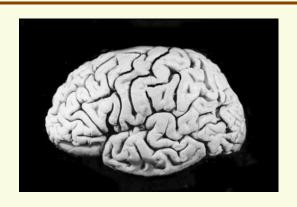
# **Multilayer Neural Networks**

### Brain vs. Computer



- Designed to solve logic and arithmetic problems
- Can solve a gazillion arithmetic and logic problems in an hour
- absolute precision
- Usually one very fast procesor
- high reliability

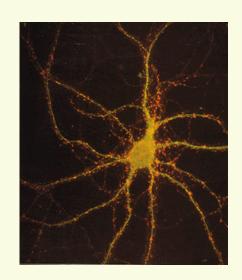


- Evolved (in a large part) for pattern recognition
- Can solve a gazillion of PR problems in an hour
- Huge number of parallel but relatively slow and unreliable processors
- not perfectly precise
- not perfectly reliable

Seek an inspiration from human brain for PR?

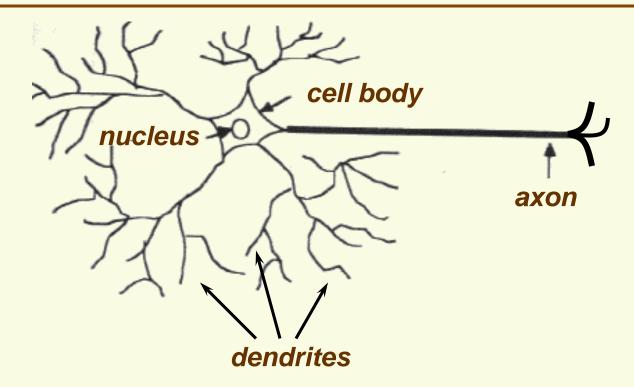
#### Neuron: Basic Brain Processor





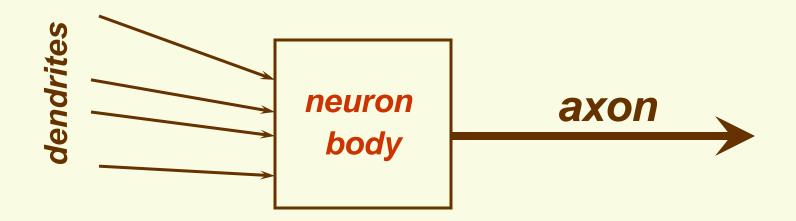
- Neurons are nerve cells that transmit signals to and from brains at the speed of around 200mph
- Each neuron cell communicates to anywhere from 1000 to 10,000 other neurons, muscle cells, glands, so on
- Have around 10<sup>10</sup> neurons in our brain (network of neurons)
- Most neurons a person is ever going to have are already present at birth

### Neuron: Basic Brain Processor



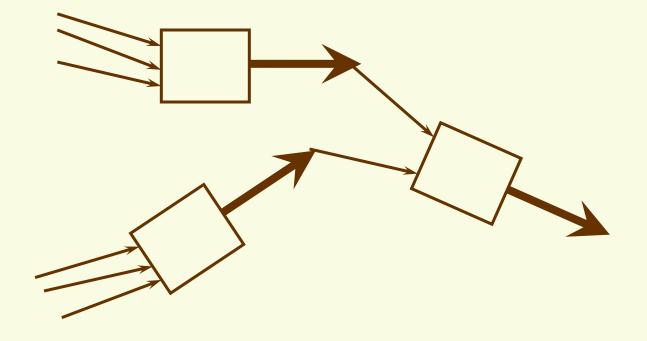
- Main components of a neuron
  - Cell body which holds DNA information in nucleus
  - Dendrites may have thousands of dendrites, usually short
  - axon long structure, which splits in possibly thousands branches at the end. May be up to 1 meter long

### Neuron in Action (simplified)



- Input: neuron collects signals from other neurons through dendrites, may have thousands of dendrites
- Processor: Signals are accumulated and processed by the cell body
- Output: If the strength of incoming signals is large enough, the cell body sends a signal (a spike of electrical activity) to the axon

### **Neural Network**



### ANN History: Birth

- 1943, famous paper by W. McCulloch (neurophysiologist) and W. Pitts (mathematician)
  - Using only math and algorithms, constructed a model of how neural network may work
  - Showed it is possible to construct any computable function with their network
  - Was it possible to make a model of thoughts of a human being?
  - Considered to be the birth of AI
- 1949, D. Hebb, introduced the first (purely pshychological) theory of learning
  - Brain learns at tasks through life, thereby it goes through tremendous changes
  - If two neurons fire together, they strengthen each other's responses and are likely to fire together in the future

### ANN History: First Successes

- 1958, F. Rosenblatt,
  - perceptron, oldest neural network still in use today
  - Algorithm to train the perceptron network (training is still the most actively researched area today)
  - Built in hardware
  - Proved convergence in linearly separable case
- 1959, B. Widrow and M. Hoff
  - Madaline
  - First ANN applied to real problem (eliminate echoes in phone lines)
  - Still in commercial use

