# QBUS6850 Lecture 9 Neural Network and Deep Learning- I

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- □ Topics covered
  - Neural network (NN) intuition
  - Neural network representation
  - Forward propagation
  - Neural network examples: Boolean functions
- □ References
  - Alpaydin (2014), Chapter 11
  - Bishop (2006), Chapter 5
  - https://am207.github.io/2017/wiki/gradientdescent.h tml#stochastic-gradient-descent



# **Learning Objectives**

- Understand the intuition of NN
- Understand the how NN can be used for regression and classification
- Understand the how forward propagation NN works
- Understand how NN can be applied to realize Boolean functions



# **Neural Network Intuition**

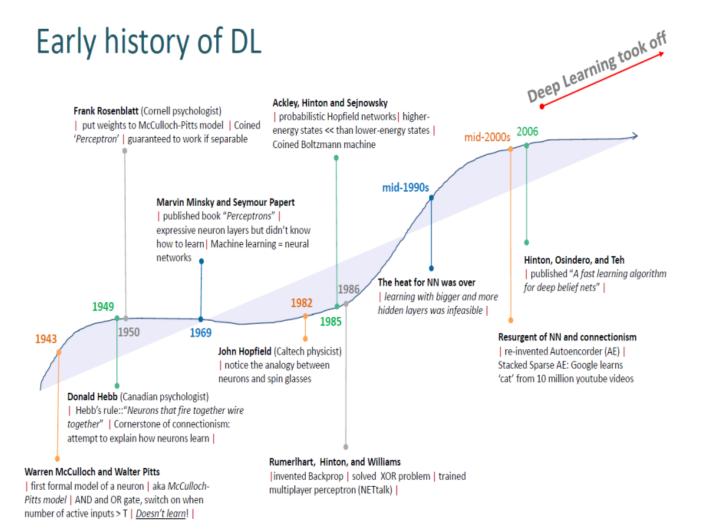


### **NN** Introduction

- Neural network is the type of algorithm that tries to simulate how human brain works
- Was widely used in 80s and 90s
- Popularity diminished in late 90s
- Recently, neural network and deep learning became the state-ofart algorithms for many application
- Especially with the High Performance Computers (HPC) and cloud computing
- Neural networks and deep neural networks (called deep learning)
  has become an exciting research and application area in the last
  few years

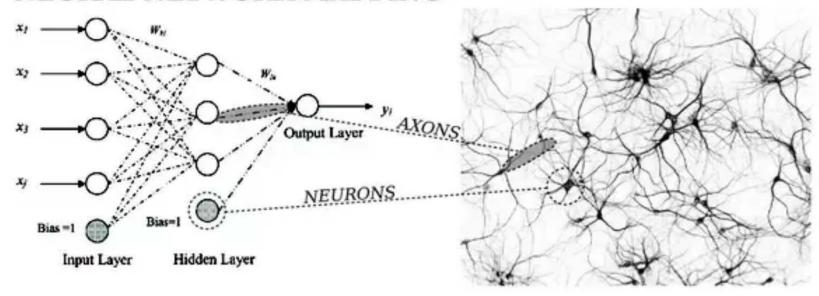


# NN and DL History





#### NEURAL NETWORK MAPPING



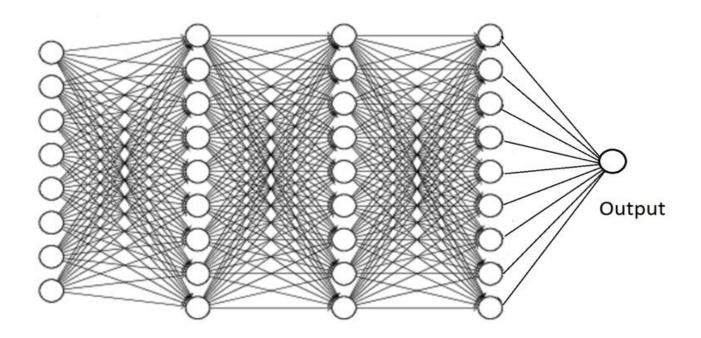
https://www.quora.com/When-will-technology-surpass-the-complexity-and-intelligence-of-the-human-brain



# Neural Network Representation

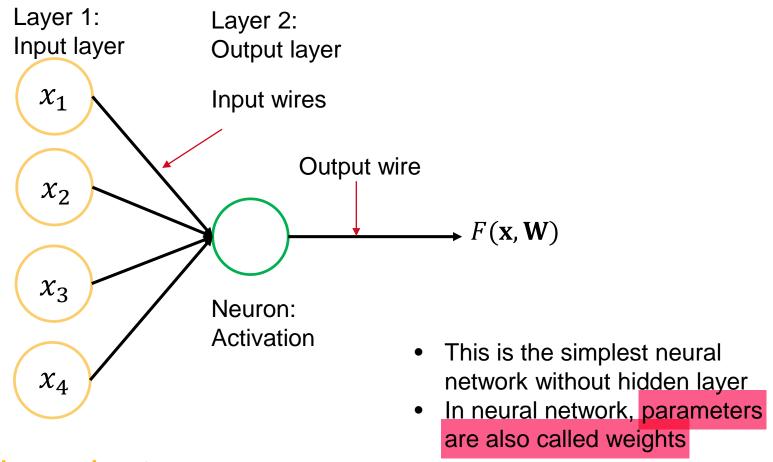


A neural network is a multi-stage **regression or classification** model, typically represented by a network diagram





