

# Machine Learning

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Useless without any pattern

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**Information** (Average level of Surprise / Uncertainty)

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Learning is involved using information, provides interpretation, understanding of unknown phenomenon.

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**Knowledge**

Learning is involved using information, provides interpretation, understanding of unknown phenomenon.

Processor uses data to generate a connected mapping using some mathematical functions / models to understand unknown data.

# Machine Learning

## Definition by Tom Mitchell (1998):

Machine Learning is the study of algorithms that

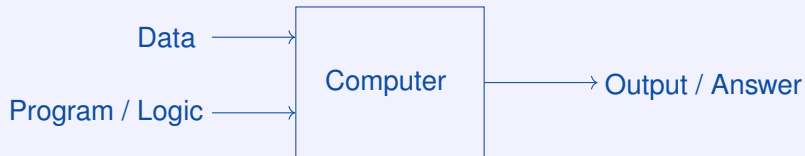
- improve their performance  $P$
- for some task  $T$
- with experience  $E$ .

A well defined learning task is given by  $\langle P, T, E \rangle$ .

Improve on task  $T$  with respect to Performance metric  $P$  based on experience  $E$



## Traditional Programming

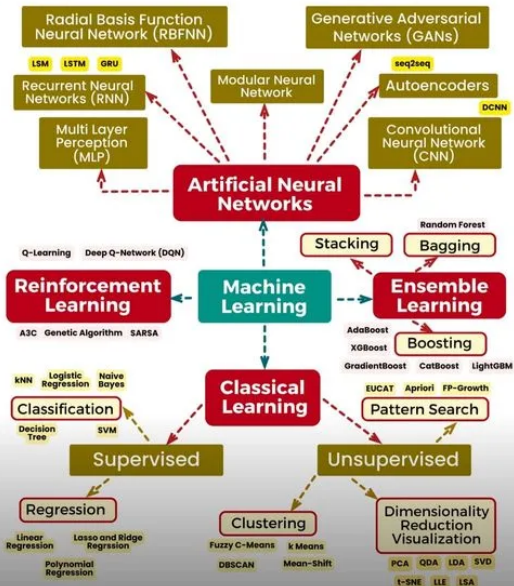


## Machine Learning



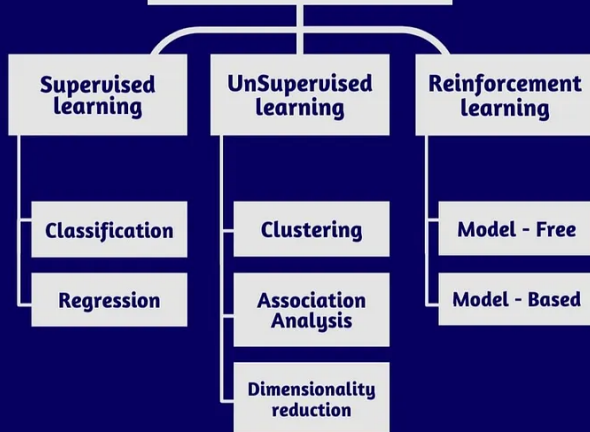
Apply the generated logic to future unknown Data to get some output / result.

# Machine Learning Algorithms





# Machine Learning



# Data Engineering

## TOOLS:

- TensorFlow: Open source ML Lib developed by Google.
- PyTorch: Open source Deep learning framework know for dynamic computation graph, intuitive design and support for dynamic NN.
- Scikit-learn: Library with collection of tools for data preprocessing, feature selection, model evaluation etc.
- Keras: A Deep learning API on the top of TensorFlow or PyTorch.

## Big data Technologies for processing and Storing ML Data

- Hadoop: Open source Big data framework includes Hadoop Distributed File System (HDFS) for distributed storage. Hadoop has the MapReduce programming model for processing large datasets.
- Apache Spark: Open source framework for distributed data processing provides libraries for various tasks including data preprocessing, ML, graph processing. Its in-memory processing capabilities accelerate computations using AI/ML. It overcomes limitations of Hadoop.

