Lecture 7: Multilayer Perceptrons

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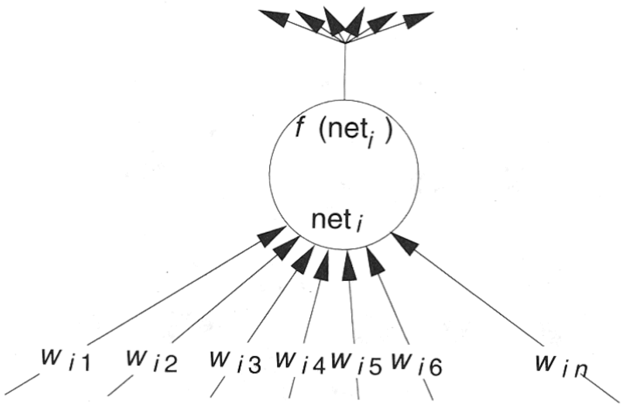
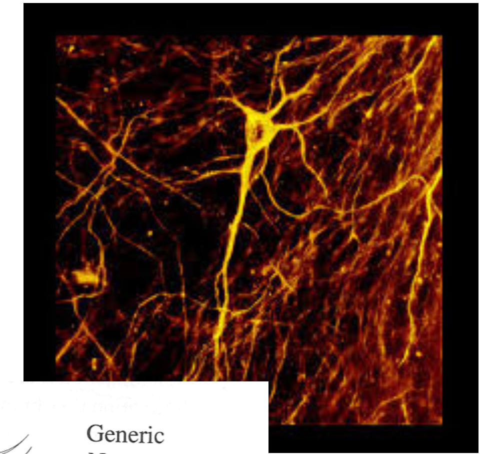
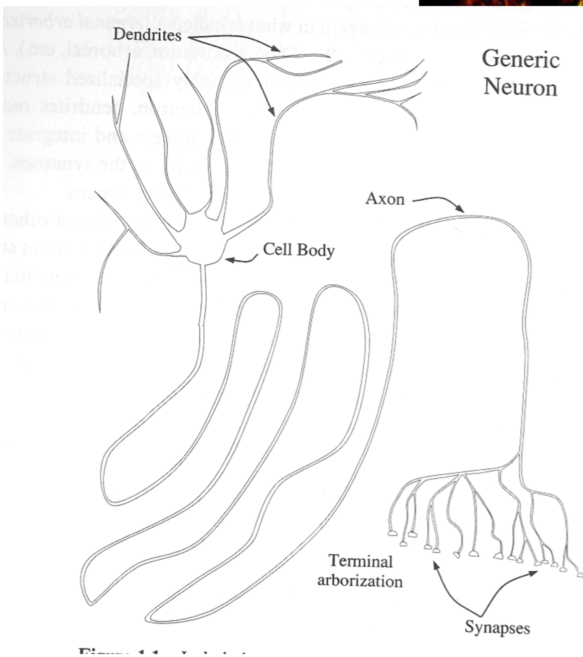
Similarity to real neurons...







- The dot product is a linear representation represented by the value *net*

$$y = net := \langle \mathbf{x} | \mathbf{w} \rangle = \sum_{j=1}^{D} w_j \cdot x_j,$$

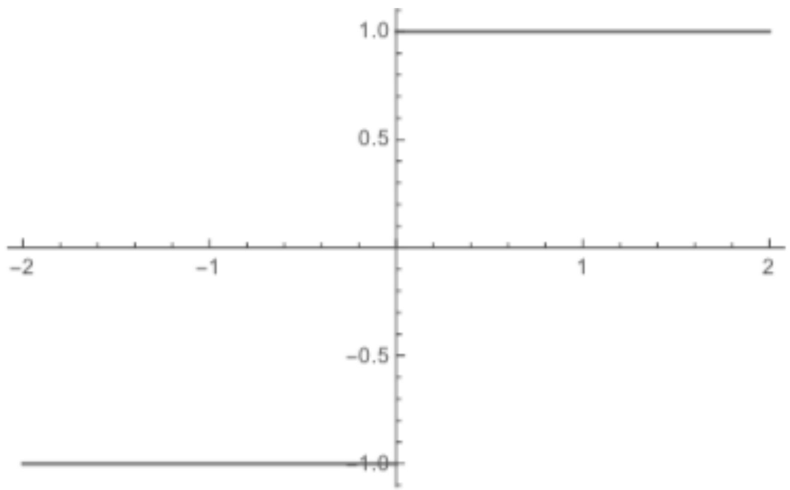
- *Non linearity* can be achieved be a non liner activation (transfer) function *φ()* with

$$o = \phi(net) = \phi(\langle \mathbf{x} | \mathbf{w} \rangle) = \phi\left(\sum_{j=1}^{D} w_j \cdot x_j\right)$$

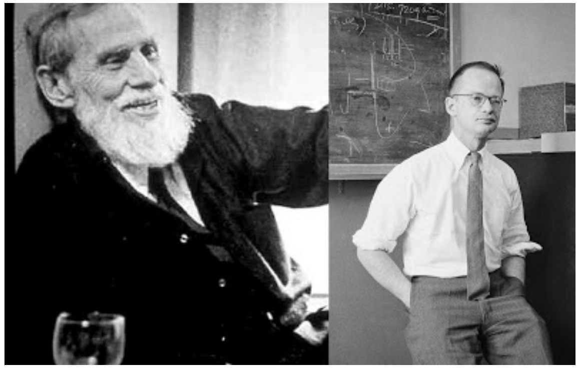
Sgn

- Examples of nonlinear transfer functions are the *sgn* function

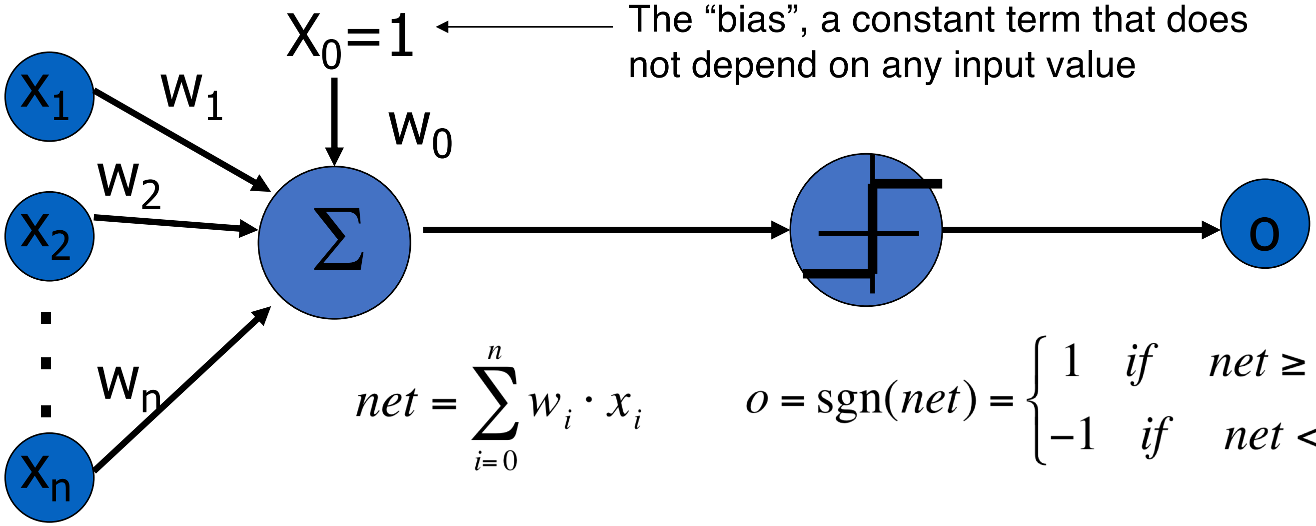
$$\phi(net) := sgn(net) = \begin{cases} 1 & \text{if} \quad net \geq 0 \\ -1 & \text{if} \quad net < 0 \end{cases}$$



Perceptron (1957)



- Linear threshold unit (LTU)

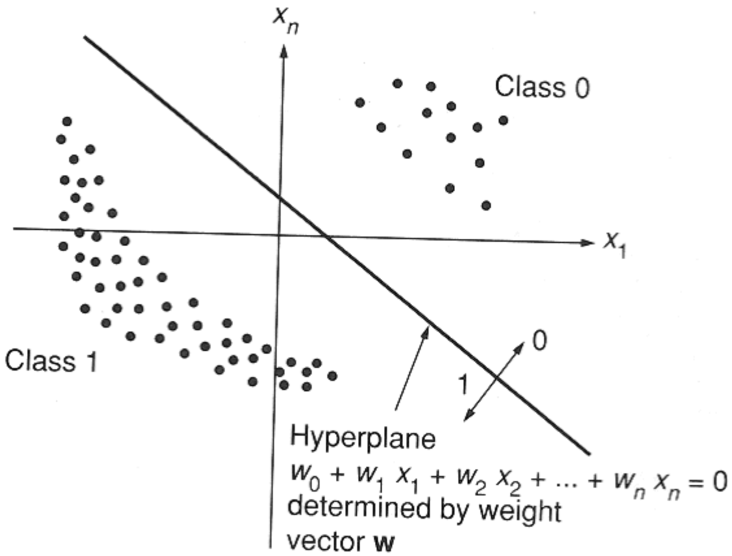


$$net = \sum_{i=0}^{n} w_i \cdot x_i \qquad o = \mathrm{sgn}(net) = \begin{cases} 1 & if \quad net \geq 0 \\ -1 & if \quad net < 0 \end{cases}$$

McCulloch-Pitts model of a neuron (1943)

Linearly separable patterns

$$o = \mathrm{sgn}(\sum_{i=0}^{n} w_i x_i)$$



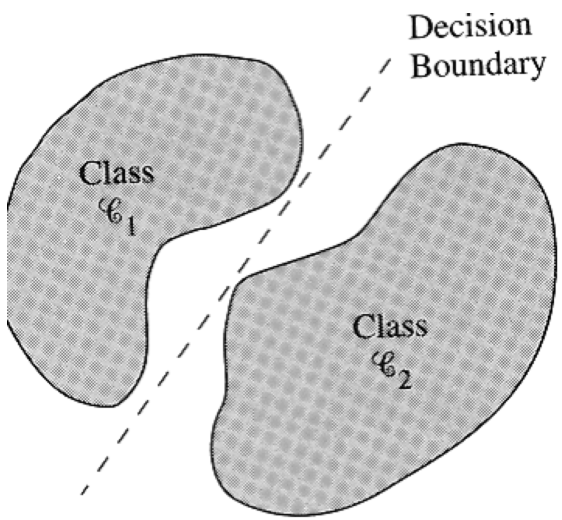
$$\sum_{i=0}^{n} w_i x_i > 0 \qquad for \quad C_0$$

$$\sum_{i=0}^{n} w_i x_i \leq 0 \qquad for \quad C_1$$

$X_0=1$, bias...