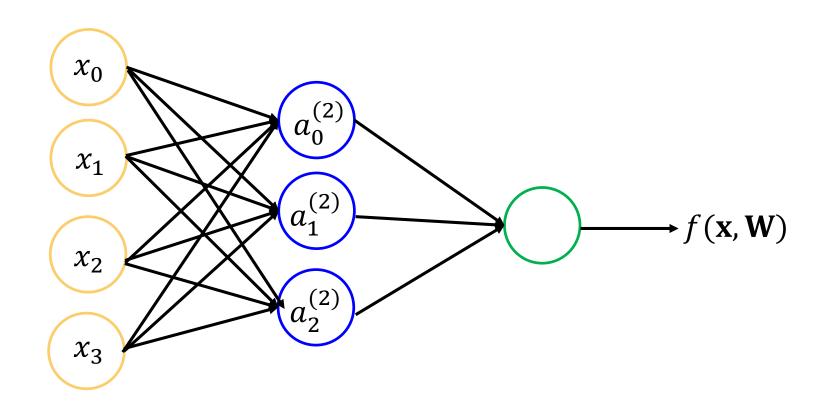
# 2 layer Neural Network



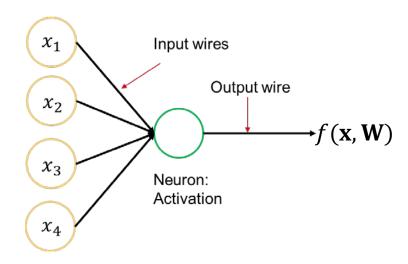
They are input, not neuron



# 3 layer Neural Network







The neuron is the basic processing element.

It has inputs that may come from the environment or may be the outputs of other neurons.

For a given dataset, we need to estimate weights, so that correct outputs are generated given the inputs.



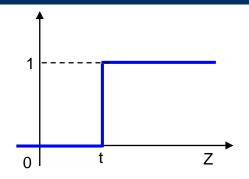
#### **Activation Functions**

- The output of a layered neural network model depends completely on the characteristics of the output layer. Units in a layer have (almost always) the same activation function.
- Typical activation functions are the sigmoid, hyperbolic tangent, and linear functions.
- The sigmoid function can only produce outputs in the range [0,1], the hyperbolic tangent produces outputs in the range [-1,1], and the linear function produces outputs in the range  $[-\infty,\infty]$
- If we need great than 1 output in NN regression, we could use linear output units and leave the non-linear sigmoid or hyperbolical tangent units for the hidden layer. Bounded nonlinearities in the output layer are best left for cases when you require "almost binary" outputs or likelihoods (probabilities).

#### **Activation Functions**

#### Threshold function

$$\sigma(z) = \begin{cases} 1 & \text{if } z \ge t \\ 0 & \text{if } z < t \end{cases}$$



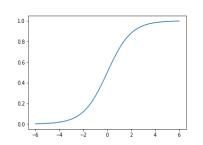
#### Generalized logistic (sigmoid) function

$$\sigma_{s,l}(z) = \frac{1}{1 + e^{-s(z-l)}}$$

s controls the steepness and l controls the location

Logistic (sigmoid) function

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



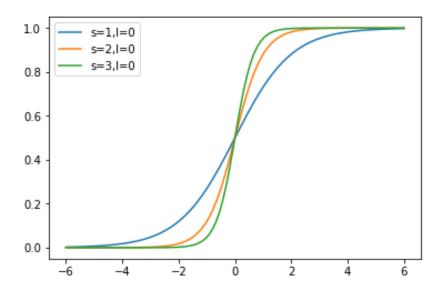
$$s = 1$$
 and  $l = 0$ 

Output range (0,1)



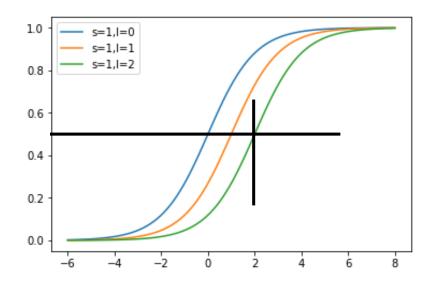
# Sigmoid Function

s controls the steepness of sigmoid function. Observations?