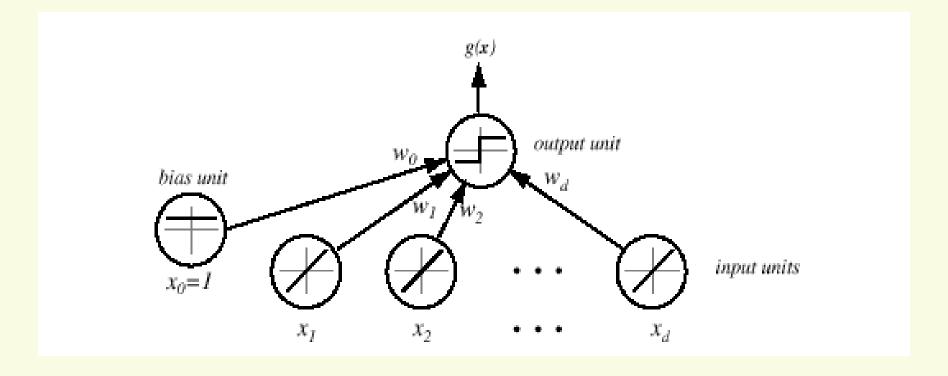
### ANN History: Stagnation

- Early success lead to a lot of claims which were not fulfilled
- 1969, M. Minsky and S. Pappert
  - Book "Perceptrons"
  - Proved that perceptrons can learn only linearly separable classes
  - In particular cannot learn very simple XOR function
  - Conjectured that multilayer neural networks also limited by linearly separable functions
- No funding and almost no research (at least in North America) in 1970's as the result of 2 things above

## ANN History: Revival

- Revival of ANN in 1980's
- 1982, J. Hopfield
  - New kind of networks (Hopfield's networks)
  - Bidirectional connections between neurons
  - Implements associative memory
- 1982 joint US-Japanese conference on ANN
  - US worries that it will stay behind
- Many examples of mulitlayer NN appear
- 1982, discovery of backpropagation algorithm
  - Allows a network to learn not linearly separable classes
  - Discovered independently by
    - 1. Y. Lecunn
    - 2. D. Parker
    - 3. Rumelhart, Hinton, Williams

### ANN: Perceptron



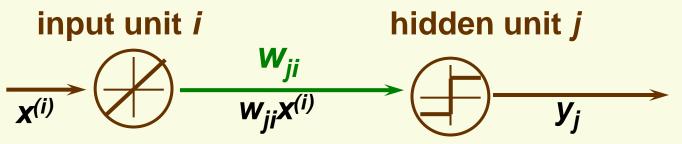
- Input and output layers
- $g(x) = w^t x + w_0$
- Limitation: can learn only linearly separable classes

### MNN: Feed Forward Operation

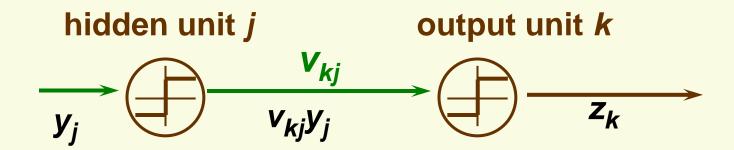
output layer: m outputs, one for each class input layer: hidden layer: **d** features  $V_{kj}$  $Z_1$  $\boldsymbol{z}_{m}$ bias unit

