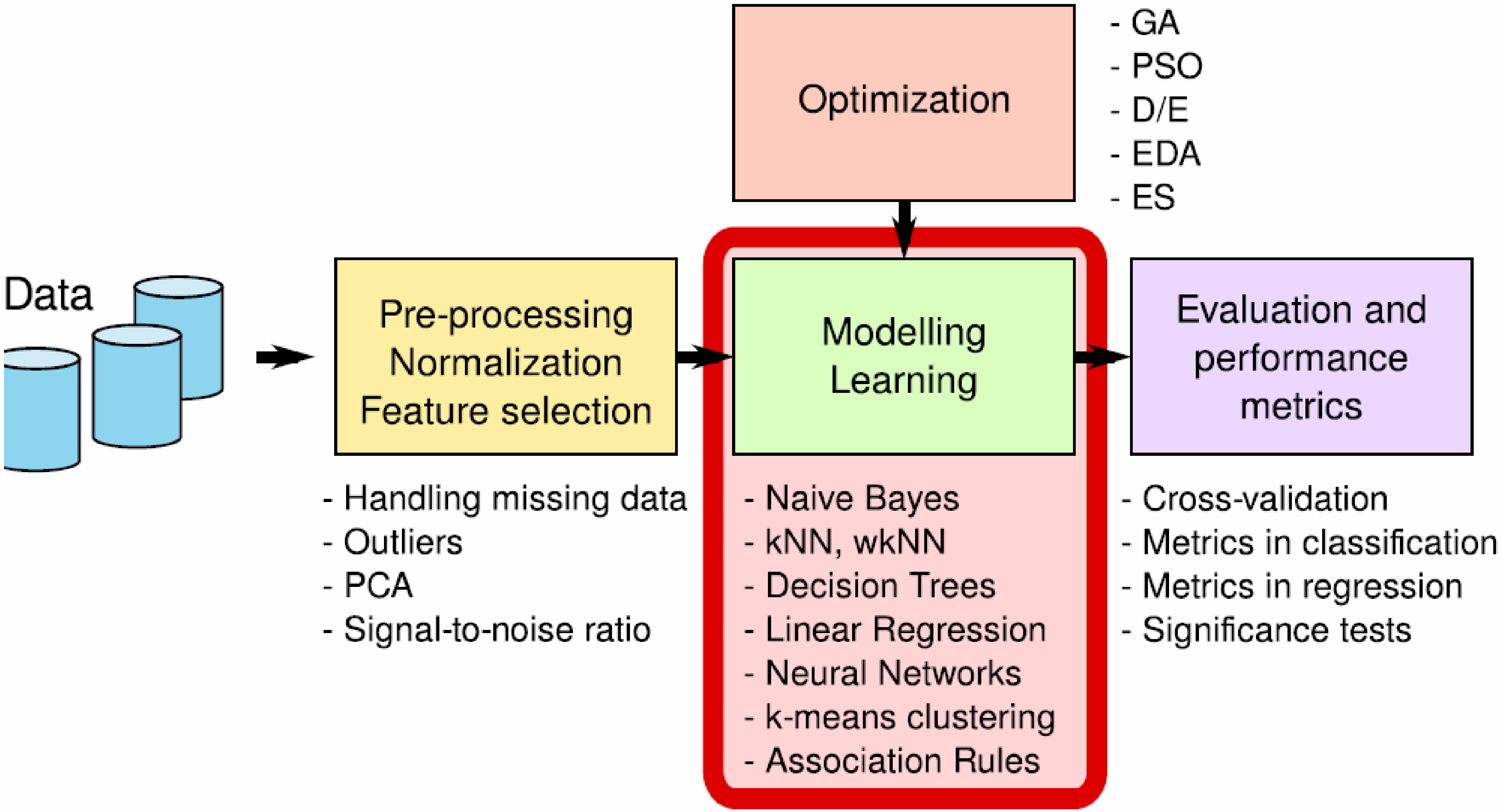
DATA MINING & MACHINE LEARNING

Artificial Neural Networks

Course Outline



Learning Outcomes

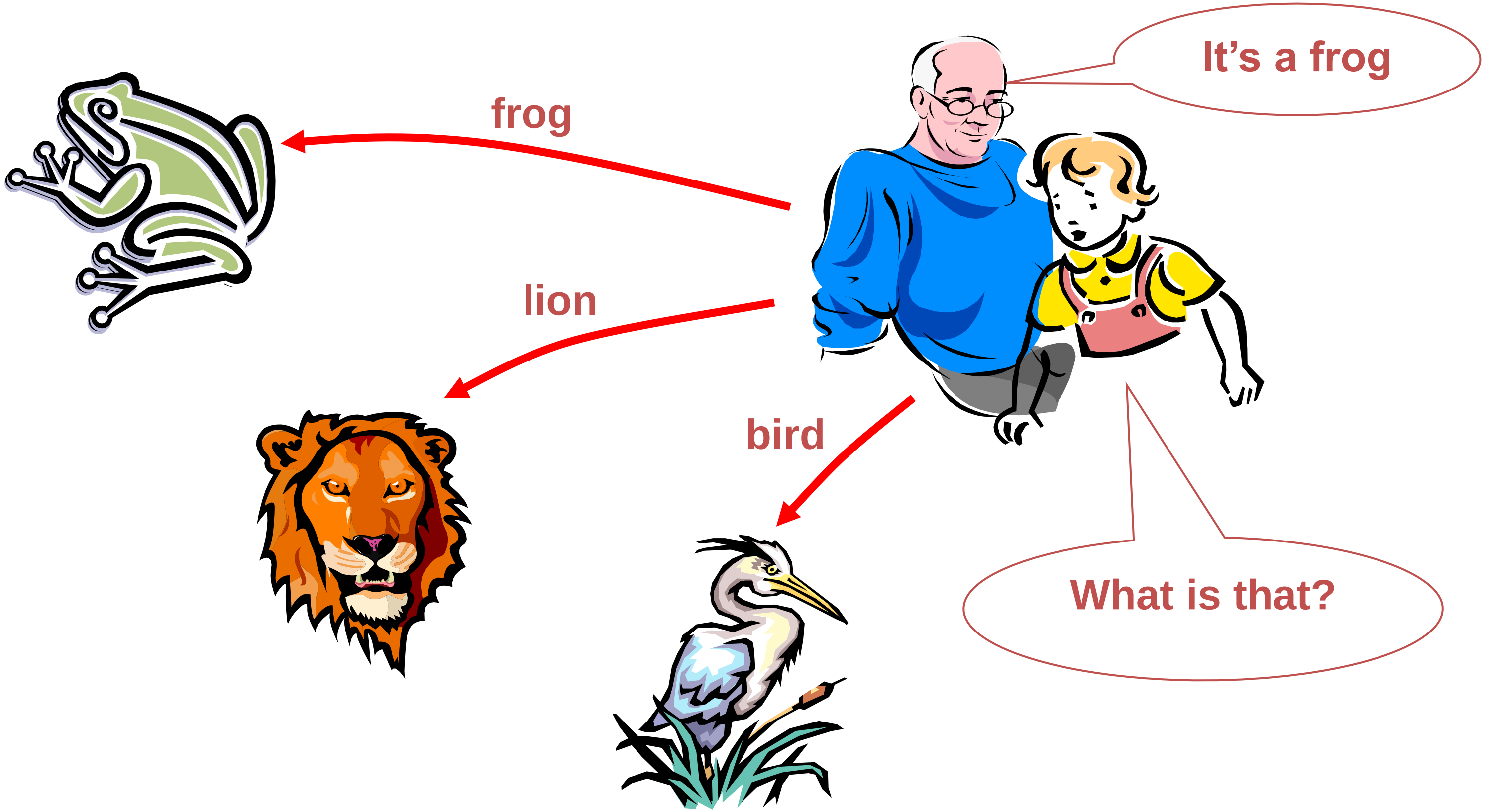
- Examine the basic principles of artificial neural networks.
- Discuss the operation of the Multi Layer Perceptron through the use of suitable examples.
- Discuss the derivation of the weight update formula through the use of *backpropagation.*

