Neural Network Lectures

ME 60033 IMS 2014-15

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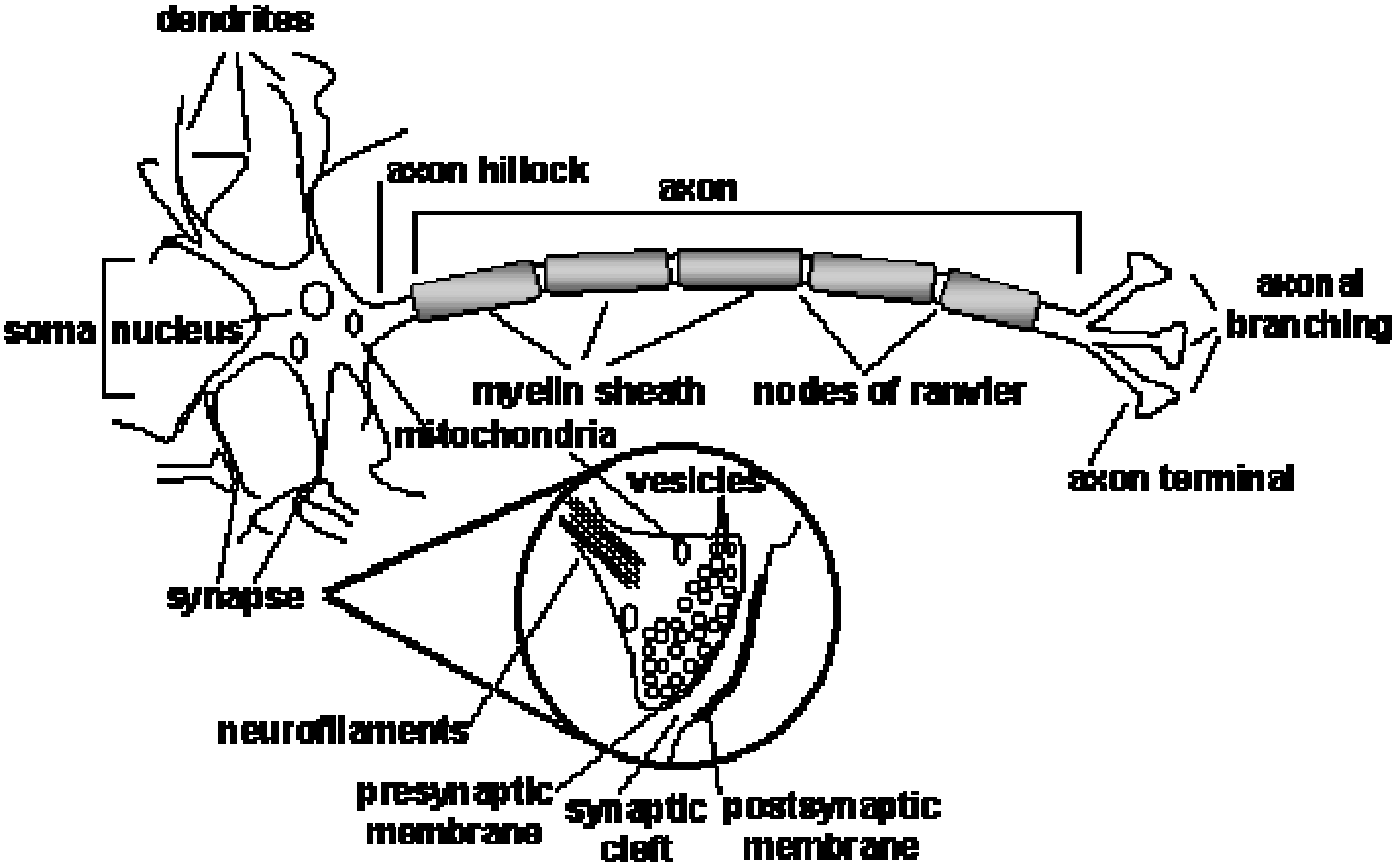
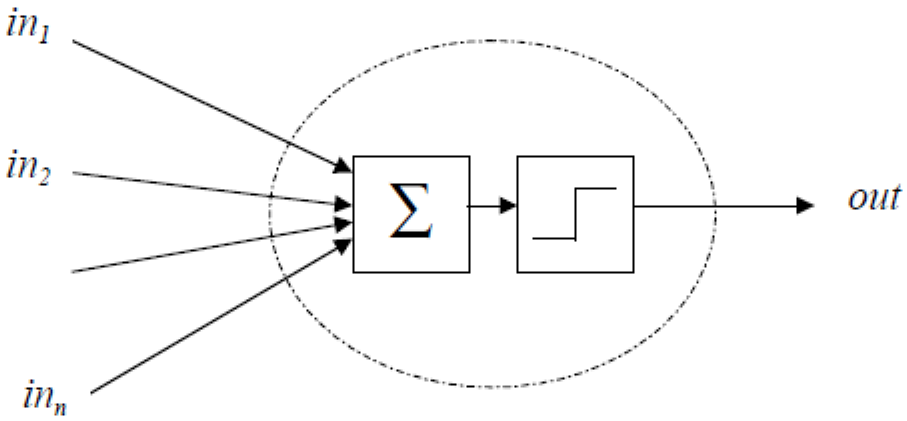
Schematic Diagram of a Biological Neuron



The McCulloch-Pitts Neuron

This vastly simplified model of real neurons is also known as a ***Threshold Logic Unit*** :



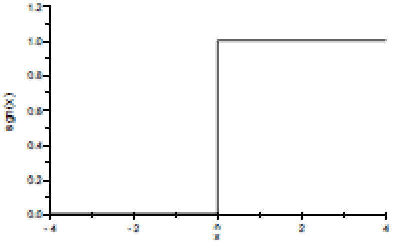
1. A set of synapses (i.e. connections) brings in activations from other neurons.
2. A processing unit sums the inputs, and then applies a non-linear activation function (i.e. squashing/transfer/threshold function).
3. An output line transmits the result to other neurons.

Some Useful Functions

A function $y = f(x)$ describes a relationship (input-output mapping) from x to y.

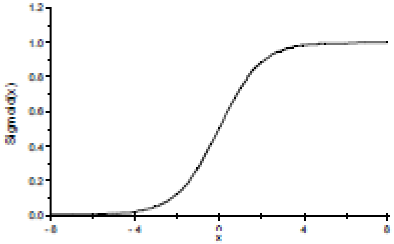
Example 1 The threshold or sign function $\mathrm{sgn}(x)$ is defined as

$$\mathrm{sgn}(x)=\begin{cases} 1 & \text{if } x\geq 0 \\ 0 & \text{if } x<0 \end{cases}$$



Example 2 The logistic or sigmoid function $\mathrm{Sigmoid}(x)$ is defined as

$$\mathrm{Sigmoid}(x) = \frac{1}{1+e^{-x}}$$



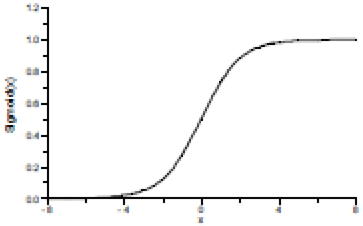
This is a smoothed (differentiable) form of the threshold function.

Other Types of Activation/Transfer Function

Sigmoid Functions These are smooth (differentiable) and monotonically increasing.

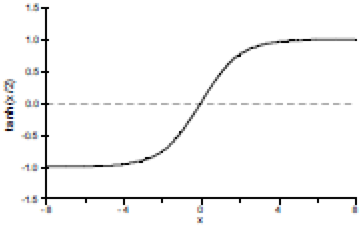
The logistic function

$$\text{Sigmoid}(x) = \frac{1}{1+e^{-x}}$$



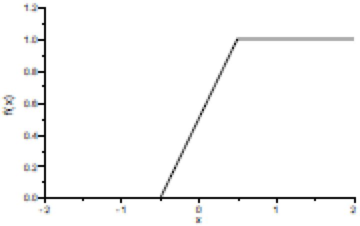
Hyperbolic tangent

$$\tanh(\tfrac{x}{2}) = \frac{1-e^{-x}}{1+e^{-x}}$$



Piecewise-Linear Functions Approximations of a sigmoid functions.

$$f(x) = \begin{cases} 1 & \text{if x} \geq 0.5 \\ x+0.5 & \text{if -}0.5 \leq \text{x} \leq 0.5 \\ 0 & \text{if x} \leq 0.5 \end{cases}$$



The McCulloch-Pitts Neuron Equation

Using the above notation, we can now write down a simple equation for the ***output*** *out* of a McCulloch-Pitts neuron as a function of its n ***inputs*** in_i :

$$out = \operatorname{sgn}(\sum_{i=1}^{n} in_i - \theta)$$

where θ is the neuron's activation ***threshold***. We can easily see that:

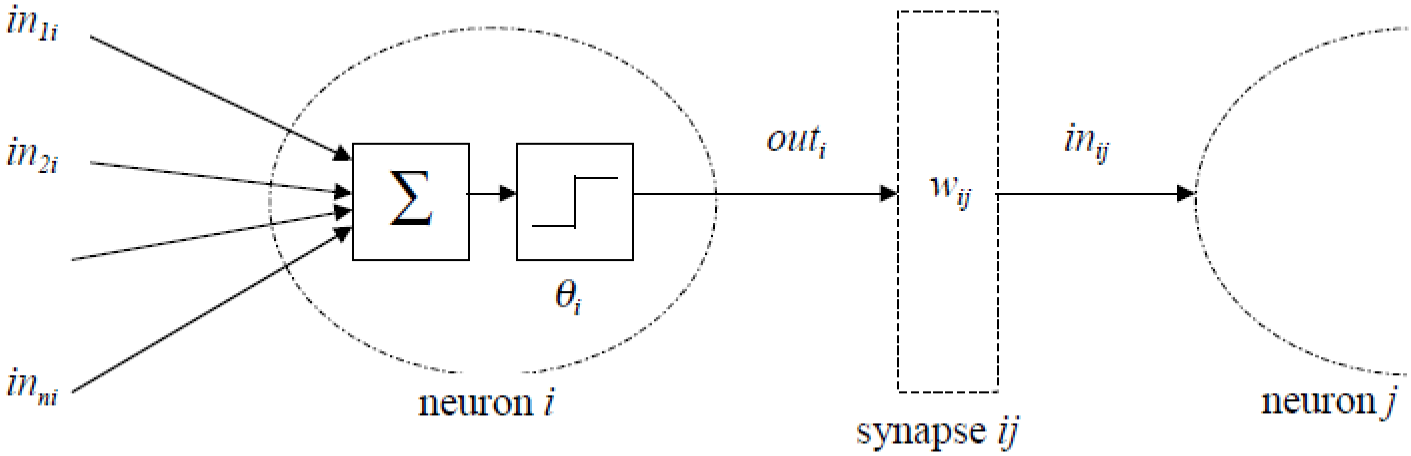
$$out = 1 \quad \text{if} \quad \sum_{k=1}^{n} in_k \geq \theta \qquad\qquad out = 0 \quad \text{if} \quad \sum_{k=1}^{n} in_k < \theta$$

Note that the McCulloch-Pitts neuron is an extremely simplified model of real biological neurons. Some of its missing features include: non-binary inputs and outputs, non-linear summation, smooth thresholding, stochasticity, and temporal information processing.

Nevertheless, McCulloch-Pitts neurons are computationally very powerful. One can show that assemblies of such neurons are capable of universal computation.

