CS840a
Learning and Computer Vision
Prof. Olga Veksler

Lecture 6

Multilayer Neural Networks

Today

- Multilayer Neural Networks
  - Inspiration from Biology
  - History
  - Perceptron
  - Multilayer perceptron

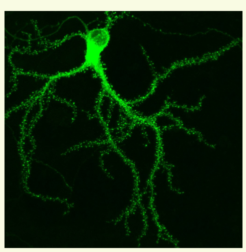
Brain vs. Computer

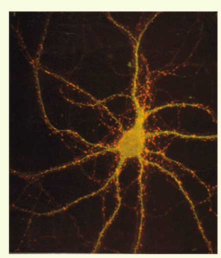
- Designed to solve logic and arithmetic problems
- Can solve a gazillion arithmetic and logic problems in an hour
- absolute precision
- Usually one very fast procesor
- high reliability

- 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?

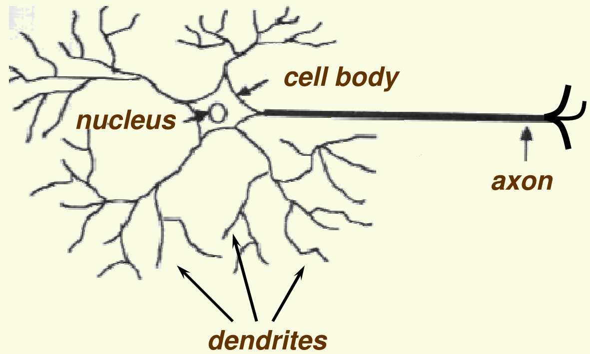
Neuron: Basic Brain Processor





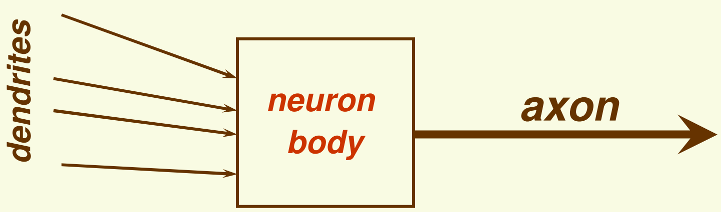
- Neurons are nerve cells that transmit signals to and from brains at the speed of around 200mph
- Each neuron cell communicates to anywhere from 1000 to 10,000 other neurons, muscle cells, glands, so on
- Have around 10^{10} neurons in our brain (network of neurons)
- Most neurons a person is ever going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

Neuron: Basic Brain Processor



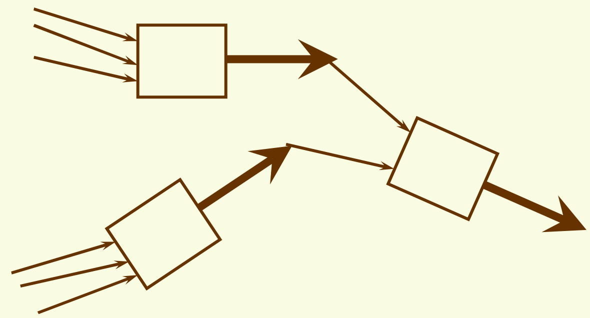
- Main components of a neuron
  - ***Cell body*** which holds DNA information in ***nucleus***
  - ***Dendrites*** may have thousands of dendrites, usually short
  - ***axon*** long structure, which splits in possibly thousands branches at the end. May be up to 1 meter long