### MNN: Notation for Weights

Use w<sub>ji</sub> to denote the weight between input unit i and hidden unit j



Use v<sub>kj</sub> to denote the weight between hidden unit j
and output unit k



### MNN: Notation for Activation

Use net; to denote the activation and hidden unit j

$$net_{j} = \sum_{i=1}^{d} x^{(i)} w_{ji} + w_{j0}$$

$$x^{(2)} w_{j2}$$

$$y_{j}$$

$$y_{j}$$

Use net\* to denote the activation at output unit k

$$net_{k}^{*} = \sum_{j=1}^{N_{H}} y_{j} v_{kj} + v_{k0}$$

$$y_{2} v_{k2}$$

$$y_{2} v_{k2}$$

$$y_{3} v_{k2}$$

$$y_{4} v_{k0}$$

$$y_{2} v_{k2}$$

$$y_{3} v_{k2}$$

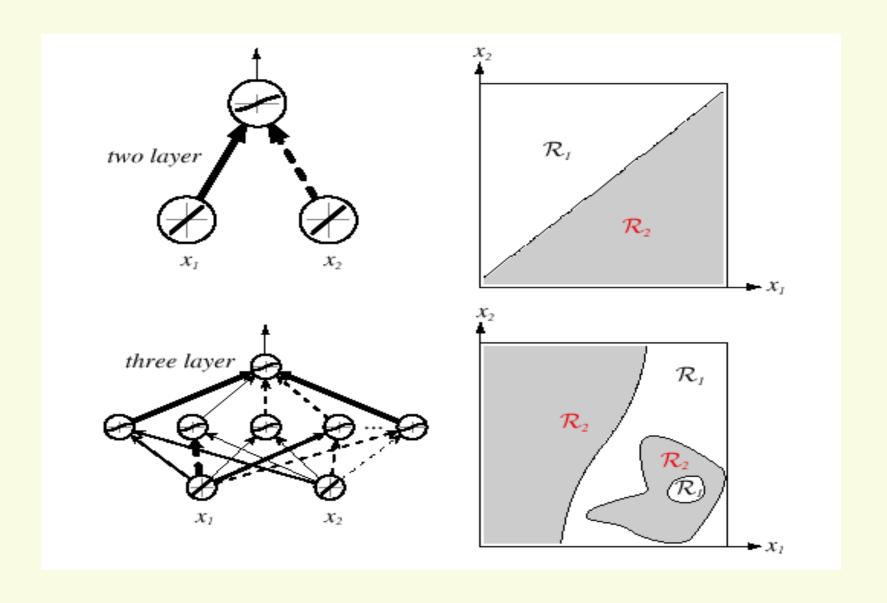
$$y_{4} v_{k0}$$

#### Discriminant Function

Discriminant function for class k (the output of the kth output unit)

$$g_{k}(x) = z_{k} =$$
activation at ith hidden unit
$$= f\left(\sum_{j=1}^{N_{H}} v_{kj} f\left(\sum_{j=1}^{d} w_{ji} x^{(i)} + w_{j0}\right) + v_{k0}\right)$$
activation at kth output unit

### **Discriminant Function**



### Expressive Power of MNN

- It can be shown that every continuous function from input to output can be implemented with enough hidden units, 1 hidden layer, and proper nonlinear activation functions
- This is more of theoretical than practical interest
  - The proof is not constructive (does not tell us exactly how to construct the MNN)
  - Even if it were constructive, would be of no use since we do not know the desired function anyway, our goal is to learn it through the samples
  - But this result does give us confidence that we are on the right track
    - MNN is general enough to construct the correct decision boundaries, unlike the Perceptron

### MNN Activation function

- Must be nonlinear for expressive power larger than that of perceptron
  - If use linear activation function at hidden layer, can only deal with linearly separable classes
  - Suppose at hidden unit j, h(u)=aiu

$$g_{k}(x) = f\left(\sum_{j=1}^{N_{H}} v_{kj} h\left(\sum_{i=1}^{d} w_{ji} x^{(i)} + w_{j0}\right) + v_{k0}\right)$$

$$= f\left(\sum_{j=1}^{N_{H}} v_{kj} a_{j} \left(\sum_{i=1}^{d} w_{ji} x^{(i)} + w_{j0}\right) + v_{k0}\right)$$

$$= f\left(\sum_{i=1}^{d} \sum_{j=1}^{N_{H}} \left(v_{kj} a_{j} w_{ji} x^{(i)} + v_{kj} a_{j} w_{j0}\right) + v_{k0}\right)$$

$$= f\left(\sum_{i=1}^{d} x^{(i)} \sum_{j=1}^{N_{H}} v_{kj} a_{j} w_{ji}\right) + \left(\sum_{j=1}^{N_{H}} v_{kj} a_{j} w_{j0}\right) + v_{k0}$$

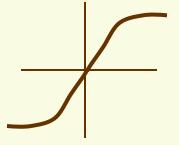
### MNN Activation function

could use a discontinuous activation function

$$f(net_k) = \begin{cases} 1 & if \ net_k \ge 0 \\ -1 & if \ net_k < 0 \end{cases}$$



 However, we will use gradient descent for learning, so we need to use a continuous activation function sigmoid function



From now on, assume f is a differentiable function

### MNN: Modes of Operation

Network have two modes of operation:

#### Feedforward

The feedforward operations consists of presenting a pattern to the input units and passing (or feeding) the signals through the network in order to get outputs units (no cycles!)

#### Learning

The supervised learning consists of presenting an input pattern and modifying the network parameters (weights) to reduce distances between the computed output and the desired output

### MNN

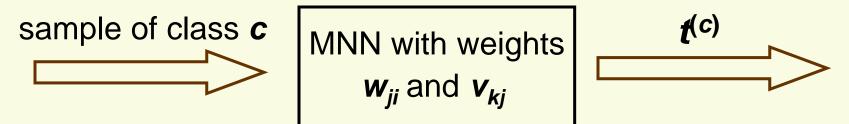
- Can vary
  - number of hidden layers
  - Nonlinear activation function
    - Can use different function for hidden and output layers
    - Can use different function at each hidden and output node

### MNN: Class Representation

- Training samples x<sub>1</sub>,..., x<sub>n</sub> each of class 1,...,m
- Let network output z represent class c as target t<sup>(c)</sup>

$$\mathbf{z} = \begin{bmatrix} \mathbf{z}_1 \\ \vdots \\ \mathbf{z}_c \\ \vdots \\ \mathbf{z}_m \end{bmatrix} = \mathbf{t}^{(c)} = \begin{bmatrix} \mathbf{0} \\ \vdots \\ \mathbf{1} \\ \vdots \\ \mathbf{0} \end{bmatrix}$$
 cth row

