# Introduction to Artificial Intelligence Multilayer Perceptron 

Andres Mendez-Vazquez

March 11, 2019

## Outline

(1) Introduction

- The XOR Problem
(2) Multi-Layer Perceptron
- Architecture
- Back-propagation
- Gradient Descent
- Hidden-to-Output Weights
- Input-to-Hidden Weights
- Total Training Error
- About Stopping Criteria
- Final Basic Batch Algorithm
(3) Using Matrix Operations to Simplify
- Using Matrix Operations to Simplify the Pseudo-Code
- Generating the Output $z_{k}$
- Generating $z_{k}$
- Generating the Weights from Hidden to Output Layer
- Generating the Weights from Input to Hidden Layer
- Activation Functions

4 Heuristic for Multilayer Perceptron

- Maximizing information content
- Activation Function
- Target Values
- Normalizing the inputs
- Virtues and limitations of Back-Propagation Layer


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## Do you remember?

The Perceptron has the following problem
Given that the perceptron is a linear classifier

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Given that the perceptron is a linear classifier

## It is clear that

It will never be able to classify stuff that is not linearly separable

## Example: XOR Problem

## The Problem



Class 2

## The Perceptron cannot solve it

## Because

The perceptron is a linear classifier!!!

## The Perceptron cannot solve it

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## Thus

Something needs to be done!!!

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## Thus

Something needs to be done!!!

## Maybe <br> Add an extra layer!!!

## A little bit of history

## It was first cited by Vapnik

Vapnik cites (Bryson, A.E.; W.F. Denham; S.E. Dreyfus. Optimal programming problems with inequality constraints. I: Necessary conditions for extremal solutions. AIAA J. 1,11 (1963) 2544-2550) as the first publication of the backpropagation algorithm in his book "Support Vector Machines."

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Arthur E. Bryson and Yu-Chi Ho described it as a multi-stage dynamic system optimization method in 1969.

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## It was first used by

Arthur E. Bryson and Yu-Chi Ho described it as a multi-stage dynamic system optimization method in 1969.

## However

It was not until 1974 and later, when applied in the context of neural networks and through the work of Paul Werbos, David E. Rumelhart, Geoffrey E. Hinton and Ronald J. Williams that it gained recognition.

## Then

## Something Notable

It led to a "renaissance" in the field of artificial neural network research.

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## Nevertheless

During the 2000s it fell out of favour but has returned again in the 2010s, now able to train much larger networks using huge modern computing power such as GPUs.

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## Multi-Layer Perceptron (MLP)

Multi-Layer Architecture.


## Information Flow

## We have the following information flow



## Explanation

Problems with Hidden Layers
(1) Increase complexity of Training

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(2) It is necessary to think about "Long and Narrow" network vs "Short and Fat" network.

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## Advantages

It has been proven that an MLP with one hidden layer can learn any nonlinear function of the input.

## The Process

## We have something like this



Layer 2


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## Remember!!! The Quadratic Learning Error function

## Cost Function our well know error at pattern $m$

$$
\begin{equation*}
J(m)=\frac{1}{2} e_{k}^{2}(m) \tag{1}
\end{equation*}
$$

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## Delta Rule or Widrow-Hoff Rule

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\begin{equation*}
\Delta w_{k j}(m)=-\eta e_{k}(m) x_{j}(m) \tag{2}
\end{equation*}
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$$

Actually this is know as Gradient Descent

$$
\begin{equation*}
w_{k j}(m+1)=w_{k j}(m)+\Delta w_{k j}(m) \tag{3}
\end{equation*}
$$

## Back-propagation

## Setup

Let $t_{k}$ be the $k$-th target (or desired) output and $z_{k}$ be the $k$-th computed output with $k=1, \ldots, d$ and $\boldsymbol{w}$ represents all the weights of the network

## Back-propagation

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Training Error for a single Pattern or Sample!!!

$$
\begin{equation*}
J(\boldsymbol{w})=\frac{1}{2} \sum_{k=1}^{c}\left(t_{k}-z_{k}\right)^{2}=\frac{1}{2}\|\boldsymbol{t}-\boldsymbol{z}\|^{2} \tag{4}
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## Gradient Descent

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## Reducing the Error

The weights are initialized with pseudo-random values and are changed in a direction that will reduce the error:

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\begin{equation*}
\Delta \boldsymbol{w}=-\eta \frac{\partial J}{\partial \boldsymbol{w}} \tag{5}
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$$

## Where

$\eta$ is the learning rate which indicates the relative size of the change in weights:

$$
\begin{equation*}
w(m+1)=w(m)+\Delta w(m) \tag{6}
\end{equation*}
$$

where $m$ is the $m$-th pattern presented

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## Multilayer Architecture

Multilayer Architecture: hidden-to-output weights


## Observation about the activation function

## Hidden Output is equal to

$$
y_{j}=f\left(\sum_{i=1}^{d} w_{j i} x_{i}\right)
$$

Observation about the activation function

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Output is equal to

$$
z_{k}=f\left(\sum_{j=1}^{y_{n_{H}}} w_{k j} y_{j}\right)
$$

## Hidden-to-Output Weights

Error on the hidden-to-output weights

$$
\begin{equation*}
\frac{\partial J}{\partial w_{k j}}=\frac{\partial J}{\partial n e t_{k}} \cdot \frac{\partial n e t_{k}}{\partial w_{k j}}=-\delta_{k} \cdot \frac{\partial n e t_{k}}{\partial w_{k j}} \tag{7}
\end{equation*}
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## $n^{n} t_{k}$

