Course 395: Machine Learning - Lectures

Lecture 1-2: Concept Learning (M. Pantic)

Lecture 3-4: Decision Trees & CBC Intro (M. Pantic & S. Petridis)

Lecture 5-6: Evaluating Hypotheses (S. Petridis)

➢ Lecture 7-8: Artificial Neural Networks I (S. Petridis)

Lecture 9-10: Artificial Neural Networks II (S. Petridis)

Lecture 11-12: Instance Based Learning (M. Pantic)

Lecture 13-14: Genetic Algorithms (M. Pantic)

Neural Networks

Reading:

- *Machine Learning (Tom Mitchel) Chapter 4*

- *Pattern Classification (Duda, Hart, Stork) Chapter 6 (strongly to advised to read 6.1, 6.2, 6.3, 6.8)*

Further Reading:

- *Pattern Recognition and Machine Learning by C. Bishop, Springer, 2006 (chapter: 5)*

- *Neural Networks (Haykin)*

- *Neural Networks for Pattern Recognition (C. Bishop)*

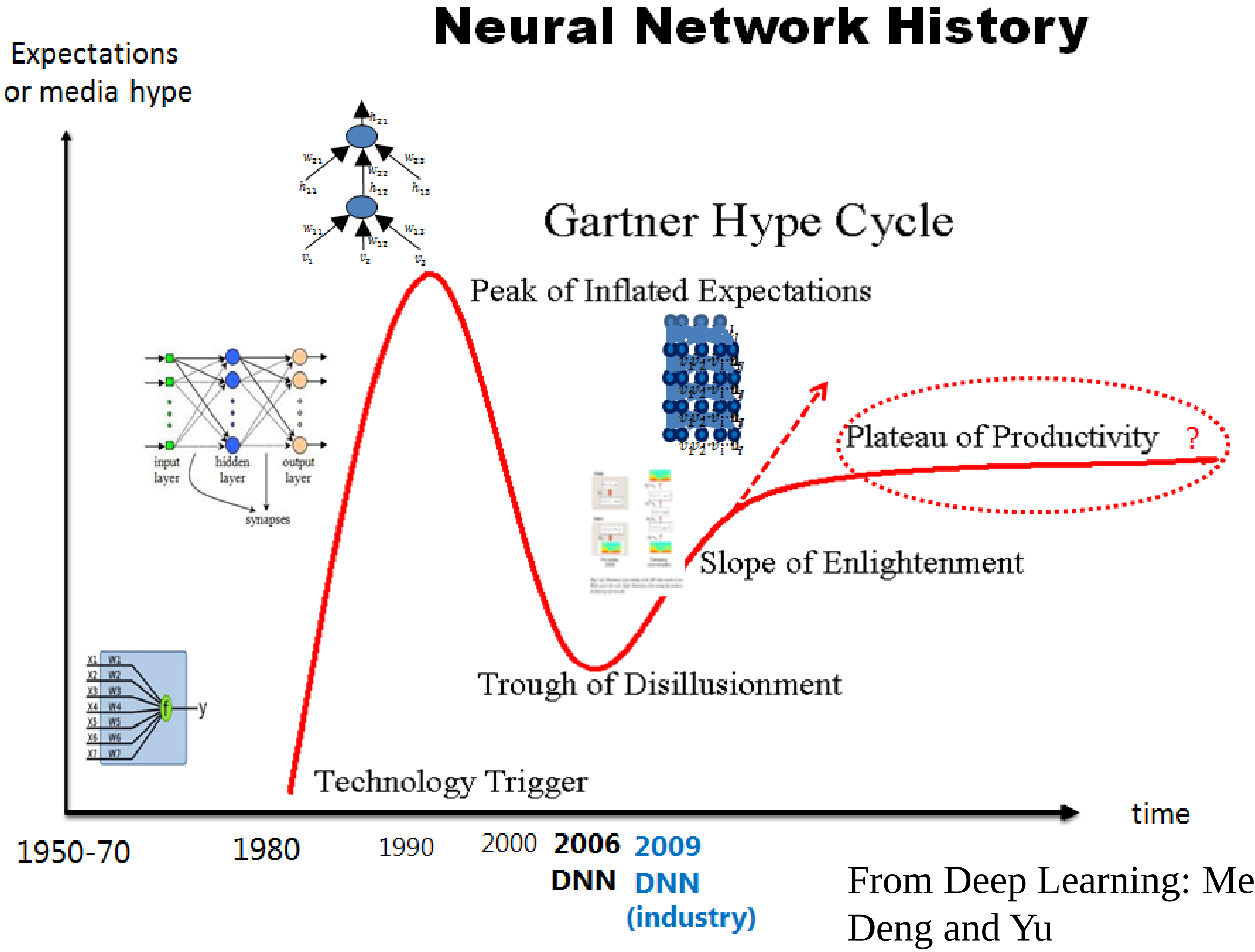
History

- *1st generation Networks: Perceptron 1957 – 1969*
  - *Perceptron is useful only for examples that are linearly separable*

- *2nd generation Networks: Feedforward Networks and other variants, beginning of 1980s to middle/end of 1990s*
  - *Difficult to train, many parameters, similar performance to SVMs*

- *3rd generation Networks: Deep Networks 2006 - ?*
  - *New approach to train networks with multiple layers*
  - *State of the art in object recognition / speech recognition*

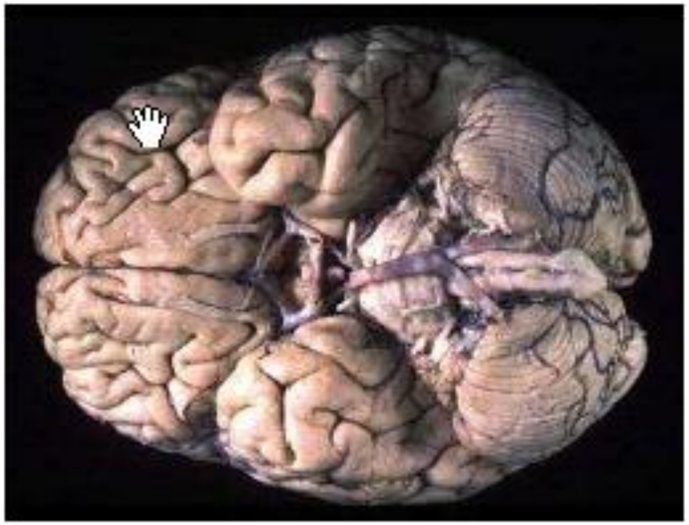
Hype Cycle



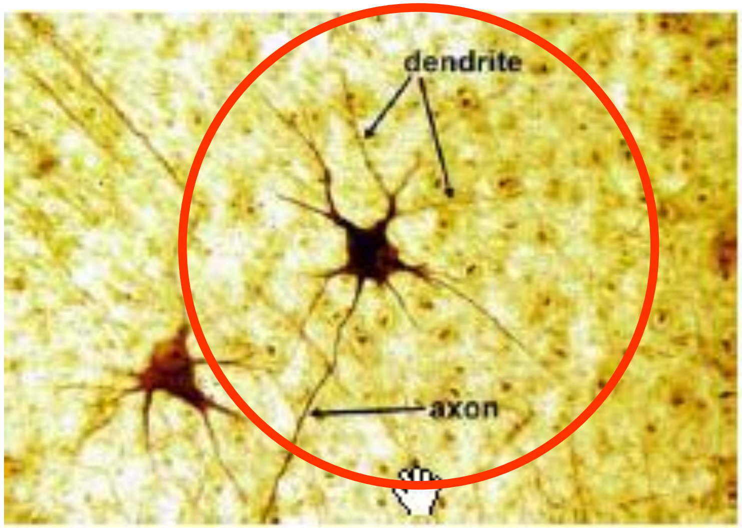
From Deep Learning: Methods and Applications, Deng and Yu

What are Neural Networks?

The real thing!



10 billion neurons

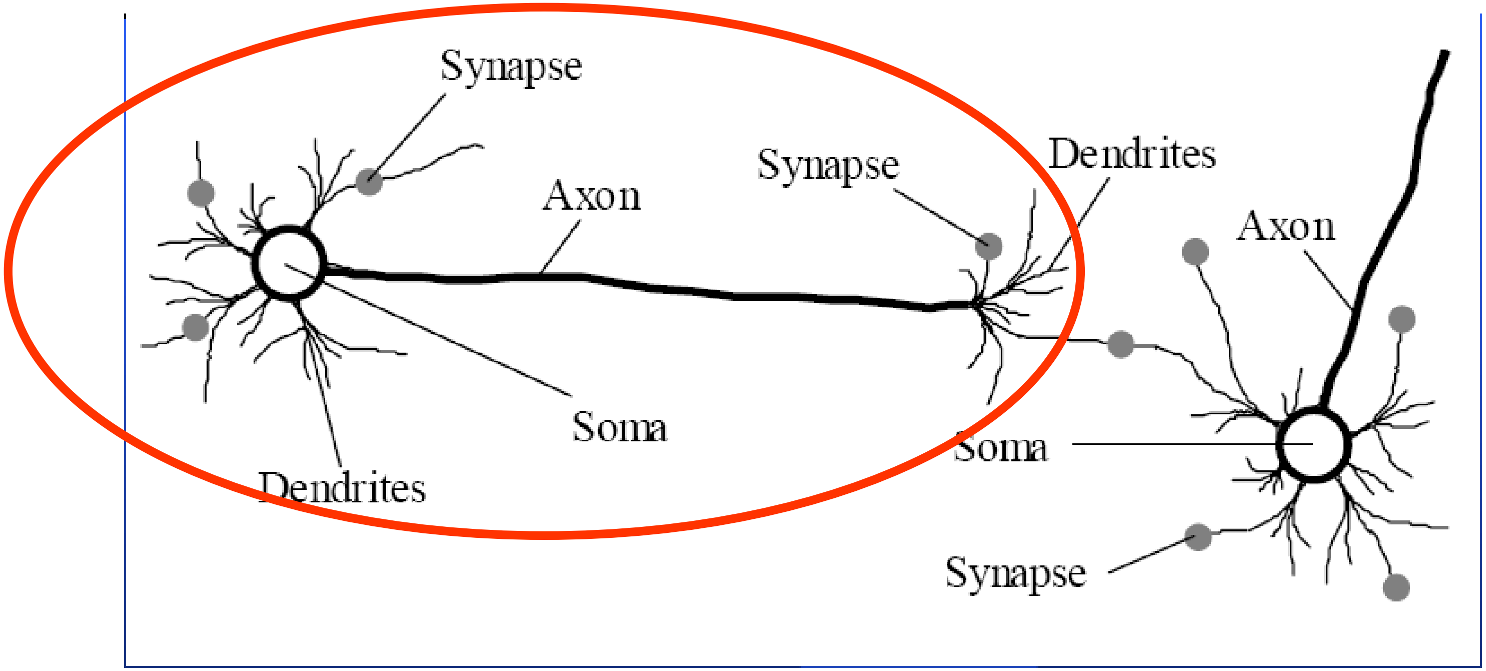


Local computations on **interconnected** elements (neurons)

Parallel computation

• neuron switch time 0.001sec
• recognition tasks performed in 0.1 sec.

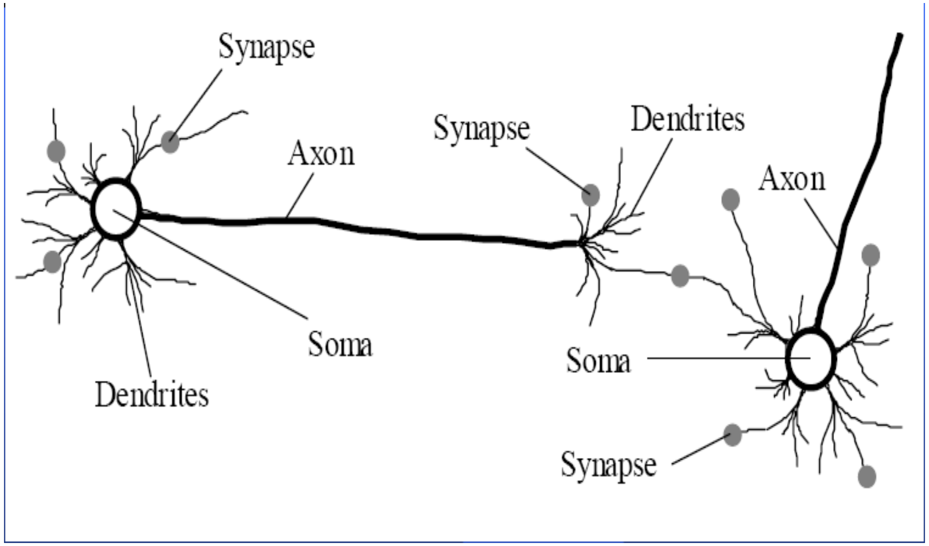
Biological Neural Networks

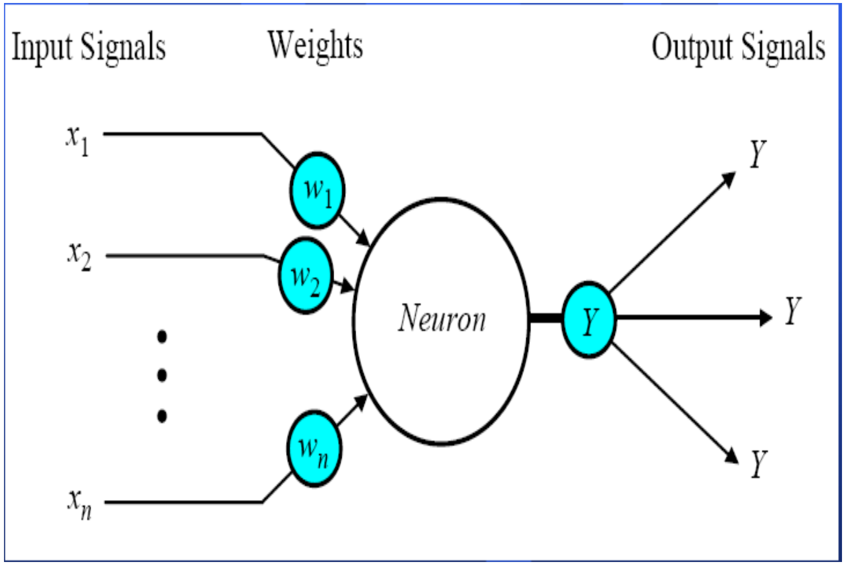


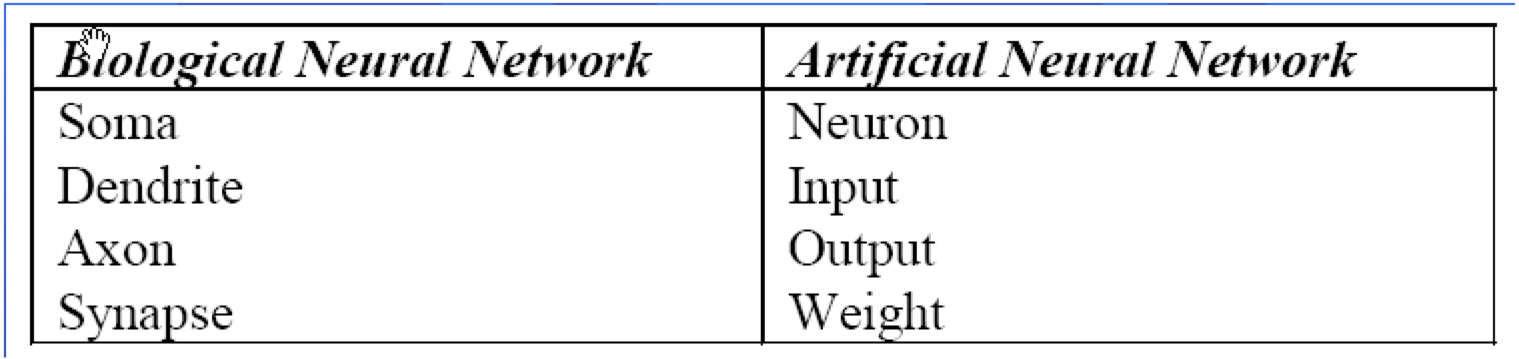
A network of interconnected biological neurons.

