Neural Computation : Revision Lecture

1. Module Aims and Learning Outcomes
2. Biological and Artificial Neural Networks
3. Training Methods for Multi Layer Perceptrons
4. Bias + Variance and Improving Generalization
5. Applications of Multi-Layer Perceptrons
6. Recurrent Neural Networks
7. Radial Basis Function Networks
8. Self Organizing Maps and Learning Vector Quantization
9. Committee Machines and Evolutionary Optimization

L1 : Module Aims and Learning Outcomes

Aims

1. Introduce some of the fundamental techniques and principles of neural computation.
2. Investigate some common neural-based models and their applications.
3. Present neural network models in the larger context of state-of-the-art techniques of automated learning.

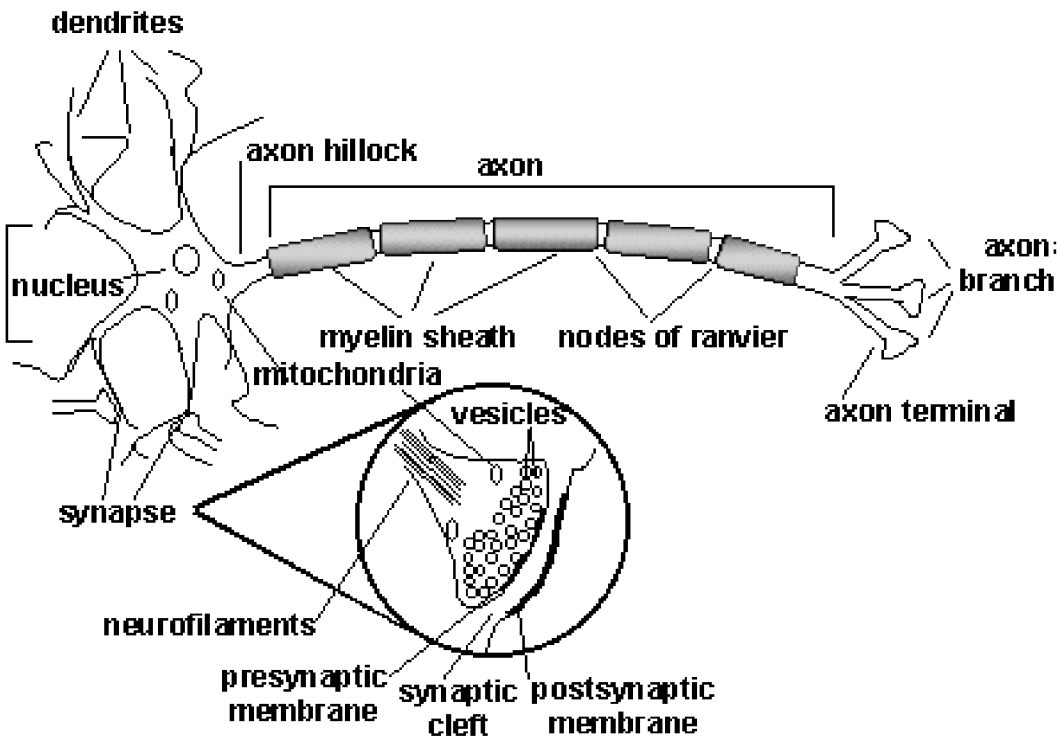
Learning Outcomes

1. Understand the relationship between real brains and simple artificial neural network models.
2. Describe and explain some of the principal architectures and learning algorithms of neural computation.
3. Explain the learning and generalization aspects of neural computation.
4. Demonstrate an understanding of the benefits and limitations of neural-based learning techniques in context of other state-of-the-art methods of automated learning.
5. Apply neural computation algorithms to specific technical and scientific problem. [L4 only]

Why are Artificial Neural Networks worth studying?

1. Even though individual artificial neurons are very simple, networks of them can be shown to be extremely powerful computational devices (Turing equivalent, universal computers).
2. Very simple ANNs can be set up to learn and generalize well – so they can perform difficult tasks without the need for enormous feats of programming.
3. Their massive parallelism can make them very efficient.
4. They are particularly fault tolerant – this is equivalent to the "graceful degradation" found in biological brains.
5. They are very noise tolerant – so they can cope with situations where normal symbolic (rule-based) systems would have difficulty.
6. In principle, they can do anything a symbolic/logic system can do, and a lot more. Though, in practice, getting them to do it can be rather difficult…
7. They are useful for both the scientific goal of modelling how real brains work, and the engineering goal of building efficient systems for real world applications.