#### Our Ultimate Goal For FeedForward Operation

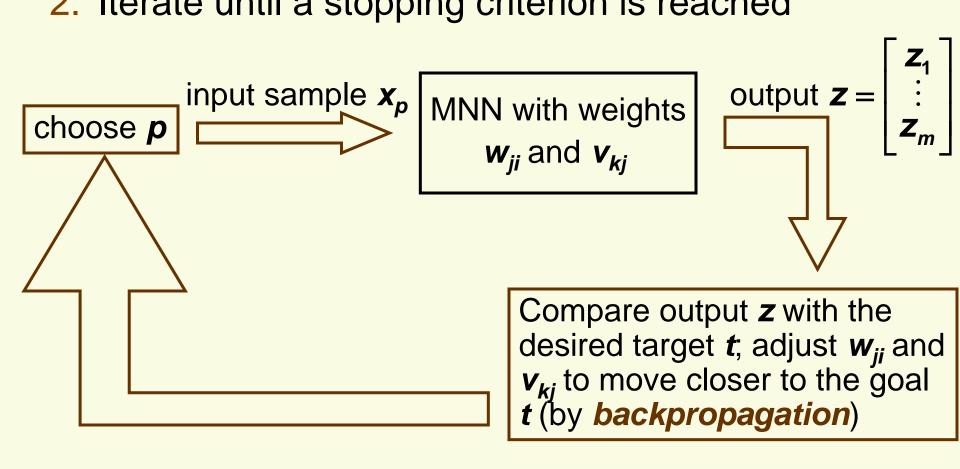


#### MNN training to achieve the Ultimate Goal

Modify (learn) MNN parameters  $w_{ji}$  and  $v_{kj}$  so that for each *training* sample of class c MNN output  $z = t^{(c)}$ 

# Network Training (learning)

- 1. Initialize weights  $\mathbf{w}_{ii}$  and  $\mathbf{v}_{ki}$  randomly but not to 0
- 2. Iterate until a stopping criterion is reached



- Learn  $w_{ii}$  and  $v_{ki}$  by minimizing the training error
- What is the training error?
- Suppose the output of MNN for sample x is z and the target (desired output for x) is t
- Error on one sample:  $J(w,v) = \frac{1}{2} \sum_{c=1}^{m} (t_c z_c)^2$
- Training error:  $J(w,v) = \frac{1}{2} \sum_{i=1}^{n} \sum_{c=1}^{m} (t_c^{(i)} z_c^{(i)})^2$

Use gradient descent:

$$\mathbf{v}^{(0)}, \mathbf{w}^{(0)} = \text{random}$$
 $repeat until convergence:$ 
 $\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \nabla_{w} J(\mathbf{w}^{(t)})$ 
 $\mathbf{v}^{(t+1)} = \mathbf{v}^{(t)} - \eta \nabla_{v} J(\mathbf{v}^{(t)})$ 

For simplicity, first take training error for one sample X;

$$J(w,v) = \frac{1}{2} \sum_{c=1}^{m} (t_c - z_c)^2$$
 function of w,v  
fixed constant

$$z_k = f\left(\sum_{j=1}^{N_H} \mathbf{v}_{kj} f\left(\sum_{i=1}^d \mathbf{w}_{ji} \mathbf{x}^{(i)} + \mathbf{w}_{j0}\right) + \mathbf{v}_{k0}\right)$$

- Need to compute
  - 1. partial derivative w.r.t. hidden-to-output weights  $\frac{\partial J}{\partial v_{ki}}$
  - 2. partial derivative w.r.t. input-to-hidden weights  $\frac{\partial \mathbf{J}}{\partial \mathbf{w}_{ii}}$

### BackPropagation: Layered Model

activation at hidden unit j

output at hidden unit j

activation at output unit **k** 

activation at output unit **k** 

objective function

$$net_{j} = \sum_{i=1}^{d} x^{(i)} w_{ji} + w_{j0}$$

$$y_{j} = f(net_{j})$$

$$net_{k}^{*} = \sum_{j=1}^{N_{H}} y_{j} v_{kj} + v_{k0}$$

$$\sum_{j=1}^{N_{H}} v_{j} v_{kj} + v_{k0}$$

$$\sum_{j=1}^{d} v_{kj} v_{kj} + v_{k0}$$

∂W ii

$$net_{k}^{*} = \sum_{j=1}^{N_{H}} y_{j} v_{kj} + v_{k0} \implies z_{k} = f(net_{k}^{*}) \implies J(w,v) = \frac{1}{2} \sum_{c=1}^{m} (t_{c} - z_{c})^{2}$$