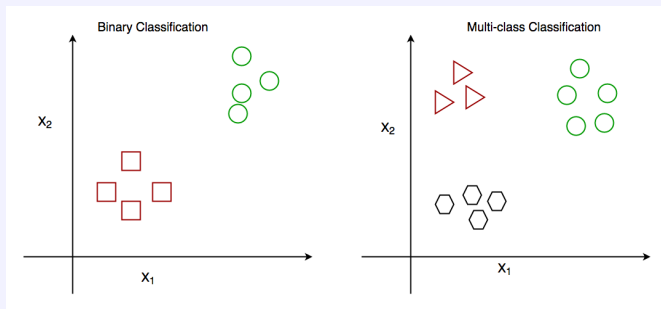
## Data / Outliers / Anomalies

- Outliers: Distribution or dataset having unusual input for training.
- Overfitting: Outliers cause Overfitting.
- Sorting, grouping may help to detect Outliers.
- Anomaly may represent distribution or pattern but does not accurately reflect dataset. Outliers may be Anomalies while Anomalies are not Outliers.

## Classification Algorithm: Supervised Learning

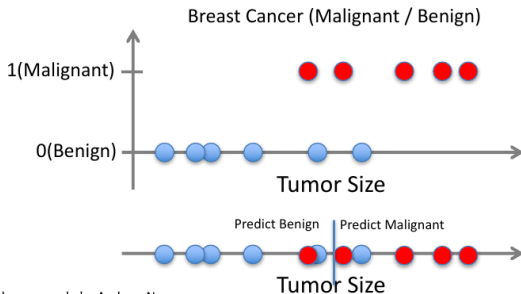
Classification problem:

Model or function to separate data into multiple categorical classes *i.e.* discrete values.



# Supervised Learning: Classification

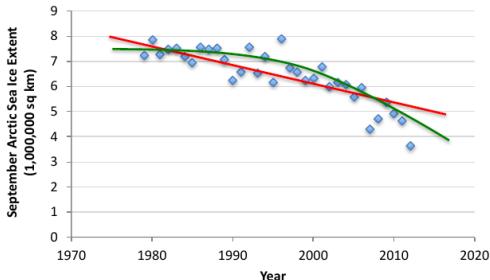
- Given  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$
- Learn a function  $f(x)$  to predict  $y$  given  $x$ 
  - $y$  is categorical == classification



Based on example by Andrew Ng

# Supervised Learning: Regression

- Given  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$
- Learn a function  $f(x)$  to predict  $y$  given  $x$ 
  - $y$  is real-valued == regression

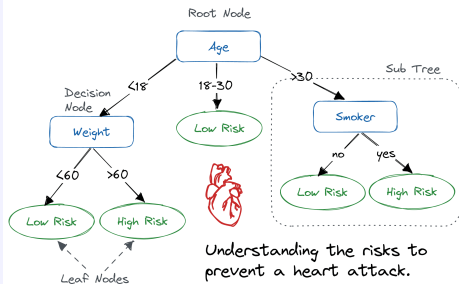


Data from G. Witt. Journal of Statistics Education, Volume 21, Number 1 (2013)

## Decision Tree : Classification

- Consecutive set of questions (nodes).
  - Only TWO possible answers per question.
  - Each question depends on previous answers.
  - Final verdict (leaf) is reached after a given maximum number of nodes.
- Easy to understand/interpret
  - Good with multivariate data
  - Fast training
  - Single tree is NOT very strong  $\Rightarrow$  Random Forests

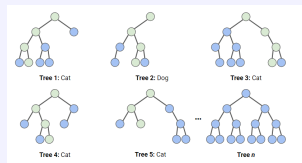
# Decision Tree : Classification



- The topmost node is called Root Node.
- Root node learns to make partition on the basis of attribute values.
- Partitioning is done in recursive manner.
- Best attribute selection is heuristic and best attribute becomes a decision node.
- Easily capture non-linear patterns.
- It can be used for feature engineering to predict missing data etc.
- Sensitive to noisy data and may overfit.
- Small variation may produce different tree which can be fixed by bagging and boosting.