Networks of McCulloch-Pitts Neurons

One neuron can't do much on its own. Usually we will have many neurons labelled by indices *k*, *i*, *j* and activation flows between them via synapses with strengths w_{ki}, w_{ij}:

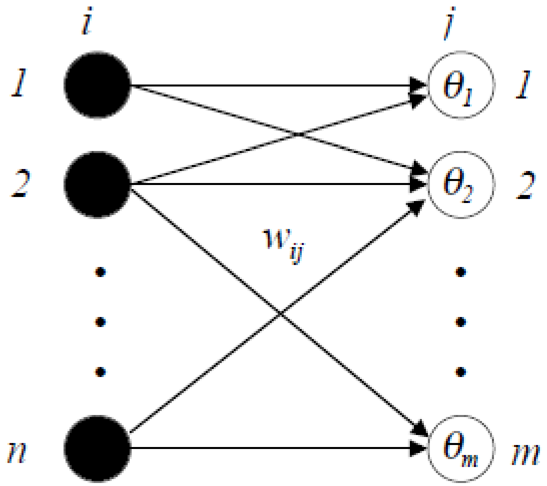


$$in_{ki} = out_k w_{ki} \qquad out_i = \mathrm{sgn}\left(\sum_{k=1}^{n} in_{ki} - \theta_i\right) \qquad in_{ij} = out_i w_{ij}$$

The Perceptron

We can connect any number of McCulloch-Pitts neurons together in any way we like.

An arrangement of one input layer of McCulloch-Pitts neurons feeding forward to one output layer of McCulloch-Pitts neurons is known as a ***Perceptron***.



$$out_j = \operatorname{sgn}\left(\sum_{i=1}^{n} out_i w_{ij} - \theta_j\right)$$

Already this is a powerful computational device. Later we shall see variations that make it even more powerful.

ANN Architectures/Structures/Topologies

Mathematically, ANNs can be represented as ***weighted directed graphs***. For our purposes, we can simply think in terms of activation flowing between processing units via one-way connections. Three common ANN architectures are:

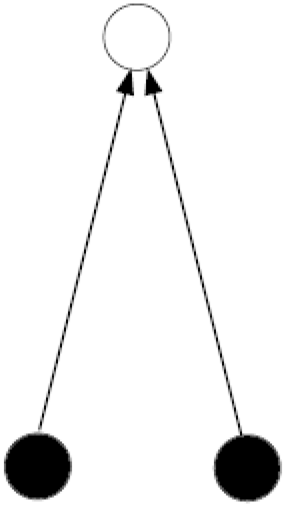
Single-Layer Feed-forward NNs One input layer and one output layer of processing units. No feed-back connections. (For example, a simple Perceptron.)

Multi-Layer Feed-forward NNs One input layer, one output layer, and one or more hidden layers of processing units. No feed-back connections. The hidden layers sit in between the input and output layers, and are thus *hidden* from the outside world. (For example, a Multi-Layer Perceptron.)

Recurrent NNs Any network with at least one feed-back connection. It may, or may not, have hidden units. (For example, a Simple Recurrent Network.)

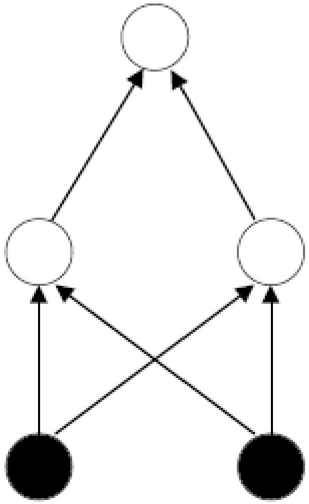
Examples of Network Architectures

Single Layer Feed-forward



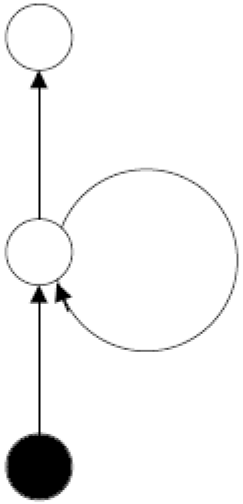
Single-Layer Perceptron

Multi-Layer Feed-forward



Multi-Layer Perceptron

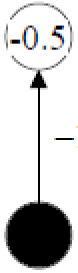
Recurrent Network



Simple Recurrent Network

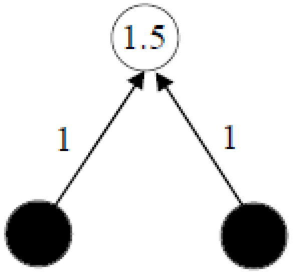
NOT

in	*out*
0	1
1	0



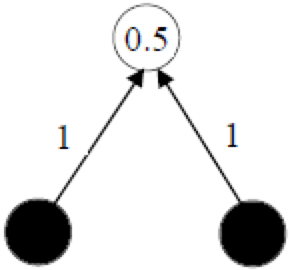
AND

in_1	in_2	*out*
0	0	0
0	1	0
1	0	0
1	1	1



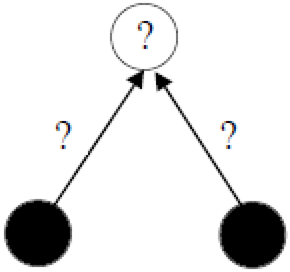
OR

in_1	in_2	*out*
0	0	0
0	1	1
1	0	1
1	1	1



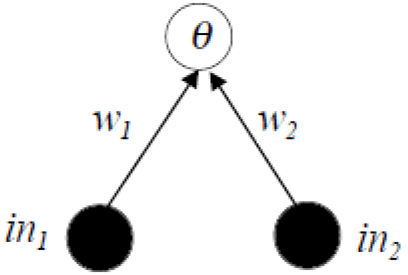
XOR

in_1	in_2	*out*
0	0	0
0	1	1
1	0	1
1	1	0



Decision Boundaries in Two Dimensions

For simple logic gate problems, it is easy to visualise what the neural network is doing. It is forming ***decision boundaries*** between classes. Remember, the network output is:



$$out = \mathrm{sgn}(w_1 in_1 + w_2 in_2 - \theta)$$

The decision boundary (between $out = 0$ and $out = 1$) is at

$$w_1 in_1 + w_2 in_2 - \theta = 0$$

i.e. along the straight line:

$$in_2 = \left(\frac{-w_1}{w_2}\right) in_1 + \left(\frac{\theta}{w_2}\right)$$

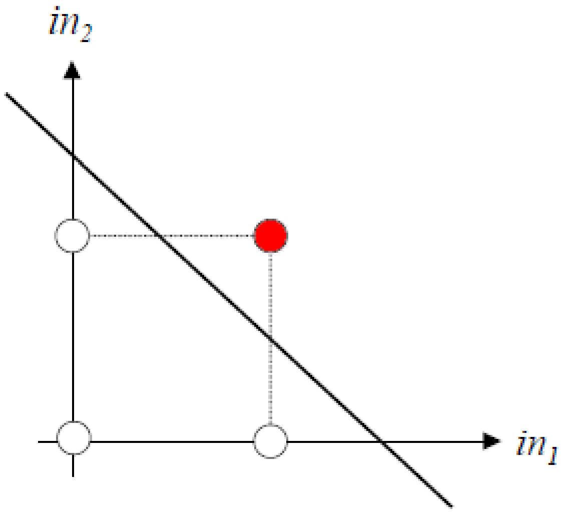
So, in two dimensions the decision boundaries are always straight lines.

Decision Boundaries for AND and OR

We can easily plot the decision boundaries we found by inspection last lecture:

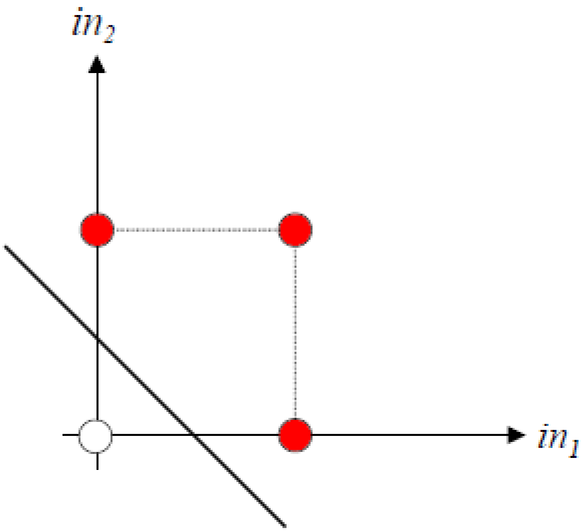
AND

$w_1 = 1,\ \ w_2 = 1,\ \ \theta = 1.5$



OR

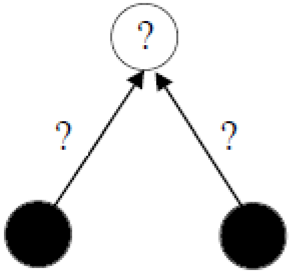
$w_1 = 1,\ \ w_2 = 1,\ \ \theta = 0.5$

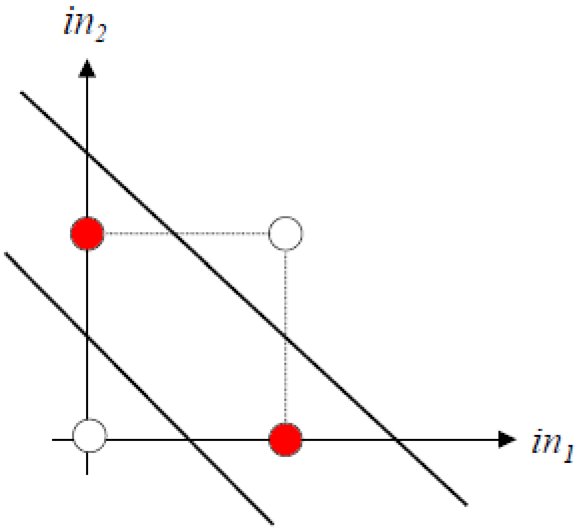


The extent to which we can change the weights and thresholds without changing the output decisions is now clear.

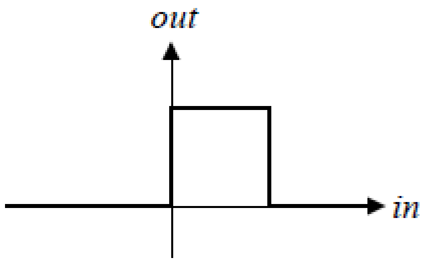
XOR

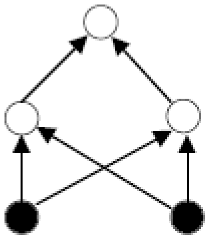
in_1	in_2	out
0	0	0
0	1	1
1	0	1
1	1	0





⇒
e.g.





Decision Hyperplanes and Linear Separability

If we have two inputs, then the weights define a decision boundary that is a one dimensional straight line in the two dimensional ***input space*** of possible input values.

If we have *n* inputs, the weights define a decision boundary that is an *n-1* dimensional ***hyperplane*** in the *n* dimensional input space:

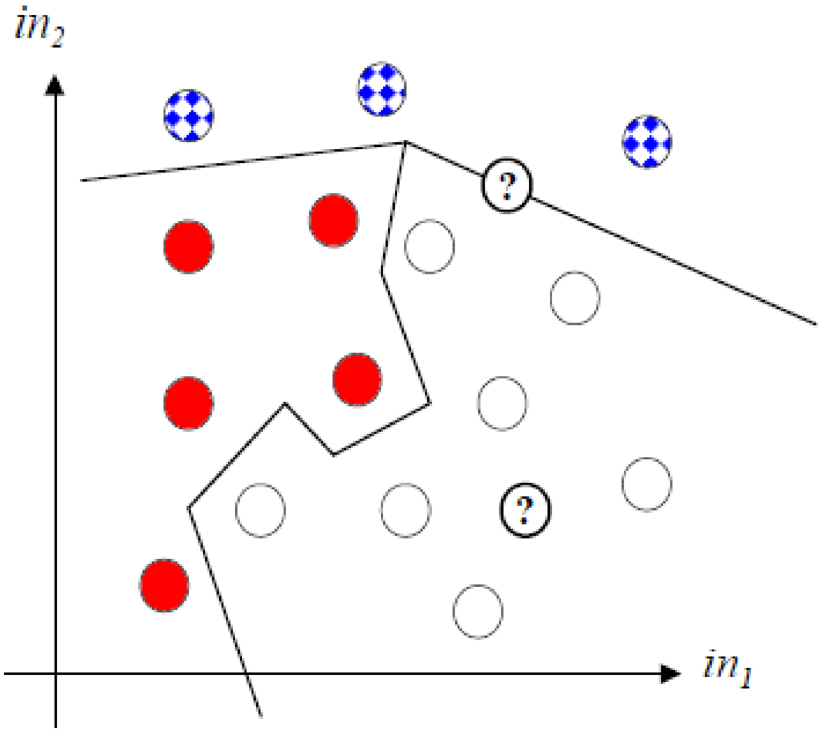
$$w_1 in_1 + w_2 in_2 + \ldots + w_n in_n - \theta = 0$$

This hyperplane is clearly still linear (i.e. straight/flat) and can still only divide the space into two regions. We still need more complex transfer functions, or more complex networks, to deal with XOR type problems.

