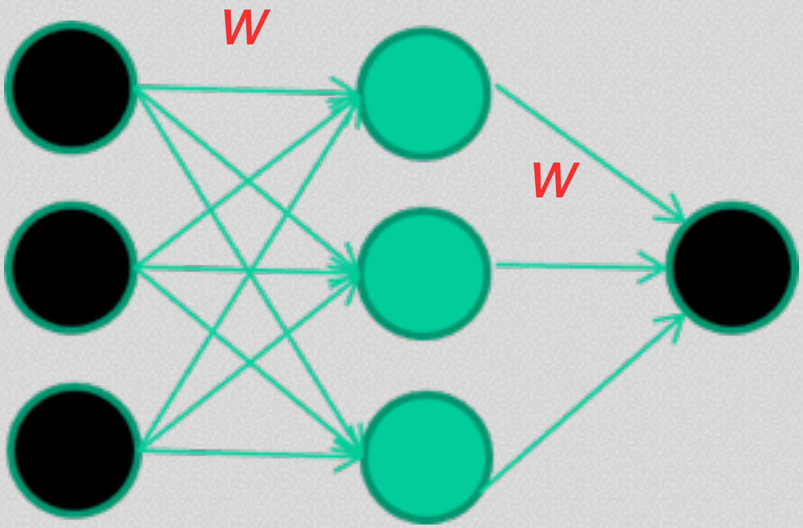
Multilayer Percetrons

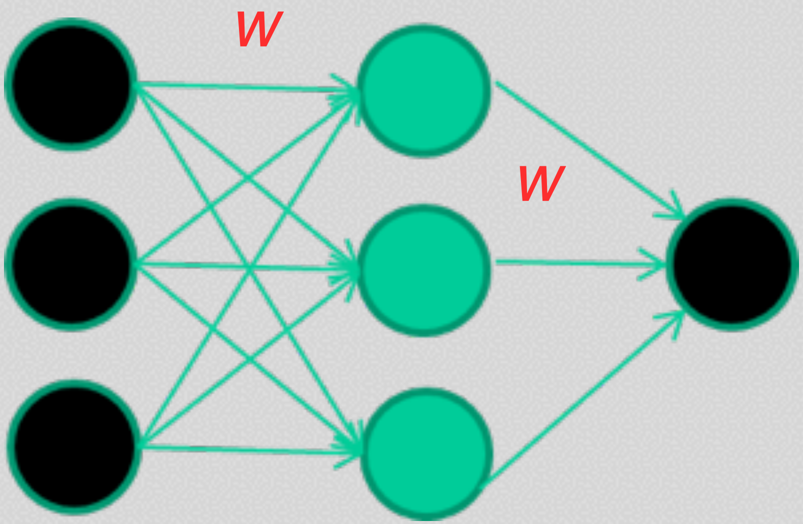
A dataset

Fields			***class***
2.5	3.8	2.0	0
4.9	4.5	4.3	0
7.5	3.9	2.8	1
3.6	1.2	1.3	0
etc …			



Training the neural network

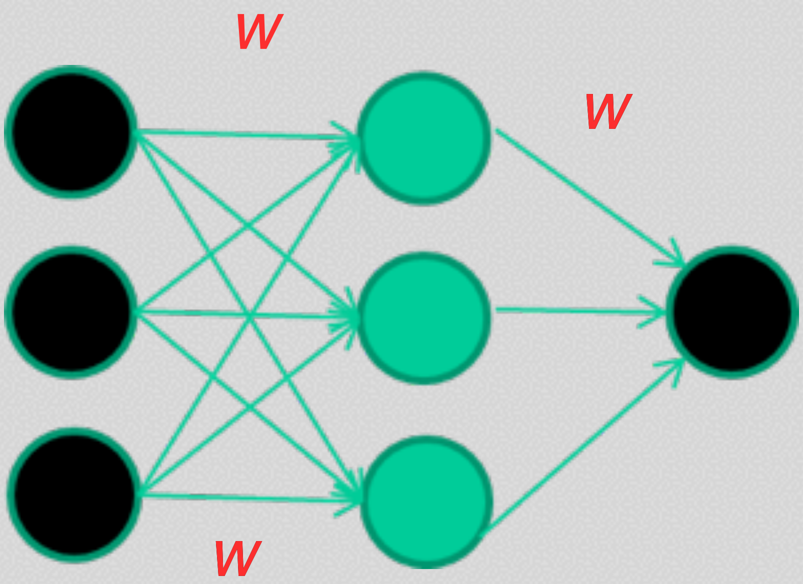
Fields			***class***
2.5	3.8	2.0	0
4.9	4.5	4.3	0
7.5	3.8	2.8	1
3.6	1.2	1.3	0
etc …			



Training the neural network

Fields			***class***
2.5	3.8	2.0	0
4.9	4.5	4.3	0
7.5	3.8	2.8	1
3.6	1.2	1.3	0
etc …			

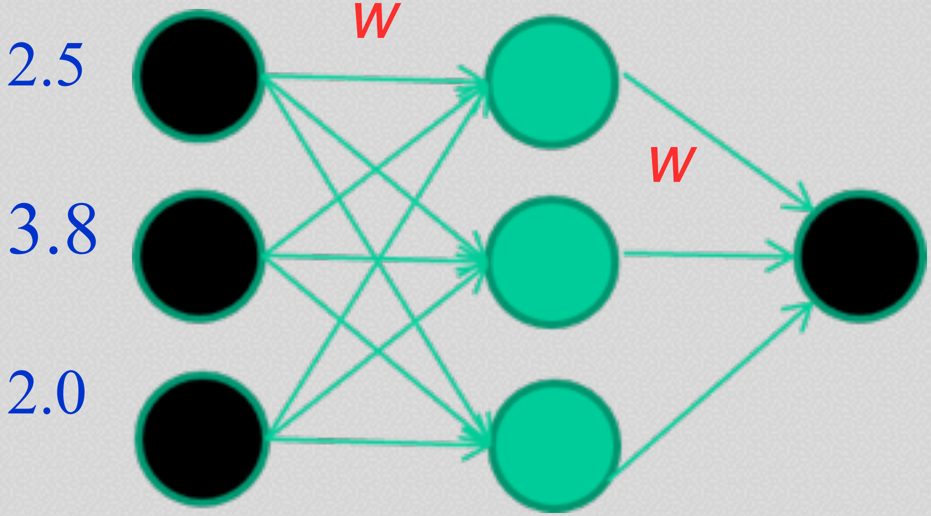
Initialise with random weights



Training the neural network

Fields			***class***
2.5	3.8	2.0	0
4.9	4.5	4.3	0
7.5	3.8	2.8	1
3.6	1.2	1.3	0
etc …			

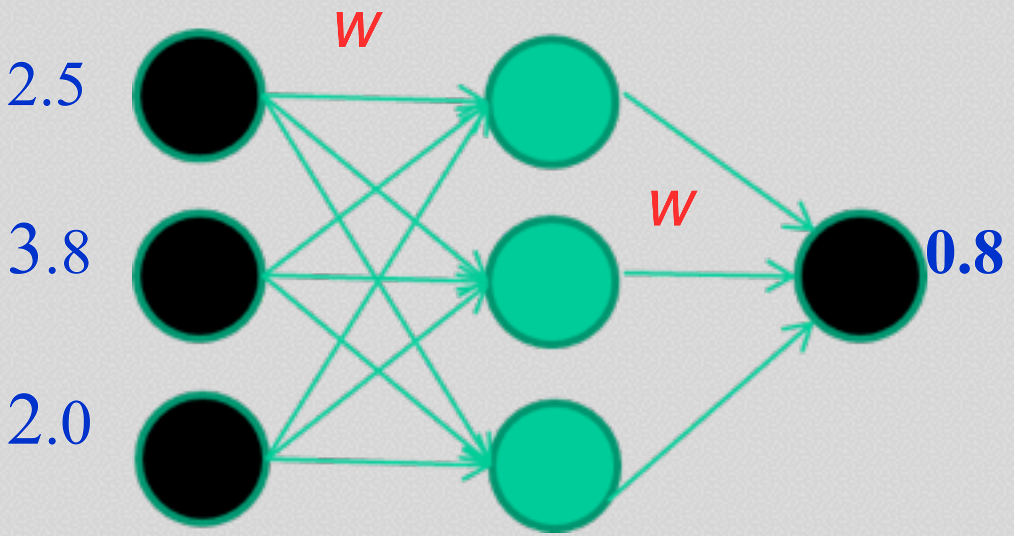
Input the training pattern



Training the neural network

Fields			***class***
2.5	3.8	2.0	0
4.9	4.5	4.3	0
7.5	3.8	2.8	1
3.6	1.2	1.3	0
etc …			

Feed it through to get output

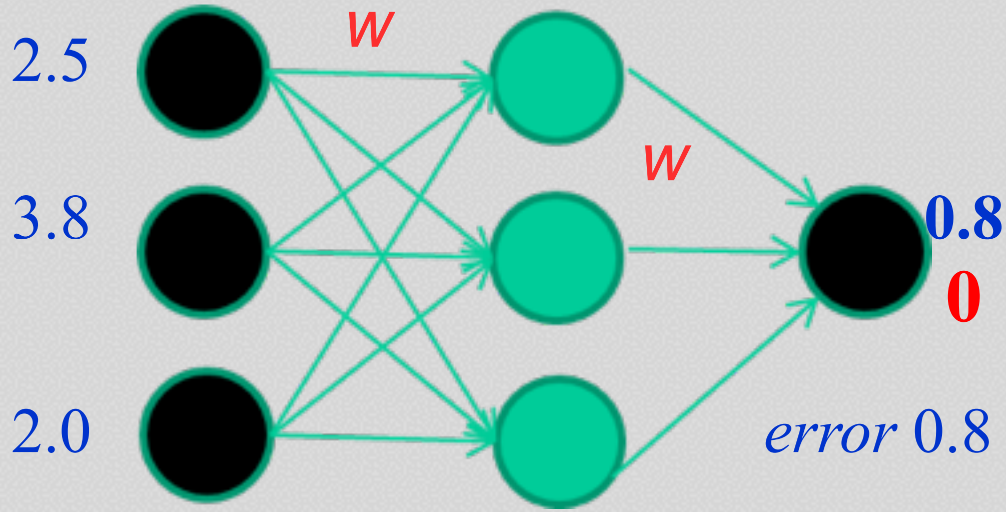


Training the neural network

Fields			***class***
2.5	3.8	2.0	0
4.9	4.5	4.3	0
7.5	3.8	2.8	1
3.6	1.2	1.3	0

etc …

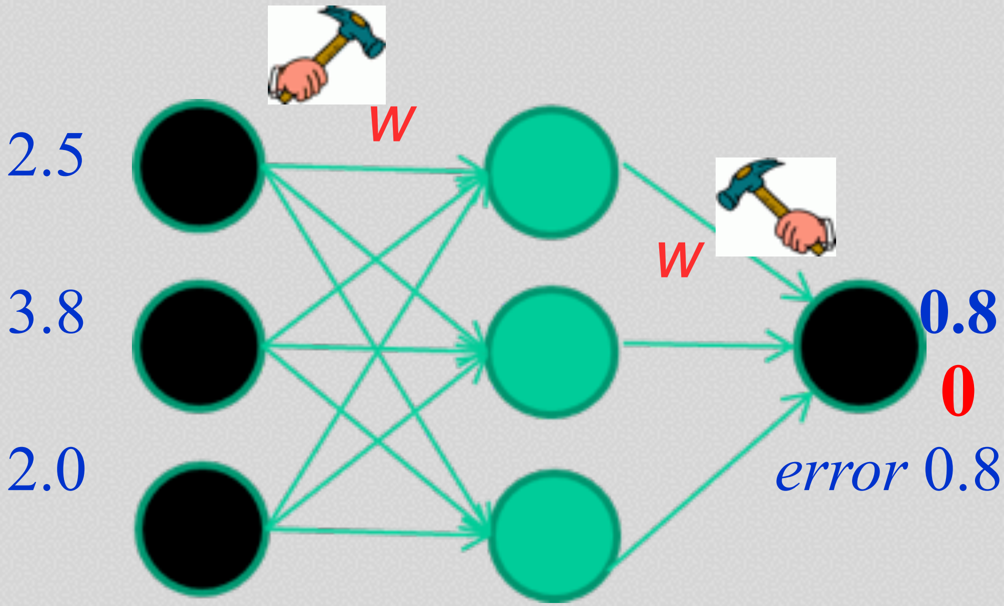
Compare with target output



Training the neural network

Fields			***class***
2.5	3.8	2.0	0
4.9	4.5	4.3	0
7.5	3.8	2.8	1
3.6	1.2	1.3	0
etc …			

