Neural Networks

Some slides were adapted/taken from various sources, including Prof. Andrew Ng's Coursera Lectures, Stanford University, Prof. Kilian Q. Weinberger's lectures on Machine Learning, Cornell University, Prof. Sudeshna Sarkar's Lecture on Machine Learning, IIT Kharagpur, Prof. Bing Liu's lecture, University of Illinois at Chicago (UIC), CS231n: Convolutional Neural Networks for Visual Recognition lectures, Stanford University and many more. We thankfully acknowledge them. Students are requested to use this material for their study only and **NOT** to distribute it.

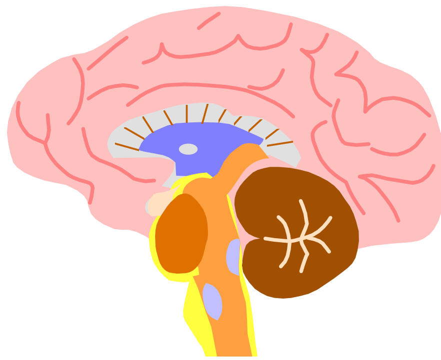
Outline

- The Brain
- Perceptrons
- Gradient descent
- Multi-layer networks
- Backpropagation

Artificial Neural Networks

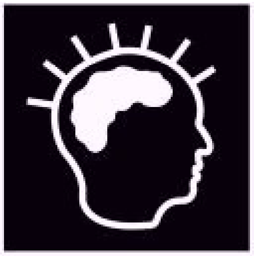
- Other terms/names
  - connectionist
  - parallel distributed processing
  - neural computation
  - adaptive networks..
- History
  - 1943-McCulloch & Pitts are generally recognised as the designers of the first neural network
  - 1949-First learning rule
  - 1969-Minsky & Papert - perceptron limitation - Death of ANN
  - 1980’s - Re-emergence of ANN - multi-layer networks

The biological inspiration



- The brain has been extensively studied by scientists.
- Vast complexity prevents all but rudimentary understanding.
- Even the behaviour of an individual neuron is extremely complex

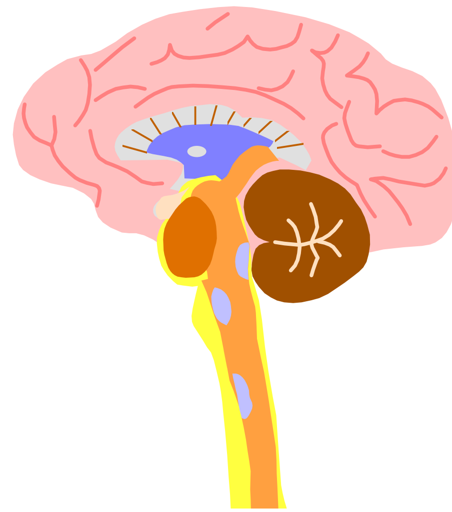
Features of the Brain

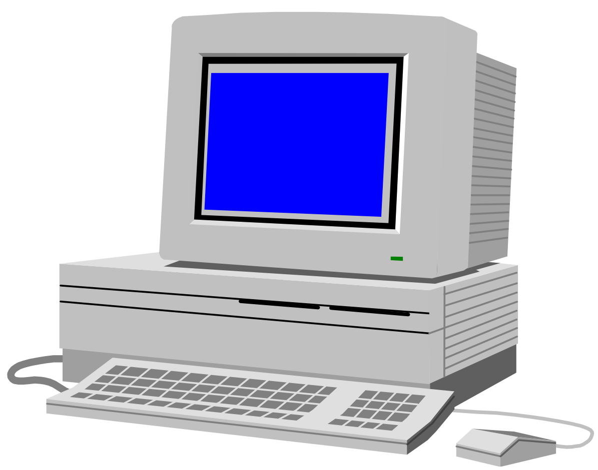


- Ten billion (10^{10}) neurons
- Neuron switching time $>10^{-3}$secs
- Face Recognition ~0.1secs
- On average, each neuron has several thousand connections
- Hundreds of operations per second
- High degree of parallel computation
- Distributed representations
- Die off frequently (never replaced)
- Compensated for problems by massive parallelism

Brain and Machine

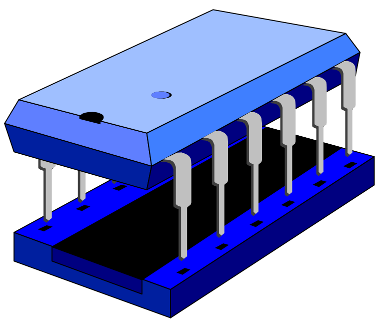
- The Brain
  - Pattern Recognition
  - Association
  - Complexity
  - Noise Tolerance





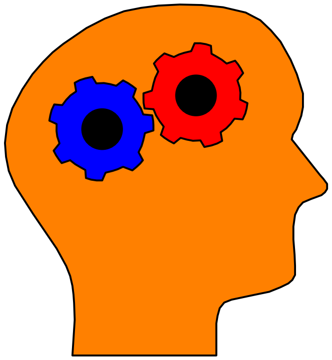
- The Machine
  - Calculation
  - Precision
  - Logic

The contrast in architecture

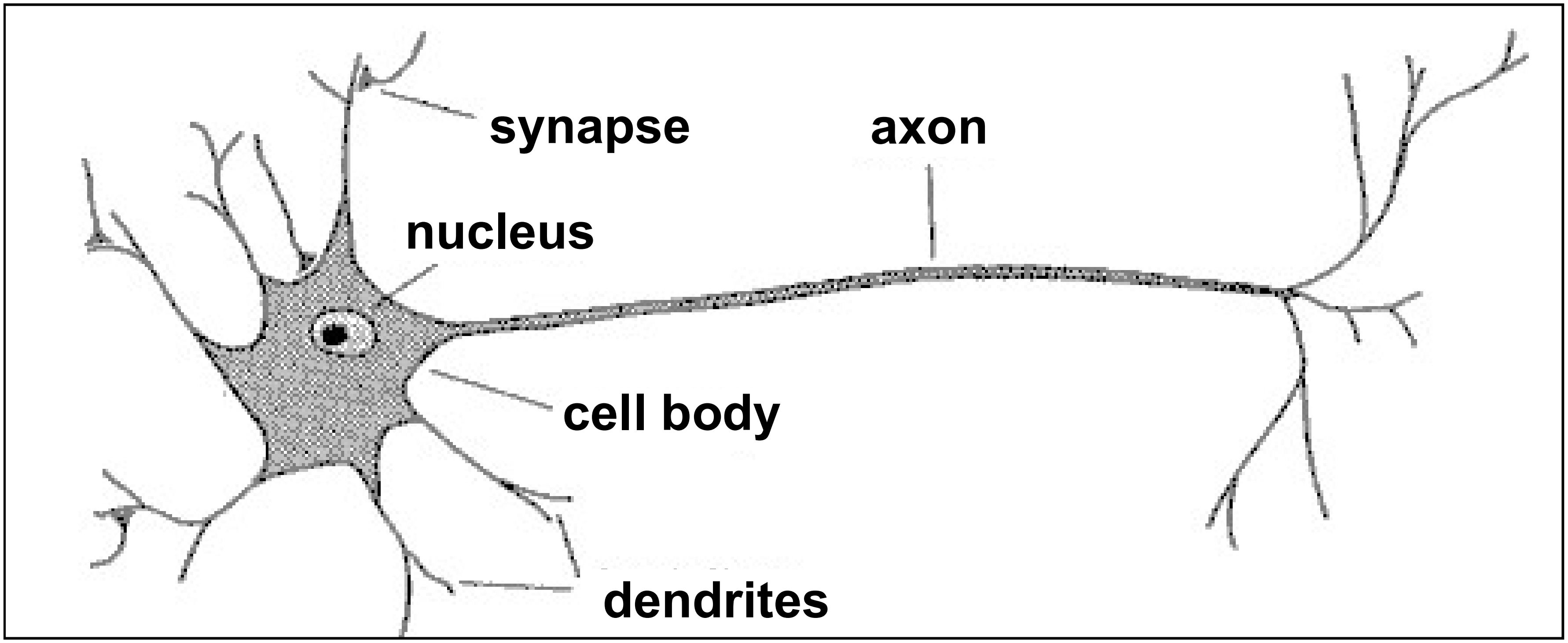


- The Von Neumann architecture uses a single processing unit;
  - Tens of millions of operations per second
  - Absolute arithmetic precision

- The brain uses many slow unreliable processors acting in parallel



The Structure of Neurons



The Structure of Neurons

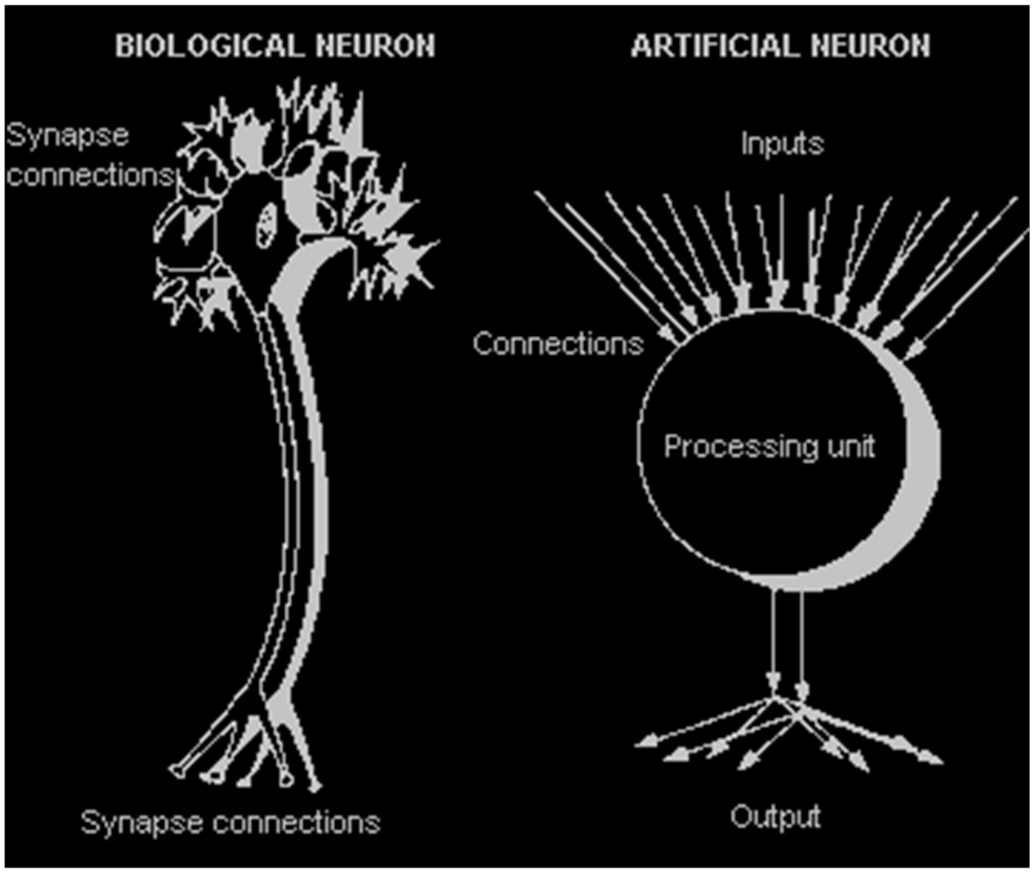
- A neuron only fires if its input signal exceeds a certain amount (the threshold) in a short time period.
- Synapses vary in strength
  - Good connections allowing a large signal
  - Slight connections allow only a weak signal.
  - Synapses can be either excitatory or inhibitory.