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

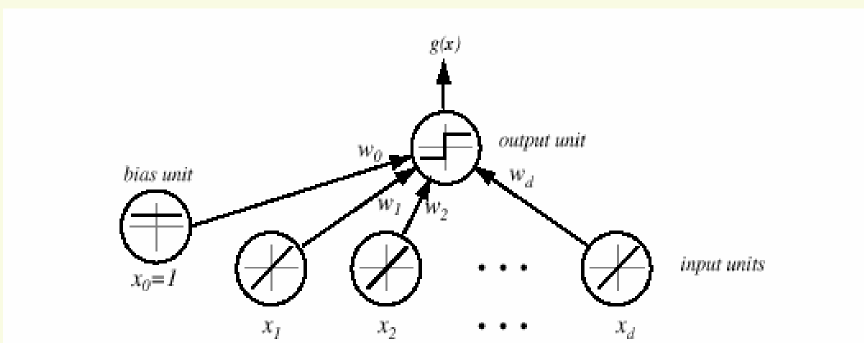
ANN History: Stagnation

- 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

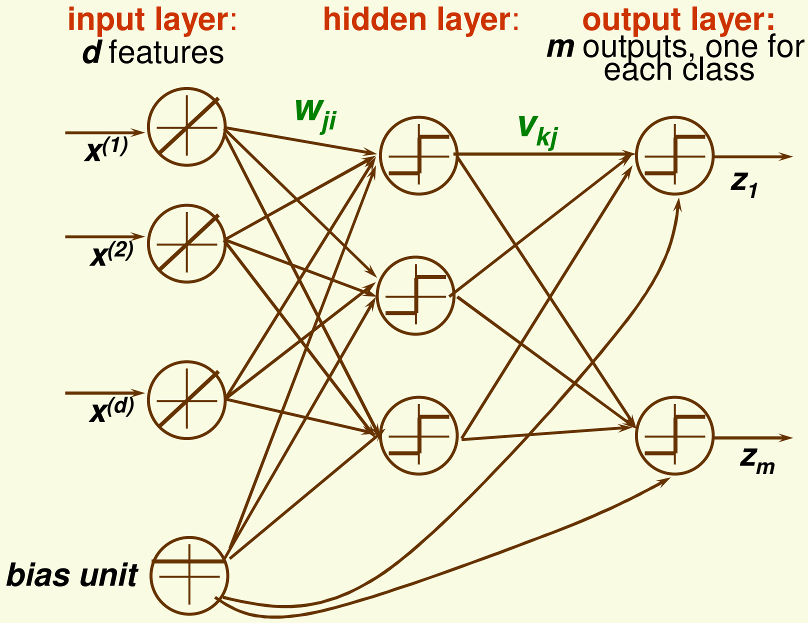
- Revival of ANN in 1980's
- 1982, J. Hopfield
  - New kind of networks (Hopfield's networks)
  - Bidirectional connections between neurons
  - Implements associative memory
- 1982 joint US-Japanese conference on ANN
  - US worries that it will stay behind
- Many examples of mulitlayer NN appear
- 1982, 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



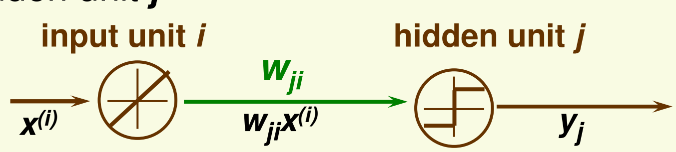
- Input and output layers
- $\boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{w}^t\boldsymbol{x} + \boldsymbol{w}_0$
- Limitation: can learn only linearly separable classes

MNN: Feed Forward Operation

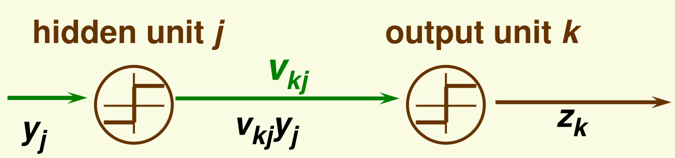


MNN: Notation for Weights

- Use w_{ji} to denote the weight between input unit i and hidden unit j



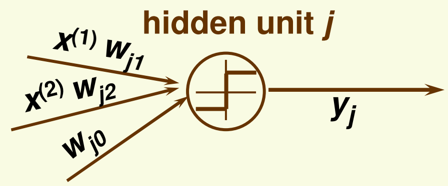
- Use v_{kj} to denote the weight between hidden unit j and output unit k



MNN: Notation for Activation

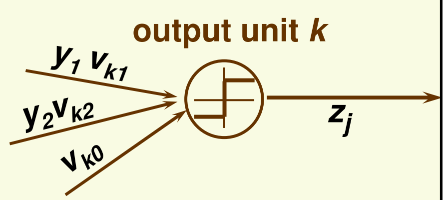
- Use net_j to denote the activation and hidden unit j