• First compute hidden-to-output derivatives  $\frac{\partial J}{\partial v_{ki}}$ 

$$\frac{\partial J}{\partial \mathbf{v}_{kj}} = \frac{1}{2} \sum_{c=1}^{m} \frac{\partial}{\partial \mathbf{v}_{kj}} (t_c - \mathbf{z}_c)^2 = \sum_{c=1}^{m} (t_c - \mathbf{z}_c) \frac{\partial}{\partial \mathbf{v}_{kj}} (t_c - \mathbf{z}_c)$$

$$= (t_k - \mathbf{z}_k) \frac{\partial}{\partial \mathbf{v}_{kj}} (t_k - \mathbf{z}_k) = -(t_k - \mathbf{z}_k) \frac{\partial}{\partial \mathbf{v}_{kj}} (\mathbf{z}_k)$$

$$= -(t_k - \mathbf{z}_k) \frac{\partial \mathbf{z}_k}{\partial \mathbf{net}_k^*} \frac{\partial \mathbf{net}_k^*}{\partial \mathbf{v}_{kj}}$$

$$= \begin{cases} -(t_k - \mathbf{z}_k) \mathbf{f}'(\mathbf{net}_k^*) \mathbf{y}_j & \text{if } j \neq 0 \\ -(t_k - \mathbf{z}_k) \mathbf{f}'(\mathbf{net}_k^*) & \text{if } j = 0 \end{cases}$$

# Gradient Descent Single Sample Update Rule for hidden-to-output weights $v_{ki}$

$$j > 0$$
:  $v_{kj}^{(t+1)} = v_{kj}^{(t)} + \eta (t_k - z_k) f'(net_k^*) y_j$ 

$$j = 0$$
 (bias weight):  $v_{k0}^{(t+1)} = v_{k0}^{(t)} + \eta(t_k - z_k)f'(net_k^*)$ 

Now compute input-to-hidden

$$\frac{\partial \mathbf{J}}{\partial \mathbf{w}_{ji}}$$

$$\frac{\partial J}{\partial W_{ji}} = \sum_{k=1}^{m} (t_k - z_k) \frac{\partial}{\partial W_{ji}} (t_k - z_k)$$

$$=-\sum_{k=1}^{m} (t_k-z_k) \frac{\partial z_k}{\partial w_{ji}} = -\sum_{k=1}^{m} (t_k-z_k) \frac{\partial z_k}{\partial net_k^*} \frac{\partial net_k^*}{\partial w_{ji}}$$

$$=-\sum_{k=1}^{m}(t_{k}-z_{k})f'(net_{k}^{*})\frac{\partial net_{k}^{*}}{\partial y_{j}}\frac{\partial y_{j}}{\partial w_{ji}}$$

$$= -\sum_{k=1}^{m} (t_k - z_k) f'(net_k^*) v_{kj} \frac{\partial y_j}{\partial net_j} \frac{\partial net_j}{\partial w_{ji}}$$

$$= \begin{cases} -\sum_{k=1}^{m} (t_k - z_k) f'(net_k^*) v_{kj} f'(net_j) x^{(i)} & \text{if } i \neq 0 \\ -\sum_{k=1}^{m} (t_k - z_k) f'(net_k^*) v_{kj} f'(net_j) & \text{if } i = 0 \end{cases}$$

$$net_h = \sum_{h=1}^{d} x^{(i)} w_{hi} + w_{h0}$$

$$y_j = f(net_j)$$

$$net_{k}^{*} = \sum_{s=1}^{N_{H}} y_{s} v_{ks} + v_{k0}$$

$$\mathbf{z}_{k} = f(\mathbf{net}_{k}^{*})$$

$$1 \frac{1}{2}$$

$$J(w,v) = \frac{1}{2} \sum_{c=1}^{m} (t_c - z_c)^2$$

$$\frac{\partial J}{\partial W_{ji}} = \begin{cases} -f'(net_j)x^{(i)} \sum_{k=1}^{m} (t_k - z_k) f'(net_k^*) v_{kj} & \text{if } i \neq 0 \\ -f'(net_j) \sum_{k=1}^{m} (t_k - z_k) f'(net_k^*) v_{kj} & \text{if } i = 0 \end{cases}$$

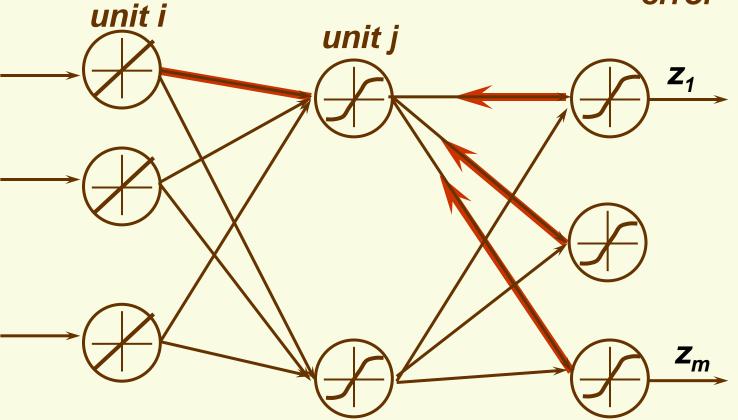
# Gradient Descent Single Sample Update Rule for input-to-hidden weights w<sub>ii</sub>