Problems with input patterns which can be classified using a single hyperplane are said to be ***linearly separable***. Problems (such as XOR) which cannot be classified in this way are said to be ***non-linearly separable***.

General Decision Boundaries

Generally, we will want to deal with input patterns that are not binary, and expect our neural networks to form complex decision boundaries, e.g.



We may also wish to classify inputs into many classes (such as the three shown here).

Learning and Generalization

A network will also produce outputs for input patterns that it was not originally set up to classify (shown with question marks), though those classifications may be incorrect.

There are two important aspects of the network's operation to consider:

Learning The network must learn decision surfaces from a set of ***training patterns*** so that these training patterns are classified correctly.

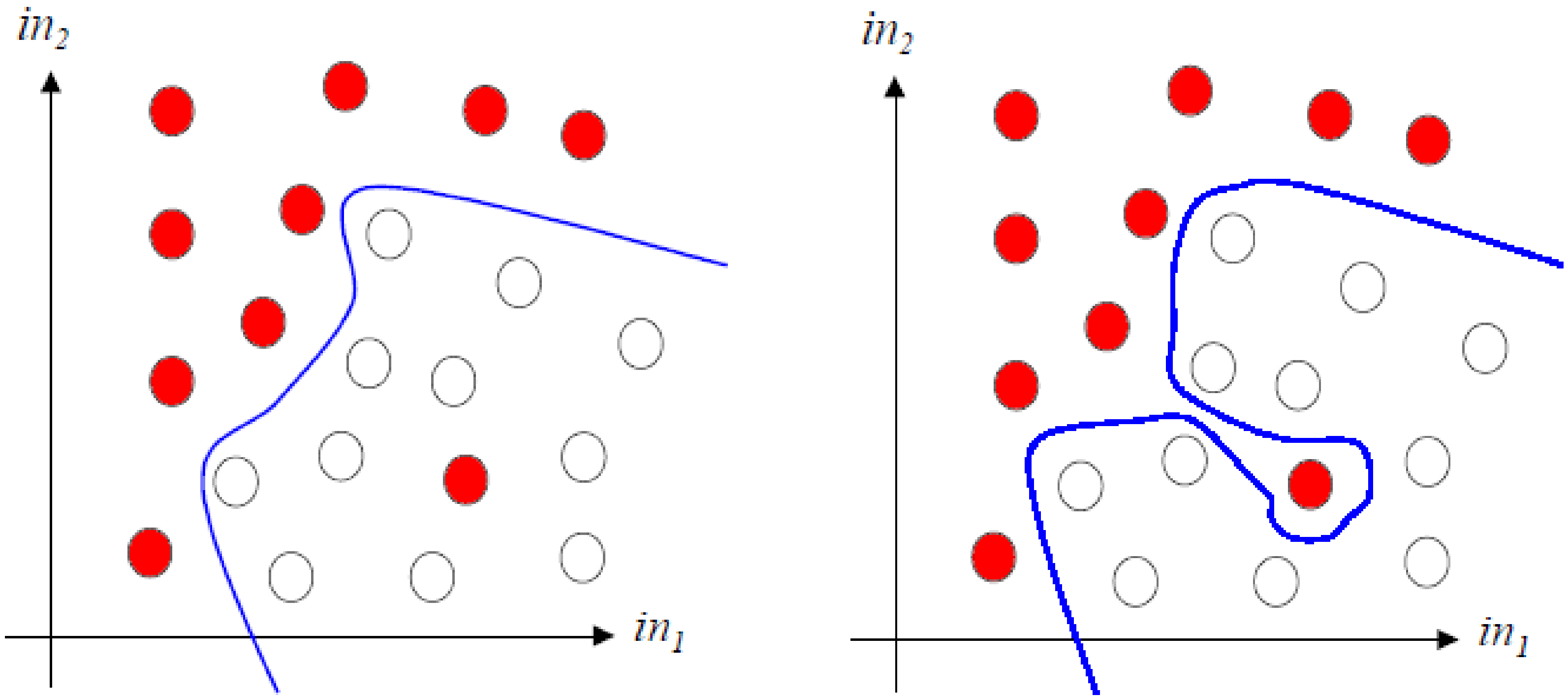
Generalization After training, the network must also be able to generalize, i.e. correctly classify ***test patterns*** it has never seen before.

Usually we want our neural networks to learn well, and also to generalize well.

Sometimes, the training data may contain errors (e.g. noise in the experimental determination of the input values, or incorrect classifications). In this case, learning the training data perfectly may make the generalization worse. There is an important ***trade-off*** between learning and generalization that arises quite generally.

Generalization in Classification

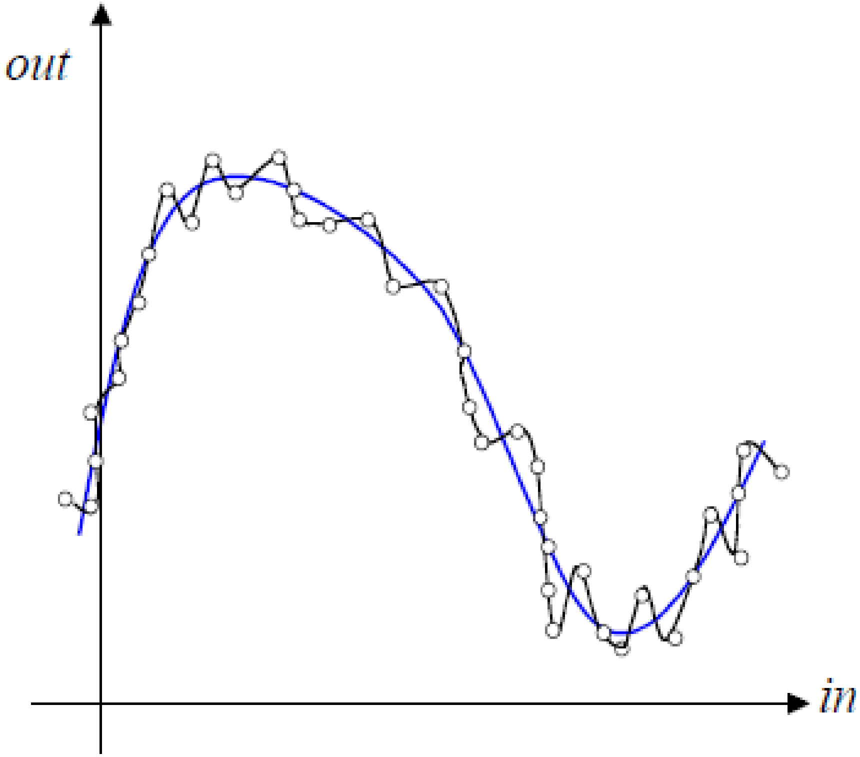
Suppose the task of our network is to learn a classification decision boundary:



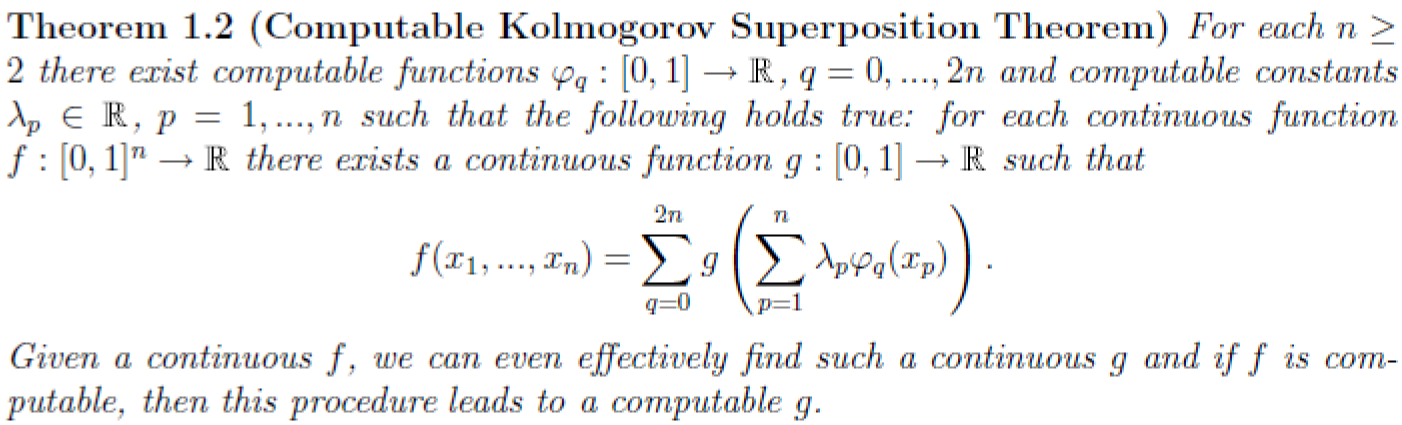
Our aim is for the network to generalize to classify new inputs appropriately. If we know that the training data contains noise, we don't necessarily want the training data to be classified totally accurately, as that is likely to reduce the generalization ability.

Generalization in Function Approximation

Suppose we wish to recover a function for which we only have noisy data samples:



We can expect the neural network output to give a better representation of the underlying function if its output curve does not pass through all the data points. Again, allowing a larger error on the training data is likely to lead to better generalization.



Theorem 1.2 (Computable Kolmogorov Superposition Theorem) *For each $n \geq 2$ there exist computable functions $\varphi_q : [0,1] \to \mathbb{R}$, $q = 0, ..., 2n$ and computable constants $\lambda_p \in \mathbb{R}$, $p = 1, ..., n$ such that the following holds true: for each continuous function $f : [0,1]^n \to \mathbb{R}$ there exists a continuous function $g : [0,1] \to \mathbb{R}$ such that*

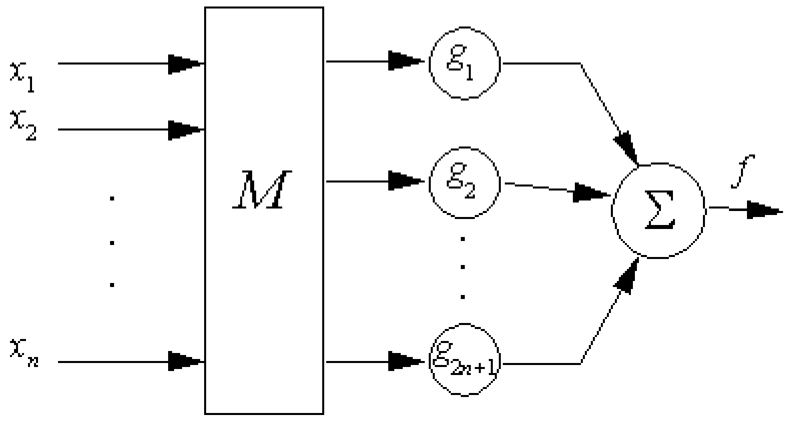
$$f(x_1, ..., x_n) = \sum_{q=0}^{2n} g\left(\sum_{p=1}^{n} \lambda_p \varphi_q(x_p)\right).$$

Given a continuous f, we can even effectively find such a continuous g and if f is computable, then this procedure leads to a computable g.

Hecht Nelson 1987,1990; Leppmann 1987 , Spreecher 1993

$$f(x_1,x_2,...,x_n) = \sum_{j=1}^{2n+1} g_j\left(\sum_{i=1}^{n} \phi_{ij}(x_i)\right)$$

Multivariable function



Neural network representation

Training a Neural Network

Whether our neural network is a simple Perceptron, or a much more complicated multi-layer network with special activation functions, we need to develop a systematic procedure for determining appropriate connection weights.