It describes how the overall error changes with the activation of the unit's net:

$$
\begin{equation*}
\operatorname{net}_{k}=\sum_{j=1}^{y_{n}} w_{k j} y_{j}=\boldsymbol{w}_{k}^{T} \cdot \boldsymbol{y} \tag{8}
\end{equation*}
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$$

## Now

$$
\begin{equation*}
\delta_{k}=-\frac{\partial J}{\partial n e t_{k}}=-\frac{\partial J}{\partial z_{k}} \cdot \frac{\partial z_{k}}{\partial n e t_{k}}=\left(t_{k}-z_{k}\right) f^{\prime}\left(n e t_{k}\right) \tag{9}
\end{equation*}
$$

## Hidden-to-Output Weights

## Why?

$$
\begin{equation*}
z_{k}=f\left(\text { net }_{k}\right) \tag{10}
\end{equation*}
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$$

Since $\operatorname{net}_{k}=\boldsymbol{w}_{k}^{T} \cdot \boldsymbol{y}$ therefore:

$$
\begin{equation*}
\frac{\partial n e t_{k}}{\partial w_{k j}}=y_{j} \tag{12}
\end{equation*}
$$

## Finally

The weight update (or learning rule) for the hidden-to-output weights is:

$$
\begin{equation*}
\triangle w_{k j}=\eta \delta_{k} y_{j}=\eta\left(t_{k}-z_{k}\right) f^{\prime}\left(n e t_{k}\right) y_{j} \tag{13}
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## Multi-Layer Architecture

Multi-Layer Architecture: Input-to-Hidden weights


## Input-to-Hidden Weights

Error on the Input-to-Hidden weights

$$
\begin{equation*}
\frac{\partial J}{\partial w_{j i}}=\frac{\partial J}{\partial y_{j}} \cdot \frac{\partial y_{j}}{\partial n e t_{j}} \cdot \frac{\partial n e t_{j}}{\partial w_{j i}} \tag{14}
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$$

Thus

$$
\begin{aligned}
\frac{\partial J}{\partial y_{j}} & =\frac{\partial}{\partial y_{j}}\left[\frac{1}{2} \sum_{k=1}^{c}\left(t_{k}-z_{k}\right)^{2}\right] \\
& =-\sum_{k=1}^{c}\left(t_{k}-z_{k}\right) \frac{\partial z_{k}}{\partial y_{j}} \\
& =-\sum_{k=1}^{c}\left(t_{k}-z_{k}\right) \frac{\partial z_{k}}{\partial n e t_{k}} \cdot \frac{\partial n e t_{k}}{\partial y_{j}} \\
& =-\sum_{k=1}^{c}\left(t_{k}-z_{k}\right) \frac{\partial f\left(\text { net }_{k}\right)}{\partial n e t_{k}} \cdot w_{k j}
\end{aligned}
$$

## Input-to-Hidden Weights

## Finally

$$
\begin{equation*}
\frac{\partial J}{\partial y_{j}}=-\sum_{k=1}^{c}\left(t_{k}-z_{k}\right) f^{\prime}\left(n e t_{k}\right) \cdot w_{k j} \tag{15}
\end{equation*}
$$

## Remember

$$
\begin{equation*}
\delta_{k}=-\frac{\partial J}{\partial n e t_{k}}=\left(t_{k}-z_{k}\right) f^{\prime}\left(n e t_{k}\right) \tag{16}
\end{equation*}
$$

## What is $\frac{\partial y_{j}}{\partial n e t_{j}} ?$

## First

$$
\begin{equation*}
n e t_{j}=\sum_{i=1}^{d} w_{j i} x_{i}=\boldsymbol{w}_{j}^{T} \cdot \boldsymbol{x} \tag{17}
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\frac{\partial y_{j}}{\partial n e t_{j}}=\frac{\partial f\left(\text { net }_{j}\right)}{\partial n e t_{j}}=f^{\prime}\left(\text { net }_{j}\right)
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By defying the sensitivity for a hidden unit:

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\delta_{j}=f^{\prime}\left(n e t_{j}\right) \sum_{k=1}^{c} w_{k j} \delta_{k} \tag{18}
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$$

## Which means that:

"The sensitivity at a hidden unit is simply the sum of the individual sensitivities at the output units weighted by the hidden-to-output weights $w_{k j}$; all multiplied by $f^{\prime}\left(\right.$ net $\left._{j}\right)$ "

What about $\frac{\partial \text { net }_{j}}{\partial w_{j i}}$ ?

We have that

$$
\frac{\partial n e t_{j}}{\partial w_{j i}}=\frac{\partial \boldsymbol{w}_{j}^{T} \cdot \boldsymbol{x}}{\partial w_{j i}}=\frac{\partial \sum_{i=1}^{d} w_{j i} x_{i}}{\partial w_{j i}}=x_{i}
$$

## Finally

The learning rule for the input-to-hidden weights is:

$$
\begin{equation*}
\Delta w_{j i}=\eta x_{i} \delta_{j}=\eta\left[\sum_{k=1}^{c} w_{k j} \delta_{k}\right] f^{\prime}\left(\text { net }_{j}\right) x_{i} \tag{19}
\end{equation*}
$$

## Basically, the entire training process has the following steps

Initialization

Assuming that no prior information is available, pick the synaptic weights and thresholds

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Compute the induced function signals of the network by proceeding forward through the network, layer by layer.

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Compute the local gradients of the network.

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## Forward Computation

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Compute the local gradients of the network.

## Finally

Adjust the weights!!!

