# Machine Learning

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# **5.1. Multi-Layer Perceptron (MLP)**



- Feed-forward structure: inputs from the previous layer and outputs to the next layer
- Output layer: sigmoid activation function for classification problems and linear activation function for regression problems
- Figure: two-layer network (two layer of weights)

#### **Architecture of MLP (N-H-M): Forward Propagation**



# **5.2. Representational Power of MLP**

- MLP with two layers can represent arbitrary function
	- Each hidden unit represents a soft threshold function in the input space
	- Combine two opposite-facing threshold functions to make a ridge
	- Combine two perpendicular ridges to make a bump
	- Add bumps of various sizes and locations to fit any surface



- Universal approximator
	- Given a sufficiently large number of hidden units , a two layer (linear output) network can approximate any continuous function on a compact input domain to arbitrary accuracy.

#### **5.3. Training of MLP : Error Back-Propagation Algorithm**

**of MLP**<br>  $\begin{aligned} &\frac{1}{2}, x_2, \cdots, \\ &\frac{1}{2}, y_2, \cdots, \\ &\frac{1}{2} \text{cot} \mathbf{r} \cdot \mathbf{t} = \\ &\frac{1}{2} \sum_{k=1}^{2} \left( \frac{1}{2} \sum_{k=1}^{2} \mathbf{r}^k \right) \mathbf{r}^k. \end{aligned}$ **MLP :**<br> $x_2, \dots, x_N$ <br> $y_1, y_2, \dots,$ <br> $y_k$ )<sup>2</sup><br> $\delta_k^{(out)} h_j$ The  $\left[\begin{array}{c} \mathbf{Error} \\ \mathbf{y} \end{array}\right]^{T}$ <br>  $\left[\begin{array}{c} \mathbf{y}_{M} \end{array}\right]^{T}$ <br>  $\mathbf{y}_{M}$  is the sum where 2  $1 \qquad \qquad$ **MLP : Error Back-F**<br>  $\begin{bmatrix} y_2, \cdots, x_N \end{bmatrix}^T$ <br>  $\begin{bmatrix} y_2, \cdots, y_M \end{bmatrix}^T$ <br>  $\begin{bmatrix} \mathbf{t} = [t_1, t_2, \cdots, t_M]^T \end{bmatrix}^T$ <br>
unction:<br>  $\begin{bmatrix} y_1^{(out)} & \mathbf{h}_j \end{bmatrix}^T$  where  $\delta_k^{(out)} = \begin{bmatrix} y_1^{(hid)} & x_i \end{bmatrix}^T$  where  $\delta_j^{(hid)} = \begin{$ **5.3. Training of MLP : Error Back-P**<br>
Input Pattern:  $\mathbf{x} = [x_1, x_2, \dots, x_N]^T$ <br>
Output Vector:  $\mathbf{y} = [y_1, y_2, \dots, y_M]^T$ <br>
Desired Output Vector:  $\mathbf{t} = [t_1, t_2, \dots, t_M]^T$ <br>
Mean-Squared Error Function:<br>  $E_m(\mathbf{x}) = \frac{1}{2} \sum_{$ **5.3. Training of MLP :**<br>
Input Pattern:**x** = [ $x_1, x_2, \dots, x_i$ <br>
Output Vector: **y** = [ $y_1, y_2, \dots$ <br>
Desired Output Vector: **t** = [*t*<br>
Mean-Squared Error Functio:<br>  $E_m(\mathbf{x}) = \frac{1}{2} \sum_{k=1}^{M} (t_k - y_k)^2$ <br>  $\Delta v_{kj} = -\eta \frac{\partial E_m(\mathbf$ ing of MLP : Error Back-Propag<br>  $\mathbf{x} = [x_1, x_2, \dots, x_N]^T$ <br>  $\therefore \mathbf{y} = [y_1, y_2, \dots, y_M]^T$ <br>