L2 : Biological Neural Networks



1. The majority of ***neurons*** encode their outputs or activations as a series of brief electical pulses (i.e. spikes or action potentials).
2. ***Dendrites*** are the receptive zones that receive activation from other neurons.
3. The ***cell body (soma)*** of the neuron's processes the incoming activations and converts them into output activations.
4. ***Axons*** are transmission lines that send activation to other neurons.
5. ***Synapses*** allow weighted transmission of signals (using ***neurotransmitters***) between axons and dendrites to build up large neural networks.

Rate Coding versus Spike Time Coding

When sufficient input is received, the neuron generates an action potential or 'spike' (i.e. it 'fires'). In biological networks, the individual spike timings are often important. So "***spike time coding***" is the most realistic representation for artificial neural networks.

However, averages of spike rates across time or populations of neurons carry a lot of the useful information, and so "***rate coding***" is a useful approximation.

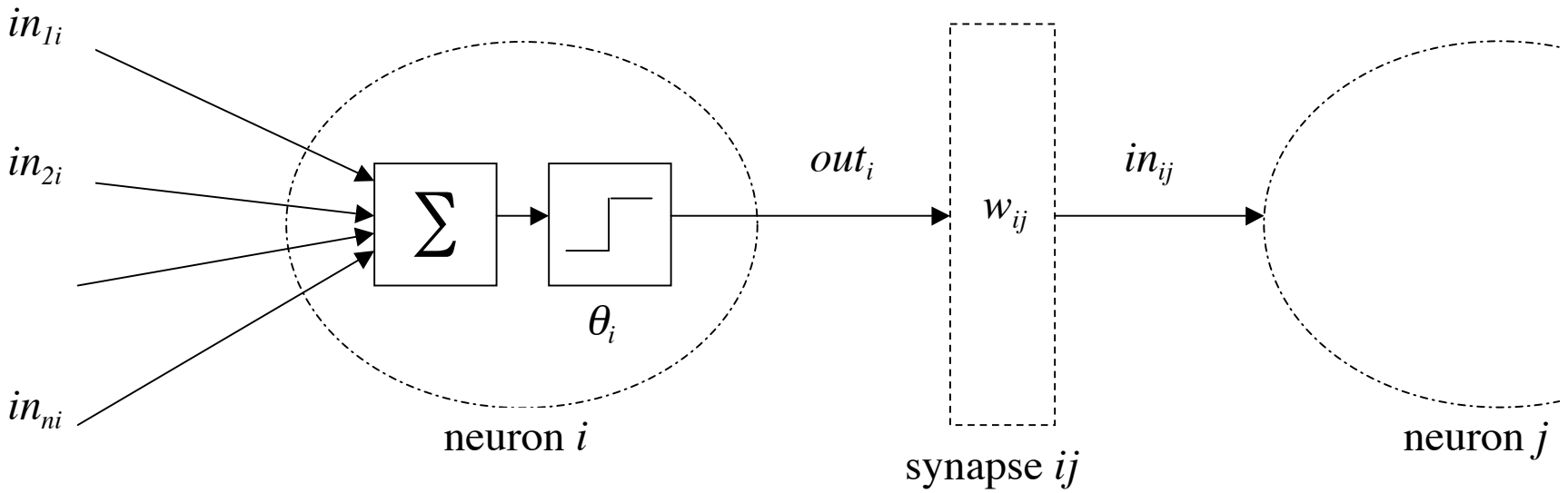
Spike coding is more powerful, but the computer models are much more complicated and more difficult to train.

Rate coding blurs the information coded in individual neurons, but usually leads to simpler models with differentiable outputs, which is important for generating efficient learning algorithms.

Sigmoid shaped activation functions in the rate coding approach follow from the cumulative effect of Gaussian distributed spikes.