Neural Networks

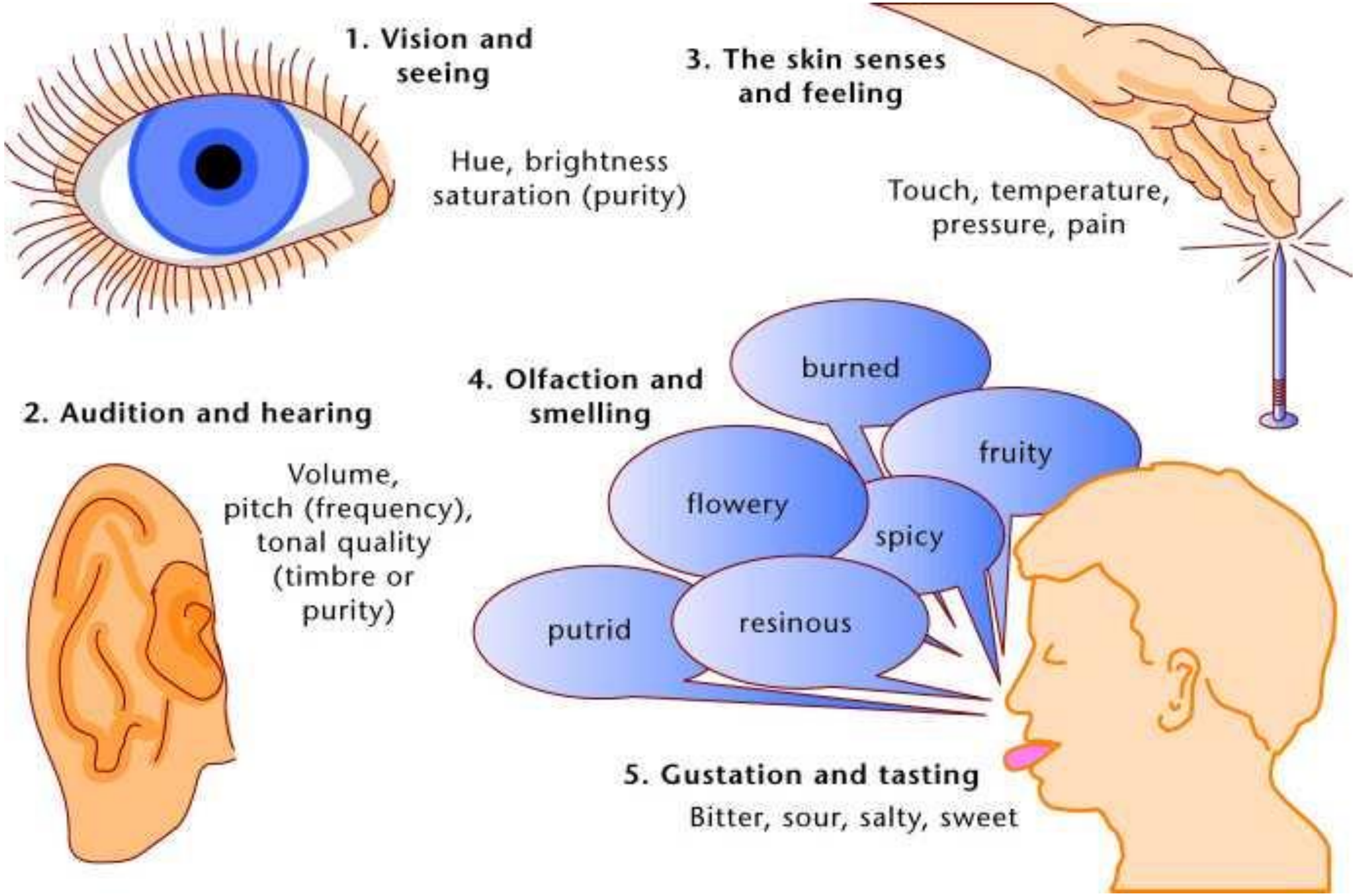
- Biologically inspired family of algorithms that is inspired by the human brain
- Neural Networks are used for *classification*, *clustering* and *numeric prediction* tasks.
- Most popular types are
  - Multi Layer Perceptron (MLP) used for classification
  - Radial Basis Function (RBF) used for classification and numeric prediction
  - Self Organizing Map (SOM) used for clustering
  - Convolutional Neural Network (CNN)used for image classification
  - Long Short Term Memory (LSTM) used for modelling time series

The idea of ANNs..?

- NNs learn relationship between cause and effect or organize large volumes of data into orderly and informative patterns.



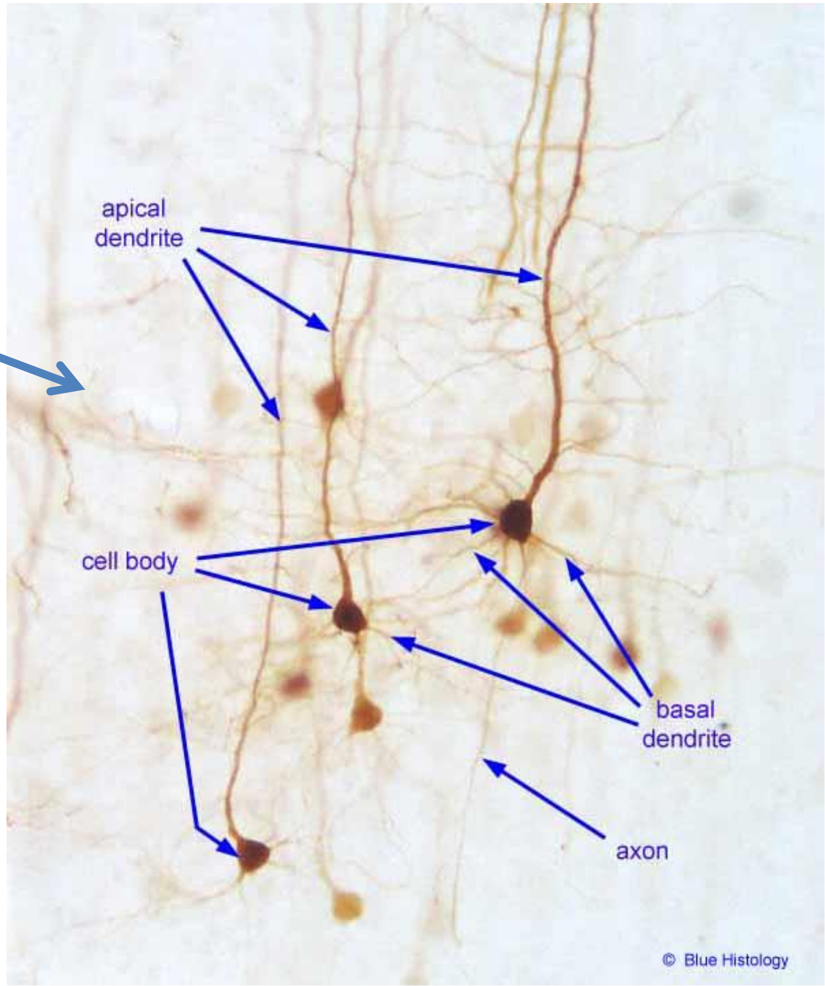
Brain performs classifications, predictions and associations

