Application of Computer in Chemistry SSC 3533

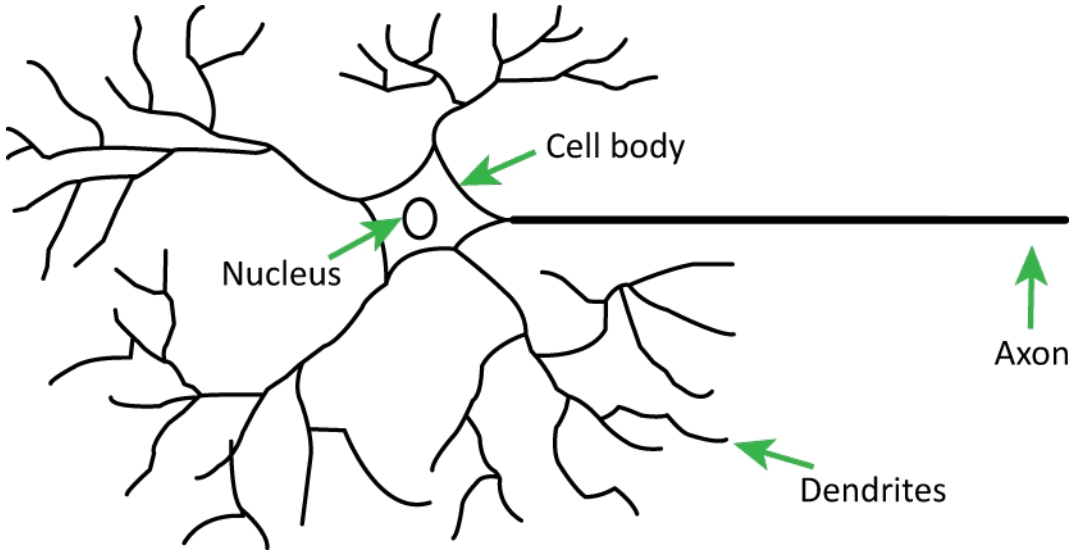
NEURAL NETWORKS

Prof. Mohamed Noor Hasan
Dr. Hasmerya Maarof
Department of Chemistry

Introduction

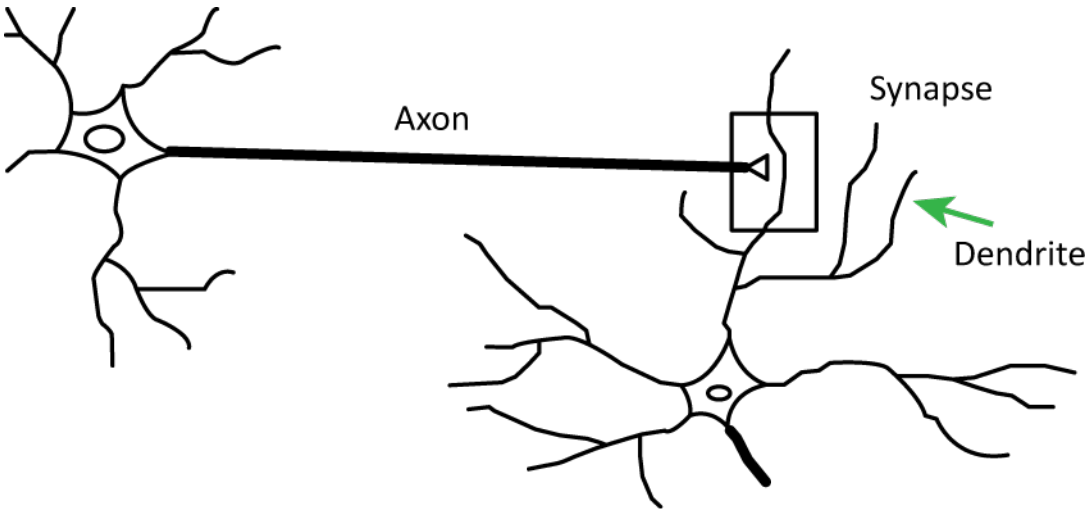
- A new technique for processing information
- Based on the operation in human nervous system
- Consist of processing units (cells) which are connected to one another (network)