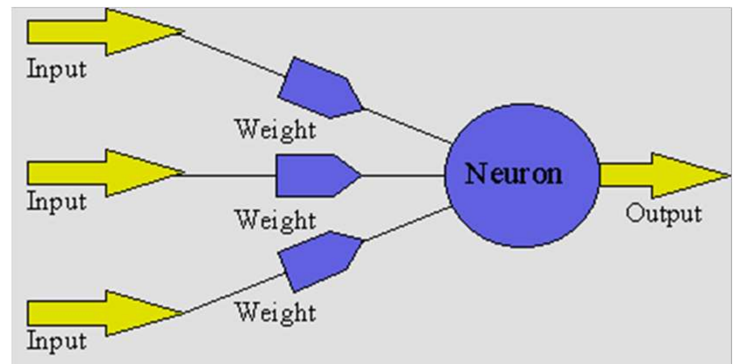
The Structure of Neurons

A neuron has a cell body, a branching **i**nput structure (the dendr**I**te) and a branching **o**utput structure (the ax**O**n)

- Axons connect to dendrites via synapses.
- Electro-chemical signals are propagated from the dendritic input, through the cell body, and down the axon to other neurons

Properties of Artificial Neural Nets (ANNs)





Properties of Artificial Neural Nets (ANNs)

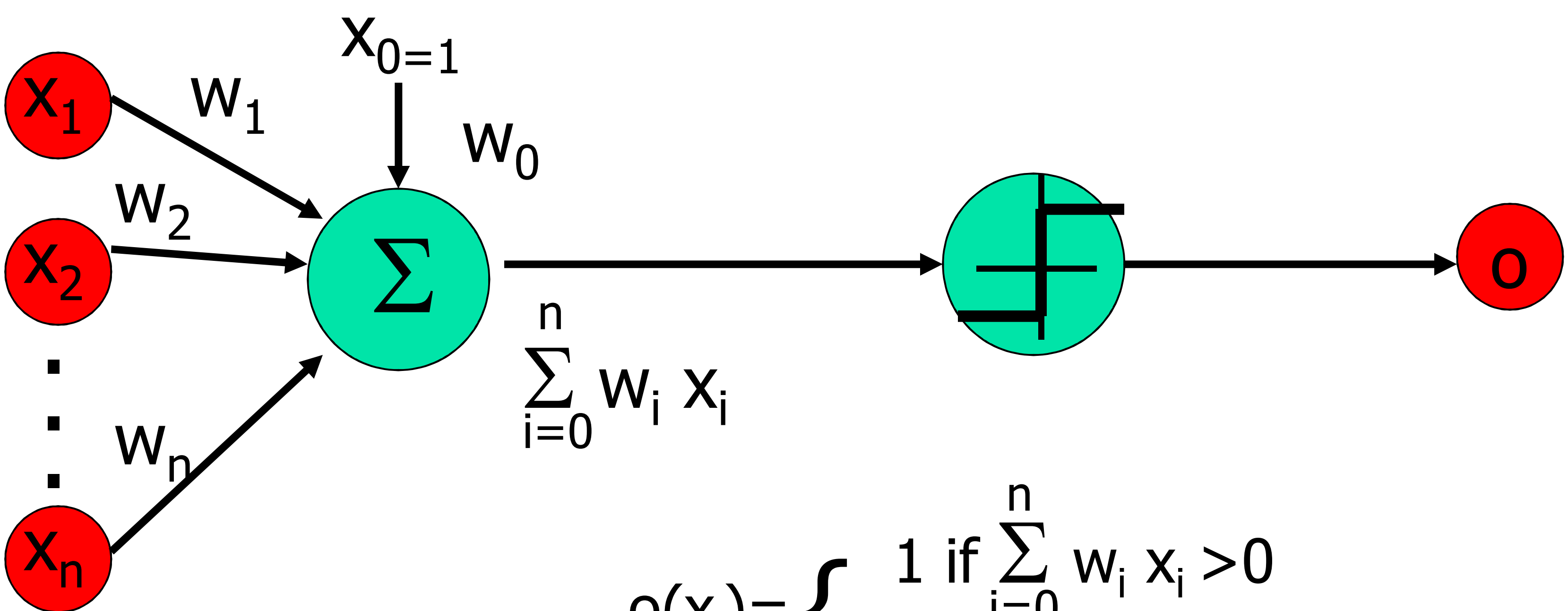
- Many simple neuron-like threshold switching units
- Many weighted interconnections among units
- Highly parallel, distributed processing
- Learning by tuning the connection weights

Appropriate Problem Domains for Neural Network Learning

- Input is high-dimensional discrete or real-valued (e.g. raw sensor input)
- Output is discrete or real valued
- Output is a vector of values
- Form of target function is unknown
- Humans do not need to interpret the results (black box model)

Perceptron

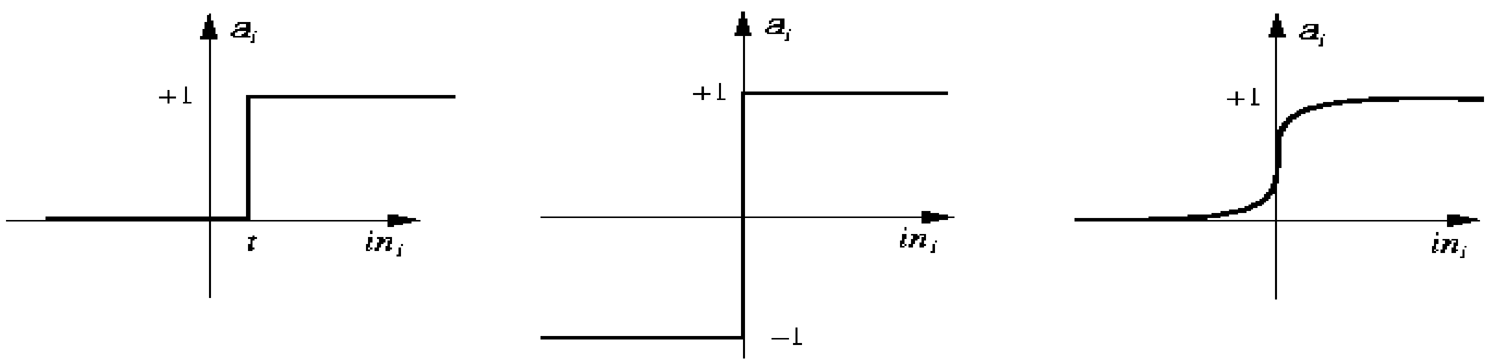
- Linear treshold unit (LTU)



$$o(x_i) = \begin{cases} 1 \text{ if } \sum_{i=0}^{n} w_i x_i > 0 \\ -1 \text{ otherwise} \end{cases}$$

Activation functions

- Transforms neuron's input into output.
- Features of activation functions:
  - A squashing effect is required
    - Prevents accelerating growth of activation levels through the network.



(a) Step function (b) Sign function (c) Sigmoid function

Standard activation functions

- The hard-limiting threshold function
  - Corresponds to the biological paradigm
    - either fires or not
- Sigmoid functions ('S'-shaped curves)
  - The logistic function

$$\phi(x) = \frac{1}{1 + e^{-ax}}$$

  - The hyperbolic tangent (symmetrical)
  - Both functions have a simple differential
  - Only the shape is important

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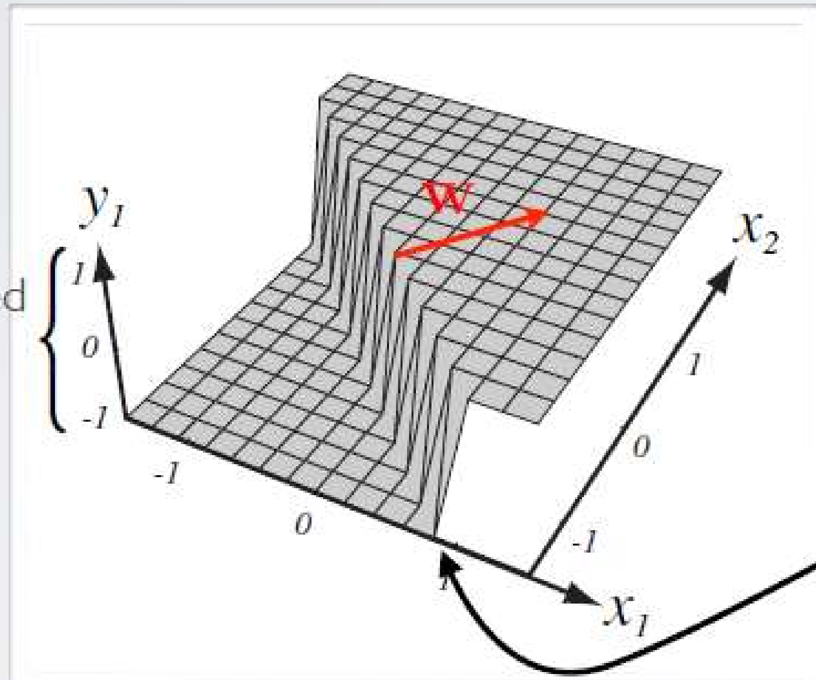
Topics: connection weights, bias, activation function

range determined by $g(\cdot)$



bias b only changes the position of the riff

(from Pascal Vincent's slides)

Perceptron Learning Rule

$w_i = w_i + \Delta w_i$ (weight updation)

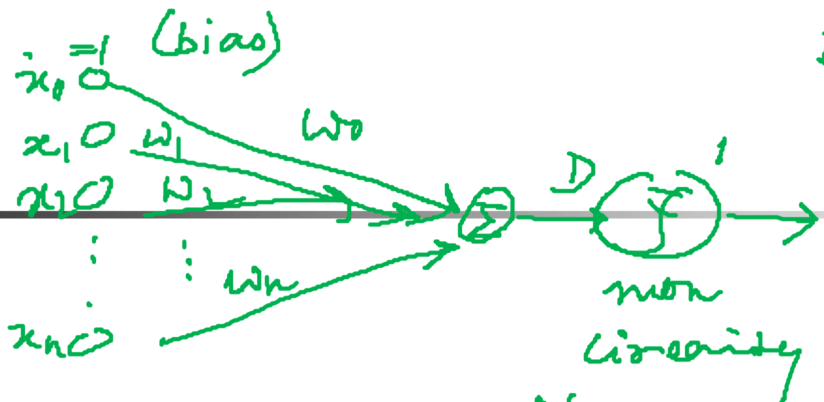
$\boxed{\Delta w_i = \eta\ (t - o)\ x_i}$

$t=c(x)$ is the target value

o is the perceptron output

η Is a small constant (e.g. 0.1) called *learning rate*

- If the output is correct ($t=o$) the weights w_i are not changed
- If the output is incorrect ($t \neq o$) the weights w_i are changed such that the output of the perceptron for the new weights is *closer* to t.
- The algorithm converges to the correct classification
  - if the training data is linearly separable
  - and η is sufficiently small



$b, \underline{w_1, w_2, \ldots w_n}$

Initialize randomly

$$\underline{D} = \sum_{i=0}^{N} w_i x_i \quad , \quad \text{~~target o/p~~} = d$$

Mean square error

$$E = \frac{1}{2}(D-d)^2 \quad , \quad \text{minimize Error } (E) \text{ with respect } w_i\text{'s.}$$

Error gradient

$$\frac{\partial E}{\partial w_i} = (D-d)\left[\frac{\partial (D-d)}{\partial w_i}\right]$$

$d =$ const. independent of i

$$\frac{\partial (D-d)}{\partial (w_i)} = \frac{\partial}{\partial w_i}(D)$$

$$= \frac{\partial}{\partial w_i}\left[\sum_{i=0}^{N} x_i w_i\right] = x_i$$

$$\underline{\frac{\partial E}{\partial w_i} = (D-d)\, x_i}$$

$w_i(0)$ = initialized randomly.

$$W_i(k+1) = w_i(k) - \eta \frac{\partial E}{\partial w_i}$$

$$= w_i(k) - \underline{\underline{\eta}} (D-d) x_i$$

2-class Problem

updation rule of weight at step $k+1$

η = learning rate

Extend to Multi-class Problem

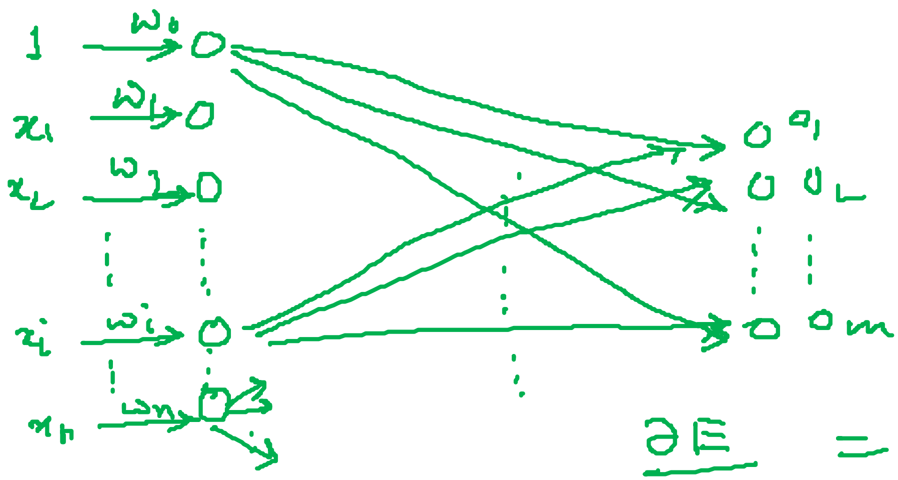
= rate of convergence.

for $\forall$ w_i

$$g_i(x) > g_j(x) \quad \forall j \neq i$$

$\Rightarrow x \in w_i$

Multi-class classification



$$E = \frac{1}{2}\sum_{j=1}^{n}(D_j - d_j)^2$$

$$\frac{\partial E}{\partial w_{ij}} = (D_j - d_j)x_i$$

Training algo

$w_{ij}(0) \leftarrow$ initialized randomly

$$w_{ij}(k+1) = w_{ij}(k) - \eta (D_j - d_j)x_i$$

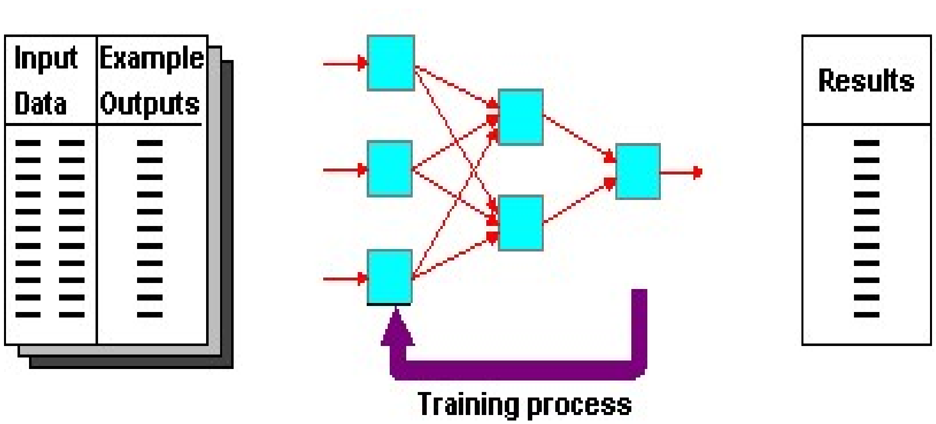
weight updation rule.