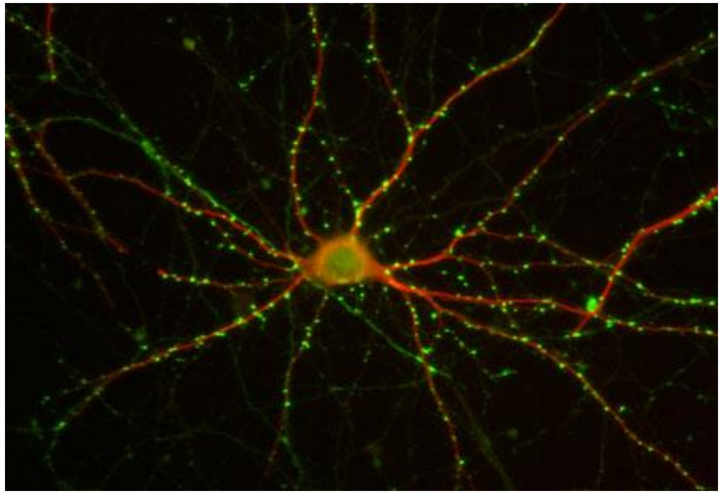


Neural Networks

Huge complexity: 10^{11} of neurons in the brain

Huge connectivity: each neuron sends and receives 10^4 of synapses (contacts)



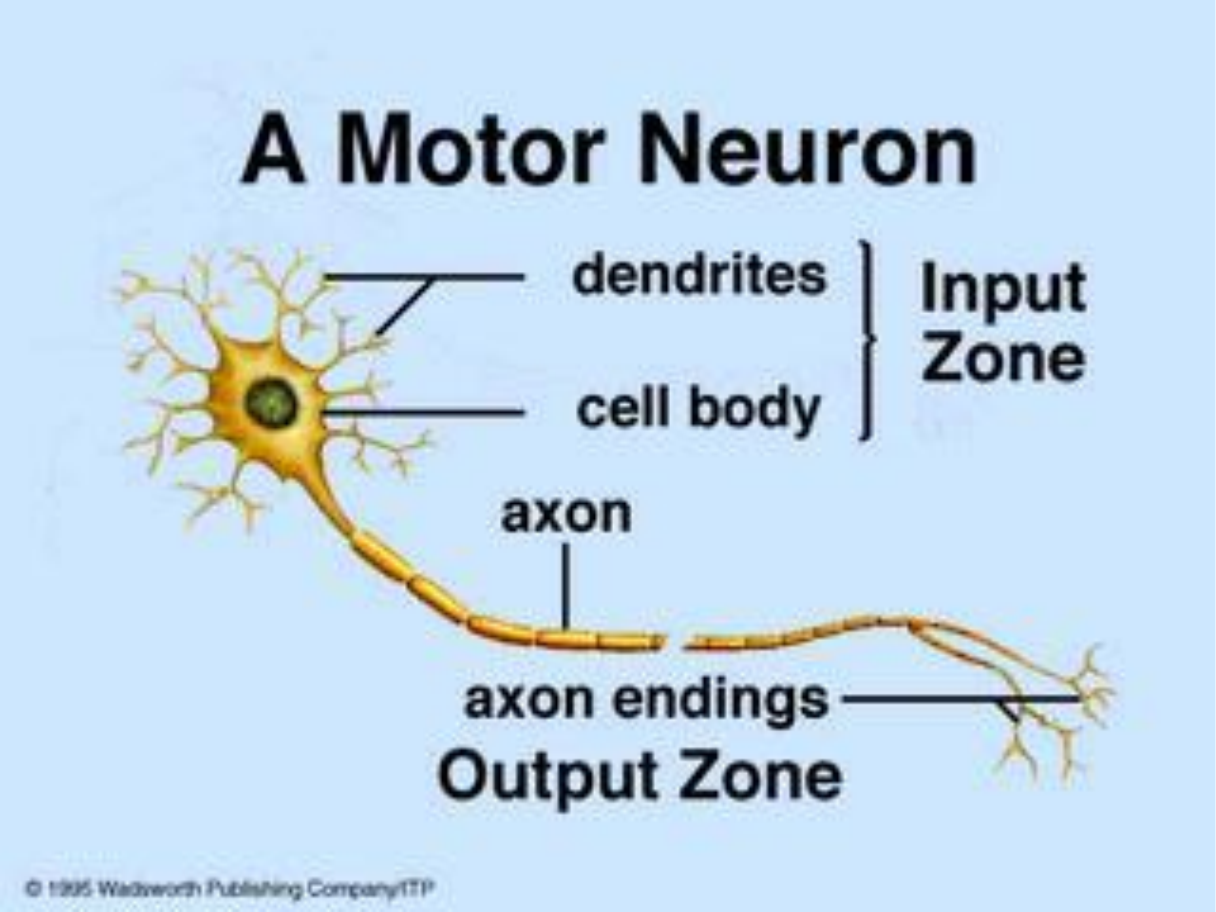


Biological Neural Networks

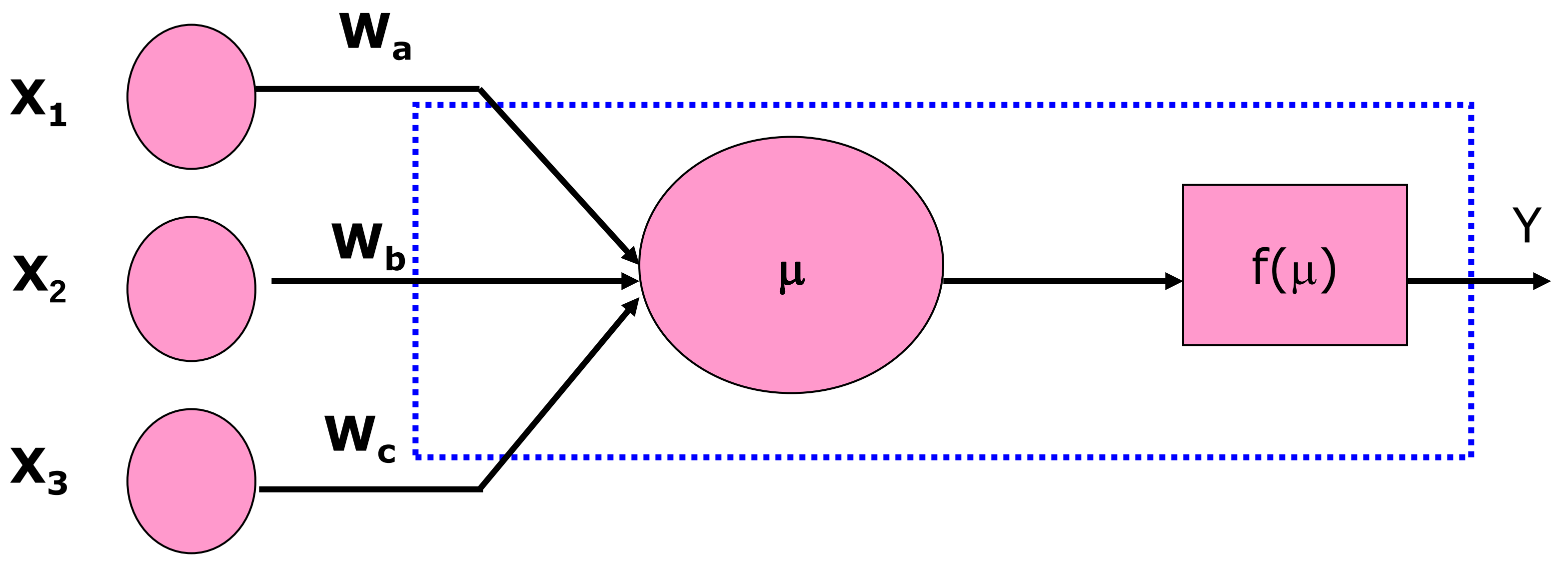
A biological neuron has three types of main components;

- *Dendrites,*
- *Soma (or cell body)*
- *Axon.*

- Dendrites receives signals from other neurons.
- The soma, sums the incoming signals. When sufficient input is received, the cell fires; that is it transmit a signal over its axon to other cells.