## Random Forest: (Classification & Regression)



Green circle is hypothetical path the tree took to reach decision

- Random forest can be used for Regression (numeric target) and Classification (categorical target).
- Multiple decision trees are created using different random sets of data and features.
- Predictions are made by voting for classification and by averaging for regression.



## Supervised Learning

### Supervised Learning:

Training data :  $\{(x_1, y_1), \dots, (x_N, y_N)\}$

$x_i$ : feature vector,  $y_i$ : label (class) of  $i^{th}$  data,  $g \in G$ : Hypothesis space.

A learning algorithm seeks a function  $g : X \rightarrow Y$ , where  $X$  is input space and  $Y$  is output space.

### Logistic Regression Model:

1. Estimates the probability of occurrence of an event based on given dataset of independent variables.
2. It is probability of a class.
3. Since outcome is probability, dependent variable is bounded in  $[0, 1]$



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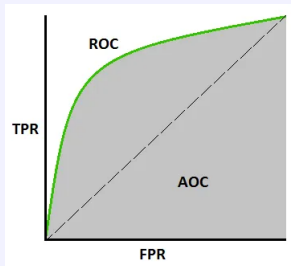
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### Support Vector Machine (SVM):

1. Goal is to create decision boundary segregating n-dim space into classes.
2. Best decision boundary is called Hyperplane.
3. SVM : (a) Linear and (b) Non-linear.

## Performance Measurement for Classification

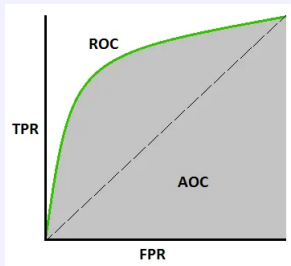


AUC-ROC :Performance measurement.

AUC:- Area Under the Curve.

ROC:- Receiver Operating Characteristics.

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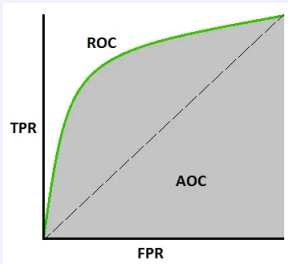
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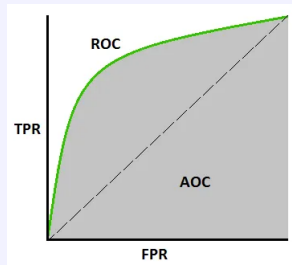
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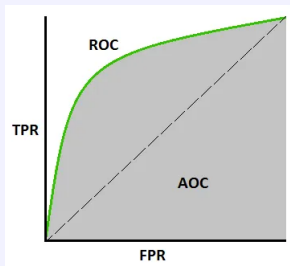
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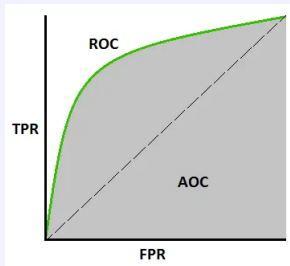
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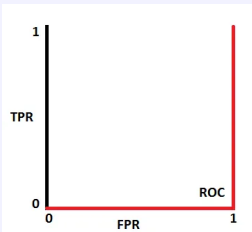
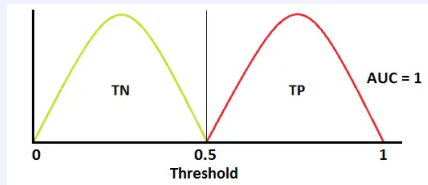
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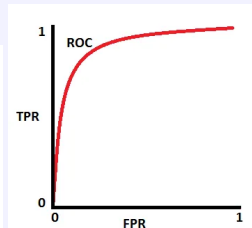
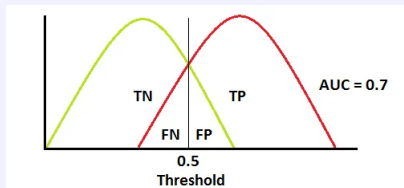
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A Good model has AUC → 1 means good separability of classes.