Supervised Learning

This is a linear discreminate fn

if the classes are linearly separable, using SLP, we can get a linear decision boundary.

Every neuron o/p actually gives an eqn of a st. line.



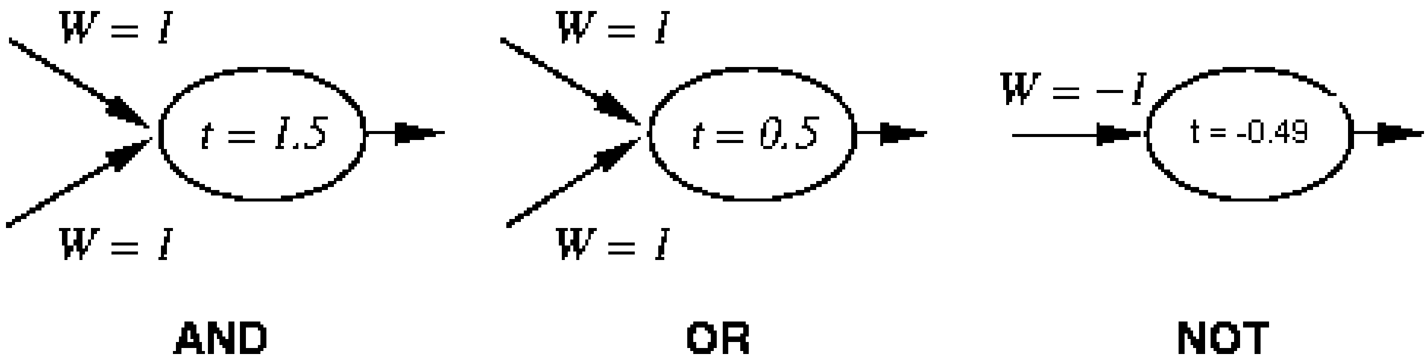
$y = \sum w_i x_i + b$

$y = mx + c$ st-line eqn.

Decision boundary is a st. line

Sepal length	Sepal width	Petal length	Petal width	Class
5.1	3.5	1.4	0.2	0
4.9	3.0	1.4	0.2	2
4.7	3.2	1.3	0.2	0
4.6	3.1	1.5	0.2	1

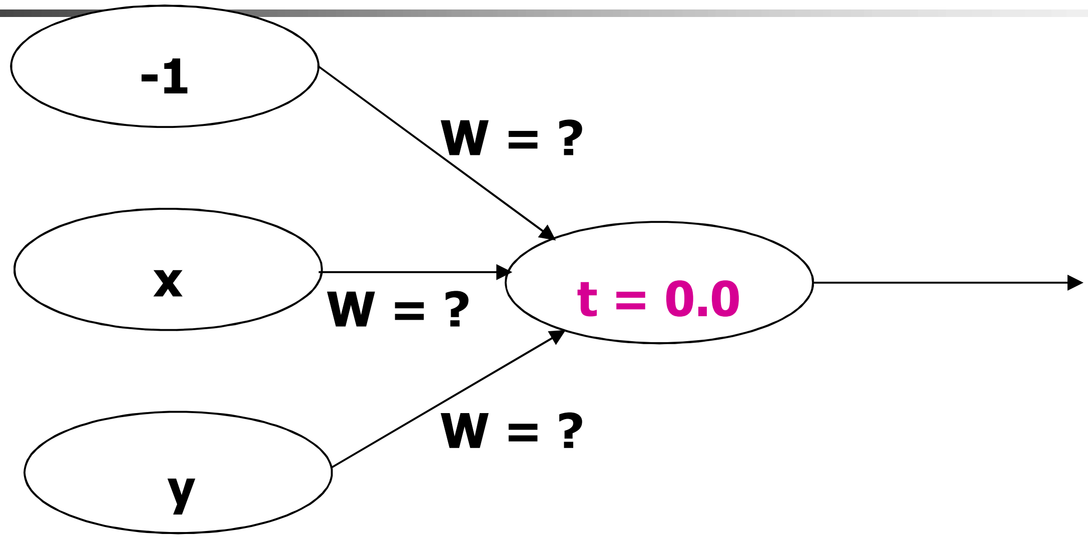
Perceptron Training



$$\text{Output}=\begin{cases} 1 \text{ if } \sum_{i=0} w_i\, x_i > t \\ 0 \text{ otherwise} \end{cases}$$

- Linear threshold is used.
- W - weight value
- t - threshold value

Training Perceptrons

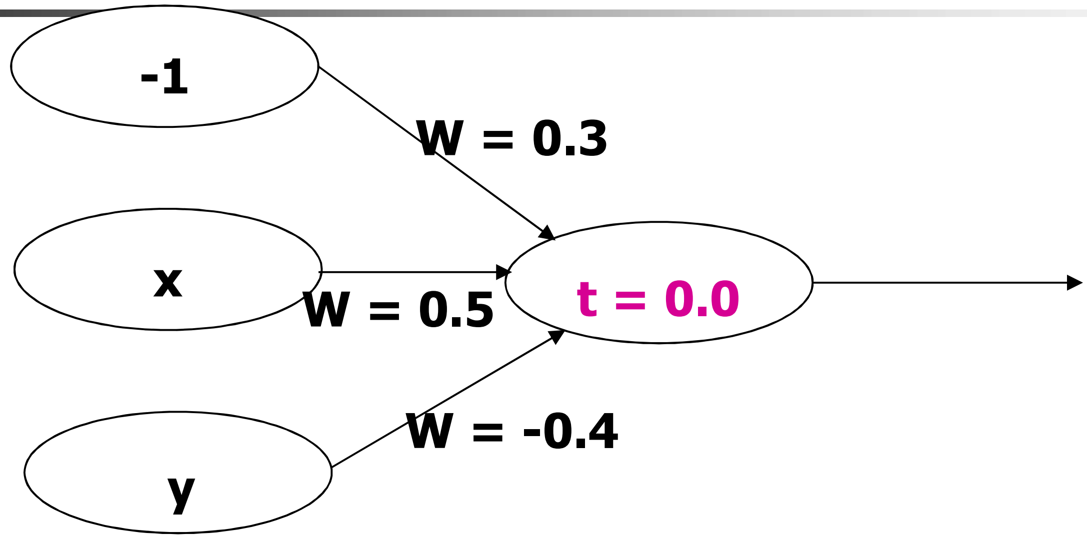


For AND

A	B	Output
0	0	0
0	1	0
1	0	0
1	1	1

- What are the weight values?
- Initialize with random weight values

Training Perceptrons



For AND

A	B	Output
0	0	0
0	1	0
1	0	0
1	1	1

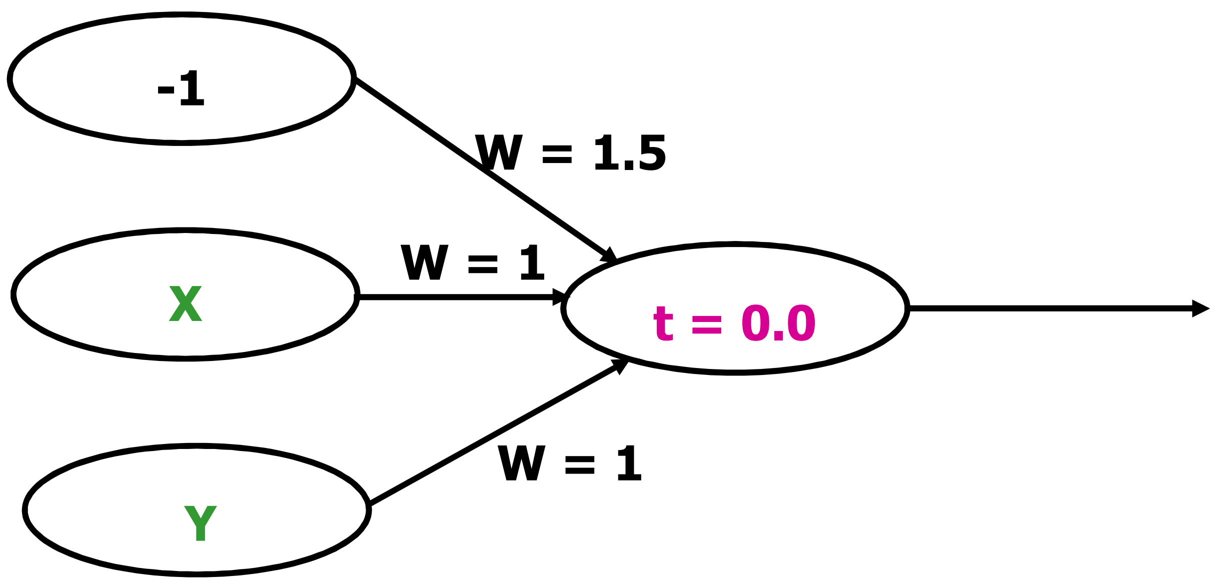
I_1	I_2	I_3	Summation	Output
-1	0	0	(-1*0.3) + (0*0.5) + (0*-0.4) = -0.3	0
-1	0	1	(-1*0.3) + (0*0.5) + (1*-0.4) = -0.7	0
-1	1	0	(-1*0.3) + (1*0.5) + (0*-0.4) = 0.2	1
-1	1	1	(-1*0.3) + (1*0.5) + (1*-0.4) = -0.2	0

Simple network

$$\text{output} = \begin{cases} 1 & \text{if } \sum_{i=0} w_i x_i > t \\ 0 & \text{otherwise} \end{cases}$$

For AND

A	B	Output
0	0	0
0	1	0
1	0	0
1	1	1



Learning algorithm

Epoch : Presentation of the entire training set to the neural network.
In the case of the AND function an epoch consists of four sets of inputs being presented to the network (i.e. [0,0], [0,1], [1,0], [1,1])

Error: The error value is the amount by which the value output by the network differs from the target value. For example, if we required the network to output 0 and it output a 1, then Error = -1

Learning algorithm

Target Value, T : When we are training a network we not only present it with the input but also with a value that we require the network to produce. For example, if we present the network with [1,1] for the AND function the training value will be 1

Output , O : The output value from the neuron

I_j : Inputs being presented to the neuron

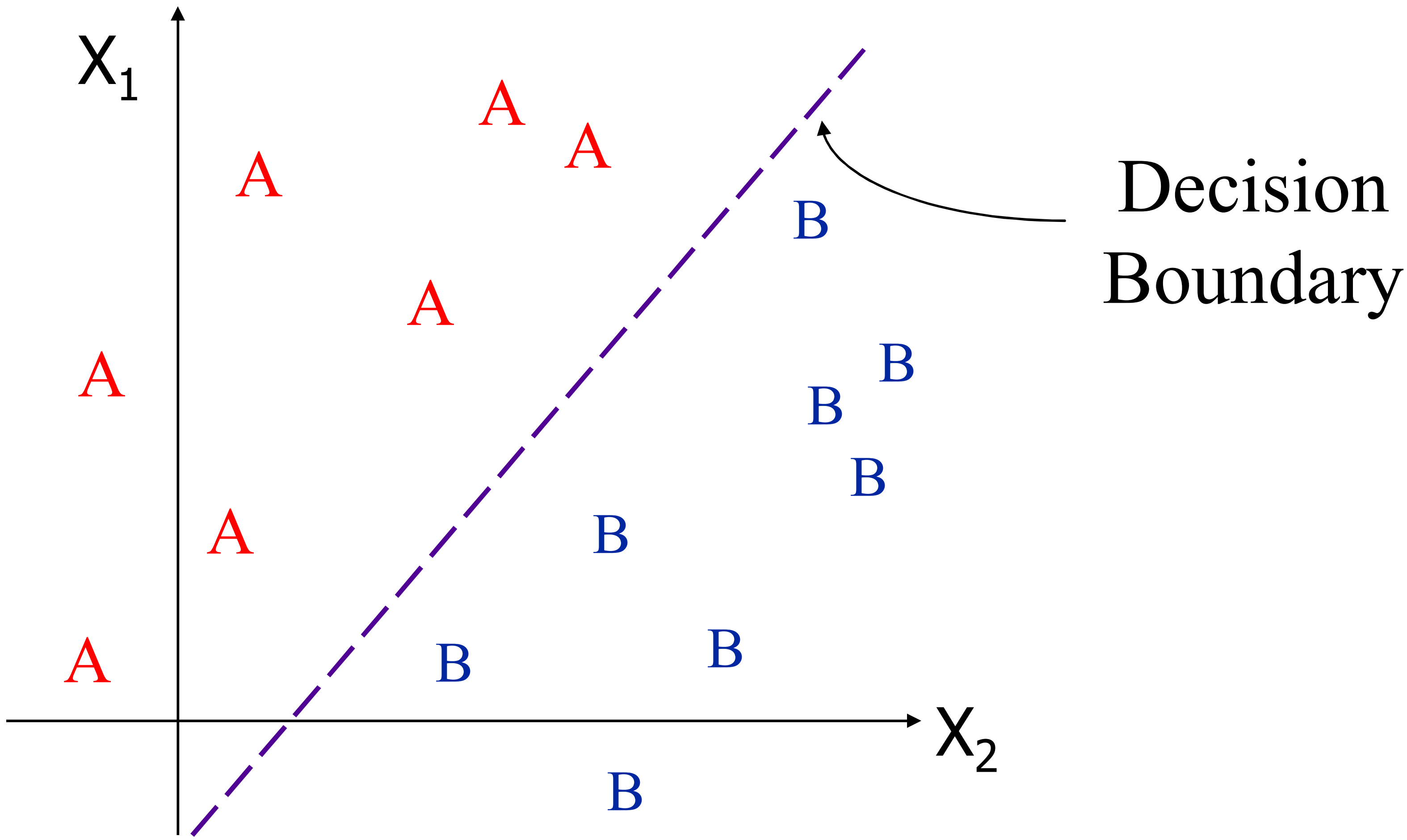
W_j : Weight from input neuron (I_j) to the output neuron

LR : The learning rate. This dictates how quickly the network converges. It is set by a matter of experimentation. It is typically 0.1

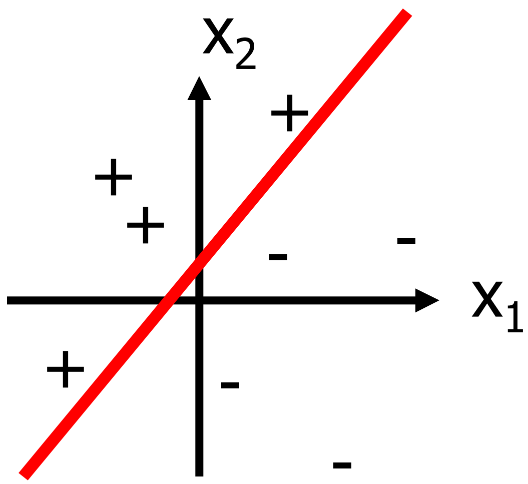
Decision boundaries

- In simple cases, divide feature space by drawing a hyperplane across it.
- Known as a decision boundary.
- Discriminant function: returns different values on opposite sides. (straight line)
- Problems which can be thus classified are linearly separable.