$$i > 0$$
:  $w_{ji}^{(t+1)} = w_{ji}^{(t)} + \eta f'(net_j) x^{(i)} \sum_{k=1}^{m} (t_k - z_k) f'(net_k^*) v_{kj}^{(t)}$ 

$$i = 0$$
 (bias weight):  $w_{j0}^{(t+1)} = w_{j0}^{(t)} + \eta f'(net_j) \sum_{k=1}^{m} (t_k - z_k) f'(net_k^*) v_{kj}^{(t)}$ 

### BackPropagation of Errors

$$\frac{\partial J}{\partial w_{ji}} = -f'(net_j)x^{(i)}\sum_{k=1}^{m} (t_k - z_k)f'(net_k^*)v_{kj} \qquad \frac{\partial J}{\partial v_{kj}} = -(t_k - z_k)f'(net_k^*)y_j$$



 Name "backpropagation" because during training, errors propagated back from output to hidden layer

Consider update rule for hidden-to-output weights:

$$\boldsymbol{v}_{kj}^{(t+1)} = \boldsymbol{v}_{kj}^{(t)} + \eta (\boldsymbol{t}_k - \boldsymbol{z}_k) \boldsymbol{f}' (\boldsymbol{net}_k^*) \boldsymbol{y}_j$$

- Suppose  $t_k z_k > 0$
- Then output of the kth hidden unit is too small:  $t_k > z_k$
- Typically activation function f is s.t. f' > 0
- Thus  $(t_k z_k)f'(net_k^*) > 0$

 $z_k$ 

- There are 2 cases:
  - 1.  $y_j > 0$ , then to increase  $z_k$ , should increase weight  $v_{kj}$  which is exactly what we do since  $\eta(t_k z_k)f'(net_k^*)y_j > 0$
  - 2.  $y_j < 0$ , then to increase  $z_k$ , should decrease weight  $v_{kj}$  which is exactly what we do since  $\eta(t_k z_k)f'(net_k^*)y_j < 0$

- The case  $t_k z_k < 0$  is analogous
- Similarly, can show that input-to-hidden weights make sense
- Important: weights should be initialized to random nonzero numbers

$$\frac{\partial J}{\partial w_{ji}} = -f'(net_j)x^{(i)}\sum_{k=1}^{m}(t_k - z_k)f'(net_k^*)v_{kj}$$

• if  $\mathbf{v}_{kj} = 0$ , input-to-hidden weights  $\mathbf{w}_{ji}$  never updated

### **Training Protocols**

- How to present samples in training set and update the weights?
- Three major training protocols:

#### 1. Stochastic

 Patterns are chosen randomly from the training set, and network weights are updated after every sample presentation

#### 2. Batch

weights are update based on all samples; iterate weight update

#### 3. Online

 each sample is presented only once, weight update after each sample presentation

## Stochastic Back Propagation

- 1. Initialize
  - number of hidden layers n<sub>H</sub>
  - weights w, v
  - convergence criterion  $\theta$  and learning rate  $\eta$
  - time t = 0
- 2. <u>do</u>

```
x \leftarrow \text{ randomly chosen training pattern}
\underline{for \ all} \quad 0 \le i \le d, \quad 0 \le j \le n_H, \quad 0 \le k \le m
v_{kj} = v_{kj} + \eta(t_k - z_k) f'(net_k^*) y_j
v_{k0} = v_{k0} + \eta(t_k - z_k) f'(net_k^*)
w_{jj} = w_{jj} + \eta f'(net_j) x^{(i)} \sum_{k=1}^{m} (t_k - z_k) f'(net_k^*) v_{kj}
w_{j0} = w_{j0} + \eta f'(net_j) \sum_{k=1}^{m} (t_k - z_k) f'(net_k^*) v_{kj}
```

$$t = t + 1$$
until  $||J|| < \theta$ 

3. <u>return</u> v, w

### **Batch Back Propagation**

- This is the *true* gradient descent, (unlike stochastic propagation)
- For simplicity, derived backpropagation for a single sample objective function:

$$J(w,v) = \frac{1}{2} \sum_{c=1}^{m} (t_c - z_c)^2$$

The full objective function:

$$J(w,v) = \frac{1}{2} \sum_{i=1}^{n} \sum_{c=1}^{m} (t_c^{(i)} - z_c^{(i)})^2$$

Derivative of full objective function is just a sum of derivatives for each sample:

$$\frac{\partial}{\partial W}J(W,V) = \frac{1}{2}\sum_{i=1}^{n}\frac{\partial}{\partial W}\left(\sum_{c=1}^{m}\left(t_{c}^{(i)}-Z_{c}^{(i)}\right)^{2}\right)$$

already derived this

## **Batch Back Propagation**

For example,

$$\frac{\partial J}{\partial \mathbf{w}_{ii}} = \sum_{p=1}^{n} -f'(\mathbf{net}_{j}) \mathbf{x}_{p}^{(i)} \sum_{k=1}^{m} (t_{k} - \mathbf{z}_{k}) f'(\mathbf{net}_{k}^{*}) \mathbf{v}_{kj}$$