Or we can see that *s* controls activation rate. larger *s* amounts to a shaper activation (closer to the threshold function)

*l* controls the location of sigmoid function

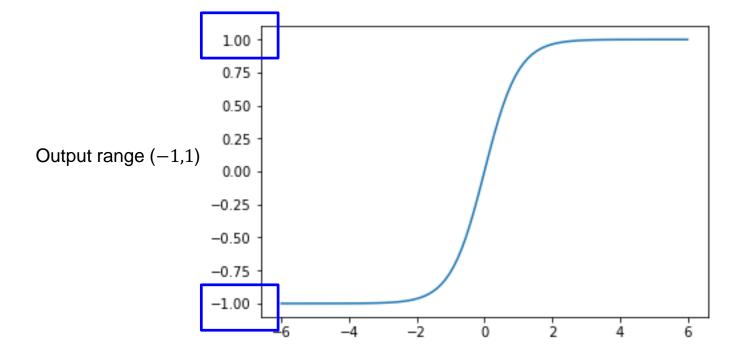


l shifts activation threshold.

#### **Hyperbolic Tangent Function**

This function is defined as the ratio of the difference and sum of two exponential functions in the points z and -z:

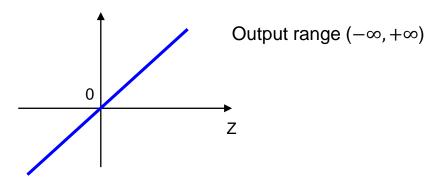
$$\sigma(z) = \frac{2}{1 + e^{-2z}} - 1 = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$



## **Identity Activation Function**

The simplest activation function, one that is commonly used for the output layer activation function in regression problems, is the identity/linear activation function:

$$\sigma(z) = z$$



Why use an identity activation function?

For example, a multi-layer network that has nonlinear activation functions amongst
the hidden units and an output layer that uses the identity activation function
implements a powerful form of nonlinear regression. Specifically, the network can
predict continuous target values using a linear combination of signals that arise
from one or more layers of nonlinear transformations of the input.

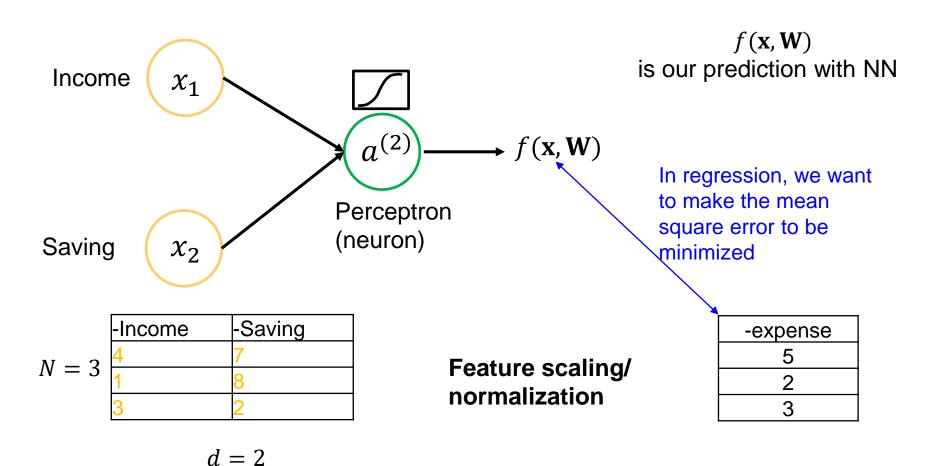


# Forward Propagation 2 Layer Neural Network



# 2 Layer NN

Let's start with a 2 layer NN for regression





#### Feature scaling/ normalization

$$N = 3 \begin{array}{c|c} -Income & -Saving \\ \hline 4 & 7 \\ \hline 1 & 8 \\ \hline 3 & 2 \\ \end{array}$$

$$d = 2$$

0.25

-Saving
0.875
1

-expense		
5		
2		
3		

Divide by maximum of  $x_1, x_2, t$  respectively

-expense	
1	
0.4	
0.6	

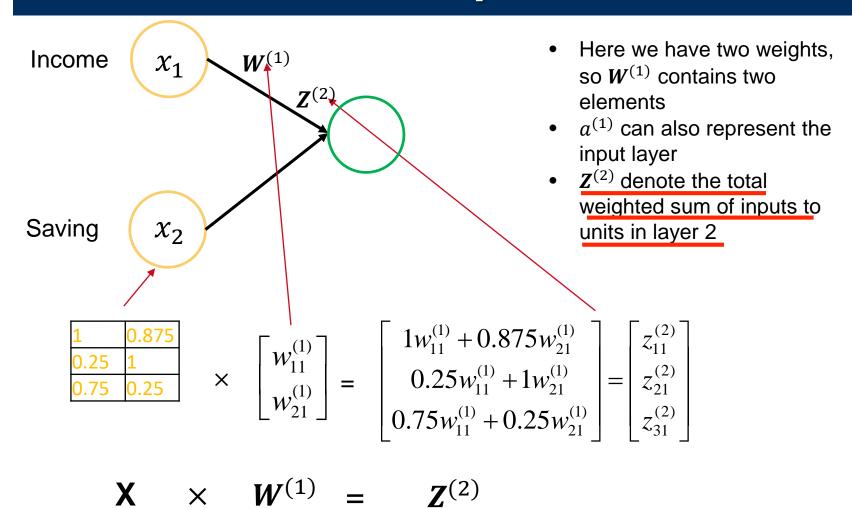
#### Why scaling?