Model Of A Neuron



Input units (dendrite)

Connection weights (synapse)

Summing function

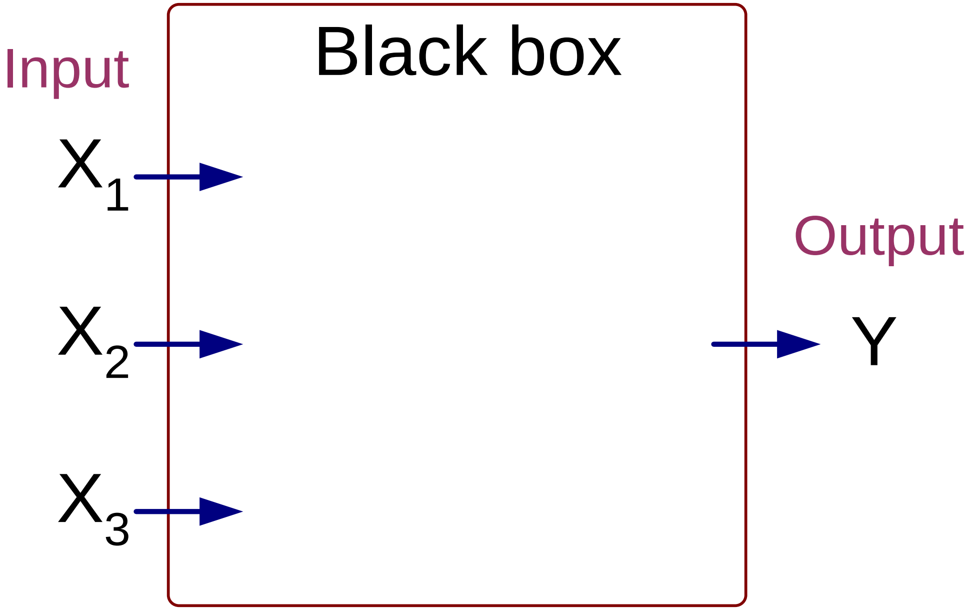
computation

$\underbrace{\text{Summing function} \quad \text{computation}}_{\text{(soma)}}$

(axon)

Artificial Neural Networks (ANN)

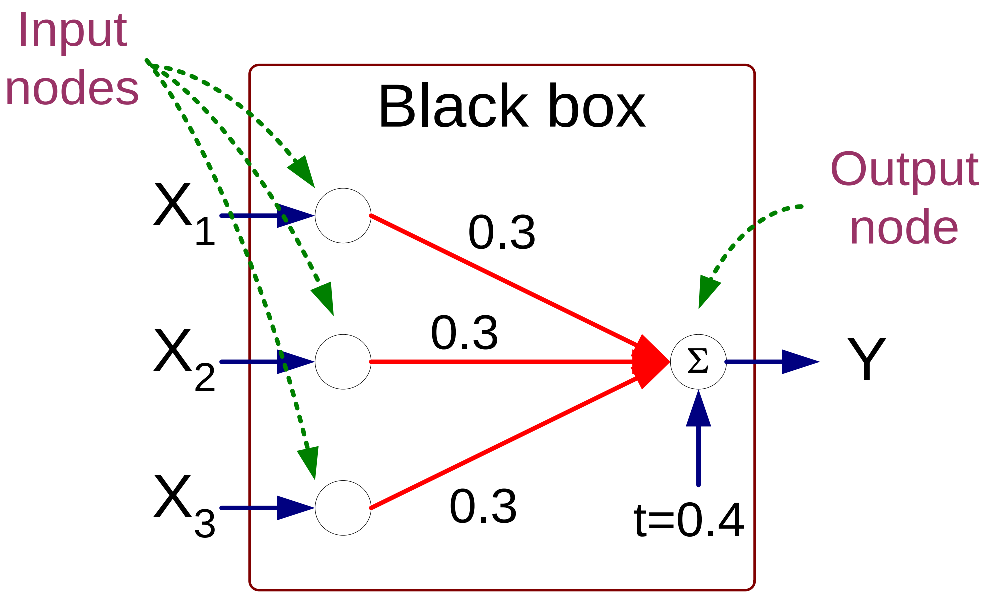
X_1	X_2	X_3	Y
1	0	0	0
1	0	1	1
1	1	0	1
1	1	1	1
0	0	1	0
0	1	0	0
0	1	1	1
0	0	0	0



Output Y is 1 if at least two of the three inputs are equal to 1.

Artificial Neural Networks (ANN)

X_1	X_2	X_3	Y
1	0	0	0
1	0	1	1
1	1	0	1
1	1	1	1
0	0	1	0
0	1	0	0
0	1	1	1
0	0	0	0

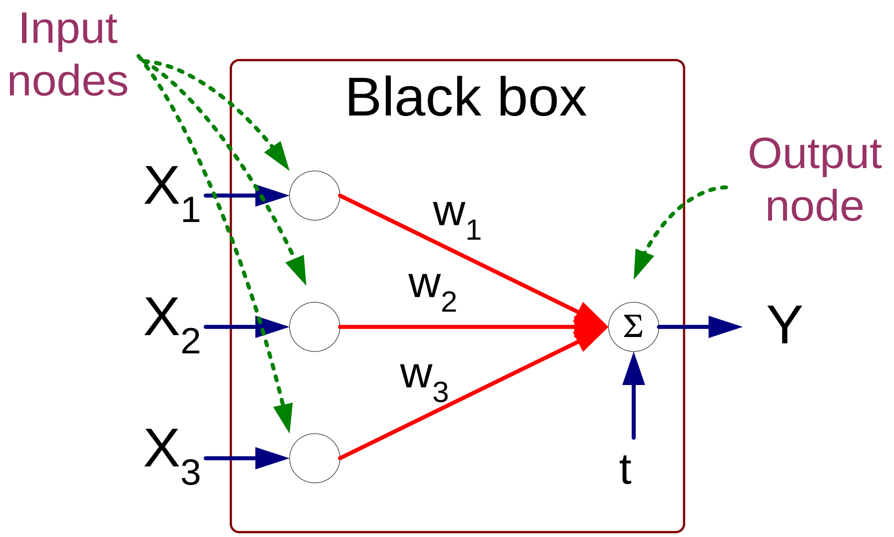


$$Y = I(0.3X_1 + 0.3X_2 + 0.3X_3 - 0.4 > 0)$$

$$\text{where } I(z) = \begin{cases} 1 & \text{if } z \text{ is true} \\ 0 & \text{otherwise} \end{cases}$$

Artificial Neural Networks (ANN)

- Model is an assembly of inter-connected nodes and weighted links
- Output node sums up each of its input value according to the weights of its links
- Compare output node against some threshold t



