction of the axes with most variance .
- Eigenvalue = amount of variance attached in each PC.
- Percentage of variance = Eigenvalues / total sum of Eigenvalues



Neural Network

- Introduction
- ANN Structure
- How ANN Works
- Activation Functions

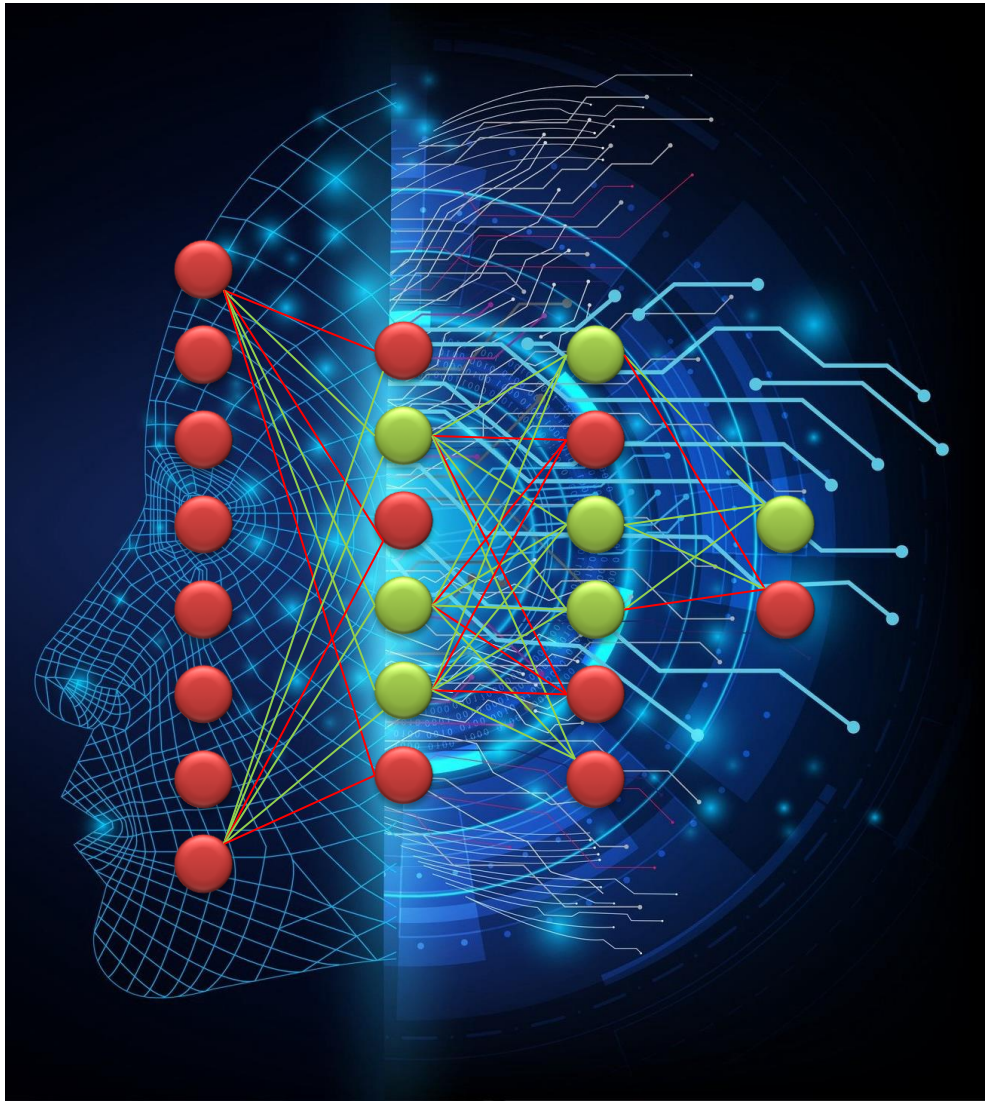
Neural Network - Introduction

- In 1943, Warren McCulloch and Walter Pitts first made a trial to create a computational model from human neural networks.

