## 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 200 mph
- Each neuron cell communicates to anywhere from 1000 to 10,000 other neurons, muscle cells, glands, so on
- Have around $\mathbf{1 0}^{10}$ 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
- $\boldsymbol{g}(\boldsymbol{x})=w^{t} \boldsymbol{x}+w_{0}$
- Limitation: can learn only linearly separable classes


## MNN: Feed Forward Operation



## MNN: Notation for Weights

- Use $\boldsymbol{w}_{j i}$ to denote the weight between input unit $\boldsymbol{i}$ and hidden unit $\boldsymbol{j}$
input unit $i \quad$ hidden unit $j$

- Use $\boldsymbol{v}_{\boldsymbol{k} j}$ to denote the weight between hidden unit $\boldsymbol{j}$ and output unit $\boldsymbol{k}$
hidden unit $\boldsymbol{j}$



## MNN: Notation for Activation

- Use $\boldsymbol{n e t}_{\boldsymbol{i}}$ to denote the activation and hidden unit $\boldsymbol{j}$

$$
\text { net }_{j}=\sum_{i=1}^{d} x^{(i)} w_{j i}+w_{j 0} \xrightarrow[w_{j i 0}]{\frac{x^{(1)} w_{j i}}{x^{(2)} w_{j 2}}}
$$

- Use $\boldsymbol{n e t}{ }^{*}{ }_{k}$ to denote the activation at output unit $\boldsymbol{k}$

$$
\operatorname{net}_{k}^{*}=\sum_{j=1}^{N_{H}} y_{j} \boldsymbol{v}_{k j}+\boldsymbol{v}_{k 0}
$$



## Discriminant Function

- Discriminant function for class $\boldsymbol{k}$ (the output of the $k$ th output unit)

$$
\begin{aligned}
\boldsymbol{g}_{\boldsymbol{k}}(\boldsymbol{x}) & =\boldsymbol{z}_{\boldsymbol{k}}=\begin{array}{c}
\begin{array}{c}
\text { activation at } \\
\text { jth hidden unit }
\end{array} \\
\\
\end{array}=\boldsymbol{f}(\underbrace{\sum_{j=1}^{\boldsymbol{N}_{H}} \boldsymbol{v}_{\boldsymbol{k} \boldsymbol{j}} \boldsymbol{f}\left(\sum_{i=1}^{\left.\sum_{i=1} \boldsymbol{w}_{j \boldsymbol{i}} \boldsymbol{x}^{(\boldsymbol{i})}+\boldsymbol{w}_{j \boldsymbol{j}}\right)+\boldsymbol{v}_{\boldsymbol{k} \mathbf{0}}}\right)}_{\text {activation at kth output unit }}
\end{aligned}
$$

## 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 $\boldsymbol{j}, \boldsymbol{h}(\boldsymbol{u})=\mathbf{a}_{\boldsymbol{j}} \boldsymbol{u}$

$$
\begin{aligned}
& \boldsymbol{g}_{k}(\boldsymbol{x})=\boldsymbol{f}\left(\sum_{j=1}^{N_{H}} \boldsymbol{v}_{k j} \boldsymbol{h}\left(\sum_{i=1}^{d} \boldsymbol{w}_{j i} \boldsymbol{X}^{(i)}+\boldsymbol{w}_{j 0}\right)+\boldsymbol{v}_{\mathrm{k} 0}\right) \\
& =f\left(\sum_{j=1}^{N_{H}} \boldsymbol{v}_{k j} a_{j}\left(\sum_{i=1}^{d} w_{j i} x^{(i)}+w_{j 0}\right)+v_{k 0}\right) \\
& =f\left(\sum_{i=1}^{d} \sum_{j=1}^{N_{H}}\left(v_{k j} a_{j} \boldsymbol{w}_{j i} x^{(i)}+v_{k j} a_{j} \boldsymbol{w}_{j 0}\right)+v_{k 0}\right) \\
& =f\left(\sum_{i=1}^{d} x^{(i)} \sum_{j=1}^{N_{H}} \boldsymbol{w}_{i j} a_{i} \boldsymbol{w}_{j i}+\left(\sum_{j=1}^{N_{H}} \boldsymbol{W}_{k j} a_{j} \boldsymbol{w}_{j 0}+V_{k 0}\right)\right)
\end{aligned}
$$