Perceptron Model

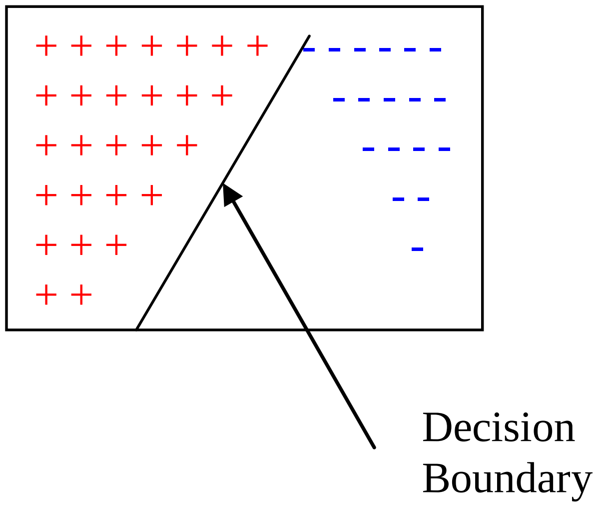
$$Y = I\left(\sum_i w_i X_i - t\right) \quad \text{or}$$

$$Y = sign\left(\sum_i w_i X_i - t\right)$$

Limitations of Simple Perceptron

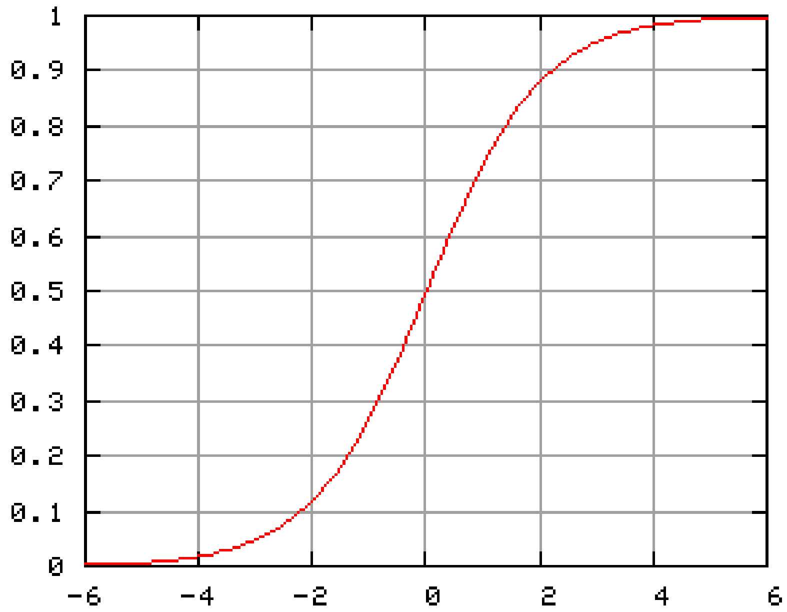
- Simple perceptron can be used to classify problems which are linearly separable

- For such problems a single line can be drawn which separates the two classes with zero (or near zero) error

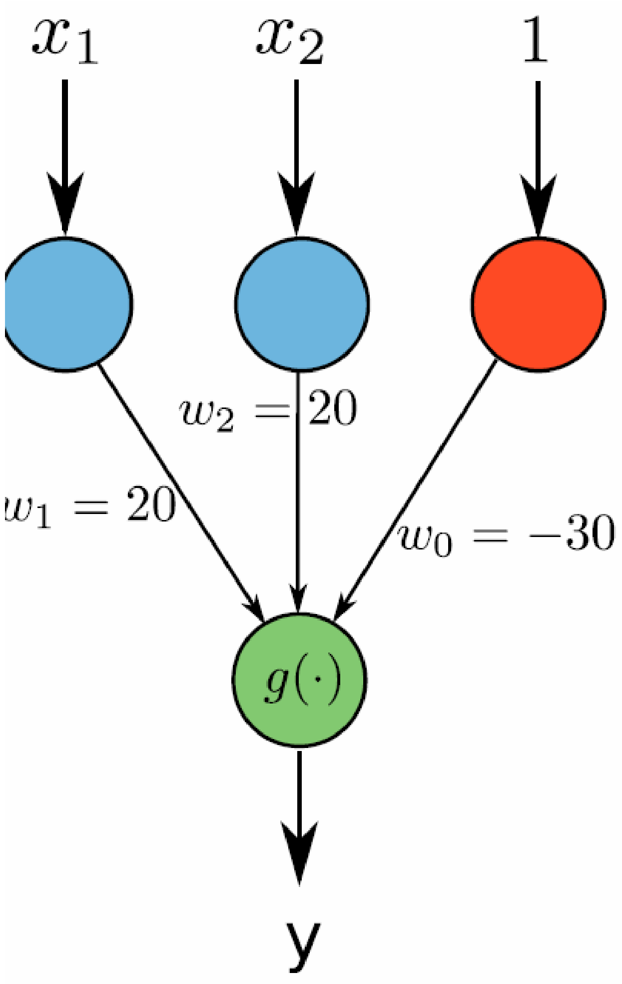


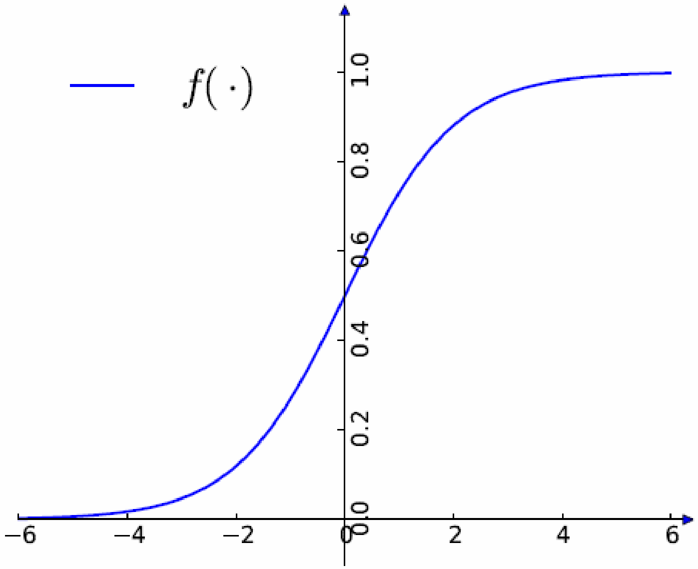
Activation Functions

- Just as with human neurons, the neurons in the hidden layer are activated only when the input they receive is above a certain threshold value
- To model this situation the sigmoid function is commonly used as an activation function
- $\sigma(x) = \frac{1}{1+e^{-x}}$