-Income

0.25

• There are a variety of practical reasons why scaling the inputs can make training faster and reduce the chances of getting stuck in local optima.

# Step 1



 $3 \times 1$ 

 $2 \times 1$ 

 $3 \times 2$ 



# Step 2

$$\begin{array}{c}
\mathbf{Z}^{(2)} \\
\hline
 a_1^{(2)} \\
\end{array} \qquad f(\mathbf{X}, \mathbf{W})$$

$$\mathbf{Z}^{(2)} = \begin{bmatrix} z_{11}^{(2)} \\ z_{21}^{(2)} \\ z_{31}^{(2)} \end{bmatrix}$$

3 × 1 matrix (vector), Each row represents one example Each column represents one hidden

unit, here we only have one hidden unit

$$f(\mathbf{x}, \mathbf{W}) = \mathbf{a}^{(2)} = \sigma(\mathbf{Z}^{(2)})$$

Apply activation function for **EACH** element of the matrix  $\mathbf{Z}^{(2)}$  to produce the prediction  $f(\mathbf{x}, \mathbf{W}) = a^{(2)}$  (3 × 1)

Loss function of regression:

$$L(\mathbf{W}) = \frac{1}{2N} \sum_{n=1}^{N} (f(\mathbf{x}_n, \mathbf{W}) - t_n)^2$$

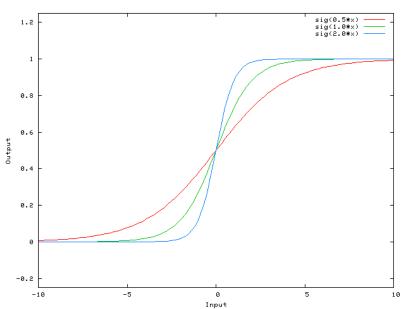


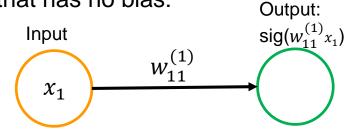
# **Bias Unit Impact**



- Note that bias units don't have inputs or connections going into them, since they always output the value +1
- Biases are almost always helpful. In effect, a bias value allows you to shift the activation function to the left or right, which may be critical for successful learning.

Consider this 1-input, 1-output network that has no bias:

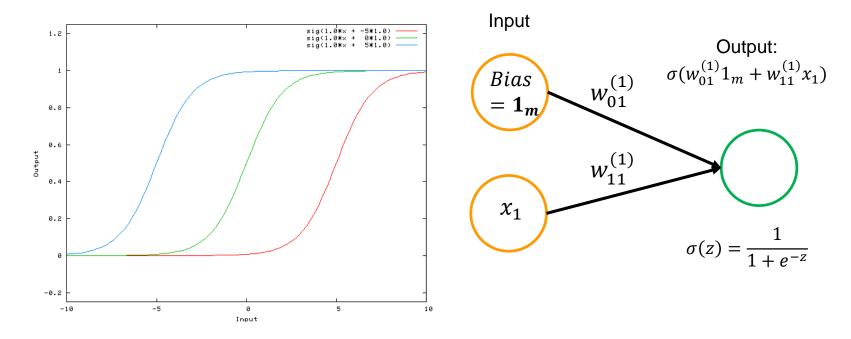




$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

Changing the weight  $w_{11}^{(1)}$  essentially changes the "steepness" of the sigmoid. That's useful, but what if you wanted the network to output 0 when  $x_1$  is 2? Just changing the steepness of the sigmoid won't really work -- you want to be able to shift the entire curve to the right.

If we add a bias unit to this network, then the output of the network becomes  $\sigma(w_{01}^{(1)}1_m + w_{11}^{(1)}x_1)$ . Here is what the output of the network looks like for various values of  $w_{01}^{(1)}$ :



- Having a weight of -5 for  $w_{01}^{(1)}$  shifts "location" of the curve to the right, which allows us to have a network that outputs 0 when  $x_1$  is 2.
- Connect and compare this with generalized logistic (sigmoid) function.