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



- Use net^*_k to denote the activation at output unit k

$$net^*_k = \sum_{j=1}^{N_H} y_j v_{kj} + v_{k0}$$



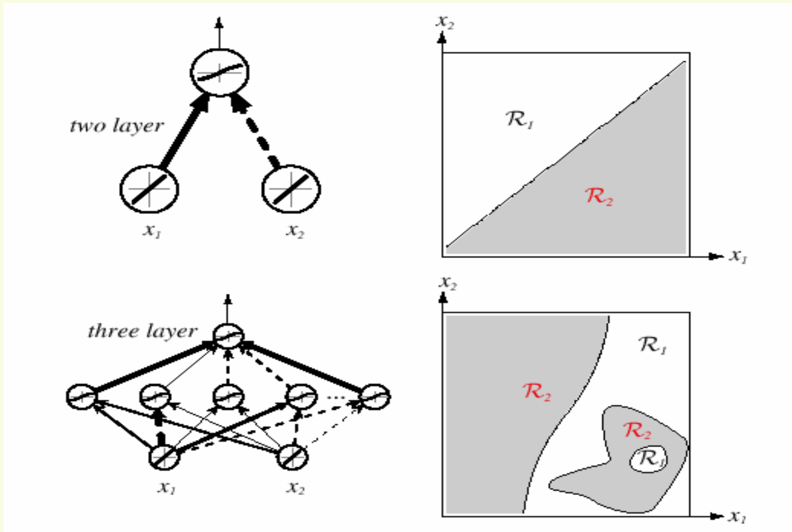
Discriminant Function

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

$$g_k(x) = z_k =$$

$$= f\left(\underbrace{\sum_{j=1}^{N_H} v_{kj} f\left(\overbrace{\sum_{i=1}^{d} w_{ji} x^{(i)} + w_{j0}}^{\text{activation at jth hidden unit}} \right) + v_{k0}}_{\text{activation at kth output unit}} \right)$$

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

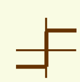
- Must be nonlinear for expressive power larger than that of perceptron
  - If use linear activation function at hidden layer, can only deal with linearly separable classes
  - Suppose at hidden unit ***j***, $h(u)=a_j u$

$$
\begin{aligned}
g_k(x) &= f\left(\sum_{j=1}^{N_H} v_{kj}\, h\left(\sum_{i=1}^{d} w_{ji} x^{(i)} + w_{j0}\right) + v_{k0}\right) \\
&= f\left(\sum_{j=1}^{N_H} v_{kj}\, a_j \left(\sum_{i=1}^{d} w_{ji} x^{(i)} + w_{j0}\right) + v_{k0}\right) \\
&= f\left(\sum_{i=1}^{d}\sum_{j=1}^{N_H}\left(v_{kj} a_j w_{ji} x^{(i)} + v_{kj} a_j w_{j0}\right) + v_{k0}\right) \\
&= f\left(\sum_{i=1}^{d} x^{(i)} \overbrace{\sum_{j=1}^{N_H} v_{kj} a_j w_{ji}}^{w_i^{new}} + \overbrace{\left(\sum_{j=1}^{N_H} v_{kj} a_j w_{j0} + v_{k0}\right)}^{w_0^{new}}\right)
\end{aligned}
$$

MNN Activation function

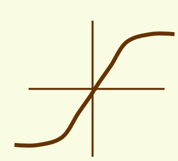
- could use a discontinuous activation function

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



- 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

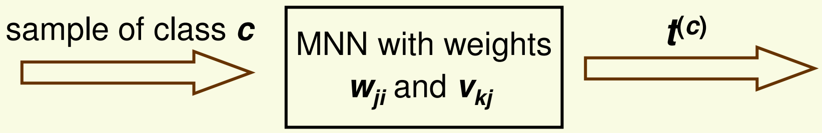
- Can vary
  - number of hidden layers
  - Nonlinear activation function
    - Can use different function for hidden and output layers
    - Can use different function at each hidden and output node

MNN: Class Representation

- Training samples $\boldsymbol{x_1}, \ldots, \boldsymbol{x_n}$ each of class $\boldsymbol{1}, \ldots, \boldsymbol{m}$
- Let network output $\boldsymbol{z}$ represent class $\boldsymbol{c}$ as **target $\boldsymbol{t^{(c)}}$**

$$z = \begin{bmatrix} z_1 \\ \vdots \\ z_c \\ \vdots \\ z_m \end{bmatrix} = t^{(c)} = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \leftarrow c\text{th row}$$