## ROC: Probability Curve.

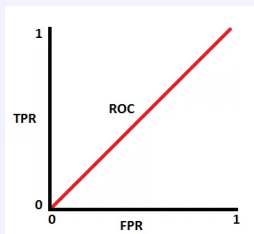
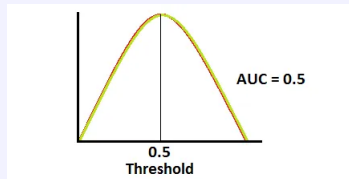


Ideal measure of probability. Positive class (e.g. patient with disease, Negative class (e.g. No disease))

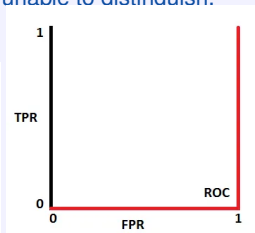
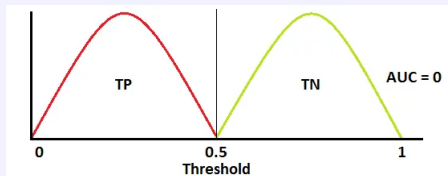


AUC=0.7 means the model may separate classes with 70% probability.

## ROC: Probability Curve.



AUC=0.5 is the worst situation where model is unable to distinguish.

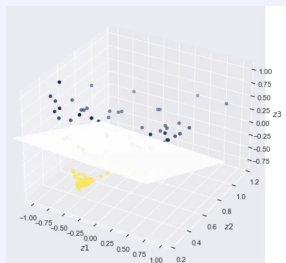
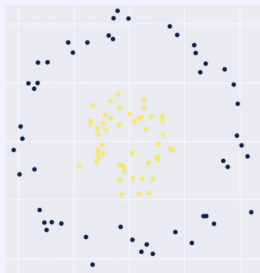


AUC=0 means the model is recognising a positive class as negative and vice versa.

## The Kernels

- Kernels (function) are a set of algorithms used for pattern matching.
- Usually non-linear problems are solved by linear classifier - “Kernel Tricks” « SVM ».
- The kernel function is applied on each data instance to map the original non-linear observations into a higher-dimensional space in which they become separable without computing the coordinates of the data in a higher dimensional space.
- Kernel Trick allows us to operate in the original feature space .

# Kernels



- 2D dataset with 2 classes. Function to separate 2 classes is required. Data is NOT linearly separable into 2 classes.
- One can fit a complex polynomial function to separate the data.
- Data may be transformed into 3D.
- A linear decision boundary may be found by fitting a linear classifier (a plane separating data) - *Hyperplane* .
- Map the linear decision boundary back into 2D space. The result will be a non-linear decision boundary in 2D

Let us consider a regression model:

$$y_i = w_0 + w_1 x_i + w_2 x_i + \epsilon_i$$

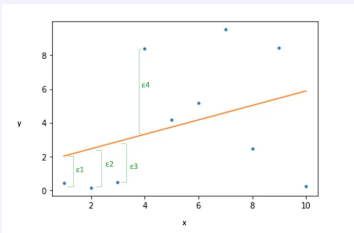
$$y_i = W^T x_i + \epsilon_i,$$

where,  $W = \{w_0, w_1, w_2\}$  are weights.

Error:  $\epsilon_i = (W^T x_i - y_i)$ .

Let  $x_a = [x_{a1}, x_{a2}]$  and  $x_b = [x_{b1}, x_{b2}] \in \mathcal{R}^2$ .