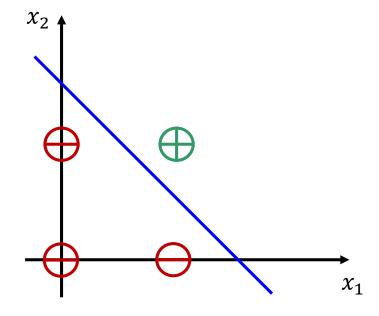
# Forward Propagation 2 Layer Neural Network Example



# **Example: AND Function**

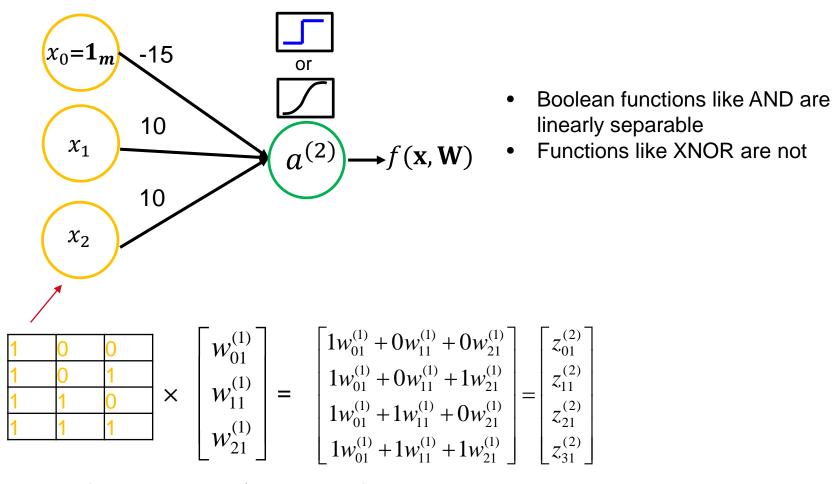
$x_1$	$x_2$		t
0	0	0	$\Theta$
0	1	0	$\Theta$
1	0	0	Ŏ
1	1	1	$\oplus$

We want to find the blue decision boundary: **above it predict 1**; below it predict 0





## Example



- Role of the intercept term/bias unit here?
- Note that bias units don't have inputs or connections going into them, since they always output the value +1

# Sigmoid Activation Function

Suppose we have 
$$\begin{bmatrix} w_{01}^{(1)} \\ w_{11}^{(1)} \\ w_{21}^{(1)} \end{bmatrix} = \begin{bmatrix} -15 \\ 10 \\ 10 \end{bmatrix}$$
 How to estimate?

$$a^{2} = \sigma(\mathbf{Z}^{(2)}) = \begin{bmatrix} \approx 0 \\ \approx 0 \\ \approx 0 \\ \approx 0 \\ \approx 1 \end{bmatrix}$$

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

Predictions 
$$f(\mathbf{x}, \mathbf{W}) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$
 Actual observations

#### Threshold Activation Function

# $\sigma(z) = \begin{cases} 1 & \text{if } z \ge 0 \\ 0 & \text{if } z < 0 \end{cases}$ $\begin{bmatrix} 1 \\ 0 \\ 10 \end{bmatrix} \times \begin{bmatrix} -15 \\ 10 \\ 10 \end{bmatrix} = \begin{bmatrix} z_{01}^{(2)} \\ z_{11}^{(2)} \\ z_{21}^{(2)} \\ z_{21}^{(2)} \end{bmatrix} = \begin{bmatrix} -15 \\ -5 \\ -5 \\ 5 \end{bmatrix}$ $a^{2} = \sigma(\mathbf{Z}^{(2)}) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$

0 is the threshold

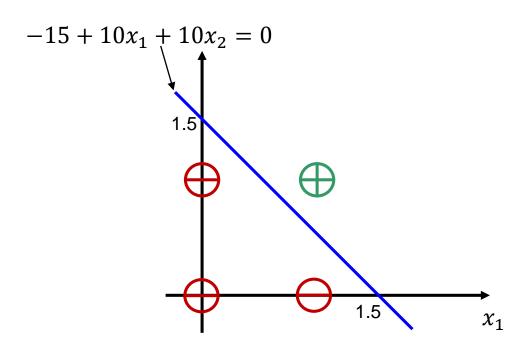
$$\sigma(z) = \begin{cases} 1 & \text{if } z \ge 0 \\ 0 & \text{if } z < 0 \end{cases}$$

$$a^{2} = \sigma(\mathbf{Z}^{(2)}) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Predictions 
$$f(\mathbf{x}, \mathbf{W}) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$
 Actual observations  $\begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$ 

# **AND Function Summary**

$x_1$	<i>x</i> <sub>2</sub>	t
0	0	0
0	1	0
1	0	0
1	1	1



$$-15 + 10x_1 + 10x_2 = 0$$
 is the decision boundary.

$$-15 + 10x_1 + 10x_2 \ge 0$$
, predict 1

$$-15 + 10x_1 + 10x_2 < 0$$
, predict 0

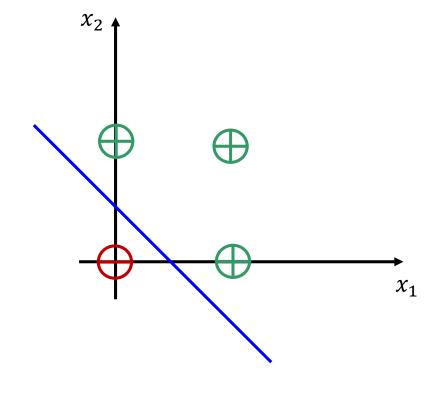
We will talk about how to estimate the parameters next week