The general procedure is to have the network ***learn*** the appropriate weights from a representative set of training data.

In all but the simplest cases, however, direct computation of the weights is intractable.

Instead, we usually start off with ***random initial weights*** and adjust them in small steps until the required outputs are produced.

Perceptron Learning

For simple Perceptrons performing classification, we have seen that the decision boundaries are hyperplanes, and we can think of ***learning*** as the process of shifting around the hyperplanes until each training pattern is classified correctly.

Somehow, we need to formalise that process of "shifting around" into a systematic algorithm that can easily be implemented on a computer.

The "shifting around" can conveniently be split up into a number of small steps.

If the network weights at time t are $w_{ij}(t)$, then the shifting process corresponds to moving them by an amount $\Delta w_{ij}(t)$ so that at time $t+1$ we have weights

$$w_{ij}(t+1) = w_{ij}(t) + \Delta w_{ij}(t)$$

It is convenient to treat the thresholds as weights, as discussed previously, so we don't need separate equations for them.

Formulating the Weight Changes

Suppose the target output of unit j is $targ_j$ and the actual output is $out_j = \text{sgn}(\sum in_i w_{ij})$, where in_i are the activations of the previous layer of neurons (e.g. the network inputs). Then we can just go through all the possibilities to work out an appropriate set of small weight changes, and put them into a common form:

If $out_j = targ_j$ do nothing — Note $targ_j - out_j = 0$

so $w_{ij} \rightarrow w_{ij}$

If $out_j = 1$ and $targ_j = 0$ — Note $targ_j - out_j = -1$

then $\sum in_i w_{ij}$ is too large

first when $in_i = 1$ decrease w_{ij}

so $w_{ij} \rightarrow w_{ij} - \eta = w_{ij} - \eta \, in_i$

and when $in_i = 0$ w_{ij} doesn't matter

so $w_{ij} \rightarrow w_{ij} - 0 = w_{ij} - \eta \, in_i$

so $w_{ij} \rightarrow w_{ij} - \eta \, in_i$

Convergence of Perceptron Learning

The weight changes Δw_{ij} need to be applied repeatedly – for each weight w_{ij} in the network, and for each training pattern in the training set. One pass through all the weights for the whole training set is called one ***epoch*** of training.

Eventually, usually after many epochs, when all the network outputs match the targets for all the training patterns, all the Δw_{ij} will be zero and the process of training will cease. We then say that the training process has ***converged*** to a solution.

It can be shown that if there does exist a possible set of weights for a Perceptron which solves the given problem correctly, then the Perceptron Learning Rule will find them in a finite number of iterations

Moreover, it can be shown that if a problem is linearly separable, then the Perceptron Learning Rule will find a set of weights in a finite number of iterations that solves the problem correctly.

Hebbian Learning

In 1949 neuropsychologist Donald Hebb postulated how biological neurons learn:

> "When an axon of cell A is near enough to excite a cell B and repeatedly or persistently takes part in firing it, some growth process or metabolic change takes place on one or both cells such that A's efficiency as one of the cells firing B, is increased."

In other words:

1. If two neurons on either side of a synapse (connection) are activated simultaneously (i.e. synchronously), then the strength of that synapse is selectively increased.

This rule is often supplemented by:

2. If two neurons on either side of a synapse are activated asynchronously, then that synapse is selectively weakened or eliminated.

so that chance coincidences do not build up connection strengths.

Hebbian versus Perceptron Learning

In the notation used for Perceptrons, the ***Hebbian learning*** weight update rule is:

$$\Delta w_{ij} = \eta \,.\, out_j \,.\, in_i$$

There is strong physiological evidence that this type of learning does take place in the region of the brain known as the *hippocampus*.

Recall that the ***Perceptron learning*** weight update rule we derived was:

$$\Delta w_{ij} = \eta .\, (targ_j - out_j) \,.\, in_i$$

There is some similarity, but it is clear that Hebbian learning is not going to get our Perceptron to learn a set of training data.

The are variations of Hebbian learning that do provide powerful learning techniques for biologically plausible networks, such as ***Contrastive Hebbian Learning***, but we shall adopt another approach for formulating learning algorithms for our networks.

Learning by Error Minimisation

The Perceptron Learning Rule is an algorithm for adjusting the network weights w_{ij} to minimise the difference between the actual outputs out_j and the desired outputs $targ_j$.

We can define an ***Error Function*** to quantify this difference:

$$E(w_{ij}) = \tfrac{1}{2} \sum_p \sum_j \left(targ_j - out_j \right)^2$$

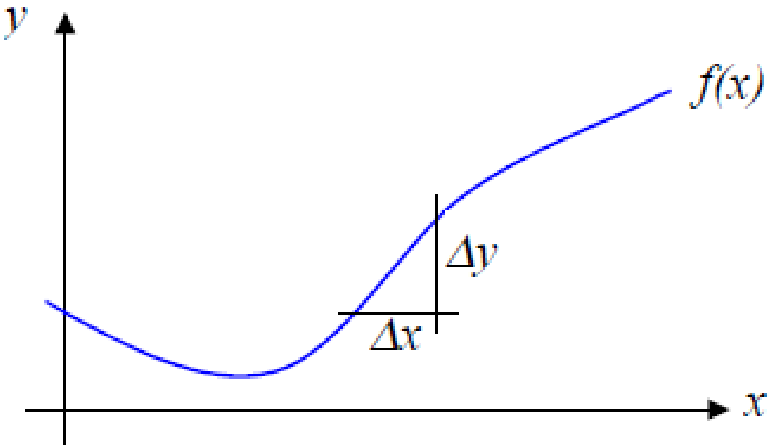
For obvious reasons this is known as the ***Sum Squared Error*** function. It is the total squared error summed over all output units j and all training patterns p.

The aim of ***learning*** is to minimise this error by adjusting the weights w_{ij}. Typically we make a series of small adjustments to the weights $w_{ij} \to w_{ij} + \Delta w_{ij}$ until the error $E(w_{ij})$ is 'small enough'.

A systematic procedure for doing this requires the knowledge of how the error $E(w_{ij})$ varies as we change the weights w_{ij}, i.e. the ***gradient*** of E with respect to w_{ij}.

Computing Gradients and Derivatives

There is a whole branch of mathematics concerned with computing gradients – it is known as ***Differential Calculus***. The basic idea is simple. Consider a function *y = f(x)*



The gradient, or rate of change, of *f(x)* at a particular value of *x*, as we change *x* can be approximated by *Δy/Δx*. Or we can write it exactly as

$$\frac{\partial f(x)}{\partial x} = \operatorname*{Lim}_{\Delta x \to 0} \frac{\Delta y}{\Delta x} = \operatorname*{Lim}_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

which is known as the ***partial derivative*** of *f(x)* with respect to *x*.

Examples of Computing Derivatives Analytically

Some simple examples should make this clearer:

$$f(x) = a.x + b \quad \Rightarrow \quad \frac{\partial f(x)}{\partial x} = \operatorname*{Lim}_{\Delta x \to 0} \frac{[a.(x+\Delta x)+b]-[a.x+b]}{\Delta x} = a$$

$$f(x) = a.x^2 \quad \Rightarrow \quad \frac{\partial f(x)}{\partial x} = \operatorname*{Lim}_{\Delta x \to 0} \frac{\left[a.(x+\Delta x)^2\right]-\left[a.x^2\right]}{\Delta x} = 2ax$$

$$f(x) = g(x) + h(x) \Rightarrow \frac{\partial f(x)}{\partial x} = \operatorname*{Lim}_{\Delta x \to 0} \frac{(g(x+\Delta x)+h(x+\Delta x))-(g(x)+h(x))}{\Delta x} = \frac{\partial g(x)}{\partial x} + \frac{\partial h(x)}{\partial x}$$

Other derivatives can be computed in the same way. Some useful ones are:

$$f(x) = a.x^n \Rightarrow \frac{\partial f(x)}{\partial x} = nax^{n-1}$$

$$f(x) = \log_e(x) \Rightarrow \frac{\partial f(x)}{\partial x} = \frac{1}{x}$$

$$f(x) = e^{ax} \Rightarrow \frac{\partial f(x)}{\partial x} = ae^{ax}$$

$$f(x) = \sin(x) \Rightarrow \frac{\partial f(x)}{\partial x} = \cos(x)$$

Gradient Descent Minimisation

Suppose we have a function *f(x)* and we want to change the value of *x* to minimise *f(x)*. What we need to do depends on the gradient of *f(x)*. There are three cases to consider:

If $\frac{\partial f}{\partial x} > 0$ then *f(x)* increases as *x* increases so we should decrease *x*

If $\frac{\partial f}{\partial x} < 0$ then *f(x)* decreases as *x* increases so we should increase *x*

If $\frac{\partial f}{\partial x} = 0$ then *f(x)* is at a maximum or minimum so we should not change *x*

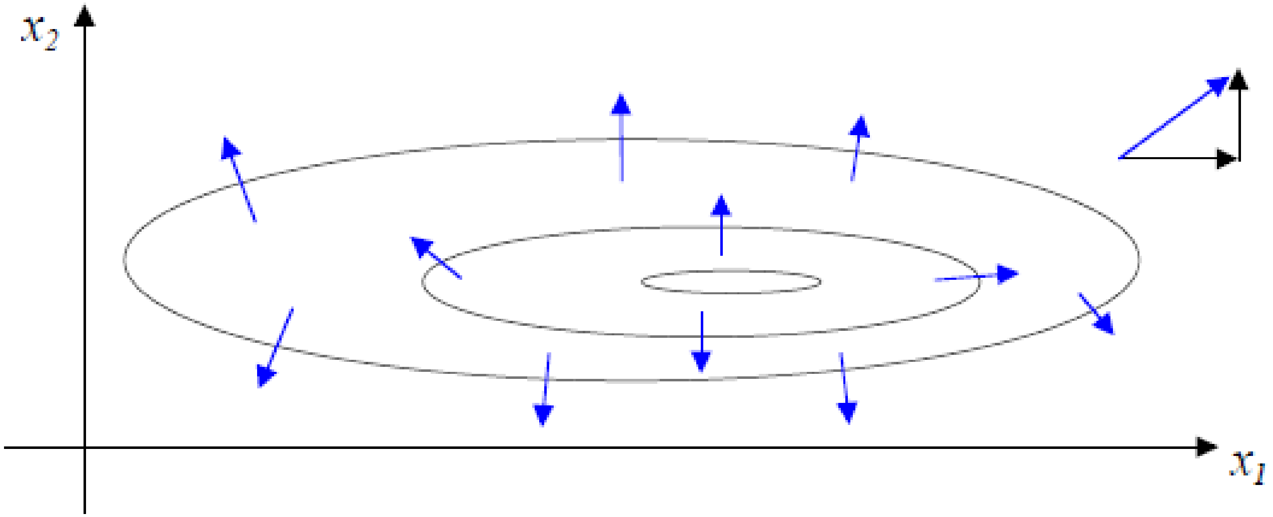
In summary, we can decrease *f(x)* by changing *x* by the amount:

$$\Delta x = x_{new} - x_{old} = -\eta \frac{\partial f}{\partial x}$$

where η is a small positive constant specifying how much we change *x* by, and the derivative $\partial f / \partial x$ tells us which direction to go in. If we repeatedly use this equation, *f(x)* will (assuming η is sufficiently small) keep descending towards its minimum, and hence this procedure is known as ***gradient descent minimisation***.

Gradients in More Than One Dimension

Is it obvious that we need the gradient/derivative itself in the weight update equation, rather than just the sign of the gradient? Consider the two dimensional function shown as a ***contour plot*** with its minimum inside the smallest ellipse:



A few representative gradient vectors are shown. By definition, they will always be perpendicular to the contours, and the closer the contours, the larger the vectors. It is now clear that we need to take the relative magnitudes of the x_1 and x_2 components of the gradient vectors into account if we are to head towards the minimum efficiently.