## MNN Activation function

- could use a discontinuous activation function

$$
f\left(\text { net }_{k}\right)=\left\{\begin{array}{rrr}
1 & \text { if } \text { net }_{k} \geq 0 \\
-1 & \text { if } \text { net }_{k}<0
\end{array}\right.
$$

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


- From now on, assume $\boldsymbol{f}$ 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 $\boldsymbol{x}_{\mathbf{1}}, \ldots, \boldsymbol{x}_{\boldsymbol{n}}$ each of class $\mathbf{1}, \ldots, \boldsymbol{m}$
- Let network output $\boldsymbol{z}$ represent class $\boldsymbol{c}$ as target $\boldsymbol{t}^{(c)}$

$$
\boldsymbol{z}=\left[\begin{array}{c}
z_{1} \\
\vdots \\
z_{c} \\
\vdots \\
\boldsymbol{z}_{m}
\end{array}\right]=\boldsymbol{t}^{(c)}=\left[\begin{array}{c}
0 \\
\vdots \\
1 \\
\vdots \\
0
\end{array}\right] \rightarrow c \text { th row }
$$

Our Ultimate Goal For FeedForward Operation sample of class $c$


MNN with weights
$\boldsymbol{w}_{\boldsymbol{j i}}$ and $\boldsymbol{v}_{\boldsymbol{k} j}$

## MNN training to achieve the Ultimate Goal

 Modify (learn) MNN parameters $\boldsymbol{w}_{\boldsymbol{j} \boldsymbol{i}}$ and $\boldsymbol{v}_{\boldsymbol{k j}}$ so that for each training sample of class $\boldsymbol{c}$ MNN output $\boldsymbol{z}=\boldsymbol{t}^{(c)}$
## Network Training (learning)

1. Initialize weights $\boldsymbol{w}_{\boldsymbol{j} \boldsymbol{i}}$ and $\boldsymbol{v}_{\boldsymbol{k j}}$ randomly but not to 0
2. Iterate until a stopping criterion is reached


## BackPropagation

- Learn $w_{j i}$ and $v_{k j}$ by minimizing the training error
- What is the training error?
- Suppose the output of MNN for sample $\boldsymbol{x}$ is $\boldsymbol{z}$ and the target (desired output for $\boldsymbol{x}$ ) is $\boldsymbol{t}$
- Error on one sample: $J(w, v)=\frac{1}{\mathbf{2}} \sum_{c=1}^{m}\left(\boldsymbol{t}_{c}-z_{c}\right)^{2}$
- Training error: $J(w, v)=\frac{1}{2} \sum_{i=1}^{n} \sum_{c=1}^{m}\left(t_{c}^{(i)}-z_{c}^{(i)}\right)^{2}$
- Use gradient descent:

$$
\boldsymbol{v}^{(0)}, \boldsymbol{w}^{(0)}=\text { random }
$$

repeat until convergence:

$$
\begin{aligned}
& \boldsymbol{w}^{(t+1)}=\boldsymbol{w}^{(t)}-\eta \nabla_{w} \boldsymbol{J}\left(\mathbf{w}^{(t)}\right) \\
& \boldsymbol{v}^{(t+1)}=\boldsymbol{v}^{(t)}-\eta \nabla_{v} \boldsymbol{J}\left(\boldsymbol{v}^{(t)}\right)
\end{aligned}
$$

## BackPropagation

- For simplicity, first take training error for one sample $\boldsymbol{x}_{\boldsymbol{i}}$

$$
\begin{aligned}
& J(w, v)=\frac{1}{2} \sum_{c=1}^{m}\left(t_{c}-z_{c}\right)^{2} \text { function of } w, v \\
& \text { fixed constant }
\end{aligned}
$$

$$
z_{k}=f\left(\sum_{j=1}^{N_{H}} v_{k j} f\left(\sum_{i=1}^{d} w_{j i} x^{(i)}+w_{j 0}\right)+v_{k 0}\right)
$$

- Need to compute

1. partial derivative w.r.t. hidden-to-output weights $\frac{\partial J}{\partial \boldsymbol{v}_{k j}}$
2. partial derivative w.r.t. input-to-hidden weights $\frac{\partial J}{\partial \boldsymbol{w}_{j}}$