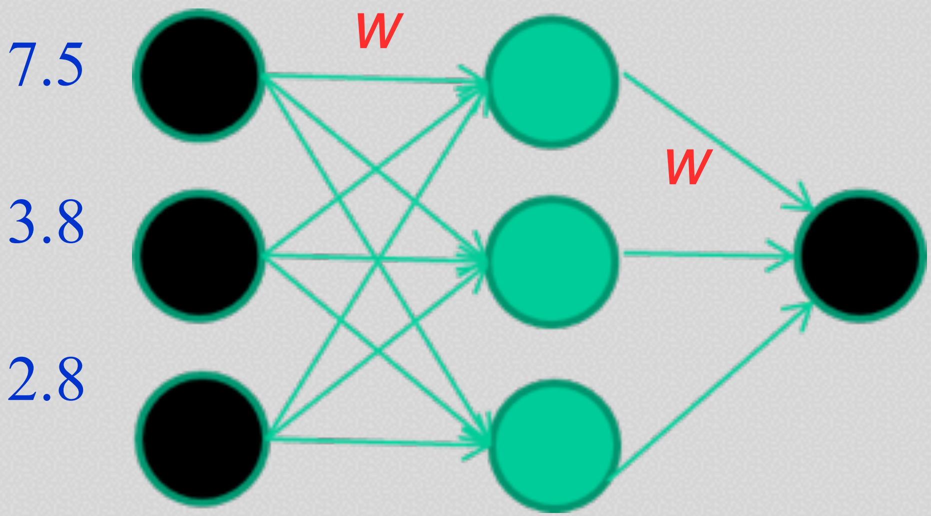
Adjust weights based on error



Training the neural network

Fields			***class***
2.5	3.8	2.0	0
4.9	4.5	4.3	0
7.5	3.8	2.8	1
3.6	1.2	1.3	0
etc …			

Present a training pattern

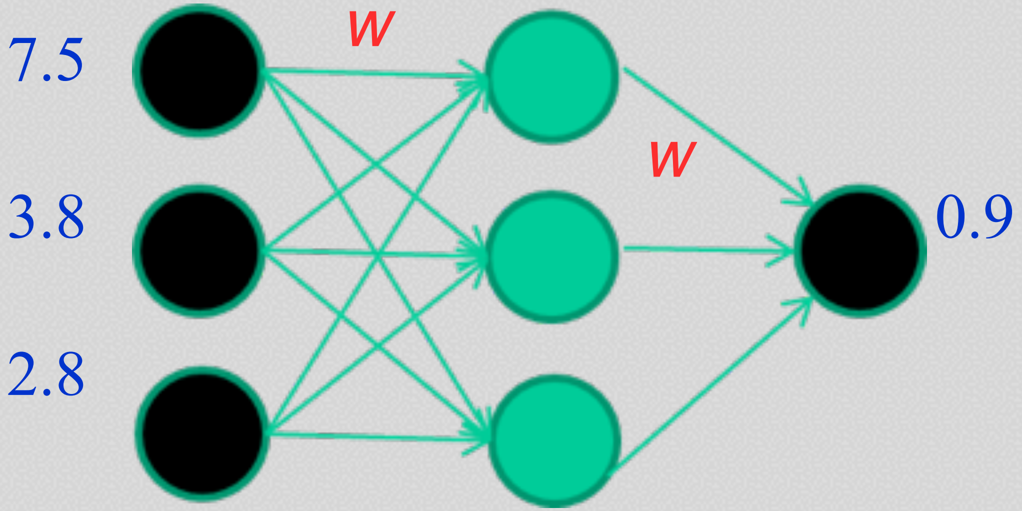


Training the neural network

Fields			***class***
2.5	3.8	2.0	0
4.9	4.5	4.3	0
7.5	3.8	2.8	1
3.6	1.2	1.3	0

etc …

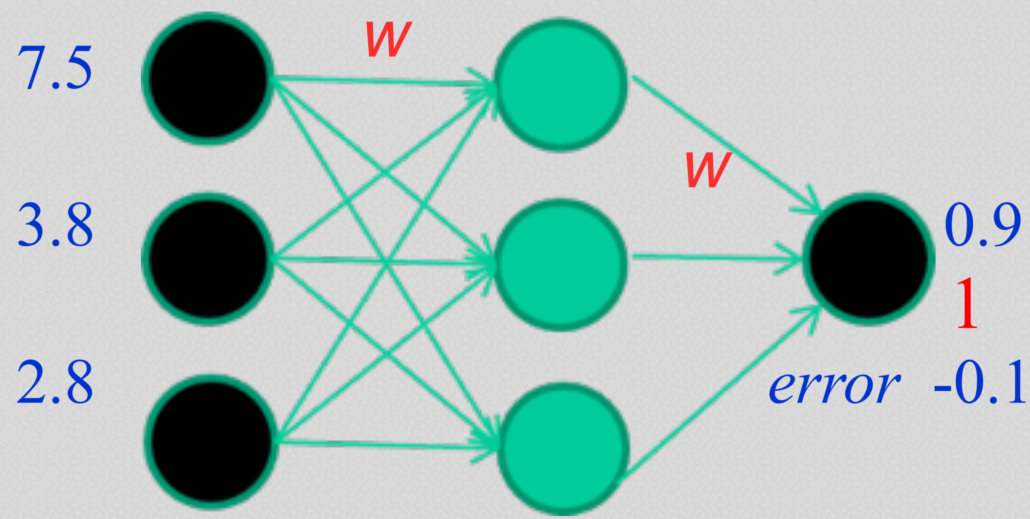
Feed it through to get output



Training the neural network

Fields			***class***
2.5	3.8	2.0	0
4.9	4.5	4.3	0
7.5	3.8	2.8	1
3.6	1.2	1.3	0
etc …			

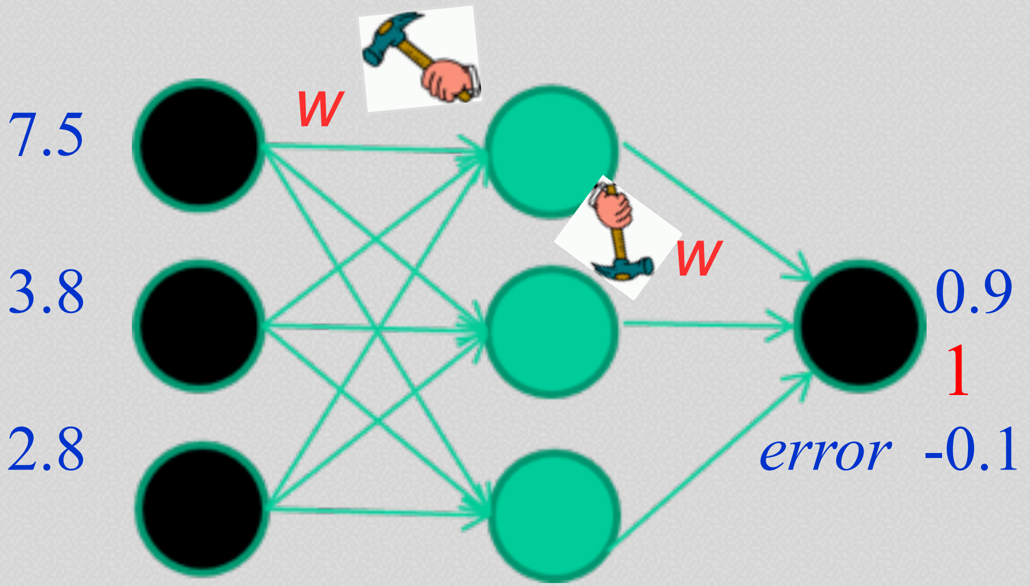
Compare with target output



Training the neural network

Fields			***class***
2.5	3.8	2.0	0
4.9	4.5	4.3	0
7.5	3.8	2.8	1
3.6	1.2	1.3	0
etc …			

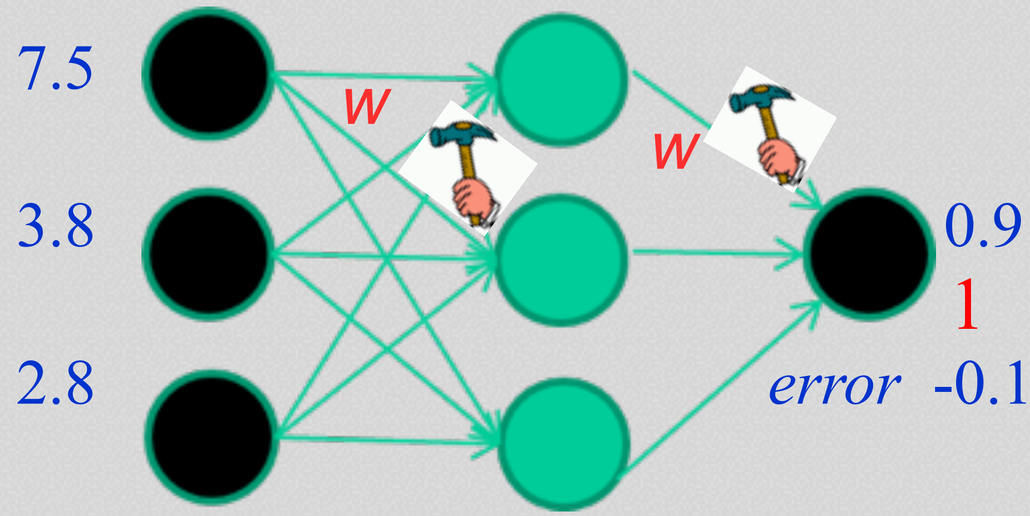
Adjust weights based on error



Training the neural network

Fields			***class***
2.5	3.8	2.0	0
4.9	4.5	4.3	0
7.5	3.8	2.8	1
3.6	1.2	1.3	0
etc …			

And so on ….