Biological Nerve Cell



Dendrites bring signal in, axon takes signal out

Synapse

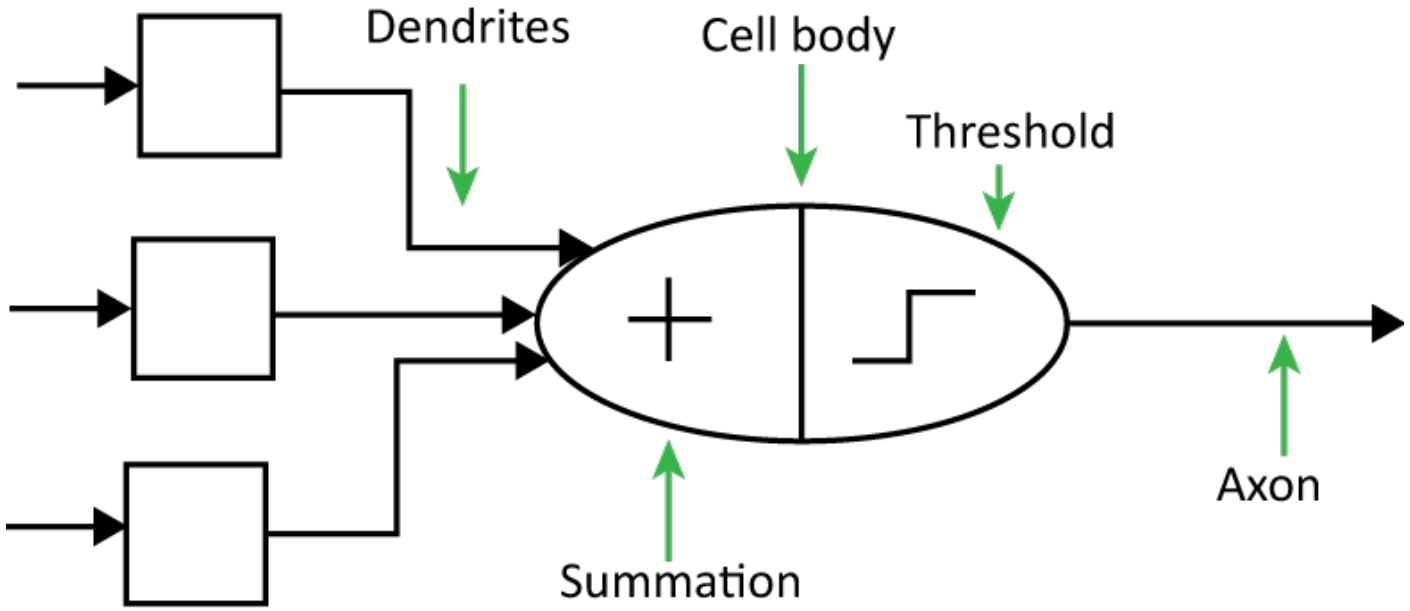


Synapse – signal is transferred from one cell to another

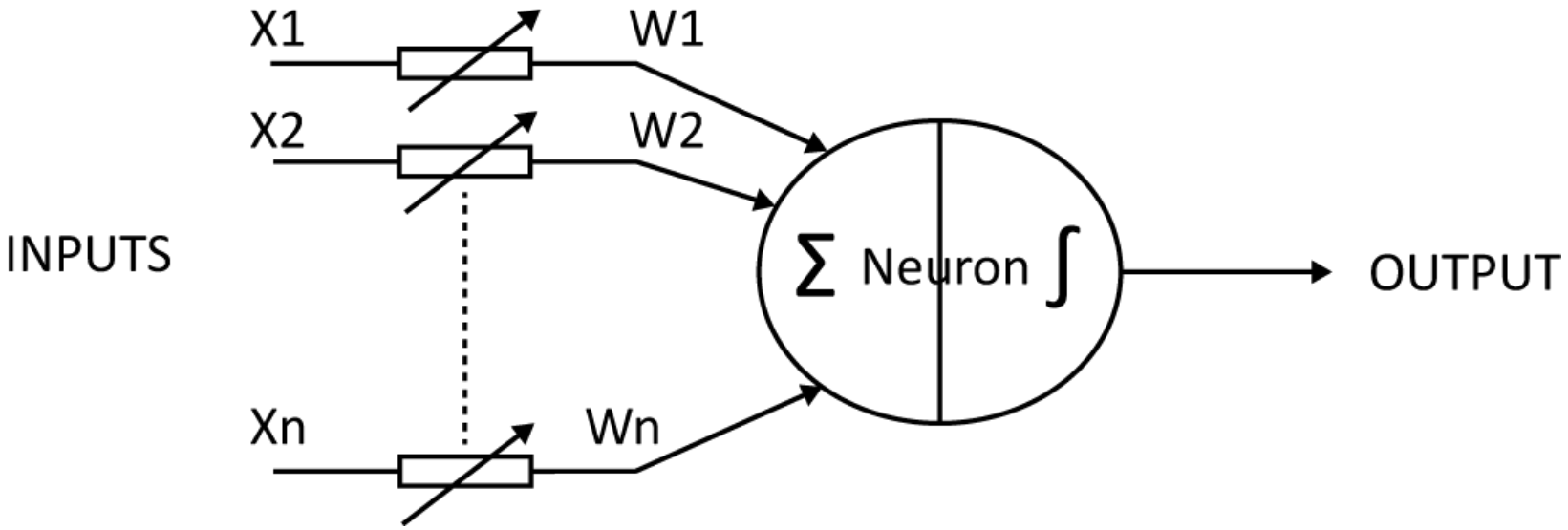
The signal must be larger than certain threshold before it can be passed to other cells