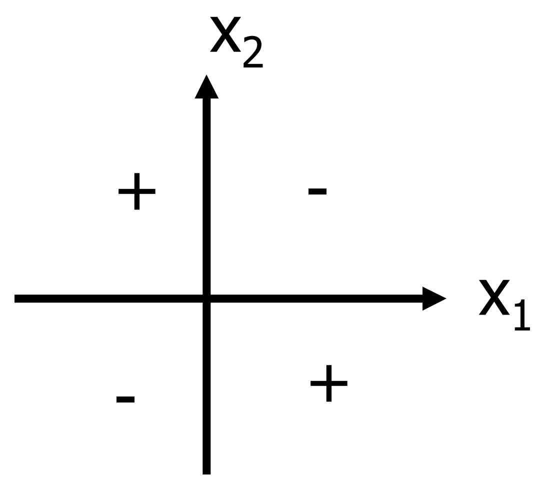
Linear Separability



Decision Surface of a Perceptron



Linearly separable



Non-Linearly separable

- Perceptron is able to represent some useful functions
- AND(x_1,x_2) choose weights w_0=-1.5, w_1=1, w_2=1
- But functions that are not linearly separable (e.g. XOR) are not representable

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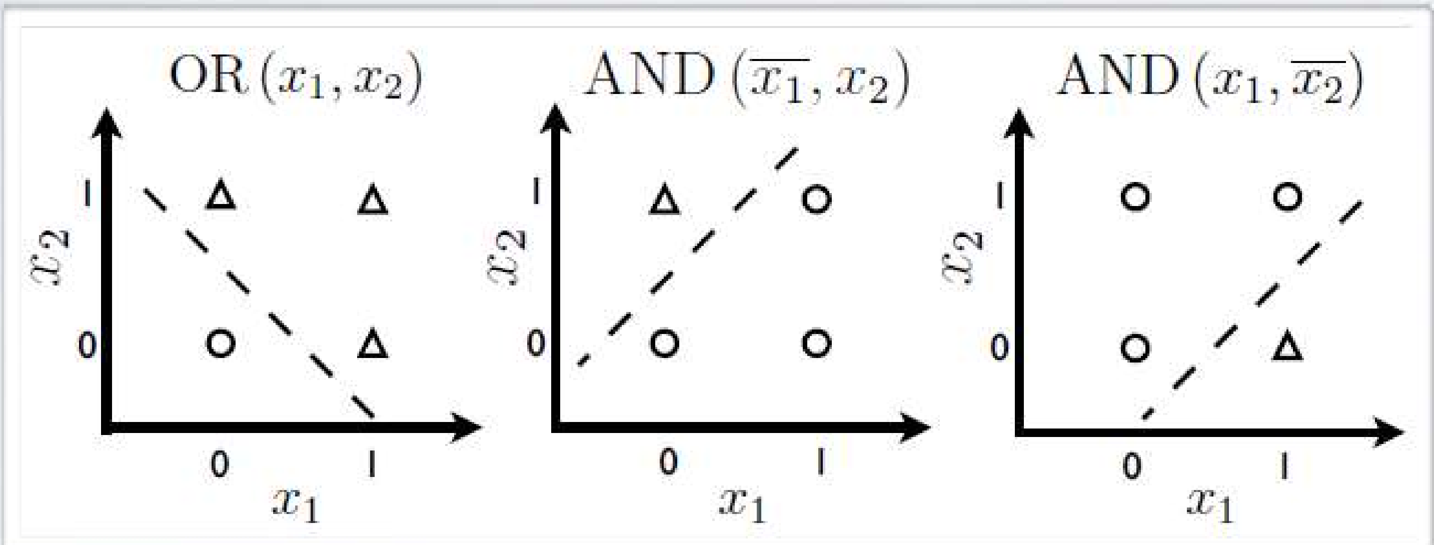
Topics: capacity of single neuron

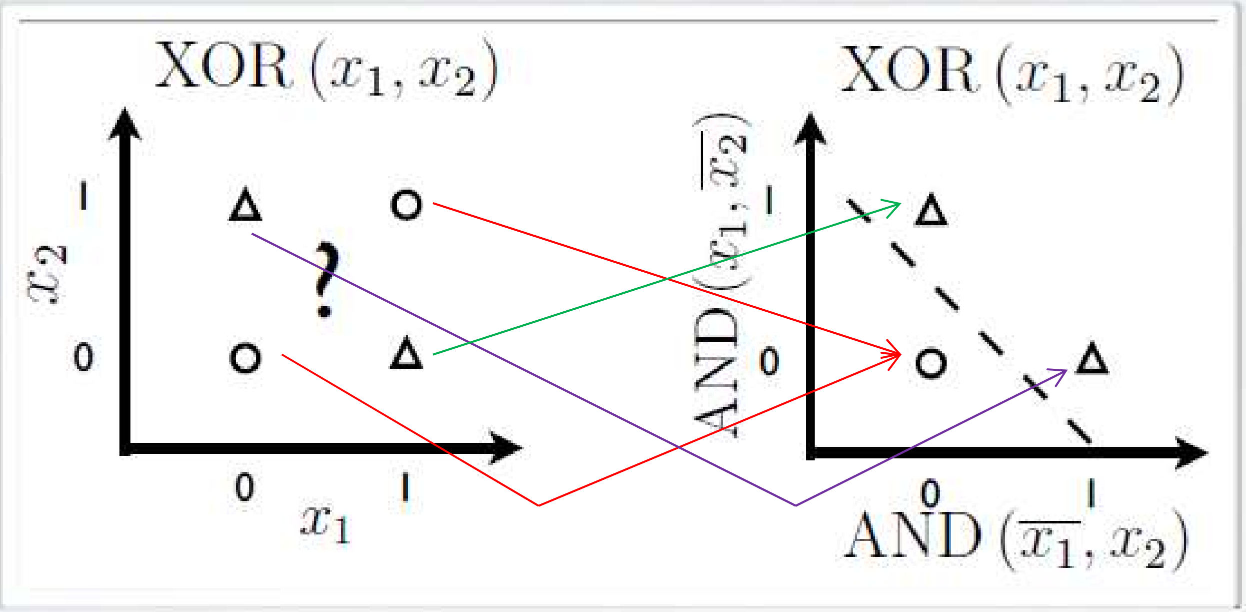
- Can solve linearly separable problems



ARTIFICIAL NEURON

Topics: capacity of single neuron

- Can't solve non linearly separable problems...

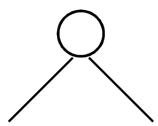
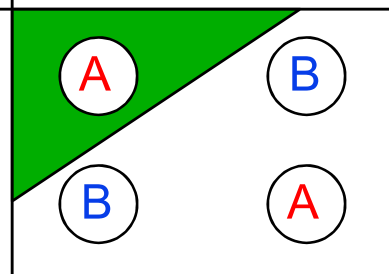
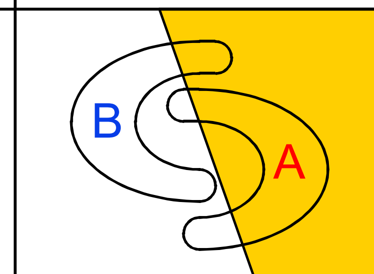
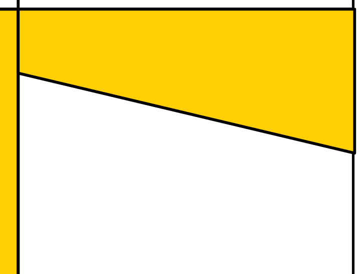
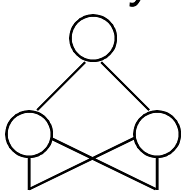
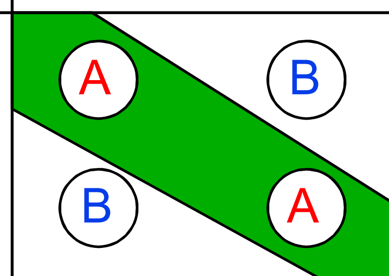
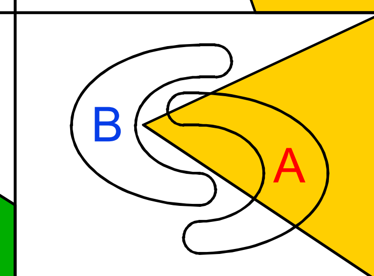
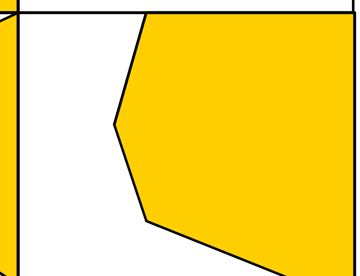
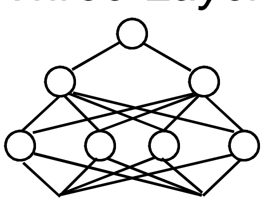
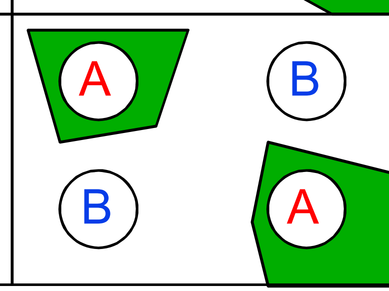
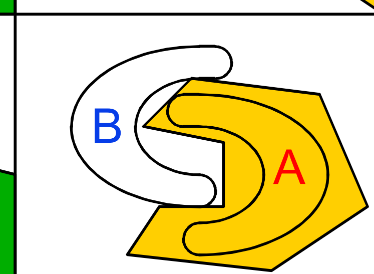
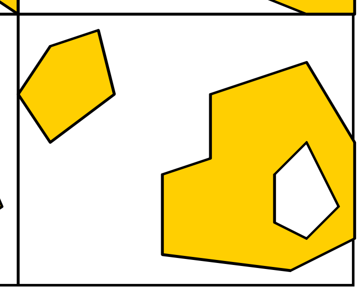


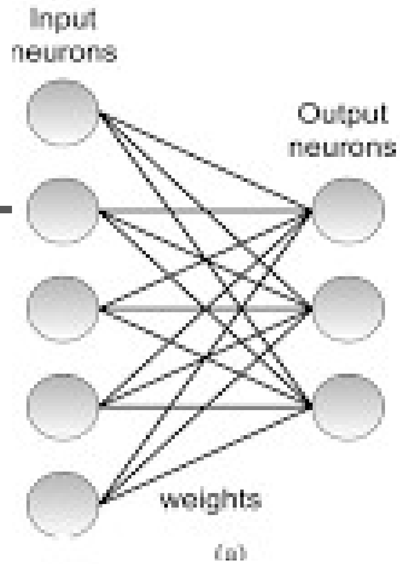
- ... unless the input is transformed in a better representation

Hyperplane partitions

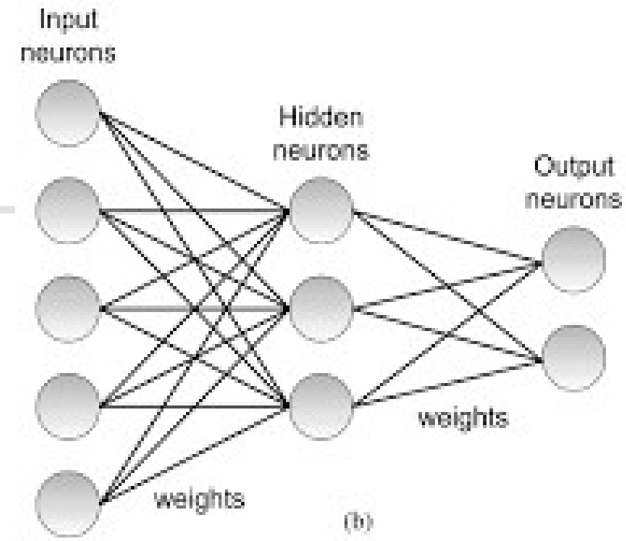
- An extra layer models a convex hull
  - "An area with no dents in it"
  - Perceptron models, but can't learn
  - Sigmoid function learning of convex hulls
  - Two layers add convex hulls together
  - Sufficient to classify anything "sane".
- In theory, further layers add nothing
- In practice, extra layers may be better