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## Now, Calculating Total Change

We have for that<br>The Total Training Error is the sum over the errors of $N$ individual patterns

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## The Total Training Error

$$
\begin{equation*}
J=\sum_{p=1}^{N} J_{p}=\frac{1}{2} \sum_{p=1}^{N} \sum_{k=1}^{d}\left(t_{k}^{p}-z_{k}^{p}\right)^{2}=\frac{1}{2} \sum_{p=1}^{n}\left\|\boldsymbol{t}^{p}-\boldsymbol{z}^{p}\right\|^{2} \tag{20}
\end{equation*}
$$

## About the Total Training Error

## Remarks

- A weight update may reduce the error on the single pattern being presented but can increase the error on the full training set.


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- A weight update may reduce the error on the single pattern being presented but can increase the error on the full training set.
- However, given a large number of such individual updates, the total error of equation (20) decreases.


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## Therefore

It is necessary to have a way to stop when the change of the weights is enough!!!

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- The algorithm terminates when the change in the criterion function $J(\boldsymbol{w})$ is smaller than some preset value $\Theta$.

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- The algorithm terminates when the change in the criterion function $J(\boldsymbol{w})$ is smaller than some preset value $\Theta$.

$$
\begin{equation*}
\Delta J(\boldsymbol{w})=|J(\boldsymbol{w}(t+1))-J(\boldsymbol{w}(t))| \tag{21}
\end{equation*}
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\Delta J(\boldsymbol{w})=|J(\boldsymbol{w}(t+1))-J(\boldsymbol{w}(t))| \tag{21}
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$$

- There are other stopping criteria that lead to better performance than this one.


## Other Stopping Criteria

## Norm of the Gradient

The back-propagation algorithm is considered to have converged when the Euclidean norm of the gradient vector reaches a sufficiently small gradient threshold.

$$
\begin{equation*}
\left\|\nabla_{\boldsymbol{w}} J(m)\right\|<\Theta \tag{22}
\end{equation*}
$$

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\end{equation*}
$$

## Rate of change in the average error per epoch

The back-propagation algorithm is considered to have converged when the absolute rate of change in the average squared error per epoch is sufficiently small.

$$
\begin{equation*}
\left|\frac{1}{N} \sum_{p=1}^{N} J_{p}\right|<\Theta \tag{23}
\end{equation*}
$$

## About the Stopping Criteria

## Observations

(1) Before training starts, the error on the training set is high.

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(1) Before training starts, the error on the training set is high.

- Through the learning process, the error becomes smaller.


## About the Stopping Criteria

## Observations

(1) Before training starts, the error on the training set is high.

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(2) The error per pattern depends on the amount of training data and the expressive power (such as the number of weights) in the network.


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## About the Stopping Criteria

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(3) The average error on an independent test set is always higher than on the training set, and it can decrease as well as increase.
(9) A validation set is used in order to decide when to stop training.
- We do not want to over-fit the network and decrease the power of the classifier generalization "we stop training at a minimum of the error on the validation set"


## Some More Terminology

## Epoch

As with other types of backpropagation, 'learning' is a supervised process that occurs with each cycle or 'epoch' through a forward activation flow of outputs, and the backwards error propagation of weight adjustments.

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## Epoch

As with other types of backpropagation, 'learning' is a supervised process that occurs with each cycle or 'epoch' through a forward activation flow of outputs, and the backwards error propagation of weight adjustments.

## In our case

I am using the batch sum of all correcting weights to define that epoch.

## Outline

(1) Introduction

- The XOR Problem
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- Input-to-Hidden Weights
- Total Training Error
- About Stopping Criteria
- Final Basic Batch Algorithm

3 Using Matrix Operations to Simplify

- Using Matrix Operations to Simplify the Pseudo-Code
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## Final Basic Batch Algorithm

## Perceptron $(\boldsymbol{X})$

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## Perceptron $(\boldsymbol{X})$

(1) Initialize random $\boldsymbol{w}$, number of hidden units $n_{H}$, number of outputs $\boldsymbol{z}$, stopping criterion $\Theta$, learning rate $\eta$, epoch $m=0$

## Final Basic Batch Algorithm

## Perceptron $(\boldsymbol{X})$

(1) Initialize random $\boldsymbol{w}$, number of hidden units $n_{H}$, number of outputs $\boldsymbol{z}$, stopping criterion $\Theta$, learning rate $\eta$, epoch $m=0$
(2) do

## Final Basic Batch Algorithm

## Perceptron $(\boldsymbol{X})$

(1) Initialize random $\boldsymbol{w}$, number of hidden units $n_{H}$, number of outputs $\boldsymbol{z}$, stopping criterion $\Theta$, learning rate $\eta$, epoch $m=0$
(2) do
(3) $m=m+1$

## Final Basic Batch Algorithm

## Perceptron $(\boldsymbol{X})$

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(2) do
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$$

(4)

$$
\text { for } s=1 \text { to } N
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## Final Basic Batch Algorithm

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m=0
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(2) do
(3)

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(4)

$$
\text { for } s=1 \text { to } N
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(5)

$$
\boldsymbol{x}(m)=\boldsymbol{X}(:, s)
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(6)
for $k=1$ to $c$

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for $k=1$ to $c$

$$
\delta_{k}=\left(t_{k}-z_{k}\right) f^{\prime}\left(\boldsymbol{w}_{k}^{T} \cdot \boldsymbol{y}\right)
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$$
n e t_{j}=\boldsymbol{w}_{j}^{T} \cdot \boldsymbol{x} ; y_{j}=f\left(\text { net }_{j}\right)
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(11)

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\delta_{j}=f^{\prime}\left(n e t_{j}\right) \sum_{k=1}^{c} w_{k j} \delta_{k}
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## Outline