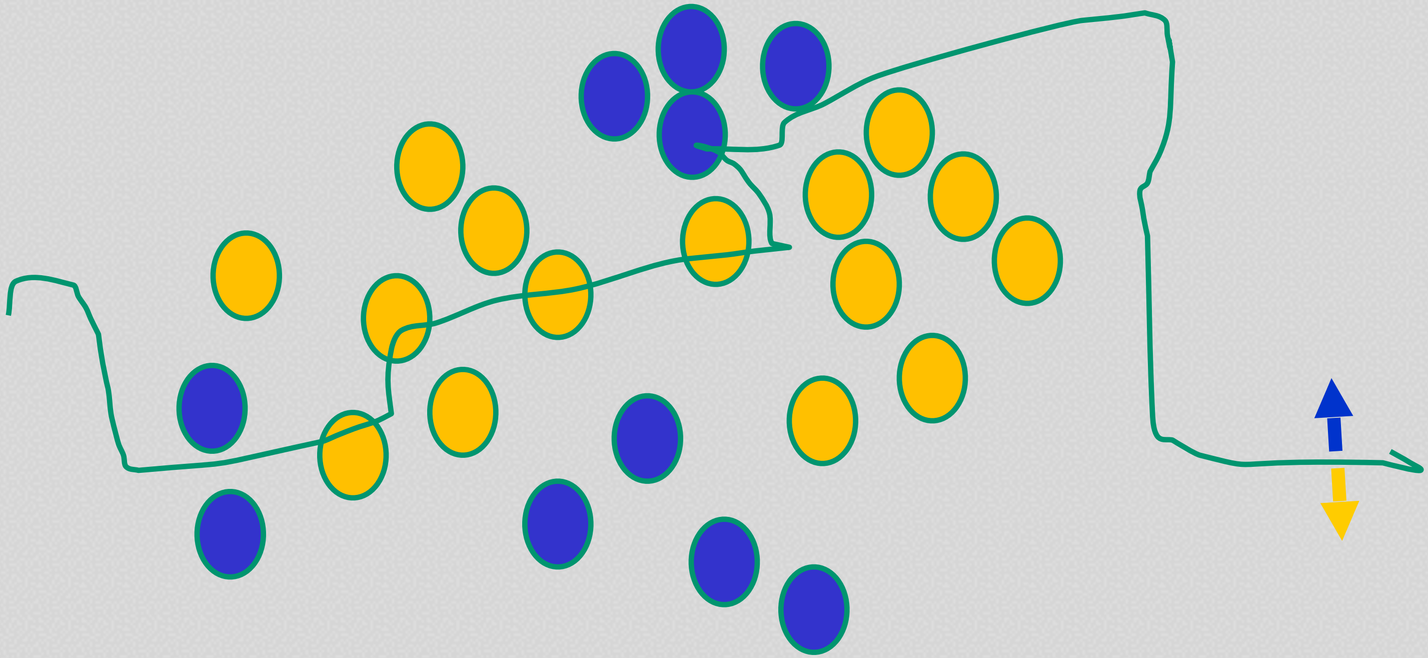


Repeat this thousands, maybe millions of times – each time taking a random training instance, and making slight weight adjustments

Algorithms for weight adjustment are designed to make changes that will reduce the error