at Vector:  $\mathbf{t} = [t_1, t_2, \dots, t_M]^T$ <br>  $\mathbf{d}$  Error Function:<br>  $\frac{d}{dt} (t_k - y_k)^2$ <br>  $(\mathbf{x}) = \eta \delta_k^{(out)} h_j$  where  $\delta_k^{(out)} = -\frac{\partial E_m(t_k)}{\partial \hat{$ *T*  $\mathbf{x} = [x_1, x_2, \cdots, x_N]^T$ *T*  $\mathbf{y} = [y_1, y_2, \cdots, y_M]^{T}$  $T$  –  $\frac{2}{9}$ <sup>6,025</sup>  $M$  **J** *M* **.3. Training of MLF**<br>the Pattern: **x** = [ $x_1, x_2, \cdots$ <br>put Vector: **y** = [ $y_1, y_2, \cdots$ <br>ired Output Vector: **t** =<br> $\ln$ -Squared Error Funct<br> $m(\mathbf{x}) = \frac{1}{2} \sum_{k=1}^{M} (t_k - y_k)^2$ <br> $= -\eta \frac{\partial E_m(\mathbf{x})}{\partial v_{kj}} = \eta \delta_k^{(out)}$ <br> $= -\eta \frac{\partial E_m$ **5.3. Training of MLP : Error Back-Propagatic**<br>
out Pattern:**x** = [ $x_1, x_2, \dots, x_N$ ]<sup>*r*</sup><br>
ttput Vector: **y** = [ $y_1, y_2, \dots, y_M$ ]<sup>*r*</sup><br>
sired Output Vector: **t** = [ $t_1, t_2, \dots, t_M$ ]<sup>*r*</sup><br>
sinced Output Vector: **t** = [ $t_1, t_$ *kj* of MLP : Error<br> *x*<sub>1</sub>, *x*<sub>2</sub>, ···, *x<sub>N</sub>*]<sup>*T*</sup><br>
= [*y*<sub>1</sub>, *y*<sub>2</sub>, ···, *y<sub>M</sub>*]<sup>*T*</sup><br>
= ctor: **t** = [*t*<sub>1</sub>, *t*<sub>2</sub>, ···<br>
or Function:<br>  $-y_k$ )<sup>2</sup><br>
=  $\eta \delta_k^{(out)} h_j$  wher **f MLP : Error E**<br>  $x_2, \dots, x_N$ ]<sup>T</sup><br>  $y_1, y_2, \dots, y_M$ ]<sup>T</sup><br>
(or: **t** = [ $t_1, t_2, \dots, t_k$ <br>
Function:<br>  $y_k$ )<sup>2</sup><br>  $\eta \delta_k^{(out)} h_j$  where  $\delta_k$ <br>  $\eta \delta_j^{(hid)} x_i$  where  $\delta_k$ **: Error Bac**<br> $\begin{bmatrix} t_N \end{bmatrix}^T$ <br> $t_1, t_2, \dots, t_M \end{bmatrix}^T$ <br>on:<br>where  $\delta_k^{(out)}$ <br>where  $\delta_j^{(hid)}$ **5.3. Training of MLP : Error Back-Propagation**<br>
pput Pattern: $\mathbf{x} = [x_1, x_2, \dots, x_N]^T$ <br>
vutput Vector:  $\mathbf{y} = [y_1, y_2, \dots, y_M]^T$ <br>
essired Output Vector:  $\mathbf{t} = [t_1, t_2, \dots, t_M]^T$ <br>
flean-Squared Error Function:<br>  $E_m(\mathbf{x}) = \$ **Training of MLP : Error Back-Propagation Algorithm**<br>
attern:**x** = [ $x_1, x_2, \dots, x_N$ ]<sup>T</sup><br>
Vector: **y** = [ $y_1, y_2, \dots, y_M$ ]<sup>T</sup><br>
(Output Vector: **t** = [ $t_1, t_2, \dots, t_M$ ]<sup>T</sup><br>
(Output Vector: **t** = [ $t_1, t_2, \dots, t_M$ ]<sup>T</sup><br>
( $\theta$ )<br>  $=1$  ${\bf t} = [t_1, t_2, \cdots]$ **5.3. Training of MLP : Error Back-Propagation Algorithm**<br>
Input Pattern:**x** = [ $x_1, x_2, \dots, x_N$ ]<sup>T</sup><br>
Output Vector: **y** = [ $y_1, y_2, \dots, y_M$ ]<sup>T</sup><br>
Desired Output Vector: **t** = [ $t_1, t_2, \dots, t_M$ ]<sup>T</sup><br>
Mean-Squared Error Functio **x**) =  $\frac{1}{2}$   $\sum (t_k - y_k)^2$ **x**) **Training of MLP : Error Back-Propagatio**<br>
Pattern:**x** =  $[x_1, x_2, \dots, x_n]^T$ <br> **t** Vector: **y** =  $[y_1, y_2, \dots, y_M]^T$ <br> **d** Output Vector: **t** =  $[t_1, t_2, \dots, t_M]^T$ <br> **Squared Error Function:**<br> **x**) =  $\frac{1}{2} \sum_{k=1}^M (t_k - y_k)^2$ <br>  $-\$  $\frac{1}{2} \sum_{k=1}^{M} (t_k - y_k)^2$ <br> $\frac{E_m(\mathbf{x})}{\partial v_k} = \eta \delta_k^{(out)} h_j$  where ALP : Error Back-Propagation Algorithm<br>  $y_2, ..., y_M$ <sup>T</sup><br>  $t = [t_1, t_2, ..., t_M]$ <sup>T</sup><br>
( $t = [t_1, t_2, ..., t_M]$ <sup>T</sup><br>
(metion:<br>  $y^2$ <br>
(mai)  $h_j$  where  $\delta_k^{(out)} = -\frac{\partial E_m(\mathbf{x})}{\partial \hat{y}_k} = (t_k - y_k) f'(\hat{y}_k)$ <br>