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## Example of Architecture to be used

Given the following Architecture and assuming $N$ samples


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## Generating the output $z_{k}$

Given the input

$$
\boldsymbol{X}=\left[\begin{array}{llll}
x_{1} & x_{2} & \cdots & x_{N}
\end{array}\right]
$$

## Generating the output $z_{k}$

Given the input

$$
\boldsymbol{X}=\left[\begin{array}{llll}
\boldsymbol{x}_{1} & \boldsymbol{x}_{2} & \cdots & \boldsymbol{x}_{N} \tag{24}
\end{array}\right]
$$

## Where

$\boldsymbol{x}_{i}$ is a vector of features

$$
\boldsymbol{x}_{i}=\left(\begin{array}{c}
x_{1 i}  \tag{25}\\
x_{2 i} \\
\vdots \\
x_{d i}
\end{array}\right)
$$

## Therefore

## We must have the following matrix for the input to hidden inputs

$$
\boldsymbol{W}_{I H}=\left(\begin{array}{cccc}
w_{11} & w_{12} & \cdots & w_{1 d}  \tag{26}\\
w_{21} & w_{22} & \cdots & w_{2 d} \\
\vdots & \vdots & \ddots & \vdots \\
w_{n_{H} 1} & w_{n_{H} 2} & \cdots & w_{n_{H} d}
\end{array}\right)=\left(\begin{array}{c}
\boldsymbol{w}_{1}^{T} \\
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\vdots \\
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\end{array}\right)
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\end{array}\right)
$$

Given that $\boldsymbol{w}_{j}=\left(\begin{array}{c}w_{j 1} \\ w_{j 2} \\ \vdots \\ w_{j d}\end{array}\right)$

## Thus

We can create the $\boldsymbol{n e t}_{\boldsymbol{j}}$ for all the inputs by simply

$$
\boldsymbol{n e t}_{j}=\boldsymbol{W}_{I H} \boldsymbol{X}=\left(\begin{array}{cccc}
\boldsymbol{w}_{1}^{T} \boldsymbol{x}_{1} & \boldsymbol{w}_{1}^{T} \boldsymbol{x}_{2} & \cdots & \boldsymbol{w}_{1}^{T} \boldsymbol{x}_{N}  \tag{27}\\
\boldsymbol{w}_{2}^{T} \boldsymbol{x}_{1} & \boldsymbol{w}_{2}^{T} \boldsymbol{x}_{2} & \cdots & \boldsymbol{w}_{2}^{T} \boldsymbol{x}_{N} \\
\vdots & \vdots & \ddots & \vdots \\
\boldsymbol{w}_{n_{H}}^{T} \boldsymbol{x}_{1} & \boldsymbol{w}_{n_{H}}^{T} \boldsymbol{x}_{2} & \cdots & \boldsymbol{w}_{n_{H}}^{T} \boldsymbol{x}_{N}
\end{array}\right)
$$

Now, we need to generate the $\boldsymbol{y}_{k}$

We apply the activation function element by element in $\boldsymbol{n e t}_{j}$

$$
\boldsymbol{y}_{1}=\left(\begin{array}{cccc}
f\left(\boldsymbol{w}_{1}^{T} \boldsymbol{x}_{1}\right) & f\left(\boldsymbol{w}_{1}^{T} \boldsymbol{x}_{2}\right) & \cdots & f\left(\boldsymbol{w}_{1}^{T} \boldsymbol{x}_{N}\right)  \tag{28}\\
f\left(\boldsymbol{w}_{2}^{T} \boldsymbol{x}_{1}\right) & f\left(\boldsymbol{w}_{2}^{T} \boldsymbol{x}_{2}\right) & \cdots & f\left(\boldsymbol{w}_{2}^{T} \boldsymbol{x}_{N}\right) \\
\vdots & \vdots & \ddots & \vdots \\
f\left(\boldsymbol{w}_{n_{H}}^{T} \boldsymbol{x}_{1}\right) & f\left(\boldsymbol{w}_{n_{H}}^{T} \boldsymbol{x}_{2}\right) & \cdots & f\left(\boldsymbol{w}_{n_{H}}^{T} \boldsymbol{x}_{N}\right)
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## IMPORTANT about overflows!!!

- Be careful about the numeric stability of the activation function.

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## IMPORTANT about overflows!!!

- Be careful about the numeric stability of the activation function.
- I the case of python, we can use the ones provided by scipy.special


## However, We can create a Sigmoid function

## It is possible to use the following pseudo-code

Sigmoid $(x)$
(1)
if $x<-B I G R E A L$
(2)
return 0

## However, We can create a Sigmoid function

## It is possible to use the following pseudo-code

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4) return 1

## However, We can create a Sigmoid function

## It is possible to use the following pseudo-code

Sigmoid $(x)$
(1) if $x<-$ BIGREAL
(2)
return 0
(3) else if $x>B I G R E A L$
(9) return 1
(5) else
©

$$
\begin{aligned}
& \text { return } \frac{1.0}{1.0+\exp \{-\alpha x\}} \triangleleft 1.0 \text { refers to the floating point (Rationals } \\
& \triangleleft \text { trying to represent Reals) }
\end{aligned}
$$

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- Maximizing information content
- Activation Function
- Target Values
- Normalizing the inputs
- Virtues and limitations of Back-Propagation Layer

For this, we get $\boldsymbol{n e t}_{k}$
For this, we obtain the $W_{H O}$

$$
\boldsymbol{W}_{H O}=\left(\begin{array}{llll}
w_{11}^{o} & w_{12}^{o} & \cdots & w_{1 n_{H}}^{o}
\end{array}\right)=\left(\begin{array}{l}
\boldsymbol{w}_{o}^{T} \tag{29}
\end{array}\right)
$$