- The goal of a perceptron is to correctly classify the set of pattern $\boldsymbol{D}=\{\mathbf{x}_1,\mathbf{x}_2,..\mathbf{x}_m\}$ into one of the classes C_1 and C_2
- The output for class C_1 is $o=1$ and for C_2 is $o=-1$

  - For $n=2$ ➔



Perceptron learning rule

- Consider linearly separable problems
- How to find appropriate weights
  - Initialize each vector ***w*** to some small *random* values
- Look if the output pattern *o* belongs to the desired class, has the desired value *d*

$$w^{new} = w^{old} + \Delta w \qquad \Delta w = \eta \cdot (d - o) \cdot x$$

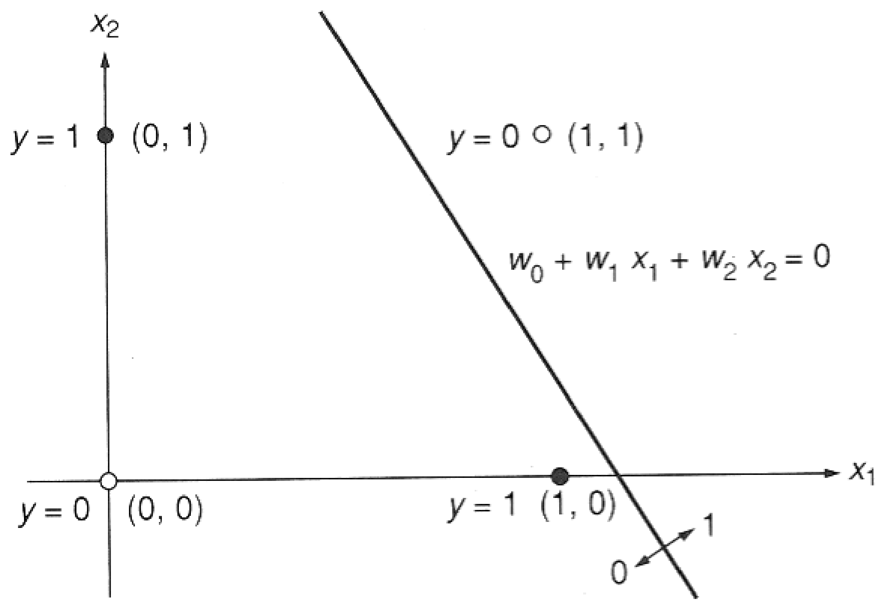
- η is called the **learning rate**
- $0 < \eta \leq 1$

- In supervised learning the network has its output compared with known correct answers
  - Supervised learning
  - Learning with a teacher
- *(d-o)* plays the role of the error signal

- The algorithm converges to the correct classification
  - if the training data is linearly separable
  - and η is sufficiently small

XOR problem and Perceptron

- By Minsky and Papert in mid 1960



Multi-layer Networks

- The limitations of simple perceptron do not apply to feed-forward networks with intermediate or „hidden“ nonlinear units
- A network with just one hidden unit can represent any Boolean function
- The great power of multi-layer networks was realized long ago
  - But it was only in the eighties it was shown how to make them learn

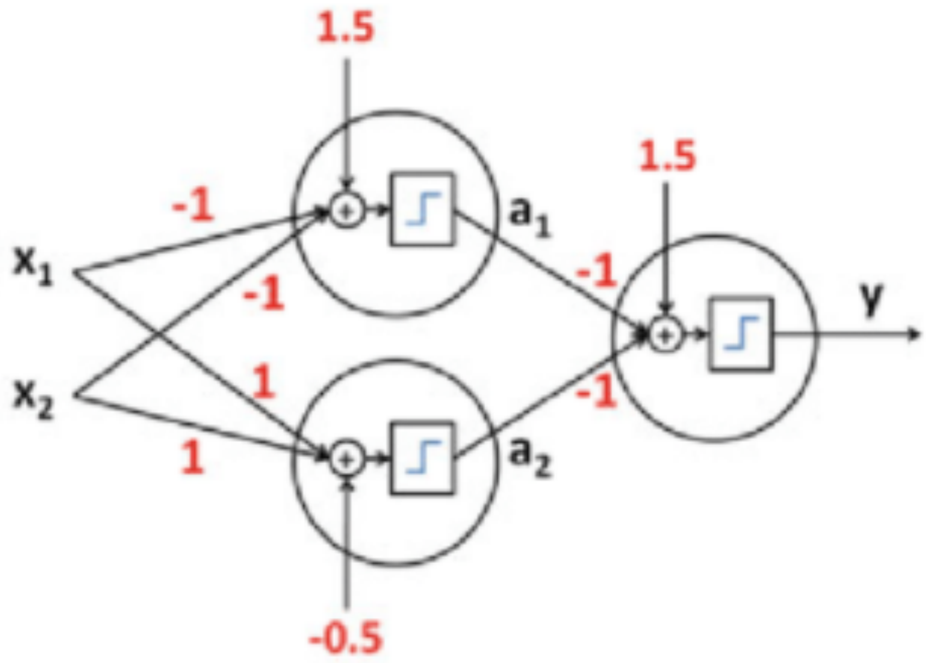
XOR-example

Knowl Inf Syst (2012) 30:135–154
DOI 10.1007/s10115-011-0392-6

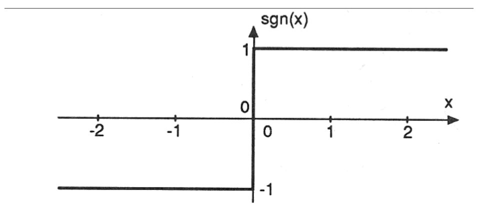
REGULAR PAPER

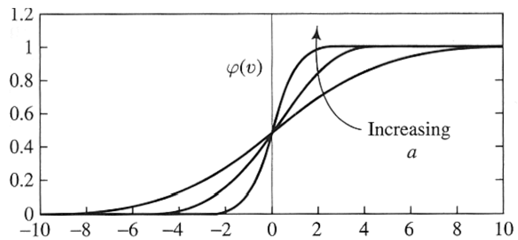
A general insight into the effect of neuron structure on classification

Hadi Sadoghi Yazdi · Alireza Rowhanimanesh · Hamidreza Modares



- Multiple layers of cascade linear units still produce only linear functions
- We search for networks capable of representing nonlinear functions
  - Units should use nonlinear activation functions
  - Examples of nonlinear activation functions





Gradient Descent for one Unit

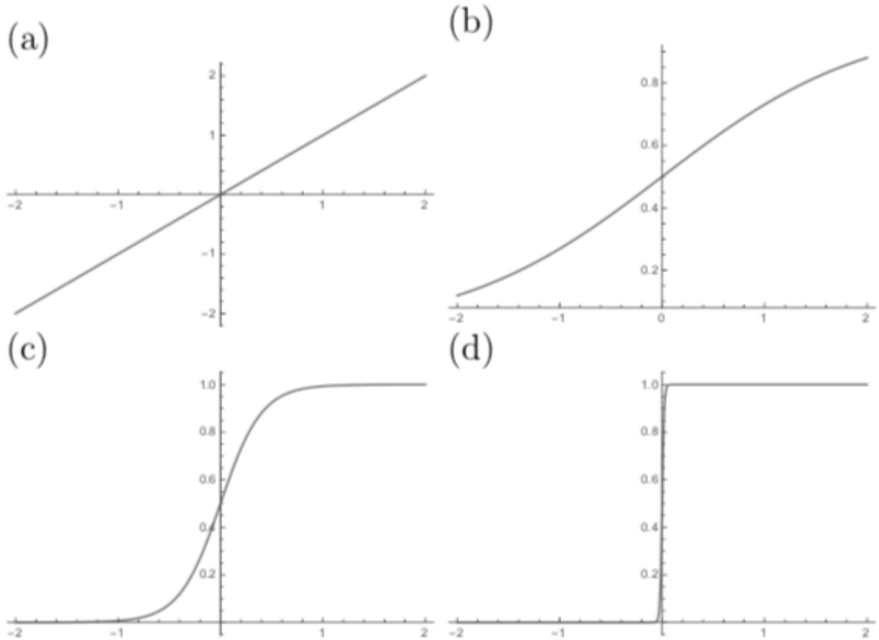


Figure 1.1: (a) Linear activation function. (b) The function $\sigma(net)$ with $\alpha = 1$. (c) The function $\sigma(net)$ with $\alpha = 5$. (d) The function $\sigma(net)$ with $\alpha = 10$ is very similar to $sgn_0(net)$, bigger α make it even more similar.

Linear Unit

$$o_k = \sum_{j=0}^{D} w_j \cdot x_{k,j}$$

The update rule for gradient decent is given by

$$\Delta w_j = \eta \cdot \sum_{k=1}^{N} (t_k - o_k) \cdot x_{k,j}.$$

Sigmoid Unit

$$\sigma(net) = \frac{1}{1 + e^{(-\alpha \cdot net)}} = \frac{e^{(\alpha \cdot net)}}{1 + e^{(\alpha \cdot net)}}$$

$$o_k = \sigma\left(\sum_{j=0}^{N} w_j \cdot x_{k,j}\right)$$

$$\frac{\partial E}{\partial w_j} = -\alpha \cdot \sum_{k=1}^{N} (t_k - o_k) \cdot \sigma\left(net_{k,j}\right) \cdot \left(1 - \sigma\left(net_{k,j}\right)\right) \cdot x_{k,j}.$$

$$\Delta w_j = \eta \cdot \alpha \cdot \sum_{k=1}^{N} (t_k - o_k) \cdot \sigma\left(net_{k,j}\right) \cdot \left(1 - \sigma\left(net_{k,j}\right)\right) \cdot x_{k,j}$$

Logistic Regression

$$p(C_1|\mathbf{x}) = \sigma(net) = \frac{1}{1+e^{(-net)}} = \frac{e^{(net)}}{1+e^{(net)}}$$

$$p(C_1|\mathbf{x}) = \sigma\left(\sum_{j=0}^{N} w_j \cdot x_j\right) = \sigma\left(\mathbf{w}^T \cdot \mathbf{x}\right)$$

Error function is defined by negative logarithm of the likelihood which leads to the update rule where the target t_k can be only one or zero (a constraint)

The update rule for gradient decent is given for target $t_k \in \{0, 1\}$

$$\Delta w_j = \eta \cdot \sum_{k=1}^{N} (t_k - o_k) \cdot x_{k,j}.$$

Sigmoid Unit versus Logistic Regression

Sigmoid Unit is with target, should be positive (between zero and one):

$$\Delta w_j = \eta \cdot \alpha \cdot \sum_{k=1}^{N} (t_k - o_k) \cdot \sigma\left(net_{k,j}\right) \cdot \left(1 - \sigma\left(net_{k,j}\right)\right) \cdot x_{k,j}$$

Logistic Regression is with target $t_k \in \{0, 1\}$

$$\Delta w_j = \eta \cdot \sum_{k=1}^{N} (t_k - o_k) \cdot x_{k,j}.$$

If we assume $\alpha = 1$ then the difference between sigmoid unit and the logistic regression that was derived by maximising the negative logarithm of the likelihood is

$$\sigma\left(net_{k,j}\right) \cdot \left(1 - \sigma\left(net_{k,j}\right)\right) \geq 0$$

the step size in the direction of gradient. Does it mean that Sigmoid Unit converge faster?

Linear Unit versus Logistic Regression

Target can be any value and can be solved by closed-form solution, by pseudo inverse

$$o_k = \sum_{j=0}^{D} w_j \cdot x_{k,j}$$

Target $t_k \in \{0, 1\}$ cannot be solved by closed-form solution

$$o_k = \frac{1}{1 + e^{\left(-\alpha \cdot \left(\sum_{j=0}^{N} w_j \cdot x_{k,j}\right)\right)}}$$

$$\Delta w_j = \eta \cdot \sum_{k=1}^{N} (t_k - o_k) \cdot x_{k,j}.$$

Logistic Regression as well as the sigmoid unit gives a better decision boundary.