Different Non-Linearly Separable Problems

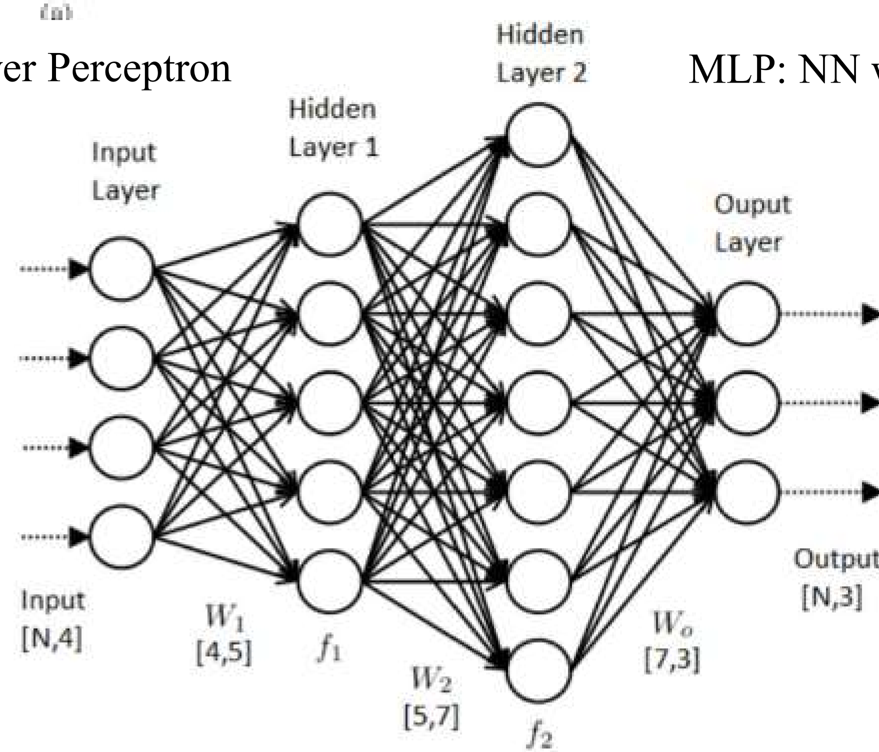
Structure	*Types of Decision Regions*	*Exclusive-OR Problem*	*Classes with Meshed regions*	*Most General Region Shapes*
Single-Layer 	*Half Plane Bounded By Hyperplane*			
Two-Layer 	*Convex Open Or Closed Regions*			
Three-Layer 	Arbitrary (Complexity Limited by No. of Nodes)			



SLP: Single Layer Perceptron



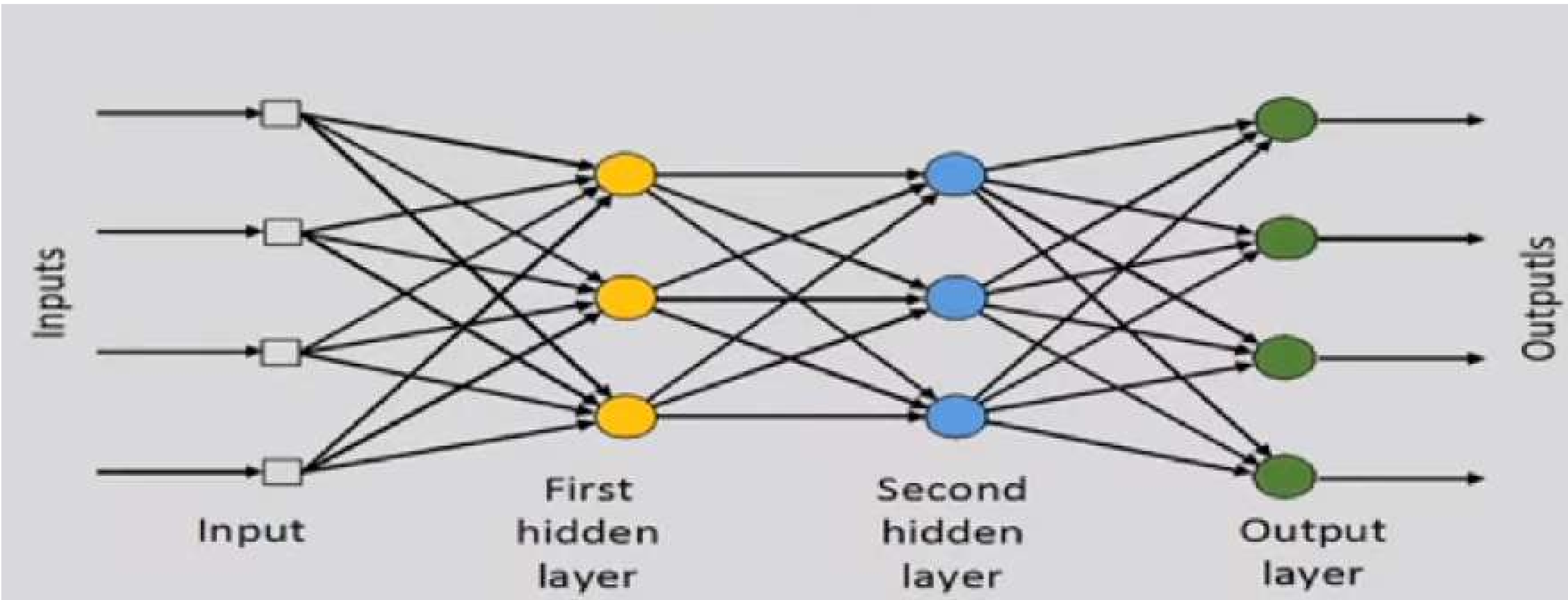
MLP: NN with single hidden layer

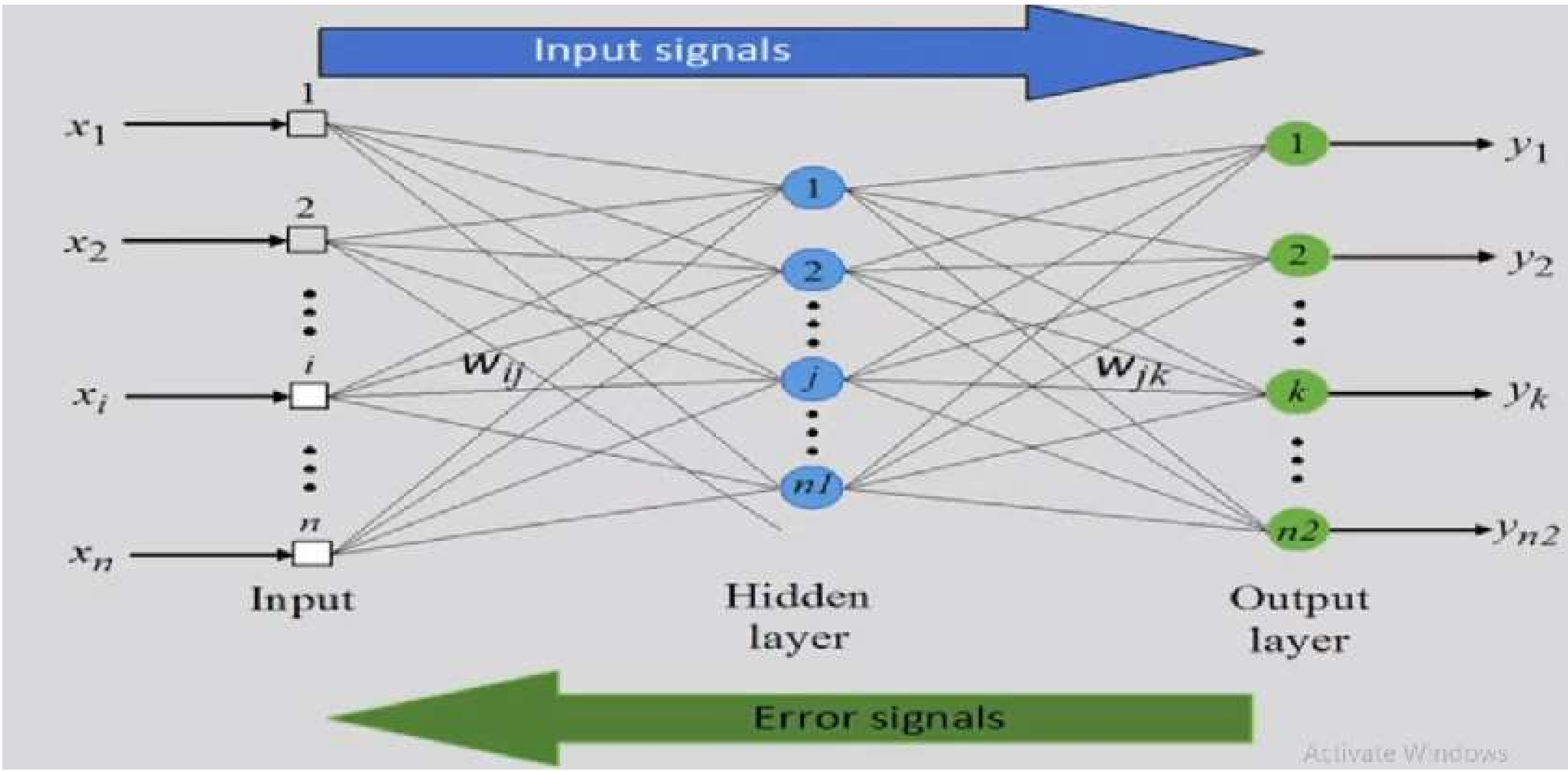


MLP: NN with two hidden layer

Representation of the Neural Network

- Single layer nets have limited representation power (linear separability problem). Multi layer nets of (or nets with non linear hidden unit) may overcome linear inseparability problem.
- Every Boolean function can be realized by a network with single hidden layer.
- Every bounded continuous function can be approximated with arbitrary small error, by network with one hidden layer.
- Any function can be approximated to arbitrary accuracy by a neural network having two hidden layer.


Inputs
Input
First
hidden
layer
Second
hidden
layer
Output
layer
Outputis



Input signals
x_1
x_2
x_i
x_n
1
2
i
n
w_{ij}
w_{jk}
1
2
j
n1
1
2
k
n2
y_1
y_2
y_k
y_{n2}
Input
Hidden layer
Output layer
Error signals

Multi Layer Perceptron (MLP)

Topics: single hidden layer neural network

- Hidden layer pre-activation:

$$\mathbf{a}(\mathbf{x}) = \mathbf{b}^{(1)} + \mathbf{W}^{(1)}\mathbf{x}$$

$$\left(a(\mathbf{x})_i = b_i^{(1)} + \textstyle\sum_j W_{i,j}^{(1)} x_j\right)$$

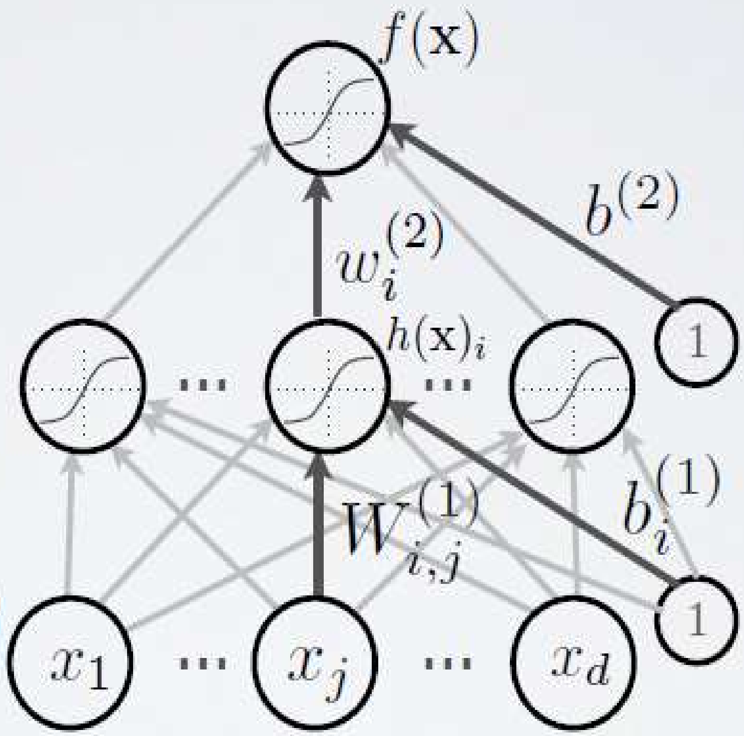
- Hidden layer activation:

$$\mathbf{h}(\mathbf{x}) = \mathbf{g}(\mathbf{a}(\mathbf{x}))$$

- Output layer activation:

$$f(\mathbf{x}) = o\left(b^{(2)} + \mathbf{w}^{(2)\top}\mathbf{h}^{(1)}\mathbf{x}\right)$$

output activation function



Multi Layer Perceptron (MLP)

Topics: softmax activation function

- For multi-class classification:
  - we need multiple outputs (1 output per class)
  - we would like to estimate the conditional probability $p(y = c|\mathbf{x})$
- We use the softmax activation function at the output:

$$\mathbf{o}(\mathbf{a}) = \mathrm{softmax}(\mathbf{a}) = \left[\frac{\exp(a_1)}{\sum_c \exp(a_c)} \cdots \frac{\exp(a_C)}{\sum_c \exp(a_c)} \right]^\top$$