Our Ultimate Goal For FeedForward Operation

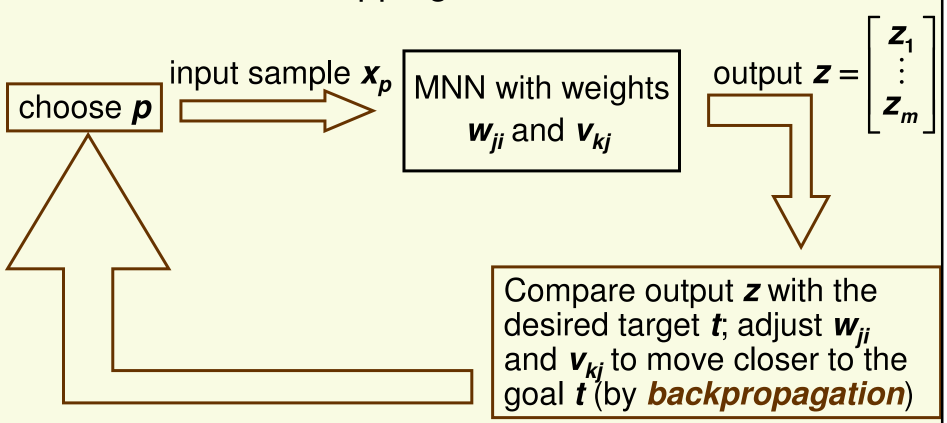


MNN training to achieve the Ultimate Goal

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

Network Training (learning)

1. Initialize weights $\boldsymbol{w_{ji}}$ and $\boldsymbol{v_{kj}}$ randomly **but not to 0**
2. Iterate until a stopping criterion is reached



BackPropagation

- Learn w_{ji} and v_{kj} 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: $J(w,v)=\frac{1}{2}\sum_{i=1}^{n}\sum_{c=1}^{m}\left(t_c^{(i)} - z_c^{(i)}\right)^2$
- Use gradient descent:

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

repeat until convergence:

$$w^{(t+1)} = w^{(t)} - \eta \nabla_w J\left(w^{(t)}\right)$$
$$v^{(t+1)} = v^{(t)} - \eta \nabla_v J\left(v^{(t)}\right)$$

BackPropagation

- For simplicity, first take training error for one sample x_i

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

function of w,v

fixed constant

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

- Need to compute
  1. partial derivative w.r.t. hidden-to-output weights $\frac{\partial J}{\partial v_{kj}}$
  2. partial derivative w.r.t. input-to-hidden weights $\frac{\partial J}{\partial w_{ji}}$

BackPropagation: Layered Model

activation at hidden unit ***j***

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

$$\Downarrow$$

output at hidden unit ***j***

$$y_j = f(net_j)$$

$$\Downarrow$$

activation at output unit ***k***

$$net_k^* = \sum_{j=1}^{N_H} y_j v_{kj} + v_{k0}$$

$$\Downarrow$$

activation at output unit ***k***

$$z_k = f(net_k^*)$$

$$\Downarrow$$

objective function

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

chain rule $\dfrac{\partial J}{\partial v_{kj}}$

chain rule $\dfrac{\partial J}{\partial w_{ji}}$

BackPropagation

$$net_k^* = \sum_{j=1}^{N_H} y_j v_{kj} + v_{k0} \Rightarrow z_k = f(net_k^*) \Rightarrow J(w,v) = \frac{1}{2}\sum_{c=1}^{m}(t_c - z_c)^2$$

- First compute hidden-to-output derivatives $\dfrac{\partial J}{\partial v_{kj}}$

$$\frac{\partial J}{\partial v_{kj}} = \frac{1}{2}\sum_{c=1}^{m}\frac{\partial}{\partial v_{kj}}(t_c - z_c)^2 = \sum_{c=1}^{m}(t_c - z_c)\frac{\partial}{\partial v_{kj}}(t_c - z_c)$$

$$= (t_k - z_k)\frac{\partial}{\partial v_{kj}}(t_k - z_k) = -(t_k - z_k)\frac{\partial}{\partial v_{kj}}(z_k)$$

$$= -(t_k - z_k)\frac{\partial z_k}{\partial net_k^*}\frac{\partial net_k^*}{\partial v_{kj}}$$

$$= \boxed{\begin{cases} -(t_k - z_k) f'(net_k^*) y_j & \text{if } j \neq 0 \\ -(t_k - z_k) f'(net_k^*) & \text{if } j = 0 \end{cases}}$$