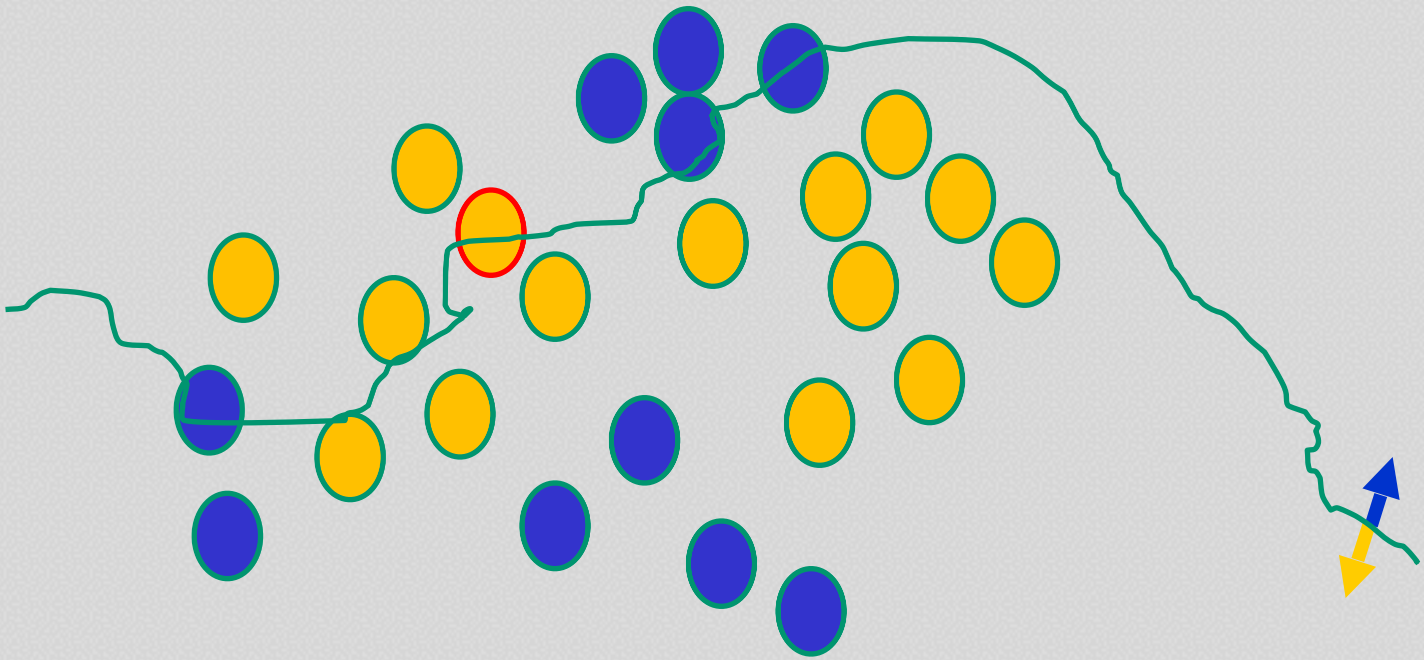
The decision boundary perspective…

Initial random weights



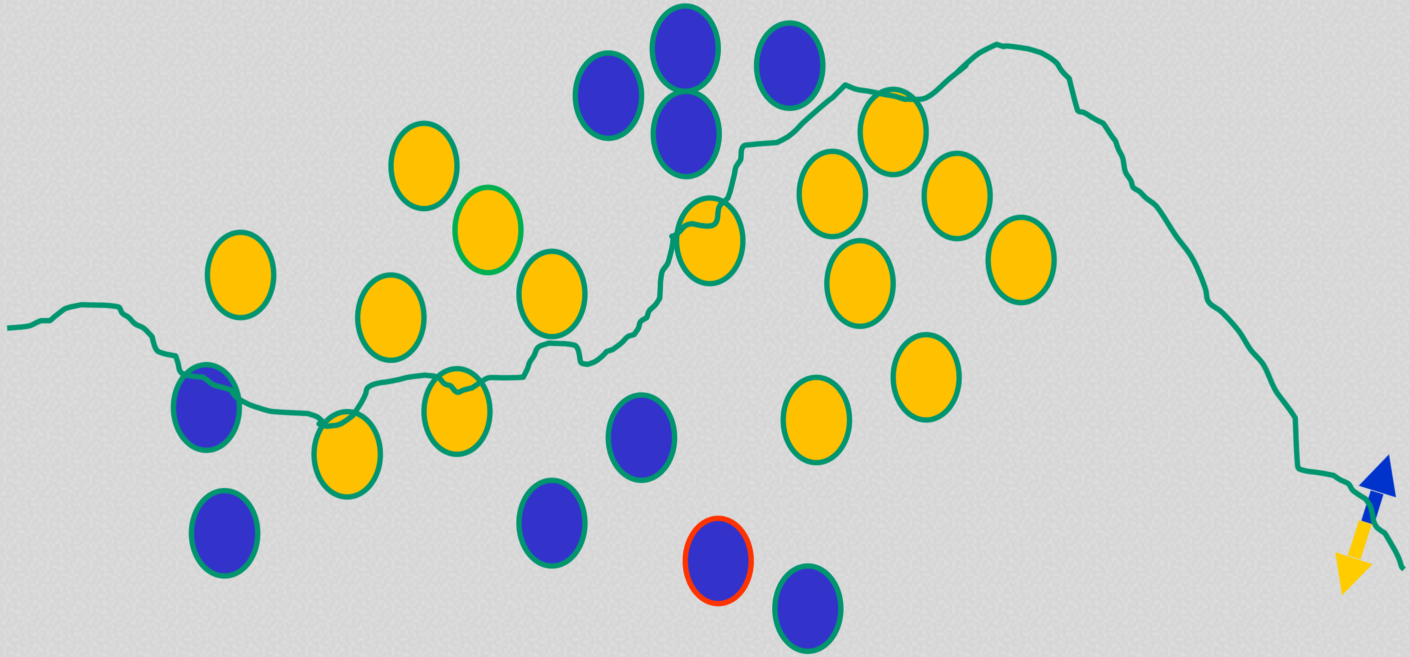
The decision boundary perspective…

Present a training instance / adjust the weights



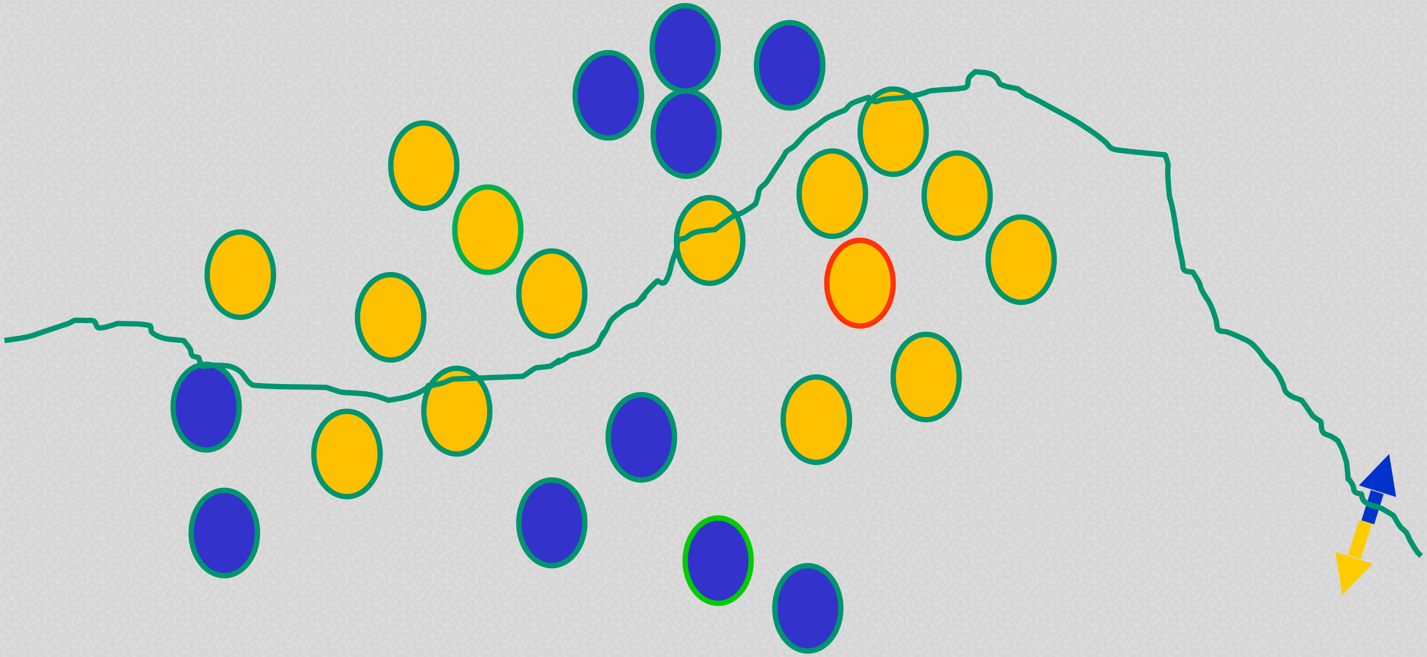
The decision boundary perspective…

Present a training instance / adjust the weights



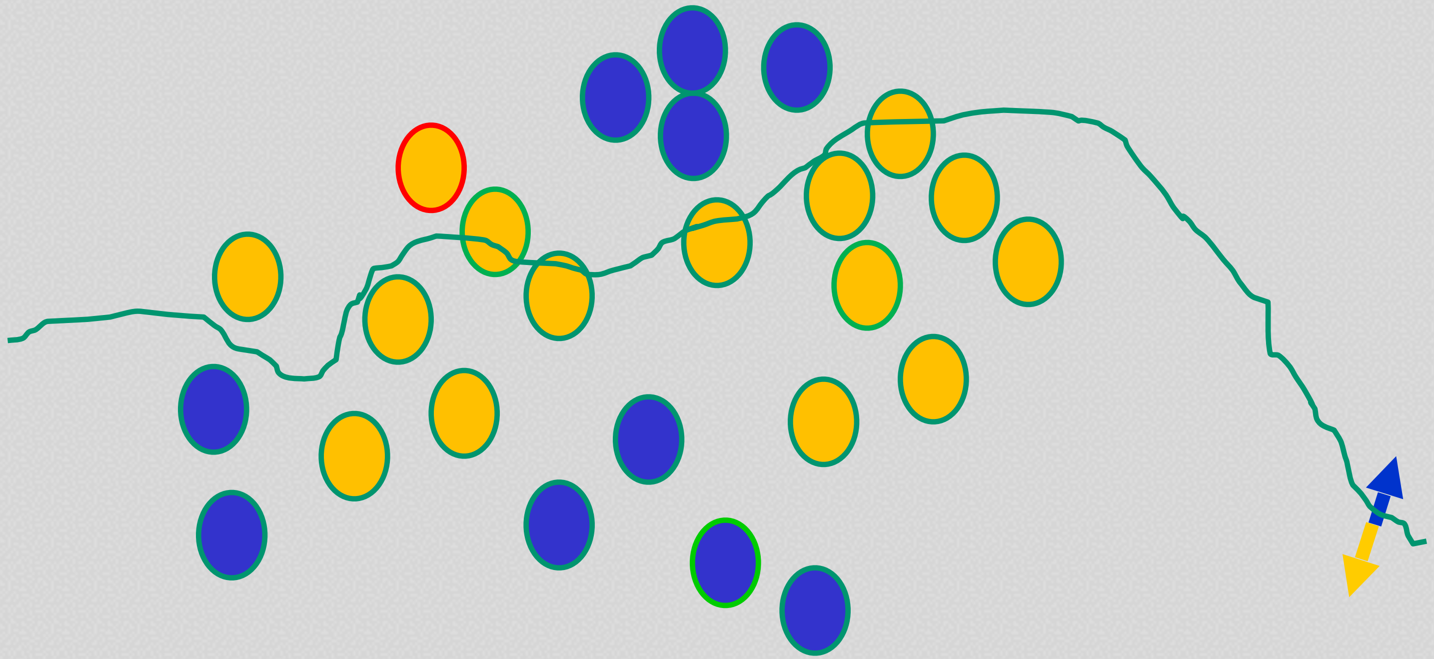
The decision boundary perspective…

Present a training instance / adjust the weights



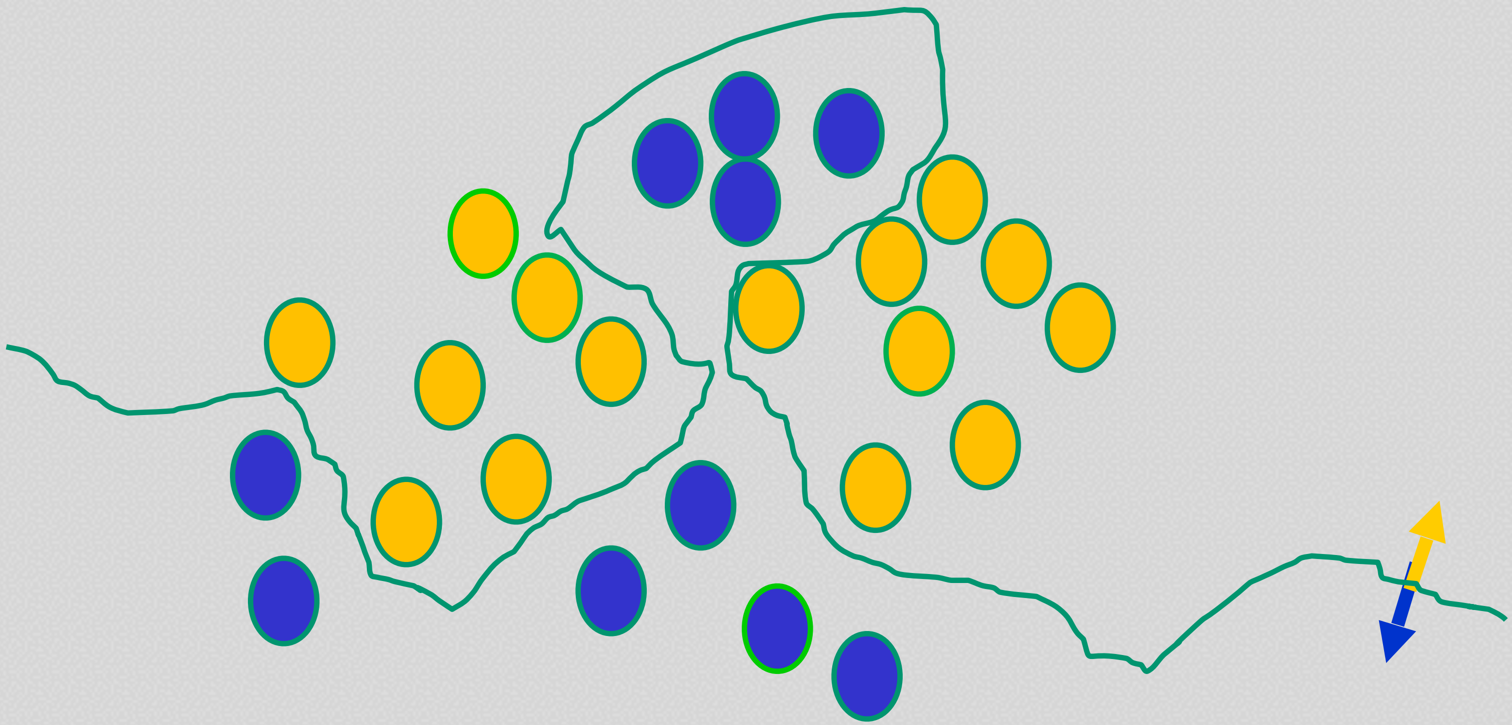
The decision boundary perspective…

Present a training instance / adjust the weights



The decision boundary perspective…

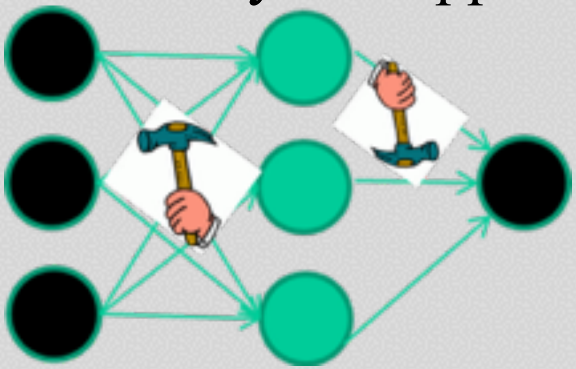
Eventually ….



Learning Algo.,

- weight-learning algorithms for NNs
- They work by making thousands and thousands of tiny adjustments, each making the network do better at the most recent pattern, but perhaps a little worse on many others
- But, by dumb luck, eventually this tends to be good enough to

learn effective classifiers for many real applications



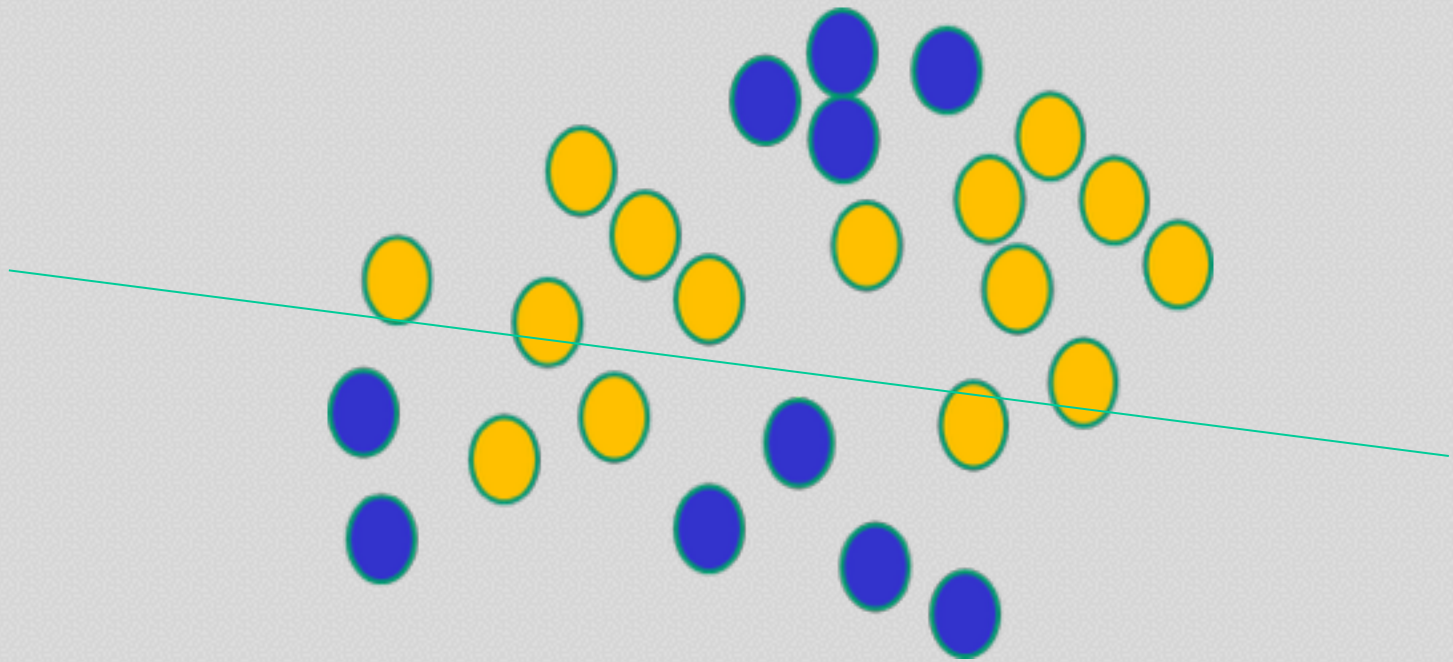
Some other points

Detail of a standard NN weight learning algorithm

If $f(x)$ is non-linear, a network with 1 hidden layer can, in theory, learn perfectly any classification problem. A set of weights exists that can produce the targets from the inputs. The problem is finding them.