(hid)  $x_i$  where  $\delta_j^{(hid)} = -\frac{\partial E_m(\mathbf{x$  $\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$ on Algorithm<br>
<br>
(  $(t_k - y_k) f'(\hat{y}_k)$ <br>  $f'(\hat{h}_j) \sum_{k=1}^M v_{kj} \delta_k^{(out)}$  $\hat{\mathbf{y}}_k$ ng of MLP : Error Back-Propagation<br>  $x = [x_1, x_2, \dots, x_N]^T$ <br>  $\vdots y = [y_1, y_2, \dots, y_M]^T$ <br>  $\vdots y = [y_1, y_2, \dots, y_M]^T$ <br>  $\vdots$   $\vdots$  $\hat{h}$ Error Back-Propagation Algorit<br>  $\begin{pmatrix} y_M \end{pmatrix}^T$ <br>  $\begin{pmatrix} y_M \end{pmatrix}^T$ <br>  $\begin{pmatrix} y_M \end{pmatrix}^T$ <br>  $\begin{pmatrix} y_M \end{pmatrix}^T$ <br>  $\begin{pmatrix} y_M \end{pmatrix}^T = \frac{\partial E_m(\mathbf{x})}{\partial \hat{y}_k} = (t_k - y_k) f'(\mathbf{x})$ <br>
where  $\delta_j^{(mid)} = -\frac{\partial E_m(\mathbf{x})}{\partial \hat{h}_j} = f'(\hat{h}_j) \sum_{k=$ **Algorithm**<br> **k**  $\theta$  *M* **ing of MLP : Error Back-Propagation Algorithm**<br>  $\mathbf{x} = [x_1, x_2, \dots, x_N]^T$ <br>  $\text{or: } \mathbf{y} = [y_1, y_2, \dots, y_M]^T$ <br>  $\text{at Vector: } \mathbf{t} = [t_1, t_2, \dots, t_M]^T$ <br>  $\text{d Error Function:}$ <br>  $\sum_{k=1}^M (t_k - y_k)^2$ <br>  $\sum_{v_{kj}}^m (x_k - y_k)^2 = \eta \delta_k^{(out)} h_j$  where  $\delta_k^{(out)}$ **j.3. Training of MLP : Error Back-Propagation Algorithm**<br>
ut Pattern:**x** = [ $x_1, x_2, \dots, x_N$ ]<sup>*r*</sup><br>
tput Vector: **y** = [ $y_1, y_2, \dots, y_M$ ]<sup>*r*</sup><br>
sired Output Vector: **t** = [ $t_1, t_2, \dots, t_M$ ]<sup>*r*</sup><br>
an-Squared Error Function:<br>  $\frac{E_m(\mathbf{x})}{\partial w_{ji}} = \eta \delta_j^{(hid)} x_i$  where  $\delta_j^{(hid)} = -\frac{\partial E_m(\mathbf{x})}{\partial \hat{h}_j} = f'(\hat{h}_j) \sum_{k=1}^M v_{kj} \delta_k$ *t y f y* **5.3. Training of MLP : Error Back-Propagation Algorithm**<br> *y wutput Vector:*  $\mathbf{y} = [x_1, x_2, \dots, x_N]^T$ *<br>
<i>y w w westerd Output Vector:*  $\mathbf{t} = [t_1, t_2, \dots, t_M]^T$ *<br> E <i>w w*  $\mathbf{y} = -\eta \frac{\partial E_m(\mathbf{x})}{\partial v_{ij}} = \eta \delta_i^{(wa)} h$ **5.3. Training of MLP : Error Back-Propagation Algorithm**<br>
Input Pattern:**x** = [ $x_1, x_2, \dots, x_N$ ]<sup>T</sup><br>
Output Vector: **y** = [ $y_1, y_2, \dots, y_M$ ]<sup>T</sup><br>
Desired Output Vector: **t** = [ $t_1, t_2, \dots, t_M$ ]<sup>T</sup><br>
Mean-Squared Error Functio **x**) **x** =  $[x_1, x_2, \dots, x_N]^T$ <br> **y** =  $[y_1, y_2, \dots, y_M]^T$ <br> **y** =  $[y_1, y_2, \dots, y_M]^T$ <br>
Vector: **t** =  $[t_1, t_2, \dots, t_M]^T$ <br>
Error Function:<br>  $(t_k - y_k)^2$ <br> **x**) =  $\eta \delta_k^{(out)} h_j$  where  $\delta_k^{(out)} = -\frac{\partial E_m(\mathbf{x})}{\partial \hat{y}_k} = (t_k - \frac{\mathbf{x}}{i}) = \eta \delta_j^{(mid)} x_i$  $(y_k) f'(\hat{y}_k)$  $\partial \hat{y}_k$ **Training of MLP : Error Back-Propagatic**<br>
<sup>2</sup> attern:**x** = [ $x_1, x_2, ..., x_N$ ]<sup>*T*</sup><br> **1** Output Vector: **t** = [ $t_1, t_2, ..., t_M$ ]<sup>*T*</sup><br> **5** Squared Error Function:<br> **x**) =  $\frac{1}{2} \sum_{k=1}^{M} (t_k - y_k)^2$ <br>  $-\eta \frac{\partial E_m(\mathbf{x})}{\partial v_{kj}} = \eta \delta_k$ 