Gradient Descent Error Minimisation

Remember that we want to train our neural networks by adjusting their weights w_{ij} in order to minimise the error function:

$$E(w_{ij}) = \tfrac{1}{2}\sum_p \sum_j \left(targ_j - out_j\right)^2$$

We now see it makes sense to do this by a series of gradient descent weight updates:

$$\Delta w_{kl} = -\eta \frac{\partial E(w_{ij})}{\partial w_{kl}}$$

If the transfer function for the output neurons is *f(x)*, and the activations of the previous layer of neurons are in_i, then the outputs are $out_j = f(\sum_i in_i w_{ij})$, and

$$\Delta w_{kl} = -\eta \frac{\partial}{\partial w_{kl}} \left[\tfrac{1}{2}\sum_p \sum_j \left(targ_j - f(\sum_i in_i w_{ij}) \right)^2 \right]$$

Dealing with equations like this is easy if we use the chain rules for derivatives.

Chain Rules for Computing Derivatives

Computing complex derivatives can be done in stages. First, suppose *f(x) = g(x).h(x)*

$$\frac{\partial f(x)}{\partial x} = \operatorname*{Lim}_{\Delta x \to 0} \frac{g(x+\Delta x).h(x+\Delta x) - g(x).h(x)}{\Delta x} = \operatorname*{Lim}_{\Delta x \to 0} \frac{\left(g(x) + \frac{\partial g(x)}{\partial x}\Delta x\right).\left(h(x) + \frac{\partial h(x)}{\partial x}\Delta x\right) - g(x).h(x)}{\Delta x}$$

$$\frac{\partial f(x)}{\partial x} = \frac{\partial g(x)}{\partial x}h(x) + g(x)\frac{\partial h(x)}{\partial x}$$

We can similarly deal with nested functions. Suppose *f(x) = g(h(x))*

$$\frac{\partial f(x)}{\partial x} = \operatorname*{Lim}_{\Delta x \to 0} \frac{g(h(x+\Delta x)) - g(h(x))}{\Delta x} = \operatorname*{Lim}_{\Delta x \to 0} \frac{g(h(x) + \frac{\partial h(x)}{\partial x}\Delta x) - g(h(x))}{\Delta x}$$

$$\frac{\partial f(x)}{\partial x} = \operatorname*{Lim}_{\Delta x \to 0} \frac{g(h(x)) + \frac{\partial g(x)}{\partial h(x)}\Delta h(x) - g(h(x))}{\Delta x} = \operatorname*{Lim}_{\Delta x \to 0} \frac{g(h(x)) + \frac{\partial g(x)}{\partial h(x)}\left(\frac{\partial h(x)}{\partial x}\Delta x\right) - g(h(x))}{\Delta x}$$

$$\frac{\partial f(x)}{\partial x} = \frac{\partial g(h(x))}{\partial h(x)} \cdot \frac{\partial h(x)}{\partial x}$$

Using the Chain Rule on our Weight Update Equation

The algebra gets rather messy, but after repeated application of the chain rule, and some tidying up, we end up with a very simple weight update equation:

$$\Delta w_{kl} = -\eta \frac{\partial}{\partial w_{kl}} \left[\tfrac{1}{2} \sum_{p} \sum_{j} \left(targ_j - f\left(\sum_{i} in_i w_{ij}\right) \right)^2 \right]$$

$$\Delta w_{kl} = -\eta \left[\tfrac{1}{2} \sum_{p} \sum_{j} \frac{\partial}{\partial w_{kl}} \left(targ_j - f\left(\sum_{i} in_i w_{ij}\right) \right)^2 \right]$$

$$\Delta w_{kl} = -\eta \left[\tfrac{1}{2} \sum_{p} \sum_{j} 2 \left(targ_j - f\left(\sum_{i} in_i w_{ij}\right) \right) \left(-\frac{\partial}{\partial w_{kl}} f\left(\sum_{m} in_m w_{mj}\right) \right) \right]$$

$$\Delta w_{kl} = \eta \left[\sum_{p} \sum_{j} \left(targ_j - f\left(\sum_{i} in_i w_{ij}\right) \right) \left(f'\left(\sum_{n} in_n w_{nj}\right) \frac{\partial}{\partial w_{kl}} \left(\sum_{m} in_m w_{mj}\right) \right) \right]$$

$$\Delta w_{kl} = \eta\left[\sum_p\sum_j\left(targ_j - f(\sum_i in_i w_{ij})\right)\left(f'(\sum_n in_n w_{nj})(\sum_m in_m \frac{\partial w_{mj}}{\partial w_{kl}})\right)\right]$$

$$\Delta w_{kl} = \eta\left[\sum_p\sum_j\left(targ_j - f(\sum_i in_i w_{ij})\right)\left(f'(\sum_n in_n w_{ij})(\sum_m in_m \delta_{mk}\delta_{jl})\right)\right]$$

$$\Delta w_{kl} = \eta\left[\sum_p\sum_j\left(targ_j - f(\sum_i in_i w_{ij})\right)\left(f'(\sum_n in_n w_{nj})(in_k \delta_{jl})\right)\right]$$

$$\Delta w_{kl} = \eta\left[\sum_p\left(targ_l - f(\sum_i in_i w_{il})\right)\left(f'(\sum_n in_n w_{nl})(in_k)\right)\right]$$

$$\Delta w_{kl} = \eta\sum_p (targ_l - out_l).f'(\sum_n in_n w_{nl}).in_k$$

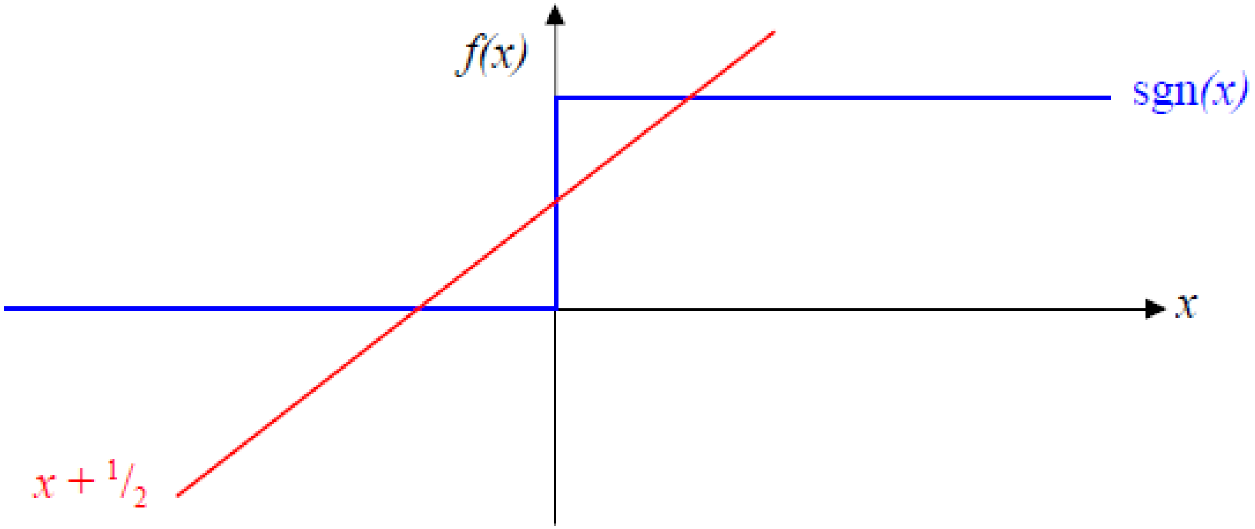
The *prime notation* is defined such that f' is the derivative of f. We have also used the *Kronecker Delta* symbol δ_{ij} defined such that $\delta_{ij} = 1$ when $i = j$ and $\delta_{ij} = 0$ when $i \neq j$.

The Delta Rule

We now have the basic gradient descent learning algorithm for single layer networks:

$$\Delta w_{kl} = \eta \sum_{p} \left(targ_l - out_l \right).f'(\sum_{i} in_i w_{il}).in_k$$

Notice that it still involves the derivative of the transfer function *f(x)*. This is clearly problematic for the simple Perceptron that uses the step function sgn(x) as its threshold function, because this has zero derivative everywhere except at $x = 0$ where it is infinite.



Fortunately, there is a ***clever trick*** we can use that will be apparent from the above graph. Suppose we had the transfer $f(x) = x + {}^1/_2$, then when the target is 1 the network will learn $x = {}^1/_2$, and when the target is 0 it will learn $x = -{}^1/_2$. It is clear that these values will also result in the right values of sgn(x), and so the Perceptron will work properly.

In other words, we can use the gradient descent learning algorithm with $f(x) = x + {}^1/_2$ to get our Perceptron to learn the right weights. In this case $f'(x) = 1$ and so the weight update equation becomes:

$$\Delta w_{kl} = \eta \sum_p \left(targ_l - out_l \right).in_k$$

This is known as the ***Delta Rule*** because it depends on the discrepancy

$$\delta_l = targ_l - out_l$$

Delta Rule vs. Perceptron Learning Rule

We can see that the Delta Rule and the Perceptron Learning Rule for training Single Layer Perceptrons have exactly the same weight update equation:

$$\Delta w_{kl} = \eta \sum_{p} \left(targ_l - f\left(\sum_i in_i w_{il} \right) \right) .in_k$$

However, there are significant underlying differences. The Perceptron Learning Rule uses the actual activation function $f(x) = \mathrm{sgn}(x)$, whereas the Delta Rule uses the linear function $f(x) = x + {}^1/_2$. The two algorithms were also obtained from very different theoretical starting points. The Perceptron Learning Rule was derived from a consideration of how we should shift around the decision hyper-planes, while the Delta Rule emerged from a gradient descent minimisation of the Sum Squared Error.

The Perceptron Learning Rule will converge to zero error and no weight changes in a finite number of steps if the problem is linearly separable, but otherwise the weights will keep oscillating. On the other hand, the Delta Rule will (for sufficiently small η) always converge to a set of weights for which the error is a minimum, though the convergence to the precise values of $x = \pm{}^1/_2$ will generally proceed at an ever decreasing rate.

Gradient Descent Learning

It is worth summarising all the factors involved in Gradient Descent Learning:

1. The purpose of neural network learning or training is to minimise the output errors on a particular set of training data by adjusting the network weights w_{ij}.
2. We define an Error Function $E(w_{ij})$ that "measures" how far the current network is from the desired (correctly trained) one.
3. Partial derivatives of the error function $\partial E(w_{ij})/\partial w_{ij}$ tell us which direction we need to move in weight space to reduce the error.
4. The learning rate η specifies the step sizes we take in weight space for each iteration of the weight update equation.
5. We keep stepping through weight space until the errors are 'small enough'.
6. If we choose neuron activation functions with derivatives that take on particularly simple forms, we can make the weight update computations very efficient.

These factors lead to powerful learning algorithms for training our neural networks:

Training a Single Layer Feed-forward Network

Now we understand how gradient descent weight update rules can lead to minimisation of a neural network's output errors, it is straightforward to train any network:

1. Take the set of training patterns you wish the network to learn

   $\{in_i^p, out_j^p : i = 1 \ldots ninputs, j = 1 \ldots noutputs, p = 1 \ldots npatterns\}$

2. Set up your network with *ninputs* input units fully connected to *noutputs* output units via connections with weights w_{ij}

3. Generate random initial weights, e.g. from the range [–*smwt*, +*smwt*]

4. Select an appropriate error function $E(w_{ij})$ and learning rate η

5. Apply the weight update $\Delta w_{ij} = -\eta \, \partial E(w_{ij})/\partial w_{ij}$ to each weight w_{ij} for each training pattern *p*. One set of updates of all the weights for all the training patterns is called one ***epoch*** of training.

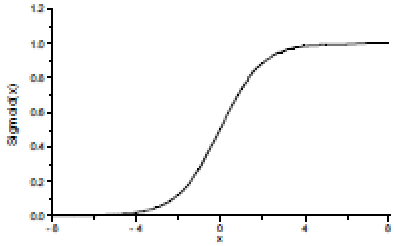
6. Repeat step 5 until the network error function is 'small enough'.