- Neural Network structure is composed of :
  - Input Layer
  - Hidden Layers
  - Output Layers

- Composed of two algorithmic stages :
  - Forward Propagation
  - Backward Propagation

- Neural Network can be used for prediction or classification based on the nature of the output layer.



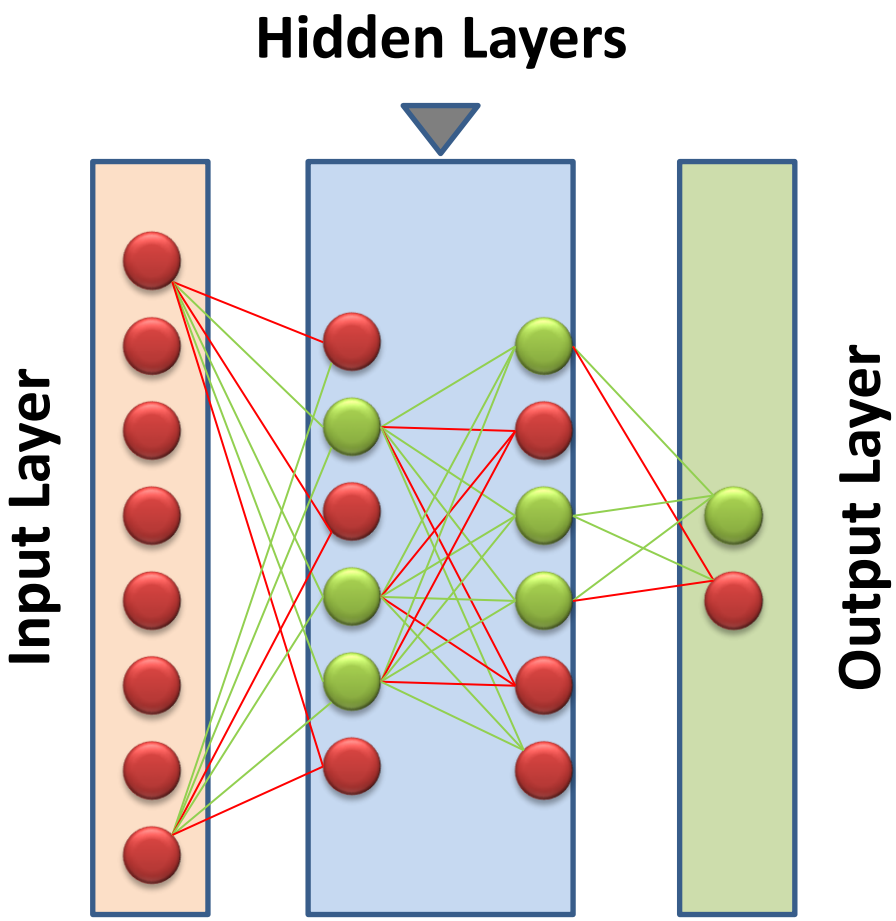
Neural Network - Structure

Input Layer:

- Number of nodes is equal to number of input variables.
- Each node is associated with a randomly selected weight.

Hidden Layer(s):

- Number of layers and Nodes are dependent on the problem.
- Each connection is passing through Activation function that affects the next layer



Output Layer:

- **In case of prediction**,
  - the output layer will be consisting of 1 node that result in the predication.
- **In case of classification:**
  - the number of nodes will be equal to the classes we need to predict associated with probabilities for each class.
  - The higher probability will be the predicted class.