L3 : Networks of McCulloch-Pitts Neurons

Artificial neurons have the same basic components as biological neurons. The simplest ANNs consist of a set of ***McCulloch-Pitts neurons*** labelled by indices k, i, j and activation flows between them via synapses with strengths w_{ki}, w_{ij}:



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

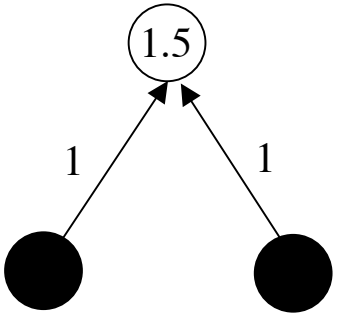
Implementation of Simple Logic Gates

We have inputs in_i and output $out = \text{step}(w_1\, in_1 + w_2\, in_2 - \theta)$ and need to solve for w_1 and θ:

AND

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

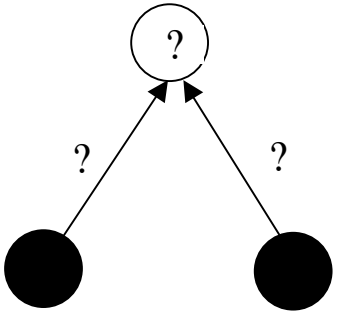
$$w_1\,0 + w_2\,0 - \theta < 0$$
$$w_1\,0 + w_2\,1 - \theta < 0$$
$$w_1\,1 + w_2\,0 - \theta < 0$$
$$w_1\,1 + w_2\,1 - \theta > 0$$
$$\theta > 0\ ,\ w_1\ ,\ w_2 < \theta\ ,\ w_1 + w_2 > \theta$$



XOR

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

$$w_1\,0 + w_2\,0 - \theta < 0$$
$$w_1\,0 + w_2\,1 - \theta > 0$$
$$w_1\,1 + w_2\,0 - \theta > 0$$
$$w_1\,1 + w_2\,1 - \theta < 0$$
$$\theta > 0\ ,\ w_1\ ,\ w_2 > \theta\ ,\ w_1 + w_2 < \theta$$



Solutions only exist for ***linearly separable*** problems, but since the simple gates (AND, OR, NOT) can be linked together to solve arbitrarily complex mappings, they are very powerful.

Building an Artificial Neural Network

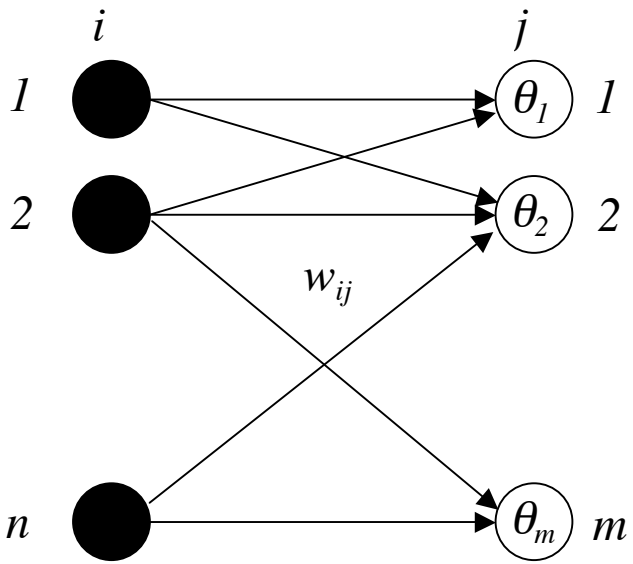
Formulating neural network solutions for particular problems is a multi-stage process:

1. Understand and specify the problem in terms of ***inputs and required outputs***, e.g. outputs are binary class vectors for classification or real valued vectors for regression.
2. Take the ***simplest form of network*** you think might be able to solve the problem.
3. Try to find appropriate ***connection weights*** (including neuron thresholds) so that the network produces the right outputs for each input in its training data.
4. Make sure that the network works on its ***training data***, and test its generalization performance by checking how well it works on previously unseen ***testing data***.
5. If the network doesn't perform well enough, go back to stage 3 and try harder.
6. If the network still doesn't perform well enough, go back to stage 2 and try harder.
7. If the network still doesn't perform well enough, go back to stage 1 and try harder.
8. Either the problem is solved or admit defeat – move on to the next problem.

After training, the network is usually expected to ***generalize*** well, i.e. produce appropriate outputs for ***test patterns*** it has never seen before.

L4 : The Perceptron and the Perceptron Learning Rule

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



Network Activations:

$$out_j = step(\sum_{i=1}^{n} in_i w_{ij} - \theta_j)$$

Perceptron Learning Rule:

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

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

The ***Perceptron Learning Rule*** iteratively shifts around the weights w_{ij} and hence the decision boundaries to give the target outputs for each input. If the problem is ***linearly separable***, the required weights will be found in a finite number of iterations.