Connections per neuron 10^4 - 10^5

Biological vs Artificial Neural Networks

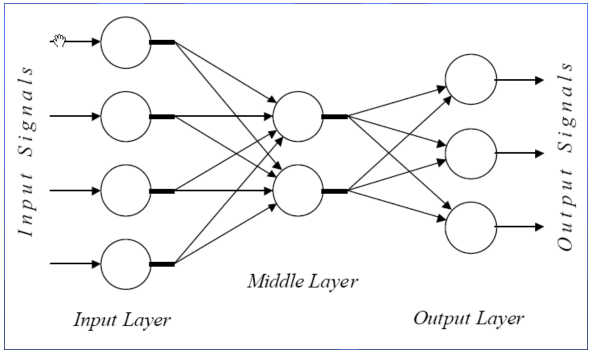






Biological Neural Network	*Artificial Neural Network*
Soma	Neuron
Dendrite	Input
Axon	Output
Synapse	Weight

Artificial Neural Networks: the dimensions



Architecture

How are the neurons connected

The Neuron

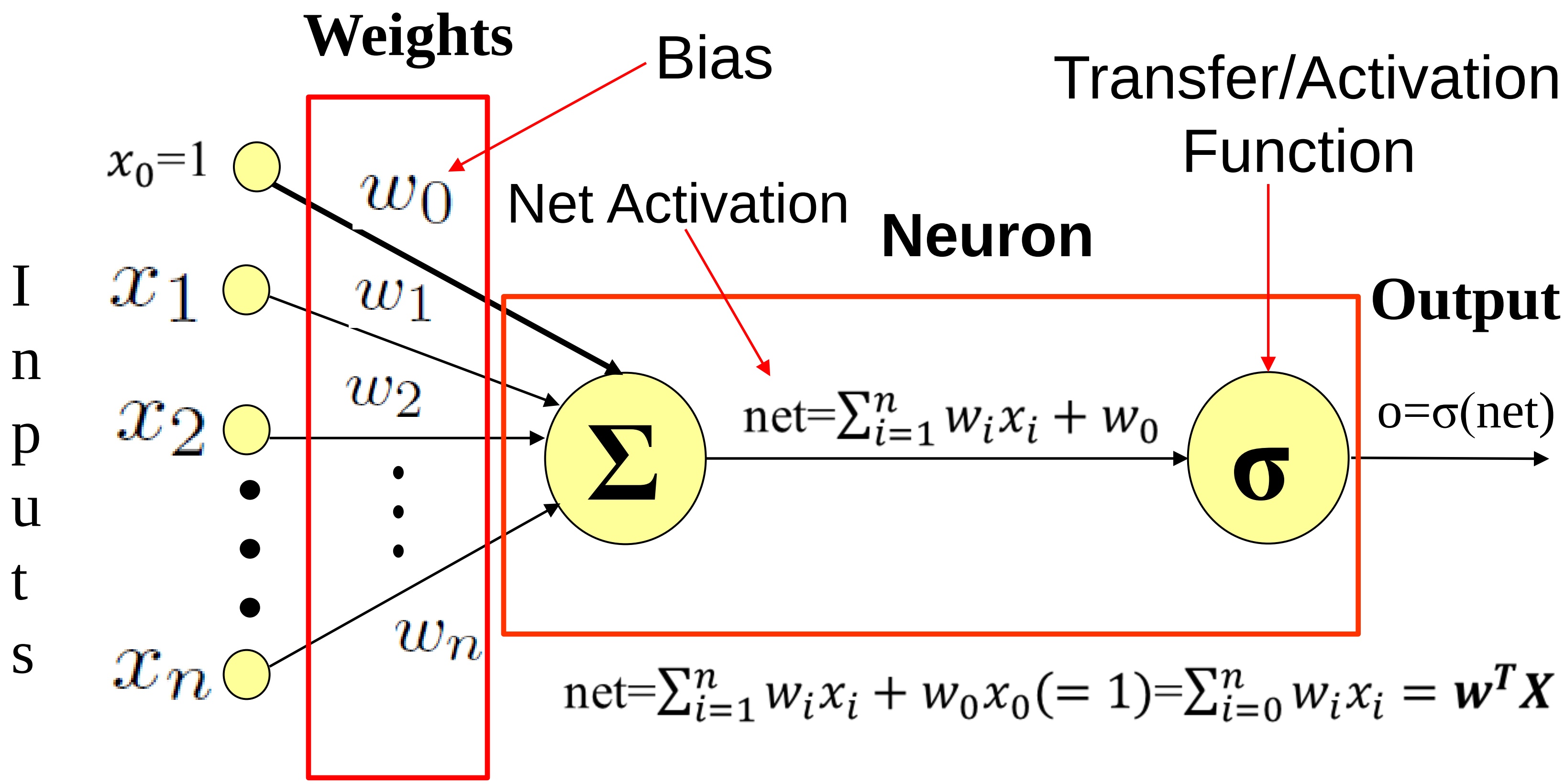
How information is processed in each unit. output = f(input)

Learning algorithms

How a Neural Network modifies its **weights** in order to solve a particular **learning task** in a set of **training examples**

The goal is to have a Neural Network that **generalizes** well, that is, that it generates a ‘correct’ output on a set of **test/new examples/inputs**.

The Neuron

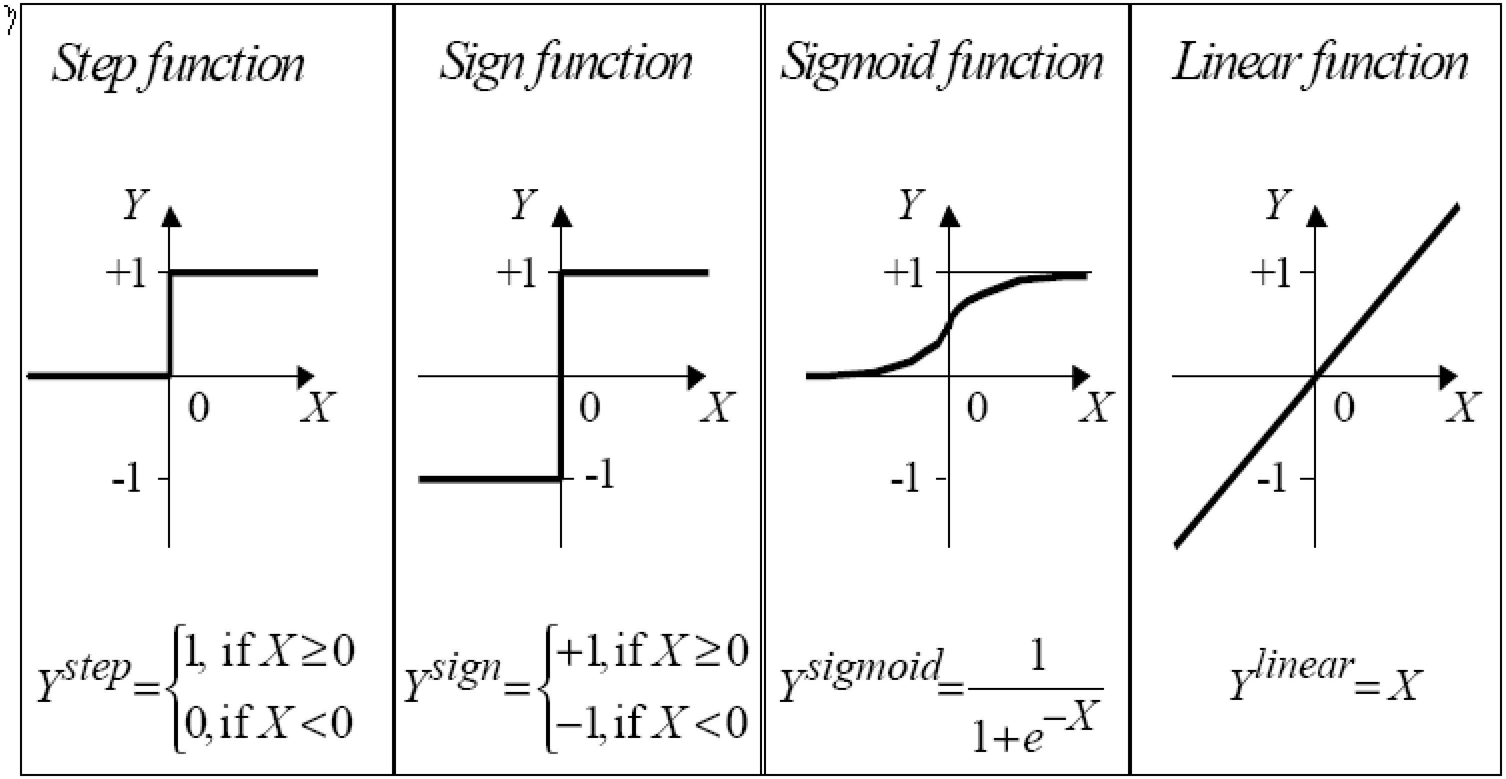


$$\text{net}=\sum_{i=1}^{n} w_i x_i + w_0 x_0 (= 1)=\sum_{i=0}^{n} w_i x_i = \boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{X}$$

$$\text{o} = \sigma(\text{net}) = \sigma(\boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{X})$$

- Main building block of any neural network

Activation functions



Step function

$$Y^{step} = \begin{cases} 1, \text{ if } X \geq 0 \\ 0, \text{ if } X < 0 \end{cases}$$

Sign function

$$Y^{sign} = \begin{cases} +1, \text{ if } X \geq 0 \\ -1, \text{ if } X < 0 \end{cases}$$

Sigmoid function

$$Y^{sigmoid} = \frac{1}{1+e^{-X}}$$

Linear function

$$Y^{linear} = X$$

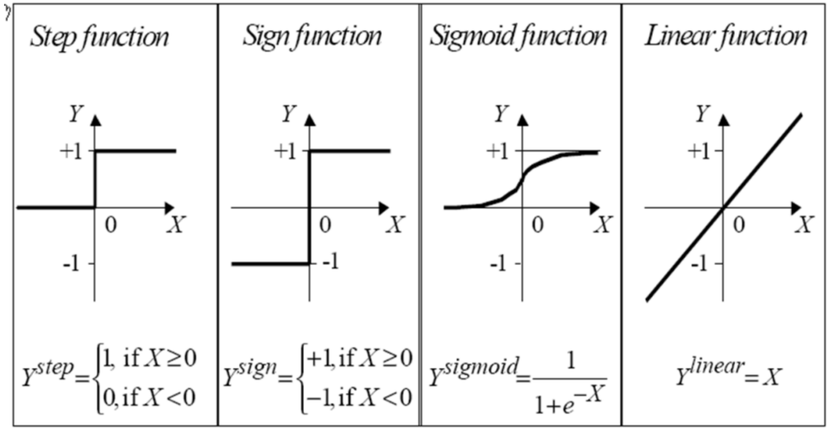
$$X = net = \sum_{i=1}^{n} w_i x_i + w_0, \quad Y = o = \sigma(net)$$

Role of Bias

$$net = \sum_{i=1}^{n} w_i x_i + w_0 x_0 (= 1)$$

$$\text{o} = \sigma(net)$$

$$w_0 = \text{-}\theta$$

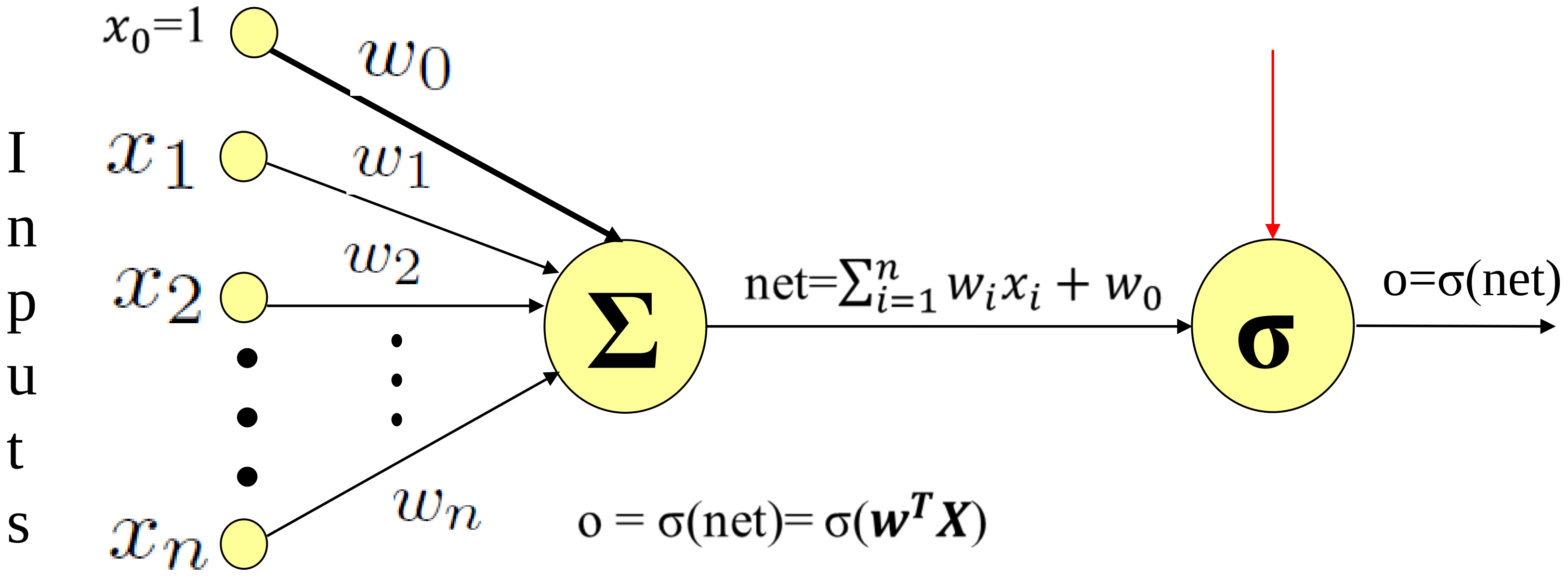


- The threshold where the neuron fires should be adjustable
- Instead of adjusting the threshold we add the bias term
- Defines how strong the neuron input should be before the neuron fires

$$o = \begin{cases} 1 \; if \;\; \sigma\left(\sum_{i=1}^{n} w_i x_i\right) \geq \theta \\ 0 \; if \;\; \sigma\left(\sum_{i=1}^{n} w_i x_i\right) < \theta \end{cases}$$

$$o = \begin{cases} 1 \; if \;\; \sigma\left(\sum_{i=1}^{n} w_i x_i - \theta\right) \geq 0 \\ 0 \; if \;\; \sigma\left(\sum_{i=1}^{n} w_i x_i - \theta\right) < 0 \end{cases}$$