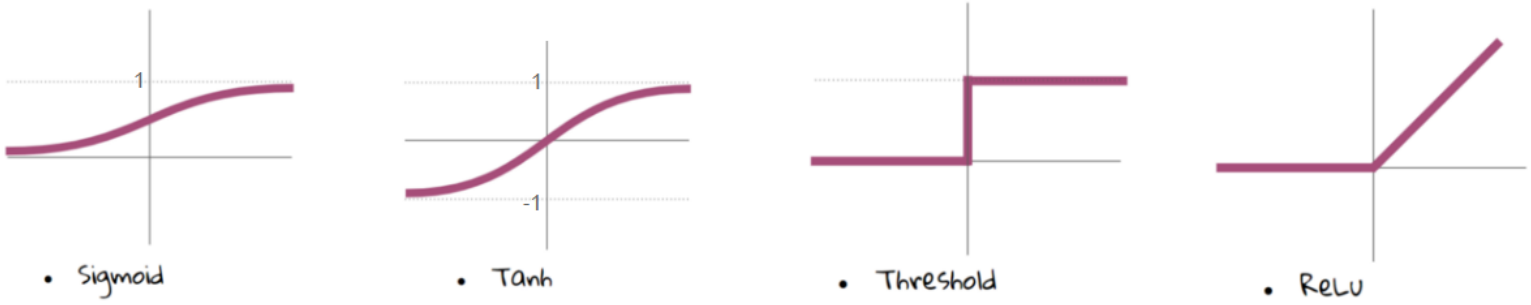
Neural Network – How it works

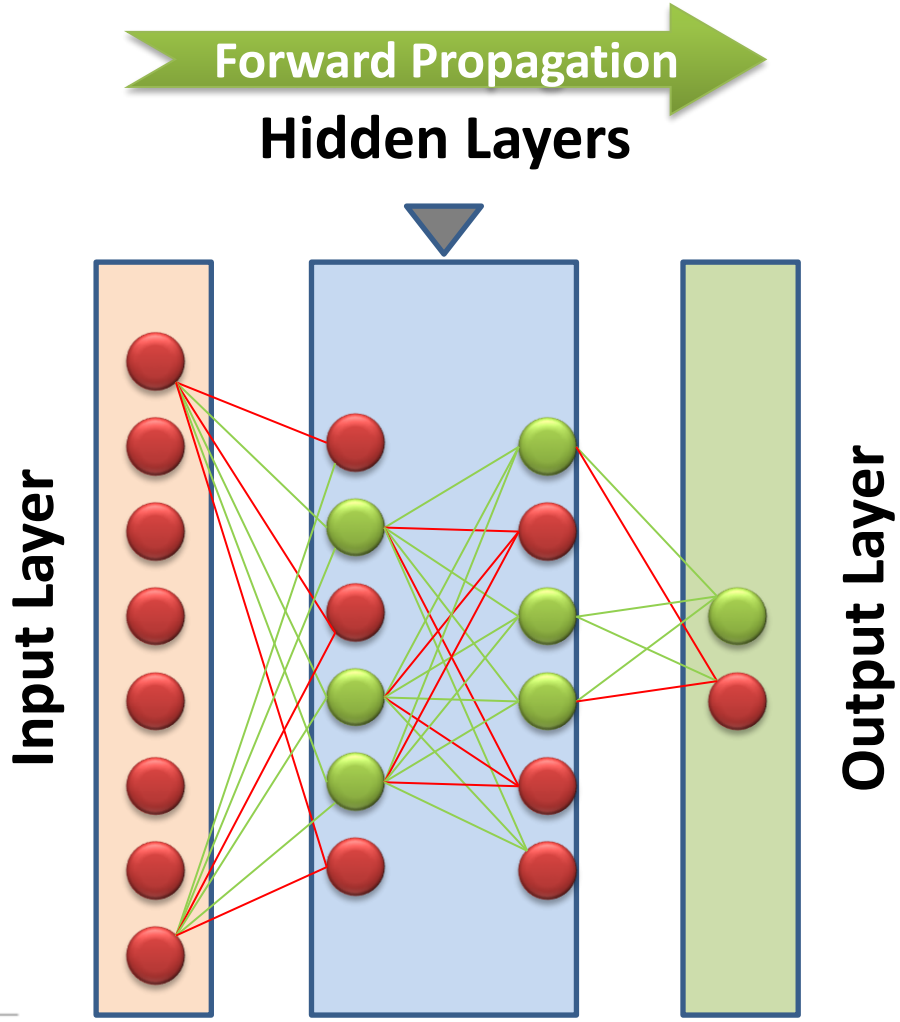
1. Forward propagation:

- Random weights assigned to inputs nodes
- ***Activation function*** applied to each node to change the weight.