You thus end up with a trained neural network. But step 5 can still be difficult…

The Derivative of a Sigmoid

We noted earlier that the Sigmoid is a smooth (i.e. differentiable) threshold function:

$$f(x) = \text{Sigmoid}(x) = \frac{1}{1+e^{-x}}$$

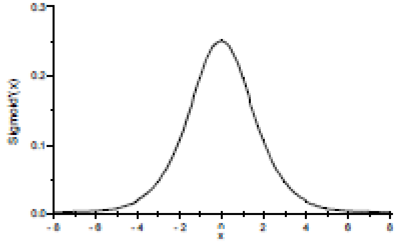


We can use the chain rule by putting *f(x)* = *g(h(x))* with *g(h)* = h^{-1} and *h(x)* = 1 + e^{-x} so

$$\frac{\partial g(h)}{\partial h} = -\frac{1}{h^2} \quad \text{and} \quad \frac{\partial h(x)}{\partial x} = -e^{-x}$$

$$\frac{\partial f(x)}{\partial x} = -\frac{1}{(1+e^{-x})^2} \cdot (-e^{-x}) = \left(\frac{1}{1+e^{-x}}\right) . \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)$$

$$f'(x) = \frac{\partial f(x)}{\partial x} = f(x).(1-f(x))$$



This simple relation will make our equations much easier and save a lot of computing time!

The Generalised Delta Rule

We can avoid using tricks for deriving gradient descent learning rules, by making sure we use a differentiable activation function such as the Sigmoid. This is also more like the threshold function used in real brains, and has several other nice mathematical properties.

If we use the Sigmoid activation function, a single layer network has outputs given by

$$out_l = \mathrm{Sigmoid}(\sum_i in_i w_{il})$$

and, due to the properties of the Sigmoid derivative, the general weight update equation

$$\Delta w_{kl} = \eta \sum_p \left(targ_l - out_l\right).f'(\sum_i in_i w_{il}).in_k$$

simplifies so that it only contains neuron activations and no derivatives:

$$\Delta w_{kl} = \eta \sum_p \left(targ_l - out_l\right).out_l.(1 - out_l).in_k$$

This is known as the ***Generalized Delta Rule*** for training sigmoidal networks.

Practical Considerations for Gradient Descent Learning

From the above discussion, it is clear that there remain a number of important questions about training single layer neural networks that still need to be resolved:

1. Do we need to pre-process the training data? If so, how?
2. How do we choose the initial weights from which we start the training?
3. How do we choose an appropriate learning rate η?
4. Should we change the weights after each training pattern, or after the whole set?
5. Are some activation/transfer functions better than others?
6. How can we avoid flat spots in the error function?
7. How can we avoid local minima in the error function?
8. How do we know when we should stop the training?

Pre-processing the Training Data

In principle, we can just use any raw input-output data to train our networks. However, in practice, it often helps the network to learn appropriately if we carry out some pre-processing of the training data before feeding it to the network.

We should make sure that the training data is representative – it should not contain too many examples of one type at the expense of another. On the other hand, if one class of pattern is easy to learn, having large numbers of patterns from that class in the training set will only slow down the over-all learning process.

If the training data is continuous, rather than binary, it is generally a good idea to re-scale the input values. Simply shifting the zero of the scale so that the mean value of each input is near zero, and normalising so that the standard deviation of the values for each input are roughly the same, can make a big difference. It will require more work, but de-correlating the inputs before normalising is often also worthwhile.

If we are using on-line training rather than batch training, we should usually make sure we shuffle the order of the training data each epoch.

Choosing the Initial Weights

The gradient descent learning algorithm treats all the weights in the same way, so if we start them all off with the same values, all the hidden units will end up doing the same thing and the network will never learn properly.

For that reason, we generally start off all the weights with small random values. Usually we take them from a flat distribution around zero [–*smwt*, +*smwt*], or from a Gaussian distribution around zero with standard deviation *smwt*.

Choosing a good value of *smwt* can be difficult. Generally, it is a good idea to make it as large as you can without saturating any of the sigmoids.

We usually hope that the final network performance will be independent of the choice of initial weights, but we need to check this by training the network from a number of different random initial weight sets.

In networks with hidden layers, there is no real significance to the order in which we label the hidden neurons, so we can expect very different final sets of weights to emerge from the learning process for different choices of random initial weights.

Choosing the Learning Rate

Choosing a good value for the learning rate η is constrained by two opposing facts:

1. If η is too small, it will take too long to get anywhere near the minimum of the error function.
2. If η is too large, the weight updates will over-shoot the error minimum and the weights will oscillate, or even diverge.

Unfortunately, the optimal value is very problem and network dependent, so one cannot formulate reliable general prescriptions. Generally, one should try a range of different values (e.g. $\eta = 0.1, 0.01, 1.0, 0.0001$) and use the results as a guide.

There is no necessity to keep the learning rate fixed throughout the learning process. Typical variable learning rates that prove advantageous are:

$$\eta(t) = \frac{\eta(1)}{t} \qquad\qquad \eta(t) = \frac{\eta(0)}{1 + t/\tau}$$

Similar age dependent learning rates are found to exist in human children.

Batch Training *vs.* On-line Training

The gradient descent learning algorithm contains a sum over all training patterns *p*

$$\Delta w_{kl} = \eta \sum_p \left(targ_l - out_l \right).f'(\sum_i in_i w_{il}).in_k$$

When we add up the weight changes for all the training patterns like this, and apply them in one go, it is called ***Batch Training***.

A natural alternative is to update all the weights immediately after processing each training pattern. This is called ***On-line Training*** (or ***Sequential Training***).

On-line learning does not perform true gradient descent, and the individual weight changes can be rather erratic. Normally a much lower learning rate η will be necessary than for batch learning. However, because each weight now has *npatterns* updates per epoch, rather than just one, overall the learning is often much quicker. This is particularly true if there is a lot of redundancy in the training data, i.e. many training patterns containing similar information.

Choosing the Transfer Function

We have already seen that having a differentiable transfer/activation function is important for the gradient descent algorithm to work. We have also seen that, in terms of computational effeciency, the standard sigmoid (i.e. logistic function) is a particularly convenient replacement for the step function of the Simple Perceptron.

The logistic function ranges from 0 to 1. There is some evidence that an anti-symmetric transfer function, i.e. one that satisfies $f(-x) = -f(x)$, enables the gradient descent algorithm to learn faster. To do this we must use targets of +1 and –1 rather than 0 and 1. A convenient alternative to the logistic function is then the hyperbolic tangent

$$f(x) = \tanh(x) \qquad f(-x) = -f(x) \qquad f'(x) = 1 - f(x)^2$$

which, like the logistic function, has a particularly simple derivative.

When the outputs are required to be non-binary, i.e. continuous real values, having sigmoidal transfer functions no longer makes sense. In these cases, a simple linear transfer function $f(x) = x$ is appropriate.

Classification Outputs as Probabilities

Another powerful feature of neural network classification systems is that non-binary outputs can be interpreted as the probabilities of the corresponding classifications. For example, an output of 0.9 on a unit corresponding to a particular class would indicate a 90% chance that the input data represents a member of that class.

The mathematics is rather complex, but one can show that for two classes represented as activations of 0 and 1 on a single output unit, the activation function that allows us to do this is none other than our ***Sigmoid*** activation function.

If we have more than two classes, and use one output unit for each class, we should employ a generalization of the Sigmoid known as the ***Softmax*** activation function:

$$out_j = e^{-\sum_i in_i w_{ij}} \Big/ \sum_k e^{-\sum_n in_n w_{nk}}$$

In either case, we use a ***Cross Entropy*** error measure rather than Sum Squared Error.

Flat Spots in the Error Function

The gradient descent weight changes depend on the gradient of the error function. Consequently, if the error function has flat spots, the learning algorithm can take a long time to pass through them.

A particular problem with the sigmoidal transfer functions is that the derivative tends to zero as it saturates (i.e. gets towards 0 or 1). This means that if the outputs are totally wrong (i.e. 0 instead of 1, or 1 instead of 0), the weight updates are very small and the learning algorithm cannot easily correct itself. There are two simple solutions:

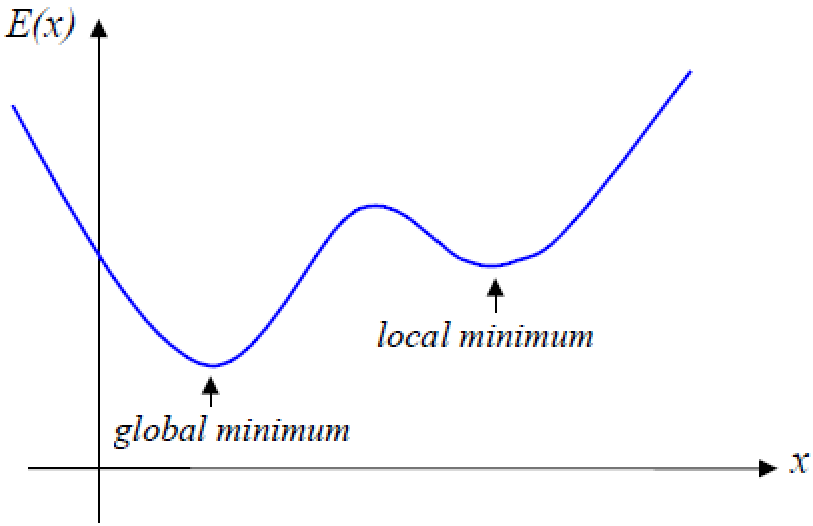
Target Off-sets Use targets of 0.1 and 0.9 (say) instead of 0 and 1. The sigmoids will no longer saturate and the learning will no longer get stuck.

Sigmoid Prime Off-set Add a small off-set (of 0.1 say) to the sigmoid prime (i.e. the sigmoid derivative) so that it is no longer zero when the sigmoids saturate.

We can now see why we should keep the initial network weights small enough that the sigmoids are not saturated before training. Off-setting the targets also has the effect of stopping the network weights growing too large.

Local Minima

Error functions can quite easily have more than one minimum:



If we start off in the vicinity of the local minimum, we may end up at the local minimum rather than the global minimum. Starting with a range of different initial weight sets increases our chances of finding the global minimum. Any variation from true gradient descent will also increase our chances of stepping into the deeper valley.

When to Stop Training

The Sigmoid(x) function only takes on its extreme values of 0 and 1 at $x = \pm\infty$. In effect, this means that the network can only achieve its binary targets when at least some of its weights reach $\pm\infty$. So, given finite gradient descent step sizes, our networks will never reach their binary targets.