L5 : Learning by Gradient Descent Error Minimisation

The Perceptron learning rule is an algorithm that adjusts the network weights w_{ij} to minimise the difference between the actual outputs out_j and the target outputs $targ_j^p$. We can quantify this difference by defining an error function $E(w_{mn})$ over all output units j and all training patterns p, e.g. ***Cross Entropy*** for classification or ***Sum Squared Error*** for regression:

$$E_{CE} = -\sum_p \left[targ^p . \log\left(out^p\right) + \left(1 - targ^p\right) . \log\left(1 - out^p\right) \right] \quad , \quad E_{SSE} = \tfrac{1}{2} \sum_p \sum_j \left(targ_j^p - out_j^p \right)^2$$

It is the general aim of network ***learning*** to minimise the error by adjusting the weights w_{mn}. Typically we make a series of small adjustments to the weights $w_{mn} \rightarrow w_{mn} + \Delta w_{mn}$ until the error $E(w_{mn})$ is 'small enough'. We can determine which direction to change the weights in by looking at the gradients (i.e. partial derivatives) of E with respect to each weight w_{mn}. Then the ***gradient descent update equation*** (with positive learning rate η) is

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

which can be applied iteratively to minimise the error.

L6 : Practical Considerations for Gradient Descent Learning

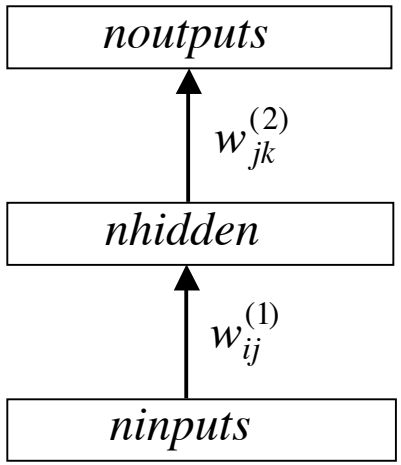
There a number of important practical/implementational considerations that must be taken into account when training neural networks:

1. Do we need to pre-process the training data? If so, how?
2. How many hidden layers with how many hidden units do we need
3. Are some activation functions better than others?
4. How do we choose the initial weights from which we start the training?
5. Should we have different learning rates for the different layers?
6. How do we choose appropriate learning rates?
7. Do we change the weights after each training pattern, or after the whole set?
8. How do we avoid local minima in the error function?
9. How do we avoid flat spots in the error function?
10. How do we know when we should stop the training?

In general, the answers to these questions are highly problem dependent.

L7 : Multi-Layer Perceptrons (MLPs)

Perceptrons specify linear decision boundaries. To deal with non-linearly separable problems (such as XOR), one could use non-monotonic activation functions, but better results are found by extending the simple Perceptron to a ***Multi-Layer Perceptron***, which includes a least one hidden layer of neurons with ***non-linear*** activations functions *f(x)* (such as sigmoids):



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

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

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

Note that if the activation on the hidden layer were linear, the network would be equivalent to a single layer network, and wouldn't be able to cope with non-linearly separable problems.

The Back-Propagation Learning Algorithm

By computing the necessary partial derivatives using the ***chain rule***, we obtain the gradient descent weight update equation for an N layer MLP. CE with sigmoid/soft-max output activations or SSE with linear output activations both lead to the same:

$$\Delta w_{hl}^{(n)} = -\eta \partial E(w_{jk}^{(n)}) \Big/ \partial w_{jk}^{(n)} = \eta \sum_{p} delta_{l}^{(n)} . out_{h}^{(n-1)}$$

with output error signal $delta_{k}^{(N)}$ simply the difference between the target and actual outputs:

$$delta_{k}^{(N)} = \left(targ_{k} - out_{k}^{(N)} \right)$$

and these error signals ***propagate back*** to give the *delta*s at earlier layers n :

$$delta_{k}^{(n)} = \left(\sum_{k} delta_{k}^{(n+1)} . w_{lk}^{(n+1)} \right) . f' \left(\sum_{j} out_{j}^{(n-1)} w_{jk}^{(n)} \right) = \left(\sum_{k} delta_{k}^{(n+1)} . w_{lk}^{(n+1)} \right) . out_{k}^{(n)} . \left(1 - out_{k}^{(n)} \right)$$

which includes the derivative of the sigmoidal hidden unit activation function f. This is the famous ***Back-Propagation*** learning algorithm for MLPs.