Perceptron



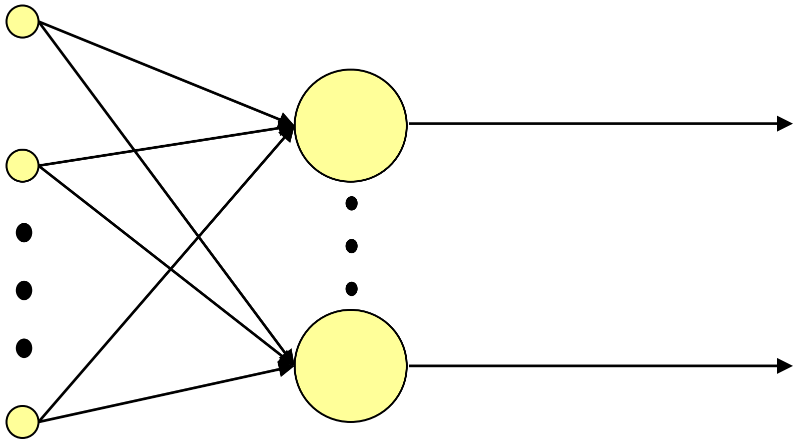
$$o = \sigma(\text{net}) = \sigma(\boldsymbol{w}^T \boldsymbol{X})$$

$$o = \sigma(\text{net}) = \begin{cases} 1 \; if \; net > 0 \\ -1 \quad otherwise \end{cases}$$

- σ = sign/step/function
- Perceptron = a neuron that its input is the dot product of W and X and uses a step function as a transfer function

Perceptron: Architecture

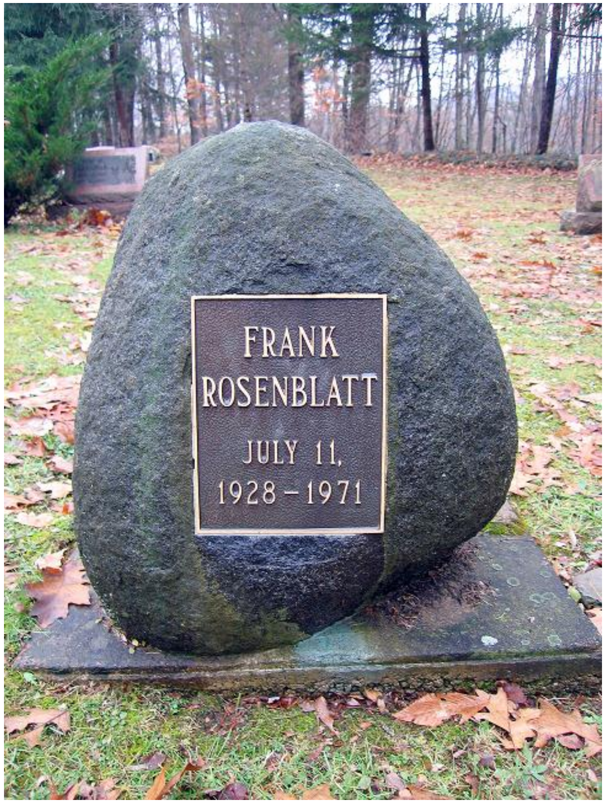
- Generalization to single layer perceptrons with more neurons is easy because:



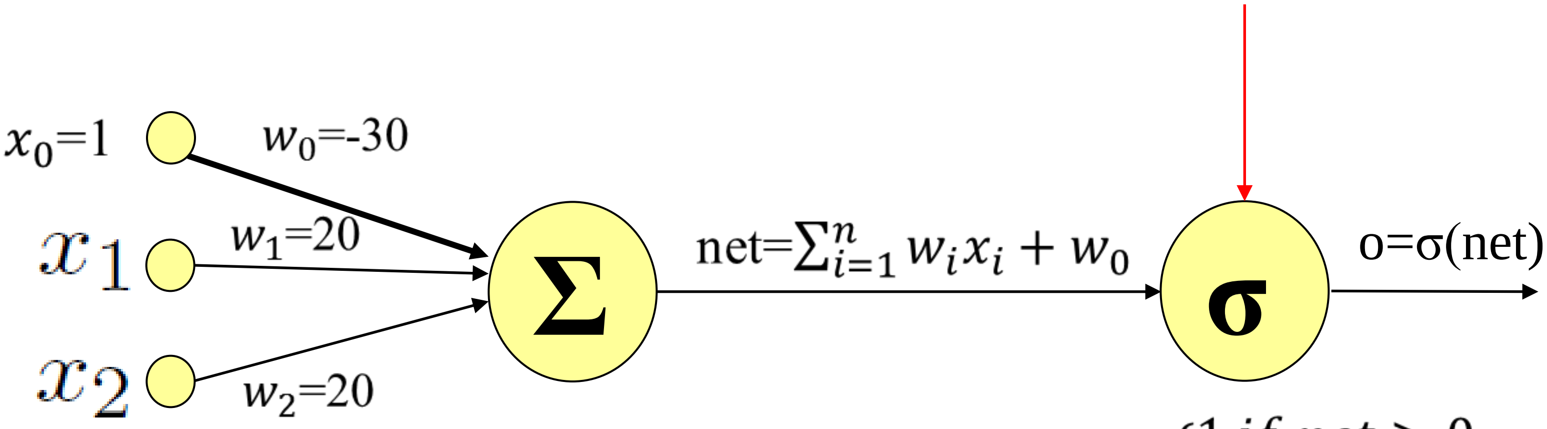
- The output units are mutually independent
- Each weight only affects one of the outputs

Perceptron

- Perceptron was invented by Rosenblatt
- *The Perceptron--a perceiving and recognizing automaton*, 1957



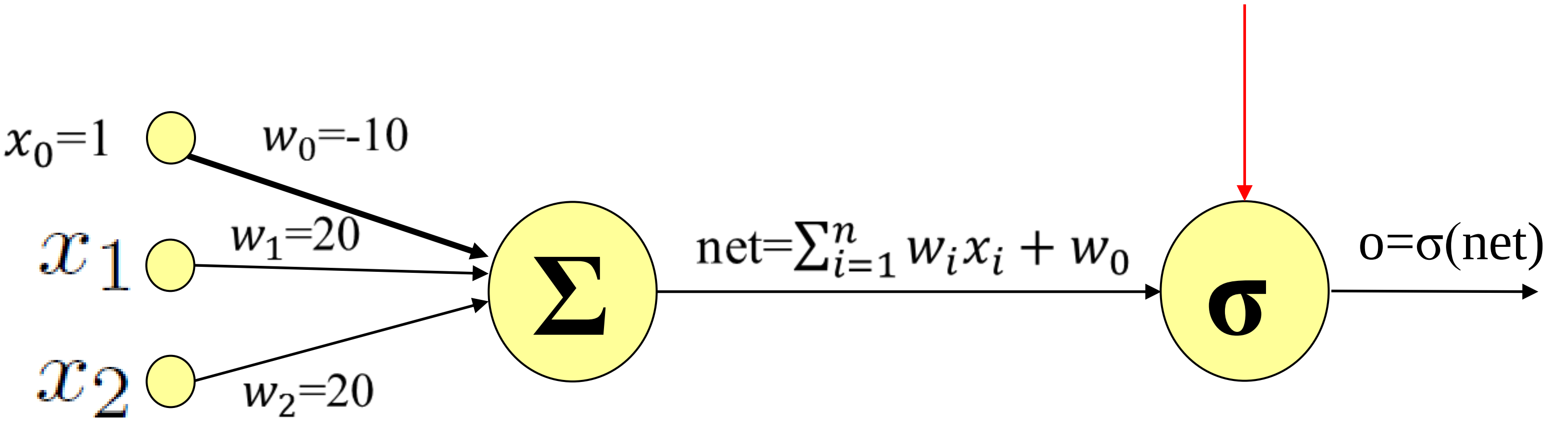
Perceptron: Example 1 - AND



$$o = \sigma(net) = \begin{cases} 1 \; if \; net > 0 \\ 0 \; otherwise \end{cases}$$

- x1 = 1, x2 = 1→ net = 20+20-30=10 →o = σ(10) = 1
- x1 = 0, x2 = 1→ net = 0+20-30 =-10 →o = σ(-10) = 0
- x1 = 1, x2 = 0→ net = 20+0-30 =-10 →o = σ(-10) = 0
- x1 = 0, x2 = 0→ net = 0+0-30 =-30 →o = σ(-10) = 0

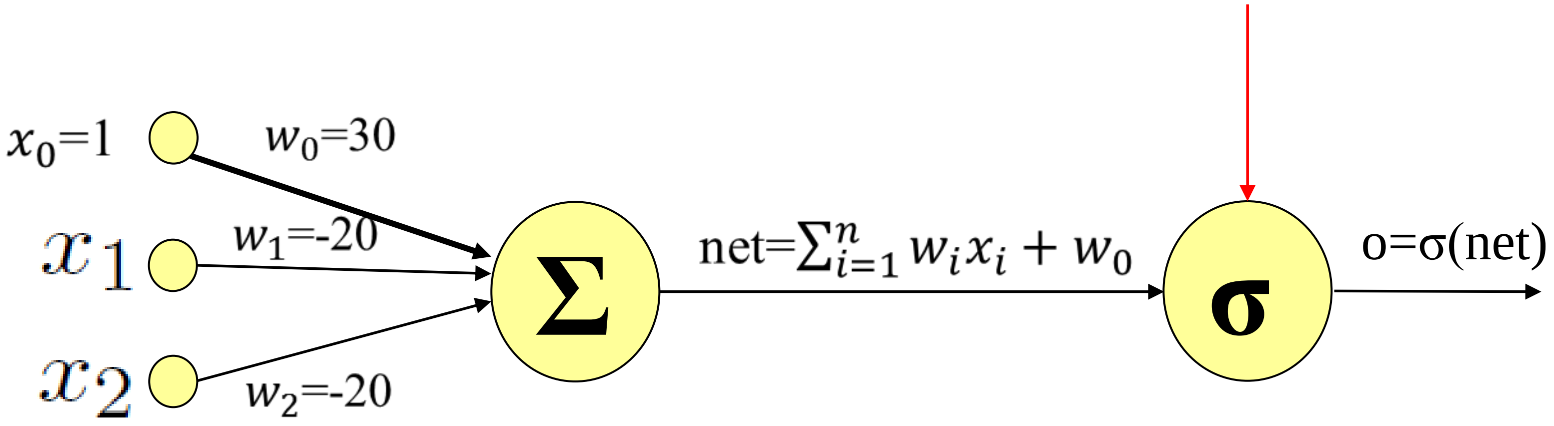
Perceptron: Example 2 - OR



$$o = \sigma(net) = \begin{cases} 1 \; if \; net > 0 \\ 0 \; otherwise \end{cases}$$

- x1 = 1, x2 = 1→ net = 20+20-10=30 →o = σ(30) = 1
- x1 = 0, x2 = 1→ net = 0+20-10 =10 →o = σ(10) = 1
- x1 = 1, x2 = 0→ net = 20+0-10 =10 →o = σ(10) = 1
- x1 = 0, x2 = 0→ net = 0+0-10 =-10 →o = σ(-10) = 0

Perceptron: Example 3 - NAND



$$o = \sigma(net) = \begin{cases} 1 \; if \; net > 0 \\ 0 \; otherwise \end{cases}$$

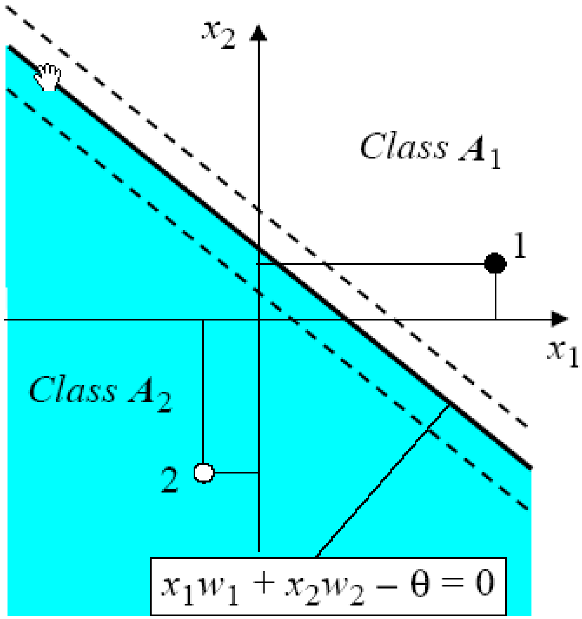
- x1 = 1, x2 = 1→ net = -20-20+30=-10 → o = σ(-10) = 0
- x1 = 0, x2 = 1→ net = 0-20+30 =10 → o = σ(10) = 1
- x1 = 1, x2 = 0→ net = -20+0+30 =10 → o = σ(10) = 1
- x1 = 0, x2 = 0→ net = 0+0+30 =30 → o = σ(30) = 1

Perceptron for classification

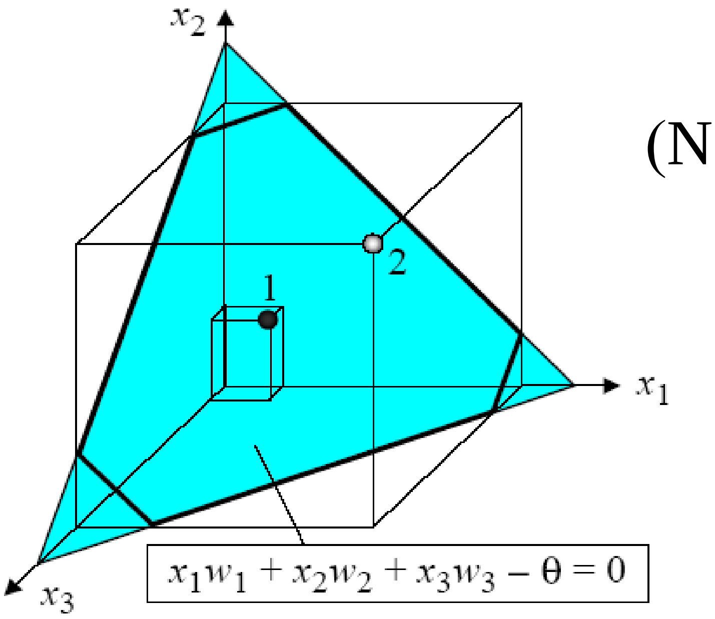
- Given training examples of classes C_1 ,C_2 train the perceptron in such a way that it classifies correctly the training examples:
  - ***If the output of the perceptron is 1 then the input is assigned to class*** C_1 ***(i.e. if*** $\sigma(\mathbf{w}^T\mathbf{x}) = 1$ ***)***
  - ***If the output is 0 then the input is assigned to class*** C_2

• Geometrically, we try to find a hyper-plane that separates the examples of the two classes. The hyper-plane is defined by the linear function

Perceptron: Geometric view



(*a*) Two-input perceptron.