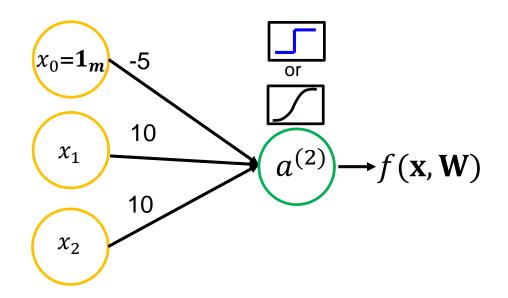
# **Example: OR Function**

We want to find the blue decision boundary: **above it predict 1**; above it predict 0. Estimated NN?

$x_1$	$x_2$	t
0	0	0
0	1	1
1	0	1
1	1	1



# **Example: OR Function**



$$\begin{bmatrix} w_{01}^{(1)} \\ w_{11}^{(1)} \\ w_{21}^{(1)} \end{bmatrix} = \begin{bmatrix} -5 \\ 10 \\ 10 \end{bmatrix}$$

This NN can achieve the OR function. Why?



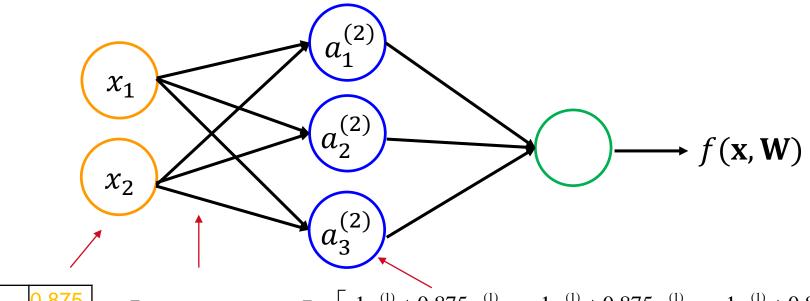
# Forward Propagation 3 Layer Neural Network

## 3 Layers Neural Network

Layer 1: Input layer Layer 2: Hidden layer

Layer 3: Output layer

No bias unit for simplicity



$$\begin{bmatrix} w_{11}^{(1)} & w_{12}^{(1)} & w_{13}^{(1)} \\ w_{21}^{(1)} & w_{22}^{(1)} & w_{23}^{(1)} \end{bmatrix}$$

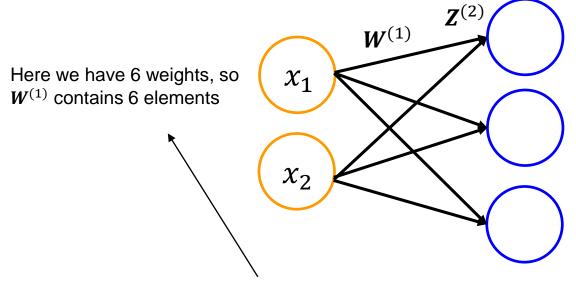
$$= \begin{bmatrix} w_{11}^{(1)} & w_{12}^{(1)} & w_{13}^{(1)} \\ w_{21}^{(1)} & w_{22}^{(1)} & w_{23}^{(1)} \end{bmatrix} = \begin{bmatrix} 1w_{11}^{(1)} + 0.875w_{21}^{(1)} & 1w_{12}^{(1)} + 0.875w_{22}^{(1)} & 1w_{13}^{(1)} + 0.875w_{23}^{(1)} \\ 0.25w_{11}^{(1)} + 1w_{21}^{(1)} & 0.25w_{12}^{(1)} + 1w_{22}^{(1)} & 0.25w_{13}^{(1)} + 1w_{23}^{(1)} \\ 0.75w_{11}^{(1)} + 0.25w_{21}^{(1)} & 0.75w_{12}^{(1)} + 0.25w_{22}^{(1)} & 0.75w_{13}^{(1)} + 0.25w_{23}^{(1)} \end{bmatrix}$$

$$1w_{12}^{(1)} + 0.875w_{22}^{(1)}$$
$$0.25w_{12}^{(1)} + 1w_{22}^{(1)}$$

$$0.25w_{12}^{(1)} + 1w_{22}^{(2)} = 0.25w_{13}^{(1)} + 1w_{23}^{(2)}$$
  
$$0.75w_{13}^{(1)} + 0.25w_{23}^{(1)} = 0.75w_{13}^{(1)} + 0.25w_{23}^{(1)}$$



# Step 1



The nice matrix representation does both multiplication and summation jobs

$$\begin{bmatrix} w_{11}^{(1)} & w_{12}^{(1)} & w_{13}^{(1)} \\ w_{21}^{(1)} & w_{22}^{(1)} & w_{23}^{(1)} \end{bmatrix}$$