For Sigmoid (Logistic) distant points from the decision boundary have the same impact

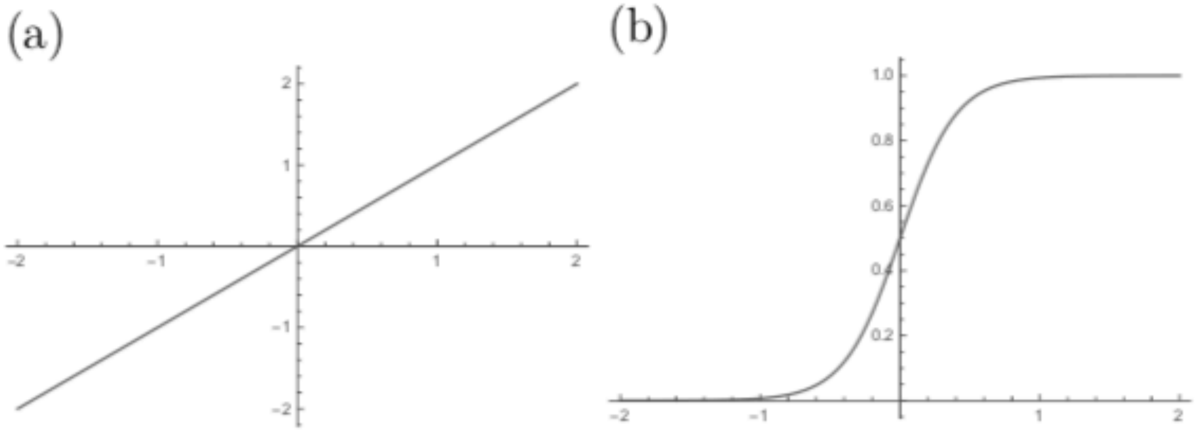
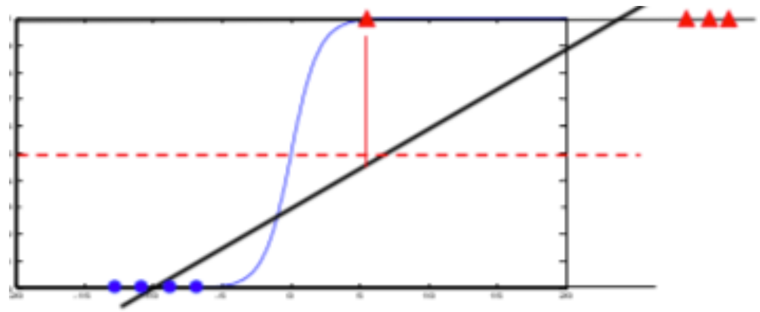
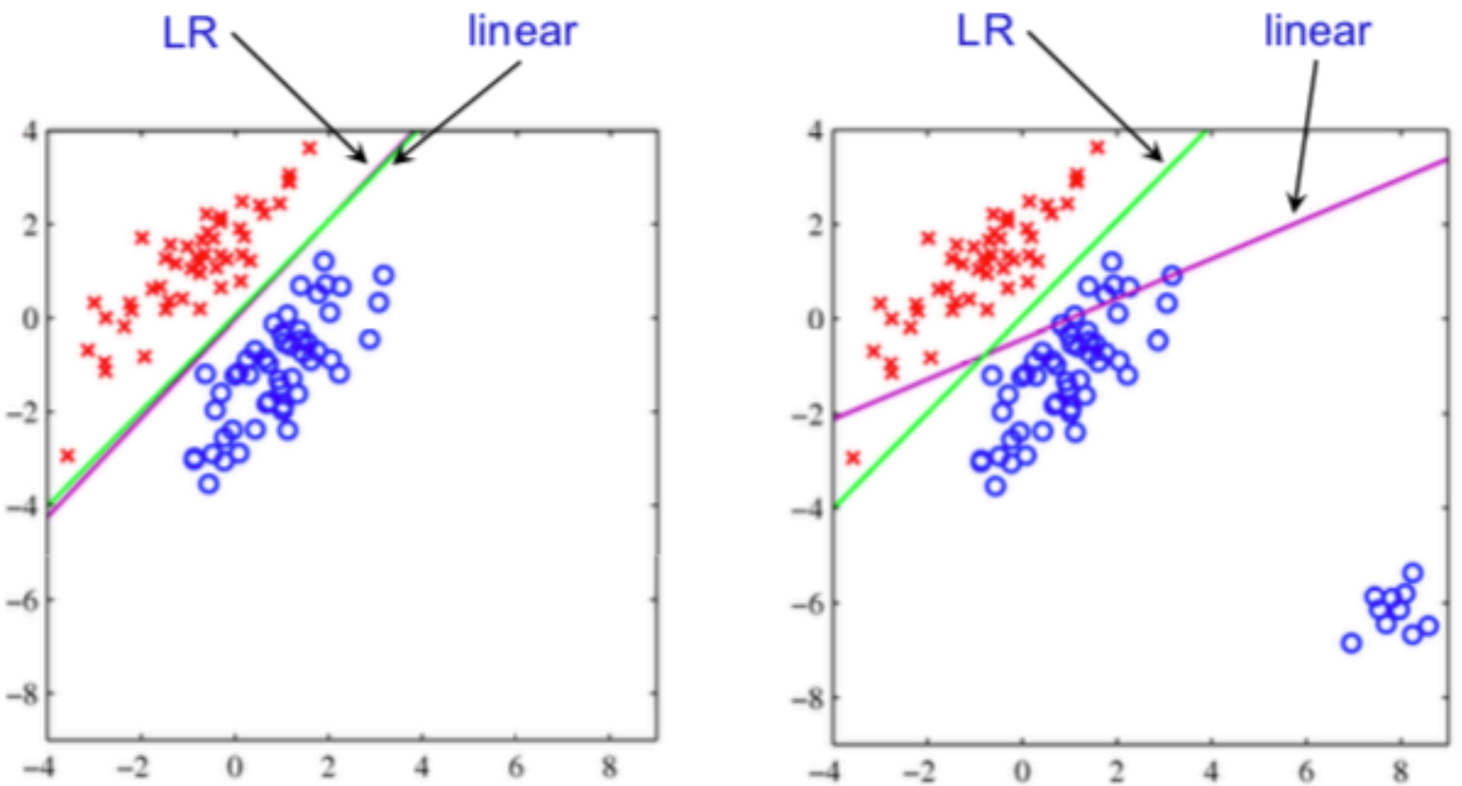


Figure 1.2: (a) Linear activation function. (b) The function $\sigma(net)$ with $\alpha = 5$

Distance



Better Decision Boundary of Logistic Regression LR (sigmoid) to Linear Unit



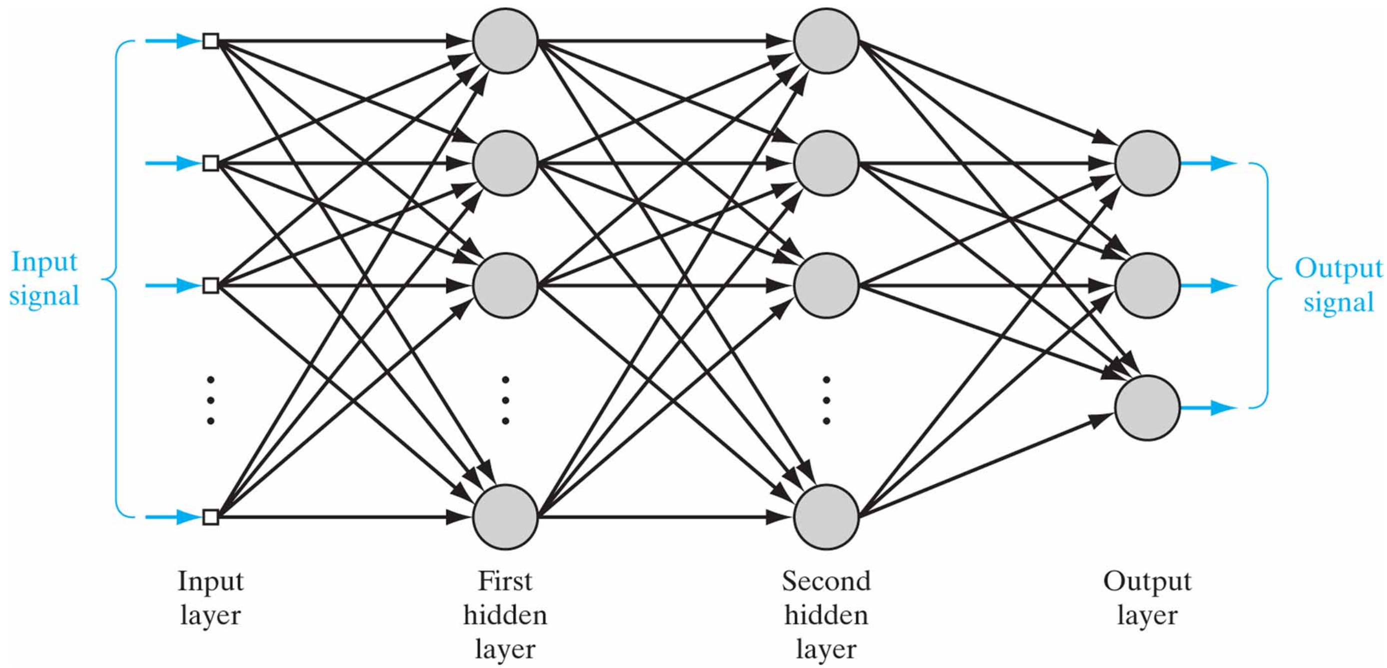
Back-propagation (1980)

- Back-propagation is a learning algorithm for multi-layer neural networks
- It was invented independently several times
  - Bryson an Ho [1969]
  - Werbos [1974]
  - Parker [1985]
  - **Rumelhart et al. [1986]**

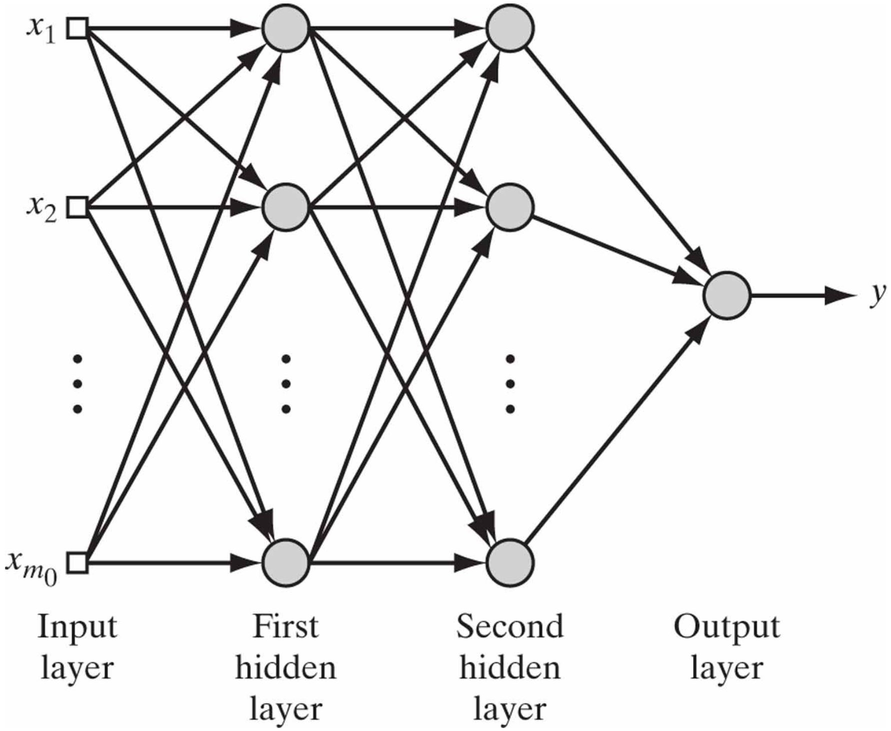
Parallel Distributed Processing - Vol. 1
Foundations
David E. Rumelhart, James L. McClelland and the PDP Research Group

What makes people smarter than computers? These volumes by a pioneering neurocomputing.....

- Feed-forward networks with hidden nonlinear units are universal approximators; they can approximate every bounded continuous function with an arbitrarily small error
- Each Boolean function can be represented by a network with a single hidden layer
  - However, the representation may require an exponential number of hidden units.
- The hidden units should be nonlinear because multiple layers of linear units can only produce linear functions.