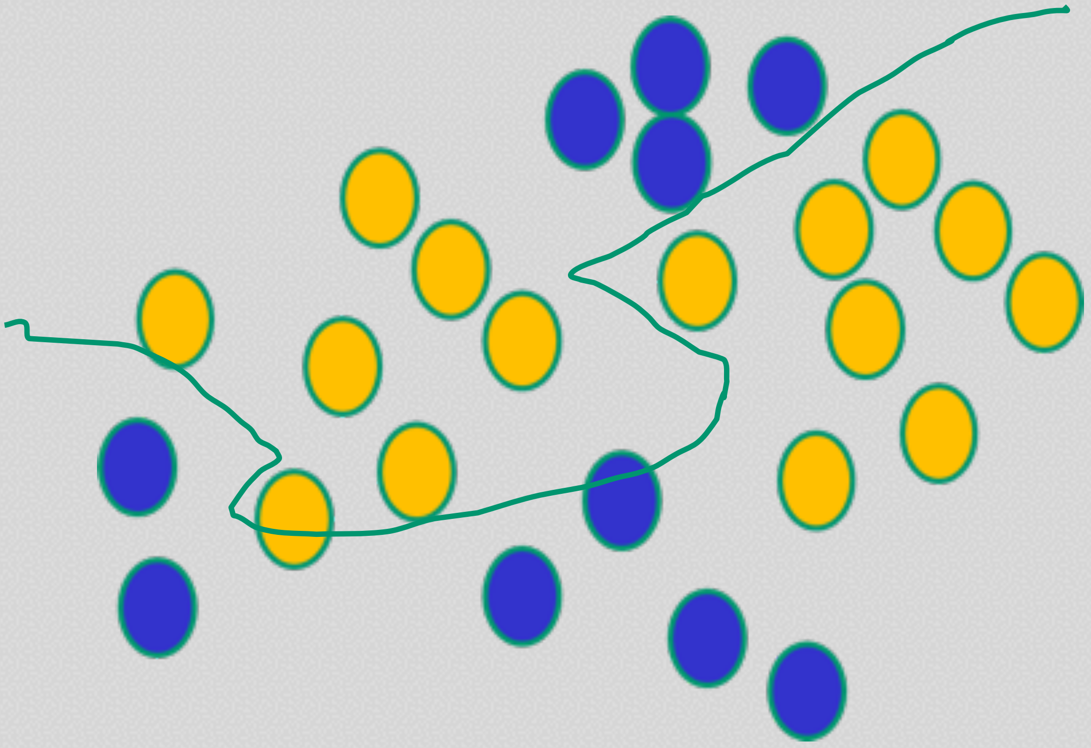
Some other 'by the way' points

If $f(x)$ is linear, the NN can **only** draw straight decision boundaries (even if there are many layers of units)



Some other ‘by the way’ points

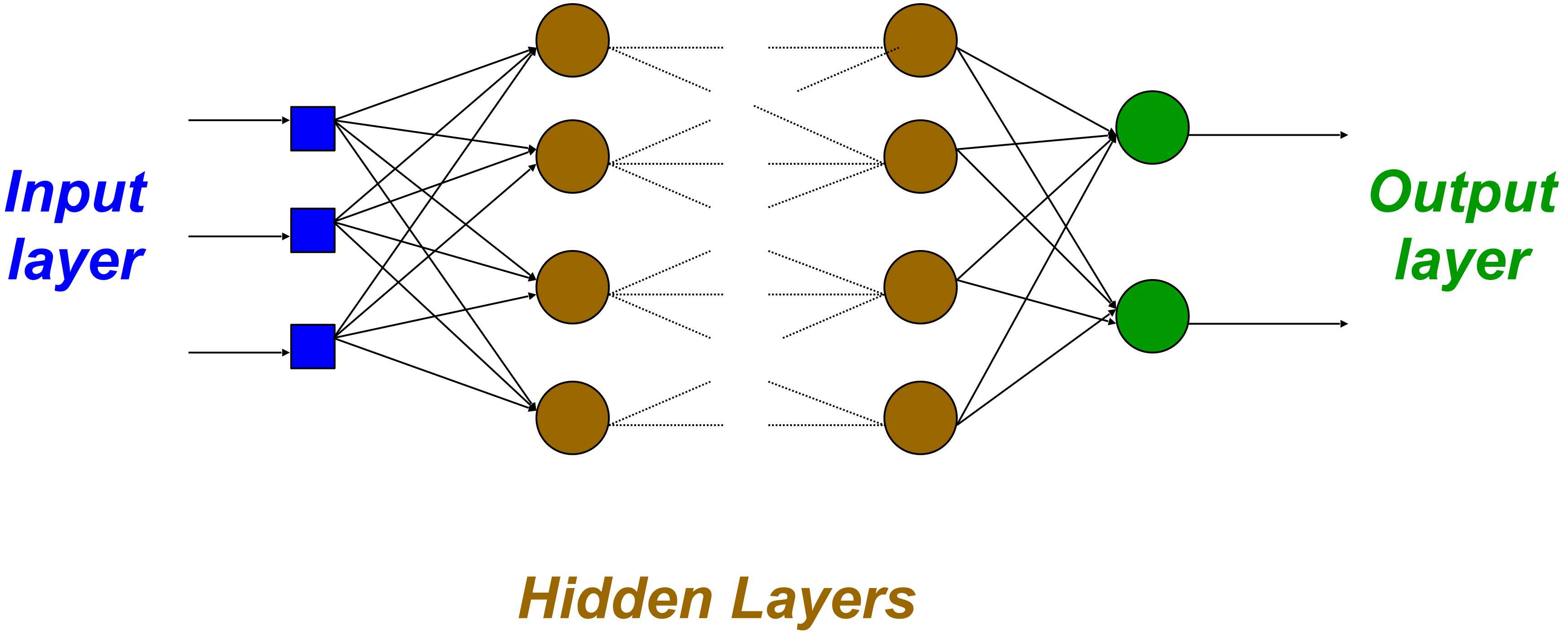
NNs use nonlinear *f*(x) so they can draw complex boundaries, but keep the data unchanged



NN and Back Propagation Algorithm

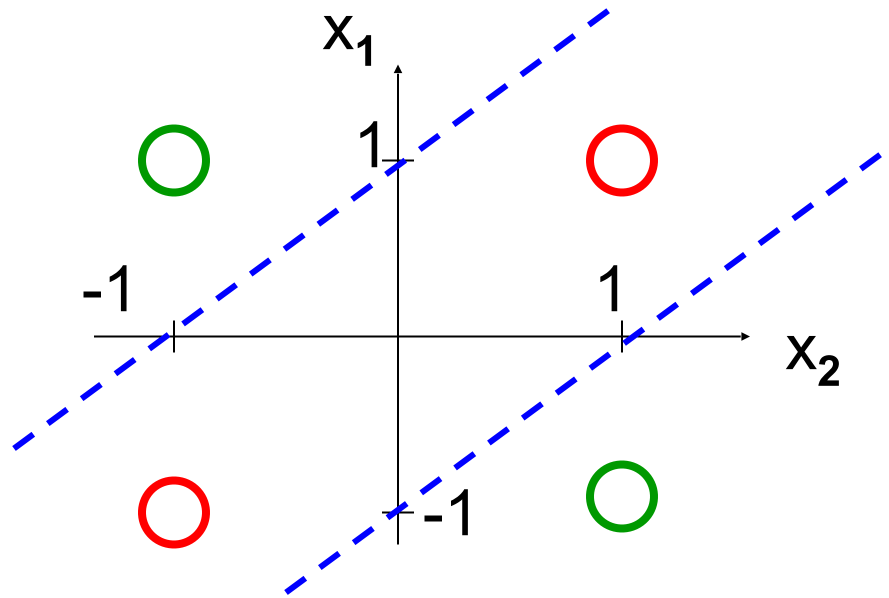
- Single layer nets have limited representation power (linear Separability problem). Multi layer nets (or nets with non-linear hidden units) may overcome linear inseparability problem.
- Every boolean function can be represented by a network with a single hidden layer
- Every bounded continuous function can be approximated with arbitrary small error, by network with one hidden layer.
- Any function can be approximated to arbitrary accuracy by a network with two hidden layers.

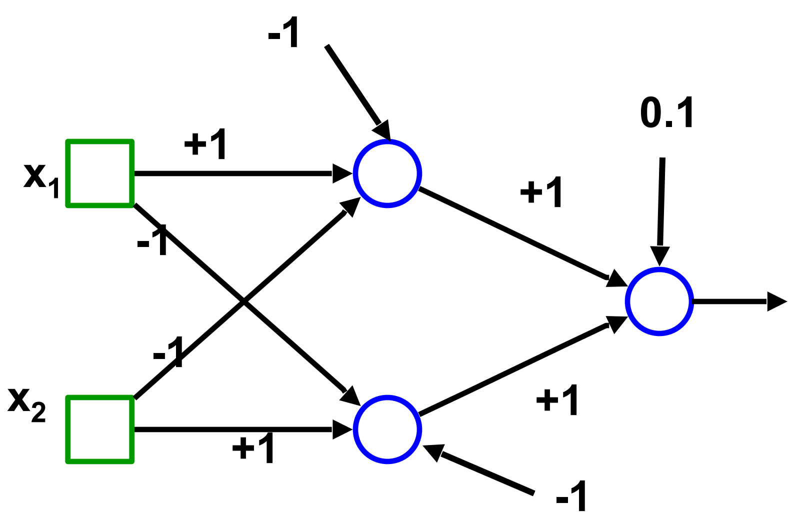
Multilayer Perceptrons Architecture



A solution for the XOR problem

x_1	x_2	x_1 xor x_2
-1	-1	-1
-1	1	1
1	-1	1
1	1	-1



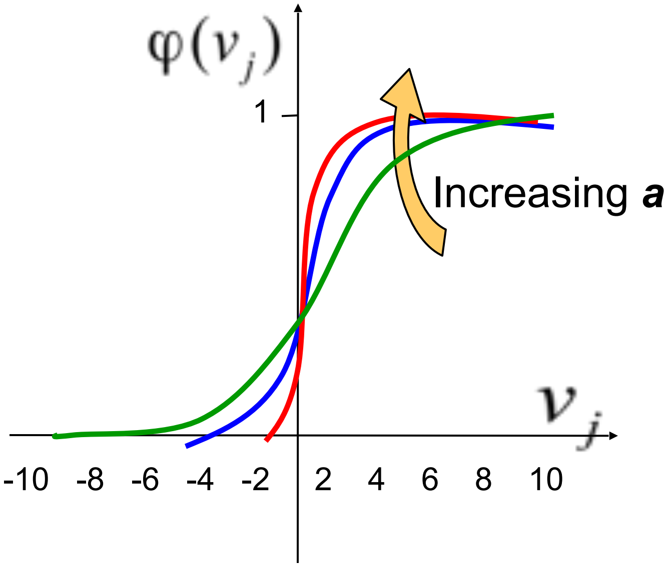


$$\varphi(v) = \begin{cases} 1 & \text{if } v > 0 \\ -1 & \text{if } v \leq 0 \end{cases}$$

φ is the sign function.

NEURON MODEL

- Sigmoidal Function



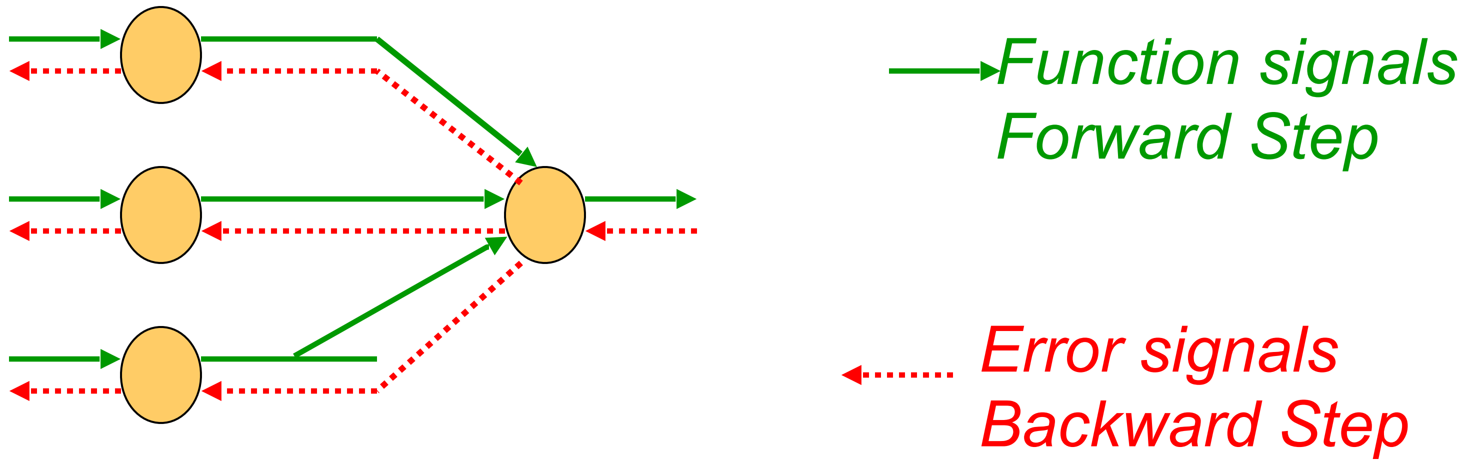
$$\boxed{\varphi(\mathrm{v}_j) = \frac{1}{1+e^{-av_j}}}$$

$$\mathrm{v}_j = \sum_{i=0,\dots,m} w_{ji} y_i$$

- v_j induced field of neuron j
- Most common form of activation function
- a $\rightarrow \infty \Rightarrow \varphi \rightarrow$ threshold function
- *Differentiable*

LEARNING ALGORITHM

- Back-propagation algorithm



- It adjusts the weights of the NN in order to minimize the average squared error.