Signals that enter a cell is proportional to the size of dendrites

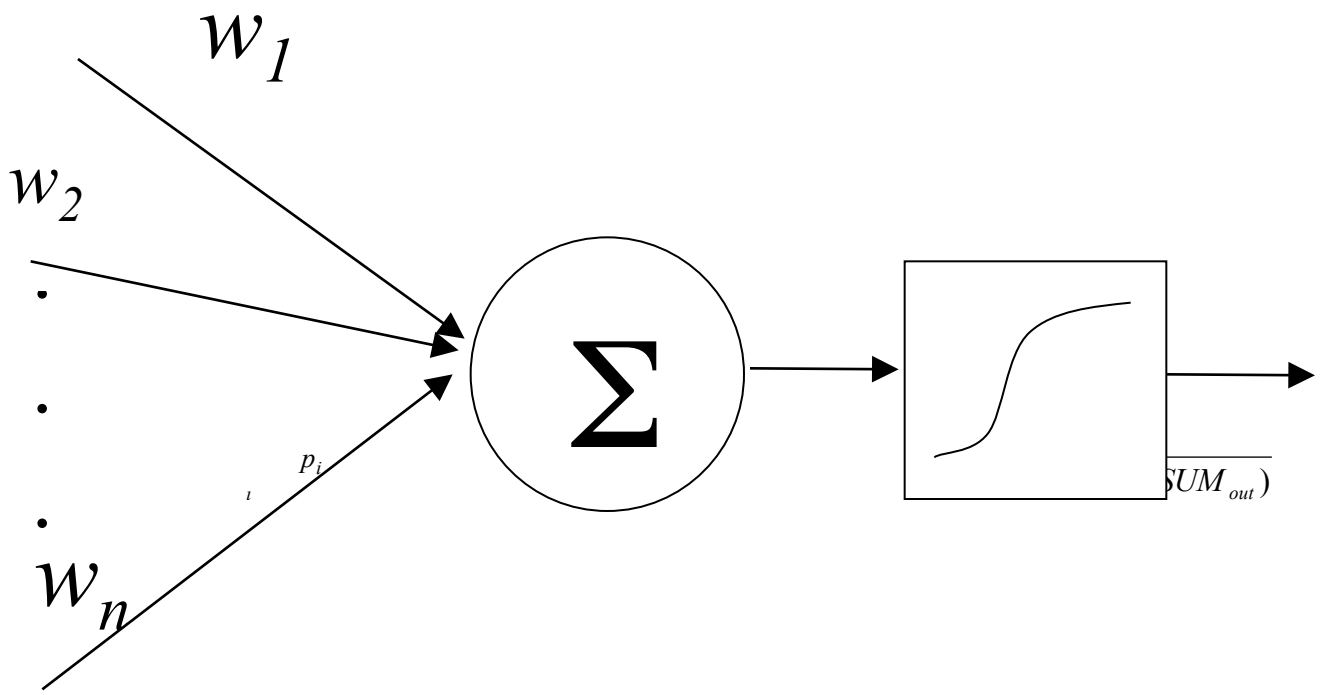
Simple Cell



Processing unit - Neuron



Neuron cell



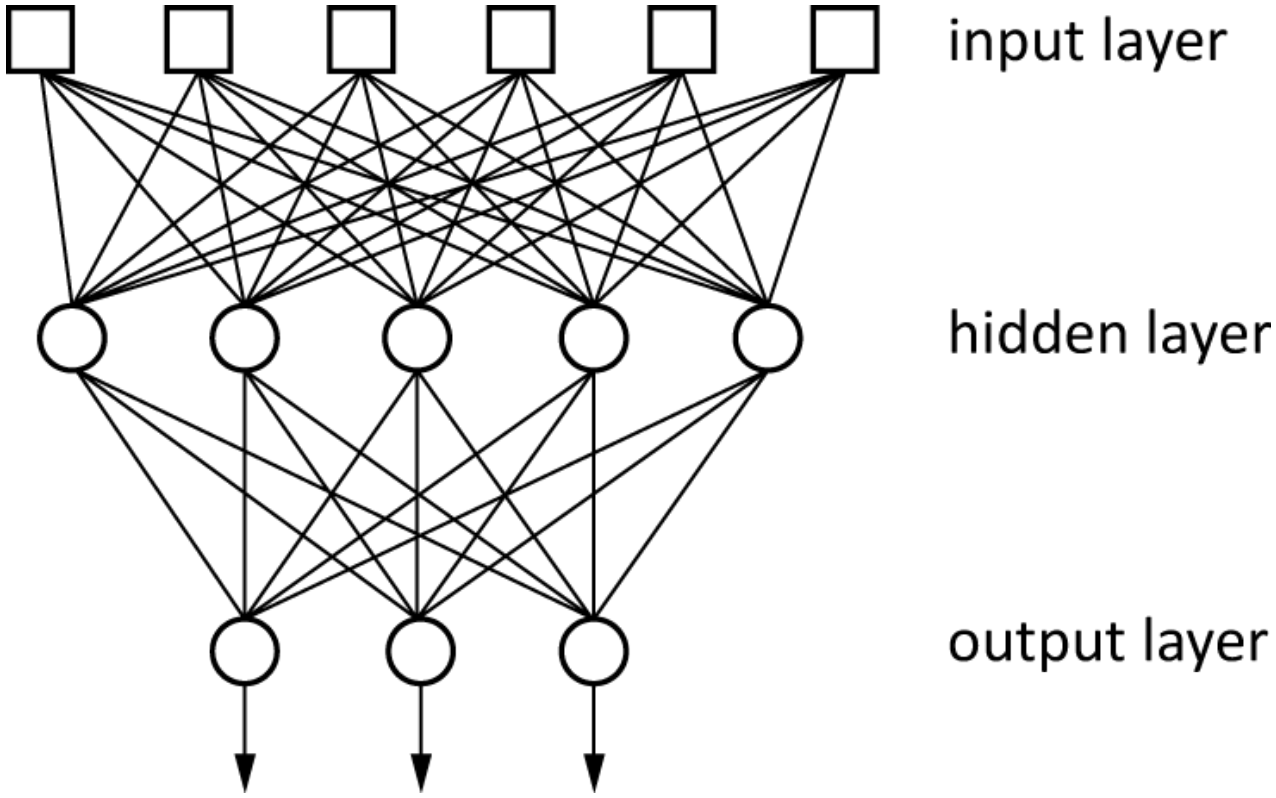
Cell activity

- Signal that enters a cell is multiplied by certain weight to determine its importance (just like the size of dendrites in nervous system)
- The input signals are summed up in the cell.