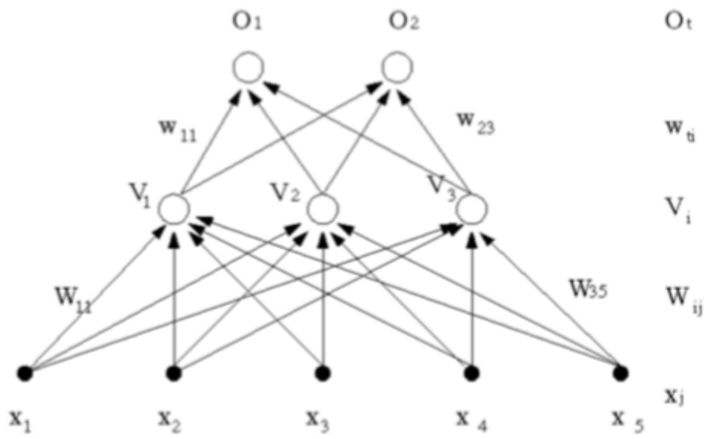
Input signal
Input layer
First hidden layer
Second hidden layer
Output layer
Output signal

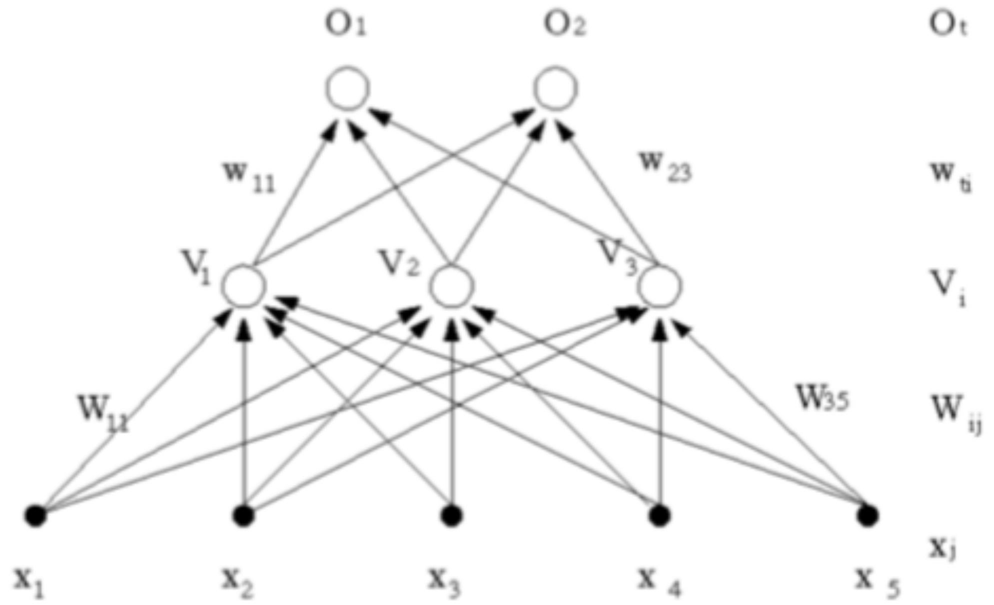


x_1
x_2
x_{m_0}
y
Input layer
First hidden layer
Second hidden layer
Output layer

Back-propagation

- The algorithm gives a prescription for changing the weights w_{ij} in any feed-forward network to learn a training set of input output pairs $\{\boldsymbol{x_k}, \boldsymbol{y_k}\}$
- We consider a simple two-layer network





- The input pattern is represented by the five-dimensional vector ***x***
- nonlinear hidden units compute the output V_1, V_2, V_3
- Two output units compute the output o_1 and o_2.
  - The units V_1, V_2, V_3 are referred to as hidden units because we cannot see their outputs and cannot directly perform error correction

- The output layer of a feed-forward network can be trained by the perceptron rule (stochastic gradient descent) since it is a Perceptron

$$\Delta w_{ti} = \eta \cdot (y_{k,t} - o_{k,t}) \cdot V_{k,i}.$$

For continuous activation function $\phi()$

$$o_{k,t} = \phi\left(\sum_{i=0}^{3} w_{ti} \cdot V_{k,i}\right).$$

$$E(\mathbf{w}) = \frac{1}{2} \cdot \sum_{t=1}^{2} \sum_{k=1}^{N} (y_{kt} - o_{kt})^2 = \frac{1}{2} \cdot \sum_{t=1}^{2} \sum_{k=1}^{N} \left(y_{kt} - \phi \left(\sum_{i=0}^{3} w_{ti} \cdot V_{k,i} \right) \right)^2$$

we get

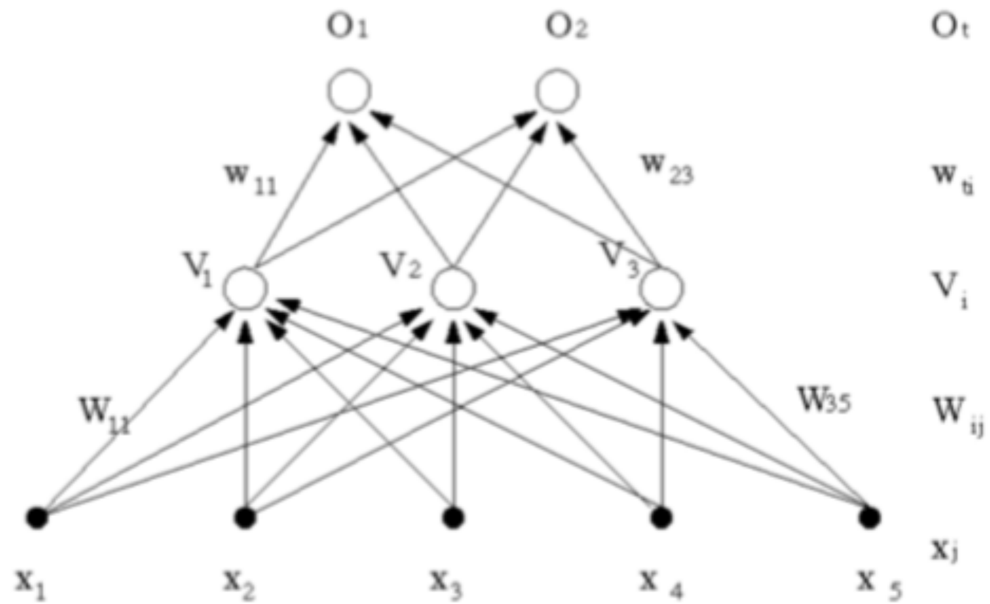
$$\frac{\partial E}{\partial w_{ti}} = - \sum_{k=1}^{N} (y_{kt} - o_{kt}) \cdot \phi' \left(\sum_{i=0}^{n} w_{ti} \cdot V_{k,i} \right) \cdot V_{k,i}.$$

For the nonlinear continuous function $\sigma()$

$$\frac{\partial E}{\partial w_{ti}} = -\alpha \cdot \sum_{k=1}^{N} (y_{kt} - o_{kt}) \cdot \sigma(net_{k,t}) \cdot (1 - \sigma(net_{k,t})) \cdot V_{k,i}$$

and

$$\Delta w_{ti} = \eta \cdot \alpha \cdot \sum_{k=1}^{N} (y_{kt} - o_{kt}) \cdot \sigma(net_{k,t}) \cdot (1 - \sigma(net_{k,t})) \cdot V_{k,i}.$$



We can determine the Δw_{ti} for the output units, but how can we determine ΔW_{ij} for the hidden units? If the hidden units use a continuous non linear activation function $\phi()$

$$V_{k,i} = \phi\left(\sum_{j=0}^{5} W_{ij} \cdot x_{k,j}\right).$$

$$V_{k,i} = \phi\left(\sum_{j=0}^{5} W_{ij} \cdot x_{k,j}\right).$$

we can define the training error for a training data set D_t of N elements with

$$E(\mathbf{w}, \mathbf{W}) =: E(\mathbf{w}) = \frac{1}{2} \cdot \sum_{k=1}^{N} \sum_{t=1}^{2} (y_{kt} - o_{kt})^2$$

$$E(\mathbf{w}, \mathbf{W}) = \frac{1}{2} \cdot \sum_{k=1}^{N} \sum_{t=1}^{2} \left(y_{kt} - \phi\left(\sum_{i=0}^{3} w_{ti} \cdot V_{k,i}\right)\right)^2$$

$$E(\mathbf{w}, \mathbf{W}) = \frac{1}{2} \cdot \sum_{k=1}^{N} \sum_{t=1}^{2} \left(y_{kt} - \phi\left(\sum_{i=0}^{3} w_{ti} \cdot \phi\left(\sum_{j=0}^{5} W_{ij} \cdot x_{k,j}\right)\right)\right)^2.$$

We already know

$$\frac{\partial E}{\partial w_{ti}} = -\sum_{k=1}^{N}(y_{kt} - o_{kt}) \cdot \phi'(net_{k,t}) \cdot V_{k,i}.$$

For $\frac{\partial E}{\partial W_{ij}}$ we can use the chain rule and we obtain

$$\frac{\partial E}{\partial W_{ij}} = \sum_{k=1}^{N} \frac{\partial E}{\partial V_{ki}} \cdot \frac{\partial V_{ki}}{\partial W_{ij}}.$$

$$E(\mathbf{w}, \mathbf{W}) = \frac{1}{2} \cdot \sum_{k=1}^{N} \sum_{t=1}^{2} \left(y_{kt} - \phi \left(\sum_{i=0}^{3} w_{ti} \cdot V_{k,i} \right) \right)^2$$

$$E(\mathbf{w}, \mathbf{W}) = \frac{1}{2} \cdot \sum_{k=1}^{N} \sum_{t=1}^{2} \left(y_{kt} - \phi \left(\sum_{i=0}^{3} w_{ti} \cdot \phi \left(\sum_{j=0}^{5} W_{ij} \cdot x_{k,j} \right) \right) \right)^2 .$$

$$\frac{\partial E}{\partial W_{ij}} = \sum_{k=1}^{N} \frac{\partial E}{\partial V_{ki}} \cdot \frac{\partial V_{ki}}{\partial W_{ij}}.$$

with

$$\frac{\partial E}{\partial V_{ki}} = -\sum_{k=1}^{N} \sum_{t=1}^{2} (y_{kt} - o_{kt}) \cdot \phi'(net_{k,t}) \cdot w_{t,i}.$$

$$V_{k,i} = \phi \left(\sum_{j=0}^{5} W_{ij} \cdot x_{k,j} \right) \longrightarrow \frac{\partial V_{ki}}{\partial W_{ij}} = \phi'(net_{k,i}) \cdot x_{k,j}$$

$$\frac{\partial E}{\partial V_{ki}} = -\sum_{k=1}^{N}\sum_{t=1}^{2}(y_{kt} - o_{kt}) \cdot \phi'(net_{k,t}) \cdot w_{t,i}.$$

$$\frac{\partial V_{ki}}{\partial W_{ij}} = \phi'(net_{k,i}) \cdot x_{k,j}$$

$$\frac{\partial E}{\partial W_{ij}} = \sum_{k=1}^{N} \frac{\partial E}{\partial V_{ki}} \cdot \frac{\partial V_{ki}}{\partial W_{ij}}.$$

$$\frac{\partial E}{\partial W_{ij}} = -\sum_{k=1}^{N}\sum_{t=1}^{2}(y_{kt} - o_{kt}) \cdot \phi'(net_{k,t}) \cdot w_{t,i} \cdot \phi'(net_{k,i}) \cdot x_{k,j}.$$

The algorithm is called back propagation because we can reuse the computation that was used to determine Δw_{ti},

$$\Delta w_{ti} = \eta \cdot \sum_{k=1}^{N} (y_{kt} - o_{kt}) \cdot \phi'(net_{k,t}) \cdot V_{k,i}.$$

and with

$$\delta_{kt} = (y_{kt} - o_{kt}) \cdot \phi'(net_{k,t})$$

we can write

$$\Delta w_{ti} = \eta \cdot \sum_{k=1}^{N} \delta_{kt} \cdot V_{k,i}.$$

$$\Delta W_{ij} = \eta \sum_{k=1}^{N} \sum_{t=1}^{2} (y_{kt} - o_{kt}) \cdot \phi'(net_{k,t}) \cdot w_{t,i} \cdot \phi'(net_{k,i}) \cdot x_{k,j}$$

we can simplify (reuse the computation) to

$$\delta_{kt} = (y_{kt} - o_{kt}) \cdot \phi'(net_{k,t})$$

$$\Delta W_{ij} = \eta \sum_{k=1}^{N} \sum_{t=1}^{2} \delta_{kt} \cdot w_{t,i} \cdot \phi'(net_{k,i}) \cdot x_{k,j}.$$

With

$$\delta_{ki} = \phi'(net_{k,i}) \cdot \sum_{t=1}^{2} \delta_{kt} \cdot w_{t,i}$$

we can simply to

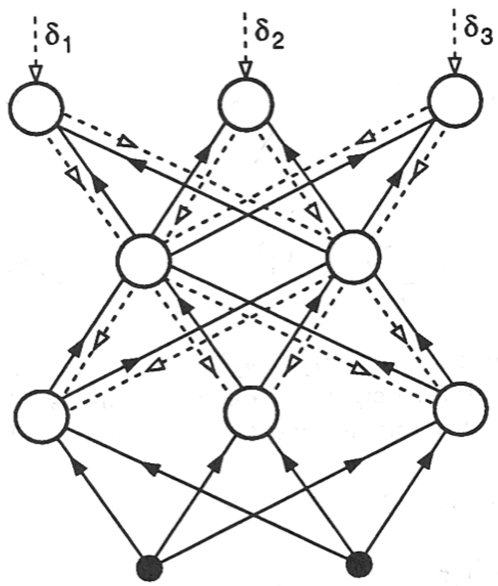
$$\Delta W_{ij} = \eta \sum_{k=1}^{N} \delta_{ki} \cdot x_{k,j}.$$