BackPropagation

Gradient Descent *Single Sample* Update Rule for hidden-to-output weights v_{kj}

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

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

BackPropagation

- Now compute input-to-hidden $\dfrac{\partial J}{\partial w_{ji}}$

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

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

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

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

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

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

$$\Downarrow$$

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

$$\Downarrow$$

$$y_j = f(net_j)$$

$$\Downarrow$$

$$net_k^* = \sum_{s=1}^{N_H} y_s v_{ks} + v_{k0}$$

$$\Downarrow$$

$$z_k = f(net_k^*)$$

$$\Downarrow$$

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

BackPropagation

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

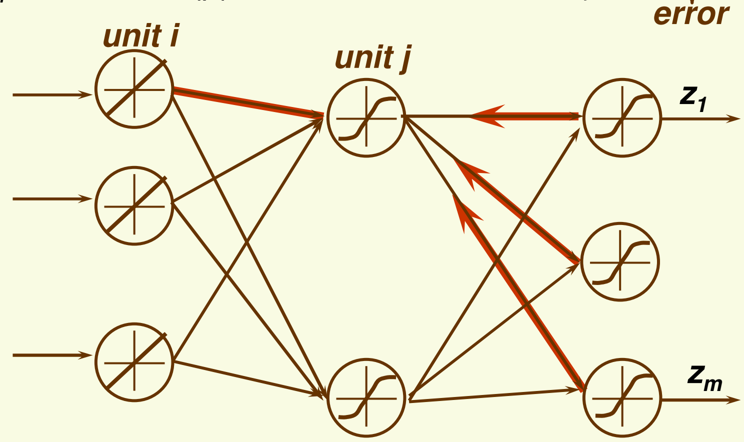
Gradient Descent *Single Sample* Update Rule for input-to-hidden weights w_{ji}

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

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

BackPropagation of Errors

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



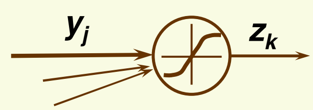
- Name "backpropagation" because during training, errors propagated back from output to hidden layer

BackPropagation

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

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

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



- 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 $\eta (t_k - z_k) f'(net_k^*) y_j < 0$

BackPropagation

- 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 $v_{kj} = 0$, input-to-hidden weights 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_H
   - weights w, v
   - convergence criterion θ and learning rate η
   - time $t = 0$
2. **do**

   $x \leftarrow$ randomly chosen training pattern

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

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

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

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

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

   $t = t + 1$

   until $\|J\| < \theta$

3. **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:

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

- The full objective function:

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

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

$$\frac{\partial}{\partial w}J(w,v) = \frac{1}{2}\sum_{i=1}^{n}\underbrace{\frac{\partial}{\partial w}\left(\sum_{c=1}^{m}\left(t_c^{(i)} - z_c^{(i)}\right)^2\right)}_{\text{already derived this}}$$

Batch Back Propagation

- For example,

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

Batch Back Propagation

1. Initialize n_H, w, v, θ, η, $t = 0$
2. ***do***

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

$$\text{one epoch} \left\{ \begin{array}{l} \underline{\textit{for all}}\ 1 \le p \le n \\ \quad \underline{\textit{for all}}\ 0 \le i \le d,\ 0 \le j \le n_H,\ 0 \le k \le m \\ \qquad \Delta v_{kj} = \Delta v_{kj} + \eta (t_k - z_k) f'(net_k^*) y_j \\ \qquad \Delta v_{k0} = \Delta v_{k0} + \eta (t_k - z_k) f'(net_k^*) \\ \qquad \Delta w_{ji} = \Delta w_{ji} + \eta f'(net_j) x_p^{(i)} \sum_{k=1}^{m} (t_k - z_k) f'(net_k^*) v_{kj} \\ \qquad \Delta w_{j0} = \Delta w_{j0} + \eta f'(net_j) \sum_{k=1}^{m} (t_k - z_k) f'(net_k^*) v_{kj} \end{array} \right.$$