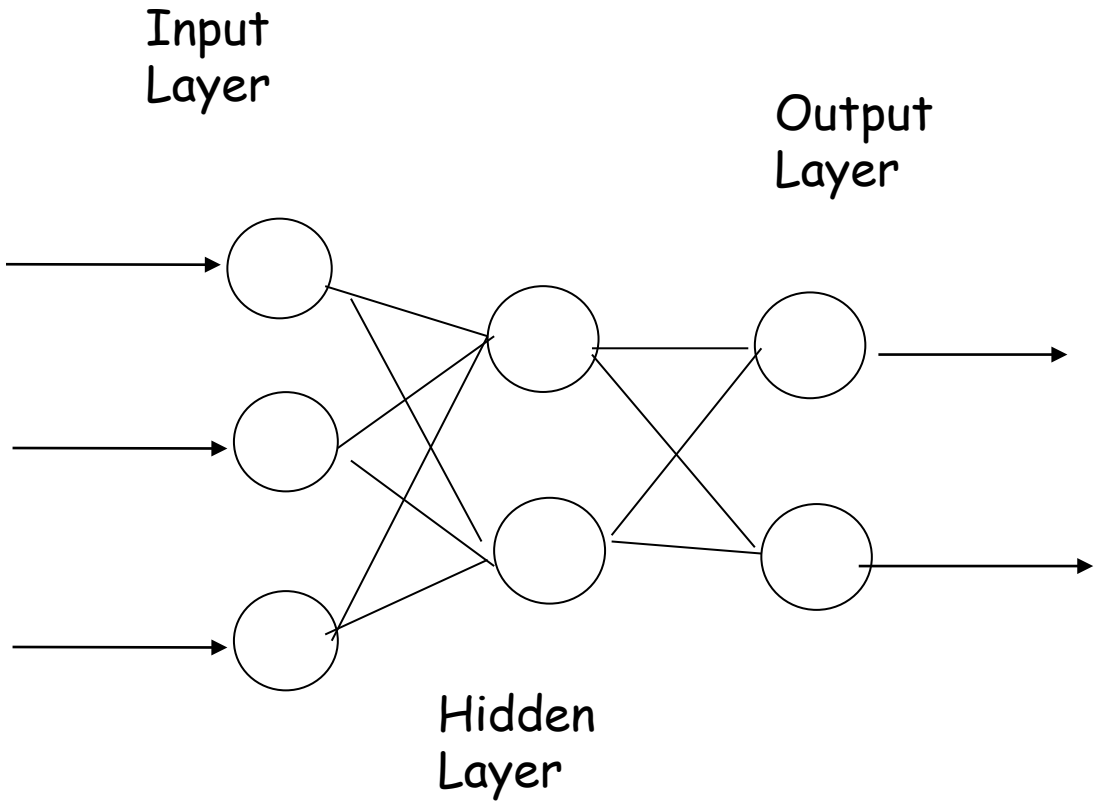
$$Net_j = \sum Inp_i . w_{ij}$$

- Signals must exceed certain threshold – will be passed to the next cell if larger that the threshold
- Output transferred to other cells – forming a network