# **Batch Back Propagation**

1. Initialize  $n_H$ , w, v,  $\theta$ ,  $\eta$ , t = 0

2. <u>do</u>

one epoch

$$\Delta v_{kj} = \Delta v_{k0} = \Delta w_{ji} = \Delta w_{j0} = 0$$

$$\underline{for \ all} \ 1 \le p \le n$$

$$\underline{for \ all} \ 0 \le i \le d, \ 0 \le j \le n_H, \ 0 \le k \le m$$

$$\Delta v_{kj} = \Delta v_{kj} + \eta(t_k - z_k) f'(net_k^*) y_j$$

$$\Delta v_{k0} = \Delta v_{k0} + \eta(t_k - z_k) f'(net_k^*)$$

$$\Delta w_{ji} = \Delta w_{ji} + \eta f'(net_j) x_p^{(i)} \sum_{k=1}^m (t_k - z_k) f'(net_k^*) v_{kj}$$

$$\Delta w_{j0} = \Delta w_{j0} + \eta f'(net_j) \sum_{k=1}^m (t_k - z_k) f'(net_k^*) v_{kj}$$

$$\mathbf{V}_{kj} = \mathbf{V}_{kj} + \Delta \mathbf{V}_{kj}; \ \mathbf{V}_{k0} = \mathbf{V}_{k0} + \Delta \mathbf{V}_{k0}; \ \mathbf{W}_{ji} = \mathbf{W}_{ji} + \Delta \mathbf{W}_{ji}; \ \mathbf{W}_{j0} = \mathbf{W}_{j0} + \Delta \mathbf{W}_{j0}$$

3. <u>return</u> v, w

## **Training Protocols**

#### 1. Batch

True gradient descent

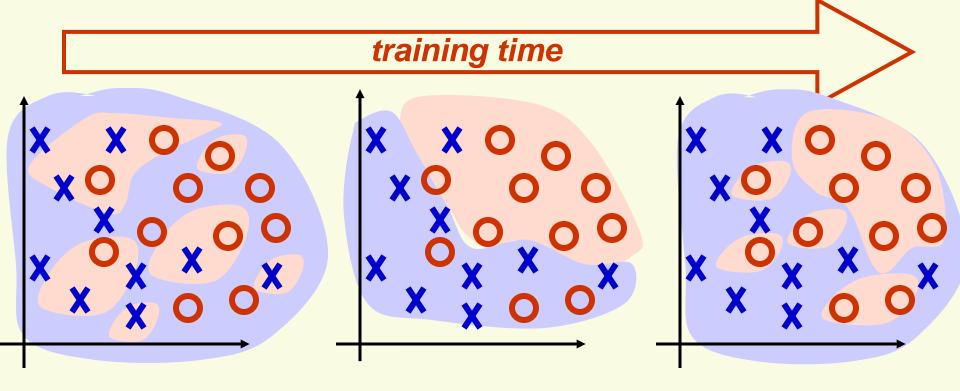
#### 2. Stochastic

- Faster than batch method
- Usually the recommended way

#### 3. Online

- Used when number of samples is so large it does not fit in the memory
- Dependent on the order of sample presentation
- Should be avoided when possible

# MNN Training



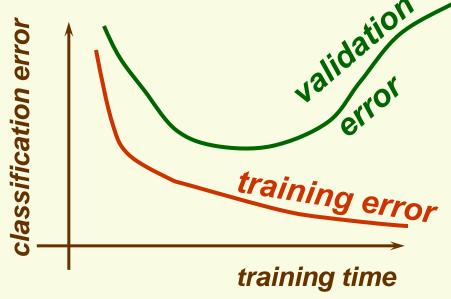
Large training error: in the beginning random decision regions

Small training error: decision regions improve with time

Zero training error: decision regions separate training data perfectly, but we overfited the network

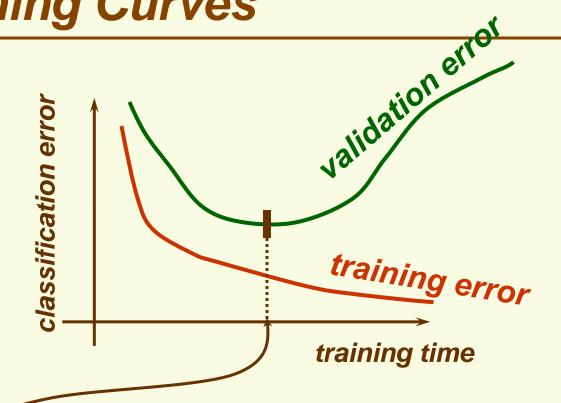
## MNN Learning Curves

- Training data: data on which learning (gradient descent for MNN) is performed
- Validation data: used to assess network generalization capabilities
- Training error typically goes down, since with enough hidden units, can find discriminant function which classifies training patterns exactly