#### **5.4. Incorrect Saturation of Output Nodes**



$$
\delta_k \equiv -\frac{\partial E_{MSE}}{\partial \hat{y_k}} = (t_k - y_k) f'(\hat{y_k})
$$
\n(5.3.4)

Correct Saturation  $y_k \approx t_k, \delta_k \approx 0$ 

Incorrect Saturation

\nIf 
$$
y_k \approx \pm 1
$$
 and  $t_k = \mp 1$ ,  $\delta_k \approx 0$  although  $|t_k - y_k| \approx 2$ 

Incorrect Saturation of Output Nodes  $\rightarrow$  Very Slow Convergence of Learning due to  $\delta_k \approx 0$ 

# **Training of MLP : Error Back-Propagation Algorithm**

$$
\delta_k^{out}(\mathbf{x}) = (t_k - y_k) f'(\hat{y}_k)
$$

. Incorrect Saturation Problem

**Training of MLP**: **E**  
\n
$$
\text{conv. MSE}
$$
  
\n $S_k^{out}(\mathbf{x}) = (t_k - y_k)f'(\hat{y}_k)$   
\nIncorrect Saturation Problem  
\n $E_m(\mathbf{x}) = \frac{1}{2} \sum_{k=1}^{M} (t_k - y_k)^2$   
\n $\text{Cross-Entropy Error} >$   
\n $S_k^{out}(\mathbf{x}) = (t_k - y_k)$   
\nOverspecialization Problem  
\n $E_{cur}(\mathbf{x}) = -\sum_{k=1}^{M} [(1+t_k) \ln(1 + y_k(\mathbf{x})) + (1-t_k)]$ 