3D mapping,  $x_i \rightarrow \phi(x_i) : x_a^T x_b \rightarrow \phi(x_a)^T \phi(x_b)$  and back to 2D,



$$K(x_a, x_b) = \phi(x_a)^T \phi(x_b)$$

$$\text{Let, } K(x_a, x_b) = (x_a^T x_b)^2 = (x_{a1} x_{b1} + x_{a2} x_{b2})^2,$$

$$= (x_{a1}^2 x_{b1}^2 + 2x_{a1} x_{a2} x_{b1} x_{b2} + x_{a2}^2 x_{b2}^2).$$

$$\text{AND can be decomposed into } \phi(x_a) = \begin{pmatrix} x_{a1}^2 \\ \sqrt{2} x_{a1} x_{a2} \\ x_{a2}^2 \end{pmatrix} \text{ and } \phi(x_b) = \begin{pmatrix} x_{b1}^2 \\ \sqrt{2} x_{b1} x_{b2} \\ x_{b2}^2 \end{pmatrix}.$$

In place of dot product we plug kernel  $K$ .

## Kernels

Vectors:  $x_a$  and  $x_b$ .

**Linear Kernel:**  $K(x_a, x_b) = x_a \cdot x_b$ .

Dot product measures similarity or distance in original feature space.

**Polynomial Kernel:**  $K(x_a, x_b) = (x_a \cdot x_b + c)^d$ ,

$d$  is the degree of the polynomial determines degree of nonlinearity.

**Gaussian Kernel :: Radial Basis Function (RBF):**  $K(x_a, x_b) = e^{-\gamma \|x_a - x_b\|^2}$ .

The  $\gamma$  tunes the performance of the Gaussian kernel.

**Laplace Kernel:**  $K(x_a, x_b) = e^{-\gamma \|x_a - x_b\|}$ .

$\|x_a - x_b\|$  is Manhattan distance or  $L_1$  norm between input vectors. It places less weight on large distance between input vectors than Gaussian kernel making it robust to Outliers.



## Kernel Characteristics

- **Mercer's condition:** Ensures that the kernel function is positive semi-definite, which means that it is always greater than or equal to zero.
- **Positive definiteness:** If kernel is always greater than zero except for when the inputs are equal to each other.
- **Non-negativity:** The kernel produces non-negative values for all inputs.
- **Symmetry:** A kernel function produces the same value regardless of the order in which the inputs are given.
- **Reproducing property:** A kernel function satisfies the reproducing property if it can be used to reconstruct the input data in the feature space.
- **Smoothness:** The kernel function produces a smooth transformation of the input data into the feature space.
- **Complexity:** More complex kernel functions may lead to over fitting and reduced generalization performance.



## Ensemble Learning : Supervised

### Ensemble Learning:

Combine the strengths of multiple models to make a single robust model less likely to overfit data.

### Techniques:

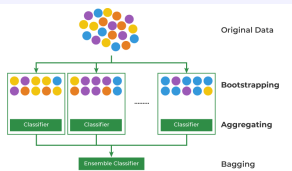
- Averaging (for regression)
- Bagging (Bootstrap Aggregation),
- Boosting and
- Stacking (Stacked Generalization)

# Bagging : Ensemble Learning

It can be used for both regression and classification.

## Bootstrap Sampling:

Randomly 'n' subsets of original data are sampled with replacement. Reduces of risks of overfitting increasing accuracy.



Original training dataset : [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]

Resampled training set #1: [2, 3, 3, 5, 6, 1, 8, 10, 9, 1]

Resampled training set #2: [1, 1, 5, 6, 3, 8, 9, 10, 2, 7]

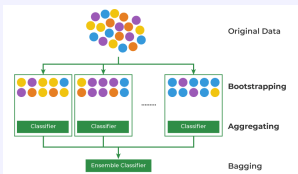
Resampled training set #3: [1, 5, 8, 9, 2, 10, 9, 7, 5, 4]

Some samples may be kept out of Sampling for verification of prediction.

## Bagging : Ensemble Learning

### Base Model Training:

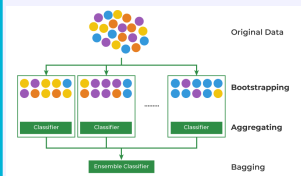
- Multiple base models are used.
- Each base model is independently trained using learning algorithm like **decision tree, SVM or Neural Networks**.
- Training is on different bootstrapped subset of data and can be parallelised.
- Each models are called "Weak Learners" as they may not be highly accurate of their own.



