## CZ4041/SC4000: Machine Learning

#### **Lesson 7: Artificial Neural Networks**

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#### **Instructor's Information**

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## **Full-time Arrangement**

- > Lectures
  - ≥3.30-5.30pm on Thursdays, LT2A
  - ➤ Weeks 7-12
- > Tutorials
  - ➤ 3.30-4.30pm on Mondays, LT2A
  - > Weeks 9, 11 and 13
  - ➤ Week 12 (3.30-4.30pm, 4 Apr), guest lecture from GovTech: Analysing Feedback on Municipal Issues with NLP and Deep Learning.

## Part-time Arrangement

- Lectures & QA sessions
  - ► 6.30-8.30pm on Thursdays, TR+3.
  - ➤ Weeks 8-13
  - > 1-hour review, followed by one hour of QA
  - It is highly recommended that you watch the lecture & tutorial videos uploaded in the previous week.

### I have questions ...

- Full-time students: Find me after the tutorials (but not the lectures)
- Part-time students: Dedicated QA time on Thursdays
- Send questions via email <u>boyang.li@ntu.edu.sg</u> or via Microsoft Teams
- Make an appointment

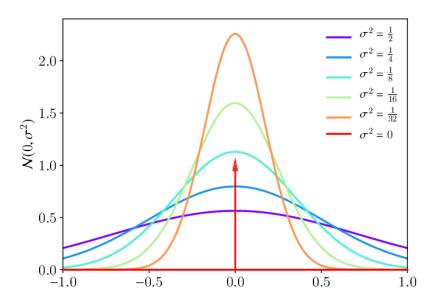
- ➤ Make Accurate Predictions
  - ➤ Which team will win a soccer match?
  - ➤ Which stock will see its price skyrocket?
  - ➤ Which patient is at higher risk?
- ➤ Usually it is difficult to write down rules manually
- Rather, we learn to make the predictions from paired data  $(x_i, y_i)$

- ➤ Make Accurate Predictions
  - ➤ Artificial Neural Networks (Week 7)
  - ➤ Support Vector Machines (Week 8)
  - ➤ Regression (Week 8)
  - ➤ Ensemble Learning (Week 9)

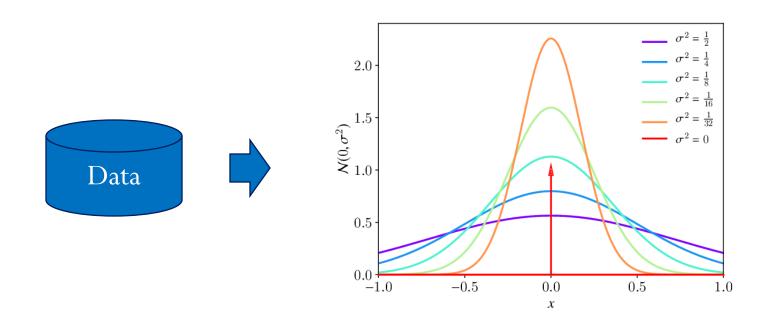
- ➤ Model Uncertainty
  - Germany will probably beat Japan, but what are the odds? 60/40, 70/30, or 80/20?
  - ➤ I'm willing to bet more money if the odds are in my favor.

➤ Often translates to: what is the shape of the

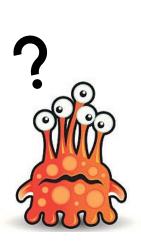
probability distribution?



- ➤ Model Uncertainty
  - ➤ Density Estimation (Week 11)



- > Pattern Discovery
  - Imagine you are an alien from another planet. You watch a soccer match. What do you observe?
  - Two groups of humans. One ball.
  - ➤ Behavior change when the ball goes into the net.





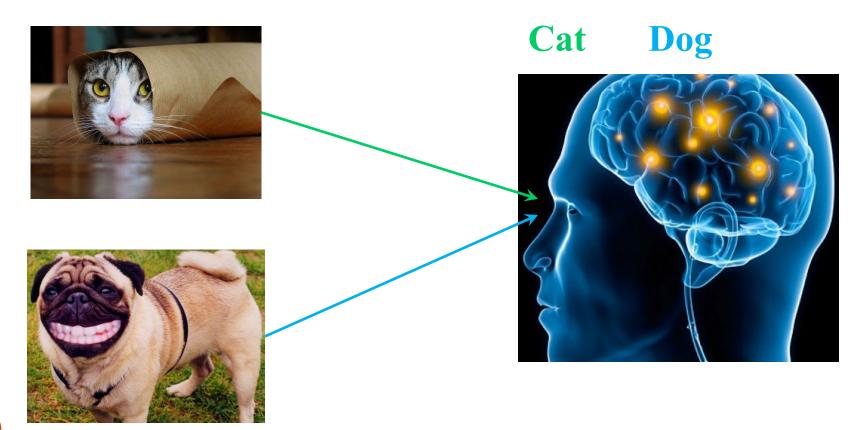
- > Pattern Discovery
  - ➤ We often have little prior experience, knowledge, or insight into the causal mechanisms that generated the data.
  - Still, with only statistical tools, we can identify many important data characteristics
  - ➤ Obviously, domain knowledge can enrich and complement statistical tools.

- > Pattern Discovery
  - ➤ Clustering (Week 10)
  - ➤ Dimensionality Reduction (Week 12)

# **Artificial Neural Networks: Perceptron**

## Artificial Neural Networks (ANN)

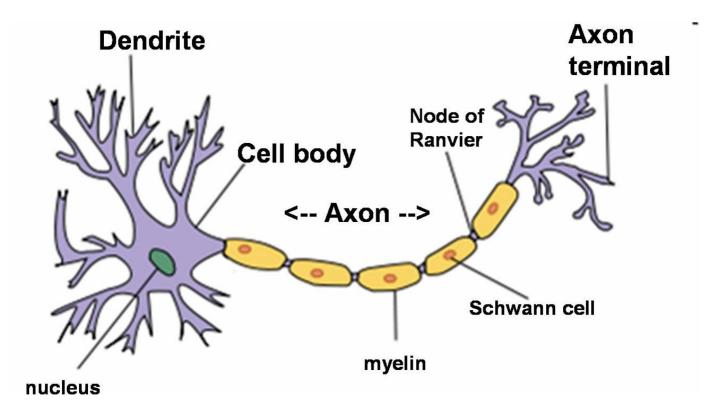
• The study of ANN was inspired by biological neural systems



## "Biology"

- Human brain is a densely interconnected network of neurons, connected to others via dendrites and axons.
- Dendrites and axons transmit electrical signals from one neuron to another
- The human brain learns by changing the strength of the synaptic connection between neurons
- An ANN is composed of an interconnected assembly of nodes and directed links.

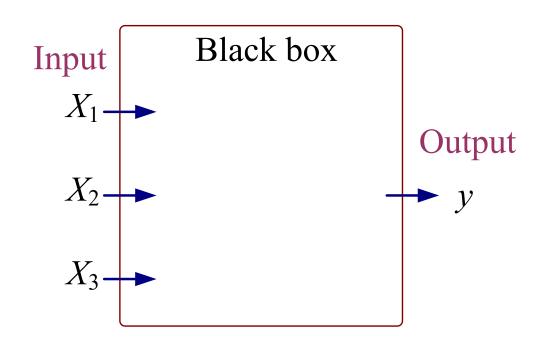
## "Biology"



• A neuron sends out a spike from the axon after receiving enough input from the dendrites.