Average Squared Error

- Error signal of output neuron ***j*** at presentation of ***n-th*** training example:

- Total error at time ***n***:

$$\boxed{e_j(n) = d_j(n) - y_j(n)}$$

- Average squared error:

$$\boxed{E(n) = \frac{1}{2} \sum_{j \in C} e_j^2(n)}$$

C: Set of neurons in output layer

- Measure of learning performance:

$$\boxed{E_{AV} = \frac{1}{N} \sum_{n=1}^{N} E(n)}$$

N: size of training set

- **Goal:** ***Adjust weights of NN to minimize E_{AV}***

Notation

e_j Error at output of neuron j

y_j Output of neuron j

$$v_j = \sum_{i=0,\dots,m} w_{ji} y_i$$ Induced local field of neuron j

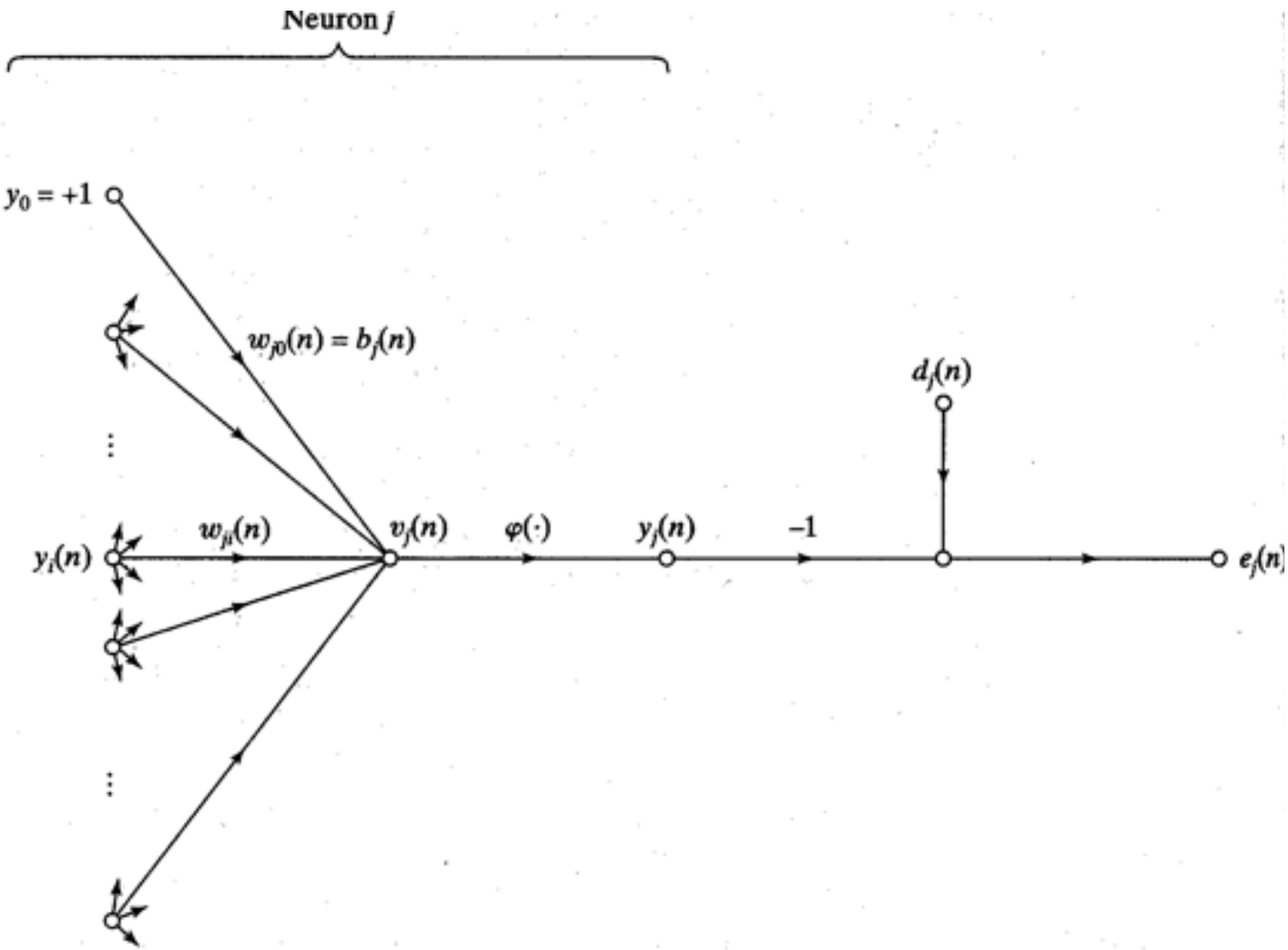
Weight Update Rule

Update rule is based on the gradient descent method take a step in the direction yielding the maximum decrease of E

$$\boxed{\Delta w_{ji} = -\eta \frac{\partial E}{\partial w_{ji}}}$$

Step in direction opposite to the gradient

Computing Model (output neuron)



Signal-flow graph highlighting the details of output neuron j.

Definition of the Local Gradient of neuron j

$$\boxed{\delta_j = -\frac{\partial E}{\partial v_j}}$$

Local Gradient

We obtain $\boxed{\delta_j = e_j \varphi'(v_j)}$

because

$$-\frac{\partial E}{\partial v_j} = -\frac{\partial E}{\partial e_j}\frac{\partial e_j}{\partial y_j}\frac{\partial y_j}{\partial v_j} = -e_j(-1)\varphi'(v_j)$$

Update Rule

- We obtain $$\boxed{\Delta w_{ji} = \eta \delta_j y_i}$$

  because

$$\frac{\partial E}{\partial w_{ji}} = \frac{\partial E}{\partial v_j} \frac{\partial v_j}{\partial w_{ji}}$$

$$-\frac{\partial E}{\partial v_j} = \delta_j \qquad \frac{\partial v_j}{\partial w_{ji}} = y_i$$

Compute local gradient of neuron j

- The key factor is the calculation of e_j
- There are two cases:
  - Case 1): j is a output neuron
  - Case 2): j is a hidden neuron

Error e_j of output neuron

- Case 1: ***j output neuron***

$$e_j = d_j - y_j$$

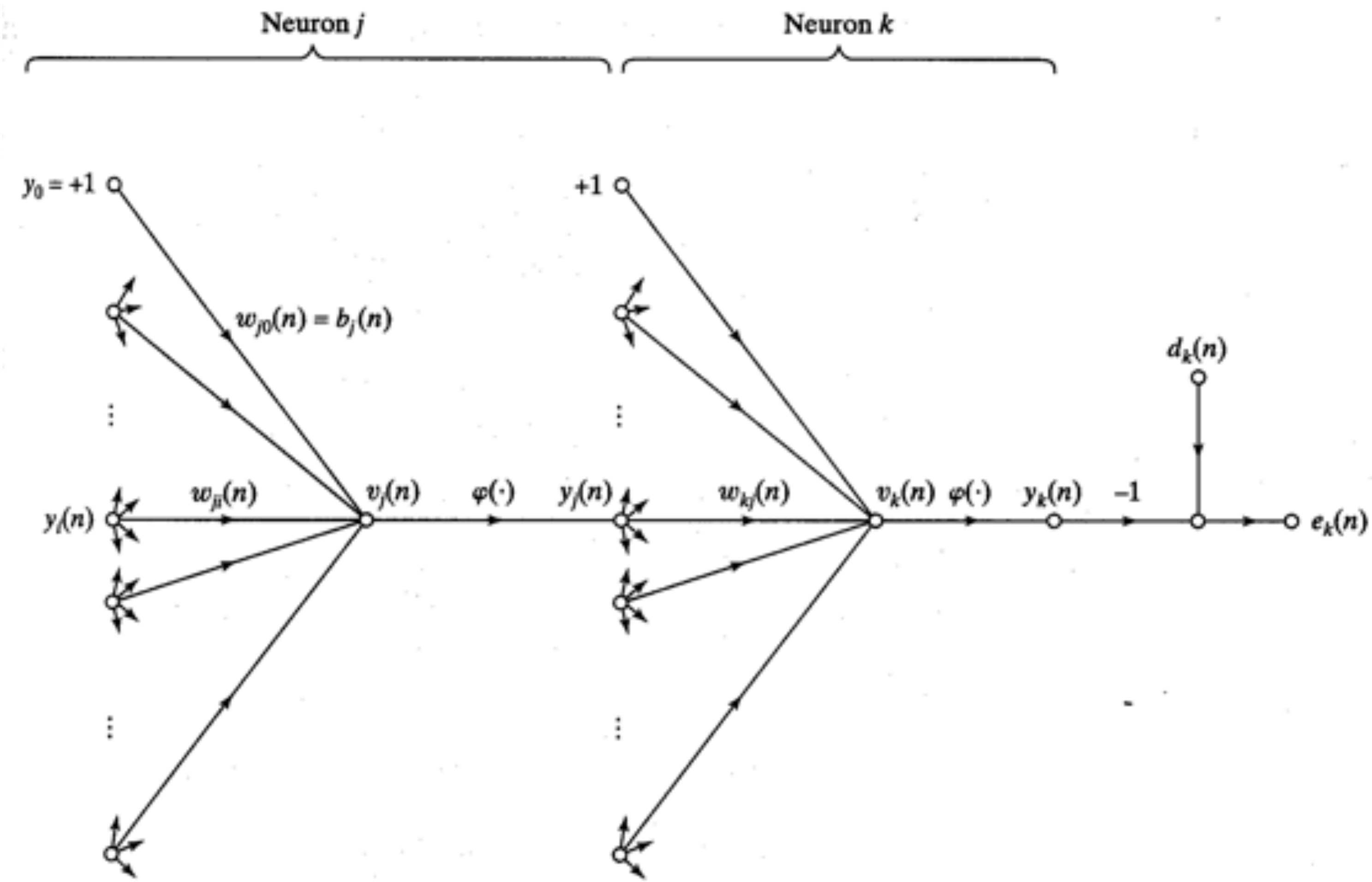
Then

$$\boxed{\delta_j = (d_j - y_j)\varphi'(v_j)}$$

Local gradient of hidden neuron

- Case 2: ***j hidden neuron***
- the local gradient for neuron j is recursively determined in terms of the local gradients of all neurons to which neuron j is directly connected

Computing model (hidden neuron)



Signal-flow graph highlighting the details of output neuron k connected to hidden neuron j.