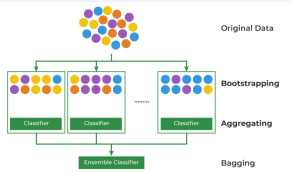
## Bagging : Ensemble Learning

### Aggregation:

- After training of all the base models, prediction is being made on unseen data.
- The Predicted class label is chosen on majority voting. <Classification>
- The final Prediction value is determined by averaging of the predictions from all base models. <Regression>



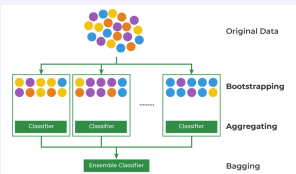
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### Out of Bag Evaluation:

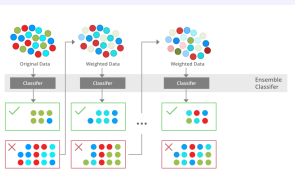
- Some samples excluded in the bootstrapping are "Out-of-Bag" Samples.
- Out-of-Bag samples may be used to estimate the model performance

## Bagging : Ensemble Learning



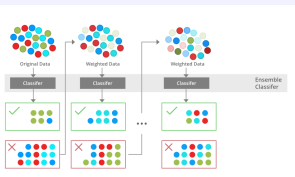
- **Improved Predictive Performance:** outperforms single classifier
- **Robustness:** Reduces impact of outliers and noises enhancing stability
- **Reduced Variances:** Since each base model is trained on different subsets, aggregated model's variance is reduced compared to individual model.
- **Parallelization:** Parallel processing of individual training reduces time.
- **Flexibility:** Wide range of algorithms can be used like DecisionTree, Random forests, support vector machine (SVM) etc.

## Boosting : Ensemble Learning



- Boosting is a sequential method

## Boosting : Ensemble Learning

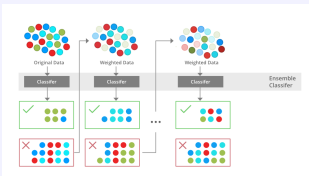


- Boosting is a sequential method
- First a model is built from training data.



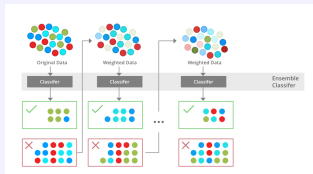
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- Second model is built with an effort to correct errors in earlier model.



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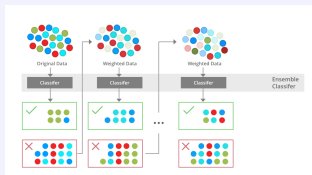
- Procedure continues

**AND**

models are added until **Either** the complete training data is predicted correctly **OR** maximum number of models have been added.

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- Types (Important): Gradient Boosting, XG-Boost, AdaBoost, CatBoost

## XGBoost (Extreme Gradient Boosting): Supervised Learning

Training data with multiple features  $x_i$  is used to predict target variable  $\hat{y}_i$  by fitting.

- Model (e.g. Linear Model): Prediction  $\hat{y}_i = \sum_j \theta_j x_{ij}$
- Training finds Best parameter  $\theta_i$  using **Objective function** measuring degree of fitness.
- Objective function:  $obj(\theta) = L(\theta) + \Omega(\theta)$ :  
 $L(\theta)$  = training loss function,  $\Omega(\theta)$  = regularization function.
- $L$ : degree of prediction w.r.t. training data.
- $\Omega$ : controls complexity of the model helping to avoid Overfitting.

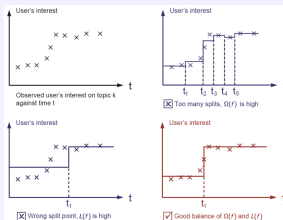
## XGBoost (Extreme Gradient Boosting): Supervised Learning

$obj(\theta)$ : (Loss  $L(\theta)$  + Regularization  $\Omega(\theta)$ ).