$$
\delta_k^{out}(\mathbf{x}) = (t_k - y_k)
$$

. Overspecialization Problem

**Training of MLP : Error Back-Pre**  
\n
$$
\begin{array}{ll}\n<\n\text{conv. MSE} >\n\\
<\n\delta_k^{out}(\mathbf{x}) = (t_k - y_k)f'(\hat{y}_k) \\
<\n\text{Incorrect Saturation Problem} \\
&E_m(\mathbf{x}) = \frac{1}{2} \sum_{k=1}^M (t_k - y_k)^2 \\
<\n\text{Cross-Entropy Error} >\n\delta_k^{out}(\mathbf{x}) = (t_k - y_k) \\
<\n\text{overspecialization Problem} \\
&E_{CE}(\mathbf{x}) = -\sum_{k=1}^M \left[ (1 + t_k) \ln(1 + y_k(\mathbf{x})) + (1 - t_k) \ln(1 - y_k(\mathbf{x})) \right] \\
<\n\delta_k^{out}(\mathbf{x}) = \frac{t_k^{n+1}(t_k - y_k)^n}{2^{n-1}} \\
&E_{nCE} = -\sum_{k=1}^M \int \frac{t_k^{n+1}(t_k - y_k)^n}{2^{n-2}(1 - y_k)(1 + y_k)} dy_k\n\end{array}
$$

 $\langle$  n-th order Extension of CE  $>$ 

$$
\delta_k^{out}(\mathbf{x}) = \frac{t_k^{n+1}(t_k - y_k)^n}{2^{n-1}}
$$

$$
<
$$
n-th order Extension of CE>
$$
S_k^{out}(\mathbf{x}) = \frac{t_k^{n+1} (t_k - y_k)^n}{2^{n-1}}
$$

$$
E_{nCE} = -\sum_{k=1}^{M} \int \frac{t_k^{n+1} (t_k - y_k)^n}{2^{n-2} (1 - y_k)(1 + y_k)} dy_k
$$



## **Error Back-Propagation Algorithm**









그림 57 필기체 숫자인식 문제의 학습 시뮬레이션 결과

예제 5.4-1

아래 그림으로 2차원 공간 상에 주어진 XOR 문제를 입력 2, 은닉노드 4, 출력 1개의 노드를

지년 다ت�에  
지년 다종파레트론으로 학'   
하가 위해여 초기 가중치를 
$$
\boldsymbol{W} = \begin{pmatrix} w_{10} \, w_{11} \, w_{12} \\ w_{20} \, w_{21} \, w_{22} \\ w_{30} \, w_{31} \, w_{32} \\ w_{40} \, w_{41} \, w_{42} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0.5 \\ 0 & 1 & 0.9 \\ 0 & 0.5 & 1 \end{pmatrix} \mathfrak{L}
$$

\n
$$
\mathbf{v} = (v_0, v_1, v_2, v_3, v_4) = (0, 0.3, 0.6, 0.9, 1.2)
$$
로 촠기회  $\mathbf{v}^4 = (1, 1)$  하였다고 가정하였다. 출력 목표! 1qは  $\mathbf{v}^1$ 과  $\mathbf{v}^4$ 에 대한 서만 −1이고 입력  $\mathbf{v}^2$ ,  $\mathbf{v}^3$ 에 대해서는 1이다. 4개의 입력 중 임의의 하나를 골라서 다승파з의 떘이어  
\nMSE, CE, nCE(n=2) 오차함수에 마른 출력노드와 첫  
\n $\mathbf{v}^2 = (1, 0)$ 은나노드의 오류신호를 구하여 보아라.\n



# **5.5. Remarks on Training**

- Convergence(?)… may oscillate or reach a local minima.
- Many epochs (thousands) may be needed for adequate training
- Termination criteria:
	- Fixed number of training epochs
	- Threshold on error of training samples
	- Increasing of error on a validation samples
- For better performance, run several trials starting from different initial random weights
	- Take the result with the best training or validation performance.
	- Build a committee of networks (ensemble technique)…Chapter 8

Data Set From  $RC$ vanny E(Validation set)<br>E(training set)  $5 - 2$ 

# **Initialization of Weights**



- Initialization of weights such that nodes are in the "linear" regions
	- To avoid the premature saturation problem
	- Keep all weights near zero, so that all sigmoid units are in their linear regions. Otherwise nodes can be initialized into flat regions of the sigmoid causing for very small gradients.⇒ Premature Saturation Problem
- Break symmetry

– Each hidden node should have different input weights so that the hidden nodes move in different directions.