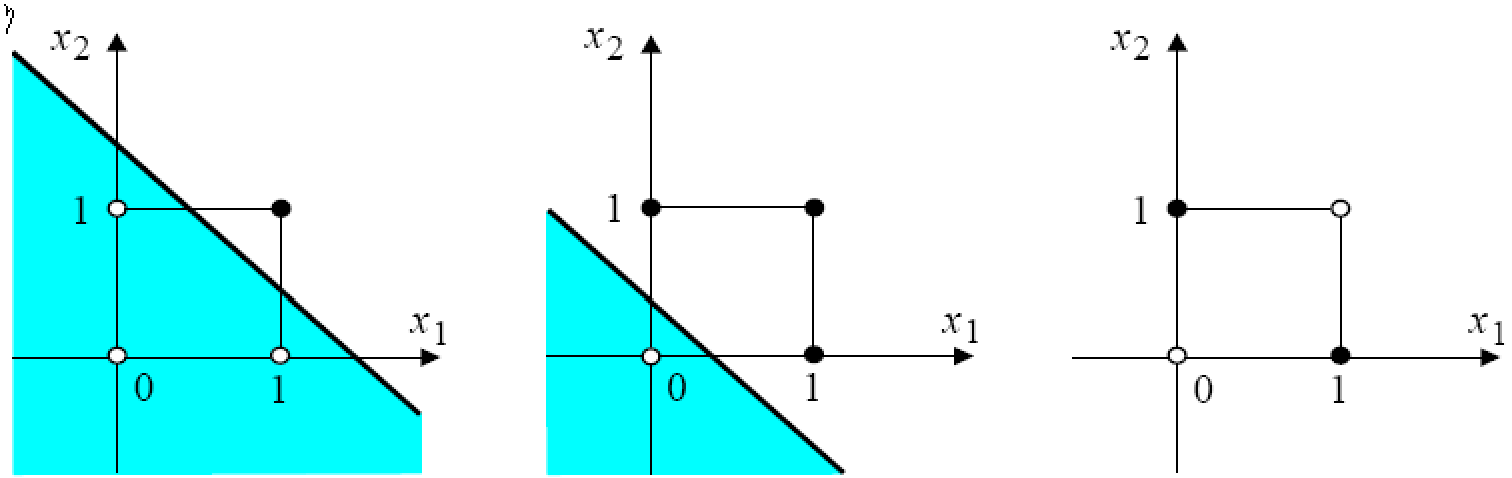
(*b*) Three-input perceptron.

(Note that $\theta = -w_0$)

$$\text{if } \; w_1 x_1 + w_2 x_2 + w_0 > 0 \; \text{ then } \; Class = A1$$
$$\text{if } \; w_1 x_1 + w_2 x_2 + w_0 < 0 \; \text{ then } \; Class = A2$$

$$\text{if } \; w_1 x_1 + w_2 x_2 + w_0 = 0 \text{ then } Class = A1 \text{ or } A2$$
depends on our definition

Perceptron: The limitations of perceptron



(a) $AND\ (x_1 \cap x_2)$

(b) $OR\ (x_1 \cup x_2)$

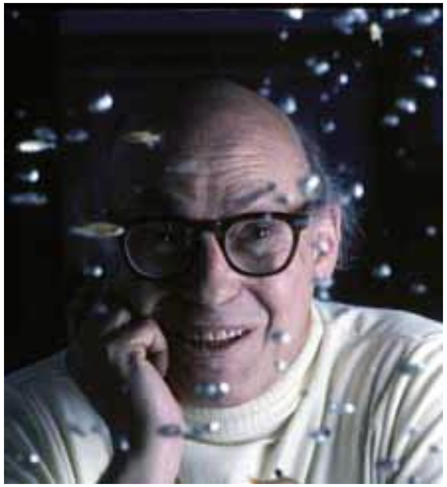
(c) $Exclusive\text{-}OR$
$(x_1 \oplus x_2)$

- Perceptron can only classify examples that are linearly separable
- The XOR is not linearly separable.
- This was a terrible blow to the field

Perceptron

- A famous book was published in 1969: **Perceptrons**
- Caused a significant decline in interest and funding of neural network research

- Marvin Minsky



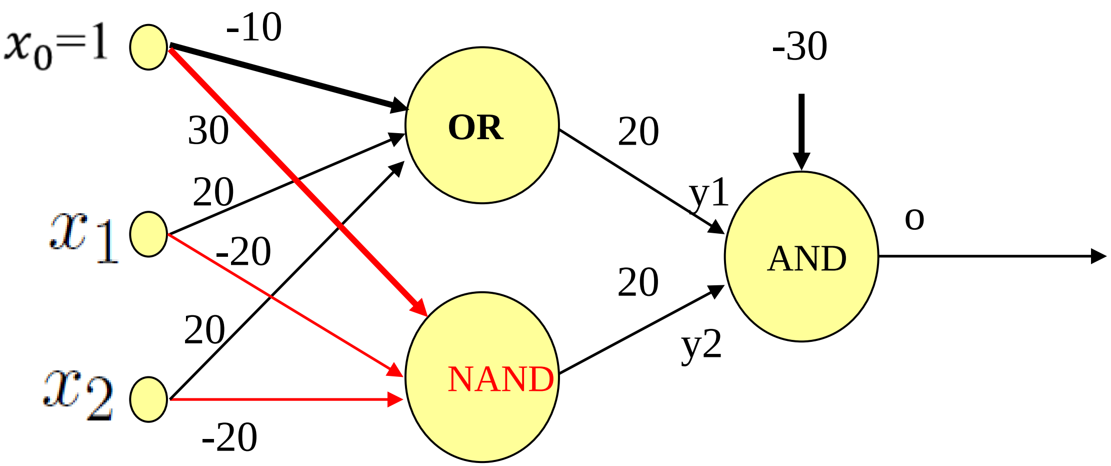
- Seymour Papert

Perceptron XOR Solution

- XOR can be expressed in terms of AND, OR, NAND

Perceptron XOR Solution

- XOR can be expressed in terms of AND, OR, NAND
- XOR = NAND (AND) OR



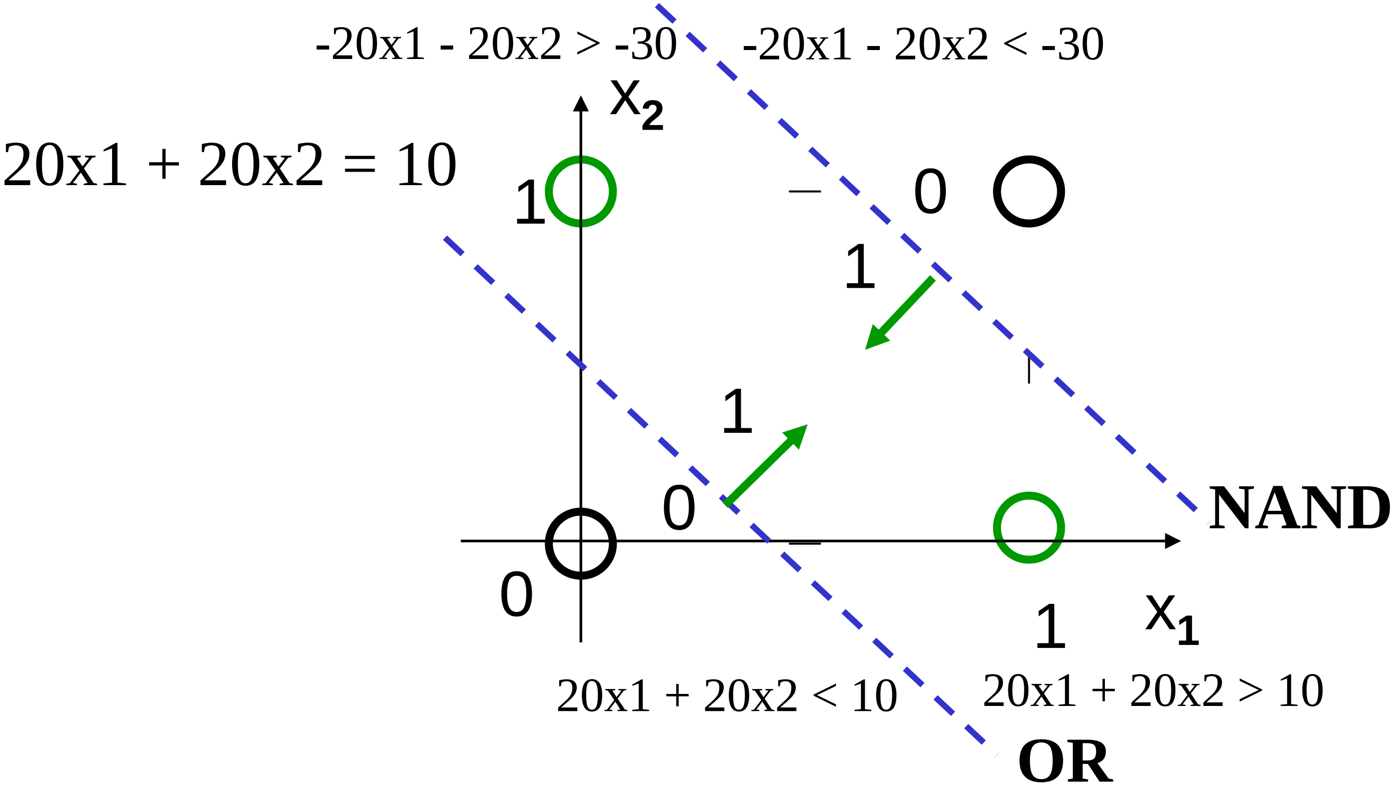
OR	**NAND**
1 1 → 1	1 1 → 0
0 1 → 1	0 1 → 1
1 0 → 1	1 0 → 1
0 0 → 0	0 0 → 1

AND
1 1 → 1
0 1 → 0
1 0 → 0
0 0 → 0

- x1=1, x2 =1→ y1=1 AND y2=0 → o = 0
- x1=1, x2 =0→ y1=1 AND y2=1 → o = 1
- x1=0, x2 =1→ y1=1 AND y2=1 → o = 1
- x1=0, x2 =0→ y1=0 AND y2=1→ o = 0

XOR

$-20x1 -20x2 = -30$



$-20x1 - 20x2 > -30$

$-20x1 - 20x2 < -30$

$20x1 + 20x2 = 10$

NAND

$20x1 + 20x2 < 10$

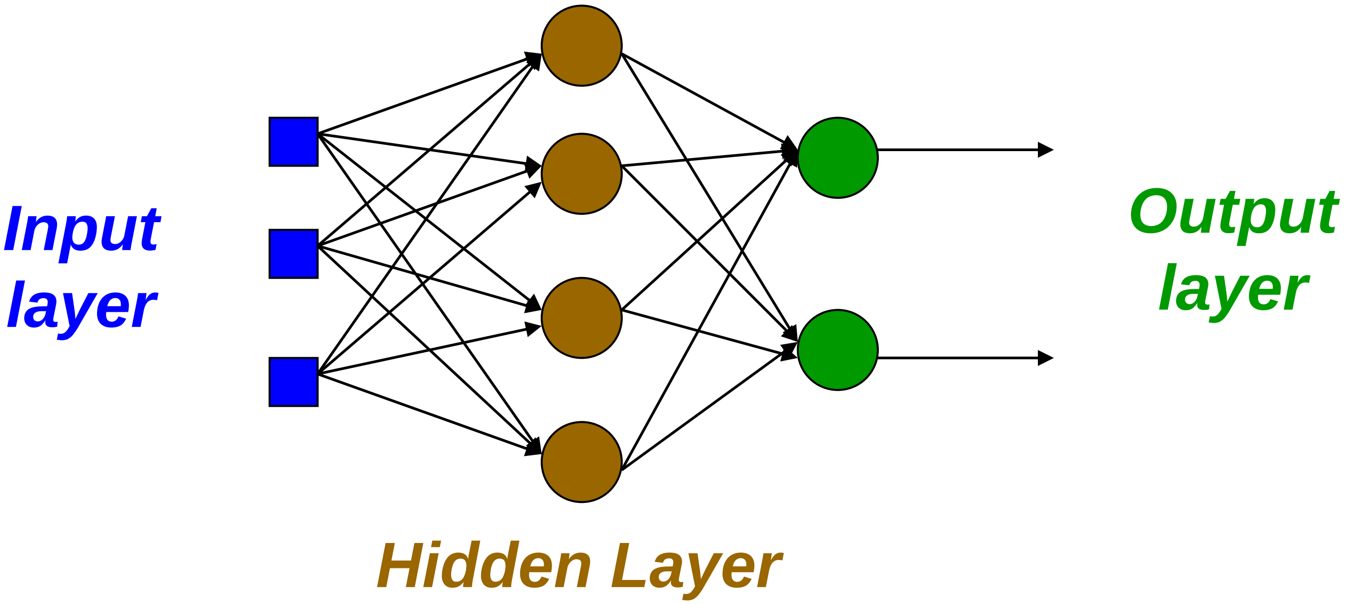
$20x1 + 20x2 > 10$

OR

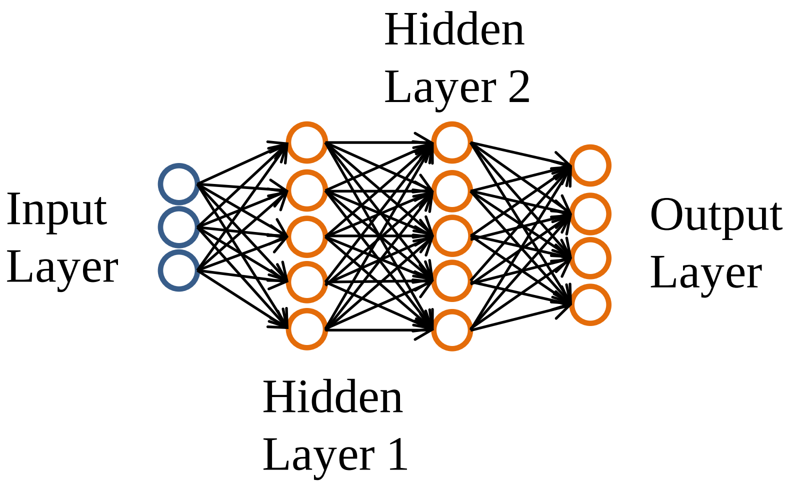
Multilayer Feed Forward Neural Network

- We consider a more general network architecture: between the input and output layers there are hidden layers, as illustrated below.

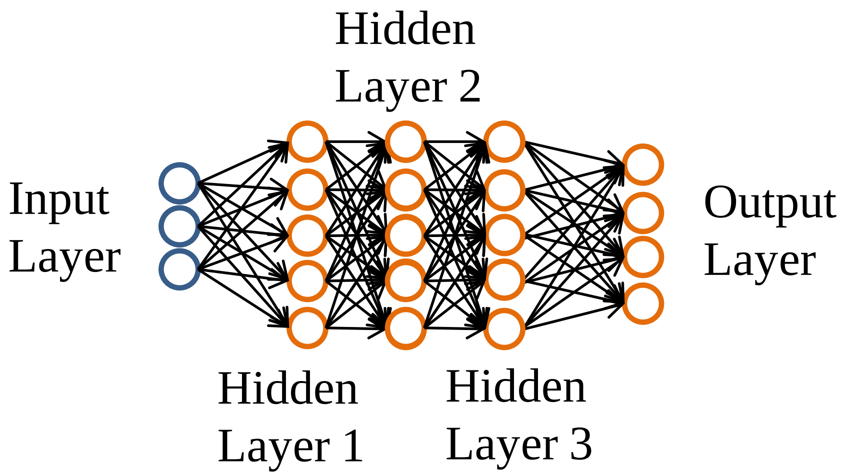
- Hidden nodes do not directly receive inputs nor send outputs to the external environment.