  - strictly positive
  - sums to one
- Predicted class is the one with highest estimated probability

Multi Layer Perceptron (MLP)

Topics: multilayer neural network

- Could have L hidden layers:
  - layer pre-activation for $k>0$ $(\mathbf{h}^{(0)}(\mathbf{x}) = \mathbf{x})$

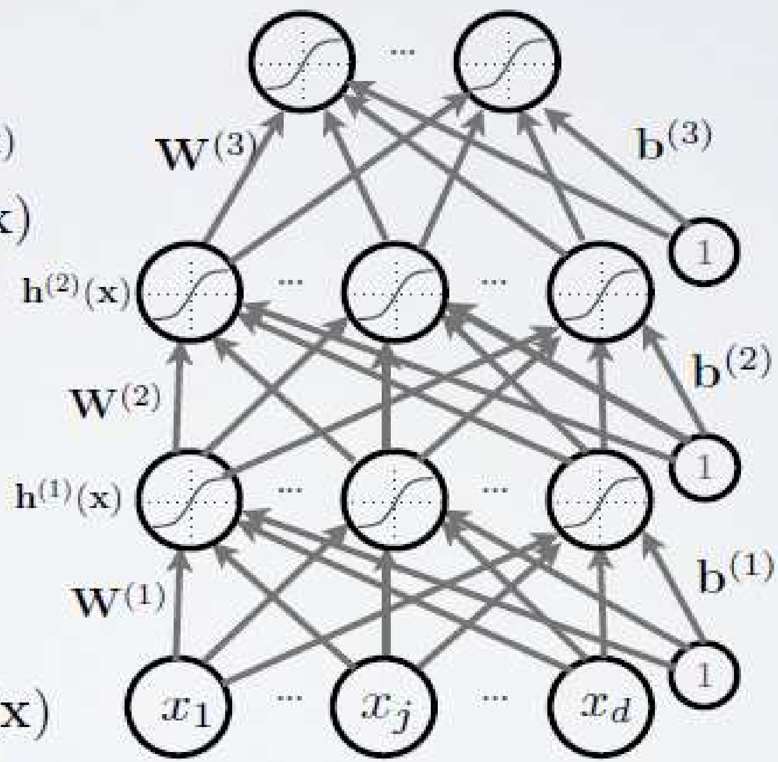
    $$\mathbf{a}^{(k)}(\mathbf{x}) = \mathbf{b}^{(k)} + \mathbf{W}^{(k)}\mathbf{h}^{(k-1)}(\mathbf{x})$$

  - hidden layer activation (k from 1 to L):

    $$\mathbf{h}^{(k)}(\mathbf{x}) = \mathbf{g}(\mathbf{a}^{(k)}(\mathbf{x}))$$

  - output layer activation ($k=L+1$):

    $$\mathbf{h}^{(L+1)}(\mathbf{x}) = \mathbf{o}(\mathbf{a}^{(L+1)}(\mathbf{x})) = \mathbf{f}(\mathbf{x})$$



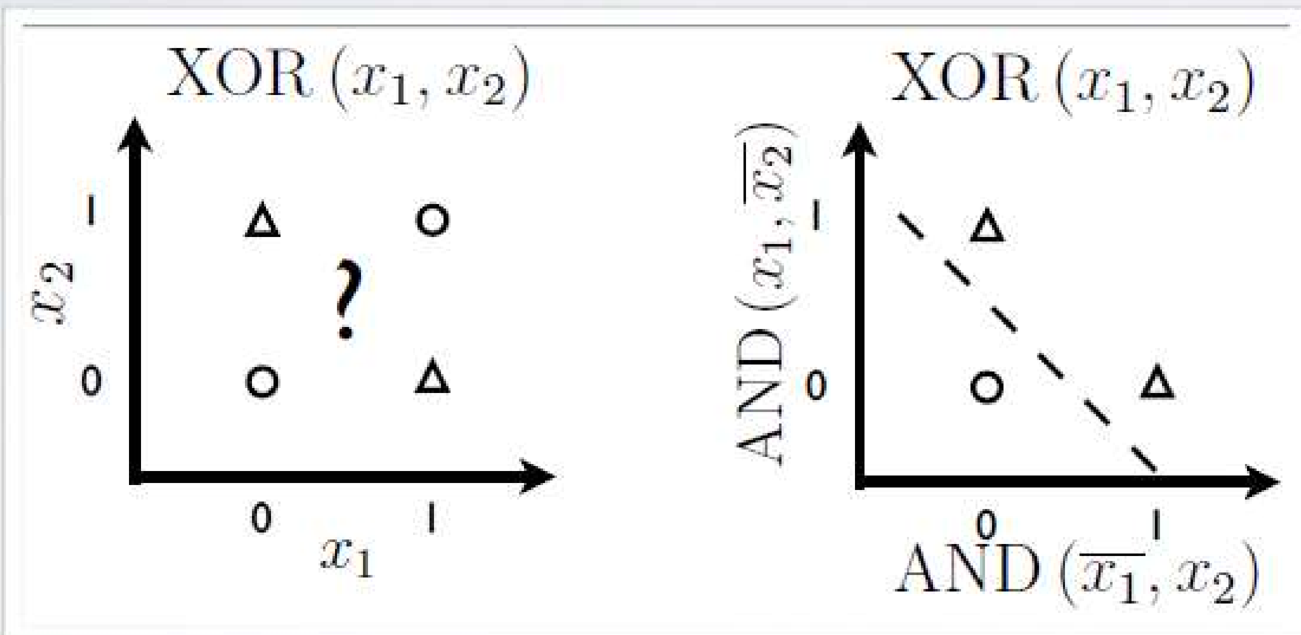
Types of Layers

- The input layer.
  - Introduces input values into the network.
  - No activation function or other processing.
- The hidden layer(s).
  - Perform classification of features
  - Two hidden layers are sufficient to solve any problem
  - Features imply more layers may be better
- The output layer.
  - Functionally just like the hidden layers
  - Outputs are passed on to the world outside the neural network.

Capacity of MLP

Topics: capacity of single neuron

- Can't solve non linearly separable problems...



- ... unless the input is transformed in a better representation

Capacity of MLP

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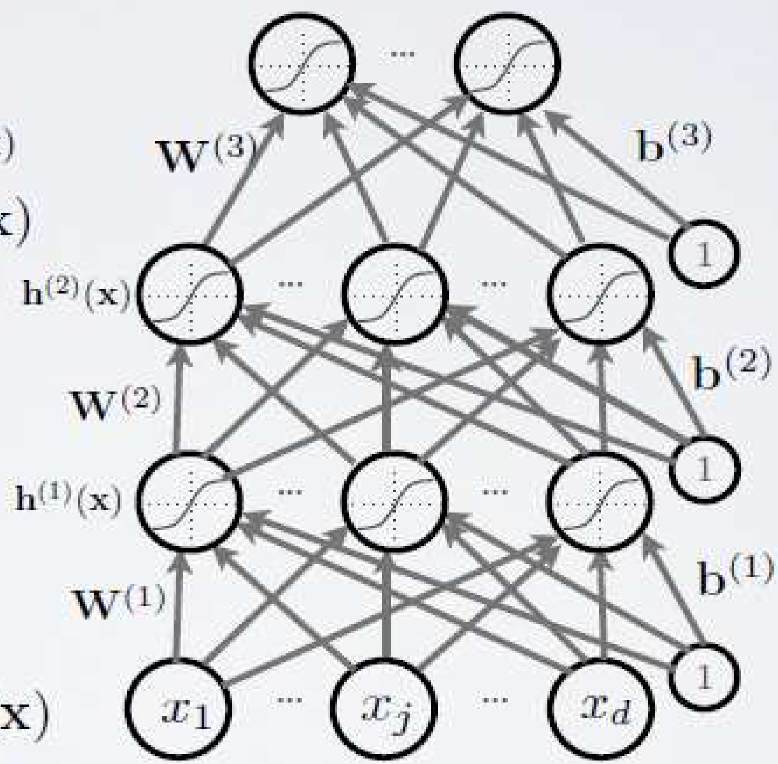
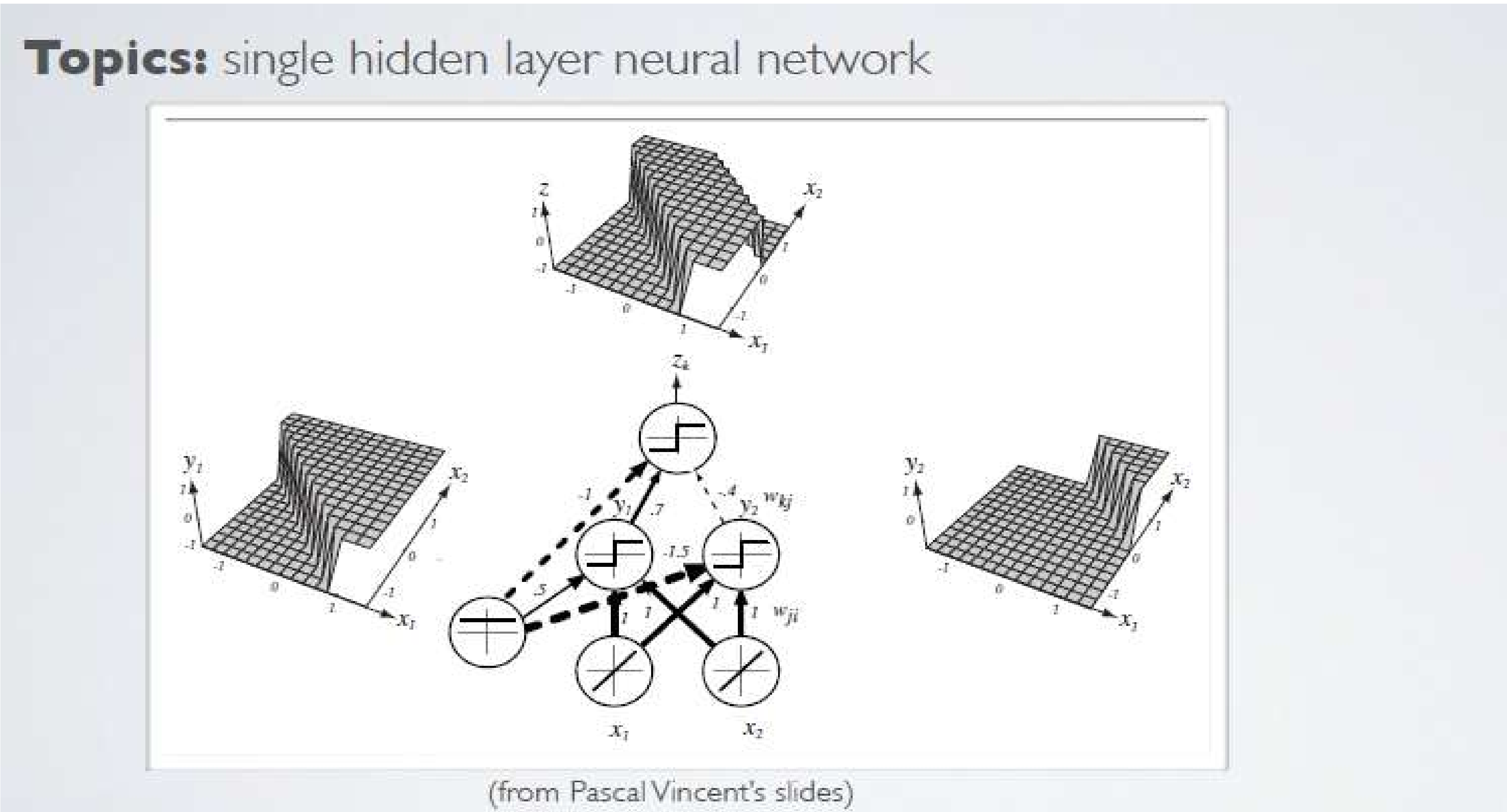
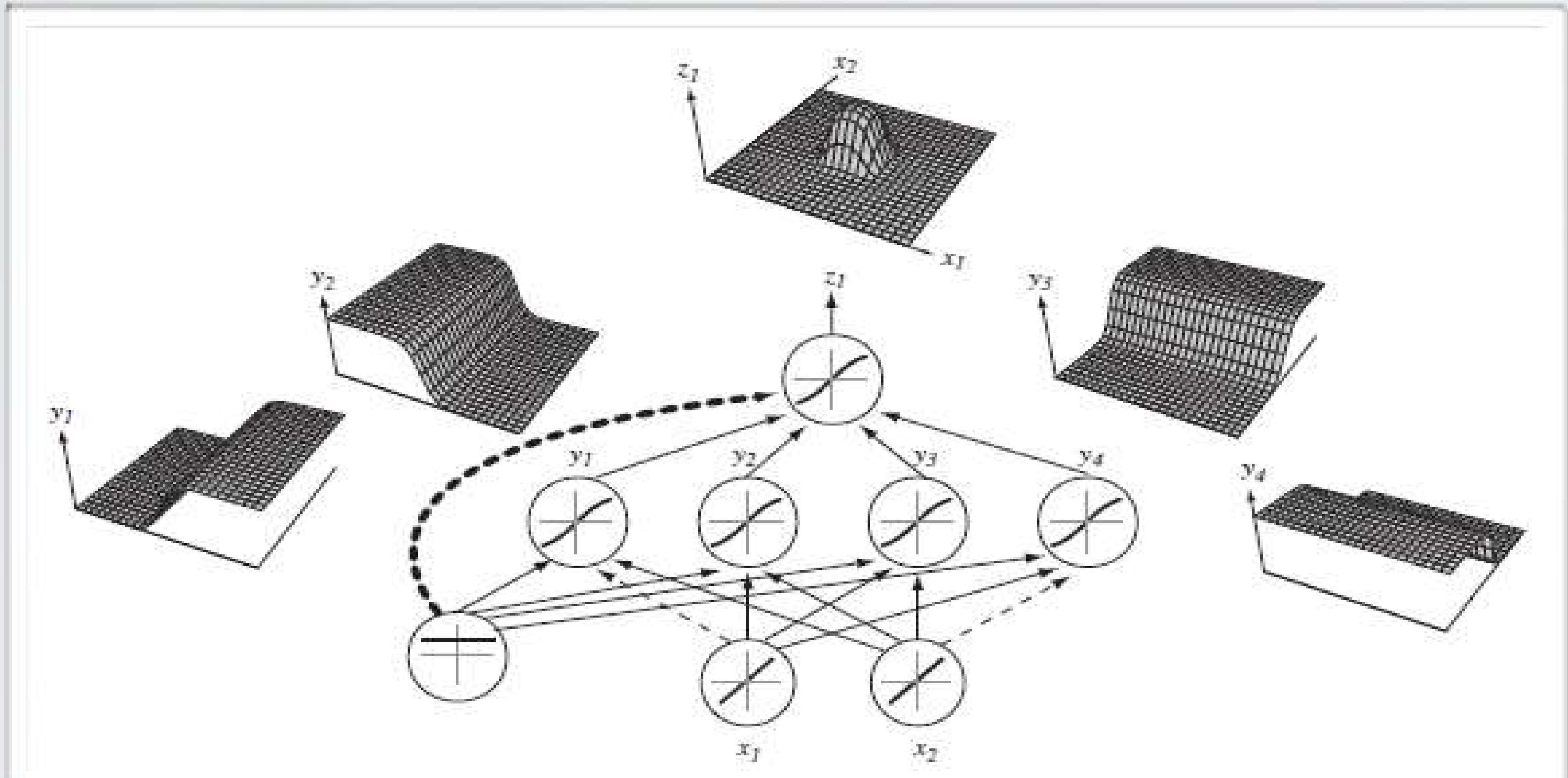