Training a Two-Layer MLP Network

The procedure for training a two layer MLP is now quite straight-forward:

1. Take the set of training (input – output) patterns the network is required to learn
   $\{in_i^p, out_j^p : i = 1 \ldots ninputs, j = 1 \ldots noutputs, p = 1 \ldots npatterns\}$.
2. Set up a network with *ninputs* input units fully connected to *nhidden* 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 connection weights, e.g. from the range [–*smwt*, +*smwt*]
4. Select an appropriate error function $E(w_{jk}^{(n)})$, e.g. CE or SSE, and learning rate η.
5. Apply the gradient descent weight update equation $\Delta w_{jk}^{(n)} = -\eta \partial E(w_{jk}^{(n)}) \big/ \partial w_{jk}^{(n)}$ 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’.

The extension to networks with more hidden layers is straightforward.

L8 : Improvements Over Back-Propagation

We can smooth out back-propagation updates by adding a ***momentum*** term $\alpha.\Delta w_{hl}^{(n)}(t-1)$ so

$$\Delta w_{hl}^{(n)}(t) = \eta.delta_{l}^{(n)}(t).out_{h}^{(n-1)}(t) + \alpha.\Delta w_{hl}^{(n)}(t-1) \ .$$

Another way to speed up learning is to compute good step sizes at each step of gradient descent by doing a ***line search*** along the gradient direction to give the best step *size(t)*, so

$$\Delta w_{hl}^{(n)}(t) = size(t).dir_{hl}^{(n)}(t)$$

There are efficient parabolic interpolation methods for doing the line searches.

A problem with using line searches on true gradient descent directions is that the subsequent steps are orthogonal, and this can cause unnecessary zig-zagging through weight space. The ***Conjugate Gradients*** learning algorithm computes better directions $dir_{hl}^{(n)}(t)$ than true gradients and then steps along them by amounts determined by line searches. This is probably the best general purpose approach to MLP training, though complex to implement.

L9 : Bias and Variance Decomposition

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 expected generalization error 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 to get the best generalization.

L10 : Improving Generalization

For networks to generalize well they need to avoid both under-fitting of the training data (high statistical bias) and over-fitting of the training data (high statistical variance).

There are a number of approaches to ***improving generalization*** – we can:

1. Arrange to have the optimum number of free parameters (independent connection weights) in the network (e.g. by fixing the number of hidden units, or weight sharing).
2. Stop the gradient descent training process just before over-fitting starts.
3. Add a regularization term $\lambda\Omega$ to the error function to smooth out the mappings that are learnt, e.g., the regularizer $\Omega = {}^1/_2 \sum (w_{ij})^2$ which corresponds to weight decay.
4. Add noise (or jitter) to the training patterns to smooth out the data points.

We can use a ***validation set*** or ***cross-validation*** as a way of estimating the generalization using only the available training data. This provides a way of optimizing any of the above procedures (e.g., the regularization parameter λ) to improve generalization.

L11: Applications of Multi-Layer Perceptrons

Neural network applications fall into two basic types:

Brain modelling The scientific goal of building models of how real brains work. This can potentially help us understand the nature of human intelligence, formulate better teaching strategies, or better remedial actions for brain damaged patients.

Artificial System Building The engineering goal of building efficient systems for real world applications. This may make machines more powerful, relieve humans of tedious tasks, and may even improve upon human performance.

We often use exactly the same networks and techniques for both. Frequently progress is made when the two approaches are allowed to feed into each other. There are fundamental differences though, e.g. the need for biological plausibility in brain modelling, and the need for computational efficiency in artificial system building. Simple neural networks (MLPs) are surprisingly effective for both. Brain models need to cover Development, Adult Performance, and Brain Damage. Real world applications include: Data Compression, Time Series Prediction, Speech Recognition, Pattern Recognition and Computer Vision.

L12 : Recurrent Network Architectures

The fundamental feature of a ***Recurrent Neural Network (RNN)*** is that the network contains at least one ***feed-back connection***, so the activations can flow round in a loop. That enables the networks to do ***temporal processing*** and ***learn sequences***, e.g., perform sequence recognition/reproduction or temporal association/prediction.