- In general, with an arbitrary number of layers, the back-propagation update rule has always the form

$$\Delta w_{ij} = \eta \sum_{d=1}^{m} \delta_{output} \cdot V_{input}$$

  - Where output and input refers to the connection concerned
  - V stands for the appropriate input (hidden unit or real input, $\boldsymbol{x}_d$)
  - δ depends on the layer concerned

- This approach can be extended to any numbers of layers
- The coefficient are usual forward, but the errors represented by δ are propagated backward



Networks with Hidden Linear Layers

Consider simple linear unit with a linear activation function

$$o_{k,t} = \sum_{i=0}^{3} w_{ti} \cdot V_{k,i} = \mathbf{w}_t^T \cdot \mathbf{V}_k$$

$$V_{k,i} = \sum_{j=0}^{5} W_{ij} \cdot x_{k,j} = \mathbf{W}_j^T \cdot \mathbf{x}_k$$

Now W is a matrix

$$\mathbf{V}_k = W \cdot \mathbf{x}_k$$

So we can write

$$o_{k,t} = \mathbf{w}_t^T \cdot W \cdot \mathbf{x}_k$$

with

$$(\mathbf{w}_t^*)^T = \mathbf{w}_t^T \cdot W$$

and we get the same discrimination power (linear separable) as a simple Perceptron

$$o_{k,t} = (\mathbf{w}_t^*)^T \cdot \mathbf{x}_k$$

However with nonlinear activation function, we cannot do the matrix multiplication

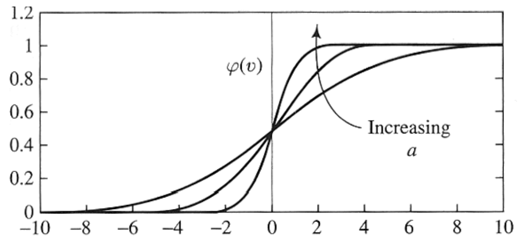
$$\mathbf{V}_k = \phi\left(W \cdot \mathbf{x}_k\right)$$

So we can write

$$o_{k,t} = \mathbf{w}_t^T \cdot \phi\left(W \cdot \mathbf{x}_k\right)$$

but we cannot simplify

- We have to use a nonlinear differentiable activation function in **hidden units**
  - Examples:



$$f(x) = \sigma(x) = \frac{1}{1 + e^{(-\alpha \cdot x)}}$$

$$f'(x) = \sigma'(x) = \alpha \cdot \sigma(x) \cdot (1 - \sigma(x))$$

$$f(x) = \tanh(\alpha \cdot x)$$

$$f'(x) = \alpha \cdot (1 - f(x)^2)$$

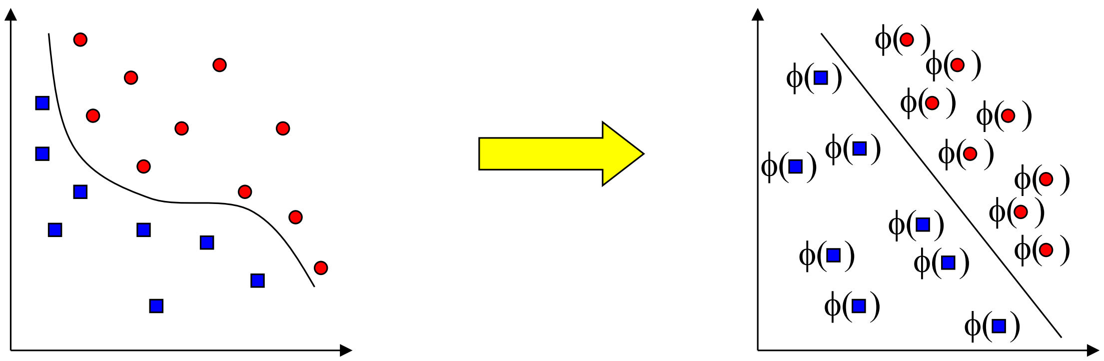
Two kind of Units

- Output Units
  - Require Bias
  - Preform **Linear Separable Problems**, means the input to them had to be somehow linearised
  - Does not require non linear activation function,
  - We **should** use sigmoid function or softmax to represent probabilities and to get **better** decision boundary.

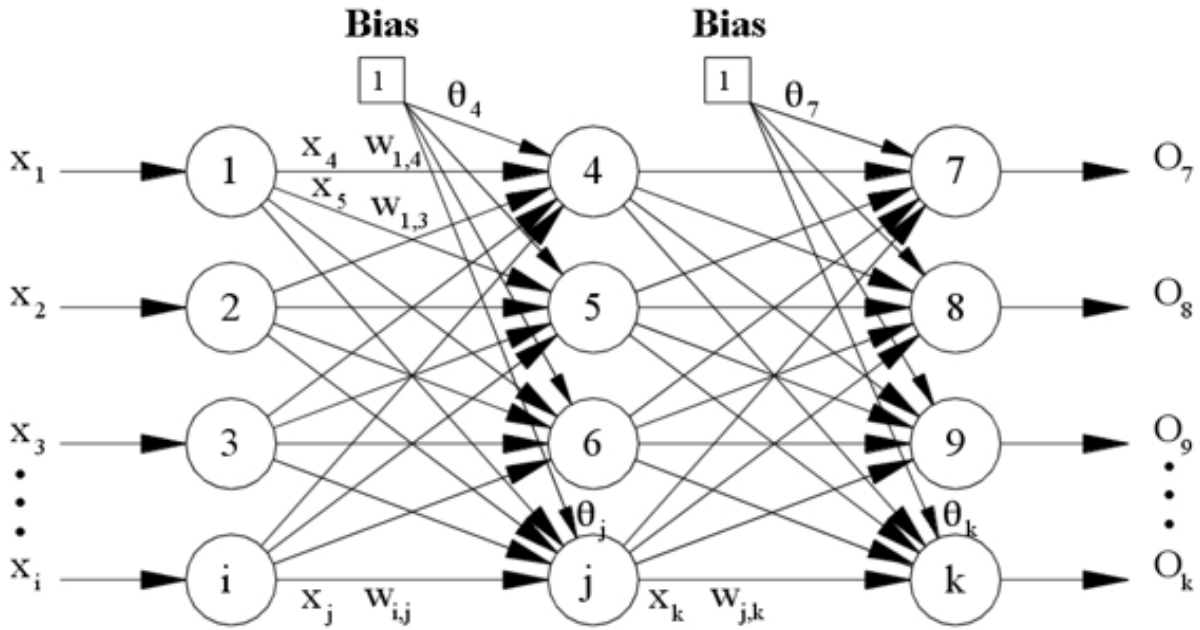
- Hidden Units
  - Nonlinear activation function
  - Feature Extraction
    Does it require Bias? It is commonly used
  - Universal Approximation Theorem uses hidden units with bias.

Output Units are linear (Perceptron)

- The hidden layer applies a nonlinear transformation from the input space to the hidden space
- In the hidden space a linear discrimination can be performed



Bias?



Bias
1
θ_4
Bias
1
θ_7
x_1
x_2
x_3
x_i
x_4 $w_{1,4}$
x_5 $w_{1,3}$
x_j $w_{i,j}$
x_k $w_{j,k}$
θ_j
θ_k
1
2
3
i
4
5
6
j
7
8
9
k
O_7
O_8
O_9
O_k

More on Back-Propagation

- Gradient descent over entire network weight vector
- Easily generalized to arbitrary directed graphs
- Will find a local, not necessarily global error minimum
  - In practice, often works well (can run multiple times)

- Gradient descent can be very slow if η is to small, and can oscillate widely if η is to large
- Often include weight *momentum* α

$$\Delta w_{pq}(t+1) = -\eta \frac{\partial E}{\partial w_{pq}} + \alpha \cdot \Delta w_{pq}(t)$$

- *Momentum* parameter α is chosen between *0* and *1, 0.9* is a good value

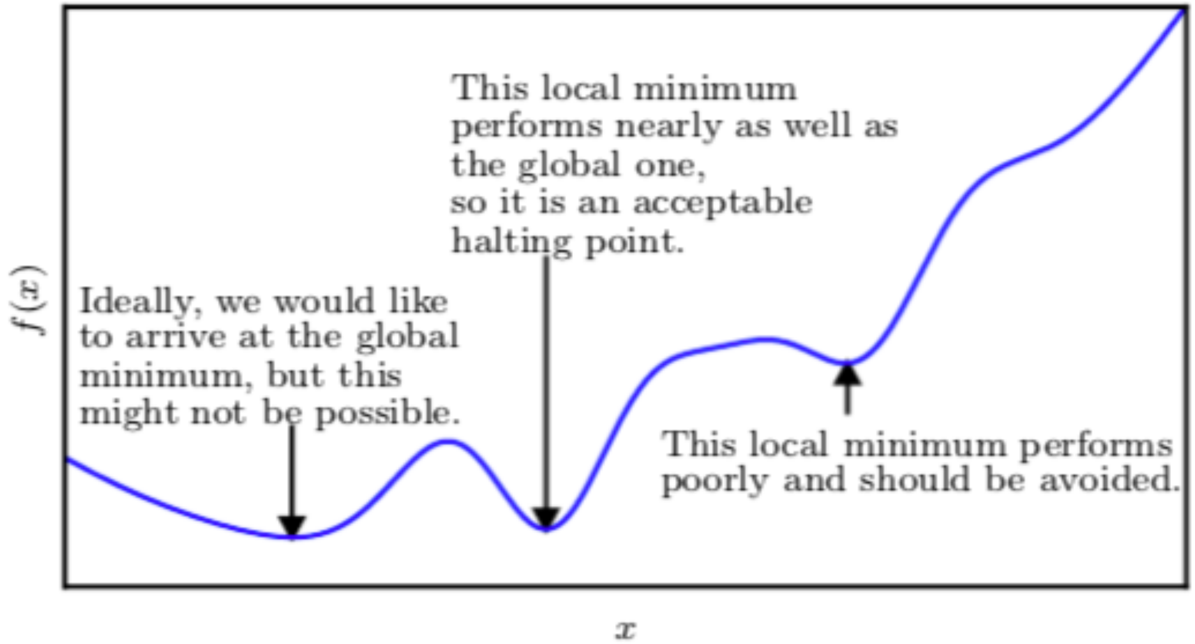
- Minimizes error over training examples
  - Will it generalize well
- Training can take thousands of iterations, it is slow!