Use the Chain Rule

$$\delta_j = -\frac{\partial E}{\partial y_j}\frac{\partial y_j}{\partial v_j} \qquad \frac{\partial y_j}{\partial v_j} = \varphi'(v_j)$$

$$\boxed{E(n) = \frac{1}{2}\sum_{k \in C} e_k^2(n)}$$

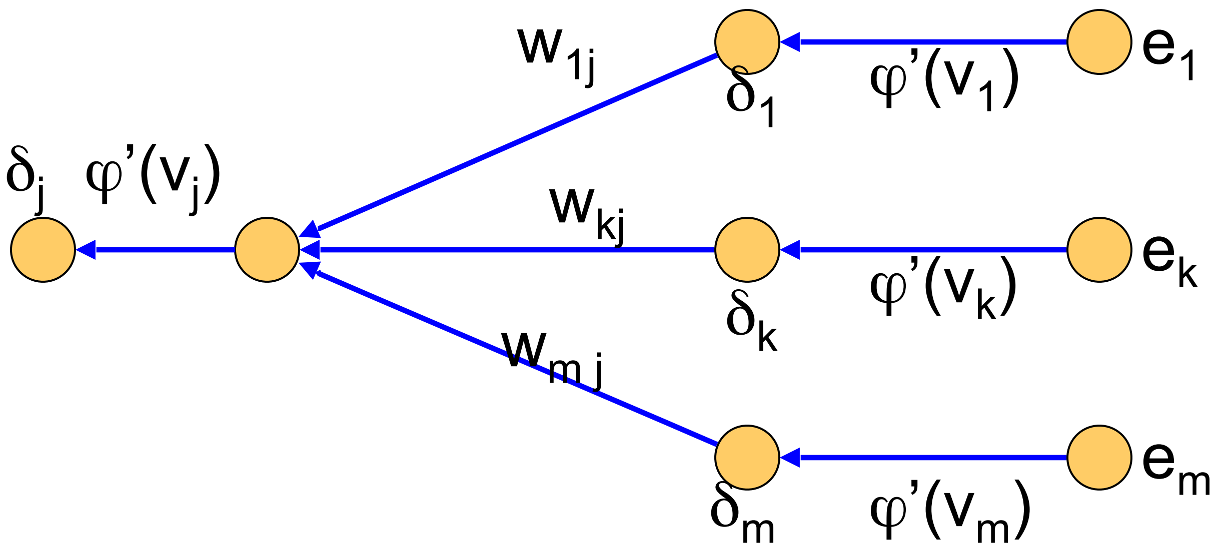
$$-\frac{\partial E}{\partial y_j} = -\sum_{k \in C} e_k \frac{\partial e_k}{\partial y_j} = \sum_{k \in C} e_k \left[-\frac{\partial e_k}{\partial v_k}\right]\frac{\partial v_k}{\partial y_j}$$

from $\quad -\frac{\partial e_k}{\partial v_k} = \varphi'(v_k) \qquad \frac{\partial v_k}{\partial y_j} = w_{kj}$

We obtain $\quad -\frac{\partial E}{\partial y_j} = \sum_{k \in C} \delta_k w_{kj}$

Local Gradient of hidden neuron j

Hence $$\boxed{\delta_j = \varphi'(v_j) \sum_{k \in C} \delta_k w_{kj}}$$



Signal-flow graph of back-propagation error signals to neuron ***j***

Delta Rule

- **Delta rule** $\Delta \boldsymbol{w}_{ji} = \eta \delta_j \boldsymbol{y}_i$

$$\delta_j = \begin{cases} \varphi'(v_j)(d_j - y_j) & \text{IF j output node} \\ \varphi'(v_j) \sum_{k \in C} \delta_k w_{kj} & \text{IF j hidden node} \end{cases}$$

C: Set of neurons in the layer following the one containing ***j***

Local Gradient of neurons

$$\varphi'(v_j) = a y_j [1 - y_j]$$

a > 0

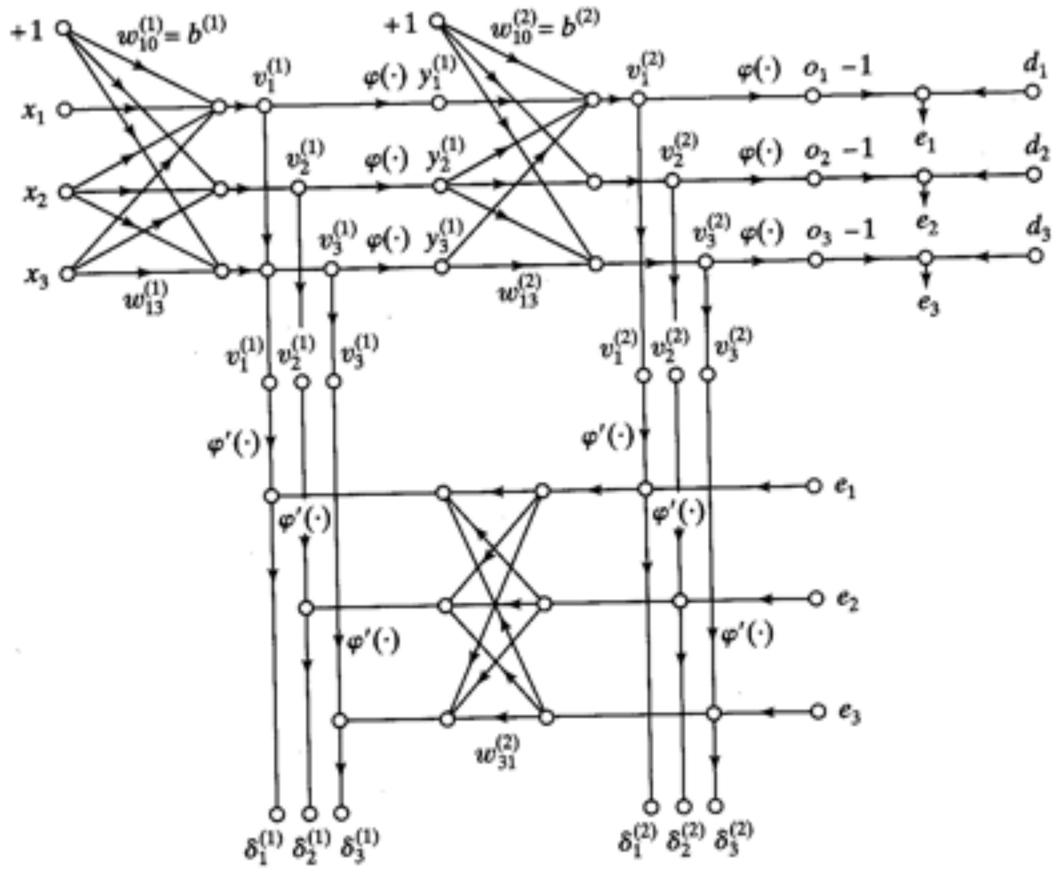
$$\delta_j = \begin{cases} a y_j [1 - y_j] \sum_k \delta_k w_{kj} & \textit{if j hidden node} \\ a y_j [1 - y_j][d_j^k - y_j] & \textit{If j output node} \end{cases}$$

Backpropagation algorithm

- Two phases of computation:
  - **Forward pass**: run the NN and compute the error for each neuron of the output layer.
  - **Backward pass**: start at the output layer, and pass the errors backwards through the network, layer by layer, by recursively computing the local gradient of each neuron.

Summary

Multilayer Perceptrons



Signal-flow graphical summary of back-propagation learning. Top part of the graph: forward pass. Bottom part of the graph: backward pass.

Training

- **Sequential mode** (on-line, pattern or stochastic mode):
  - (x(1), d(1)) is presented, a sequence of forward and backward computations is performed, and the weights are updated using the delta rule.
  - Same for (x(2), d(2)), … , (x(N), d(N)).

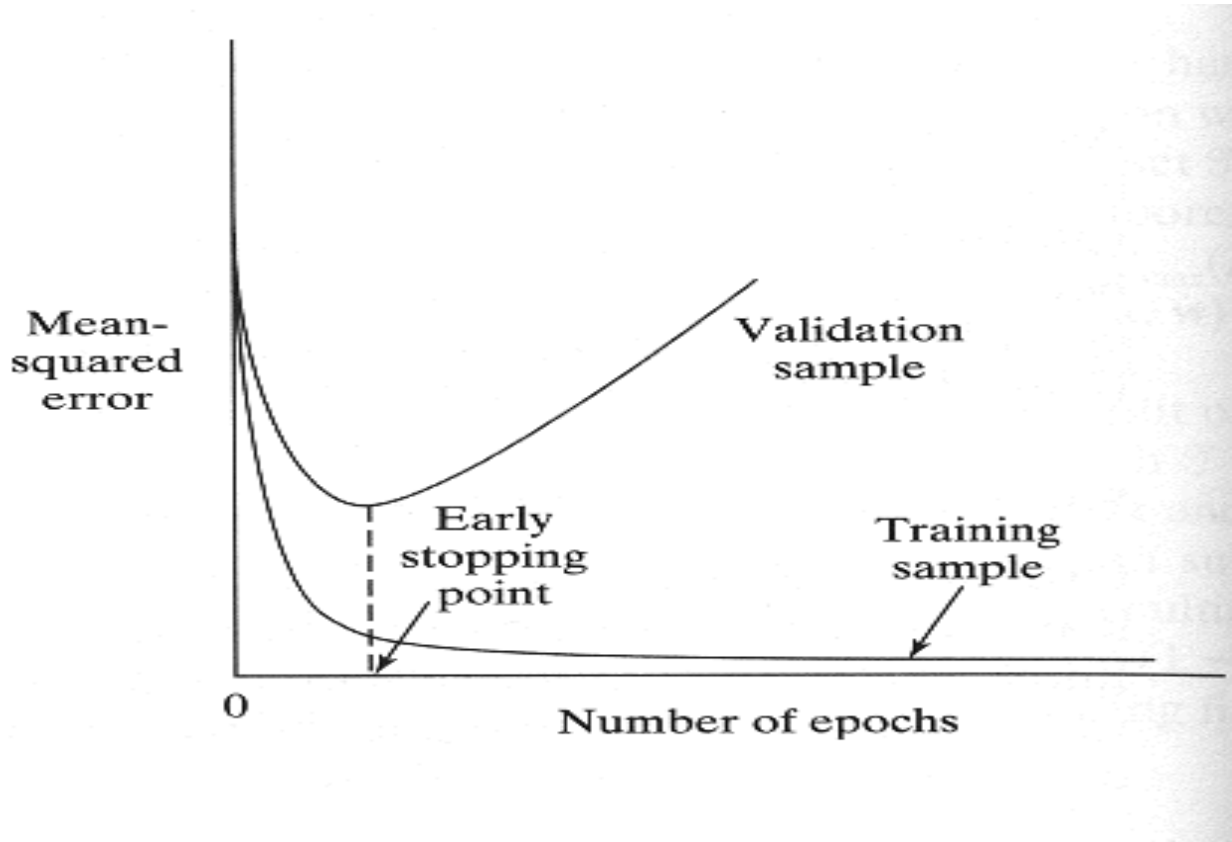
Training

- The learning process continues on an epoch-by-epoch basis until the stopping condition is satisfied.
- From one epoch to the next choose a randomized ordering for selecting examples in the training set.

Stopping criterions

- Sensible stopping criterions:
  - Average squared error change: Back-prop is considered to have converged when the absolute rate of change in the average squared error per epoch is sufficiently small (in the range [0.1, 0.01]).
  - Generalization based criterion: After each epoch the NN is tested for generalization. If the generalization performance is adequate then stop.