For this, we get $\boldsymbol{n e t}_{k}$
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\end{array}\right)=\left(\boldsymbol{w}_{o}^{T}\right)
$$

## Thus

$$
\left.w_{1 n_{H}}^{o}\right)\left(\begin{array}{cccc}
f\left(\boldsymbol{w}_{1}^{T} \boldsymbol{x}_{1}\right) & f\left(\boldsymbol{w}_{1}^{T} \boldsymbol{x}_{2}\right) & \cdots & f\left(\boldsymbol{w}_{1}^{T} \boldsymbol{x}_{N}\right)  \tag{30}\\
f\left(\boldsymbol{w}_{2}^{T} \boldsymbol{x}_{1}\right) & f\left(\boldsymbol{w}_{2}^{T} \boldsymbol{x}_{2}\right) & \cdots & f\left(\boldsymbol{w}_{2}^{T} \boldsymbol{x}_{N}\right) \\
\vdots & \vdots & \ddots & \vdots \\
\underbrace{f\left(\boldsymbol{w}_{n_{H}}^{T} \boldsymbol{x}_{1}\right)}_{\boldsymbol{y}_{k 1}} & \underbrace{f\left(\boldsymbol{w}_{n_{H}}^{T} \boldsymbol{x}_{2}\right)}_{\boldsymbol{y}_{k 2}} & \cdots & \underbrace{f\left(\boldsymbol{w}_{n_{H}}^{T} \boldsymbol{x}_{N}\right)}_{\boldsymbol{y}_{k N}}
\end{array}\right)
$$

## In matrix notation

$$
\boldsymbol{n e t}_{k}=\left(\begin{array}{cccc}
\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k 1} & \boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k 2} & \cdots & \boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k N} \tag{31}
\end{array}\right)
$$

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Now, we have

Thus, we have $\boldsymbol{z}_{k}$ (In our case $k=1$, but it could be a range of values)

$$
\boldsymbol{z}_{k}=\left(\begin{array}{llll}
f\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k 1}\right) & f\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k 2}\right) & \cdots & f\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k N}\right) \tag{32}
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\end{array}\right)
$$

Thus, we generate a vector of differences

$$
\boldsymbol{d}=\boldsymbol{t}-\boldsymbol{z}_{k}=\left(\begin{array}{llll}
t_{1}-f\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k 1}\right) & t_{2}-f\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k 2}\right) & \cdots & t_{N}-f\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k N}\right) \tag{33}
\end{array}\right)
$$

where $\boldsymbol{t}=\left(\begin{array}{llll}t_{1} & t_{2} & \cdots & t_{N}\end{array}\right)$ is a row vector of desired outputs for each sample.

Now, we multiply element wise

We have the following vector of derivatives of net

$$
\boldsymbol{D}_{f}=\left(\begin{array}{llll}
\eta f^{\prime}\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k 1}\right) & \eta f^{\prime}\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k 2}\right) & \cdots & \eta f^{\prime}\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k N}\right) \tag{34}
\end{array}\right)
$$

where $\eta$ is the step rate.

## Now, we multiply element wise

## We have the following vector of derivatives of net

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\boldsymbol{D}_{f}=\left(\begin{array}{llll}
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\end{array}\right)
$$

where $\eta$ is the step rate.

## Finally, by element wise multiplication (Hadamard Product)

$$
\begin{aligned}
\boldsymbol{d}=( & \eta\left[t_{1}-f\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k 1}\right)\right] f^{\prime}\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k 1}\right) \quad \eta\left[t_{2}-f\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k 2}\right)\right] f^{\prime}\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k 2}\right) \\
& \left.\eta\left[t_{N}-f\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k N}\right)\right] f^{\prime}\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k N}\right)\right)
\end{aligned}
$$

## Tile $\boldsymbol{d}$

Tile downward

$$
\boldsymbol{d}_{\text {tile }}=n_{H} \text { rows }\left\{\left(\begin{array}{c}
\boldsymbol{d} \\
\boldsymbol{d} \\
\vdots \\
\boldsymbol{d}
\end{array}\right)\right.
$$

## Tile $\boldsymbol{d}$

Tile downward

$$
\boldsymbol{d}_{\text {tile }}=n_{H} \text { rows }\left\{\left(\begin{array}{c}
\boldsymbol{d}  \tag{35}\\
\boldsymbol{d} \\
\vdots \\
\boldsymbol{d}
\end{array}\right)\right.
$$

Finally, we multiply element wise against $\boldsymbol{y}_{1}$ (Hadamard Product)

$$
\begin{equation*}
\Delta \boldsymbol{w}_{1 j}^{t e m p}=\boldsymbol{y}_{1} \circ \boldsymbol{d}_{t i l e} \tag{36}
\end{equation*}
$$

## We obtain the total $\Delta \boldsymbol{w}_{1 j}$

## We sum along the rows of $\Delta \boldsymbol{w}_{1 j}^{\text {temp }}$

$$
\Delta \boldsymbol{w}_{1 j}=\left(\begin{array}{c}
\eta\left[t_{1}-f\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k 1}\right)\right] f^{\prime}\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k 1}\right) y_{11}+\eta\left[t_{1}-f\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k N}\right)\right] f^{\prime}\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k N}\right) y_{1 N}  \tag{37}\\
\vdots \\
\eta\left[t_{1}-f\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k 1}\right)\right] f^{\prime}\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k 1}\right) y_{n_{H} 1}+\eta\left[t_{1}-f\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k N}\right)\right] f^{\prime}\left(\boldsymbol{w}_{o}^{T} \boldsymbol{y}_{k N}\right) y_{n_{H} N}
\end{array}\right)
$$

where $y_{h m}=f\left(\boldsymbol{w}_{h}^{T} \boldsymbol{x}_{m}\right)$ with $h=1,2, \ldots, n_{H}$ and $m=1,2, \ldots, N$.