- Using network after training is very fast

Convergence of Back-propagation

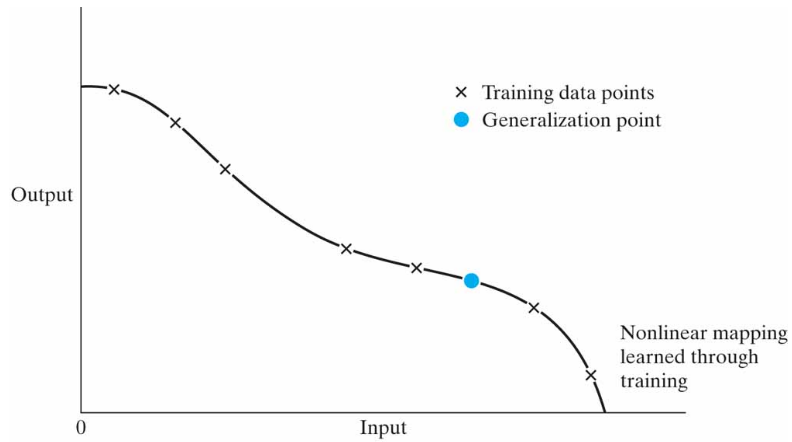
- Gradient descent to some local minimum
    - Perhaps not global minimum...
    - Add momentum
    - Stochastic gradient descent
    - Train multiple nets with different initial weights

- Nature of convergence
    - Initialize weights near zero
    - Therefore, initial networks near-linear
    - Increasingly non-linear functions possible as training progresses


This local minimum
performs nearly as well as
the global one,
so it is an acceptable
halting point.
Ideally, we would like
to arrive at the global
minimum, but this
might not be possible.
This local minimum performs
poorly and should be avoided.
$f(x)$
x

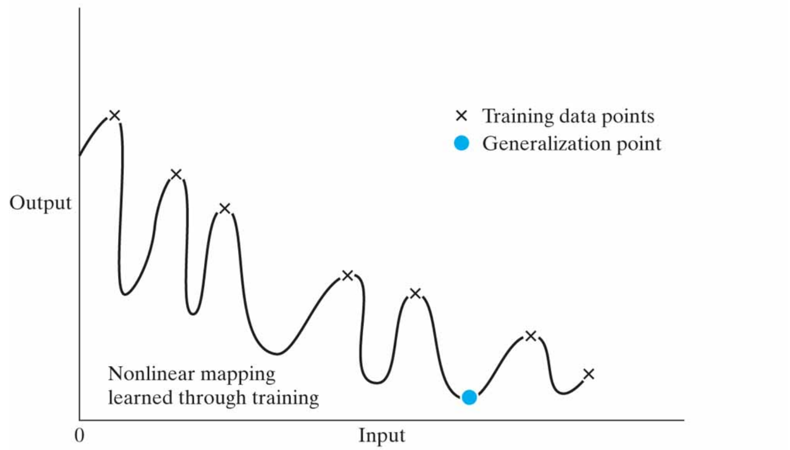
Expressive Capabilities of ANNs

- Boolean functions:
  - Every boolean function can be represented by network with single hidden layer
  - but might require exponential (in number of inputs) hidden units
- Continuous functions:
  - Every bounded continuous function can be approximated with arbitrarily small error, by network with one hidden layer [Cybenko 1989; Hornik et al. 1989]
    - See: https://en.wikipedia.org/wiki/Universal_approximation_theorem
  - Any function can be approximated to arbitrary accuracy by a network with two hidden layers [Cybenko 1988].



Training data points
Generalization point
Output
Nonlinear mapping
learned through
training
0
Input

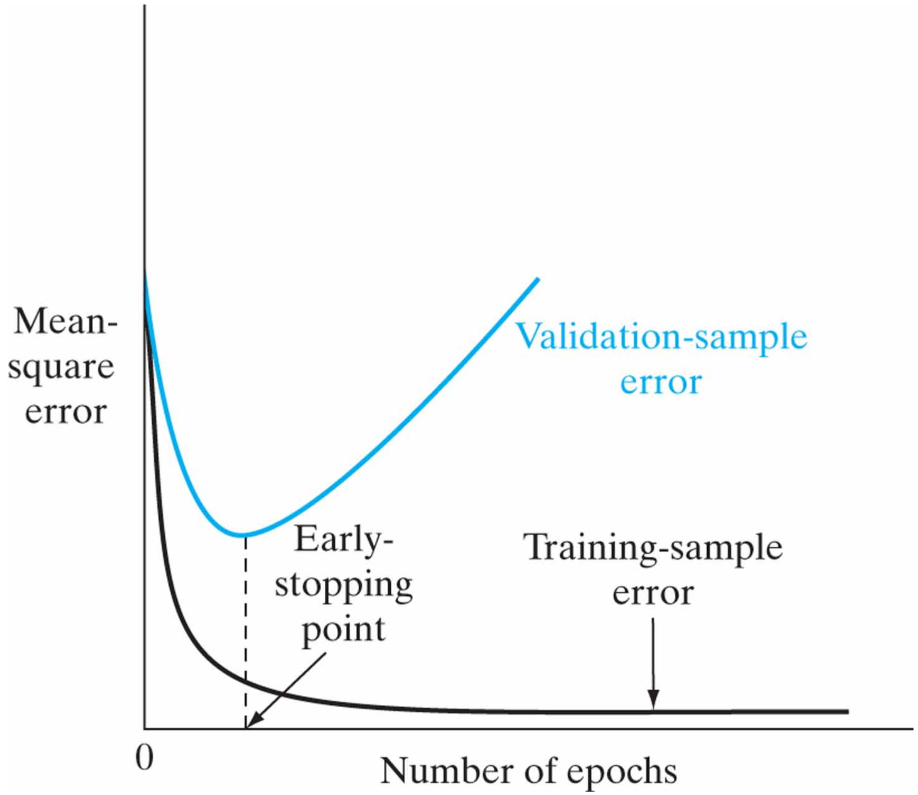
(a)

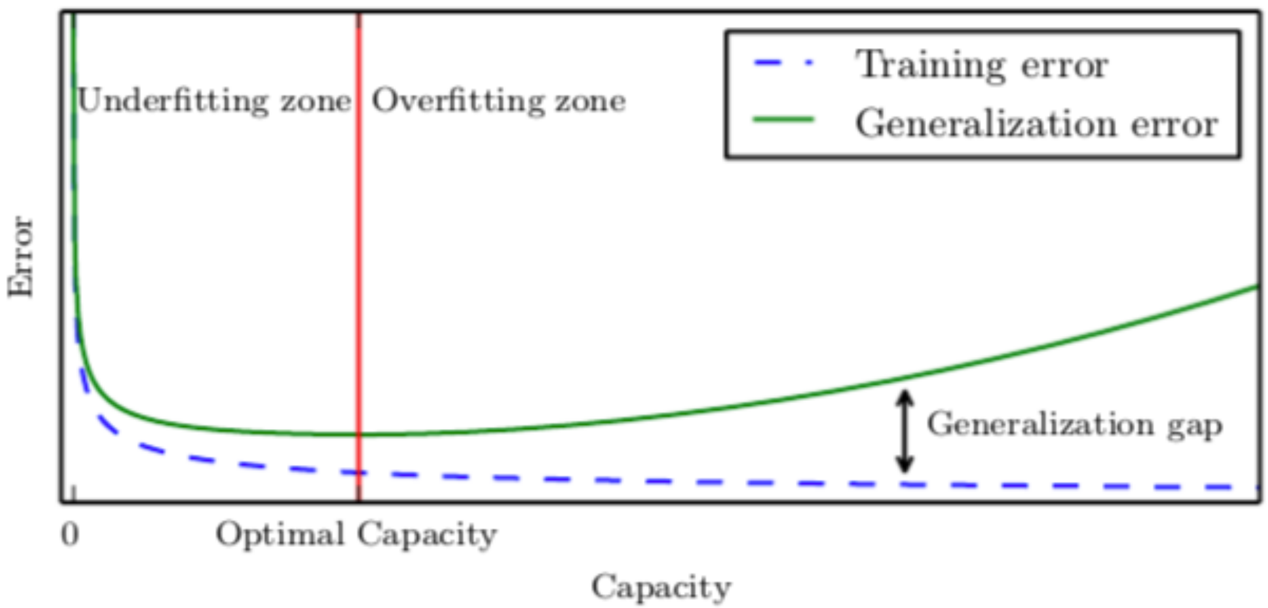


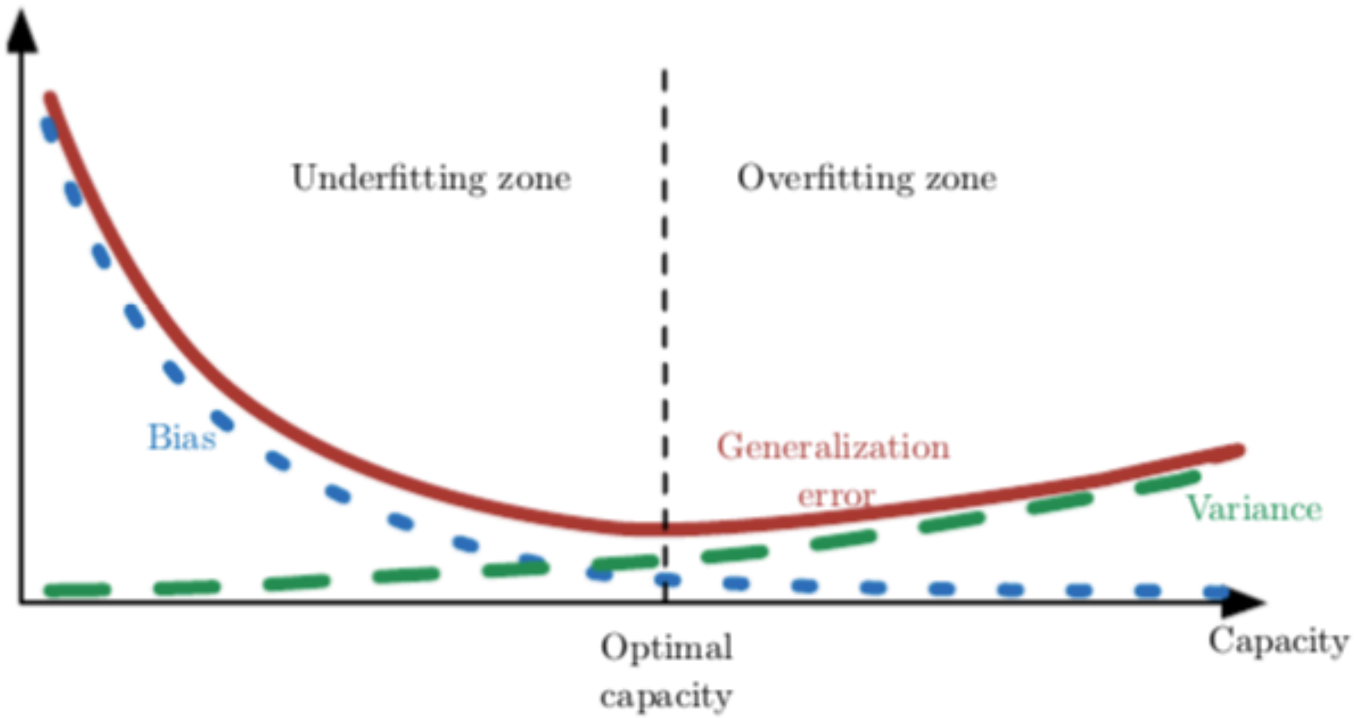
Training data points
Generalization point
Output
Nonlinear mapping
learned through training
0
Input

(b)

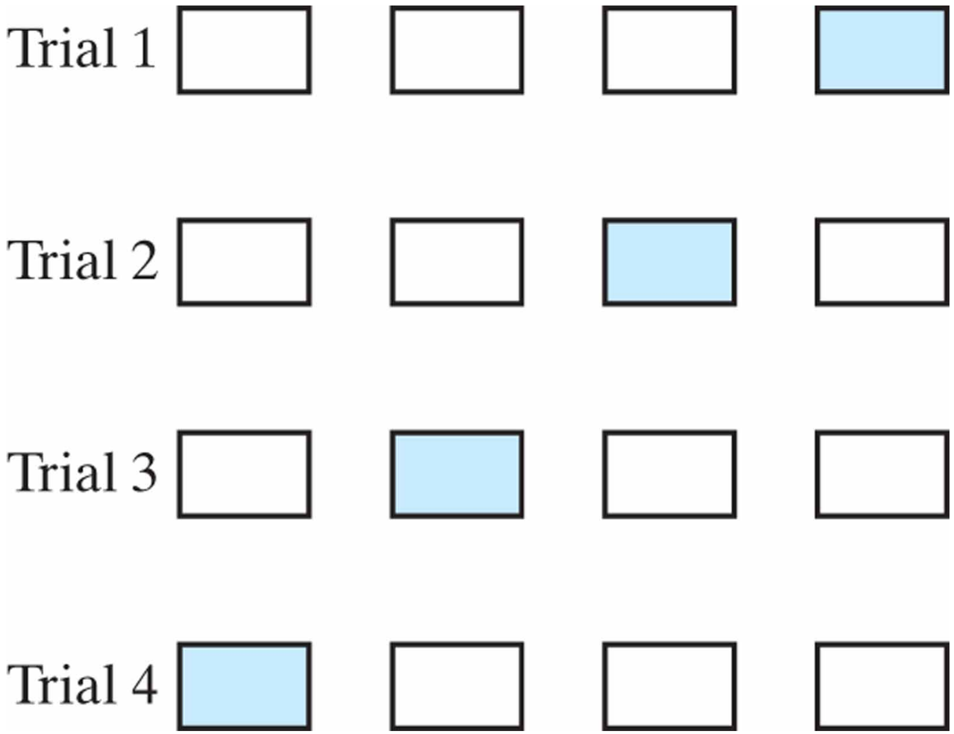
Early-Stopping Rule




Training error
Generalization error
Underfitting zone
Overfitting zone
Generalization gap
Error
0
Optimal Capacity
Capacity