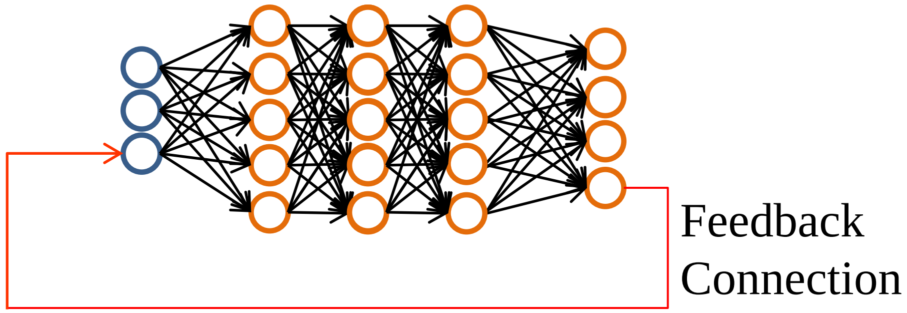
NNs: Architecture



3-layer feed-forward network



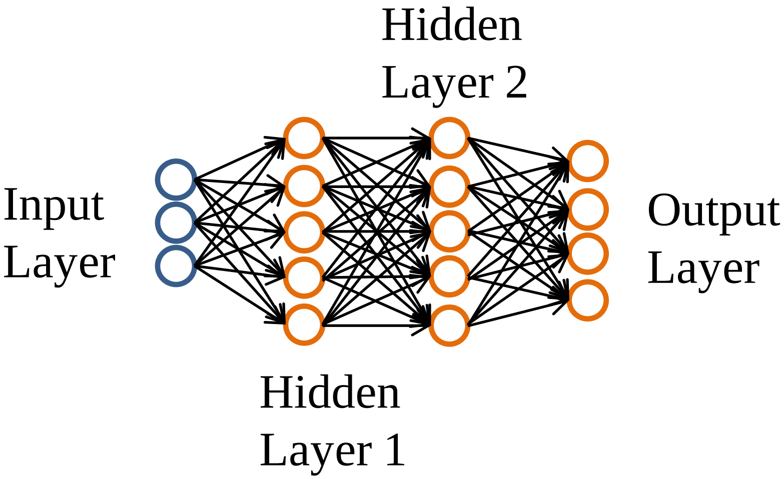
4-layer feed-forward network



4-layer recurrent network – Difficult to train

- The input layer does not count as a layer

NNs: Architecture

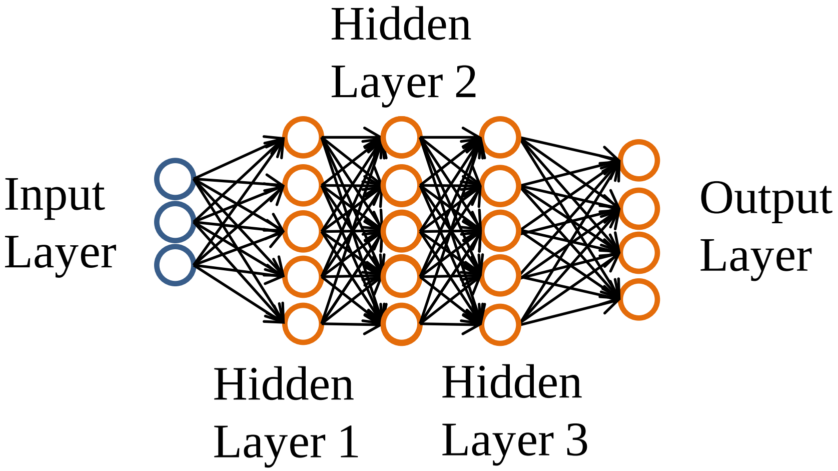

Hidden Layer 2

Input Layer

Output Layer

Hidden Layer 1

3-layer feed-forward network


Hidden Layer 2

Input Layer

Output Layer

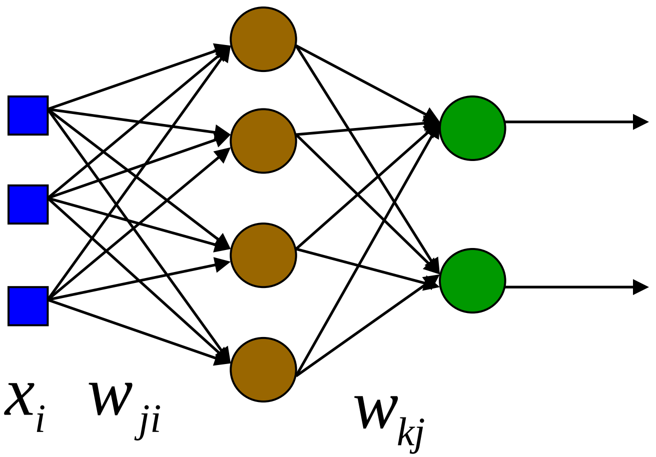
Hidden Layer 1

Hidden Layer 3

4-layer feed-forward network

- Deep networks are simply networks with many layers.
- They are trained in the same way as shallow networks but weight initialisation is done in a different way.

Multilayer Feed Forward Neural Network



w_{ji} = weight associated with *i*th input to hidden unit *j*

w_{kj} = weight associated with *j*th input to output unit *k*

y_j = output of *j*th hidden unit

o_k = output of *k*th output unit

n = number of inputs

nH = number of hidden neurons

$$y_j = \sigma\left(\sum_{i=0}^{n} x_i w_{ji}\right)$$

$$o_k = \sigma\left(\sum_{j=1}^{nH} y_j w_{kj}\right)$$

$$o_k = \sigma\left(\sum_{j=1}^{nH} \sigma\left(\sum_{i=0}^{n} x_i w_{ji}\right) w_{kj}\right)$$

Example

- http://galaxy.agh.edu.pl/~vlsi/AI/backp_t_en/backprop.html

Representational Power of Feedforward Neural Networks

- Boolean functions: Every boolean function can be represented exactly by some network with two layers

- Continuous functions: Every bounded continuous function can be approximated with arbitrarily small error by a network with 2 layers

- Arbitrary functions: Any function can be approximated to arbitrary accuracy by a network with 3 layers

- Catch: We do not know 1) what the appropriate number of hidden neurons is, 2) the proper weight values

$$o_k = \sigma\left(\sum_{j=1}^{nH} \sigma\left(\sum_{i=0}^{n} x_i w_{ji}\right) w_{kj}\right)$$

Classification /Regression with NNs

- You should think of neural networks as function approximators

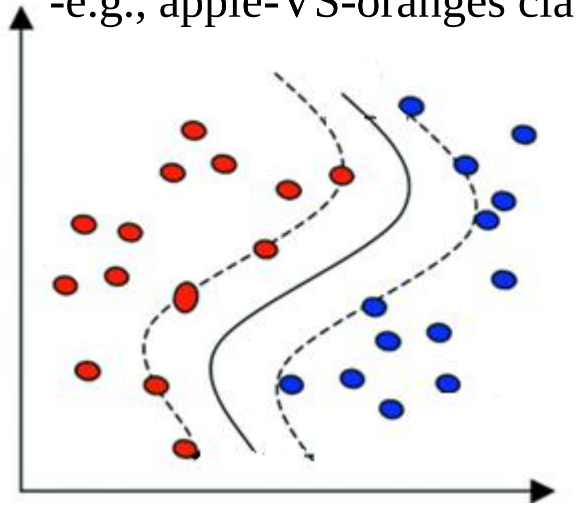
$$o_k = \sigma\left(\sum_{j=1}^{nH} \sigma\left(\sum_{i=0}^{n} x_i w_{ji}\right) w_{kj}\right)$$

Classification

-Decision boundary approximation

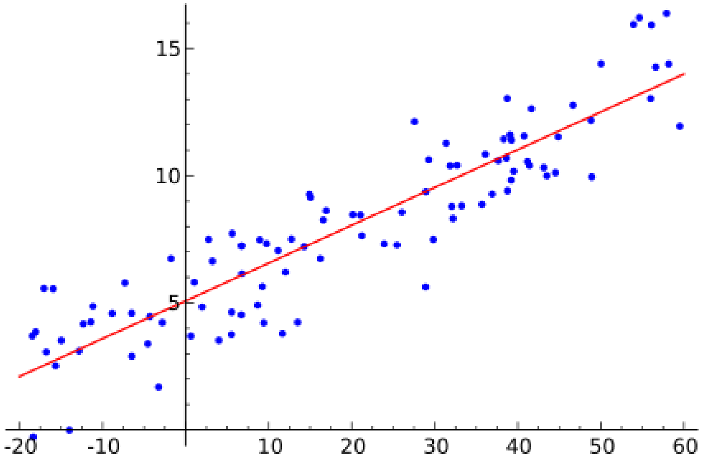
-Discrete output

-e.g., apple-VS-oranges classifier

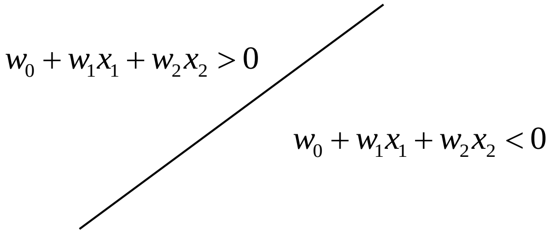


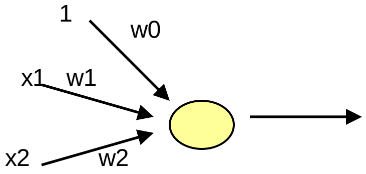
Regression

- Function approximation
- Continuous output
- e.g., house price estimation

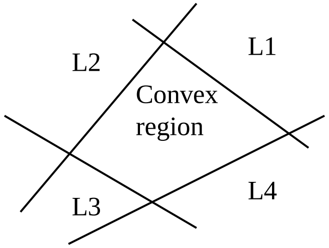


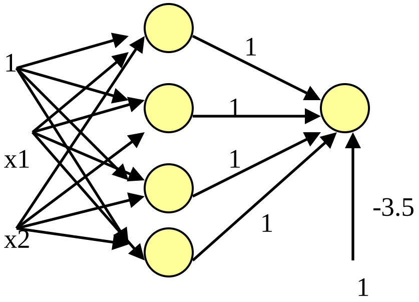
Decision boundaries



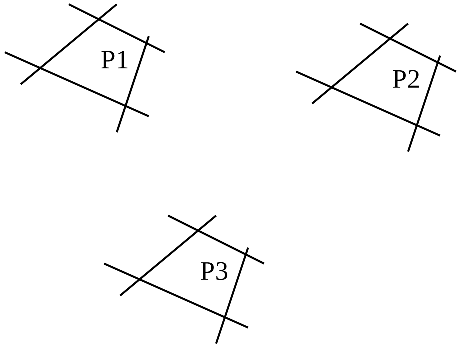


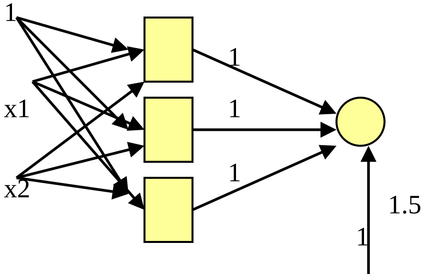
Network with a single node





One-hidden layer network that realizes the convex region: each hidden node realizes one of the lines bounding the convex region





two-hidden layer network that realizes the union of three convex regions: each box represents a one hidden layer network realizing one convex region

Output Representation

- Binary Classification

  Target Values (t): 0 (negative) and 1 (positive)

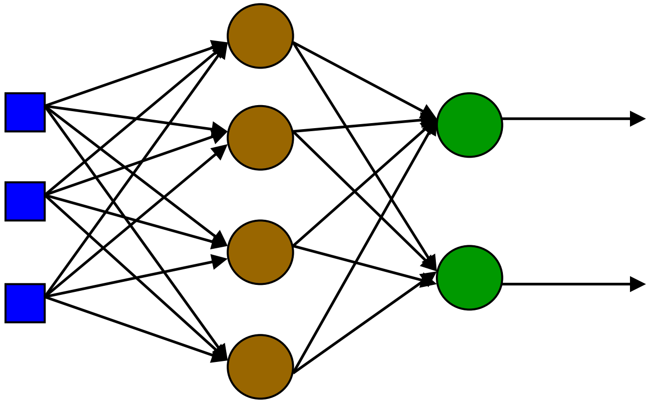
- Regression

  Target values (t): continuous values [-inf, +inf]

- Ideally o ≈ t

$$o_k = \sigma\left(\sum_{j=1}^{nH} \sigma\left(\sum_{i=0}^{n} x_i w_{ji}\right) w_{kj}\right)$$

Multiclass Classification



Target Values: vector (length=no. Classes)

$$\begin{array}{cccc} \text{Class1} & \text{Class2} & \text{Class3} & \text{Class4} \\ \begin{bmatrix}1\\0\\0\\0\end{bmatrix} & \begin{bmatrix}0\\1\\0\\0\end{bmatrix} & \begin{bmatrix}0\\0\\1\\0\end{bmatrix} & \begin{bmatrix}0\\0\\0\\1\end{bmatrix} \end{array}$$

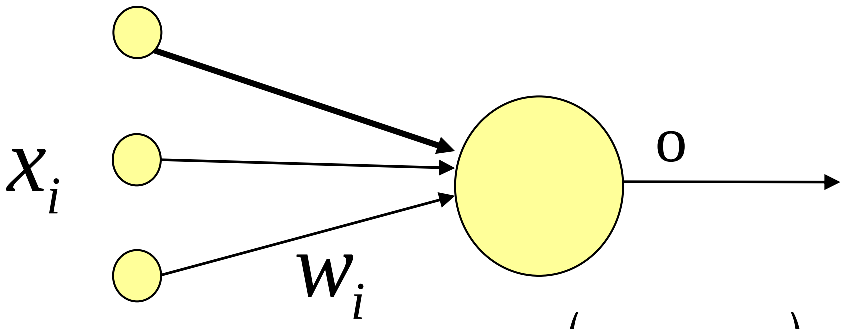
Training

- We have assumed so far that we know the weight values
- We are given a training set consisting of inputs and targets (**X, T**)
- Training: Tuning of the weights (w) so that for each input pattern (x) the output (o) of the network is close to the target values (t).

$$\mathrm{o} \approx \mathrm{t}$$

$$o \;= \sigma\left(\sum_{j=1}^{nH} \sigma\left(\sum_{i=0}^{n} x_i w_{ji}\right) w_{kj}\right)$$

Perceptron Training Rule



$$o = \sigma\left(\sum_{i=0}^{n} x_i w_i\right)$$

- Training Set: A set of input vectors $x_i, i = 1 \ldots n$ with the corresponding targets t_i

- η: learning rate, controls the change rate of the weights

• Begin with random weights

• Change the weights whenever an example is misclassified

$$w_i \leftarrow w_i + \Delta w_i$$
$$\Delta w_i = \eta (t_i - o) x_i$$

• This rule works if the examples are linearly seperable

- for every input vector *x(i)* the output is the desired target o = t

Training – Gradient Descent

- In most problems the training examples are NOT linearly seperable. Therefore, we need a different approach to adjust the weights → Gradient Descent

- Gradient Descent: A general, effective way for estimating parameters (e.g. **w**) that minimise error functions

- We need to define an error function E(w)