## Artificial Neural Networks (cont.)

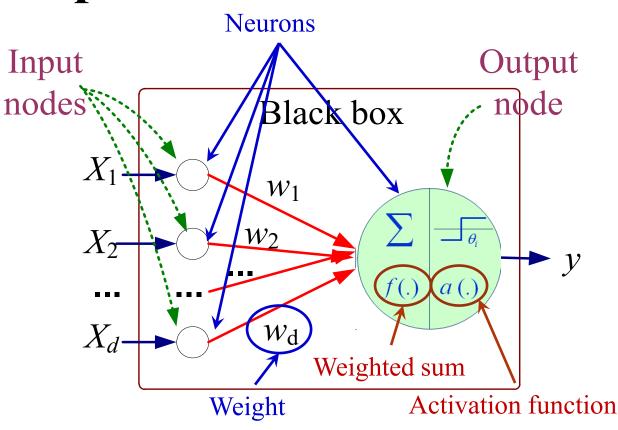
$X_1$	$X_2$	$X_3$	у
1	0	0	-1
1	0	1	1
1	1	0	1
1	1	1	1
0	0	1	-1
0	1	0	-1
0	1	1	1
0	0	0	-1



Output y is 1 if at least two of the three inputs are equal to 1

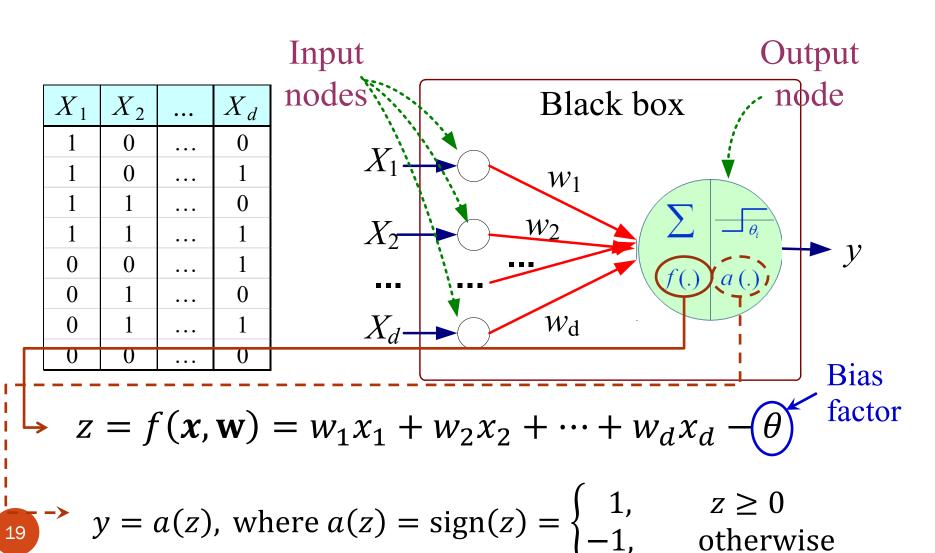
## **ANN: Perceptron**

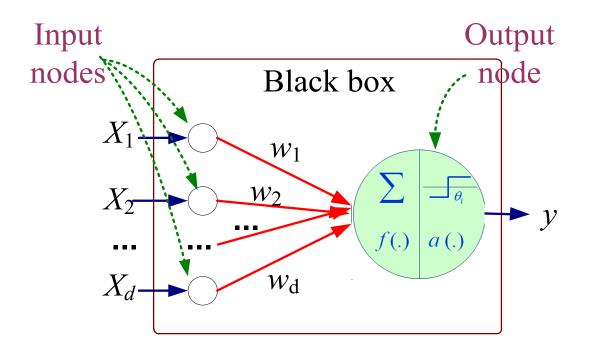
$X_1$	$X_2$	•••	$X_d$
1	0	• • •	0
1	0	• • •	1
1	1	• • •	0
1	1	• • •	1
0	0	• • •	1
0	1	• • •	0
0	1	• • •	1
0	0	•••	0



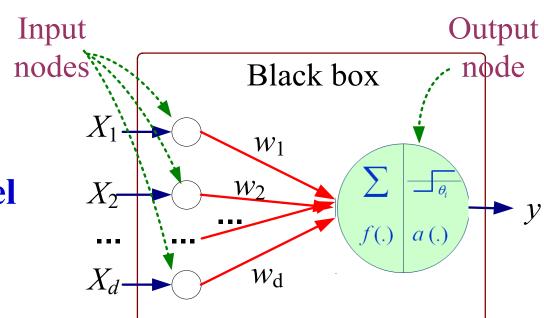
Each input node is connected via a weighted link to the output node. Weights can be positive, negative or zero (no connection)

## ANN: Perceptron (cont.)





- Model is an assembly of inter-connected nodes and weighted links
- Output node first sums up each of its input value according to the weights of its links
- Compare the weighted sum against some threshold  $\theta$
- Produce an output based on the sign of the result



#### **Perceptron Model**

$$z = \sum_{i=1}^{d} w_i x_i - \theta \longrightarrow y = a(z) = \text{sign}(z)$$

$$y = \text{sign}\left(\sum_{i=1}^{d} w_i x_i - \theta\right)$$

## ANN: Perceptron (cont.)

• Mathematically, the output of a perceptron model can be expressed in a more compact form

#### **Inner Product: Review**

• Given two vectors  $\boldsymbol{x}$  and  $\boldsymbol{z}$ , which are both of d dimensions, the <u>inner product</u> between  $\boldsymbol{x}$  and  $\boldsymbol{z}$  is defined as

$$\mathbf{x} \cdot \mathbf{z} = \sum_{i=1}^{d} x_i z_i$$

$$\mathbf{x} = (x_1, x_2, ..., x_d)$$
  $\mathbf{z} = (z_1, z_2, ..., z_d)$ 

## ANN: Perceptron (cont.)

$$y = \operatorname{sign}(\mathbf{w} \cdot \mathbf{x})$$

$$\mathbf{w} = (x_0, x_1, x_2, \dots, x_d)$$

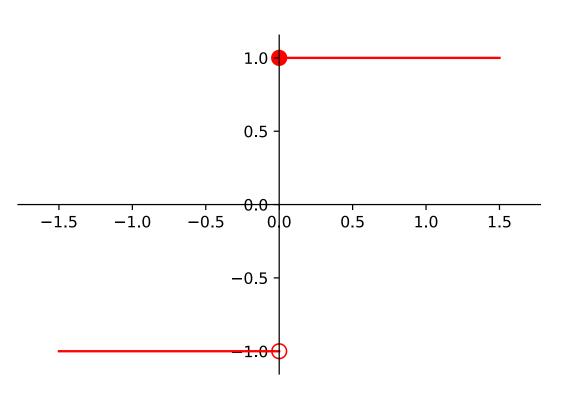
$$\mathbf{w} = (w_0, w_1, w_2, \dots, w_d)$$

$$\mathbf{w} \cdot \mathbf{x} = \sum_{i=0}^{d} (w_i x_i) = \sum_{i=1}^{d} (w_i x_i) + (w_0 x_0)$$

$$w_0 = -\theta, \text{ and } x_0 = 1$$

$$y = \operatorname{sign}\left(\sum_{i=1}^{d} w_i x_i - \theta\right) \longleftrightarrow y = \operatorname{sign}(\mathbf{w} \cdot \mathbf{x})$$

## **ANN: Sign Function**



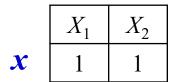
$$\operatorname{sign}(z) = \begin{cases} 1, z \ge 0 \\ -1, z < 0 \end{cases}$$

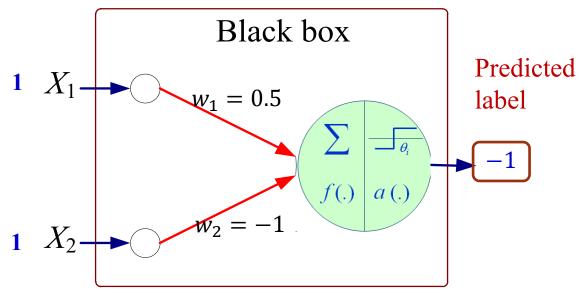
Note: the sign(z) function has derivative = 0everywhere, except at z = 0.