## BackPropagation: Layered Model

activation at
hidden unit $j$
output at
hidden unit $\boldsymbol{j}$

$$
y_{j}=f\left(\text { net }_{j}\right)
$$

activation at output unit $\boldsymbol{k}$
activation at output unit $\boldsymbol{k}$

$$
\boldsymbol{n e t}_{j}=\sum_{i=1}^{d} \boldsymbol{x}^{(i)} \boldsymbol{w}_{j i}+\boldsymbol{w}_{j 0}
$$

$$
\operatorname{net}_{k}^{*}=\sum_{j=1}^{N_{H}} \boldsymbol{y}_{j} \boldsymbol{v}_{k j}+v_{k 0}
$$

$$
z_{k}=f\left(\text { net }_{k}^{*}\right)
$$



## BackPropagation

$$
n e t_{k}^{*}=\sum_{j=1}^{N_{H}} y_{j} v_{k j}+v_{k 0} \square z_{k}=f\left(n e t_{k}^{*}\right) \quad J(w, v)=\frac{1}{2} \sum_{c=1}^{m}\left(t_{c}-z_{c}\right)^{2}
$$

- First compute hidden-to-output derivatives $\frac{\partial \boldsymbol{J}}{\partial \boldsymbol{v}_{k j}}$

$$
\begin{aligned}
& \frac{\partial \boldsymbol{J}}{\partial \boldsymbol{v}_{k j}}=\frac{\mathbf{1}}{\mathbf{2}} \sum_{c=1}^{m} \frac{\partial}{\partial \boldsymbol{v}_{k j}}\left(\boldsymbol{t}_{c}-\boldsymbol{z}_{c}\right)^{2}=\sum_{c=1}^{m}\left(\boldsymbol{t}_{c}-\boldsymbol{z}_{c}\right) \frac{\partial}{\partial \boldsymbol{v}_{k j}}\left(\boldsymbol{t}_{c}-\boldsymbol{z}_{c}\right) \\
& =\left(t_{k}-\boldsymbol{z}_{k}\right) \frac{\partial}{\partial v_{k j}}\left(t_{k}-z_{k}\right)=-\left(t_{k}-\boldsymbol{z}_{k}\right) \frac{\partial}{\partial v_{k j}}\left(z_{k}\right) \\
& =-\left(\boldsymbol{t}_{k}-\boldsymbol{z}_{k}\right) \frac{\partial \mathbf{z}_{k}}{\partial \operatorname{net}_{k}^{*}} \frac{\partial \boldsymbol{n e t}}{k} \boldsymbol{t}_{k j} \\
& = \begin{cases}-\left(t_{k}-z_{k}\right) f^{\prime}\left(\text { net }_{k}^{\prime}\right) y_{j} & \text { if } j \neq 0 \\
-\left(t_{k}-z_{k}\right) f^{\prime}\left(\text { net }_{k}^{\prime}\right) & \text { if } j=0\end{cases}
\end{aligned}
$$

## BackPropagation

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

$$
\begin{array}{r}
j>0: \quad \boldsymbol{v}_{k j}^{(t+1)}=\boldsymbol{v}_{k j}^{(t)}+\eta\left(\boldsymbol{t}_{\boldsymbol{k}}-\boldsymbol{z}_{\boldsymbol{k}}\right) \boldsymbol{f}^{\prime}\left(\boldsymbol{n e t}_{k}^{*}\right) \boldsymbol{y}_{\boldsymbol{j}} \\
j=0 \text { (bias weight): } \quad \boldsymbol{v}_{\boldsymbol{k} 0}^{(t+1)}=\boldsymbol{v}_{\boldsymbol{k} 0}^{(t)}+\eta\left(\boldsymbol{t}_{\boldsymbol{k}}-\boldsymbol{z}_{\boldsymbol{k}}\right) \boldsymbol{f}^{\prime}\left(\boldsymbol{n e t}_{k}^{*}\right)
\end{array}
$$