$L(\theta)$ :

(a) Mean Squared Error (MSE):  $L(\theta) = \sum_i (y_i - \hat{y}_i)^2$

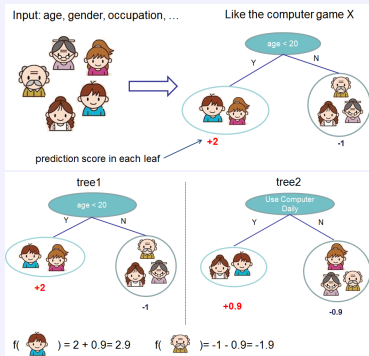
(b) Logistic:  $L(\theta) = \sum_i [y_i \ln(1 + e^{-\hat{y}_i}) + (1 - y_i) \ln(1 + e^{\hat{y}_i})]$



$\Omega(\theta)$ : Fit a step function visually given input data points. Which of the 3 solutions is best fit?

Tradeoff between  $L$  and  $\Omega$  is "**Bias-Variance trade-off**".

# XGBoost (Extreme Gradient Boosting): Supervised Learning



XGBoost: Decision Tree Ensemble: Set of Classification and Regression trees (CART).

Leaf also contains score.

2 trees complement each other:

$$\hat{y}_i = \sum_{k=1}^K f_k(x_i), f_k \in \mathcal{F}.$$

$\mathcal{F}$ : set of all possible CARTS,  $f_k$ : function in functional space  $\mathcal{F}$ ,  $K$ : number of trees.

$$obj(\theta) = \sum_i^n l(y_i, \hat{y}_i) + \sum_{k=1}^K w(f_k)$$

$w(f_k)$ : complexity depends on the scores.

**Boosted Decision Tree**      **Random Forrest!**

ONE predictive service code : Different Training.

Classify: who likes computer game.

Final score =  $\sum$  individual tree scores.

## XGBoost (Extreme Gradient Boosting): Supervised Learning

### Complexity

Define tree  $f(x) = w_{q(x)}$ ,  $w \in \mathcal{R}^T$ ,  $q : \mathcal{R}^d \rightarrow \{1, 2, 3, \dots, T\}$

$w$ =scores on leaves,  $q$ = fn assigning each data point to corresponding leaf,  
 $T$ = number of leaves.

$$w(f) = \gamma T + \frac{1}{2} \lambda \sum_{j=1}^T w_j^2.$$



# XGBoost (Extreme Gradient Boosting): Supervised Learning

Prediction values:

## Loss Function

$$\hat{y}_i^{(0)} = 0$$

$$\hat{y}_i^{(1)} = f_1(x_i) = \hat{y}_i^{(0)} + f_1(x_i)$$

$$\hat{y}_i^{(2)} = f_1(x_i) + f_2(x_i) = \hat{y}_i^{(1)} + f_2(x_i)$$

...

$$\hat{y}_i^{(t)} = \sum_{k=1}^t f_k(x_i) = \hat{y}_i^{(t-1)} + f_t(x_i)$$

At each step, tree is selected by optimized objective function.

$$obj^{(t)} = \sum_{i=1}^n l(y_i, \hat{y}_i^{(t)}) + \sum_{i=1}^t w(f_i) = \sum_{i=1}^n \left( y_i - (\hat{y}_i^{(t-1)} + f_t(x_i)) \right)^2 + \sum_{i=1}^t w(f_i), \text{ (MSE)}$$

Objective at step  $t \equiv$  goal for new tree

$$\sum_{i=1}^n \left[ g_i f_t(x_i) + \frac{1}{2} h_i f_t^2(x_i) \right] + w(f_t)$$

$$g_i = \partial_{\hat{y}_i^{(t-1)}} l(y_i, \hat{y}_i^{(t-1)}) \quad h_i = \partial_{\hat{y}_i^{(t-1)}}^2 l(y_i, \hat{y}_i^{(t-1)})$$