- Update the weights in each iteration in a direction that reduces the error the order in order to minimize E

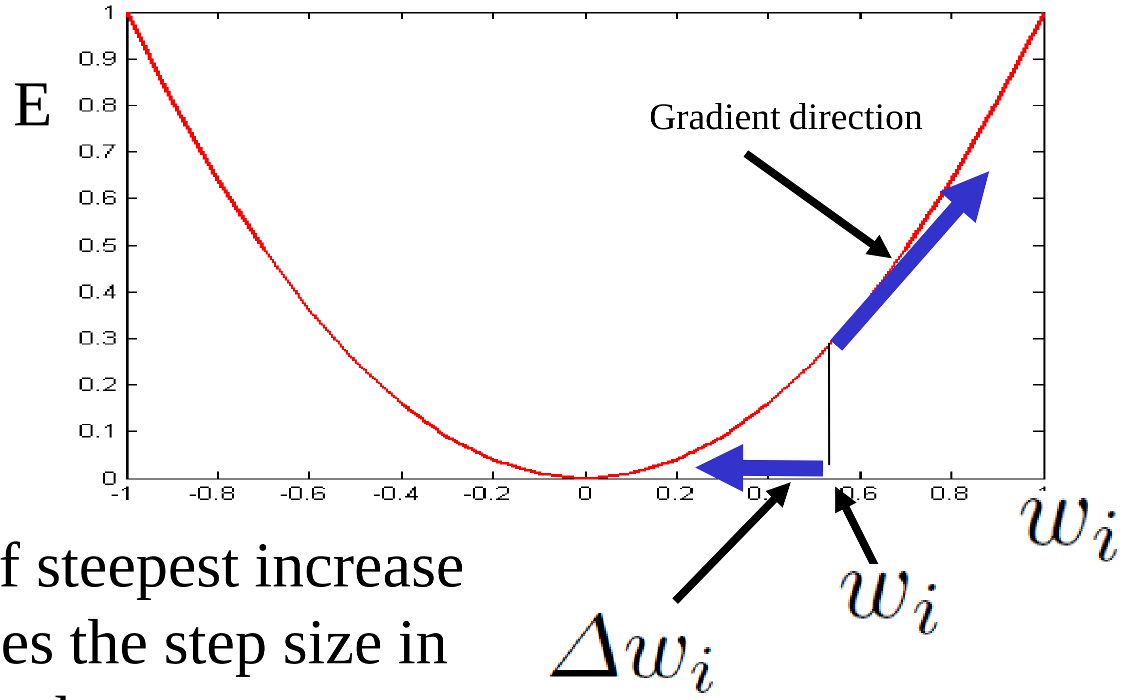
$$w_i \leftarrow w_i + \Delta w_i$$

$$\Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$

Gradient Descent

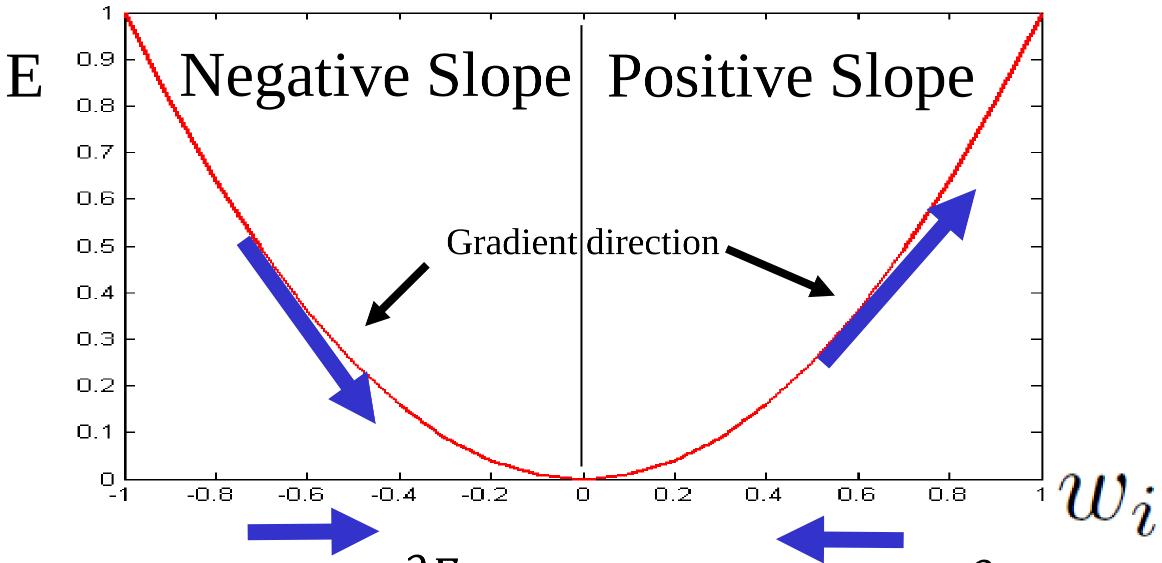
Gradient descent method: take a step in the direction that decreases the error E. This direction is the opposite of the derivative of E.

$$\Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$



- derivative: direction of steepest increase
- learning rate: determines the step size in the direction of steepest decrease

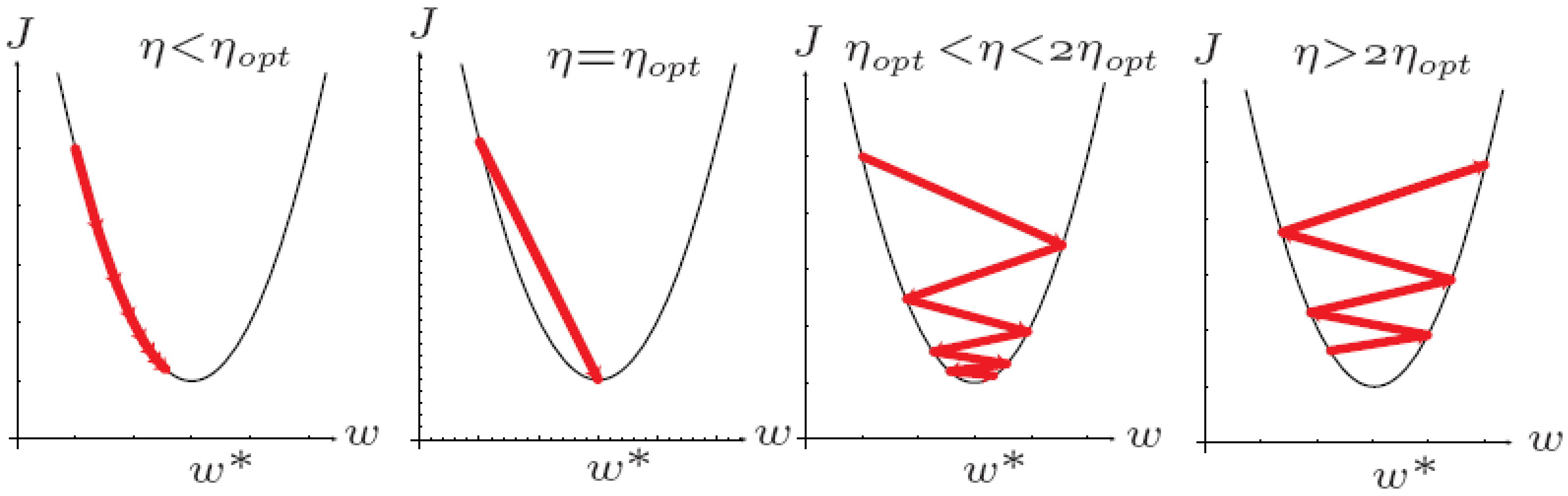
Gradient Descent – Learning Rate



$$\Delta w_i = -\eta \frac{\partial E}{\partial w_i} > 0 \qquad \Delta w_i = -\eta \frac{\partial E}{\partial w_i} < 0$$

- Derivative: direction of steepest increase
- Learning rate: determines the step size in the direction of steepest decrease. It usually takes small values, e.g. 0.01, 0.1
- If it takes large values then the weights change a lot -> network unstable

Gradient Descent –Learning Rate



Gradient Descent

- We define our error function as follows (D = number of training examples):

$$E = \frac{1}{2}\sum_{d=1}^{D}(t_d - o_d)^2$$

- We assume linear activation transfer

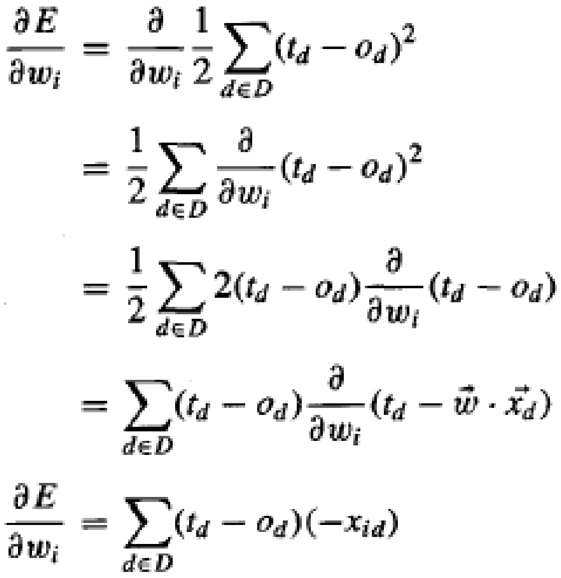
- E depends on the weights because $o_d = \sum_{i=0}^{n} x_i^d w_i$

- We wish to find the weight values that minimise E, i.e. the desired target *t* is very close to the actual output *o*.

Gradient Descent

$$E = \frac{1}{2}\sum_{d=1}^{D}\left(t_d - o_d\right)^2 \qquad \Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$

- The partial derivative can be computed as follows:



$$\begin{aligned}
\frac{\partial E}{\partial w_i} &= \frac{\partial}{\partial w_i}\frac{1}{2}\sum_{d\in D}(t_d - o_d)^2 \\
&= \frac{1}{2}\sum_{d\in D}\frac{\partial}{\partial w_i}(t_d - o_d)^2 \\
&= \frac{1}{2}\sum_{d\in D}2(t_d - o_d)\frac{\partial}{\partial w_i}(t_d - o_d) \\
&= \sum_{d\in D}(t_d - o_d)\frac{\partial}{\partial w_i}(t_d - \vec{w}\cdot\vec{x_d}) \\
\frac{\partial E}{\partial w_i} &= \sum_{d\in D}(t_d - o_d)(-x_{id})
\end{aligned}$$

- Therefore Δw is $\Delta w_i = \eta\sum_{d=1}^{D}\left(t_d - o_d\right)x_{id}$

Gradient Descent -Perceptron- Summary

1. Initialise weights randomly
2. Compute the output *o* for all the training examples
3. Compute the weight update for each weight

$$\Delta w_i = \eta \sum_{d=1}^{D} (t_d - o_d) x_{id}$$

4. Update the weights

$$w_i \leftarrow w_i + \Delta w_i$$

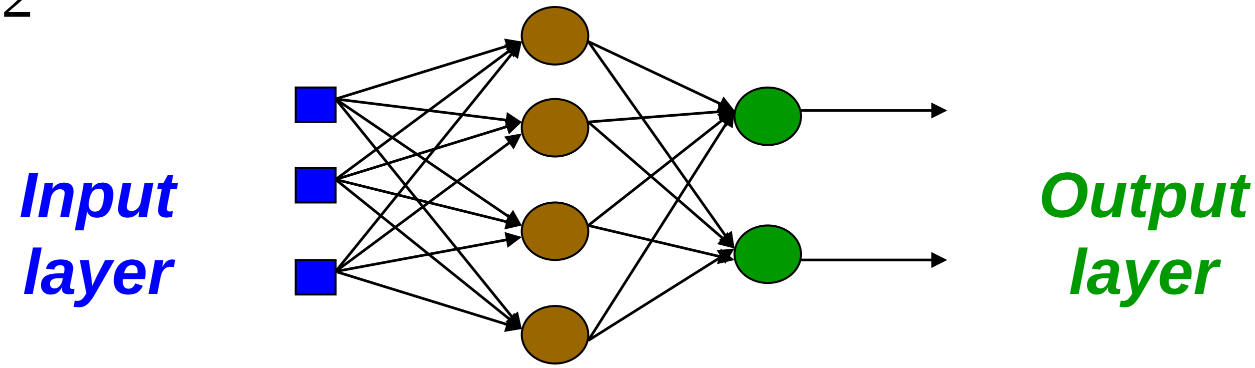
- Repeat steps 2-4 until a termination condition is met

- The algorithm will converge to a weight vector with minimum error, given that the learning rate is sufficiently small

Learning: The backpropagation algorithm

- The Backprop algorithm searches for weight values that minimize the total squared error of the network (K outputs) over the set of D training examples (training set).

$$E = \frac{1}{2}\sum_{k=1}^{K}\sum_{d=1}^{D}\left(t_{kd} - o_{kd}\right)^2$$



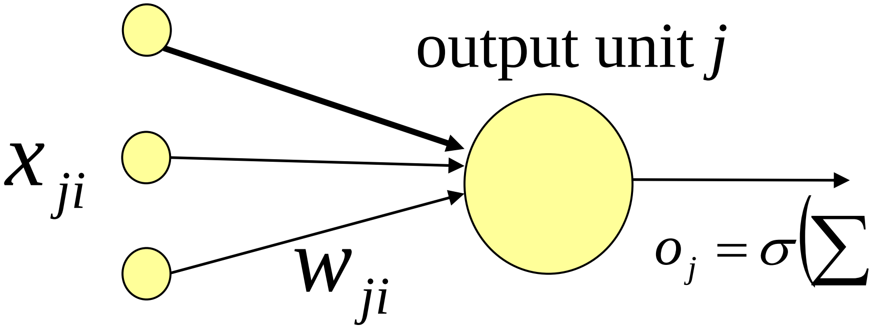
- Based on gradient descent algorithm

$$w_i \leftarrow w_i + \Delta w_i \qquad \Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$

Learning: The backpropagation algorithm

- Backpropagation consists of the repeated application of the following two passes:
  - **Forward pass**: in this step the network is activated on one example and the error of (each neuron of) the output layer is computed.
  - **Backward pass**: in this step the network error is used for updating the weights (credit assignment problem). This process is complex because hidden nodes are linked to the error not directly but by means of the nodes of the next layer. Therefore, starting at the output layer, the error is propagated backwards through the network, layer by layer.