## BackPropagation

－Now compute input－to－hidden $\frac{\partial J}{\partial \boldsymbol{w}_{j i}}$

$$
\begin{aligned}
& \frac{\partial J}{\partial \boldsymbol{w}_{j i}}=\sum_{k=1}^{m}\left(\boldsymbol{t}_{k}-\boldsymbol{z}_{k}\right) \frac{\partial}{\partial \boldsymbol{w}_{j j}}\left(\boldsymbol{t}_{k}-\boldsymbol{z}_{k}\right) \\
& =-\sum_{k=1}^{m}\left(t_{k}-z_{k}\right) \frac{\partial \boldsymbol{z}_{k}}{\partial w_{j i}}=-\sum_{k=1}^{m}\left(\boldsymbol{t}_{k}-\boldsymbol{z}_{k}\right) \frac{\partial \boldsymbol{z}_{k}}{\partial \operatorname{net}_{k}^{*}} \frac{\partial \boldsymbol{n e t}}{\hat{k}} \boldsymbol{w}_{j i} \\
& =-\sum_{k=1}^{m}\left(t_{k}-z_{k}\right) f^{\prime}\left(\text { net }_{k}^{*}\right) \frac{\partial n e t_{k}^{*}}{\partial y_{j}} \frac{\partial y_{j}}{\partial w_{j i}} \\
& =-\sum_{k=1}^{m}\left(t_{k}-z_{k}\right) f^{\prime}\left(\text { net }_{k}^{\prime}\right) \boldsymbol{v}_{k j} \frac{\partial \boldsymbol{y}_{j}}{\partial \boldsymbol{n e t}} \frac{\partial \boldsymbol{t _ { j }} \boldsymbol{t}_{j}}{\partial \boldsymbol{w}_{j i}} \\
& = \begin{cases}\left.-\sum_{k=1}^{m}\left(t_{k}-z_{k}\right) f^{\prime}\left(\text { net }_{k}^{*}\right) v_{k j} f^{\prime} \text { net }_{j}\right) x^{(i)} & \text { if } i \neq 0 \\
\left.-\sum_{k=1}^{m}\left(t_{k}-z_{k}\right) f^{\prime}\left(\text { net }_{k}^{*}\right) v_{k j} f^{\prime} \text { net }_{j}\right) & \text { if } i=0\end{cases}
\end{aligned}
$$

$$
\begin{aligned}
& \sqrt{\square} \\
& \boldsymbol{n e t}_{h}=\sum_{h=1}^{d} \boldsymbol{x}^{(i)} \boldsymbol{w}_{h i}+\boldsymbol{w}_{h 0} \\
& \urcorner \\
& y_{j}=f\left(\text { net }_{j}\right) \\
& \text { に } \\
& \operatorname{net}_{k}^{*}=\sum_{s=1}^{N_{H}} y_{s} v_{k s}+v_{k 0} \\
& \Omega \\
& z_{k}=f\left(n e t_{k}^{*}\right) \\
& \text { に } \\
& J(w, v)=\frac{\mathbf{1}}{\mathbf{2}} \sum_{c=1}^{m}\left(\boldsymbol{t}_{c}-\boldsymbol{z}_{c}\right)^{2}
\end{aligned}
$$

## BackPropagation

$$
\frac{\partial J}{\partial w_{j i}}= \begin{cases}-f^{\prime}\left(\text { net }_{j}\right) x^{(i)} \sum_{k=1}^{m}\left(t_{k}-z_{k}\right) f^{\prime}\left(\text { net }_{k}^{*}\right) v_{k j} & \text { if } i \neq 0 \\ -f^{\prime}\left(\text { net }_{j}\right) \sum_{k=1}^{m}\left(t_{k}-z_{k}\right) f^{\prime}\left(\text { net }_{k}^{*}\right) v_{k j} & \text { if } i=0\end{cases}
$$

Gradient Descent Single Sample Update Rule for input-to-hidden weights $w_{j i}$

$$
\mathrm{i}>0: \quad w_{j i}^{(t+1)}=w_{j i}^{(t)}+\eta f^{\prime}\left(\text { net }_{j}\right) x^{(i)} \sum_{k=1}^{m}\left(t_{k}-z_{k}\right) f^{\prime}\left(\text { net }_{k}^{*}\right) v_{k j}^{(t)}
$$

$\mathrm{i}=0$ (bias weight): $\boldsymbol{w}_{j 0}^{(t+1)}=\boldsymbol{w}_{j 0}^{(t)}+\eta \boldsymbol{f}^{\prime}\left(\right.$ net $\left._{j}\right) \sum_{k=1}^{m}\left(\boldsymbol{t}_{k}-\boldsymbol{z}_{k}\right) \boldsymbol{f}^{\prime}\left(\right.$ net $\left._{k}^{*}\right) \boldsymbol{v}_{k j}^{(t)}$