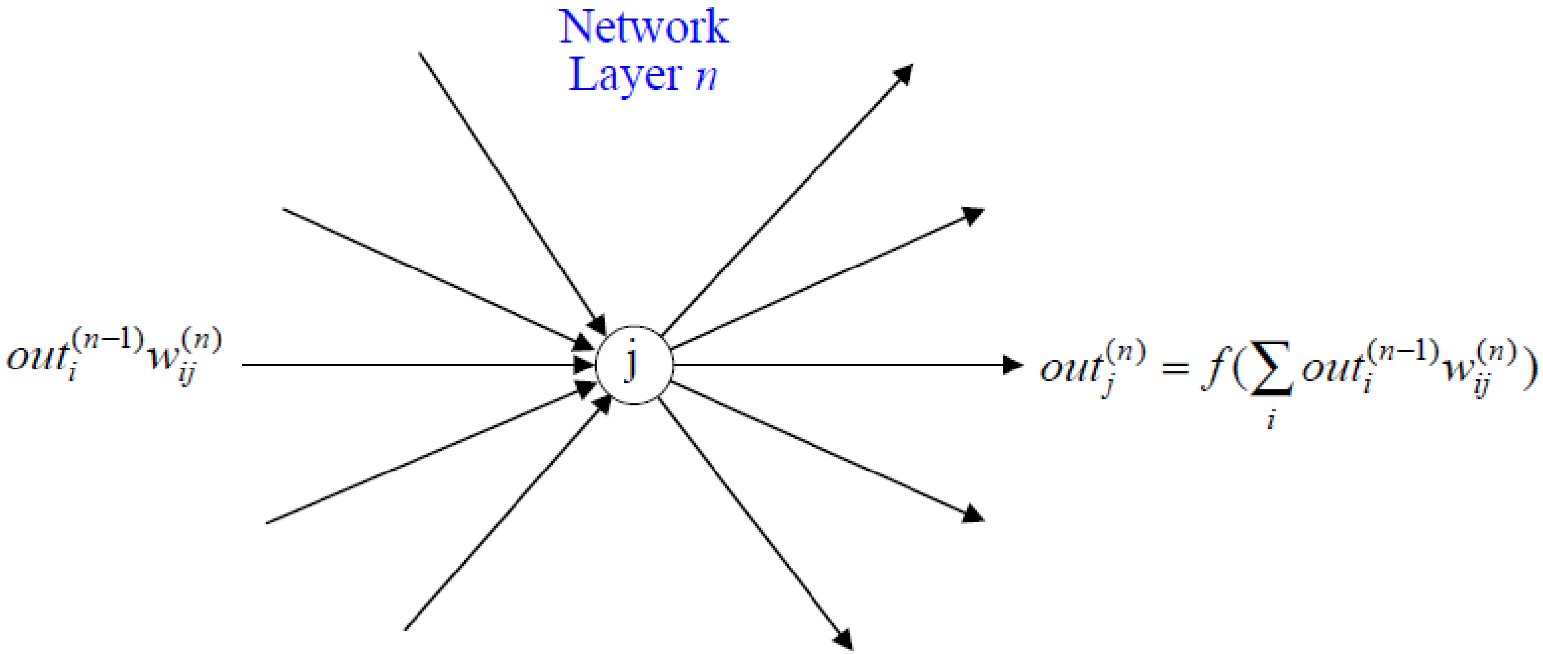
Even if we off-set the targets (to 0.1 and 0.9 say) we will generally require an infinite number of increasingly small gradient descent steps to achieve those targets.

Clearly, if the training algorithm can never actually reach the minimum, we have to stop the training process when it is 'near enough'. What constitutes 'near enough' depends on the problem. If we have binary targets, it might be enough that all outputs are within 0.1 (say) of their targets. Or, it might be easier to stop the training when the sum squared error function becomes less than a particular small value (0.2 say).

We shall see later that, when we have noisy training data, the training set error and the generalization error are related, and an appropriate stopping criteria will emerge in order to optimize the network's generalization ability.

Notation for Multi-Layer Networks

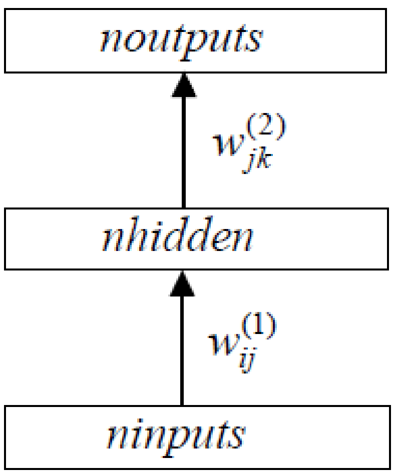
Dealing with multi-layer networks is easy if we use a sensible notation. We simply need another label *(n)* to tell us which layer in the network we are dealing with:


Network
Layer n
$out_i^{(n-1)} w_{ij}^{(n)}$
j
$out_j^{(n)} = f(\sum_i out_i^{(n-1)} w_{ij}^{(n)})$

Each unit j in layer n receives activations $out_i^{(n-1)} w_{ij}^{(n)}$ from the previous layer of processing units and sends activations $out_j^{(n)}$ to the next layer of units.

Multi-Layer Perceptrons (MLPs)

Conventionally, the input layer is layer 0, and when we talk of an *N* layer network we mean there are *N* layers of weights and *N* non-input layers of processing units. Thus a two layer Multi-Layer Perceptron takes the form:



noutputs

$w_{jk}^{(2)}$

nhidden

$w_{ij}^{(1)}$

ninputs

$$out_k^{(2)} = f(\sum_j out_j^{(1)} w_{jk}^{(2)})$$

$$out_j^{(1)} = f(\sum_i out_i^{(0)} w_{ij}^{(1)})$$

$$out_i^{(0)} = in_i$$

It is clear how we can add in further layers, though for most practical purposes two layers will be sufficient. Note that there is nothing stopping us from having different activation functions *f(x)* for different layers, or even different units within a layer.

Learning in Multi-Layer Perceptrons

We can use the same ideas as before to train our *N*-layer neural networks. We want to adjust the network weights $w_{ij}^{(n)}$ in order to minimise the sum-squared error function

$$E(w_{ij}^{(n)}) = \tfrac{1}{2}\sum_{p}\sum_{j}\left(targ_j^p - out_j^{(N)}(in_i^p)\right)^2$$

and again we can do this by a series of gradient descent weight updates

$$\Delta w_{kl}^{(m)} = -\eta \frac{\partial E(w_{ij}^{(n)})}{\partial w_{kl}^{(m)}}$$

Note that it is only the outputs $out_j^{(N)}$ of the final layer that appear in the error function. However, the final layer outputs will depend on all the earlier layers of weights, and the learning algorithm will adjust them all.

The learning algorithm automatically adjusts the outputs $out_j^{(n)}$ of the earlier (hidden) layers so that they form appropriate intermediate (hidden) representations.

Computing the Partial Derivatives

For a two layer network, the final outputs can be written:

$$out_k^{(2)} = f\left(\sum_j out_j^{(1)}.w_{jk}^{(2)}\right) = f\left(\sum_j f\left(\sum_i in_i w_{ij}^{(1)}\right).w_{jk}^{(2)}\right)$$

We can then use the chain rules for derivatives, as for the Single Layer Perceptron, to give the derivatives with respect to the two sets of weights $w_{hl}^{(1)}$ and $w_{hl}^{(2)}$:

$$\frac{\partial E(w_{ij}^{(n)})}{\partial w_{hl}^{(m)}} = -\sum_p \sum_k \left(targ_k - out_k^{(2)}\right).\frac{\partial out_k^{(2)}}{\partial w_{hl}^{(m)}}$$

$$\frac{\partial out_k^{(2)}}{\partial w_{hl}^{(2)}} = f'\left(\sum_j out_j^{(1)} w_{jk}^{(2)}\right).out_h^{(1)}.\delta_{kl}$$

$$\frac{\partial out_k^{(2)}}{\partial w_{hl}^{(1)}} = f'\left(\sum_j out_j^{(1)} w_{jk}^{(2)}\right).f'\left(\sum_i in_i w_{il}^{(1)}\right).w_{lk}^{(2)}.in_h$$

Deriving the Back Propagation Algorithm

All we now have to do is substitute our derivatives into the weight update equations

$$\Delta w_{hl}^{(2)} = \eta \sum_p \left(targ_l - out_l^{(2)}\right).f'\left(\sum_j out_j^{(1)} w_{jl}^{(2)}\right).out_h^{(1)}$$

$$\Delta w_{hl}^{(1)} = \eta \sum_p \sum_k \left(targ_k - out_k^{(2)}\right).f'\left(\sum_j out_j^{(1)} w_{jk}^{(2)}\right).f'\left(\sum_i in_i w_{il}^{(1)}\right).w_{lk}^{(2)}.in_h$$

Then if the transfer function $f(x)$ is a Sigmoid we can use $f'(x) = f(x).(1 - f(x))$ to give

$$\Delta w_{hl}^{(2)} = \eta \sum_p \left(targ_l - out_l^{(2)}\right).out_l^{(2)}.\left(1 - out_l^{(2)}\right).out_h^{(1)}$$

$$\Delta w_{hl}^{(1)} = \eta \sum_p \sum_k \left(targ_k - out_k^{(2)}\right).out_k^{(2)}.\left(1 - out_k^{(2)}\right).w_{lk}^{(2)}.out_l^{(1)}.\left(1 - out_l^{(1)}\right).in_h$$

These equations constitute the basic Back-Propagation Learning Algorithm.

Simplifying the Computation

When implementing the Back-Propagation algorithm it is convenient to define

$$delta_k^{(2)} = \left(targ_k - out_k^{(2)}\right).f'\left(\sum_j out_j^{(1)} w_{jk}^{(2)}\right) = \left(targ_k - out_k^{(2)}\right).out_k^{(2)}.\left(1 - out_k^{(2)}\right)$$

which is a generalised output deviation. We can then write the weight update rules as

$$\Delta w_{hl}^{(2)} = \eta \sum_p delta_l^{(2)}.out_h^{(1)}$$

$$\Delta w_{hl}^{(1)} = \eta \sum_p \left(\sum_k delta_k^{(2)}.w_{lk}^{(2)} \right) out_l^{(1)}.\left(1 - out_l^{(1)}\right).in_h$$

So the weight $w_{hl}^{(2)}$ between units h and l is changed in proportion to the output of unit h and the *delta* of unit l. The weight changes at the first layer now take on the same form as the final layer, but the 'error' at each unit l is ***back-propagated*** from each of the output units k via the weights $w_{lk}^{(2)}$.

Networks With Any Number of Hidden Layers

It is now becoming clear that, with the right notation, it is easy to extend our gradient descent algorithm to work for any number of hidden layers. We define

$$delta_k^{(N)} = \left(targ_k - out_k^{(N)}\right).f'\left(\sum_j out_j^{(1)} w_{jk}^{(N)}\right) = \left(targ_k - out_k^{(N)}\right).out_k^{(N)}.\left(1 - out_k^{(N)}\right)$$

as the delta for the output layer, and then back-propagate the deltas to earlier layers using

$$delta_k^{(n)} = \left(\sum_k delta_k^{(n+1)}.w_{lk}^{(n+1)}\right).f'\left(\sum_j out_j^{(n-1)} w_{jk}^{(n)}\right) = \left(\sum_k delta_k^{(n+1)}.w_{lk}^{(n+1)}\right).out_k^{(n)}.\left(1 - out_k^{(n)}\right)$$

Then each weight update equation can be written as:

$$\Delta w_{hl}^{(n)} = \eta \sum_p delta_l^{(n)}.out_h^{(n-1)}$$

The Cross Entropy Error Function

We have talked about using the ***Sum Squared Error (SSE)*** function as a measure of network performance, and as a basis for gradient descent learning algorithms. A useful alternative for classification networks is the ***Cross Entropy (CE)*** error function

$$E_{ce}(w_{ij}) = -\sum_p \sum_j \left[targ_j^p . \log\left(out_j(in_i^p)\right) + \left(1 - targ_j^p\right) . \log\left(1 - out_j(in_i^p)\right) \right]$$

This is appropriate if we want to interpret the network outputs as probabilities, and has several advantages over the *SSE* function. When we compute the partial derivatives for the gradient descent weight update equations, the sigmoid derivative cancels out leaving

$$\Delta w_{hl}^{(N)} = \eta \sum_p \left(targ_l - out_l^{(N)} \right) . out_h^{(N-1)}$$

which is easier to compute than the *SSE* equivalent, and no longer has the property of going to zero when the outputs are totally wrong (so no need for offsets, etc.).

The Need For Non-Linearity

We have noted that if the network outputs are non-binary, then it is appropriate to have a linear output activation function rather than a Sigmoid. So why not use linear activation functions on the hidden layers as well?

Recall that for an activation functions $f^{(n)}(x)$ at layer n, the outputs are given by

$$out_k^{(2)} = f^{(2)}\left(\sum_j out_j^{(1)}.w_{jk}^{(2)}\right) = f^{(2)}\left(\sum_j f^{(1)}\left(\sum_i in_i w_{ij}^{(1)}\right).w_{jk}^{(2)}\right)$$

so if the hidden layer activation is linear, i.e. $f^{(1)}(x) = x$, this simplifies to

$$out_k^{(2)} = f^{(2)}\left(\sum_i in_i.\left(\sum_j w_{ij}^{(1)} w_{jk}^{(2)}\right)\right)$$

But this is equivalent to a single layer network with weights $w_{ik} = \sum_j w_{ij}^{(1)} w_{jk}^{(2)}$ and we know that such a network cannot deal with non-linearly separable problems.