Learning: Output Layer Weights



$$o_j = \sigma\left(\sum_{i=0}^{nH} x_{ji} w_{ji}\right)$$

subscript *ji*: *i*th input to unit *j*,
i.e., input from hidden neuron *i*

- Consider the error of one pattern d: $E_d = \frac{1}{2}\sum_{k=1}^{K}(t_k - o_k)^2$
- Using exactly the same approach as in the perceptron

$$\Delta w_{ji} = \eta \underbrace{(t_j - o_j) x_{ji} \frac{\partial \sigma(net_j)}{\partial net_j}}_{-\partial E_d / \partial w_{ji}}$$

$$\Delta w_i = \eta \sum_{i=1}^{d} (t_d - o_d) x_{id}$$

perceptron Δw

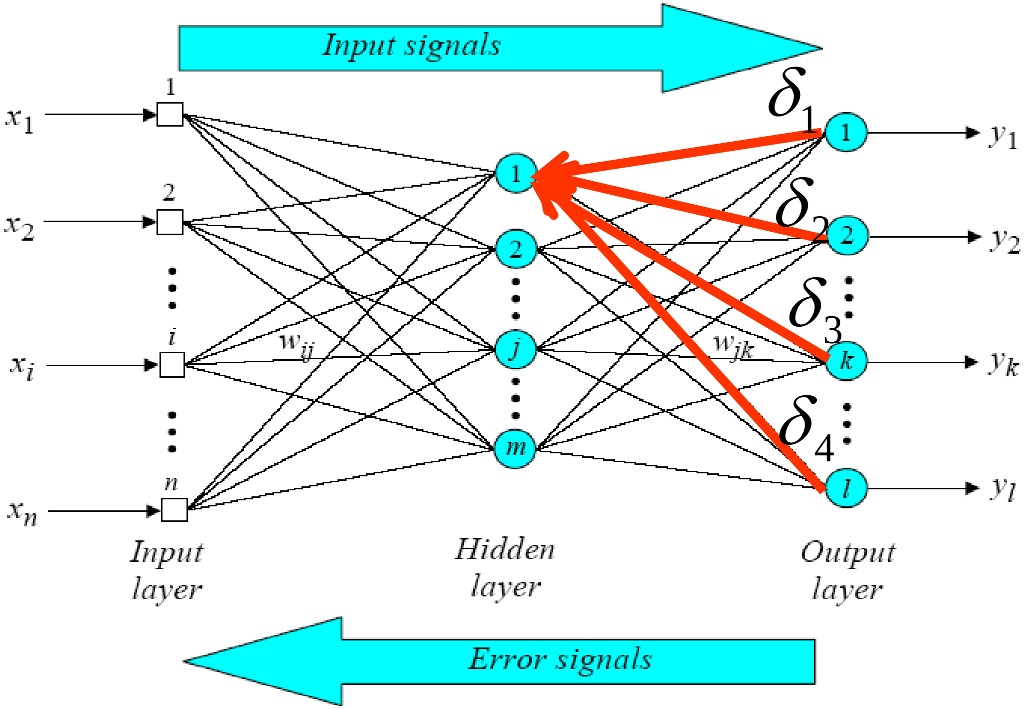
- The only difference is the partial derivative of the sigmoid activation function (we assumed linear activation → derivative =1)

Learning: Hidden Layer Weights

- We define the error term for the output *k*: $\delta_k = (t_k - o_k)\dfrac{\partial\sigma(net_k)}{\partial net_k}$

•Reminder: $\Delta w_{kj} = \eta(t_k - o_k)x_{kj}\dfrac{\partial\sigma(net_k)}{\partial net_k}$

Note that *j*→*k*, *i* →*j*, *i.e.*
j: hidden unit
k: output unit



- The error term for hidden unit *j* is:

$$\delta_j = \sum_{k=outputNeuronsConnectedToj} \delta_k w_{kj} \frac{\partial\sigma(net_j)}{\partial net_j}$$

Learning: Hidden Layer Weights

- We define the error term for the output *k*: $\delta_k = (t_k - o_k)\dfrac{\partial\sigma(net_k)}{\partial net_k}$
- Reminder: $\Delta w_{ki} = \eta(t_k - o_k)x_{ki}\dfrac{\partial\sigma(net_k)}{\partial net_k} = \eta\delta_k x_{ki}$

- x is the input to output unit *k* from hidden unit *i*

- Similarly the update rule for weights in the input layer is

$$\Delta w_{ji} = \eta\delta_j x_{ji}$$

$$\delta_j = \sum_{k=outputNeuronsConnectedToj} \delta_k w_{kj} \frac{\partial\sigma(net_j)}{\partial net_j}$$

- x is the input to hidden unit *j* from input unit *i*

Example

- http://galaxy.agh.edu.pl/~vlsi/AI/backp_t_en/backprop.html

Learning: Backpropagation Algorithm

- Finally for all training examples D

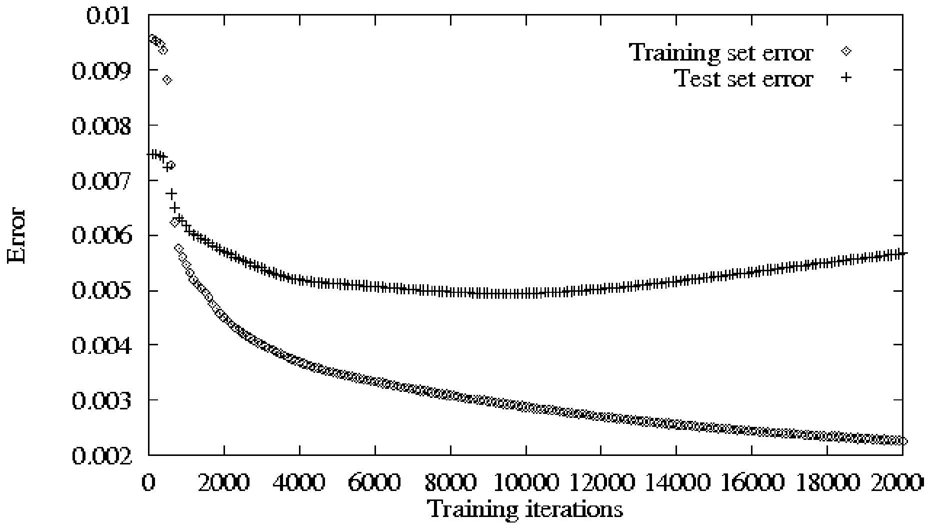
$$\Delta w_i^{for\ all\ examples} = \sum_{d=1}^{D} \Delta w_i$$

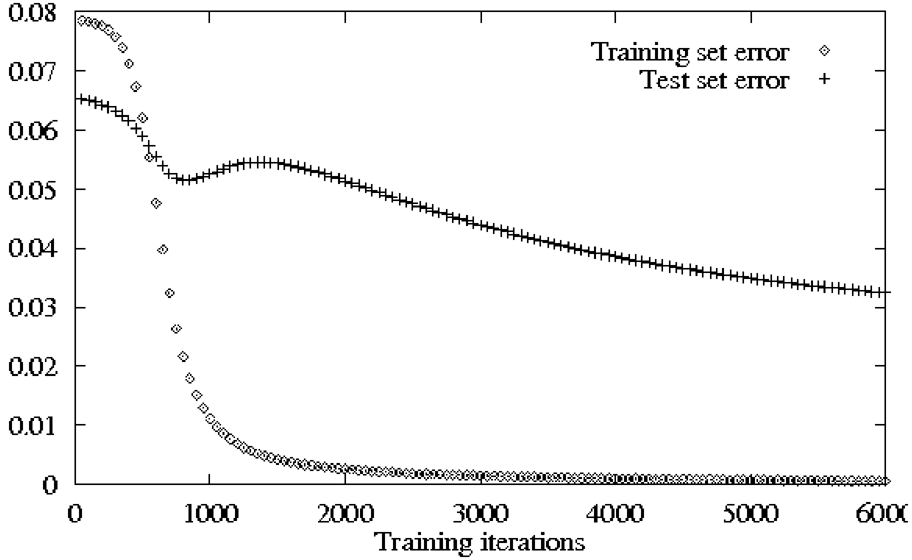
- This is called batch training because the weights are updated after all training examples have been presented to the network (=epoch)
- Matlab function: **traingd**
- Incremental training: weights are updated after each training example is presented

Backpropagation Stopping Criteria

- When the gradient magnitude (or Δw_i) is small, i.e. $\frac{\partial E}{\partial w_i} < \delta \; or \; \Delta w_i < \delta$
- When the maximum number of epochs has been reached
- When the error on the validation set increases for *n* consecutive times (this implies that we monitor the error on the validation set). This is called early stopping.

Early stopping





- Stop when the error in the validation set increases (but not too soon!)
- Error might decrease in the training set but increase in the ‘validation’ set (overfitting!)
- It is also a way to avoid overfitting.

Backpropagation Summary

1. Initialise weights randomly
2. For each input training example *x* compute the outputs (forward pass)
3. Compute the output neurons errors and then compute the update rule for output layer weights (backward pass)

$$\Delta w_{ki} = \eta \delta_k x_{ki}$$

4. Compute hidden neurons errors and then compute the update rule for hidden layer weights (backward pass)

$$\Delta w_{ji} = \eta \delta_j x_{ji}$$

Backpropagation Summary

5. Compute the sum of all Δw, once all training examples have been presented to the network

6. Update weights $w_i \leftarrow w_i + \Delta w_i$

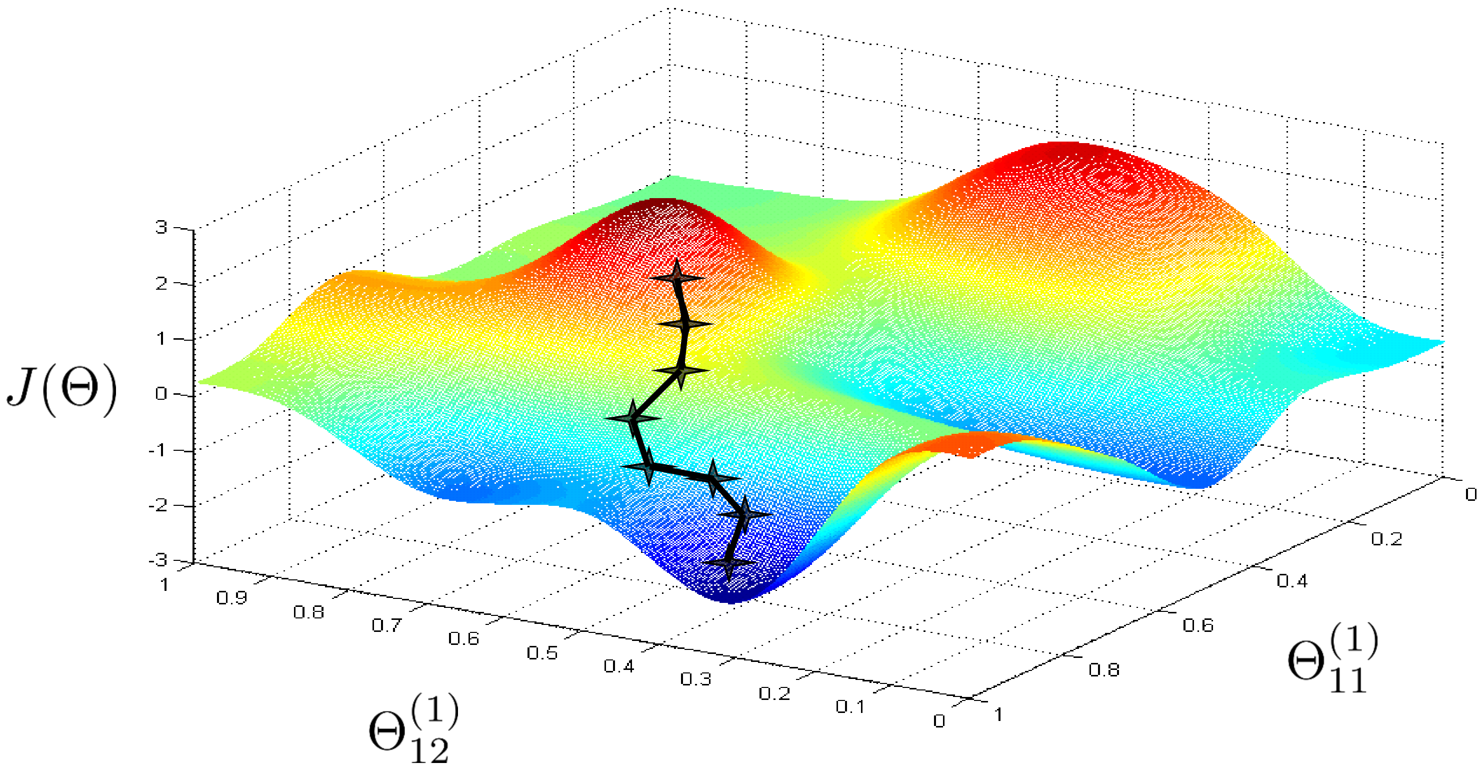
7. Repeat steps 2-6 until the stopping criterion is met

Backpropagation: Convergence

- Converges to a local minimum of the error function
  - … can be retrained a number of times
- Minimises the error over the training examples
  - …will it generalise well over unknown examples?

- Training requires thousands of iterations (slow)
  - … but once trained it can rapidly evaluate output

Backpropagation: Error Surface

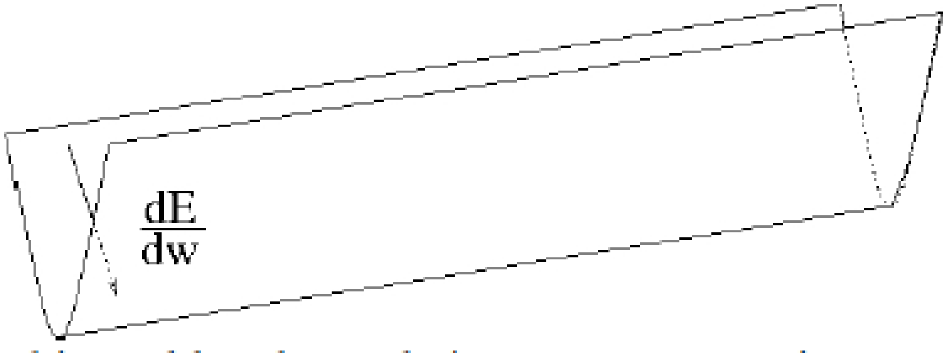


Backpropagation with momentum

- Standard backpropagation

$$w_i \leftarrow w_i + \Delta w_i \quad \Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$

- If the error surface is a long and narrow valley, gradient descent goes quickly down the valley walls, but very slowly along the valley floor.



From https://www.cs.toronto.edu/~hinton/csc2515/notes/lec6tutorial.pdf

Backpropagation with momentum

- Standard backpropagation

$$w_i \leftarrow w_i + \Delta w_i \quad \Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$

- Backpropagation with momentum

$$\Delta w_i = \mu \, \Delta w_{i-1} + (1-\mu)\left(-\eta \frac{\partial E}{\partial w_i}\right)$$

- $\mu = \text{momentum constant, usually } 0.9, 0.95$
- It is like giving momentum to the weights
- We do not take into account only the local gradient but also recent trends in the error surface
- Matlab function: **traingdm**

Backpropagation with adaptive learning rate

- It is good that the learning rate is not fixed during training

$$w_i \leftarrow w_i + \Delta w_i \quad \Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$

- Simple heuristic

1. If error decreases, increase learning rate: $\eta = \eta * \eta_{inc}$
2. If error increases, decrease learning rate and don't update the weights: $\eta = \eta * \eta_{dec}$

- Typical values for $\eta_{inc} = 1.05, 1.1$
- Typical values for $\eta_{dec} = 0.5, 0.7$
- Matlab function: **traingda**

Resilient Backpropagation

- The weight change depends on the learning rate and the value of the partial derivative. We have no control over the partial derivative.

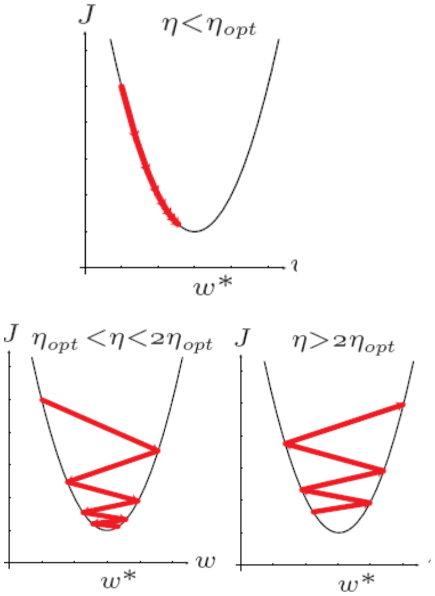
- The effect of the learning rate can be disturbed by the unforeseeable behaviour of the derivative.