Capacity of MLP



Capacity of MLP

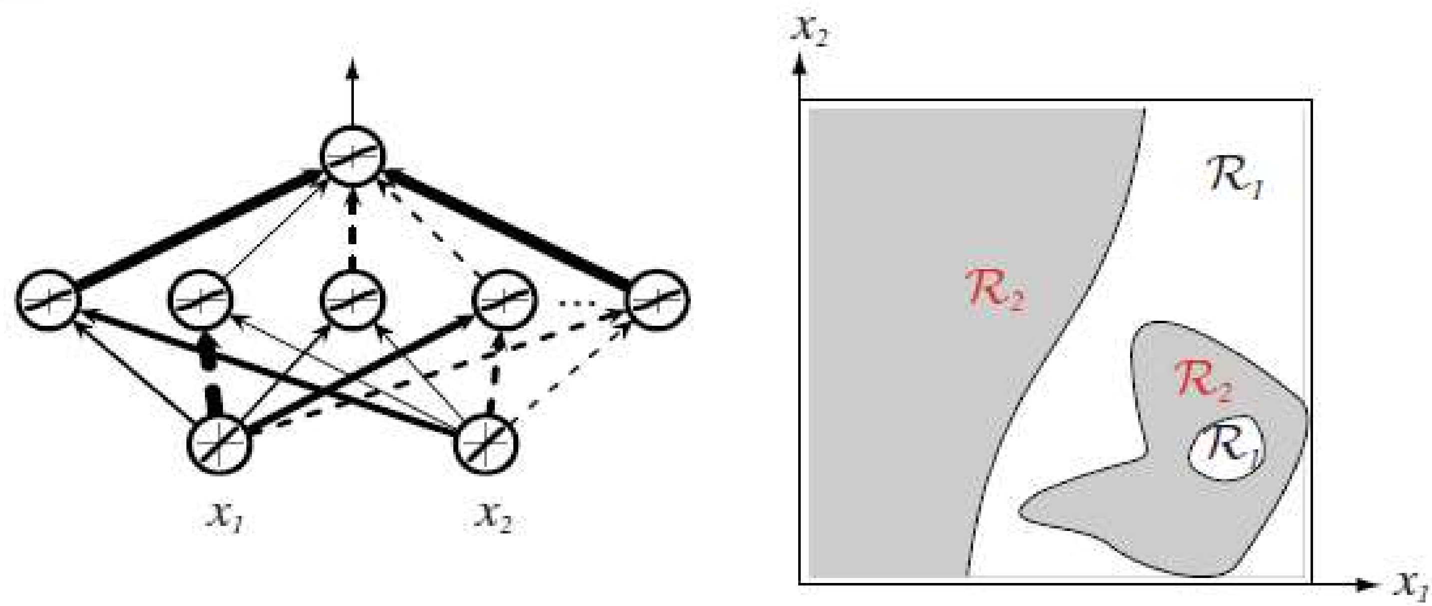
Topics: single hidden layer neural network



(from Pascal Vincent's slides)

Capacity of MLP

Topics: single hidden layer neural network



(from Pascal Vincent's slides)

Capacity of MLP

Topics: universal approximation

- Universal approximation theorem (Hornik, 1991):
  - "a single hidden layer neural network with a linear output unit can approximate any continuous function arbitrarily well, given enough hidden units"
- The result applies for sigmoid, tanh and many other hidden layer activation functions

- This is a good result, but it doesn't mean there is a learning algorithm that can find the necessary parameter values!

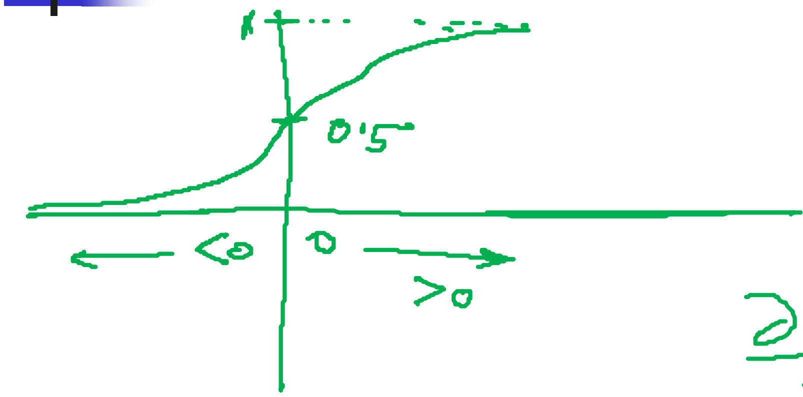
Training Algorithms

- Adjust neural network weights to map inputs to outputs.
- Use a set of sample patterns where the desired output (given the inputs presented) is known.
- The purpose is to learn to generalize
  - Recognize features which are common to good and bad exemplars

Back-Propagation

- A training procedure which allows multi-layer feedforward Neural Networks to be trained;
- Can theoretically perform “any” input-output mapping;
- Can learn to solve linearly inseparable problems.

Sigmoid fn

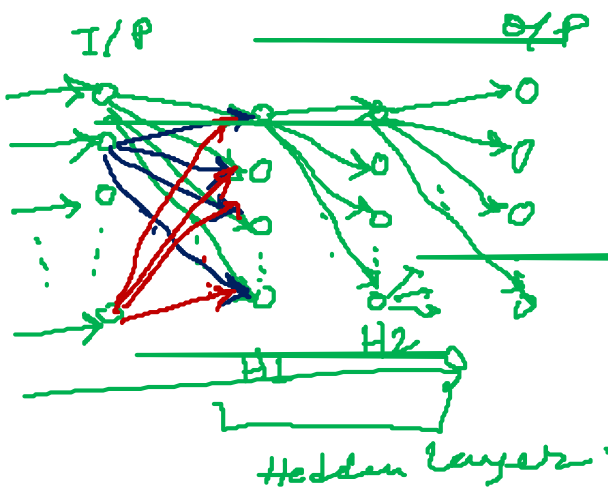


$$R(S) = \frac{1}{1+e^{-S}}$$

→ Differentiable

$$\frac{\partial R(S)}{\partial S} = R(S)\left[1 - R(S)\right]$$

MLP :-

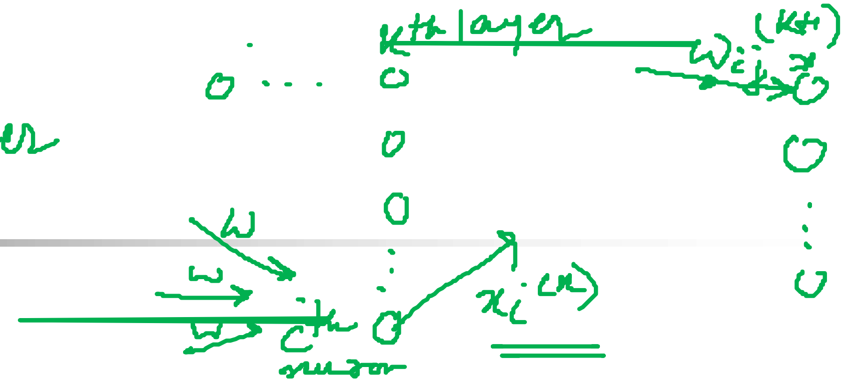


K+1 layer (1 i/p + K hidden + o/p)

→ K Layer MLP

Consider

i^{th} node k^{th} layer



$x_i^{(k)}$ = o/p of i^{th} neuron in the k^{th} layer

$$x_j^{(k+1)} = R\left(\sum_{i=0}^{M_k} w_{ij}^{(k+1)} x_i^{(k)}\right)$$

M_k = no. of node in the k^{th} hidden layer

$$E = \frac{1}{2}\sum_{j=0}^{M_k}\left[x_j^{(k)} - d_j^{(k)}\right]^2$$

at o/p layer

$$\frac{\partial E}{\partial w_{ij}^{(k)}} = \left[x_j^{(k)} - d_j^{(k)}\right]\frac{\partial x_j^{(k)}}{\partial w_{ij}^{(k)}} \quad (2)$$

$R = \text{Sigmoidal}$

$$\frac{\partial x_j^{(k)}}{\partial w_{ij}^{(k)}} = \frac{\partial}{\partial w_{ij}^{(k)}} R\left(\sum_{j=0}^{M_k-1} w_{ij}^{(k)} x_i^{(k-1)}\right)$$

$$= x_j^{(k)}\left(1 - x_j^{(k)}\right) x_i^{(k-1)}$$

$$\frac{\partial E}{\partial w_{ij}^{(k)}} = \left(x_j^{(k)} - d_j^{(k)}\right) x_j^{(k)}\left(1 - x_j^{(k)}\right) x_i^{(k-1)}$$

$$\boxed{w_{ij}(k+1) = w_{ij}(k) - \eta \, \underline{(D_j - d_j)\, x_i}}$$

$$w_{ij}^{(k)}(t+1) = w_{ij}^{(k)}(t) - \eta\, \delta_j^{(k)} x_i^{(k-1)}$$

$$\delta_j^{(k)} = \left(x_j^{(k)} - d_j^{(k)}\right) x_j^{(k)} \left(1 - x_j^{(k)}\right)$$

Feed forward Back Propagation Algo.

Back Prop. Algo.