## Perceptron: Making Prediction

• Given a learned perceptron with  $w_1 = 0.5$ ,  $w_2 = -1$ , and  $\theta = 0$ 

#### Test data:

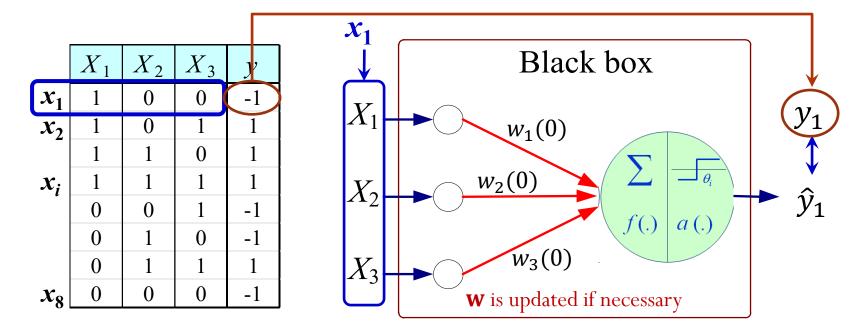


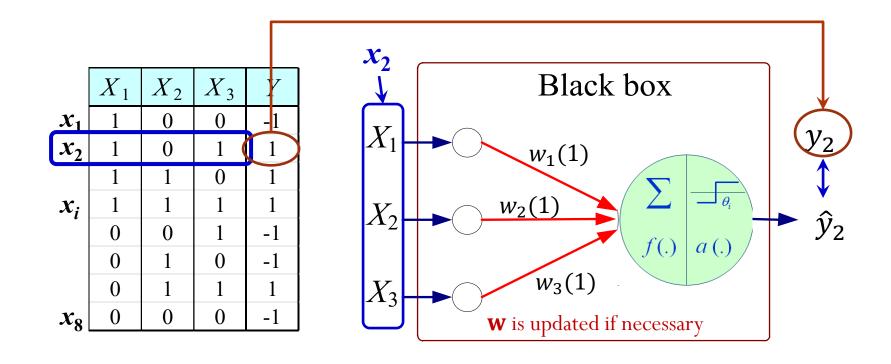


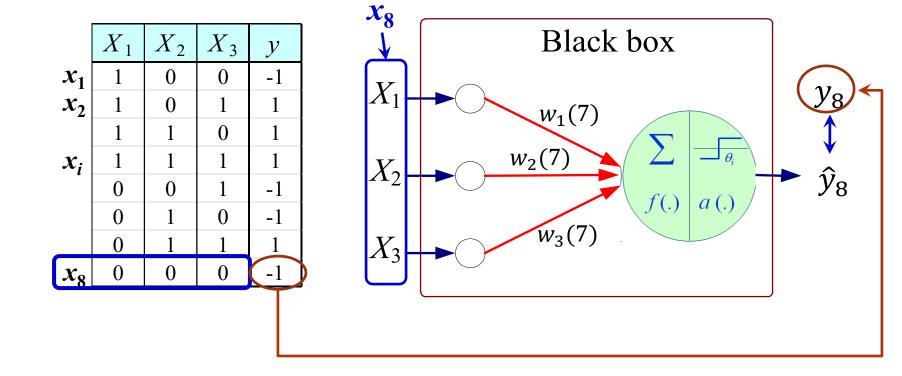
$$y = sign(1 \times 0.5 + 1 \times (-1))$$
  
=  $sign(-0.5) = -1$ 

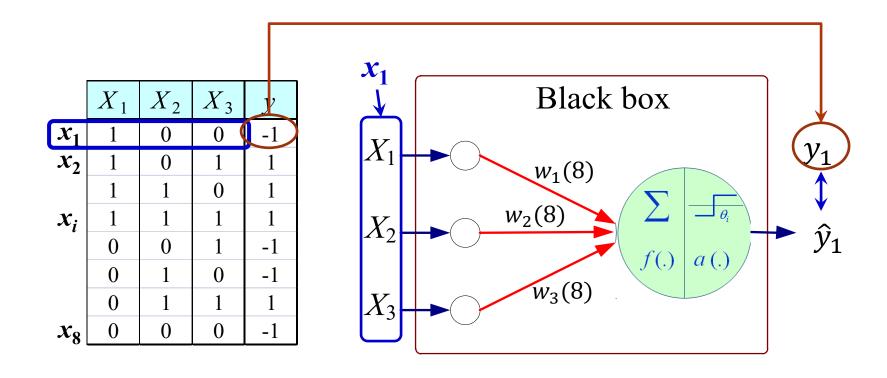
## **Perceptron: Learning**

- During training, the weight parameters **w** are adjusted until the outputs of the perceptron become consistent with the true outputs of training data
- The weight parameters **w** are updated iteratively or in an online learning manner







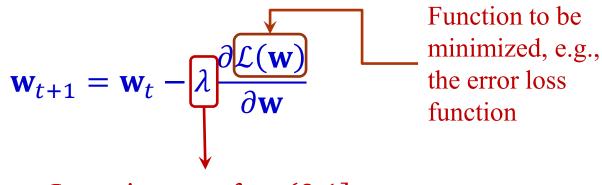


- Algorithm:  $\int_{0}^{\infty} d \operatorname{dimensions}$
- 1. Let  $D = \{(x_i, y_i) \mid i = 1, 2, ..., N\}$  be the set of training examples, t = 0
- 2. Initialize **w** with random values  $\mathbf{w}_0$
- 3. Repeat
- 4. for each training example  $(x_i, y_i)$  do
- 5. Compute the predicted output  $\hat{y}_i$
- 6. Update  $\mathbf{w}_t$  by  $\mathbf{w}_{t+1} = \mathbf{w}_t + \lambda(y_i \hat{y}_i)\mathbf{x}_i$
- 7. t = t + 1
- 8. end for
- 9. Until stopping condition is met

• Why use the following weight update rule?

$$\mathbf{w}_{t+1} = \mathbf{w}_t + \lambda (y_i - \hat{y}_i) \mathbf{x}_i$$

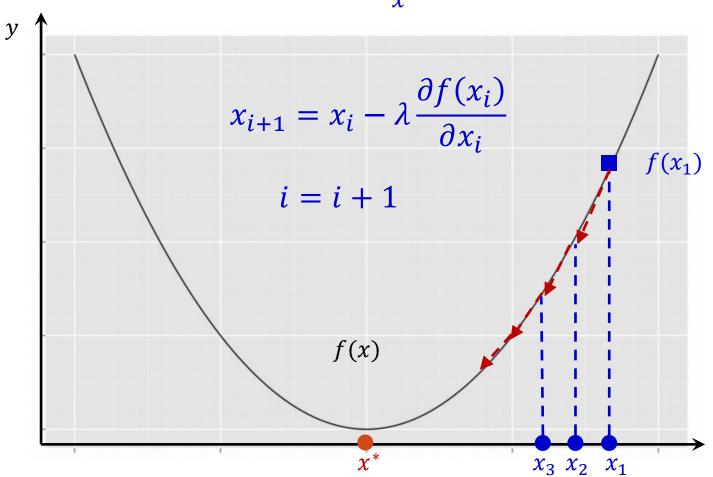
Induced based on a gradient descent method



Learning rate  $\lambda \in (0,1]$ 

#### **Gradient Descent**

$$x^* = \arg\min_{x} f(x)$$



Weight update rule

$$\mathbf{w}_{t+1} = \mathbf{w}_t + \lambda (y_i - \hat{y}_i) \mathbf{x}_i$$

• Weight update rule
$$\mathbf{w}_{t+1} = \mathbf{w}_t + \lambda(y_i - \hat{y}_i)\mathbf{x}_i \qquad \mathbf{w}_{t+1} = \mathbf{w}_t - \lambda \frac{\partial \mathcal{L}(\mathbf{w})}{\partial \mathbf{w}}$$

• Consider the loss function  $\mathcal{L}$  for each training example as  $e_i \triangleq y_i - \hat{y}_i$   $\hat{y}_i = \text{sign}(\mathbf{w}_t \cdot \mathbf{x}_i)$ 

$$\mathcal{L} = \frac{1}{2}e_i^2 = \frac{1}{2}(y_i - \hat{y}_i)^2 = \frac{1}{2}(y_i - \operatorname{sign}(\mathbf{w}_t \cdot \mathbf{x}_i))^2$$

Update the weight using a gradient descent method

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \lambda \frac{\partial \mathcal{L}(\mathbf{w})}{\partial \mathbf{w}} = \mathbf{w}_t - \lambda \underbrace{\frac{\partial \mathcal{L}(\hat{y})}{\partial \hat{y}} \frac{\partial \hat{y}(\mathbf{z})}{\partial \mathbf{z}} \frac{\partial z(\mathbf{w})}{\partial \mathbf{w}}}_{\text{Chain rule}}$$

$$\mathcal{L} = \frac{1}{2} (y - \hat{y})^2 \quad \hat{y} = \text{sign}(z) \quad z = \mathbf{w} \cdot \mathbf{x}$$