## BackPropagation of Errors

$$
\frac{\partial J}{\partial w_{j i}}=-f^{\prime}\left(n e t_{j}\right) x^{(i)} \sum_{k=1}^{m}\left(t_{k}-z_{k}\right) f^{\prime}\left(n e t_{k}^{*}\right) v_{k j} \quad \frac{\partial J}{\partial v_{k j}}=-\underbrace{t_{k}-z_{k}}_{\text {error }}) f^{\prime}\left(n e t_{k}^{*}\right) y_{j}
$$



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


## BackPropagation

- Consider update rule for hidden-to-output weights:

$$
\boldsymbol{v}_{k j}^{(t+1)}=\boldsymbol{v}_{k j}^{(t)}+\eta\left(\boldsymbol{t}_{k}-\boldsymbol{z}_{k}\right) \boldsymbol{f}^{\prime}\left(\text { net }_{k}^{*}\right) \boldsymbol{y}_{j}
$$

- Suppose $\boldsymbol{t}_{\boldsymbol{k}}-\boldsymbol{z}_{\boldsymbol{k}}>\mathbf{0}$
- Then output of the $\boldsymbol{k}$ th hidden unit is too small: $\boldsymbol{t}_{\boldsymbol{k}}>\boldsymbol{z}_{\boldsymbol{k}}$
- Typically activation function $\boldsymbol{f}$ is s.t. $\boldsymbol{f}$ ' $>\mathbf{0}$
- Thus $\left(t_{k}-z_{k}\right) f^{\prime}\left(\right.$ net $\left._{k}^{*}\right)>0$
- There are 2 cases:


1. $\boldsymbol{y}_{\boldsymbol{j}}>\mathbf{0}$, then to increase $\boldsymbol{z}_{\boldsymbol{k}}$, should increase weight $\boldsymbol{v}_{\boldsymbol{k} \boldsymbol{j}}$ which is exactly what we do since $\eta\left(\boldsymbol{t}_{k}-\boldsymbol{z}_{k}\right) \boldsymbol{f}^{\prime}\left(\right.$ net $\left._{k}^{*}\right) \boldsymbol{y}_{j}>0$
2. $\boldsymbol{y}_{\boldsymbol{j}}<\mathbf{0}$, then to increase $\boldsymbol{z}_{\boldsymbol{k}}$, should decrease weight $\boldsymbol{v}_{\boldsymbol{k} \boldsymbol{j}}$ which is exactly what we do since $\eta\left(\boldsymbol{t}_{\boldsymbol{k}}-\boldsymbol{z}_{\boldsymbol{k}}\right) \boldsymbol{f}^{\prime}\left(\boldsymbol{n e t}_{\boldsymbol{k}}^{*}\right) \boldsymbol{y}_{\boldsymbol{j}}<\mathbf{0}$

## BackPropagation

- The case $\boldsymbol{t}_{k}-\boldsymbol{z}_{k}<\mathbf{0}$ is analogous
- Similarly, can show that input-to-hidden weights make sense
- Important: weights should be initialized to random nonzero numbers

$$
\frac{\partial J}{\partial w_{j i}}=-\boldsymbol{f}^{\prime}\left(\text { net }_{j}\right) x^{(i)} \sum_{k=1}^{m}\left(t_{k}-z_{k}\right) f^{\prime}\left(\text { net }_{k}^{*}\right) v_{k j}
$$

- if $\boldsymbol{v}_{\boldsymbol{k j}}=0$, input-to-hidden weights $\boldsymbol{w}_{\boldsymbol{j} \boldsymbol{i}}$ 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 $\boldsymbol{n}_{\boldsymbol{H}}$
- weights $\boldsymbol{w}, \boldsymbol{v}$
- convergence criterion $\theta$ and learning rate $\eta$
- time $\boldsymbol{t}=0$