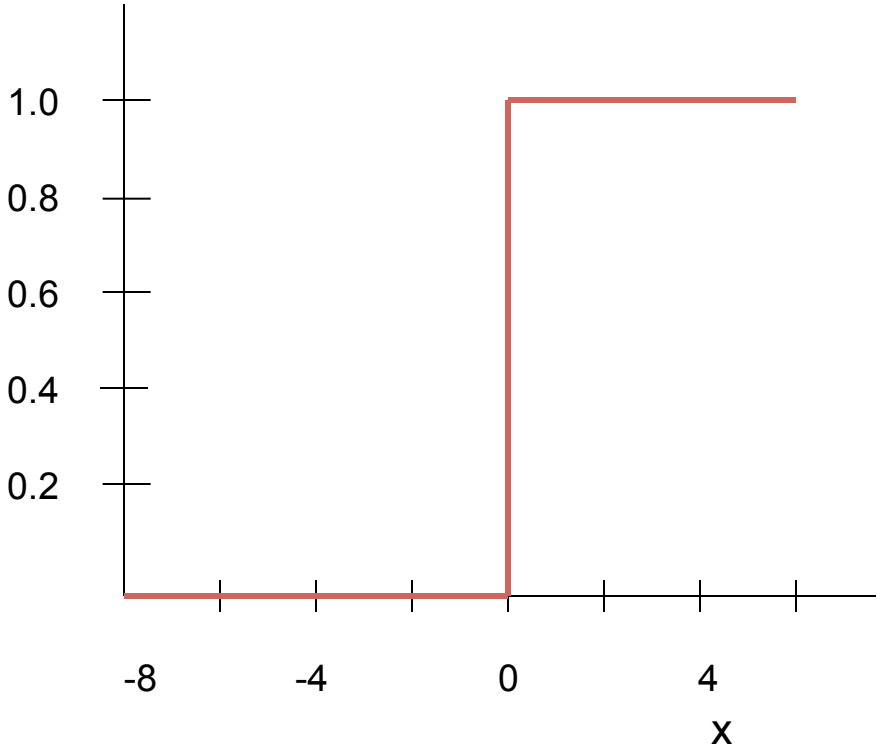
Neural Networks



Neural Networks



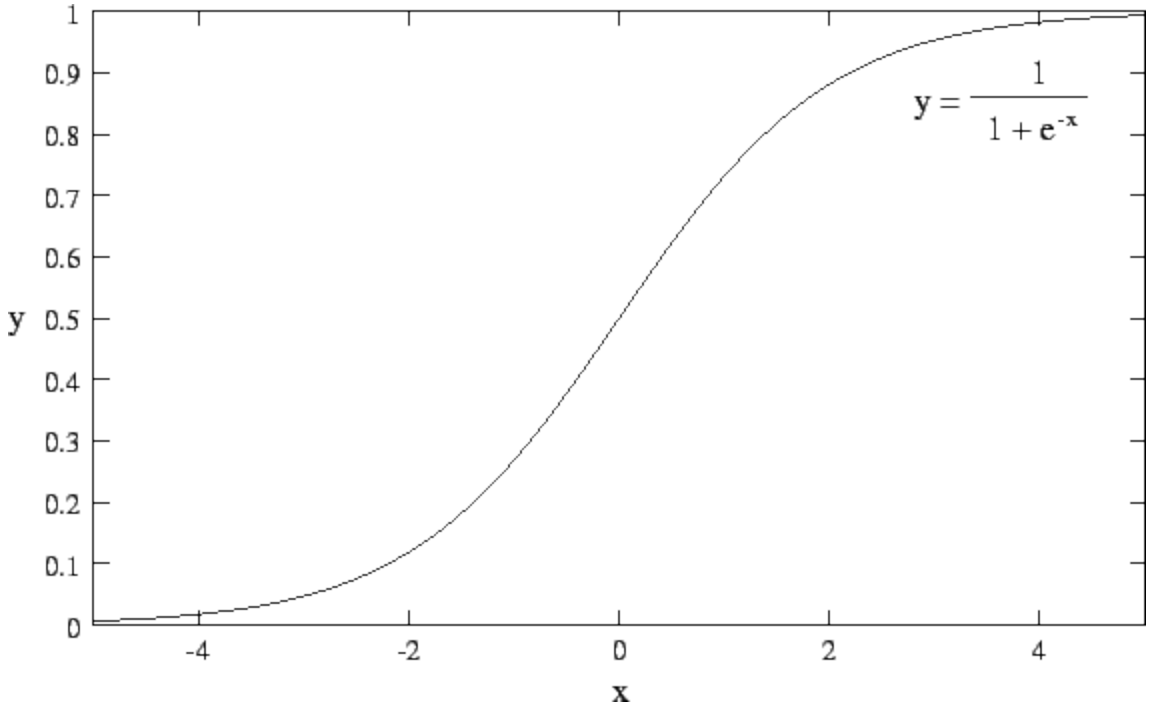
Transfer Function - Discrete



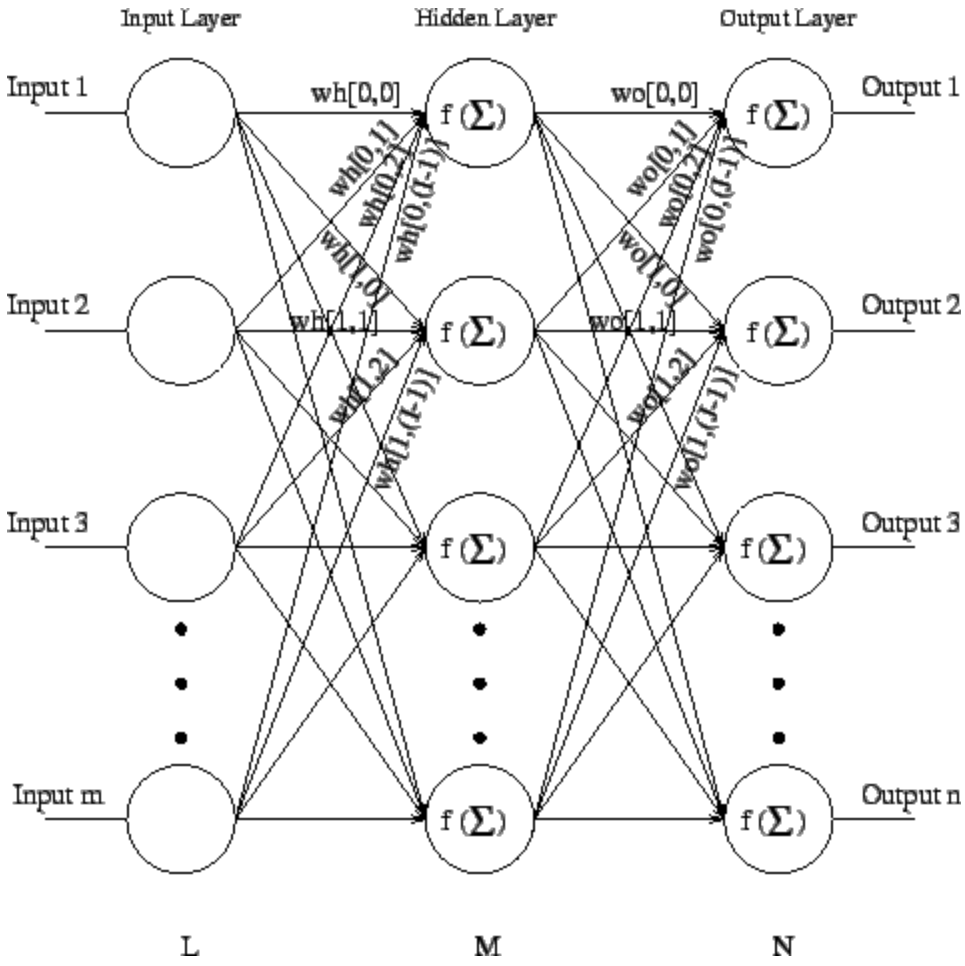
f(x) = 1 if x>0

f(x) = 0 if x<0

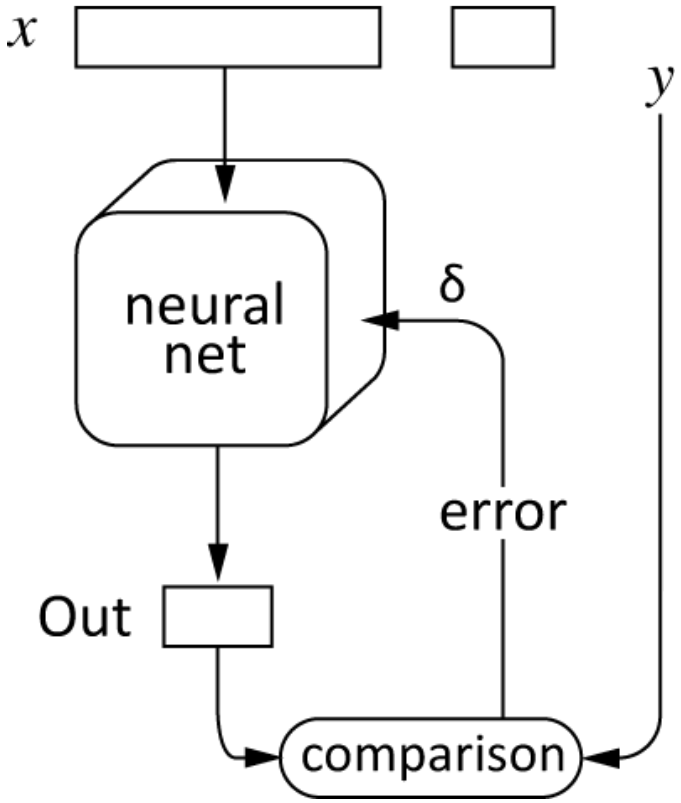
Transfer function - continuous



Network Topology

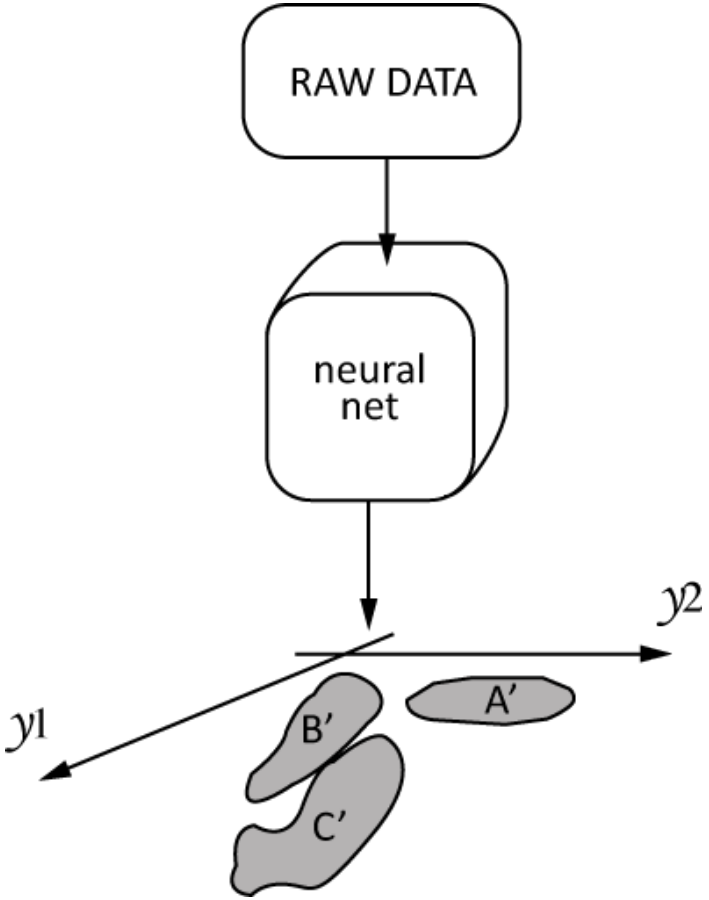


Supervised Learning



- Data **X** are entered with known value of output **Y**
- The weights are adjusted so that the output obtained are the same with the desired value.