## Chain Rule of Calculus (Review)

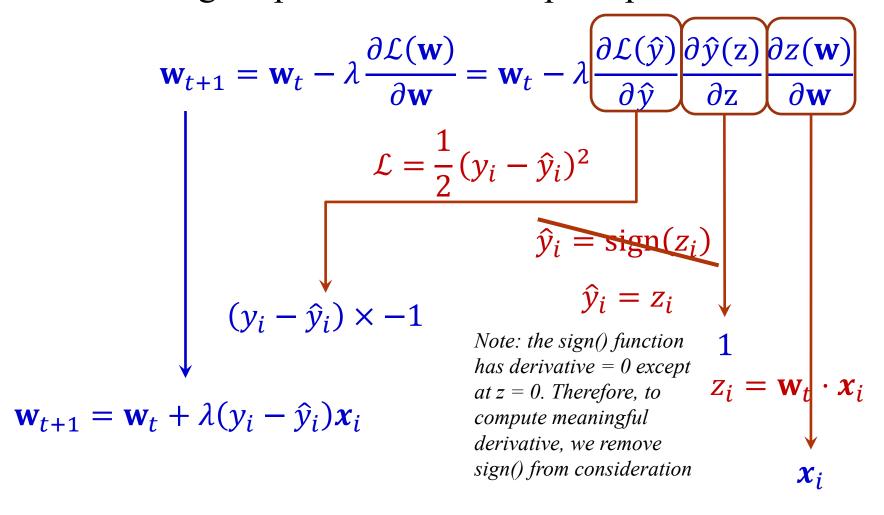
- Suppose that y = g(x) and z = f(y) = f(g(x))
- Chain rule of calculus:

$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y} \frac{\partial y}{\partial x}$$

• Generalized to the vector case: suppose  $\mathbf{x} \in \mathbb{R}^m$ ,  $\mathbf{y} \in \mathbb{R}^n$ 

$$\frac{\partial z}{\partial x_i} = \sum_{j} \frac{\partial z}{\partial y_j} \frac{\partial y_j}{\partial x_i}$$

• The weight update formula for perceptron:



# **Approximating the derivative?**

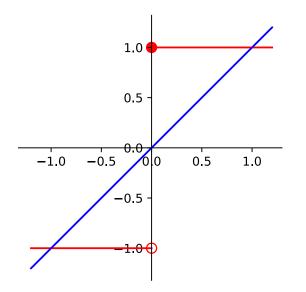
• The equation used to compute  $\hat{y}_i$  from  $z_i$ 

$$\hat{y}_i = \operatorname{sign}(z_i)$$

• The equation used to compute  $\frac{\partial \hat{y}(z)}{\partial z}$ 

$$\hat{y}_i = z_i$$

• Why? This is approximating the step function with a linear function.



While the derivative itself is incorrect, its direction is correct.

That is, if you want to increase  $\hat{y}_i$ , you should increase  $z_i$ , and vice versa.

# Perceptron Weights Update

$$\mathbf{w}_{t+1} = \mathbf{w}_t + \lambda (y_i - \hat{y}_i) \mathbf{x}_i$$

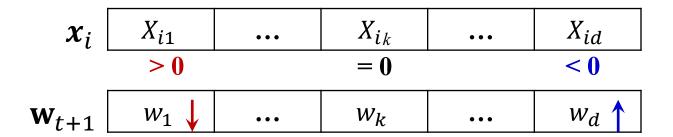
- If the prediction is correct,  $(y \hat{y}) = 0$ , then weight remains unchanged  $\mathbf{w}_{t+1} = \mathbf{w}_t$
- If y = +1 and  $\hat{y} = -1$ , then  $(y \hat{y}) = 2$
- The weights of all links with positive inputs need to be updated by increasing their values
- The weights of all links with negative inputs need to be updated by decreasing their weights

$\boldsymbol{x}_i$	$x_{i1}$	•••	$x_{ik}$	•••	$x_{id}$
	> 0		= 0		< 0
$\mathbf{V}_{t+1}$	$w_1 \uparrow$	•••	$w_k$	•••	$w_d \downarrow$

# Perceptron Weights Update (cont.)

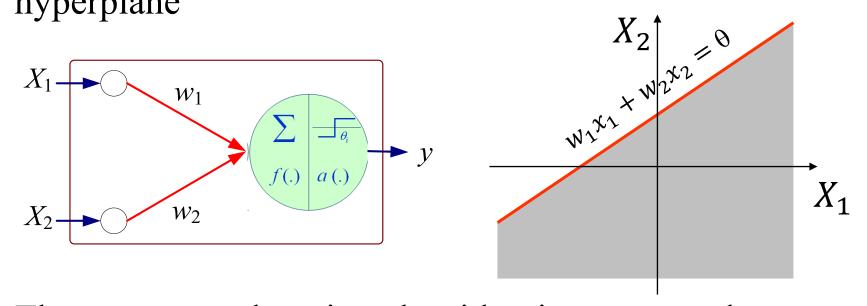
$$\mathbf{w}_{t+1} = \mathbf{w}_t + \lambda (y_i - \hat{y}_i) \mathbf{x}_i$$

- If y = -1 and  $\hat{y} = +1$ , then  $(y \hat{y}) = -2$
- The weights of all links with positive inputs need to be updated by decreasing their values
- The weights of all links with negative inputs need to be updated by increasing their weights



# Convergence

• The decision boundary of a perceptron is a linear hyperplane

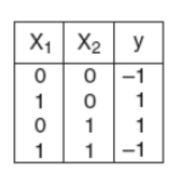


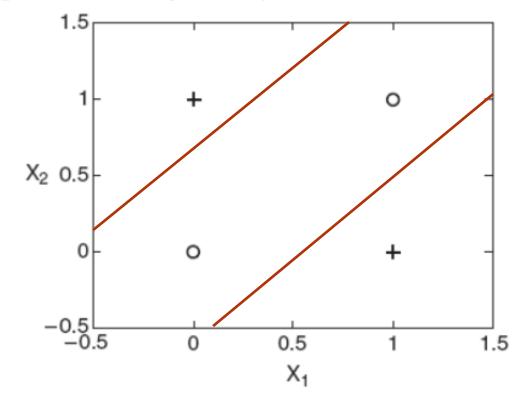
• The perceptron learning algorithm is guaranteed to converge to an optimal solution for linear classification problems

#### **Perceptron Limitation**

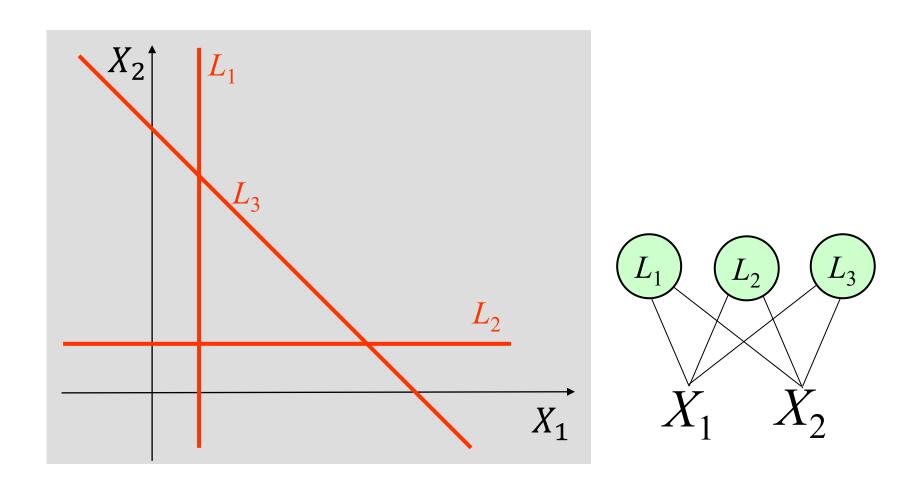
• If the problem is not linearly separable, the algorithm fails to converge

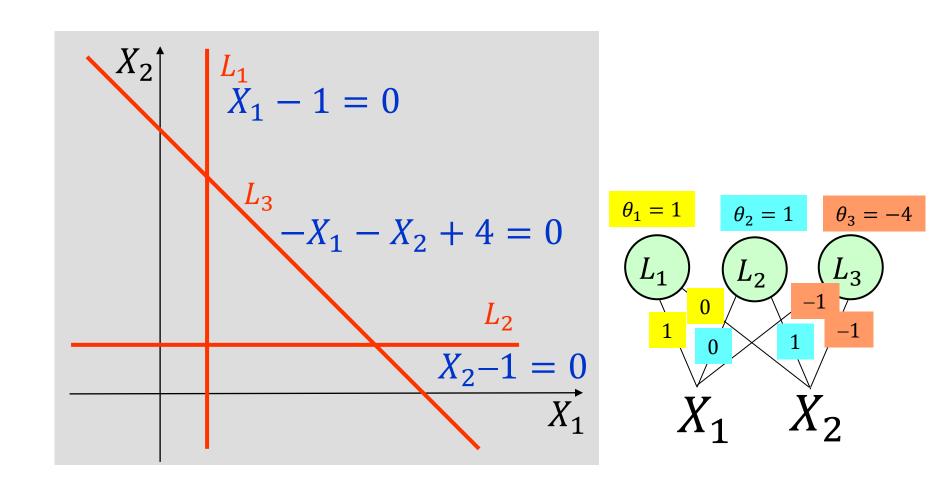
Nonlinearly separable data given by the XOR function