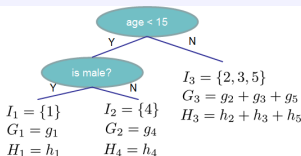


# XGBoost (Extreme Gradient Boosting): Supervised Learning

$$\begin{aligned}
 obj^{(t)} &\approx \sum_{i=1}^n \left[ g_i w_{q(x_i)} + \frac{1}{2} h_i w_{q(x_i)}^2 \right] + \gamma T + \frac{1}{2} \lambda \sum_{j=1}^T w_j^2, \\
 &= \sum_{j=1}^T \left[ w_j \sum_{i \in I_j} g_i + \frac{1}{2} \left( \sum_{i \in I_j} h_i + \lambda \right) w_j^2 \right] + \gamma T, \quad (\forall \text{ data in same leaf gets same score.}) \\
 &= \sum_{j=1}^T \left[ G_j w_j + \frac{1}{2} (H_j + \lambda) w_j^2 \right] + \gamma T \Rightarrow I_j = \{i \mid q(x_i) = j\}.
 \end{aligned}$$

Instance index    gradient statistics

1		$g_1, h_1$
2		$g_2, h_2$
3		$g_3, h_3$
4		$g_4, h_4$
5		$g_5, h_5$



$$Obj = -\sum_j \frac{G_j^2}{H_j + \lambda} + 3\gamma$$

The smaller the score is, the better the structure is

$w_j^s$  are independent.

$$w_j^* = -\frac{G_j}{H_j + \lambda}$$

$$obj^* = -\frac{1}{2} \sum_{j=1}^T \frac{G_j^2}{H_j + \lambda} + \gamma T$$

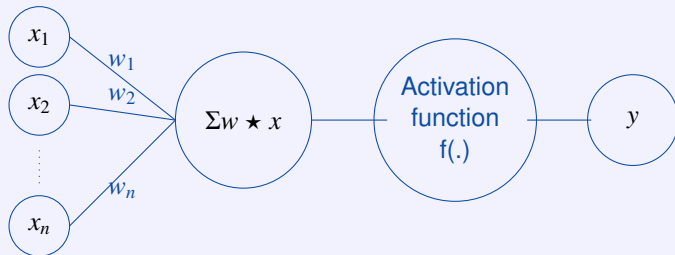
Smaller the score is,  
the better the structure is.

## AdaBoost (Adaptive Boosting) : Ensemble Learning

- Enhances weights of misclassified events after each training
- Reduces weights of correctly classified events so that future trees learn better
- Iteration continues until weight of misclassified . 50%
- Final weight is the sum of all classifiers weighted by their errors

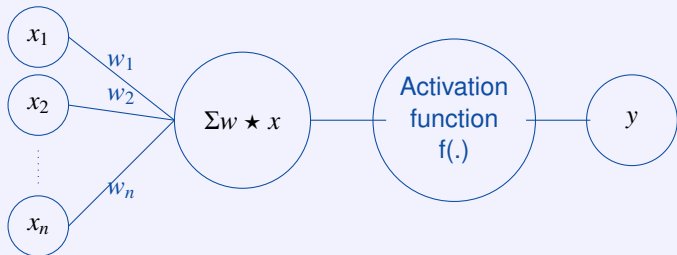
## Neural Networks

- Artificial system being inspired from biological neural networks.



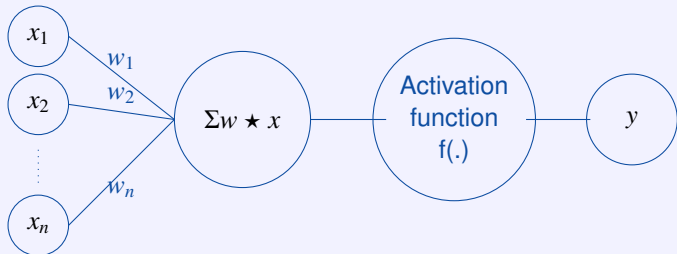
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## Neural Networks

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- It is a type of ML process that uses interconnected nodes/neurons in a layered structure called as **Deep learning**.
- Algorithm updates itself through "backpropagation" as per optimization strategy.