$$\begin{bmatrix} w_{11}^{(1)} & w_{12}^{(1)} & w_{13}^{(1)} \\ w_{21}^{(1)} & w_{22}^{(1)} & w_{23}^{(1)} \end{bmatrix} = \begin{bmatrix} 1w_{11}^{(1)} + 0.875w_{21}^{(1)} & 1w_{12}^{(1)} + 0.875w_{22}^{(1)} & 1w_{13}^{(1)} + 0.875w_{23}^{(1)} \\ 0.25w_{11}^{(1)} + 1w_{21}^{(1)} & 0.25w_{12}^{(1)} + 1w_{22}^{(1)} & 0.25w_{13}^{(1)} + 1w_{23}^{(1)} \\ 0.75w_{11}^{(1)} + 0.25w_{21}^{(1)} & 0.75w_{12}^{(1)} + 0.25w_{22}^{(1)} & 0.75w_{13}^{(1)} + 0.25w_{23}^{(1)} \end{bmatrix}$$

$$1w_{12}^{(1)} + 0.875w_{2}^{(1)}$$

$$1w_{13}^{(1)} + 0.875w_{23}^{(1)}$$

$$0.25w_{12}^{(1)} + 1w_{22}^{(1)}$$

$$0.25w_{13}^{(1)} + 1w_{23}^{(1)}$$

$$v_{21}^{(1)}$$
 (

$$0.75w_{13}^{(1)} + 0.25w_{23}^{(1)}$$

$$\times / W^{(}$$

Weights (connection) between unit 2  $(x_2)$  in input layer (layer 1) to unit 1

 $a_1^{(2)}$  in hidden layer (layer 2)

 $3 \times 3$  matrix,

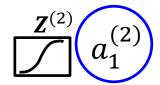
Each row represents one example

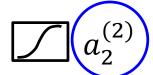
Each column represents one hidden unit



## Step 2

- a<sup>(1)</sup> can also represent the input layer
- $Z^{(2)}$  denote the total weighted sum of inputs to units in layer 2





$$\boxed{a_3^{(2)}}$$

$$\mathbf{Z}^{(2)} = \begin{bmatrix} z_{11}^{(2)} & z_{12}^{(2)} & z_{13}^{(2)} \\ z_{21}^{(2)} & z_{22}^{(2)} & z_{23}^{(2)} \\ z_{31}^{(2)} & z_{32}^{(2)} & z_{33}^{(2)} \end{bmatrix}$$

Apply activation function for **EACH** element of the  $Z^{(2)}$  matrix

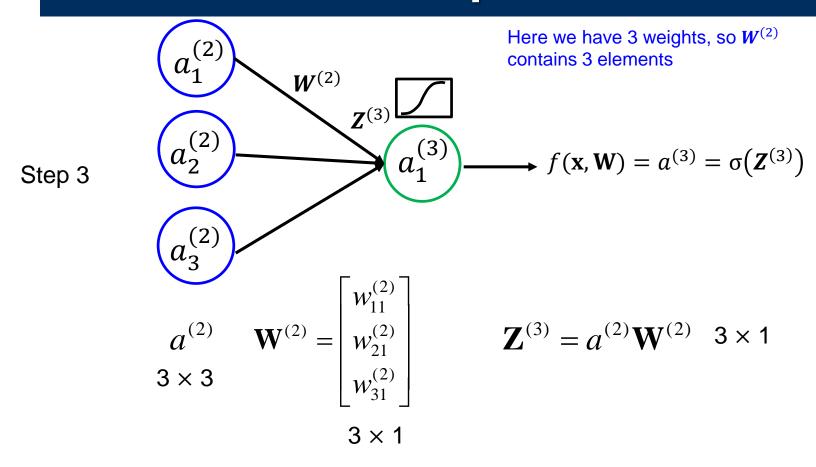
$$a^{(2)} = \sigma(\mathbf{Z}^{(2)})$$

3 by 3 matrix

Now generate the output



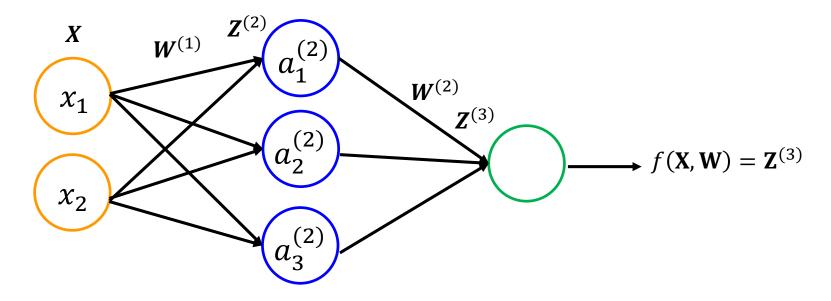
#### **Step 3&4**



Step 4 
$$f(\mathbf{x}, \mathbf{W}) = a^{(3)} = \sigma(\mathbf{Z}^{(3)})$$

Apply activation function on  $\mathbf{Z}^{(3)}$ , and generate final output/prediction  $f(\mathbf{x}, \mathbf{W}) = a^{(3)}$ 