Recurrent neural networks are fully fledged dynamical systems. One common type consists of a standard Multi-Layer Perceptron (MLP) plus added loops. This can exploit the powerful non-linear mapping capabilities of the MLP, and also have some form of ***memory***. Others have more uniform structures, potentially with every neuron connected to all the others, and may have stochastic activation functions, e.g. ***Hopfield Networks*** and ***Boltzmann Machines***.

For simple architectures and deterministic activation functions, learning can be achieved using similar gradient descent procedures to those leading to the back-propagation algorithm for feed-forward networks. Unfolding a recurrent network over time gives a feed-forward network with shared weights, and truncating that gives an Elman Network. When the activations are stochastic, simulated annealing approaches may be more appropriate.

L13 : Radial Basis Function (RBF) Mappings

These aim to learn from N data points in a multi-dimensional space with D dimensional inputs $\mathbf{x}^p = \{x_i^p : i = 1,..., D\}$ and corresponding K dimensional target outputs $\mathbf{t}^p = \{t_k^p : k = 1,..., K\}$. The output data is assumed to be given by some underlying functions $g_k(\mathbf{x})$ plus random noise. The goal is to approximate the $g_k(\mathbf{x})$ with functions $y_k(\mathbf{x})$ of the form

$$y_k(\mathbf{x}) = \sum_{j=0}^{M} w_{kj}\phi_j(\mathbf{x})$$

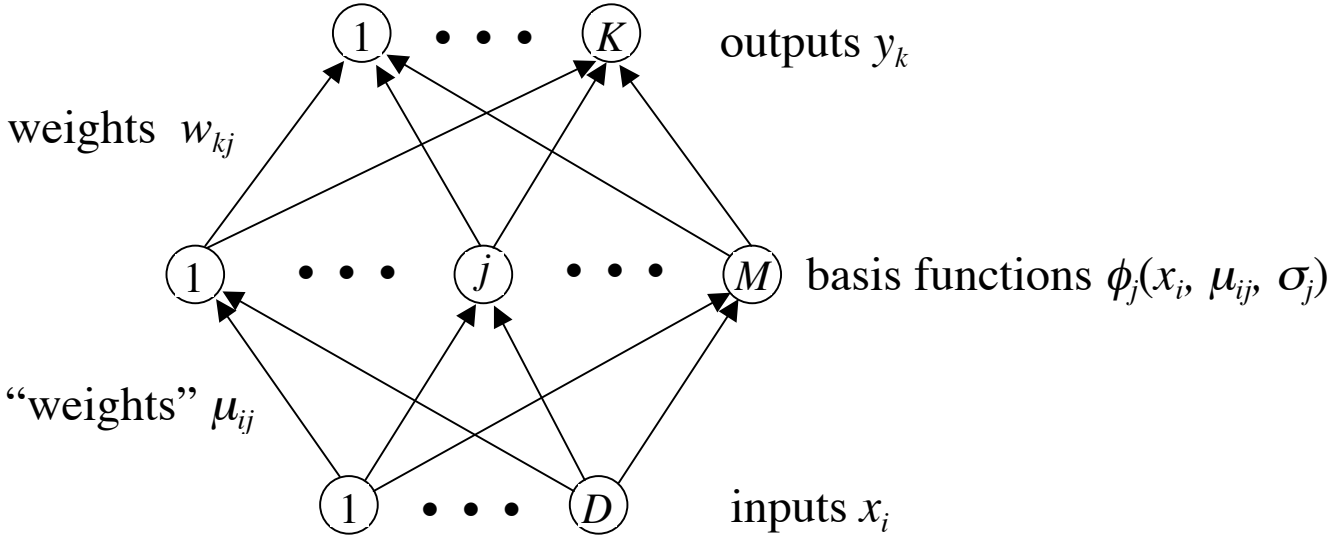
There are good computational reasons to use Gaussian radial basis functions

$$\phi_j(\mathbf{x}) = \exp\left(-\frac{\|\mathbf{x} - \boldsymbol{\mu}_j\|^2}{2\sigma_j^2}\right)$$

in which we have basis centres $\{\boldsymbol{\mu}_j\}$ and widths $\{\sigma_j\}$. If $M = N$ we can use matrix inversion techniques to perform ***exact interpolation***. But this would be computationally inefficient and not give good generalization. It is better to take a different approach with $M << N$.