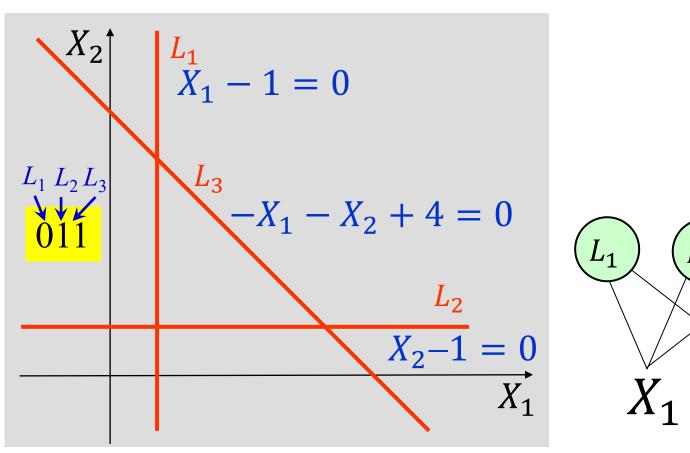


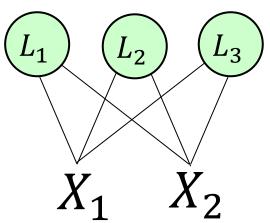


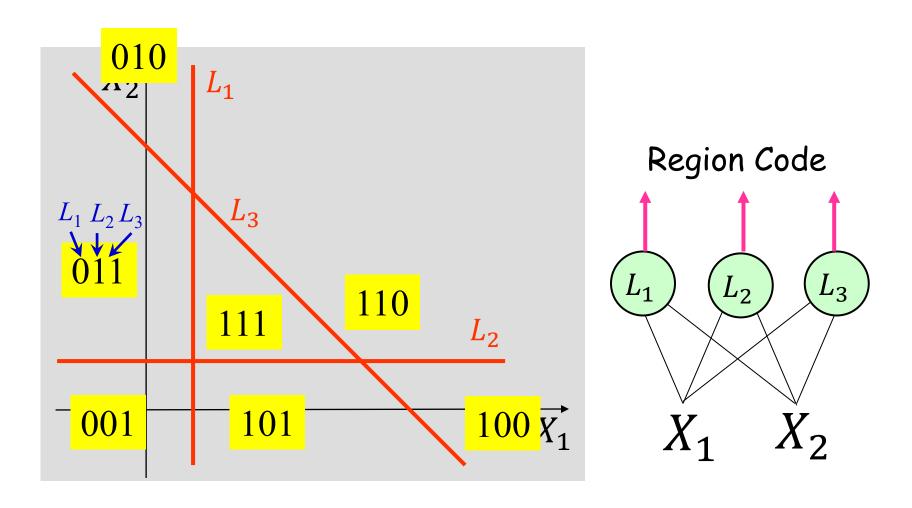
# **Multi-layer Perceptron**

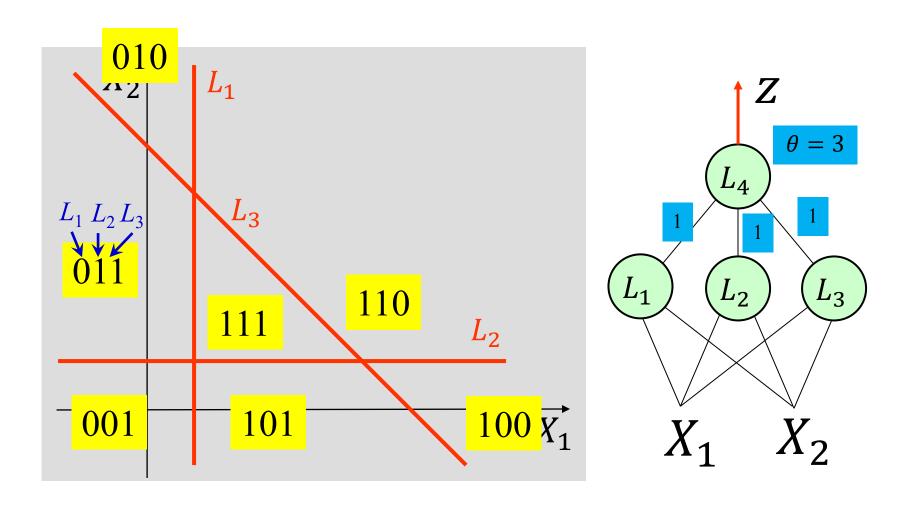


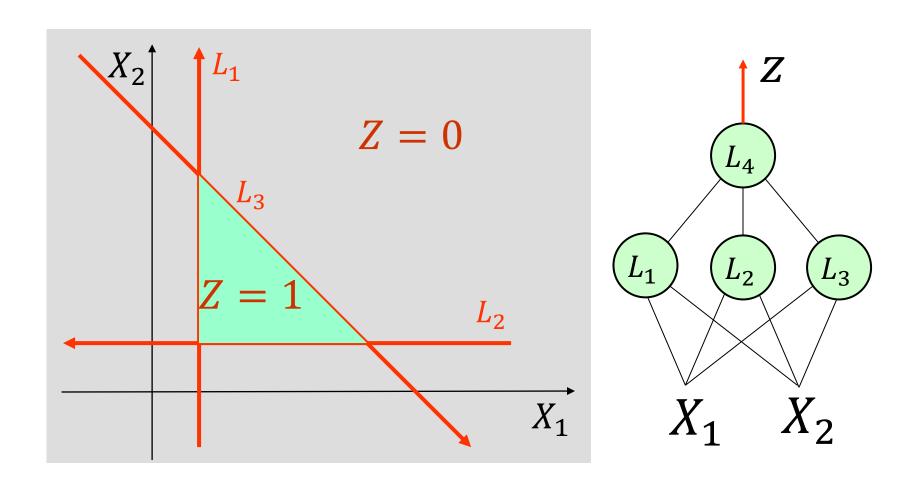




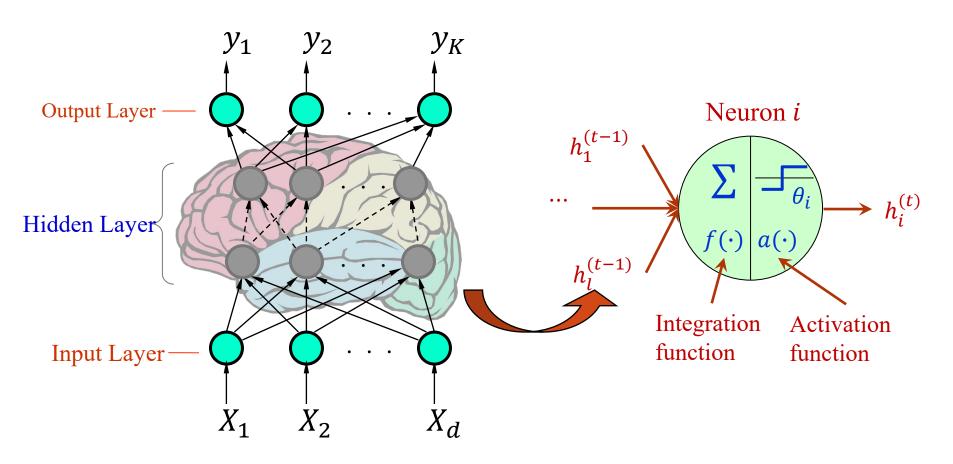








#### General Structure: Multilayer ANN



# **Integration Functions**

• Weighted sum:

$$\sum_{i=1}^{d} w_i X_i - \theta$$



Quadratic function

$$\sum_{i=1}^{d} w_i X_i^2 - \theta$$

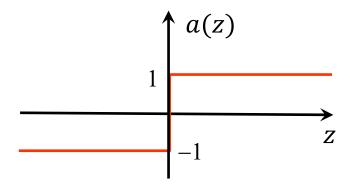
Spherical function

$$\sum_{i=1}^{d} (X_i - w_i)^2 - \theta$$

#### **Activation Functions**

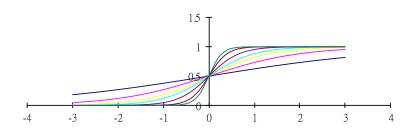
• Sign function (Threshold function)

$$a(z) = \operatorname{sign}(z) = \begin{cases} 1 & z \ge 0 \\ -1 & z < 0 \end{cases}$$