 Validation error first goes down, but then goes up since at some point we start to overfit the network to the validation data

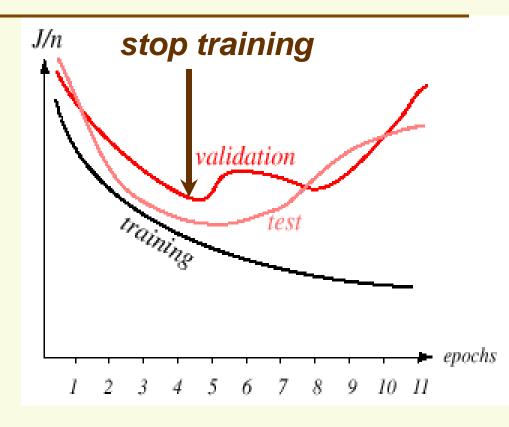
## Learning Curves



- this is a good time to stop training, since after this time we start to overfit
- Stopping criterion is part of training phase, thus validation data is part of the training data
- To assess how the network will work on the unseen examples, we still need test data

# Learning Curves

 validation data is used to determine "parameters", in this case when learning should stop



- Stop training after the first local minimum on validation data
- We are assuming performance on test data will be similar to performance on validation data

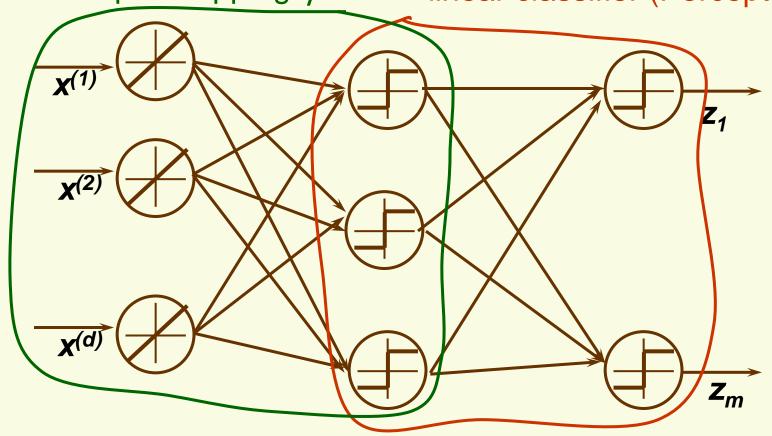
#### Data Sets

- Training data
  - data on which learning is performed
- Validation data
  - validation data is used to determine any free parameters of the classifier
    - k in the knn neighbor classifier
    - h for parzen windows
    - number of hidden layers in the MNN
    - etc
- Test data
  - used to assess network generalization capabilities

### MNN as Nonlinear Mapping

this module implements nonlinear input mapping  $\phi$ 

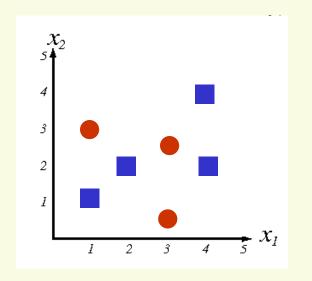
this module implements linear classifier (Perceptron)

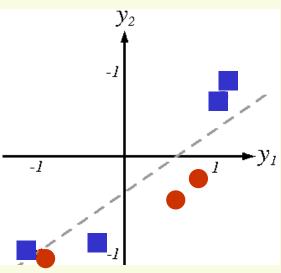


### MNN as Nonlinear Mapping

- Thus MNN can be thought as learning 2 things at the same time
  - the nonlinear mapping of the inputs
  - linear classifier of the nonlinearly mapped inputs

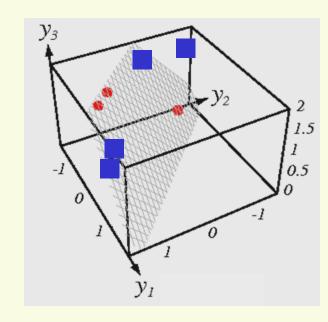
### MNN as Nonlinear Mapping





original feature space
x; patterns are not
linearly separable

MNN finds nonlinear mapping **y**=φ(**x**) to 2 dimensions (2 hidden units); patterns are almost linearly separable



MNN finds nonlinear mapping **y**=φ(**x**) to 3 dimensions (3 hidden units) that; patterns are linearly separable

### **Concluding Remarks**

#### Advantages

- MNN can learn complex mappings from inputs to outputs, based only on the training samples
- Easy to use
- Easy to incorporate a lot of heuristics

#### Disadvantages

- It is a "black box", that is difficult to analyze and predict its behavior
- May take a long time to train
- May get trapped in a bad local minima
- A lot of "tricks" to implement for the best performance