L14,15 : RBF Networks and Their Training

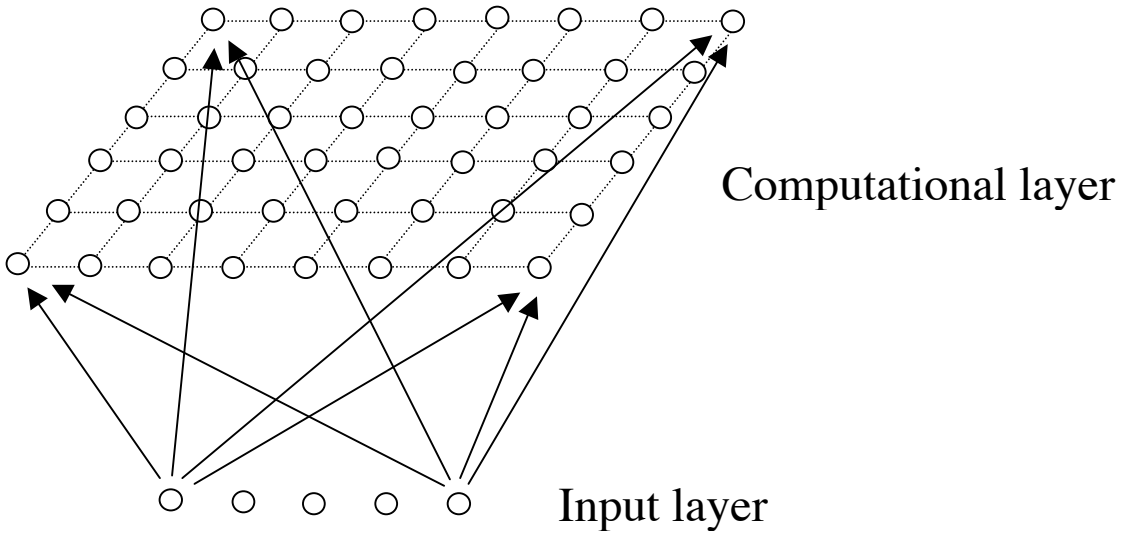
We can cast the RBF mapping into a form that looks like a neural network:



First the basis centres $\{\mu_j\}$ and widths $\{\sigma_j\}$ can be obtained by unsupervised methods, e.g., Random Training Data Points or K-Means Clustering. The output weights $\{w_{kj}\}$ can then be found analytically by solving a set of linear equations. This makes the training very quick, with no difficult to optimise learning parameters, which is a major advantage over MLPs.

L16,17 : The Kohonen Self Organizing Map (SOM)

The ***SOM*** is an ***unsupervised training*** system based on ***competitive learning***. The aim is to learn a ***feature map*** from a spatially ***continuous input space***, in which our input vectors live, to a low dimensional spatially ***discrete output space*** formed by arranging the computational neurons into a grid that is fully connected to all the input layer neurons.



This provides an approximation of the input space with ***dimensional reduction***, ***topological ordering***, ***density matching***, and ***feature selection***.

Components of Self Organization

The self-organization process has four major components:

***Initialization*:** All the connection weights are initialized with small random values.

***Competition*:** For each input pattern, each output nodes compute their respective values of a *discriminant function* which provides the basis for competition. Simple Euclidean distance between the input vector and the weight vector for each output node is suitable. The particular neuron with the smallest distance is declared the *winner*.

***Cooperation*:** The winning neuron determines the spatial location of a *topological neighbourhood* of excited neurons, thereby providing the basis for cooperation among neighbouring neurons.

***Adaptation*:** The excited neurons increase their individual values of the discriminant function in relation to the input pattern through suitable adjustment to the associated connection weights, such that the response of the winning neuron to the subsequent application of a similar input pattern is enhanced.

The SOM Algorithm

The self organising process is implemented in the SOM algorithm:

1. ***Initialization*** – Choose random values for the initial weight vectors $\mathbf{w}_j$.

2. ***Sampling*** – Draw a sample training input vector $\mathbf{x}$ from the input space.

3. ***Matching*** – Find the winning neuron $I(\mathbf{x})$ that has weight vector closest to the input vector, i.e. the minimum value of the discriminant function $d_j(\mathbf{x}) = \sum_{i=1}^{D}(x_i - w_{ji})^2$.