1. Initialize $w_{ij}^{(k)} \leftarrow$ Random values
2. Feed Training Samples
3. Feed forward

for $k = 0$ to $K-1$ compute

$$x_j^{(k+1)} = R\left(\sum_{i=0}^{M_k} w_{ij}^{(k+1)} x_{ij}^{(k)}\right)$$

for nodes $j = 1$ to $M_k + 1$

4. Back Propagation

For nodes in the o/p layer

$j = 1$ to M_K compute

$$\delta_j^{(k)} = x_j^{(k)}\left(1 - x_j^{(k)}\right)\left(x_j^{(k)} - d_j\right)$$

For layer $K-1 \ldots 1$ compute

$$\delta_i^{(k)} = x_i^{(k)}\left(1 - x_i^{(k)}\right) \sum_{j=1}^{M_{k+1}} \delta_j^{(k+1)} w_{ij}^{(k+1)}$$

For $i = 1$ to M_k

5. Updates the weights

$$w_{ij}^{(k)}(t+1) = w_{ij}^{(k)}(t) - \eta\, \delta_j^{(k)} x_i^{(k-1)}$$

Repeat - steps 2 to 5 until convergence

Activation functions and training

- For feed-forward networks:
  - A continuous function can be differentiated allowing gradient-descent.
  - Back-propagation is an example of a gradient-descent technique.
  - Reason for prevalence of sigmoid

Gradient Descent Learning Rule

- Consider linear unit without threshold and continuous output o (not just –1,1)
  - $o = w_0 + w_1 x_1 + \ldots + w_n x_n$
- Train the w_i's such that they minimize the squared error
  - $E[w_1,\ldots,w_n] = \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2$

  where D is the set of training examples

Gradient Descent

D={<(1,1),1>,<(-1,-1),1>,
<(1,-1),-1>,<(-1,1),-1>}

Gradient:
$\nabla E[w]=[\partial E/\partial w_0,\ldots\ \partial E/\partial w_n]$

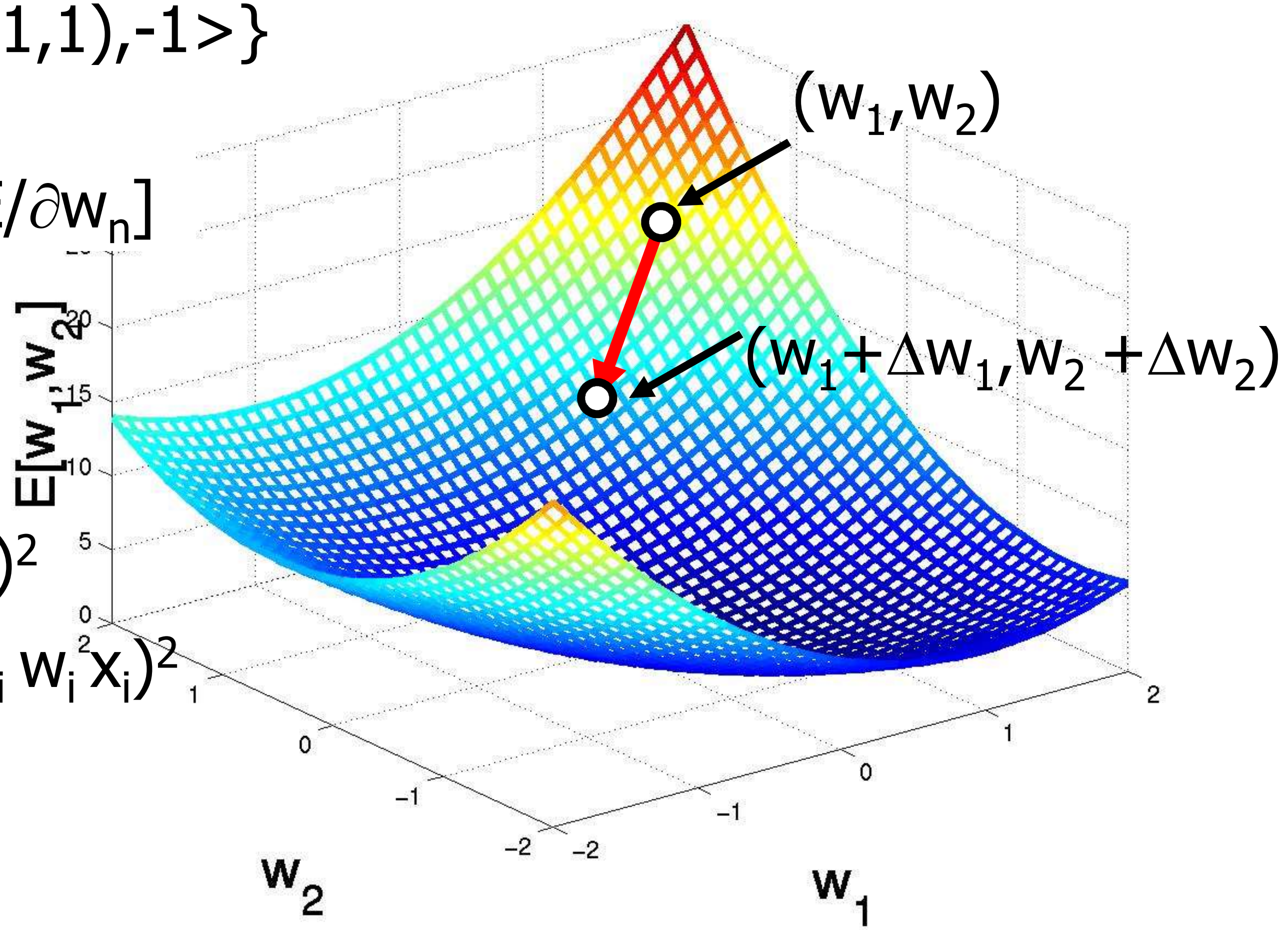
$\Delta w=-\eta\ \nabla E[w]$

$\Delta w_i=-\eta\ \partial E/\partial w_i$

$=\partial/\partial w_i\ 1/2\Sigma_d(t_d-o_d)^2$

$=\partial/\partial w_i\ 1/2\Sigma_d(t_d-\Sigma_i\ w_i\ x_i)^2$

$=\Sigma_d(t_d-\ o_d)(-x_i)$



Gradient Descent

Gradient-Descent(*training_examples*, η)

Each training example is a pair of the form <(x_1,…x_n),t> where (x_1,…,x_n) is the vector of input values, and t is the target output value, η is the learning rate (e.g. 0.1)

- Initialize each w_i to some small random value
- Until the termination condition is met, Do
  - Initialize each Δw_i to zero
  - For each <(x_1,…x_n),t> in *training_examples* Do
    - Input the instance (x_1,…,x_n) to the linear unit and compute the output o
    - For each linear unit weight w_i Do
      - $\Delta w_i = \Delta w_i + \eta$ (t-o) x_i
  - For each linear unit weight wi Do
    - $w_i = w_i + \Delta w_i$

Incremental Stochastic Gradient Descent

- Batch mode : gradient descent

  $w=w - \eta \nabla E_D[w]$ over the entire data D

  $E_D[w]=1/2\Sigma_d(t_d-o_d)^2$

- Incremental mode: gradient descent

  $w=w - \eta \nabla E_d[w]$ over individual training examples d

  $E_d[w]=1/2\ (t_d-o_d)^2$

Incremental Gradient Descent can approximate Batch Gradient Descent arbitrarily closely if η is small enough

Comparison Perceptron and Gradient Descent Rule

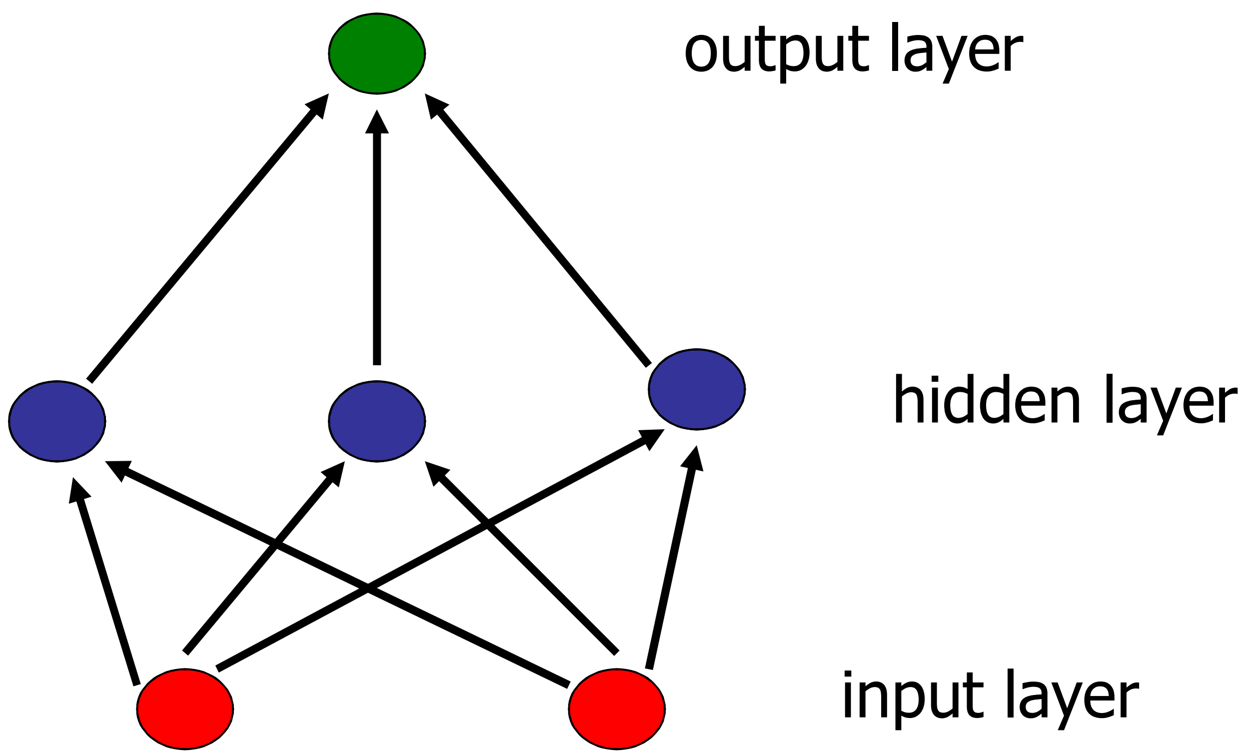
Perceptron learning rule guaranteed to succeed if

- Training examples are linearly separable
- Sufficiently small learning rate η

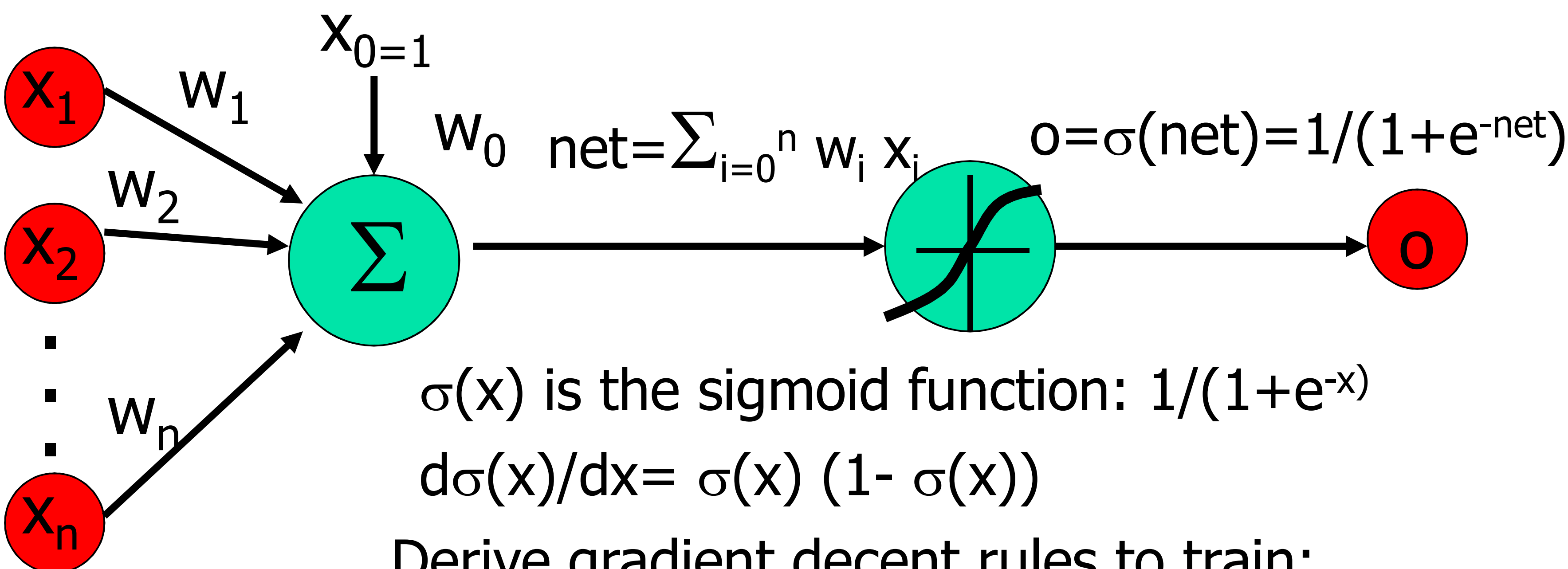
Linear unit training rules uses gradient descent

- Guaranteed to converge to hypothesis with minimum squared error
- Given sufficiently small learning rate η
- Even when training data contains noise
- Even when training data not separable by H

Multi-Layer Networks



Sigmoid Unit



$\sigma(x)$ is the sigmoid function: $1/(1+e^{-x})$

$d\sigma(x)/dx = \sigma(x)\,(1-\sigma(x))$

Derive gradient decent rules to train:

- one sigmoid function

  $\partial E/\partial w_i = -\sum_d (t_d - o_d)\, o_d\, (1-o_d)\, x_i$

- Multilayer networks of sigmoid units backpropagation:

Backpropagation Algorithm

- Initialize each w_i to some small random value
- Until the termination condition is met, Do
  - For each training example <$(x_1,\ldots x_n)$,t> Do
    - Input the instance $(x_1,\ldots,x_n)$ to the network and compute the network outputs o_k
    - For each output unit k
      - $\delta_k = o_k(1-o_k)(t_k-o_k)$
    - For each hidden unit h
      - $\delta_h = o_h(1-o_h) \sum_k w_{h,k} \delta_k$
    - For each network weight $w_{,j}$ Do
    - $w_{i,j} = w_{i,j} + \Delta w_{i,j}$ where

      $\Delta w_{i,j} = \eta \, \delta_j \, x_{i,j}$

Backpropagation

- Gradient descent over entire *network* weight vector
- Easily generalized to arbitrary directed graphs
- Will find a local, not necessarily global error minimum

  -in practice often works well (can be invoked multiple times with different initial weights)
- Often include weight *momentum* term

$$\Delta w_{i,j}(t) = \eta \, \delta_j \, x_{i,j} + \alpha \, \Delta w_{i,j}(t-1)$$

- Minimizes error training examples
  - Will it generalize well to unseen instances (over-fitting)?
- Training can be slow typical 1000-10000 iterations

  (use Levenberg-Marquardt instead of gradient descent)
- Using network after training is fast

to continue...