- Resilient backpropagation uses only the sign of the derivative!!

- For each weight w_i we define an individual update value Δ_i which depends only on the sign of the derivative and ignores its actual value

Resilient Backpropagation

$$\Delta_i(t) = \begin{cases} \Delta^{inc} * \Delta_i(t-1) \;\; if \;\; \dfrac{\partial E^{t-1}}{\partial w_i} * \dfrac{\partial E^{t}}{\partial w_i} > 0 \\ \\ \Delta^{dec} * \Delta_i(t-1) \;\; if \;\; \dfrac{\partial E^{t-1}}{\partial w_i} * \dfrac{\partial E^{t}}{\partial w_i} < 0 \end{cases}$$

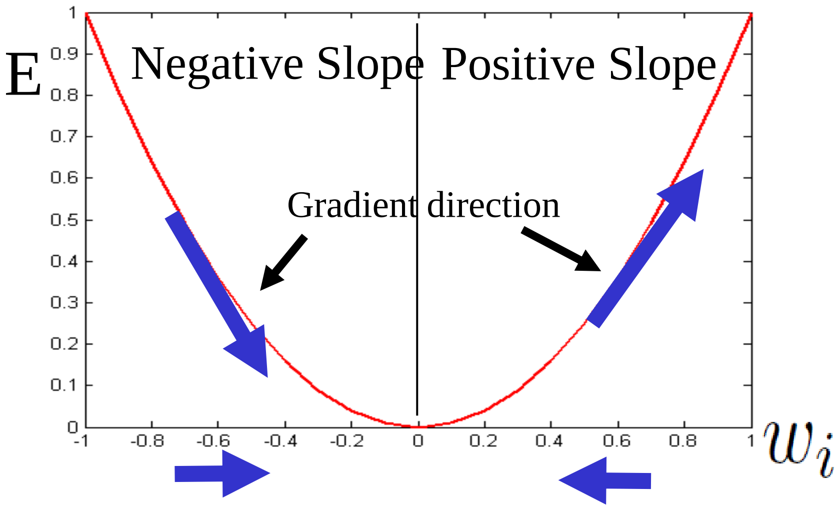


- Every time the partial derivative changes its sign, i.e., last update was too big, the update value is decreased.

- If the derivative retains its sign, the update value is increased in order to accelerate convergence.

Resilient Backpropagation

$$\Delta w_i(t) = \begin{cases} -\Delta_i(t) \ \ if \ \ \dfrac{\partial E^t}{\partial w_i} > 0 \\ \Delta_i(t) \ \ if \ \ \dfrac{\partial E^t}{\partial w_i} < 0 \end{cases}$$



- We also need to initialise the update values Δ_i
- We usually define an upper limit for Δ_i
- Typical values for $\Delta_{inc} = 1.2$
- Typical values for $\Delta_{dec} = 0.5$
- Matlab function: **trainrp**

Parameters / Weights

- Parameters are what the user specifies, e.g. number of hidden neurons, learning rate, number of epochs etc
- They need to be optimised
- Weights are the weights of the network
- They are also parameters but they are optimised automatically via gradient descent

Ways to avoid overfitting

- Early stopping (see slide 52)

- Regularisation

  - Penalise large weights, keep the weights small

$$E = \gamma\left(\frac{1}{2}\sum_{d=1}^{D}(t_d - o_d)^2\right) + (1-\gamma)\left(\frac{1}{2}\sum_{i=1}^{noWeights}(w_i)^2\right)$$

Vanishing/Exploding gradient

$$\Delta w_{ji} = \eta \delta_j x_{ji}$$

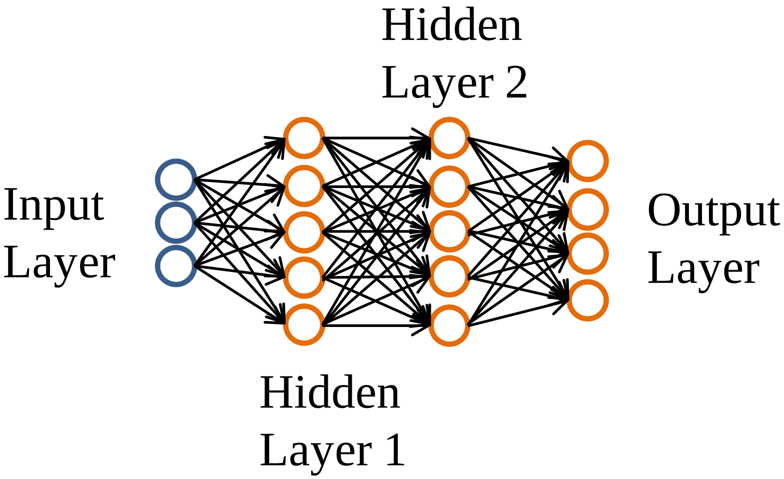
$$\delta_j = \sum_{k=outputNeuronsConnectedToj} \delta_k w_{kj} \frac{\partial \sigma(net_j)}{\partial net_j}$$

- As we backpropagate through many layers:

1. If the weights are small -> δ_i shrink exponentially
2. If the weights are big -> δ_i grow exponentially

- So either the network stops learning (case 1) or becomes unstable (case 2)
- That is why it is not possible to train deep networks with backpropagation

Deep NNs



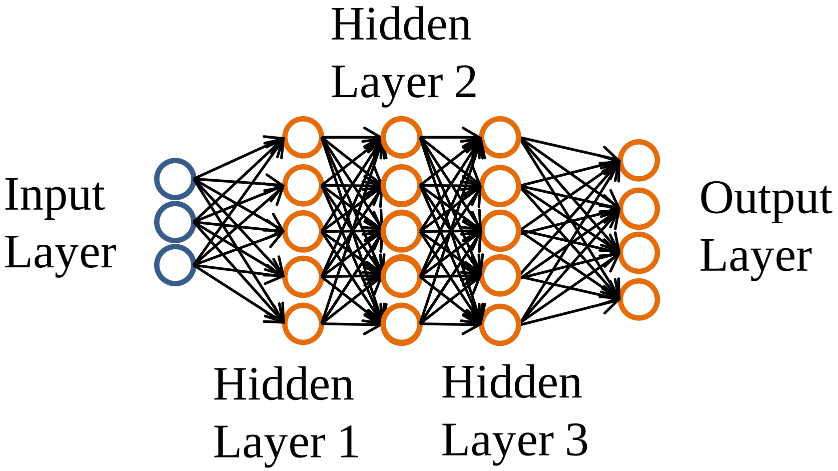
Hidden Layer 2

Input Layer

Output Layer

Hidden Layer 1

3-layer feed-forward network



Hidden Layer 2

Input Layer

Output Layer

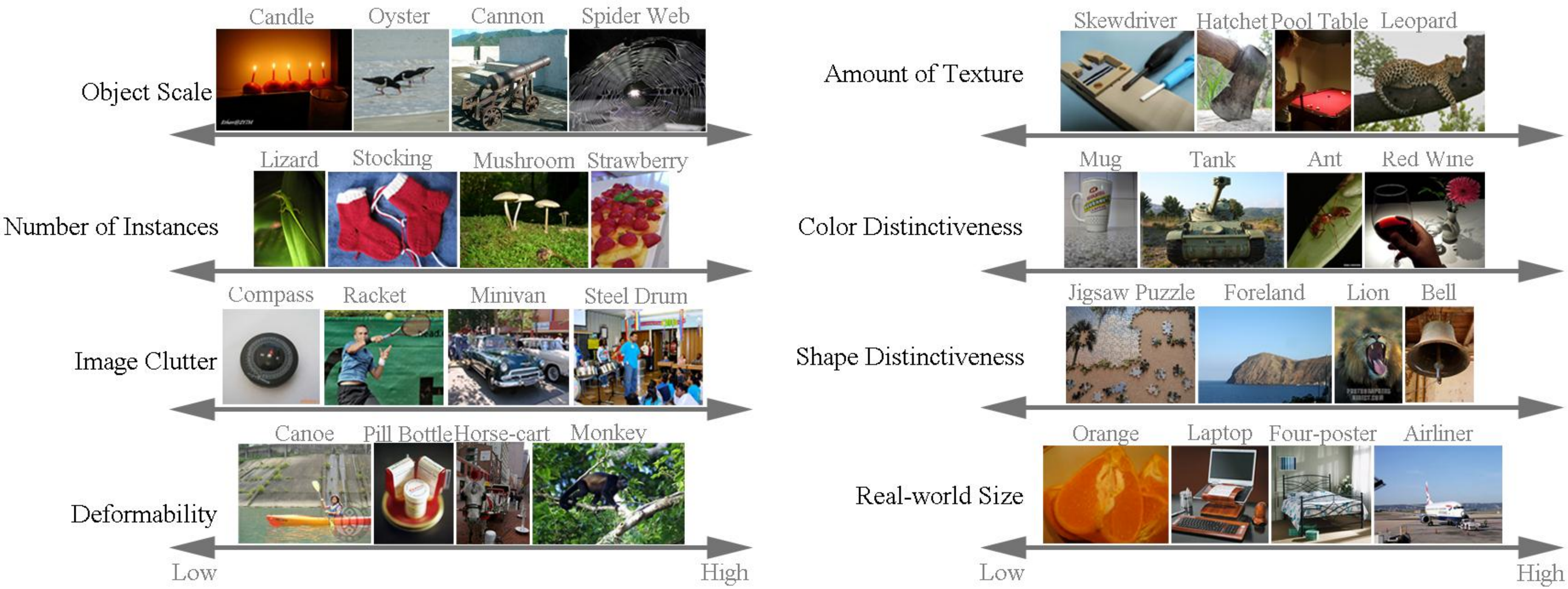
Hidden Layer 1

Hidden Layer 3

4-layer feed-forward network

- There is a pre-training phase where weights are initialised to a good starting point.
- Pre-training is performed per layer using Restricted Boltzman Machines
- Then backpropagation is used to fine-tune the weights starting from a good initialisation point.

ImageNet Competition – Object Classification



- Classification of 1000+ objects
- State-of-the-art before 2012: ~26%
- New state-of-the-art in 2012 with deep networks: ~15%

Deep NNs Applications

- Deep Face by Facebook – State of the art in Face verification

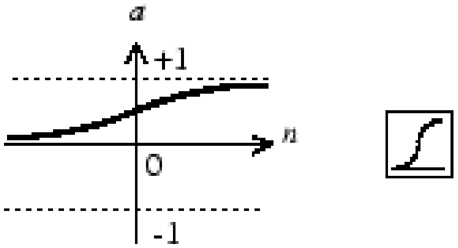
  - DeepFace: Closing the Gap to Human-Level Performance in Face Verification, Taigman, Ming, Ranzato, Wolf

- State-of-the-art performance in Speech Recognition

  - Microsoft has done a lot of research on this topic

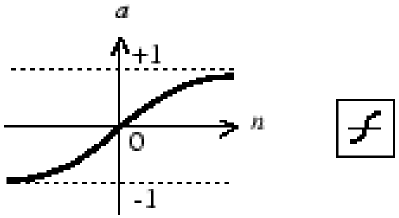
Practical Suggestions: Activation Functions

- Continuous, smooth (essential for backpropagation)
- Nonlinear
- Saturates, i.e. has a min and max value
- Monotonic (if not then additional local minima can be introduced)
- Sigmoids are good candidate (log-sig, tan-sig)



$a = logsig(n)$

Log-Sigmoid Transfer Function

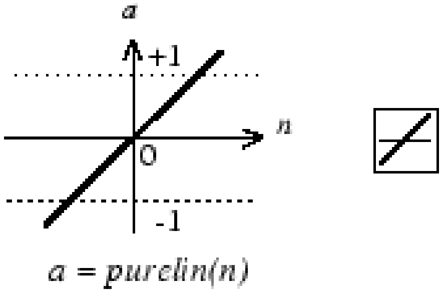


$a = tansig(n)$

Tan-Sigmoid Transfer Function

Practical Suggestions: Activation Functions

- In case of regression then output layer should have linear activation functions



Linear Transfer Function

Practical Suggestions: Scaling Inputs

- It is not desirable that some inputs are orders of magnitude larger than other inputs

- Map each input *x(i)* to [-1, +1] using this formula

$$\mathrm{y} = 2\frac{x - x_{min}}{x_{max} - x_{min}} - 1$$

- Matlab function: ***mapminmax***

  - Rows: features, columns: examples

  - Normalises each row

Practical Suggestions: Scaling Inputs

- Standardize inputs to mean=0 and 1 std. dev.=1

  $$y = \frac{x - x_{mean}}{x_{std}}$$

- Matlab function: ***mapstd***

- Scaling is needed if inputs take very different values. If e.g., they are in the range [-3, 3] then scaling is probably not needed

Practical Suggestions: Scaling Inputs

- The scaling values, x_{min}, x_{max} , $x_{mean,}$ x_{std} are computed on the training set and then applied to the validation and test sets.

- It is not correct to scale each set separately.

Practical Suggestions: Scaling Inputs

- Matlab automatically scales the inputs to [-1, 1] and removes the inputs/outputs that are constant.
- Think if you wish to scale the inputs, if not you should disable the automatic scaling
- Check *http://www.mathworks.co.uk/help/nnet/ug/choose-neural-network-input-output-processing-functions.html*

Practical Suggestions: Target Values

- Binary Classification

  - Target Values : -1/0 (negative) and 1 (positive)

  - 0 for log-sigmoid, -1 for tan-sigmoid

- Multiclass Classification

  - [0,0,1,0] or [-1, -1, 1, -1]

  - 0 for log-sigmoid, -1 for tan-sigmoid

- Regression

  Target values: continuous values [-inf, +inf]

Practical Suggestions: Number of Hidden Layers

- Networks with many hidden layers are prone to overfitting and they are also harder to train

- For most problems one hidden layer should be enough

- 2 hidden layers can sometimes lead to improvement

Division of data

- Matlab automatically divides the dataset into training/validation/test sets.

- You should force matlab to use an empty test set (you have your own) and use the same validation set as yours.
- You can provide the indices of your validation set and your test set (=empty array)

- Check *http://www.mathworks.co.uk/help/nnet/ug/divide-data-for-optimal-neural-network-training.html*

Matlab Examples

- Create feedforward network

  - net = feedforwardnet(hiddenSizes,trainFcn)

  - hiddenSizes = [10, 10, 10] – 3 layer network with 10 hidden neurons in each layer

  - trainFcn = ‘trainlm’, ‘traingdm’, ‘trainrp’ etc

- Configure (set number of input/output neurons)

  - net = configure(net,x,t)

  - x: input data, noFeatures x noExamples

  - t: target data, noClasses x noEx

Matlab Examples

- Train network
  - [net,tr] = train(net,P,T)
  - P: input data
  - T: target data
- Simulate network
  - [Y,Pf,Af,E,perf] = sim(net,P)

Matlab Examples

- Batch training: Train
- Stochastic/Incremental Training: Adapt
- Use Train for the CBC