4. ***Updating*** – Apply the weight update equation $\Delta w_{ji} = \eta(t)\, T_{j,I(\mathbf{x})}(t)\, (x_i - w_{ji})$ where $T_{j,I(\mathbf{x})}(t) = \exp(-S_{j,I(\mathbf{x})} / 2\sigma^2(t))$ is the Gaussian topological neighbourhood around the winning node $I(\mathbf{x})$ defined by the distance $S_{j,I(\mathbf{x})}$ between nodes j and $I(\mathbf{x})$ on the output grid. $\sigma(t)$ is the Gaussian's width and $\eta(t)$ is the learning rate, both of which generally decrease with time (e.g. exponentially).

5. ***Continuation*** – keep returning to step 2 until the feature map stops changing.

L18 : Learning Vector Quantization (LVQ)

The ***LVQ algorithm*** is a supervised process which starts from a trained SOM with input vectors $\{\mathbf{x}\}$ and weights (i.e. ***Vorronoi vectors***) $\{\mathbf{w}_j\}$. The classification labels of the inputs give the best classification for the nearest neighbour cell (i.e. ***Voronoi cell***) for each $\mathbf{w}_j$. It is unlikely that the cell boundaries (i.e. ***Voronoi Tesselation***) coincide with the classification boundaries. The LVQ algorithm attempts to correct this by shifting the boundaries:

1. If the input $\mathbf{x}$ and the associated Voronoi vector $\mathbf{w}_{I(\mathbf{x})}$ (i.e. the weight of the winning output node $I(\mathbf{x})$) have the same class label, then move them closer together by $\Delta\mathbf{w}_{I(\mathbf{x})}(t) = \beta(t)(\mathbf{x} - \mathbf{w}_{I(\mathbf{x})}(t))$ as in the SOM algorithm.
2. If the input $\mathbf{x}$ and associated Voronoi vector $\mathbf{w}_{I(\mathbf{x})}$ have the different class labels, then move them apart by $\Delta\mathbf{w}_{I(\mathbf{x})}(t) = -\beta(t)(\mathbf{x} - \mathbf{w}_{I(\mathbf{x})}(t))$.
3. Voronoi vectors $\mathbf{w}_j$ corresponding to other input regions are left unchanged with $\Delta\mathbf{w}_j(t) = 0$.

where $\beta(t)$ is a learning rate that decreases with the number of iterations/epochs of training. In this way we end up with better classification than by the SOM alone.

L19 : Committee Machines

Committee machines are combinations of two or more neural networks that can be made to perform better than individual networks. There are two major categories:

1. Static Structures

The outputs of several constituent networks (experts) are combined by a mechanism that does not involve the input signal, hence the designation *static*. Examples include

- ***Ensemble averaging***, where the constituent outputs are linearly combined.
- ***Boosting***, where weak learners are combined to give a strong learner.

2. Dynamic structures

The input signal is directly involved in actuating the mechanism that integrates/combines the constituent outputs, hence the designation *dynamic*. The main example is

- ***Mixtures of experts***, where the constituent outputs are non-linearly combined by some form of gating system (which may itself be a neural network).

L20 : Evolutionary Optimization

Rigorous statistical approaches are required to present results and perform model selection. The various neural network parameter values in biological systems have evolved so that they perform well. So, using simulated ***evolution by natural selection*** to automate model selection and generate high performance neural networks is becoming increasingly popular.

One takes a whole population of neural networks, each specified by some ***genotypic encoding*** of its architecture and other parameters. Each individual network is then tested on its chosen task and its ***fitness*** determined (e.g., estimated generalization performance or learning speed). The best/fittest individuals are then selected to be the parents of the next generation, with the children generated by suitable ***cross-over*** and ***mutation*** at the genotypic level.

The obvious thing to evolve is the neural network weights, but this is hard to do well, and in real brains they are not set innately, but by lifetime learning. Evolving other neural network parameters (numbers of hidden units, initial weight range ρ, learning rate η, momentum α, regularization parameter λ, epochs, etc.) consistently gives good results.

Overview and Reading

1. The module appears to have achieved its aims and learning outcomes.
2. We began by seeing how we could take simplified versions of the neural networks found in real brains to produce powerful computational devices.
3. We have seen how Multi-Layer Perceptrons, Recurrent Neural Networks, Radial Basis Function Networks, Kohonen Self Organizing Maps, Committee Machines and Evolving Neural Networks can be set up and trained.
4. We have studied the issues underlying learning and generalization in neural networks, and how we can improve them both.
5. Along the way we have considered the various implementational and practical issues that might complicate our endeavours.

Reading

1. Your lecture notes!