Underfitting zone
Overfitting zone
Bias
Generalization error
Variance
Optimal capacity
Capacity

Cross Validation to determine Parameters



Example
(different notation)

- Consider a network with M layers $m=1,2,..,M$
- $V^m{}_i$ from the output of the ith unit of the mth layer
- $V^0{}_i$ is a synonym for x_i of the ith input
- Subscript m layers m's layers, not patterns
- $W^m{}_{ij}$ mean connection from V_j^{m-1} to V_i^m

$$\Delta W_{ij} = \eta \sum_{d=1}^{m} \delta_i^d V_j^d$$

$$\Delta w_{jk} = \eta \sum_{d=1}^{m} \delta_j^d \cdot x_k^d$$

- We have same form with a different definition of δ
- *d* is the pattern identificator

- By the equation $$\delta_j^d = f^{'}(net_j^d)\sum_{i=1}^{2} W_{ij}\delta_i^d$$
- allows us to determine for a given hidden unit V_j in terms of the δ's of the unit o_i
- The coefficient are usual forward, but the errors δ are propagated backward
    - back-propagation

Stochastic Back-Propagation Algorithm

(mostly used)

1. Initialize the weights to small random values
2. Choose a pattern x^d_k and apply is to the input layer $V^0_k = x^d_k$ for all k
3. Propagate the signal through the network

$$V_i^m = f(net_i^m) = f(\sum_j w_{ij}^m V_j^{m-1})$$

4. Compute the deltas for the output layer

$$\delta_i^M = f'(net_i^M)(t_i^d - V_i^M)$$

5. Compute the deltas for the preceding layer for *m=M,M-1,..2*

$$\delta_i^{m-1} = f'(net_i^{m-1})\sum_j w_{ji}^m \delta_j^m$$

6. Update all connections

$$\Delta w_{ij}^m = \eta \delta_i^m V_j^{m-1} \qquad w_{ij}^{new} = w_{ij}^{old} + \Delta w_{ij}$$

7. Goto 2 and repeat for the next pattern

Example

$\mathbf{w}_1=\{w_{11}=0.1, w_{12}=0.1, w_{13}=0.1, w_{14}=0.1, w_{15}=0.1\}$

$\mathbf{w}_2=\{w_{21}=0.1, w_{22}=0.1, w_{23}=0.1, w_{24}=0.1, w_{25}=0.1\}$

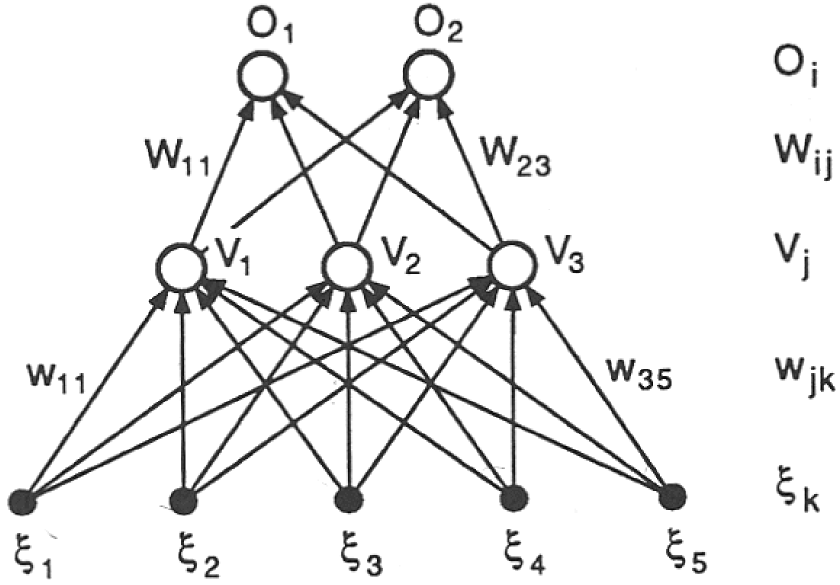
$\mathbf{w}_3=\{w_{31}=0.1, w_{32}=0.1, w_{33}=0.1, w_{34}=0.1, w_{35}=0.1\}$

$\mathbf{W}_1=\{W_{11}=0.1, W_{12}=0.1, W_{13}=0.1\}$

$\mathbf{W}_2=\{W_{21}=0.1, W_{22}=0.1, W_{23}=0.1\}$

$\mathbf{X}_1=\{1,1,0,0,0\}$; $\mathbf{t}_1=\{1,0\}$

$\mathbf{X}_2=\{0,0,0,1,1\}$; $\mathbf{t}_1=\{0,1\}$



$$f(x)=\sigma(x)=\frac{1}{1+e^{(-x)}} \qquad f^{'}(x)=\sigma^{'}(x)=\sigma(x)\cdot(1-\sigma(x))$$

$$net_1^1 = \sum_{k=1}^{5} w_{1k} x_k^1 \qquad V_1^1 = f(net_1^1) = \frac{1}{1+e^{-net_1^1}}$$

*net^1_1=1*0.1+1*0.1+0*0.1+0*0.1+0*0.1*

V^1_1=f(net^1_1)=1/(1+exp(-0.2))=0.54983

$$net_2^1 = \sum_{k=1}^{5} w_{2k} x_k^1 \qquad V_2^1 = f(net_1^1) = \frac{1}{1+e^{-net_2^1}}$$

V^1_2=f(net^1_2)=1/(1+exp(-0.2))=0.54983

$$net_3^1 = \sum_{k=1}^{5} w_{3k} x_k^1 \qquad V_3^1 = f(net_3^1) = \frac{1}{1+e^{-net_3^1}}$$

V^1_3=f(net^1_3)=1/(1+exp(-0.2))=0.54983

$$net_1^1 = \sum_{j=1}^{3} W_{1j} V_j^1 \qquad o_1^1 = f(net_1^1) = \frac{1}{1 + e^{-net_1^1}}$$

*$net^1{}_1$=0.54983*0.1+ 0.54983*0.1+ 0.54983*0.1= 0.16495*

$o^1{}_1$= f(net11)=1/(1+exp(- 0.16495))= 0.54114

$$net_2^1 = \sum_{j=1}^{3} W_{2j} V_j^1 \qquad o_2^1 = f(net_2^1) = \frac{1}{1 + e^{-net_2^1}}$$

*$net^1{}_2$=0.54983*0.1+ 0.54983*0.1+ 0.54983*0.1= 0.16495*

$o^1{}_2$= f(net11)=1/(1+exp(- 0.16495))= 0.54114

For hidden-to-output

$$\Delta W_{ij} = \eta \sum_{d=1}^{m} (t_i^d - o_i^d) f^{'}(net_i^d) \cdot V_j^d$$

- We will use **stochastic gradient** descent with *η=1*

$$\Delta W_{ij} = (t_i - o_i) f^{'}(net_i) V_j$$

$$f^{'}(x) = \sigma^{'}(x) = \sigma(x) \cdot (1 - \sigma(x))$$

$$\Delta W_{ij} = (t_i - o_i) \sigma(net_i)(1 - \sigma(net_i)) V_j$$

$$\delta_i = (t_i - o_i) \sigma(net_i)(1 - \sigma(net_i))$$
$$\Delta W_{ij} = \delta_i V_j$$

$$\delta_1 = (t_1 - o_1)\sigma(net_1)(1-\sigma(net_1))$$
$$\Delta W_{1j} = \delta_1 V_j$$

- *δ_1=(1- 0.54114)*(1/(1+exp(- 0.16495)))*(1-(1/(1+exp(- 0.16495))))= 0.11394*

$$\delta_2 = (t_2 - o_2)\sigma(net_2)(1-\sigma(net_2))$$
$$\Delta W_{2j} = \delta_2 V_j$$

- *δ_2=(0- 0.54114)*(1/(1+exp(- 0.16495)))*(1-(1/(1+exp(- 0.16495))))= -0.13437*

Input-to hidden connection

$$\Delta w_{jk} = \sum_{i=1}^{2} \delta_i \cdot W_{ij} f^{'}(net_j) \cdot x_k$$

$$\Delta w_{jk} = \sum_{i=1}^{2} \delta_i \cdot W_{ij} \sigma(net_j)(1 - \sigma(net_j)) \cdot x_k$$

$$\delta_j = \sigma(net_j)(1 - \sigma(net_j)) \sum_{i=1}^{2} W_{ij} \delta_i$$

$$\Delta w_{jk} = \delta_j \cdot x_k$$

$$\delta_1 = \sigma(net_1)(1 - \sigma(net_1)) \sum_{i=1}^{2} W_{i1}\delta_i$$

δ_1= 1/(1+exp(- 0.2))(1- 1/(1+exp(- 0.2)))*(0.1* 0.11394+0.1*(-0.13437))*

δ_1= -5.0568e-04

$$\delta_2 = \sigma(net_2)(1 - \sigma(net_2)) \sum_{i=1}^{2} W_{i2}\delta_i$$

δ_2= -5.0568e-04

$$\delta_3 = \sigma(net_3)(1 - \sigma(net_3)) \sum_{i=1}^{2} W_{i3}\delta_i$$

δ_3= -5.0568e-04

First Adaptation for $\boldsymbol{x_1}$

(one epoch, adaptation over all training patterns, in our case $\boldsymbol{x_1}$ $\boldsymbol{x_2}$)

$$\Delta w_{jk} = \delta_j \cdot x_k$$

$\delta_1 = -5.0568e\text{-}04$

$\delta_2 = -5.0568e\text{-}04$

$\delta_3 = -5.0568e\text{-}04$

$x_1 = 1$

$x_2 = 1$

$x_3 = 0$

$x_4 = 0$

$x_5 = 0$

$$\Delta W_{ij} = \delta_i V_j$$

$\delta_1 = 0.11394$

$\delta_2 = -0.13437$

$v_1 = 0.54983$

$v_2 = 0.54983$

$v_3 = 0.54983$

Learning consists of minimizing the error (loss) function [Bishop, 2006],

$$E(\mathbf{w}) = -\sum_{k=1}^{N} y_k \log o_k$$

in which $y_{kt} \in \{0,1\}$ and o_k corresponds to probabilities ($\sum_t y_{kt} = 1$). The error surface is more steeply as the error surface defined by the squared error

$$E(\mathbf{w}) = \frac{1}{2} \cdot \sum_{k=1}^{N} \sum_{t=1}^{2} (y_{kt} - o_{kt})^2$$

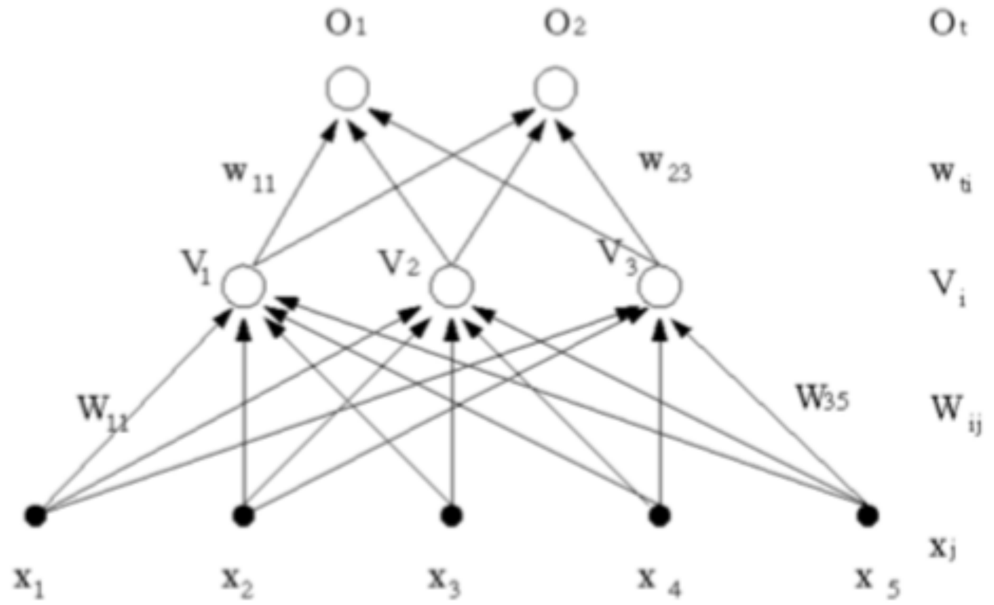
and the gradient converges faster. The cross entropy error function can be alternatively written as loss (cost) function with $\theta = \mathbf{w}$

$$L(\mathbf{x}, \mathbf{y}, \theta) = -\sum_{k=1}^{N} (y_k \log p(c_k|\mathbf{x}))$$

or as the loss function

$$J(\theta) = -\sum_{k=1}^{N} (y_k \log p(c_k|\mathbf{x})) = -\mathbb{E}_{x,y \sim p_{data}} \log p(c_k|\mathbf{x})$$

in which θ indicates the adaptive parameters of the model and $\mathbb{E}$ indicates the expectation. This notation is usually common in statistics.