• Unipolar sigmoid function:

$$a(z) = \frac{1}{1 + e^{-\lambda z}}$$



When  $\lambda = 1$ , it is called sigmoid function

#### **Update Weights for Multi-layer NNs**

- Initialize the weights in each layer  $(\mathbf{w}^{(1)}, ..., \mathbf{w}^{(k)}, ..., \mathbf{w}^{(m)})$
- Adjust the weights such that the output of ANN is consistent with class labels of training examples
  - Loss function for each training instance:

$$\mathcal{L} = \frac{1}{2}(y_i - \hat{y}_i)^2$$

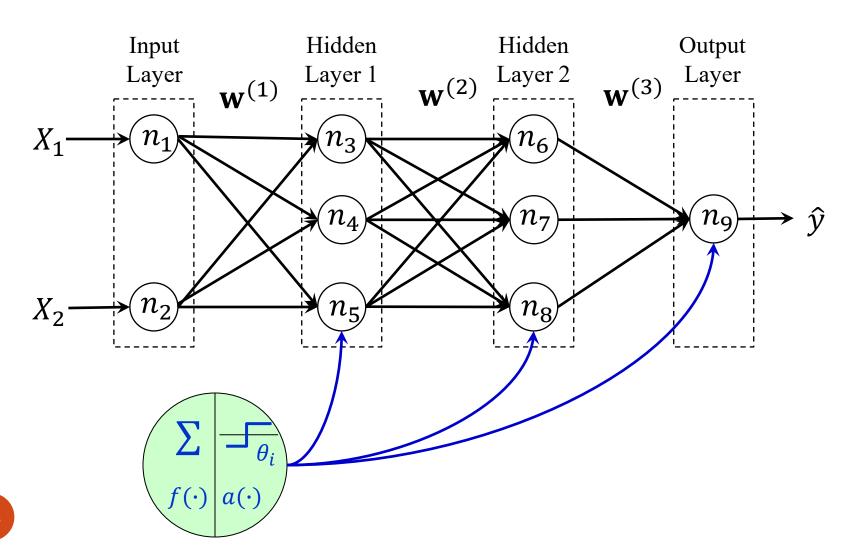
• For each layer k, update the weights,  $\mathbf{w}^{(k)}$ , by gradient descent at each iteration t:

$$\mathbf{w}_{t+1}^{(k)} = \mathbf{w}_t^{(k)} - \lambda \frac{\partial \mathcal{L}}{\partial \mathbf{w}^{(k)}}$$

• Computing the gradient w.r.t. weights in each layer is computationally expensive!

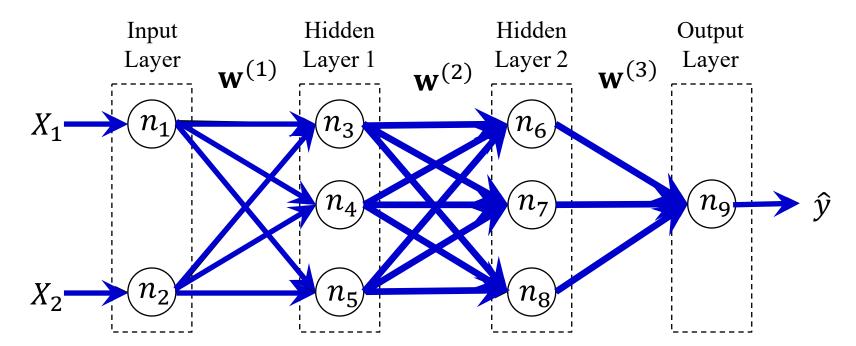
#### The Backpropagation Algorithm

# A Multi-layer Feed-forward NN



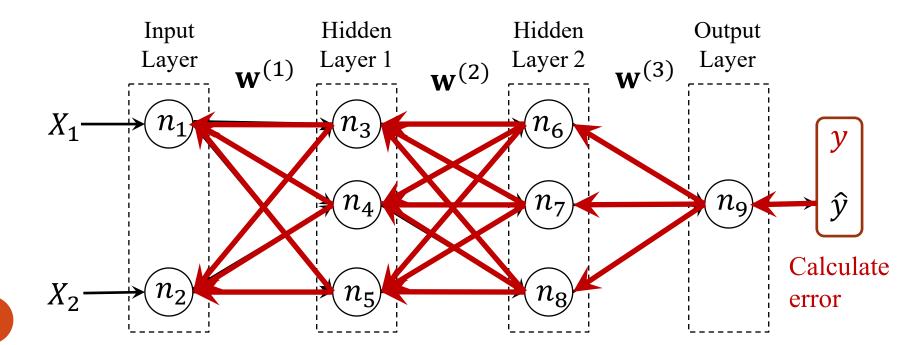
## **Backpropagation: Basic Idea**

- Initialize the weights  $(\mathbf{w}^{(1)},...,\mathbf{w}^{(3)})$
- Forward pass: each training examples  $(x_i, y_i)$  is used to compute outputs of each hidden layer and generate the final output  $\hat{y}_i$  based on the ANN

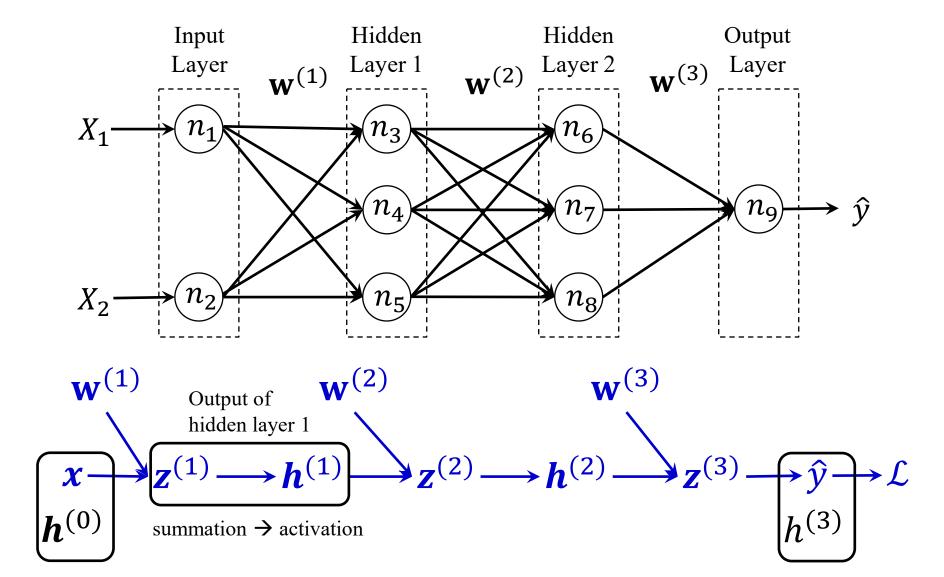


# Backpropagation: Basic Idea (cont.)

• Backpropagation: Starting with the output layer, to propagate error back to the previous layer in order to update the weights between the two layers, until the earliest hidden layer is reached



# The Computational Graph



# **Backpropagation (BP)**

- Gradient of  $\mathcal{L}$  w.r.t.  $w^{(3)}$ :  $\frac{\partial \mathcal{L}}{\partial w^{(3)}} = \left[\frac{\partial \mathcal{L}}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z^{(3)}}\right] \frac{\partial z^{(3)}}{\partial w^{(3)}}$
- Gradient of  $\mathcal{L}$  w.r.t.  $w^{(2)}$ :

$$\frac{\partial \mathcal{L}}{\partial w^{(2)}} = \underbrace{\frac{\partial \mathcal{L}}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z^{(3)}} \frac{\partial z^{(3)}}{\partial h^{(2)}} \frac{\partial h^{(2)}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial w^{(2)}}}_{\partial w^{(2)}}$$

• Gradient of  $\mathcal{L}$  w.r.t.  $w^{(1)}$ :

$$\frac{\partial \mathcal{L}}{\partial w^{(1)}} = \boxed{\frac{\partial \mathcal{L}}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z^{(3)}} \frac{\partial z^{(3)}}{\partial h^{(2)}} \frac{\partial h^{(2)}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial h^{(1)}} \frac{\partial h^{(1)}}{\partial z^{(1)}} \frac{\partial z^{(1)}}{\partial w^{(1)}}}$$