Training a Two-Layer Feed-forward Network

The training procedure for two layer networks is similar to that for single layer networks:

1. Take the set of training patterns you wish the network to learn

   $\{in_i^p, out_j^p : i = 1 \ldots ninputs, j = 1 \ldots noutputs, p = 1 \ldots npatterns\}$.

2. Set up your network with *ninputs* input units fully connected to *nhidden* non-linear hidden units via connections with weights $w_{ij}^{(1)}$, which in turn are fully connected to *noutputs* output units via connections with weights $w_{jk}^{(2)}$.

3. Generate random initial weights, e.g. from the range [–*smwt*, +*smwt*]

4. Select an appropriate error function $E(w_{jk}^{(n)})$ and learning rate η.

5. Apply the weight update equation $\Delta w_{jk}^{(n)} = -\eta \partial E(w_{jk}^{(n)}) / \partial w_{jk}^{(n)}$ to each weight $w_{jk}^{(n)}$ for each training pattern p. One set of updates of all the weights for all the training patterns is called one *epoch* of training.

6. Repeat step 5 until the network error function is 'small enough'.

Practical Considerations for Back-Propagation Learning

Most of the practical considerations necessary for general Back-Propagation learning were already covered when we talked about training single layer Perceptrons:

1. Do we need to pre-process the training data? If so, how?
2. How do we choose the initial weights from which we start the training?
3. How do we choose an appropriate learning rate η?
4. Should we change the weights after each training pattern, or after the whole set?
5. Are some activation/transfer functions better than others?
6. How can we avoid flat spots in the error function?
7. How can we avoid local minima in the error function?
8. How do we know when we should stop the training?

However, there are also two important issues that were not covered before:

9. How many hidden units do we need?
10. Should we have different learning rates for the different layers?

How Many Hidden Units?

The best number of hidden units depends in a complex way on many factors, including:

1. The number of training patterns
2. The numbers of input and output units
3. The amount of noise in the training data
4. The complexity of the function or classification to be learned
5. The type of hidden unit activation function
6. The training algorithm

Too few hidden units will generally leave high training and generalisation errors due to under-fitting. Too many hidden units will result in low training errors, but will make the training unnecessarily slow, and will result in poor generalisation unless some other technique (such as *regularisation*) is used to prevent over-fitting.

Different Learning Rates for Different Layers?

A network as a whole will usually learn most efficiently if all its neurons are learning at roughly the same speed. So maybe different parts of the network should have different learning rates η. There are a number of factors that may affect the choices:

1. The later network layers (nearer the outputs) will tend to have larger local gradients (*deltas*) than the earlier layers (nearer the inputs).
2. The activations of units with many connections feeding into or out of them tend to change faster than units with fewer connections.
3. Activations required for linear units will be different for Sigmoidal units.
4. There is empirical evidence that it helps to have different learning rates η for the thresholds/biases compared with the real connection weights.

In practice, it is often quicker to just use the same rates η for all the weights and thresholds, rather than spending time trying to work out appropriate differences. A very powerful approach is to use evolutionary strategies to determine good learning rates.

A Statistical View of the Training Data

Suppose we have a ***training data set*** *D* for our neural network:

$$D = \{\ x_i^p, y^p : i = 1 \ \ldots\ ninputs, p = 1\ \ldots\ npatterns\ \}$$

This consists of an output y^p for each input pattern x_i^p. To keep the notation simple we shall assume we only have one output unit – the extension to many outputs is obvious.

Generally, the training data will be generated by some actual function $g(x_i)$ plus random noise ε^p (which may, for example, be due to data gathering errors), so

$$y^p = g(x_i^p) + \varepsilon^p$$

We call this a ***regressive model*** of the data. We can define a statistical expectation operator $\mathcal{E}$ that averages over all possible training patterns, so

$$g(x_i) = \mathcal{E}[y \mid x_i]$$

We say that the regression function $g(x_i)$ is the *conditional mean of the model output y given the inputs* x_i.

A Statistical View of Network Training

The neural network training problem is to construct an output function $net(x_i, W, D)$ of the network weights $W = \{w_{ij}^{(n)}\}$, based on the data D, that best approximates the regression model, i.e. the underlying function $g(x_i)$.

We have seen how to train a network by minimising the sum-squared error cost function:

$$E(W) = \frac{1}{2} \sum_{p \in D} \left(y^p - net(x_i^p, W, D) \right)^2$$

with respect to the network weights $W = \{w_{ij}^{(n)}\}$. However, we have also observed that, to get good generalisation, we do not necessarily want to achieve that minimum. What we really want to do is minimise the difference between the network's outputs $net(x_i, W, D)$ and the underlying function $g(x_i) = \mathcal{E}[y \mid x_i]$.

The natural sum-squared error function, i.e. $\left(\mathcal{E}[y \mid x_i] - net(x_i, W, D) \right)^2$, depends on the specific training set D, and we really want our network training regime to produce good results averaged over all possible noisy training sets.

Bias and Variance

If we define the expectation or average operator $\mathcal{E}_D$ which takes the ***ensemble average*** over all possible training sets D, then some rather messy algebra allows us to show that:

$$\mathcal{E}_D\left[\left(\mathcal{E}[y \mid x_i] - net(x_i, W, D)\right)^2\right]$$

$$= \left(\mathcal{E}_D\left[net(x_i, W, D)\right] - \mathcal{E}[y \mid x_i]\right)^2 + \mathcal{E}_D\left[\left(net(x_i, W, D) - \mathcal{E}_D\left[net(x_i, W, D)\right]\right)^2\right]$$

$$= \qquad \text{(bias)}^2 \qquad + \qquad \text{(variance)}$$

This error function consists of two positive components:

(bias)² the difference between the average network output $\mathcal{E}_D[net(x_i, W, D)]$ and the regression function $g(x_i) = \mathcal{E}[y \mid x_i]$. This can be viewed as the ***approximation error***.

(variance) the variance of the approximating function $net(x_i, W, D)$ over all the training sets D. It represents the ***sensitivity*** of the results on the particular choice of data D.

In practice there will always be a trade-off between these two error components.

The Extreme Cases of Bias and Variance

We can best understand the concepts of ***bias*** and ***variance*** by considering the two extreme cases of what the network might learn.

Suppose our network is lazy and just generates the same constant output whatever training data we give it, i.e. $net(x_i, W, D) = c$. In this case the variance term will be zero, but the bias will be large, because the network has made no attempt to fit the data.

Suppose our network is very hard working and makes sure that it fits every data point:

$$\mathcal{E}_D\left[net(x_i, W, D)\right] = \mathcal{E}_D\left[y(x_i)\right] = \mathcal{E}_D\left[g(x_i) + \varepsilon\right] = \mathcal{E}[y \mid x_i]$$

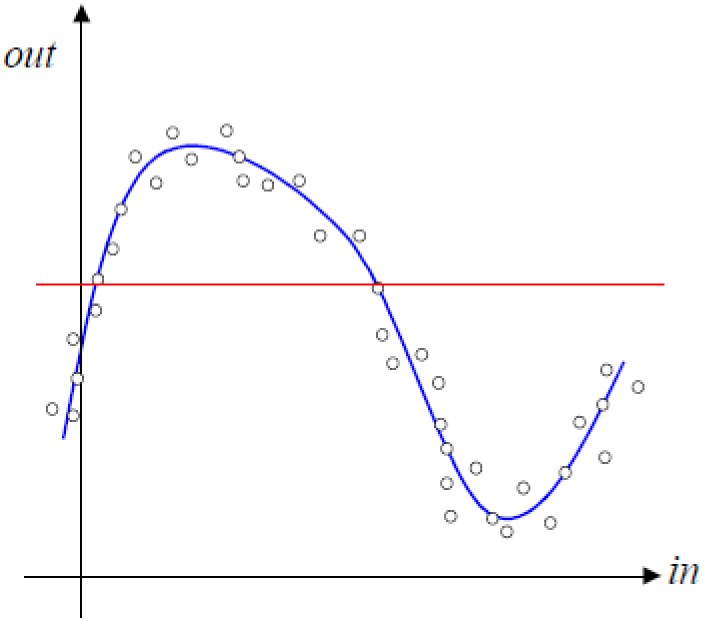
so the bias is zero, but the variance is:

$$\mathcal{E}_D\left[\left(net(x_i, W, D) - \mathcal{E}_D\left[net(x_i, W, D)\right]\right)^2\right] = \mathcal{E}_D\left[\left(g(x_i) + \varepsilon - \mathcal{E}_D\left[g(x_i) + \varepsilon\right]\right)^2\right] = \mathcal{E}_D\left[(\varepsilon)^2\right]$$

i.e. the variance of the noise on the data, which could be substantial.

Examples of the Two Extreme Cases

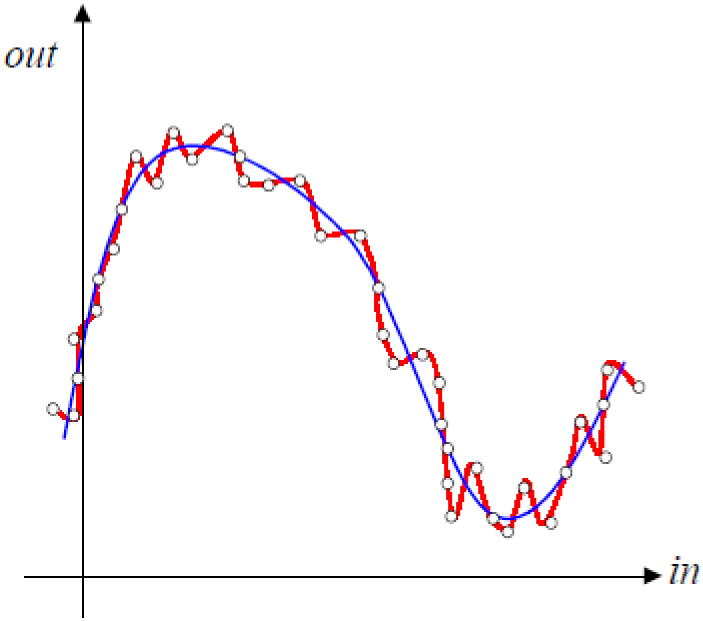
The lazy and hard-working networks approach our function approximation as follows:



Ignore the data ⇒

Big approximation errors (high bias)

No variation between data sets (no variance)



Get every data point ⇒

No approximation errors (zero bias)

Variation between data sets (high variance)

Under-fitting, Over-fitting and the Bias/Variance Trade-off

If our network is to generalize well to new data, we obviously need it to generate a good approximation to the underlying function $g(x_i) = \mathcal{E}[y \mid x_i]$, and we have seen that to do this we must minimise the sum of the bias and variance terms. There will clearly have to be a ***trade-off*** between minimising the bias and minimising the variance.

A network which is too closely fitted to the data will tend to have a large variance and hence give a large expected generalization error. We then say that ***over-fitting*** of the training data has occurred.

We can easily decrease the variance by smoothing the network outputs, but if this is taken too far, then the bias becomes large, and the expected generalization error is large again. We then say that ***under-fitting*** of the training data has occurred.

This trade-off between bias and variance plays a crucial role in the application of neural network techniques to practical applications.

Preventing Under-fitting and Over-fitting

To ***prevent under-fitting*** we need to make sure that:

1. The network has enough hidden units to represent to required mappings.
2. We train the network for long enough so that the sum squared error cost function is sufficiently minimised.

To ***prevent over-fitting*** we can:

1. Stop the training early – before it has had time to learn the training data too well.
2. Restrict the number of adjustable parameters the network has – e.g. by reducing the number of hidden units, or by forcing connections to share the same weight values.
3. Add some form of *regularization* term to the error function to encourage smoother network mappings.
4. Add noise to the training patterns to smear out the data points.