- The trained network can be used to predict value of Y for unknown

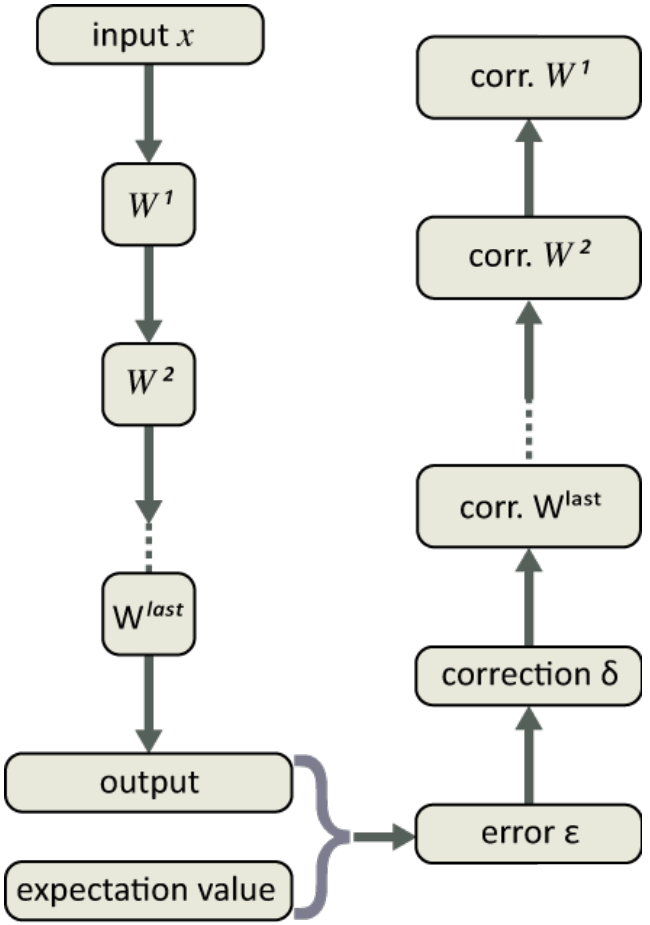
Unsupervised Learning



- Data are passed repeatedly until a stable network is obtained
- The output values will form clusters

Back Propagation Method

- The most popular neural network
- The network topology consist of many layers
- The learning method corrects errors front to the back



W Correction

- The weights are adjusted so that the desired output is obtained
- Total errors:

$$\varepsilon = \sum_{j=1}^{m} (y_j - out_j^{last})^2$$

$$\delta_j^{last} = -\partial \varepsilon / \partial Net_j^{last}$$

- Make correction on w_j proportional to the error it contributes:

$$\Delta w_{ji}^{last} = \eta \delta_j^{last} out_j^{last-1}$$

Example applications

- Spectral Interpretation
  - MS, NMR, IR, near-IR, UV-Vis, X-ray
- Pattern Recognition
  - Classification of chemical compounds
  - Predicting toxicity, biological activities

Predicting toxicity of chemical compounds

- Structures of compounds (toxic and non toxic) are entered to the computer as training set
- From the modeled molecular structures, calculate properties that can be used as variables (descriptors), for example surface area, degree of branching, log P, dipole moment, etc.
- Train the neural network using descriptors as input and weight *w* so that the class is right. Example, 1 for active, 0 for inactive.

Predicting toxicity of chemical compounds

- Adjust *w* until all compounds in the training set have the correct class.
- Enter structure of compounds with unknown toxicity and try to make classification based on the trained network.