## **Online, Batch and Learning with Momentum**

- **Online**: Take a gradient descent step with each input
- **Batch**: Sum the gradient for each example *i*. Then take a gradient descent step
- **Momentum factor**: Make the  $t+1$ -th update dependent on the  $t$ -th update

 $\varDelta v_{kj}(t)=\eta\delta_kh_j+\alpha\varDelta v_{kj}(t-1)$  $\Delta w_{ii}(t) = \eta \delta_i^{(hidden)} x_i + \alpha \Delta w_{ii}(t-1)$ 

- to keep weight moving in the same direction and improves convergence

# **Overtraining Prevention**

• Too many epochs  $\rightarrow$  over-train the network



- Use a validation set to test accuracy in some intervals of epochs
- Stop the training when the performance on the validation set decreases
- 10-fold cross-validation

# **Over-fitting Prevention**

- Too few hidden units prevent the system from adequately fitting the data and learning the concept.
- Too many hidden units leads to over-fitting.



- Trial and error
- Another approach to preventing over-fitting is **weight decay**

## **5.6. Learning Time Series Data**

• Time-delay neural networks (TDNN)



#### **5.7. Deep Neural Networks**







8

10

 $\ge 10^{-9}$ 













 $\mathcal{L}$ 

 $\mathcal{L}$ 

 $\mathcal{L}$ 

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 $\mathcal{A}$ 

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 $\mathcal{A}$ 

 $\epsilon$ 

 $\epsilon$ 

 $\mathcal{A}$ 

 $\mathcal{L}$ 



GELU는 ReLU를 매끄러운 모양으로 만들은 형태 이다. GELU는 단조함수가 아니며 모든 지점에서 곡률을 지닌 것이 ReLU 및 ELU와 다른 특징이다. 이 특징이 GELU가 ReLU 및 ELU보다 더 뛰어난 학 습 성능을 지니도록 해준다[18].

 $\sim$ 

#### 예제 5.7-1

그림 5.10과 같이 심층신경회로망이 주어졌다.  $h_i^{(l)}(l=,1,2,,.,L)$ 과 아래층 사이의 연결 가 중치를  $w_{ii}^{(l)}(l=,1,2,,.,L)$ 이라 하고 마지막층 출력노드  $y_k$ 와 아래층  $h_i^{(L)}$  사이의 연결 가 중치를  $v_{kj}$  라고 할 때, 정방향 전파의 계산 과정을 적어보아라. 또한, 출력노드의 오류신호 가  $\delta_k = t_k - y_k$ 로 주어지면 역방향 전파에 의한 은닉노드의 오류신호를 적어보아라.

#### 예제 5.7-2

SoftMax 함수는 벡터 요소들 중에서 큰 값은 더 크게, 작은 값은 더 작게 상대적으로 조정 하며 그 값들의 합은 1이 되게 한다. SoftMax 함수에 4차원 벡터 [4 10 6 5]가 입력되었을 때, SoftMax 함수를 통과한 후의 4차원 벡터를 구하여 보아라.

#### **5.8. Radial Basis Function Networks**

• Locally-tuned units:





#### **Local vs. Distributed Representation**



# **Training RBF Network**

- Hybrid learning
	- First layer centers and spreads (Unsupervised k-means)
	- Second layer weights (Supervised gradient descent)
- Fully supervised

•Similar to backpropagation in MLP, gradient descent for all parameters

## **RBF Network: Fully Supervised Method**

• Similar to backpropagation in MLP



## **RBF Network: Fully Supervised Method**

• Similar to backpropagation in MLP