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

$t = t + 1$

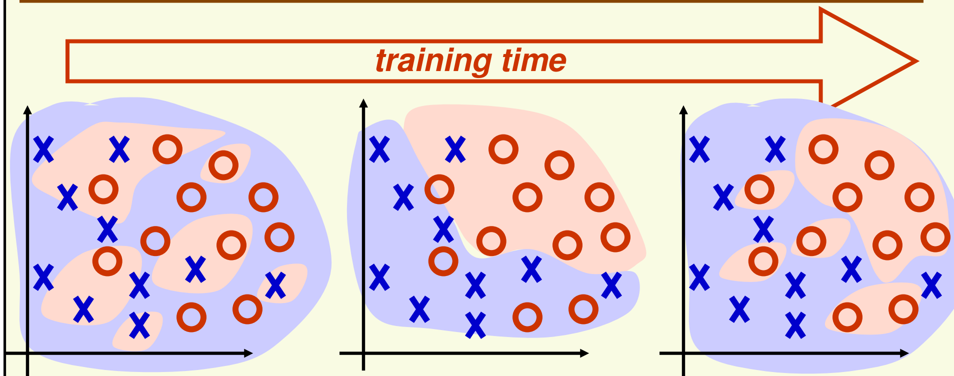
until $\|J\| < \theta$

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



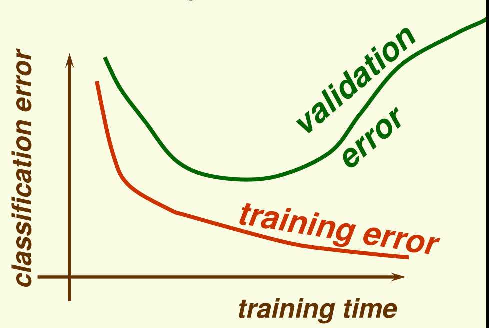
Large training error: *in the beginning random decision regions*

Small training error: *decision regions improve with time*

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

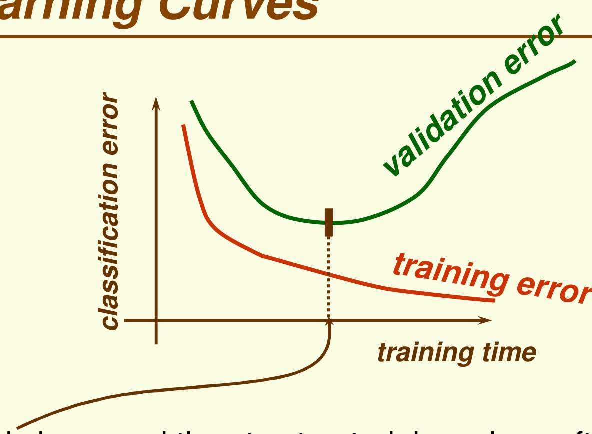
MNN Learning Curves

- ***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

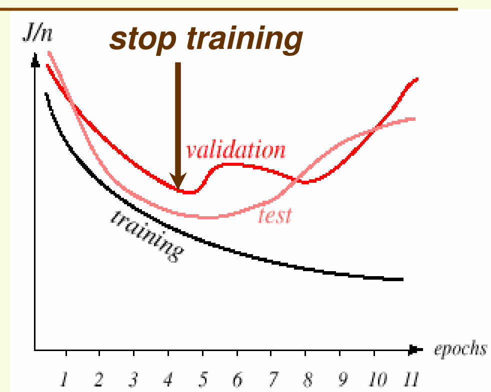
Learning Curves



- 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



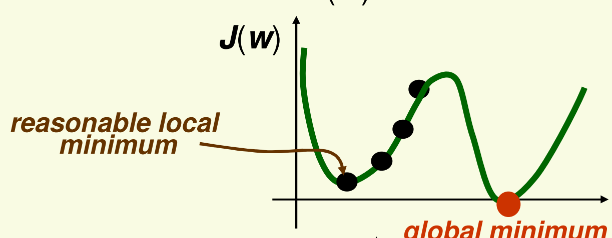
- Stop training after the first local minimum on validation data
- We are assuming performance on test data will be similar to performance on validation data

Data Sets

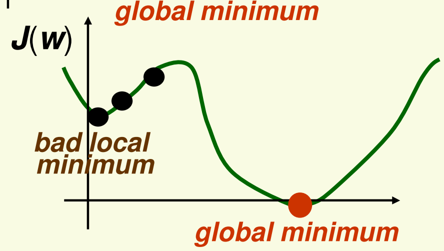
- ***Training data***
  - data on which learning is performed
- ***Validation data***
  - validation data is used to determine any free parameters of the classifier
    - ***k*** in the knn neighbor classifier
    - ***h*** for parzen windows
    - number of hidden layers in the MNN
    - etc
- ***Test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

Practical Tips for BP: Momentum

- Gradient descent finds only a local minima
  - not a problem if $\boldsymbol{J}(\boldsymbol{w})$ is small at a local minima. Indeed, we do not wish to find $\boldsymbol{w}$ s.t. $\boldsymbol{J}(\boldsymbol{w}) = 0$ due to overfitting