- The input pattern is represented by the five-dimensional vector ***x***
- nonlinear hidden units compute the output V_1, V_2, V_3
- Two output units compute the output o_1 and o_2.
  - The units V_1, V_2, V_3 are referred to as hidden units because we cannot see their outputs and cannot directly perform error correction

For simplicity we define ϕ as a sigmoid function.

For output layer it is the softmax function with

$$\phi(net) = \frac{\exp(net_k)}{\sum_{j=1}^{K} \exp(net_j)}$$

For the hidden units it is

$$\phi(net) = \sigma(net) = \frac{1}{1 + e^{(-net)}}$$

We can use different activation function, using the sigmoid function we can reuse the results which we developed when we introduced the logistic regression

We assume the target values $y_{kt} \in \{0, 1\}$

We assume the target values $y_{kt} \in \{0, 1\}$

Output unit

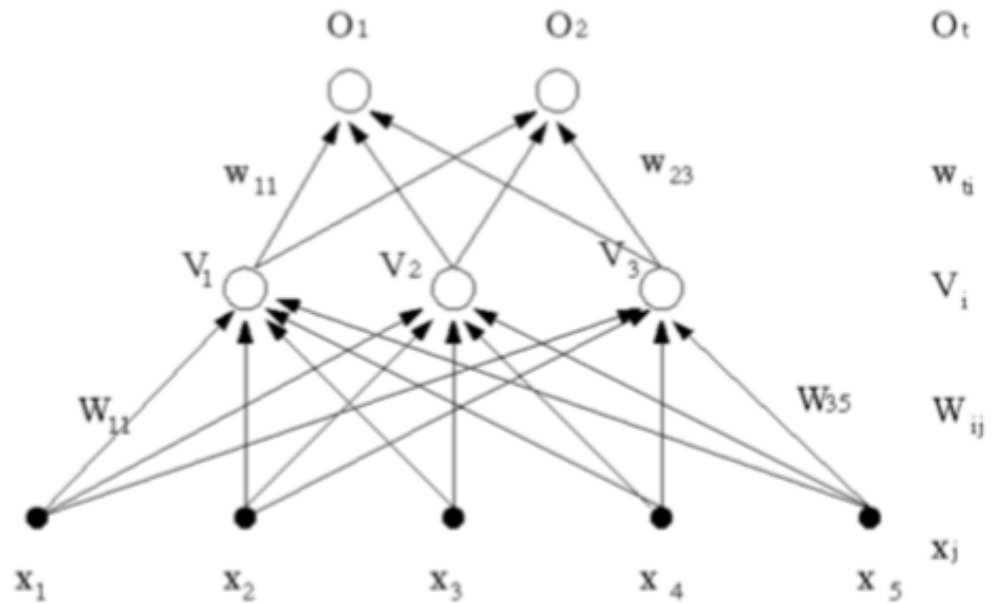
$$o_{k,t} = \phi\left(\sum_{i=0}^{3} w_{ti} \cdot V_{k,i}\right).$$

and

$$E(\mathbf{w}) = -\sum_{t=1}^{2}\sum_{k=1}^{N} y_{kt} \log o_{kt} = \sum_{t=1}^{2}\sum_{k=1}^{N} y_{kt} \log \phi\left(\sum_{i=0}^{3} w_{ti} \cdot V_{k,i}\right)$$

we get (logistic regression)

$$\frac{\partial E}{\partial w_{ti}} = -\sum_{k=1}^{N}(y_{kt} - o_{kt}) \cdot V_{k,i}.$$



We can determine the Δw_{ti} for the output units, but how can we determine ΔW_{ij} for the hidden units? If the hidden units use a continuous non linear activation function $\phi()$

$$V_{k,i} = \phi\left(\sum_{j=0}^{5} W_{ij} \cdot x_{k,j}\right).$$

$$V_{k,i} = \phi\left(\sum_{j=0}^{5} W_{ij} \cdot x_{k,j}\right).$$

we can define the training error for a training data set D_t of N elements with

$$E(\mathbf{w}, \mathbf{W}) =: E(\mathbf{w}) = -\sum_{k=1}^{N}\sum_{t=1}^{2}(y_{kt} \cdot \log o_{kt})$$

$$E(\mathbf{w}, \mathbf{W}) = -\sum_{k=1}^{N}\sum_{t=1}^{2}\left(y_{kt} \cdot \log \phi\left(\sum_{i=0}^{3} w_{ti} \cdot V_{k,i}\right)\right)$$

$$E(\mathbf{w}, \mathbf{W}) = -\sum_{k=1}^{N}\sum_{t=1}^{2}\left(y_{kt} \cdot \log \phi\left(\sum_{i=0}^{3} w_{ti} \cdot \phi\left(\sum_{j=0}^{5} W_{ij} \cdot x_{k,j}\right)\right)\right)$$

We already know

$$\frac{\partial E}{\partial w_{ti}} = -\sum_{k=1}^{N} (y_{kt} - o_{kt}) \cdot V_{k,i}.$$

For $\frac{\partial E}{\partial W_{ij}}$ we can use the chain rule and we obtain

$$\frac{\partial E}{\partial W_{ij}} = \sum_{k=1}^{N} \frac{\partial E}{\partial V_{ki}} \cdot \frac{\partial V_{ki}}{\partial W_{ij}}.$$

$$E(\mathbf{w}, \mathbf{W}) = -\sum_{k=1}^{N} \sum_{t=1}^{2} \left(y_{kt} \cdot \log \phi \left(\sum_{i=0}^{3} w_{ti} \cdot V_{k,i} \right) \right)$$

$$E(\mathbf{w}, \mathbf{W}) = -\sum_{k=1}^{N} \sum_{t=1}^{2} \left(y_{kt} \cdot \log \phi \left(\sum_{i=0}^{3} w_{ti} \cdot \phi \left(\sum_{j=0}^{5} W_{ij} \cdot x_{k,j} \right) \right) \right)$$

$$\frac{\partial E}{\partial W_{ij}} = \sum_{k=1}^{N} \frac{\partial E}{\partial V_{ki}} \cdot \frac{\partial V_{ki}}{\partial W_{ij}}.$$

$$\frac{\partial E}{\partial V_{ki}} = -\sum_{k=1}^{N} \sum_{t=1}^{2} (y_{kt} - o_{kt}) \cdot w_{t,i}.$$

$$V_{k,i} = \phi \left(\sum_{j=0}^{5} W_{ij} \cdot x_{k,j} \right) \longrightarrow \frac{\partial V_{ki}}{\partial W_{ij}} = \phi'(net_{k,i}) \cdot x_{k,j}$$

$$\frac{\partial E}{\partial W_{ij}} = \sum_{k=1}^{N} \frac{\partial E}{\partial V_{ki}} \cdot \frac{\partial V_{ki}}{\partial W_{ij}}.$$

with

$$\frac{\partial E}{\partial V_{ki}} = -\sum_{k=1}^{N}\sum_{t=1}^{2}(y_{kt} - o_{kt}) \cdot w_{t,i}.$$

and

$$\frac{\partial V_{ki}}{\partial W_{ij}} = \phi'(net_{k,i}) \cdot x_{k,j}$$

it follows

$$\frac{\partial E}{\partial W_{ij}} = -\sum_{k=1}^{N}\sum_{t=1}^{2}(y_{kt} - o_{kt}) \cdot w_{t,i} \cdot \phi'(net_{k,i}) \cdot x_{k,j}.$$

$$\frac{\partial E}{\partial W_{ij}} = -\sum_{k=1}^{N}\sum_{t=1}^{2}(y_{kt} - o_{kt}) \cdot w_{t,i} \cdot \phi'(net_{k,i}) \cdot x_{k,j}.$$

For the quadratic error it was

$$\frac{\partial E}{\partial W_{ij}} = -\sum_{k=1}^{N}\sum_{t=1}^{2}(y_{kt} - o_{kt}) \cdot \phi'(net_{k,t}) \cdot w_{t,i} \cdot \phi'(net_{k,i}) \cdot x_{k,j}.$$

You notice he difference that makes the convergence faster?

The algorithm is called back propagation because we can reuse the computation that was used to determine Δw_{ti},

$$\Delta w_{ti} = \eta \cdot \sum_{k=1}^{N} (y_{kt} - o_{kt}) \cdot V_{k,i}.$$

and with

$$\delta_{kt} = (y_{kt} - o_{kt})$$

we can write

$$\Delta w_{ti} = \eta \cdot \sum_{k=1}^{N} \delta_{kt} \cdot V_{k,i}.$$

$$\Delta W_{ij} = \eta \sum_{k=1}^{N} \sum_{t=1}^{2} (y_{kt} - o_{kt}) \cdot w_{t,i} \cdot \phi'(net_{k,i}) \cdot x_{k,j}$$

we can simplify (reuse the computation) to

$$\Delta W_{ij} = \eta \sum_{k=1}^{N} \sum_{t=1}^{2} \delta_{kt} \cdot w_{t,i} \cdot \phi'(net_{k,i}) \cdot x_{k,j}.$$

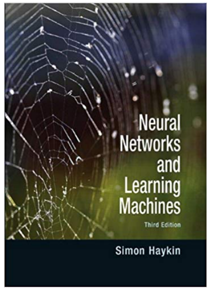
With

$$\delta_{ki} = \phi'(net_{k,i}) \cdot \sum_{t=1}^{2} \delta_{kt} \cdot w_{t,i}$$

we can simply to

$$\Delta W_{ij} = \eta \sum_{k=1}^{N} \delta_{ki} \cdot x_{k,j}.$$

Literature



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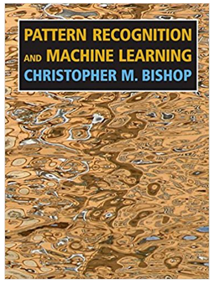

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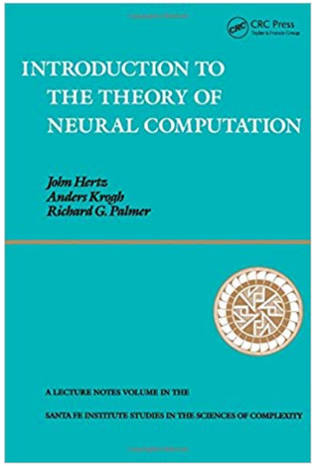
Literature (Additional)



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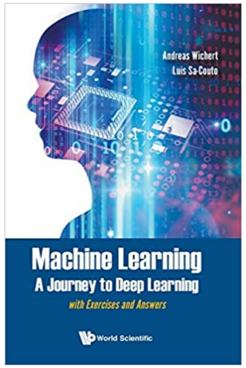
  - *Chapter 6*

Literature



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