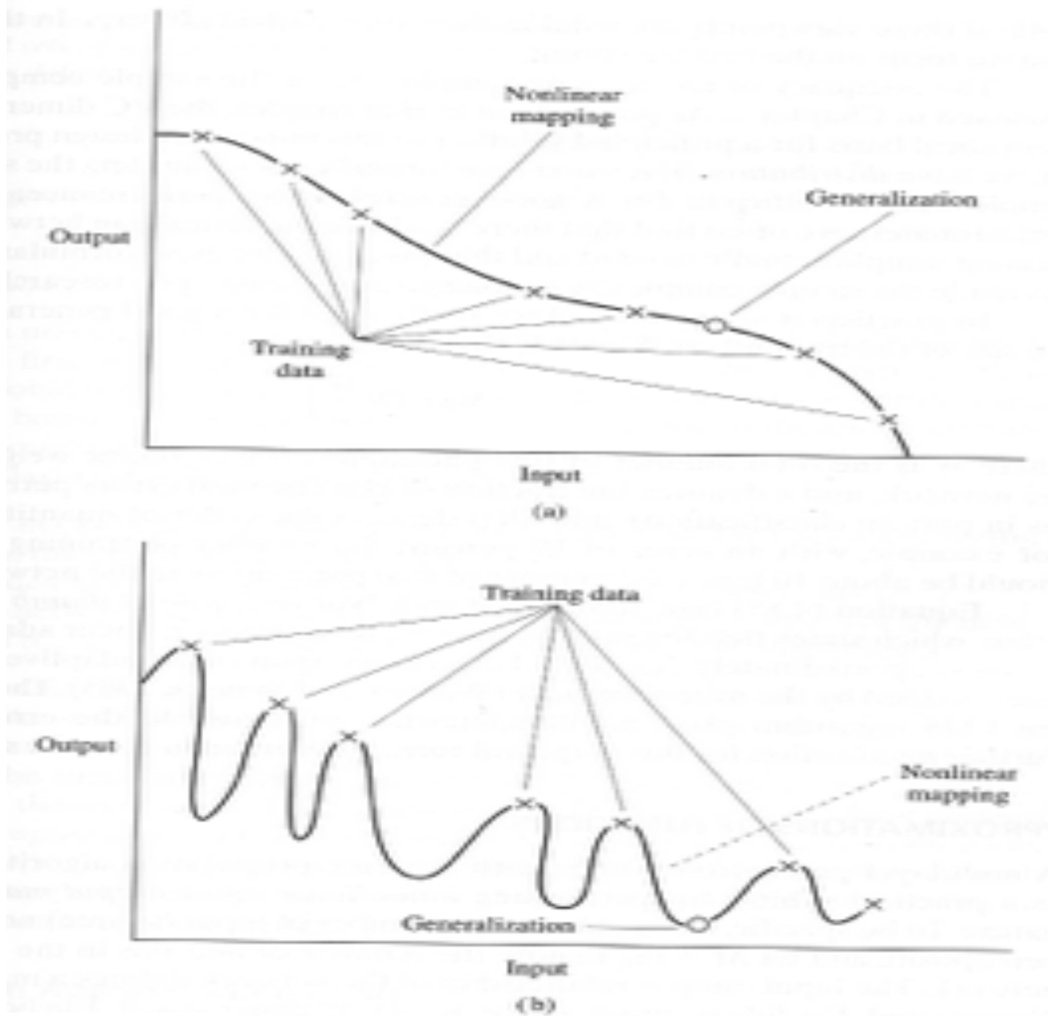
Early stopping



Generalization

- Generalization: NN generalizes well if the I/O mapping computed by the network is nearly correct for new data (test set).
- Factors that influence generalization:
  - the size of the training set.
  - the architecture of the NN.
  - the complexity of the problem at hand.
- Overfitting (overtraining): when the NN learns too many I/O examples it may end up memorizing the training data.

Generalization



(a) Properly fitted data (good generalization) (b) Overfitted data (poor generalization).

Expressive capabilities of NN

Boolean functions:

- Every boolean function can be represented by network with single hidden layer
- but might require exponential hidden units

Continuous functions:

- Every bounded continuous function can be approximated with arbitrarily small error, by network with one hidden layer
- Any function can be approximated with arbitrary accuracy by a network with two hidden layers

Generalized Delta Rule

- If η small $\Rightarrow$ Slow rate of learning
  If η large $\Rightarrow$ Large changes of weights
  $\Rightarrow$ NN can become unstable (oscillatory)
- Method to overcome above drawback:
  include a momentum term in the delta rule

$$\Delta w_{ji}(n) = \alpha \Delta w_{ji}(n-1) + \eta \delta_j(n) y_i(n)$$

Generalized delta function

momentum constant

Generalized delta rule

- the momentum accelerates the descent in steady downhill directions.
- the momentum has a stabilizing effect in directions that oscillate in time.

η adaptation

Heuristics for accelerating the convergence of the back-prop algorithm through η adaptation:

- Heuristic 1: Every weight should have its own η.
- Heuristic 2: Every η should be allowed to vary from one iteration to the next.

NN DESIGN

- Data representation
- Network Topology
- Network Parameters
- Training
- Validation

Setting the parameters

- How are the weights initialised?
- How is the learning rate chosen?
- How many hidden layers and how many neurons?
- Which activation function ?
- How to preprocess the data ?
- How many examples in the training data set?

Some heuristics (1)

- Sequential v/s Batch algorithms:
- the sequential mode (pattern by pattern) is computationally faster than the batch mode (epoch by epoch)
- Sequential also called as on line learning
- Sequential is stochastic in nature
- Tracks small changes in training data set.
- Simple to implement
- Effective solution to large scale and complex classification problems
- Cost function is instantaneous error energy

Some heuristics (2)

- Maximization of information content: every training example presented to the back propagation algorithm must maximize the information content.
  - The use of an example that results in the largest training error.
  - The use of an example that is radically different from all those previously used.

Some heuristics (3)

- Activation function: network learns faster with antisymmetric functions when compared to nonsymmetric functions.

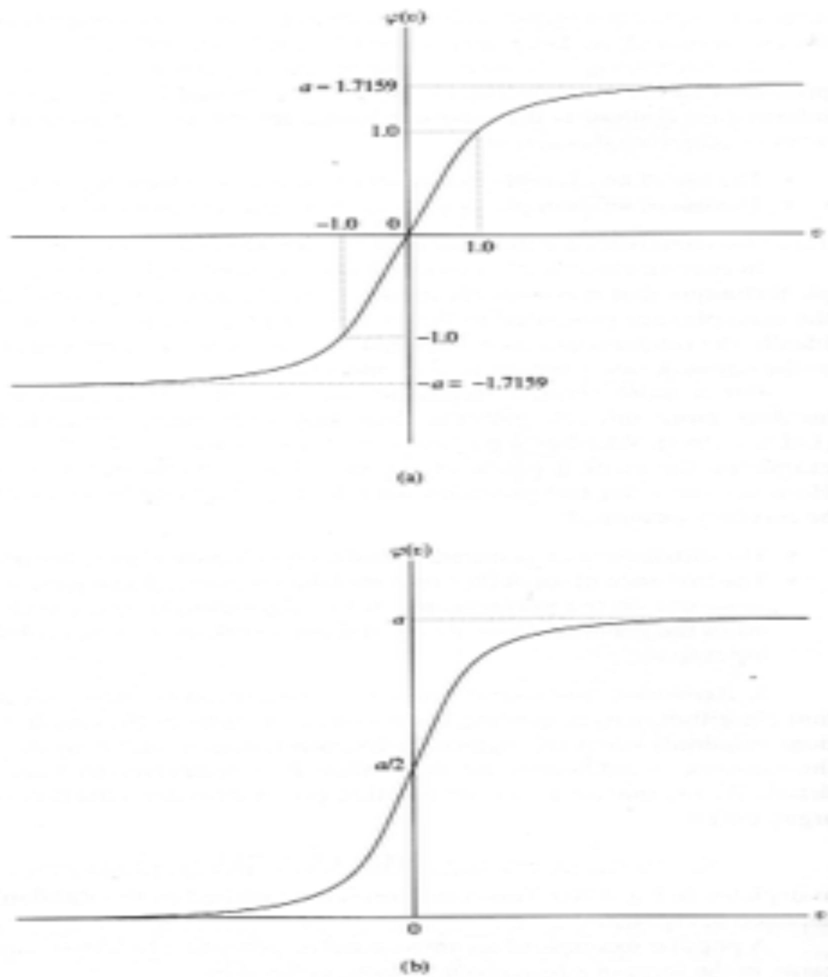
$$\varphi(\mathrm{v}) = \frac{1}{1+e^{-av}}$$

Sigmoidal function is nonsymmetric

$$\varphi(\mathrm{v}) = a\tanh(bv)$$

Hyperbolic tangent function is nonsymmetric

Some heuristics (3)



Antisymmetric activation function. (b) Nonsymmetric activation function.

Some heuristics (4)

- Target values: target values must be chosen within the range of the sigmoidal activation function.
- Otherwise, hidden neurons can be driven into saturation which slows down learning

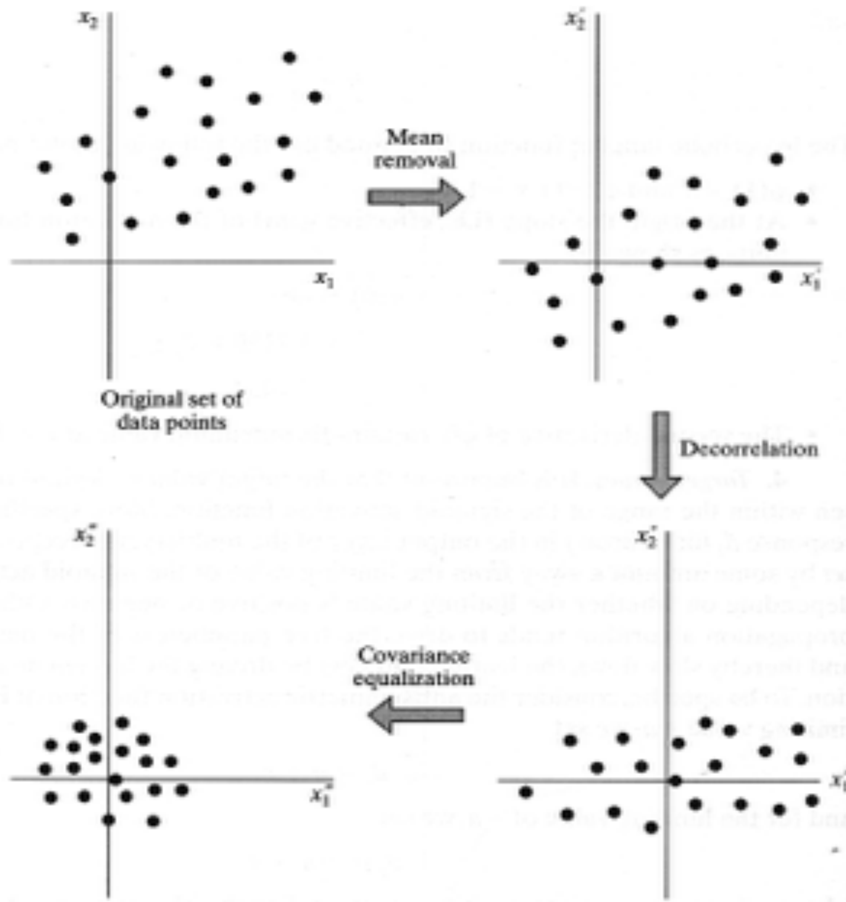
Some heuristics (4)

- For the antisymmetric activation function it is necessary to design Є
- For a+: $$d_j = a - \varepsilon$$
- For –a: $$d_j = -a + \varepsilon$$
- If a=1.7159 we can set Є=0.7159 then d=±1

Some heuristics (5)

- Inputs normalisation:
  - Each input variable should be processed so that the mean value is small or close to zero or at least very small when compared to the standard deviation.
  - Input variables should be uncorrelated.
  - Decorrelated input variables should be scaled so their covariances are approximately equal.

Some heuristics (5)



Illustrating the operation of mean removal, decorrelation, and covariance equalization for a two-dimensional input space.

Some heuristics (6)

- Initialization of weights:
  - If synaptic weights are assigned large initial values neurons are driven into saturation. Local gradients become small so learning rate becomes small.
  - If synaptic weights are assigned small initial values algorithms operate around the origin. For the hyperbolic activation function the origin is a saddle point.

Some heuristics (7)

- Learning rate:
  - The right value of η depends on the application. Values between 0.1 and 0.9 have been used in many applications.
  - Other heuristics adapt η during the training as described in previous slides.

Some heuristics (8)

- How many layers and neurons
  - The number of layers and of neurons depend on the specific task. In practice this issue is solved by trial and error.
  - Two types of adaptive algorithms can be used:
    - **start from a large network and successively remove some neurons and links until network performance degrades.**
    - **begin with a small network and introduce new neurons until performance is satisfactory.**

Some heuristics (9)

- How many training data ?
  - Rule of thumb: the number of training examples should be at least five to ten times the number of weights of the network.