  - problem if $\boldsymbol{J}(\boldsymbol{w})$ is large at a local minimum $\boldsymbol{w}$



Practical Tips for BP: Momentum

- Momentum: popular method to avoid local minima and also speeds up descent in plateau regions
  - weight update at time t is $\Delta w^{(t)} = w^{(t)} - w^{(t-1)}$
  - add temporal average direction in which weights have been moving recently

$$w^{(t+1)} = w^{(t)} + (1-\alpha)\underbrace{\left[\eta \frac{\partial J}{\partial w}\right]}_{\text{steepest descent direction}} + \alpha \underbrace{\Delta w^{(t-1)}}_{\text{previous direction}}$$

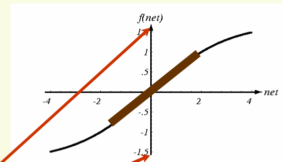
  - at $\alpha = 0$, equivalent to gradient descent
  - at $\alpha = 1$, gradient descent is ignored, weight update continues in the direction in which it was moving previously (momentum)
  - usually, α is around 0.9

Practical Tips for BP: Activation Function

- Gradient descent will work with any continuous and differentiable ***f*** **,** however some choices are better than others
- Desirable properties of ***f*** :
  - nonlinearity to express nonlinear decision boundaries
  - Saturation, that is ***f*** has minimum and maximum values (-***a*** and ***b***). Keeps and weights ***w***, ***v*** bounded, thus training time down
  - Monotonicity so that activation function itself does not introduce additional local minima
  - Linearity for a small values of net, so that network can produce linear model, if data supports it
  - antisymmetric, that is ***f***(-1) = -***f***(1), leads to faster learning

Practical Tips for BP: Activation Function

- Sigmoid activation function $\boldsymbol{f}$ satisfies all of the above properties



$$f(\boldsymbol{net}) = \alpha \frac{e^{\beta \cdot net} - e^{-\beta \cdot net}}{e^{\beta \cdot net} + e^{-\beta \cdot net}}$$

- Convenient to set $\alpha = 1.716$, $\beta = 2/3$
- Asymptotic values ∓ 1.716
- Linear range is roughly for $-1 < \boldsymbol{net} < 1$

Practical Tips for BP: Target Values

- For sigmoid function, to represent class $\boldsymbol{c}$, use

$$\begin{array}{cl} t^{(c)} = \begin{bmatrix} -1 \\ \vdots \\ 1 \\ \vdots \\ -1 \end{bmatrix} & \begin{array}{l} \\ \\ \leftarrow c\text{th row} \\ \\ \\ \end{array} \end{array}$$

- Always use values less than asymptotic values for target
  - For small error, need $\boldsymbol{t}$ to be close to $\boldsymbol{z} = \boldsymbol{f}(\boldsymbol{net})$
  - For any finite value of $\boldsymbol{net}$, $\boldsymbol{f}(\boldsymbol{net})$ never reaches the asymptotic value
  - The error will always be too large, training will never stop, and weights $\boldsymbol{w}, \boldsymbol{v}$ will go to infinity

Practical Tips for BP: Normalization

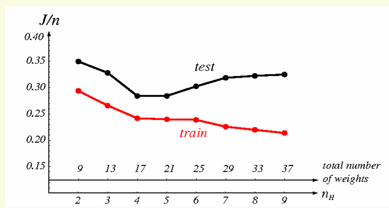
- Each feature of input data should be normalized
- Suppose we measure fish length in meters and weight in grams
  - Typical sample [length = 0.5, weight = 3000]
  - Feature length will be basically ignored by the network
  - If length is in fact important, learning will be VERY slow

Practical Tips for BP: Normalization

- Normalize each feature ***i*** to be of mean ***0*** and variance ***1***
  - First for each feature ***i***, compute ***var*** $[x^{(i)}]$ and ***mean*** $[x^{(i)}]$
  - Then $$x_k^{(i)} \leftarrow \frac{x_k^{(i)} - \mathbf{mean}\left(x^{(i)}\right)}{\sqrt{\mathbf{var}\left(x^{(i)}\right)}}$$
    - Cannot do this for online version of the algorithm since data is not available all at once
- If there are a lot of highly correlated or redundant features, can reduce dimensionality with PCA
- Test samples should be subjected to the same transformations as the training samples