Solving the Logical AND Problem

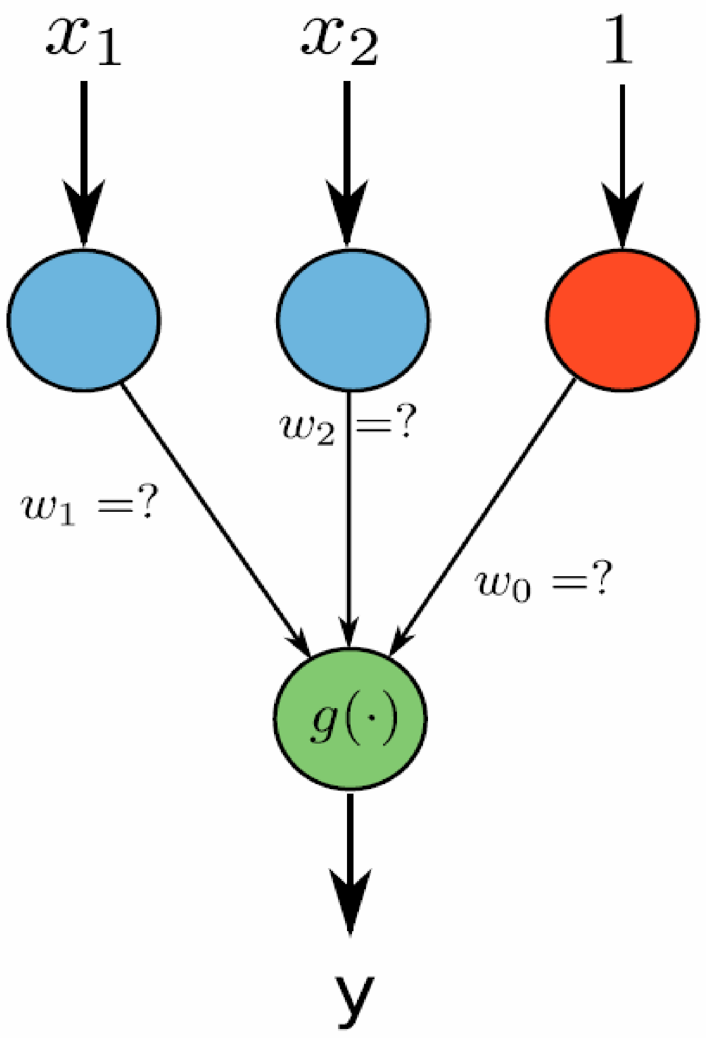


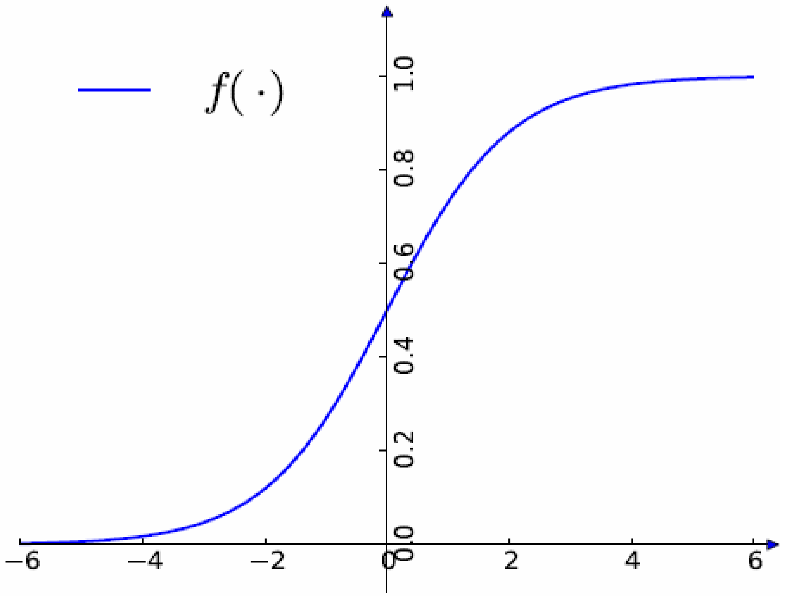


x_1	x_2	y	desired
0	0	$f(-30) \approx 0$	0
0	1	$f(-10) \approx 0$	0
1	0	$f(-10) \approx 0$	0
1	1	$f(10) \approx 1$	1

In this and the next 4 slides the functions f and the sigmoid are one and the same

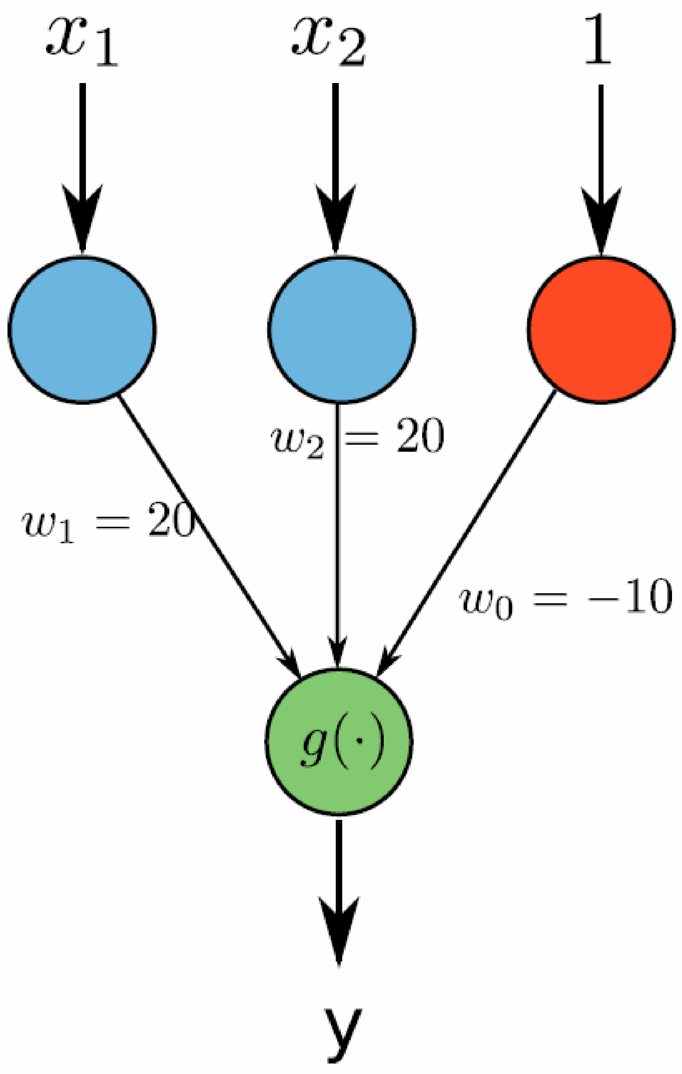
Solving the Logical OR Problem

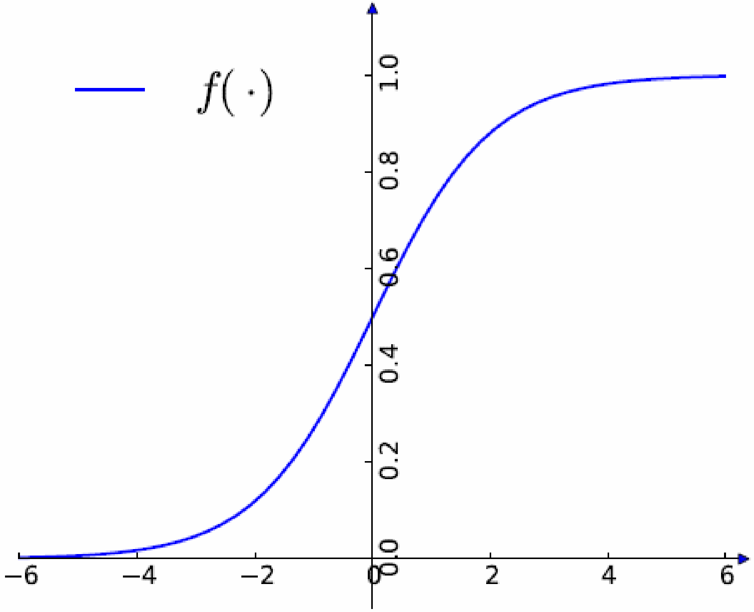




x_1	x_2	y	desired
0	0	?	0
0	1	?	1
1	0	?	1
1	1	?	1

Solving the Logical OR Problem

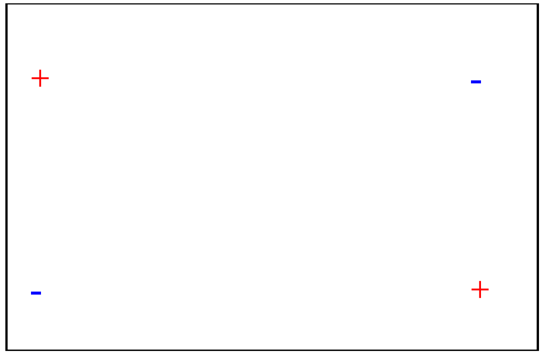




x_1	x_2	y	desired
0	0	$f(-10) \approx 0$	0
0	1	$f(10) \approx 1$	1
1	0	$f(10) \approx 1$	1
1	1	$f(30) \approx 1$	1