## Finally, we update the first weights

We have then

$$
\begin{equation*}
\boldsymbol{W}_{H O}(t+1)=\boldsymbol{W}_{H O}(t)+\Delta \boldsymbol{w}_{1 j}^{T}(t) \tag{38}
\end{equation*}
$$

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## First

We multiply element wise the $W_{H O}$ and $\Delta w_{1 j}$

$$
\begin{equation*}
\boldsymbol{T}=\Delta \boldsymbol{w}_{1 j}^{T} \circ \boldsymbol{W}_{H O}^{T} \tag{39}
\end{equation*}
$$

## First

We multiply element wise the $W_{H O}$ and $\Delta \boldsymbol{w}_{1 j}$

$$
\begin{equation*}
\boldsymbol{T}=\Delta \boldsymbol{w}_{1 j}^{T} \circ \boldsymbol{W}_{H O}^{T} \tag{39}
\end{equation*}
$$

Now, we obtain the element wise derivative of $\boldsymbol{n e} \boldsymbol{t}_{j}$

$$
\boldsymbol{D n e t}_{j}=\left(\begin{array}{cccc}
f^{\prime}\left(\boldsymbol{w}_{1}^{T} \boldsymbol{x}_{1}\right) & f^{\prime}\left(\boldsymbol{w}_{1}^{T} \boldsymbol{x}_{2}\right) & \cdots & f^{\prime}\left(\boldsymbol{w}_{1}^{T} \boldsymbol{x}_{N}\right)  \tag{40}\\
f^{\prime}\left(\boldsymbol{w}_{2}^{T} \boldsymbol{x}_{1}\right) & f^{\prime}\left(\boldsymbol{w}_{2}^{T} \boldsymbol{x}_{2}\right) & \cdots & f^{\prime}\left(\boldsymbol{w}_{2}^{T} \boldsymbol{x}_{N}\right) \\
\vdots & \vdots & \ddots & \vdots \\
f^{\prime}\left(\boldsymbol{w}_{n_{H}}^{T} \boldsymbol{x}_{1}\right) & f^{\prime}\left(\boldsymbol{w}_{n_{H}}^{T} \boldsymbol{x}_{2}\right) & \cdots & f^{\prime}\left(\boldsymbol{w}_{n_{H}}^{T} \boldsymbol{x}_{N}\right)
\end{array}\right)
$$

## Thus

## We tile to the right $T$

$$
\boldsymbol{T}_{\text {tile }}=\underbrace{\left(\begin{array}{llll}
\boldsymbol{T} & \boldsymbol{T} & \cdots & \boldsymbol{T} \tag{41}
\end{array}\right)}_{N \text { Columns }}
$$

## Thus

## We tile to the right $T$

$$
\boldsymbol{T}_{\text {tile }}=\underbrace{\left(\begin{array}{llll}
\boldsymbol{T} & \boldsymbol{T} & \cdots & \boldsymbol{T} \tag{41}
\end{array}\right)}_{N \text { Columns }}
$$

Now, we multiply element wise together with $\eta$

$$
\begin{equation*}
\boldsymbol{P}_{t}=\eta\left(\boldsymbol{D n e t}_{j} \circ \boldsymbol{T}_{\text {tile }}\right) \tag{42}
\end{equation*}
$$

where $\eta$ is constant multiplied against the result the Hadamar Product (Result a $n_{H} \times N$ matrix)

## Finally

We get use the transpose of $\boldsymbol{X}$ which is a $N \times d$ matrix

$$
\boldsymbol{X}^{T}=\left(\begin{array}{c}
\boldsymbol{x}_{1}^{T} \\
\boldsymbol{x}_{2}^{T} \\
\vdots \\
\boldsymbol{x}_{N}^{T}
\end{array}\right)
$$

(43)

## Finally

We get use the transpose of $\boldsymbol{X}$ which is a $N \times d$ matrix

$$
\boldsymbol{X}^{T}=\left(\begin{array}{c}
\boldsymbol{x}_{1}^{T}  \tag{43}\\
\boldsymbol{x}_{2}^{T} \\
\vdots \\
\boldsymbol{x}_{N}^{T}
\end{array}\right)
$$

Finally, we get a $n_{H} \times d$ matrix

$$
\begin{equation*}
\Delta \boldsymbol{w}_{i j}=\boldsymbol{P}_{t} \boldsymbol{X}^{T} \tag{44}
\end{equation*}
$$

## Finally

We get use the transpose of $\boldsymbol{X}$ which is a $N \times d$ matrix

$$
\boldsymbol{X}^{T}=\left(\begin{array}{c}
\boldsymbol{x}_{1}^{T}  \tag{43}\\
\boldsymbol{x}_{2}^{T} \\
\vdots \\
\boldsymbol{x}_{N}^{T}
\end{array}\right)
$$

Finally, we get a $n_{H} \times d$ matrix

$$
\begin{equation*}
\Delta \boldsymbol{w}_{i j}=\boldsymbol{P}_{t} \boldsymbol{X}^{T} \tag{44}
\end{equation*}
$$

Thus, given $W_{I H}$

$$
\begin{equation*}
\boldsymbol{W}_{I H}(t+1)=\boldsymbol{W}_{H O}(t)+\Delta \boldsymbol{w}_{i j}^{T}(t) \tag{45}
\end{equation*}
$$

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## We have different activation functions

The two most important
(1) Sigmoid function.