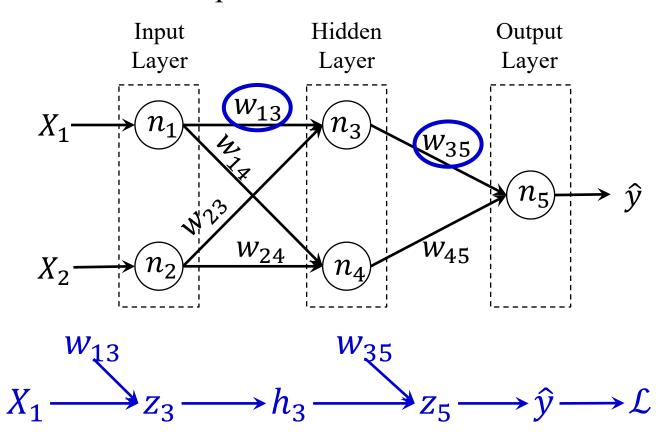
Consider each layer contains a single unit

$$w^{(1)} \qquad w^{(2)} \qquad w^{(3)}$$

$$x \longrightarrow z^{(1)} \longrightarrow h^{(1)} \longrightarrow z^{(2)} \longrightarrow h^{(2)} \longrightarrow z^{(3)} \longrightarrow \hat{y} \longrightarrow \mathcal{L}$$

#### An Example

• Consider an ANN of 1 hidden layer as follows. Suppose the sign function and the weighted sum function are used for both hidden and output nodes



$$w_{35}' = w_{35} + \lambda e_i h_3$$

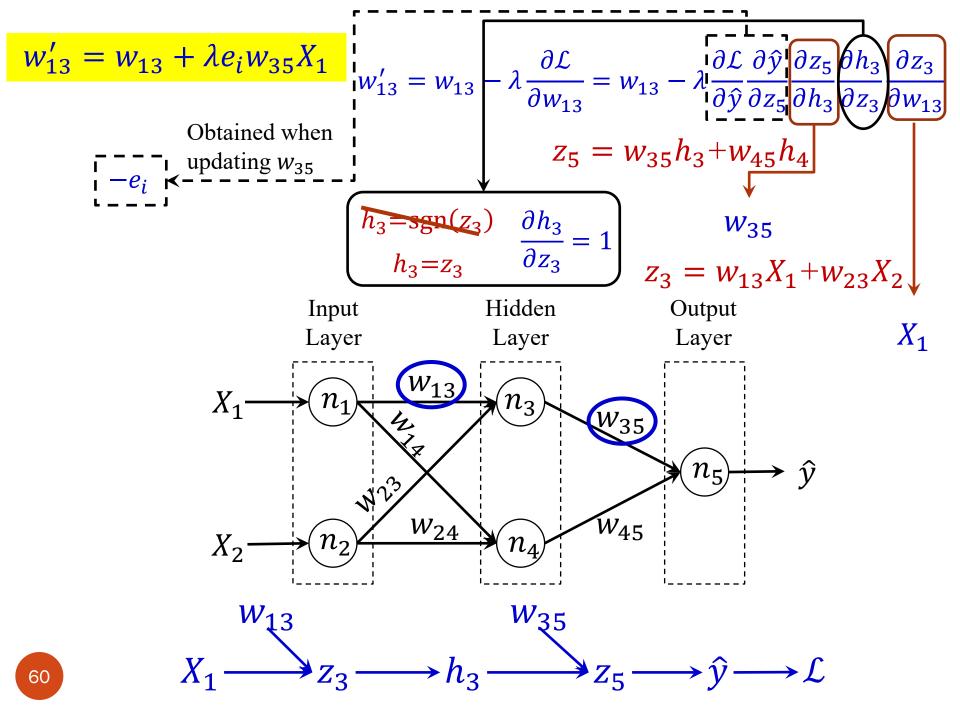
$$w_{35}' = w_{35} - \lambda \frac{\partial \mathcal{L}}{\partial w_{35}} = w_{35} - \lambda \frac{\partial \mathcal{L}}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z_5} \frac{\partial z_5}{\partial w_{35}}$$

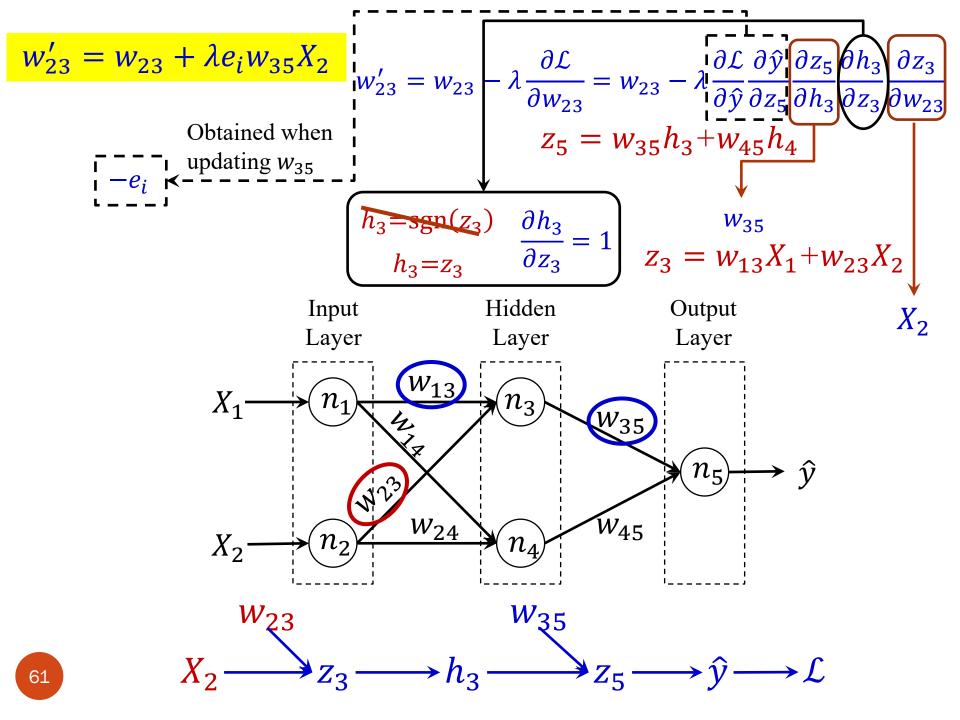
$$\mathcal{L} = \frac{1}{2} e_i^2 = \frac{1}{2} (y_i - \hat{y}_i)^2$$

$$-1 \times (y_i - \hat{y}_i) = -e_i$$

$$z_5 = w_{35} h_3 + w_{45} h_4$$

$$x_1 + w_{13} + w_{24} + w_{45} + w_{4$$





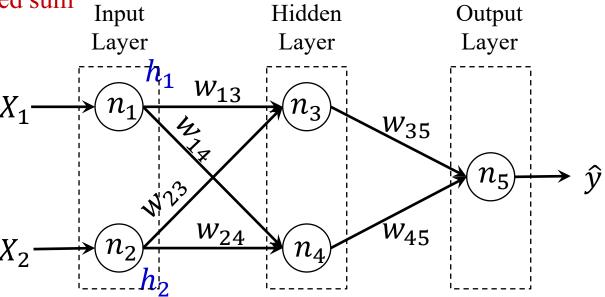
# **BP Algorithm: Example**

Activation function: sign()

Integration function: weighted sum

$$\lambda = 0.4$$
,  $\theta = 0$ 

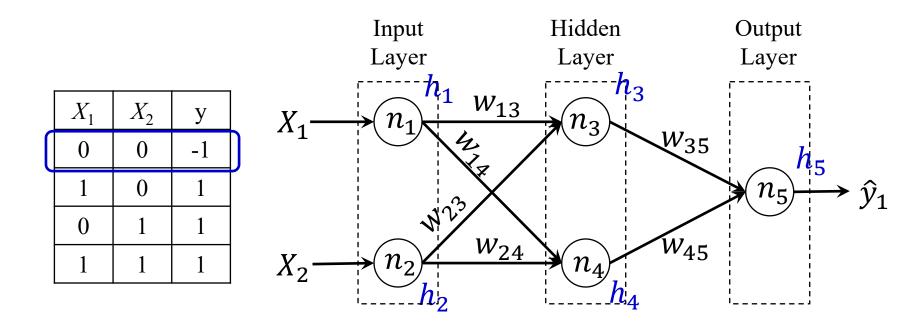
$X_1$	$X_2$	у
0	0	-1
1	0	1
0	1	1
1	1	1



#### • Initialization:

$$(w_{13} = 1, w_{14} = 1, w_{23} = 1, w_{24} = 1, w_{35} = 1, w_{45} = 1)$$

For the 1<sup>st</sup> example:  $h_1 = 0$  and  $h_2 = 0$ 

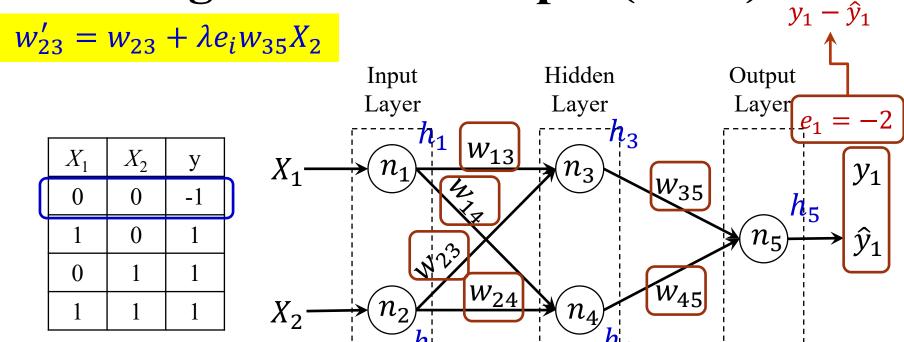


Forward pass:

$$h_3 = \text{sign}(0 \times 1 + 0 \times 1) = 1 \text{ and } h_4 = \text{sign}(0 \times 1 + 0 \times 1) = 1$$
  
Then  $\hat{y}_1 = h_5 = \text{sign}(1 \times 1 + 1 \times 1) = 1$ 

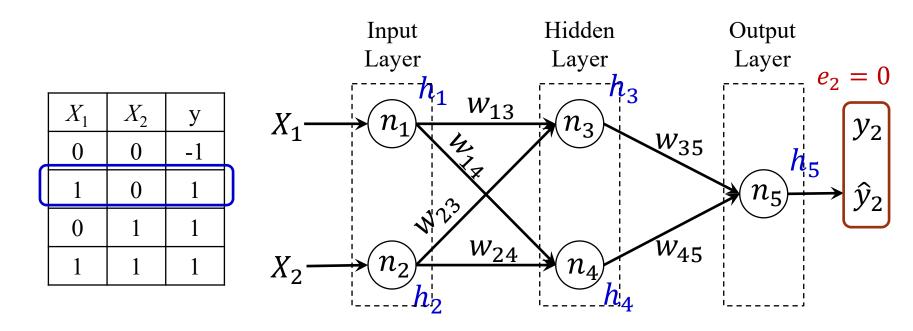
$$w_{13}' = w_{13} + \lambda e_1 w_{35} X_1$$

$$w_{35}' = w_{35} + \lambda e_1 h_3$$

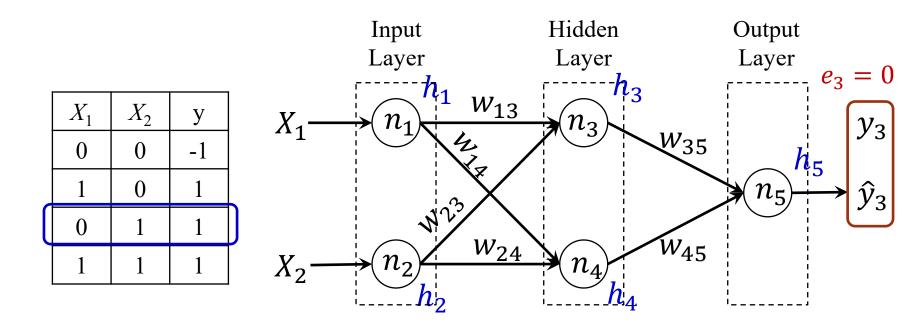


#### Backpropagation:

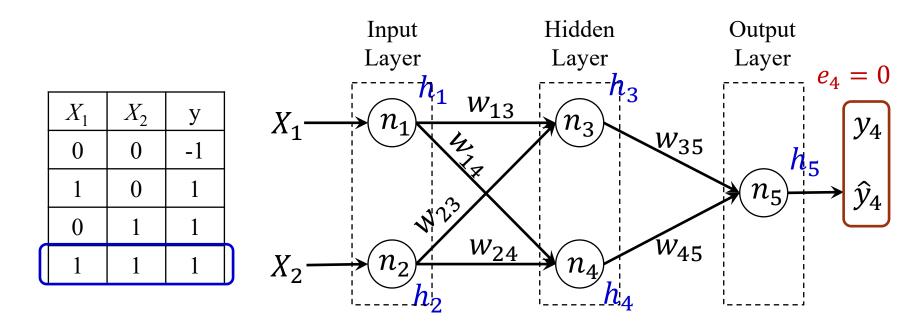
$$w_{35} = 1 + 0.4 \times (-2) \times 1 = 0.2$$
  $w_{45} = 1 + 0.4 \times (-2) \times 1 = 0.2$   $w_{13} = 1 + 0.4 \times (-2) \times 1 \times 0 = 1$   $w_{14} = 1 + 0.4 \times (-2) \times 1 \times 0 = 1$   $w_{23} = 1 + 0.4 \times (-2) \times 1 \times 0 = 1$   $w_{24} = 1 + 0.4 \times (-2) \times 1 \times 0 = 1$ 



For the 2<sup>nd</sup> example:  $h_1 = 1$  and  $h_2 = 0$   $h_3 = \text{sign}(1 \times 1 + 0 \times 1) = 1$  and  $h_4 = \text{sign}(1 \times 1 + 0 \times 1) = 1$ Then  $\hat{y}_2 = h_5 = \text{sign}(1 \times 0.2 + 1 \times 0.2) = 1$ 



For the 3<sup>rd</sup> example:  $h_1 = 0$  and  $h_2 = 1$   $h_3 = \text{sign}(0 \times 1 + 1 \times 1) = 1$  and  $h_4 = \text{sign}(0 \times 1 + 1 \times 1) = 1$ Then  $\hat{y}_3 = h_5 = \text{sign}(1 \times 0.2 + 1 \times 0.2) = 1$ 

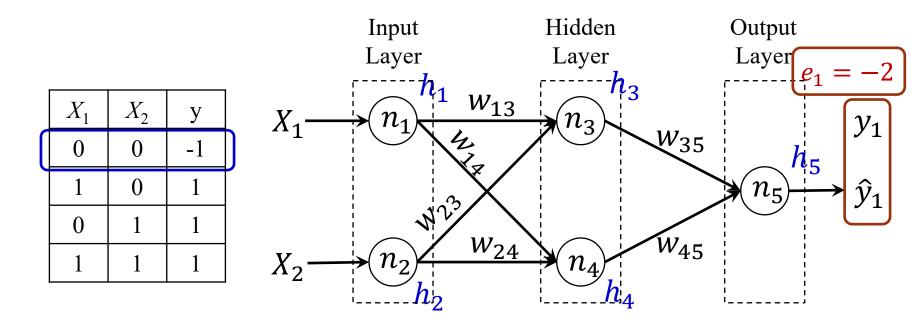


For the 4<sup>th</sup> example:  $h_1 = 1$  and  $h_2 = 1$ 

$$h_3 = \text{sign}(1 \times 1 + 1 \times 1) = 1 \text{ and } h_4 = \text{sign}(1 \times 1 + 1 \times 1) = 1$$

Then 
$$\hat{y}_4 = h_5 = \text{sign}(1 \times 0.2 + 1 \times 0.2) = 1$$

End of the 1st Epoch



For the 1<sup>st</sup> example again:  $h_1 = 0$  and  $h_2 = 0$ 

$$h_3 = \text{sign}(0 \times 1 + 0 \times 1) = 1$$
 and  $h_4 = \text{sign}(0 \times 1 + 0 \times 1) = 1$ 

Then 
$$\hat{y}_1 = h_5 = \text{sign}(0.2 \times 1 + 0.2 \times 1) = 1$$

Weights need to be further updated via backpropagation

# **Design Issues for ANN**

- The number of nodes in the input layer
  - Assign an input node to each numerical or binary input variable
- The number of nodes in the output layer
  - Binary class problem → single node
  - C-class problem  $\rightarrow$  C output nodes
- How many nodes in the hidden layer(s)?
  - Too many parameters result in networks that are too complex and overfit the data

## **Design Issues for ANN**

- How many nodes in the hidden layer(s)?
  - Too many parameters result in networks that are too complex and overfit the data
- If the network underfits
  - Try to increase the number of hidden units
- If the network overfits
  - Try to decrease the number of hidden units