Limitations of Simple Perceptrons

- However simple perceptrons cannot solve non linear classification problems such as the XOR problem



- These types of problems can only be solved by adding another layer (called the hidden layer) of neurons to the network

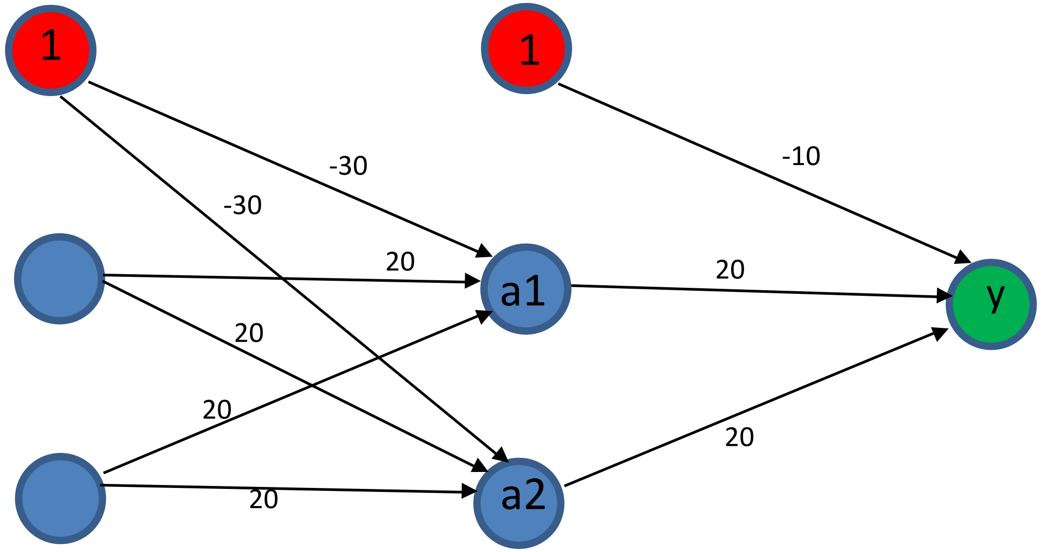
Solving the Logical XNOR Problem

- The XNOR problem is more difficult than the logical AND problem.
- It cannot be solved by a single neuron as it is a 2 stage process
- (X1 XNOR X2) = a1 OR a2 where a1=(X1 AND X2) and a2=(NOT X1 AND NOT X2)
- This can be seen from the following truth table

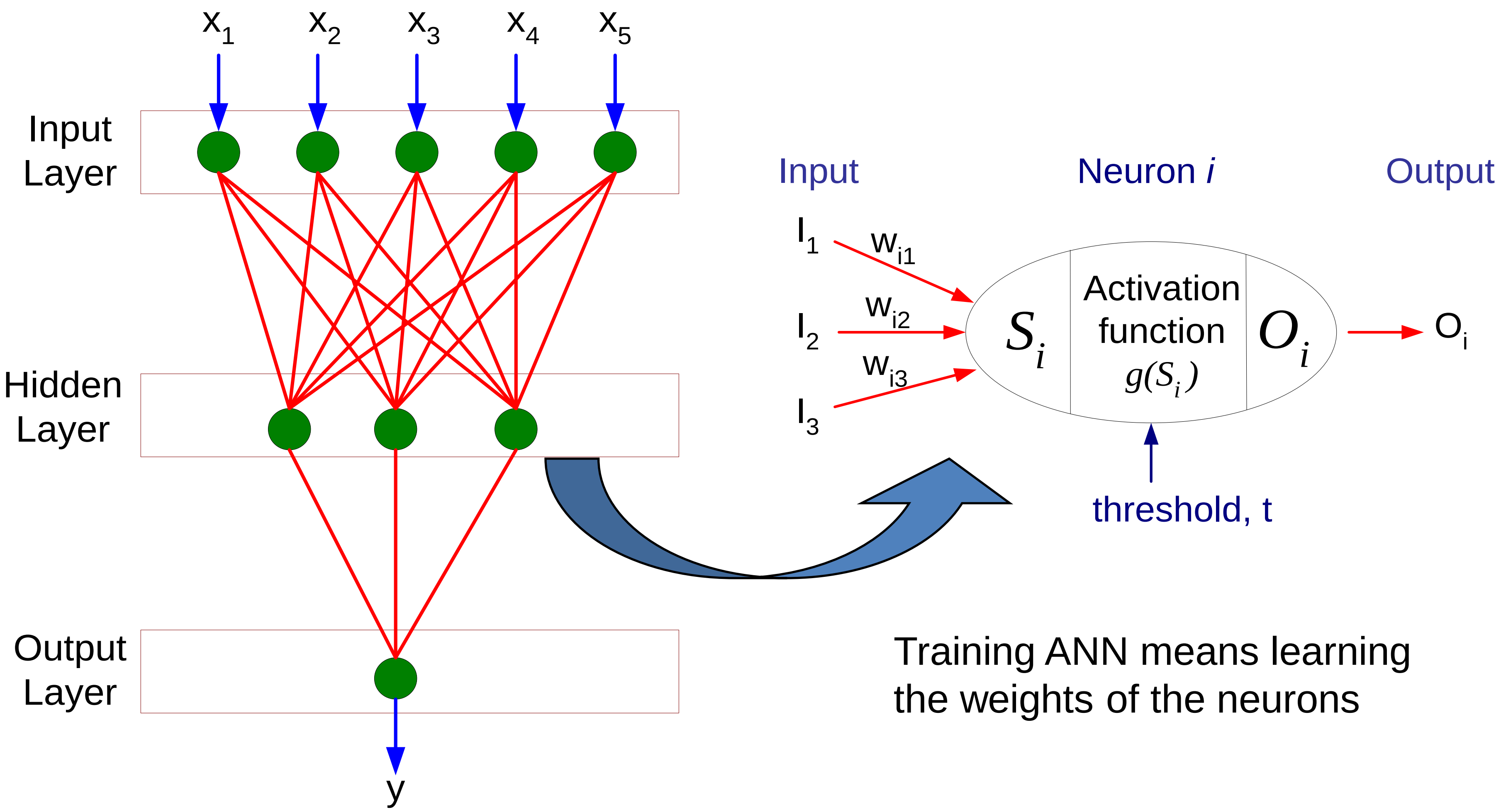
X1	X2	a1	a2	a1 OR a2	X1 XNOR X2
0	0	0	1	1	1
0	1	0	0	0	0
1	0	0	0	0	0
1	1	1	0	1	1

Neural Net for Solving the Logical XNOR Problem

- a1 and a2 can be computed in parallel and so 2 neurons can be assigned to do the computation in the hidden (intermediate layer).