## We have different activation functions

The two most important
(1) Sigmoid function.
(2) Hyperbolic tangent function

## Logistic Function

This non-linear function has the following definition for a neuron $j$

$$
\begin{equation*}
f_{j}\left(v_{j}(n)\right)=\frac{1}{1+\exp \left\{-a v_{j}(n)\right\}} a>0 \text { and }-\infty<v_{j}(n)<\infty \tag{46}
\end{equation*}
$$

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$$
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f_{j}\left(v_{j}(n)\right)=\frac{1}{1+\exp \left\{-a v_{j}(n)\right\}} a>0 \text { and }-\infty<v_{j}(n)<\infty \tag{46}
\end{equation*}
$$

## Example



The differential of the sigmoid function

Now if we differentiate, we have

$$
f_{j}^{\prime}\left(v_{j}(n)\right)=\left[\frac{1}{1+\exp \left\{-a v_{j}(n)\right\}}\right]\left[1-\frac{1}{1+\exp \left\{-a v_{j}(n)\right\}}\right]
$$

The differential of the sigmoid function

Now if we differentiate, we have

$$
\begin{aligned}
f_{j}^{\prime}\left(v_{j}(n)\right) & =\left[\frac{1}{1+\exp \left\{-a v_{j}(n)\right\}}\right]\left[1-\frac{1}{1+\exp \left\{-a v_{j}(n)\right\}}\right] \\
& =\frac{\exp \left\{-a v_{j}(n)\right\}}{\left(1+\exp \left\{-a v_{j}(n)\right\}\right)^{2}}
\end{aligned}
$$

## The outputs finish as

For the output neurons

$$
\delta_{k}=\left(t_{k}-z_{k}\right) f^{\prime}\left(\text { net }_{k}\right)
$$

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\begin{aligned}
\delta_{k} & =\left(t_{k}-z_{k}\right) f^{\prime}\left(\text { net }_{k}\right) \\
& =\left(t_{k}-f_{k}\left(v_{k}(n)\right)\right) f_{k}\left(v_{k}(n)\right)\left(1-f_{k}\left(v_{k}(n)\right)\right)
\end{aligned}
$$

## For the hidden neurons

## The outputs finish as

## For the output neurons

$$
\begin{aligned}
\delta_{k} & =\left(t_{k}-z_{k}\right) f^{\prime}\left(\text { net }_{k}\right) \\
& =\left(t_{k}-f_{k}\left(v_{k}(n)\right)\right) f_{k}\left(v_{k}(n)\right)\left(1-f_{k}\left(v_{k}(n)\right)\right)
\end{aligned}
$$

## For the hidden neurons

$$
\delta_{j}=f_{j}\left(v_{j}(n)\right)\left(1-f_{j}\left(v_{j}(n)\right)\right) \sum_{k=1}^{c} w_{k j} \delta_{k}
$$

## Hyperbolic tangent function

Another commonly used form of sigmoidal non linearity is the hyperbolic tangent function

$$
f_{j}\left(v_{j}(n)\right)=a \tanh \left(b v_{j}(n)\right)
$$

## Hyperbolic tangent function

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$$
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f_{j}\left(v_{j}(n)\right)=a \tanh \left(b v_{j}(n)\right) \tag{47}
\end{equation*}
$$

## Example



## The differential of the hyperbolic tangent

We have

$$
f_{j}\left(v_{j}(n)\right)=a b \operatorname{sech}^{2}\left(b v_{j}(n)\right)
$$

The differential of the hyperbolic tangent

We have

$$
\begin{aligned}
f_{j}\left(v_{j}(n)\right) & =a b \operatorname{sech}^{2}\left(b v_{j}(n)\right) \\
& =a b\left(1-\tanh ^{2}\left(b v_{j}(n)\right)\right)
\end{aligned}
$$

## BTW

## The differential of the hyperbolic tangent

## We have

$$
\begin{aligned}
f_{j}\left(v_{j}(n)\right) & =a b \operatorname{sech}^{2}\left(b v_{j}(n)\right) \\
& =a b\left(1-\tanh ^{2}\left(b v_{j}(n)\right)\right)
\end{aligned}
$$

## BTW

I leave to you to figure out the outputs.

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## Maximizing information content

## Two ways of achieving this, LeCun 1993

- The use of an example that results in the largest training error.


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- The use of an example that results in the largest training error.
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## For this

Randomized the samples presented to the multilayer perceptron when not doing batch training.

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Randomized the samples presented to the multilayer perceptron when not doing batch training.

## Or use an emphasizing scheme

By using the error identify the difficult vs. easy patterns:

## Maximizing information content

## Two ways of achieving this，LeCun 1993

－The use of an example that results in the largest training error．
－The use of an example that is radically different from all those previously used．

## For this

Randomized the samples presented to the multilayer perceptron when not doing batch training．

## Or use an emphasizing scheme

By using the error identify the difficult vs．easy patterns：
－Use them to train the neural network

## However!!!

## Be careful about emphasizing scheme

- The distribution of examples within an epoch presented to the network is distorted.


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- The distribution of examples within an epoch presented to the network is distorted.
- The presence of an outlier or a mislabeled example can have a catastrophic consequence on the performance of the algorithm.


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## Be careful about emphasizing scheme

- The distribution of examples within an epoch presented to the network is distorted.
- The presence of an outlier or a mislabeled example can have a catastrophic consequence on the performance of the algorithm.