2. do
$\boldsymbol{x} \leftarrow$ randomly chosen training pattern
for all $0 \leq i \leq d, 0 \leq j \leq n_{H}, 0 \leq k \leq m$

$$
\begin{aligned}
& v_{k j}=v_{k j}+\eta\left(t_{k}-z_{k}\right) f^{\prime}\left(\text { net }_{k}^{*}\right) y_{j} \\
& v_{k 0}=v_{k 0}+\eta\left(t_{k}-z_{k}\right) f^{\prime}\left(\text { net }_{k}^{*}\right) \\
& w_{j i}=w_{j i}+\eta f^{\prime}\left(\text { net }_{j}\right) x^{(i)} \sum_{k=1}^{m}\left(t_{k}-z_{k}\right) f^{\prime}\left(\text { net }_{k}^{*}\right) v_{k j} \\
& w_{j 0}=w_{j 0}+\eta f^{\prime}\left(\text { net }_{j}\right) \sum_{k=1}^{m}\left(t_{k}-z_{k}\right) f^{\prime}\left(\text { net }_{k}^{*}\right) v_{k j}
\end{aligned}
$$

$$
t=t+1
$$

until $\|J\|<\theta$
3. return $v, w$

## Batch Back Propagation

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

$$
J(w, v)=\frac{1}{2} \sum_{c=1}^{m}\left(t_{c}-z_{c}\right)^{2}
$$

- The full objective function:

$$
J(w, v)=\frac{1}{2} \sum_{l=1}^{n} \sum_{c=1}^{m}\left(t_{c}^{(i)}-z_{c}^{(i)}\right)^{2}
$$

- 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,

$$
\frac{\partial J}{\partial w_{j i}}=\sum_{p=1}^{n}-f^{\prime}\left(\text { net }_{j}\right) x_{p}^{(i)} \sum_{k=1}^{m}\left(t_{k}-z_{k}\right) f^{\prime}\left(\text { net }_{k}^{*}\right) v_{k j}
$$

## Batch Back Propagation

1. Initialize $\boldsymbol{n}_{H}, \boldsymbol{w}, \boldsymbol{v}, \boldsymbol{\theta}, \boldsymbol{\eta}, \boldsymbol{t}=\mathbf{0}$
2. do

$$
\Delta v_{k j}=\Delta v_{k 0}=\Delta w_{j i}=\Delta w_{j 0}=0
$$

for all $1 \leq p \leq n$
for all $0 \leq i \leq d, \quad 0 \leq \boldsymbol{j} \leq \boldsymbol{n}_{H}, \mathbf{0} \leq \boldsymbol{k} \leq \boldsymbol{m}$

$$
\Delta \boldsymbol{v}_{k j}=\Delta \boldsymbol{v}_{k j}+\eta\left(\boldsymbol{t}_{k}-\boldsymbol{z}_{k}\right) f^{\prime}\left(n e t_{k}^{*}\right) \boldsymbol{y}_{j}
$$

$$
\Delta v_{k 0}=\Delta v_{k 0}+\eta\left(t_{k}-z_{k}\right) f^{\prime}\left(\operatorname{net}_{m}^{*}\right)
$$

$$
\Delta w_{j i}=\Delta w_{j i}+\eta f^{\prime}\left(\text { net }_{j}\right) x_{p}^{(i)} \sum_{k=1}^{m}\left(t_{k}-z_{k}\right) f^{\prime}\left(\text { net }_{k}^{*}\right) v_{k j}
$$

$$
\Delta w_{j 0}=\Delta w_{j 0}+\eta f^{\prime}\left(n e t_{j}\right) \sum_{k=1}^{m}\left(t_{k}-z_{k}\right) f^{\prime}\left(n e t_{k}^{*}\right) v_{k j}
$$

$$
v_{k j}=v_{k j}+\Delta v_{k j} ; v_{k 0}=v_{k 0}+\Delta v_{k 0} ; w_{j i}=w_{j i}+\Delta w_{j i} ; w_{j 0}=w_{j 0}+\Delta w_{j 0}
$$

$$
t=t+1
$$

until || $\mathrm{J} \|<\theta$
3. return $v, w$

## 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




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
- $\boldsymbol{k}$ in the knn neighbor classifier
- $\boldsymbol{h}$ 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 $\varphi$
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 $\boldsymbol{y}=\varphi(\boldsymbol{x})$ to 2 dimensions (2 hidden units); patterns are almost linearly separable


MNN finds nonlinear mapping $\boldsymbol{y}=\varphi(\boldsymbol{x})$ 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