General Structure of ANN

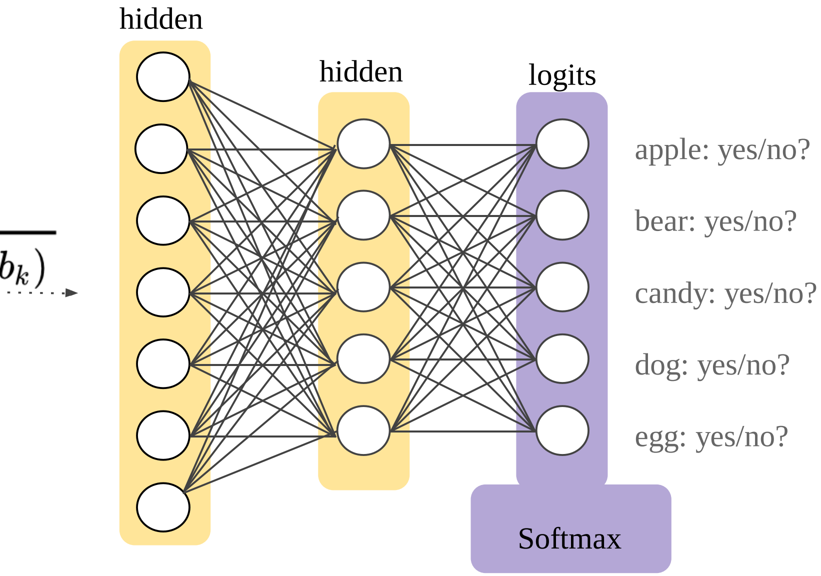


Training ANN means learning the weights of the neurons

Solving classification problems with Softmax

- Classification problems involving more than two classes are solved through the Softmax function which is implemented as an additional layer

$$p(y = j|\mathbf{x}) = \frac{e^{(\mathbf{w}_j^T \mathbf{x} + b_j)}}{\sum_{k \in K} e^{(\mathbf{w}_k^T \mathbf{x} + b_k)}}$$



General Algorithm for learning ANN

- Initialize the weights (w_0, w_1, ..., w_k)
- Compute the error at each output node (k), and the hidden node (j) connected to it.
- Now adjust the weights w_{jk} such that

$$w_{jk}(new) = w_{jk}(current) + \Delta w_{jk}$$

where $\Delta w_{jk} = rError(k)O_j$

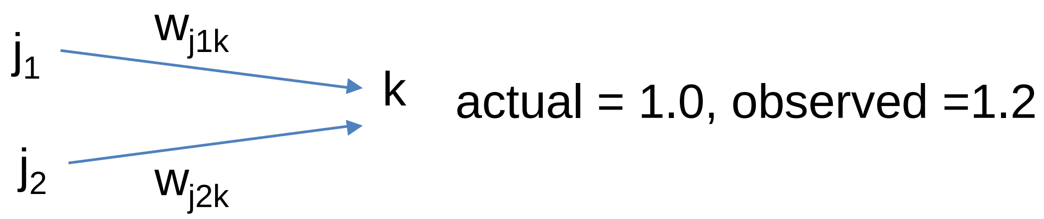
r = learning rate parameter ($0<r<1$)

Error(k) = the computed error at node k

O = output of node j

Algorithm for learning ANN

- Thus it can be seen that the observed errors are used to adjust the weights so that the overall error is minimized
- For example if the desired output at node k is 1 and the actual output is 1.2, then the error = (1-1.2) = -0.2, so we need to decrease the weight of all incoming links starting from all nodes (e.g. j1, j2) that feed into node k



- The weight adjustment process is done iteratively until the error is below some specified threshold – this will involve scanning the data many times over

The Loss function in Backpropagation Learning

- Backpropagation uses gradient descent with Loss as the objective function to minimize.
- The Loss L is defined as follows:
- $L = \frac{\sum_{i=1}^{k}(E_i - P_i)^2}{k}$, thus the loss value is the average squared difference between the expected value E_i (i.e. the actual class value) at the output node i and the predicted value P_i at that node.
- The loss is therefore a measure of error but is not exactly the same as classification error
- Python supports the computation of the loss during the training phase of the MLPClassifier – see the sklearn documentation online

Backpropagation learning

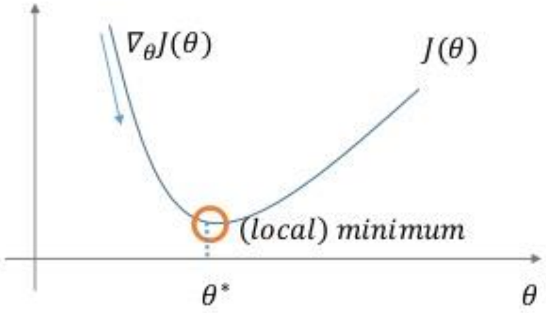
- A rigorous derivation of the weight update expression using the method of *gradient descent* available from: Backprop Algorithm
- Gradient descent is a commonly used for minimizing a function

Gradient Descent

- Gradient descent is a way to minimize an objective function $J(\theta)$
  - $J(\theta)$: Objective function
  - $\theta \in R^d$: Model's parameters
  - η : Learning rate. This determines the size of the steps we take to reach a (local) minimum.

Update equation

$$\theta = \theta - \eta * \nabla_\theta J(\theta)$$



Major Parameters for Multi Layer Perceptrons

1. *Learning rate* – this determines the size of the “steps taken” in the weight adjustment process – larger steps means learning takes place quicker but accuracy may suffer
2. *Number of epochs* – the number of times that the training dataset is scanned – larger the value the more accurate the model (generally 100 or more)
3. The *number of hidden neurons* used – generally chosen as (attributes+classes)/2
4. *Momentum* – some implementations add a term called the momentum to the current weight – this is a small fraction of the update value from the previous iteration; the momentum makes the learning process smoother

Neural Networks - Strengths

NON-LINEARITY

- *It can model non-linear systems*

INPUT-OUTPUT MAPPING

- *It can derive a relationship between a set of input & output responses*

ADAPTIVITY

- *The ability to learn allows the network to adapt to changes in the surrounding environment*

EVIDENTIAL RESPONSE

- *It can provide a confidence level to a given solution*
- *Neural Nets work well with datasets containing noise*
- *Have consistently good accuracy rates across several domains*
- *Can be used for both supervised (classification and numeric prediction) as well as unsupervised learning*

Neural Networks - Weaknesses

- Lack the ability to explain their behaviour (unlike Decision Trees and Naïve Bayes)

- In some cases, overtraining can cause over fitting

- With large datasets training time can be large – very much larger than the Decision Tree and Naïve Bayes methods

Overfitting with MLP

- With the Diabetes dataset: with number of neurons set to 300, Python produced 79% accuracy on the training segment and 71% accuracy on the test segment

- With number of neurons set to 100, Python produced 76% accuracy on both training and test segments

- This shows overfitting is taking place when the number of hidden neurons is high – in this case an accurate model is learn on existing data but the model cannot predict very well on new data that is arriving

ANN Applications

Neural Network Applications

- In general can be used for classification as well as for numeric prediction
- For classification has been used for recognizing both printed and handwritten digits
- For numeric prediction has been used for forecasting time series such as weather data (temperature, pressure, wind speed, etc), stock market prices, etc.
    - *Neural Network handwritten recognition:* *http://myselph.de/neuralNet.html*
    - *Neural Nets play Pong:* *http://www.youtube.com/watch?v=LD6OgKEj5JE*
    - *An interactive demo*