Activation Function:

- The model needs non-linear change to the values before submitting the next outcome values in hidden layer.
- Helps the model to capture non-linearities within the data.
- Different types of activation functions:





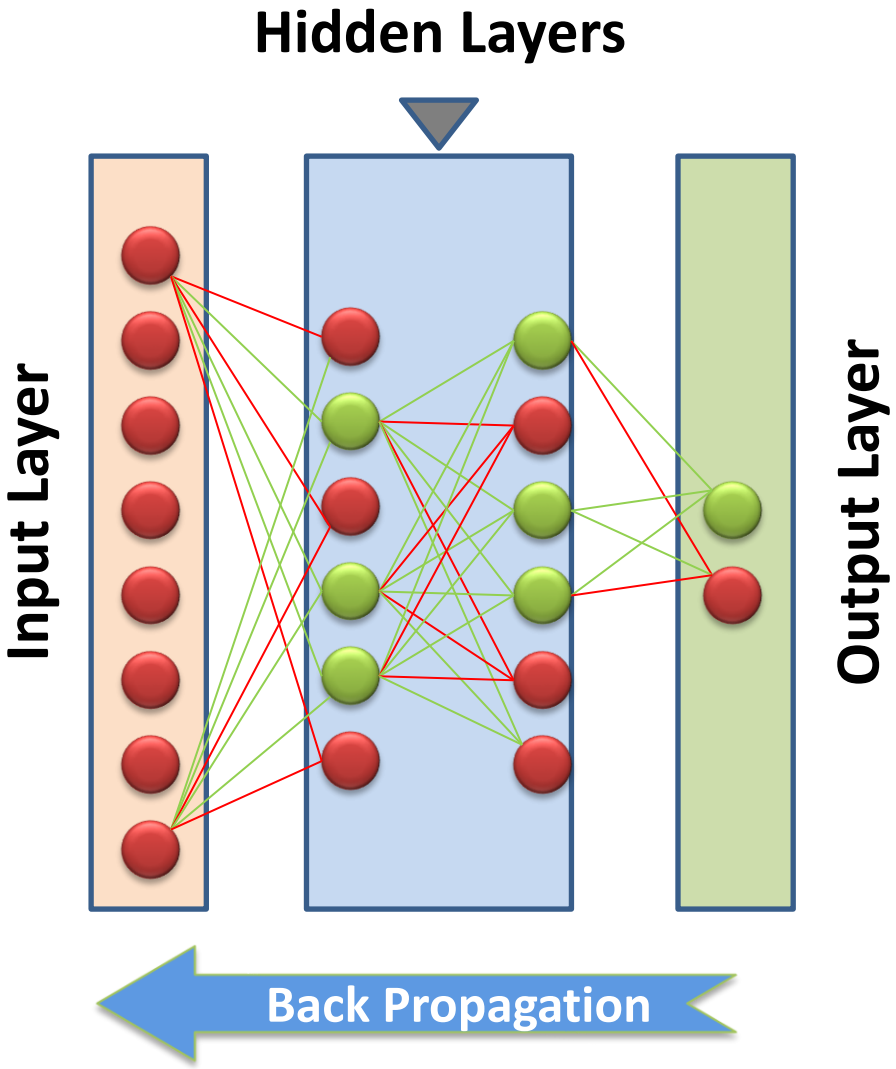
Neural Network – How it works

2. **Back propagation:**
   - Cost function estimation.
   - Update the weights by the errors difference, then
   - Iterate…..

That's called **EPOCH**

EPOCH:
Is the time consumed to do one feed forward propagation and backpropagation in any Neural Network.

Let's see how it works step by step



Thank You for Your Attention

Amr Moslim

Machine Learning Application Examples

- Facies Classification
- Porosity Prediction using seismic attributes
- Permeability Prediction using Petrophysical volumes
- Classification using K-means

Confusion Matrix

- ***Confusion Matrix KPI:***
  - ***Precision:*** *true positive rate*

$$\frac{TP}{TP + FP}$$

  - ***Recall:*** *true positive over the 1 class predict*

$$\frac{TP}{TP + FN}$$

  - ***F1 Score:***

$$\frac{2 * precision * Recall}{Precision + Recall}$$

  - ***Accuracy:***

$$\frac{TP + TN}{TP + TN + FP + FN}$$