Practical Tips for BP: # of Hidden Units

- # of input units = number of features, # output units = # classes. How to choose N_H, the # of hidden units?
- N_H determines the expressive power of the network
  - Too small N_H may not be sufficient to learn complex decision boundaries
  - Too large N_H may overfit the training data resulting in poor generalization



Practical Tips for BP: # of Hidden Units

- Choosing N_H is not a solved problem
- Rule of thumb
  - if total number of training samples is n, choose N_H so that the total number of weights is $n/10$
  - total number of weights = (# of w) + (# of v)
- Can choose N_H which gives the best performance on the validation data

Practical Tips for BP: Initializing Weights

- Do not set either ***w*** or ***v*** to 0
- Rule of thumb for our sigmoid function
  - Choose random weights from the range

$$-\frac{1}{\sqrt{d}} < w_{ji} < \frac{1}{\sqrt{d}}$$

$$-\frac{1}{\sqrt{N_H}} < v_{kj} < \frac{1}{\sqrt{N_H}}$$

Practical Tips for BP: Learning Rate

- As any gradient descent algorithm, backpropagation depends on the learning rate η
- Rule of thumb $\eta = 0.1$
- However we can adjust η at the training time
- The objective function ***J*** should decrease during gradient descent
  - If it oscillates, η is too large, decrease it
  - If it goes down but very slowly, η is too small,increase it

Practical Tips for BP: Weight Decay

- To simplify the network and avoid overfitting, it is recommended to keep the weights small
- Implement weight decay after each weight update:

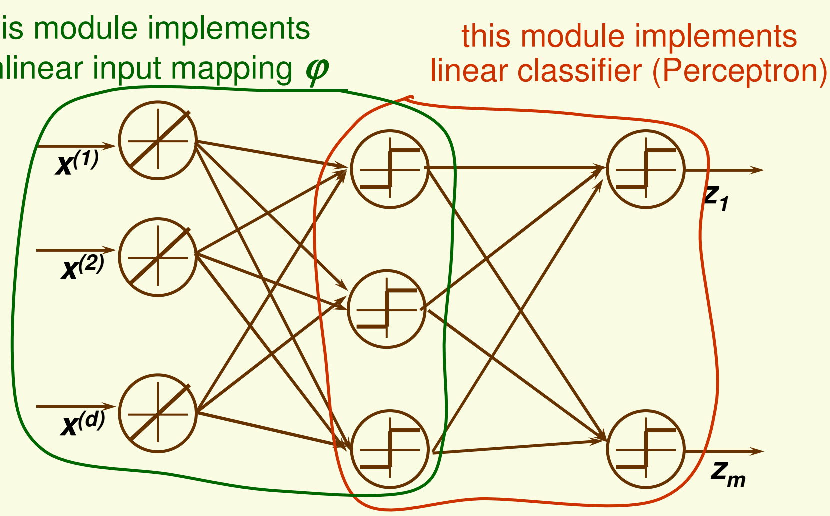
$$w^{new} = w^{old}(1-\varepsilon), \quad 0 < \varepsilon < 1$$

- Additional benefit is that “unused” weights grow small and may be eliminated altogether
  - A weight is “unused” if it is left almost unchanged by the backpropagation algorithm

Practical Tips for BP: # Hidden Layers

- Network with 1 hidden layer has the same expressive power as with several hidden layers
- For some applications, having more than 1 hidden layer may result in faster learning and less hidden units overall
- However networks with more than 1 hidden layer are more prone to the local minima problem

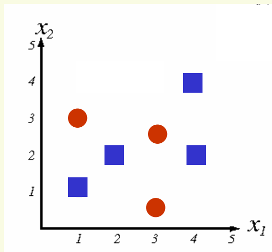
MNN as Nonlinear Mapping



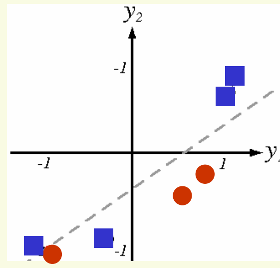
MNN as Nonlinear Mapping

- 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

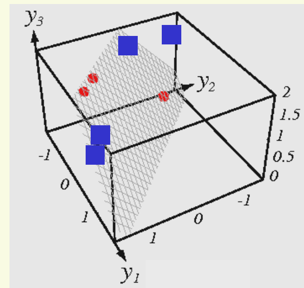
MNN as Nonlinear Mapping



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