## Definition of Outlier

An outlier is an observation that lies outside the overall pattern of a distribution (Moore and McCabe 1999).


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## Activation Function

We say that
An activation function $f(v)$ is antisymmetric if $f(-v)=-f(v)$

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## Example: The hyperbolic tangent



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## Target Values

## Important

- It is important that the target values be chosen within the range of the sigmoid activation function.


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## Important

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## Specifically

- The desired response for neuron in the output layer of the multilayer perceptron should be offset by some amount $\epsilon$


## For example

## Given the $a$ limiting value



## For example

## Given the $a$ limiting value



## We have then

- If we have a limiting value $+a$, we set $t=a-\epsilon$.


## For example

## Given the $a$ limiting value



## We have then

- If we have a limiting value $+a$, we set $t=a-\epsilon$.
- If we have a limiting value $-a$, we set $t=-a+\epsilon$.


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## Normalizing the inputs

## Something Important (LeCun, 1993)

Each input variable should be preprocessed so that:

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## Something Important (LeCun, 1993)

Each input variable should be preprocessed so that:

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## Example



## The normalization must include two other measures

## Uncorrelated

We can use the principal component analysis

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## Uncorrelated

We can use the principal component analysis

## Example



## In addition

## Quite interesting

- The decorrelated input variables should be scaled so that their covariances are approximately equal.


## In addition

## Quite interesting

- The decorrelated input variables should be scaled so that their covariances are approximately equal.


## Why?

- This makes that different synaptic weights in network to learn at approximately the same speed.


## There are other heuristics

- Initialization


## There are other heuristics

As

- Initialization
- Learning form hints


## There are other heuristics

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- Initialization
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- etc


## In addition

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- Network growing
- You start with a small network and add neurons and layers to accomplish the learning task.


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## In section 4.15, Simon Haykin

We have the following techniques:

- Network growing
- You start with a small network and add neurons and layers to accomplish the learning task.
- Network pruning
- Start with a large network, then prune weights that are not necessary in an orderly fashion.


## Outline

(1) Introduction

- The XOR Problem
(2) Multi-Layer Perceptron
- Architecture
- Back-propagation
- Gradient Descent
- Hidden-to-Output Weights
- Input-to-Hidden Weights
- Total Training Error
- About Stopping Criteria
- Final Basic Batch Algorithm
(3) Using Matrix Operations to Simplify
- Using Matrix Operations to Simplify the Pseudo-Code
- Generating the Output $z_{k}$
- Generating $z_{k}$
- Generating the Weights from Hidden to Output Layer
- Generating the Weights from Input to Hidden Layer
- Activation Functions
(4) Heuristic for Multilayer Perceptron
- Maximizing information content
- Activation Function
- Target Values
- Normalizing the inputs
- Virtues and limitations of Back-Propagation Layer


## Virtues and limitations of Back-Propagation Layer

## Something Notable

- The back-propagation algorithm has emerged as the most popular algorithm for the training of multilayer perceptrons.


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## It has two distinct properties

- It is simple to compute locally.
- It performs stochastic gradient descent in weight space when doing pattern-by-pattern training


## Connectionism

## Back-propagation

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## Back-propagation

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This constraint
It is known as the locality constraint

## Why this is advocated in Artificial Neural Networks

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The use of local computations permits a graceful degradation in performance due to hardware errors, and therefore provides the basis for a fault-tolerant network design.

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The use of local computations permits a graceful degradation in performance due to hardware errors, and therefore provides the basis for a fault-tolerant network design.

## Third

Local computations favor the use of parallel architectures as an efficient method for the implementation of artificial neural networks.

However, all this has been seriously questioned on the following grounds(Shepherd, 1990b; Crick, 1989; Stork, 1989)

## First

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## First

- The reciprocal synaptic connections between the neurons of a multilayer perceptron may assume weights that are excitatory or inhibitory.
- In the real nervous system, neurons usually appear to be the one or the other.


## Second

In a multilayer perceptron, hormonal and other types of global communications are ignored.

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## Third

- In back-propagation learning, a synaptic weight is modified by a presynaptic activity and an error (learning) signal independent of postsynaptic activity.

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## Fourth

- In a neurobiological sense, the implementation of back-propagation learning requires the rapid transmission of information backward along an axon.
- It appears highly unlikely that such an operation actually takes place in the brain.

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## Fifth

- Back-propagation learning implies the existence of a "teacher," which in the con text of the brain would presumably be another set of neurons with novel properties.

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## Fifth

- Back-propagation learning implies the existence of a "teacher," which in the con text of the brain would presumably be another set of neurons with novel properties.
- The existence of such neurons is biologically implausible.


## Computational Efficiency

## Something Notable

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Taking in account the total number of synapses, $W$ including biases
We have $\triangle w_{k j}=\eta \delta_{k} y_{j}=\eta\left(t_{k}-z_{k}\right) f^{\prime}\left(\right.$ net $\left._{k}\right) y_{j}$ (Backward Pass)

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## We have that for this step

(1) We need to calculate $n e t_{k}$ linear in the number of weights.
(2) We need to calculate $y_{j}=f\left(n e t_{j}\right)$ which is linear in the number of weights.

## Computational Efficiency

## Now the Forward Pass

$$
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## Clearly all this takes to have memory

In addition the calculation of the derivatives of the activation functions, but assuming a constant time.

## We have that

The Complexity of the multi-layer perceptron is

## $O(W)$ Complexity

## Exercises

We have from NN by Haykin
4.2, 4.3, 4.6, 4.8, 4.16, 4.17, 3.7