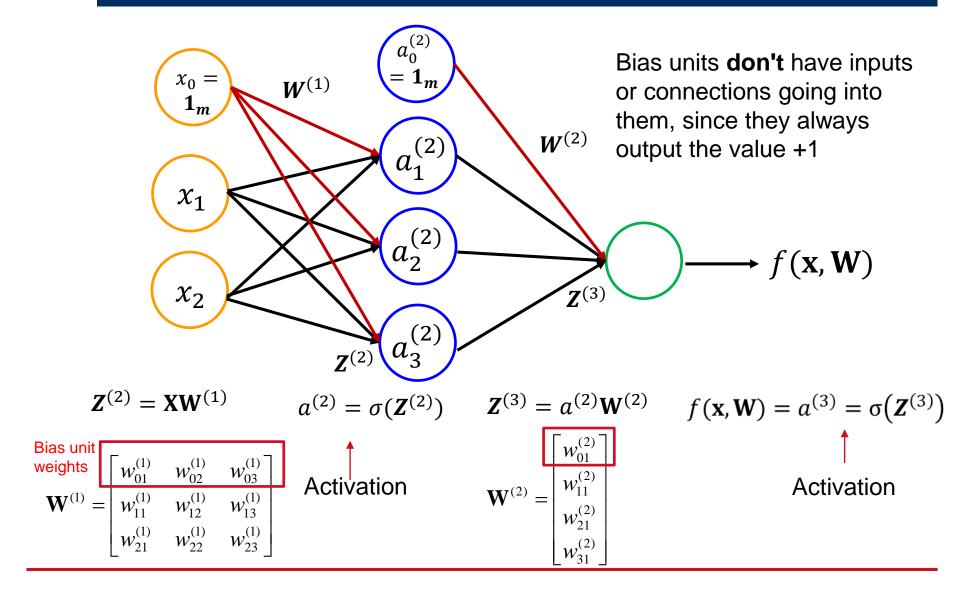
# Sum it up- no bias unit

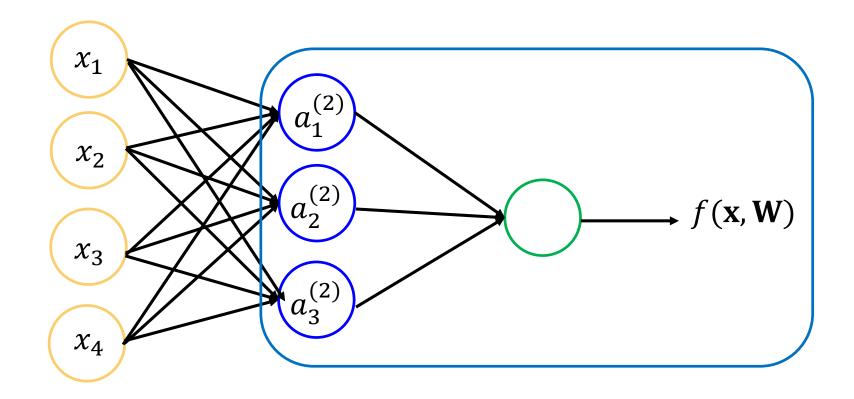


$$\mathbf{Z}^{(2)} = \mathbf{X}\mathbf{W}^{(1)}$$
  $a^{(2)} = \sigma(\mathbf{Z}^{(2)})$   $\mathbf{Z}^{(3)} = a^{(2)}\mathbf{W}^{(2)}$   $f(\mathbf{x}, \mathbf{W}) = a^{(3)} = \sigma(\mathbf{Z}^{(3)})$  Activation

- $a_i^{(j)}$ : "activation" of unit i in layer j
- $\mathbf{W}^{(j)}$ : weight matrix that controls function mapping from layer j to layer j+1
- σ() is the activation function
- No bias unit

# Sum it up- with bias unit

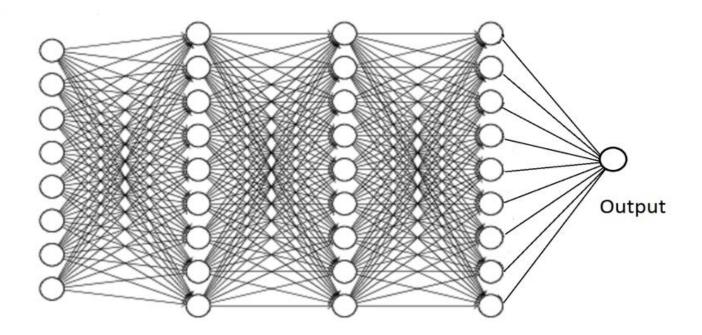




NN is learning its own features  $a_1^{(2)}$ ,  $a_2^{(2)}$ ,  $a_3^{(2)}$ 

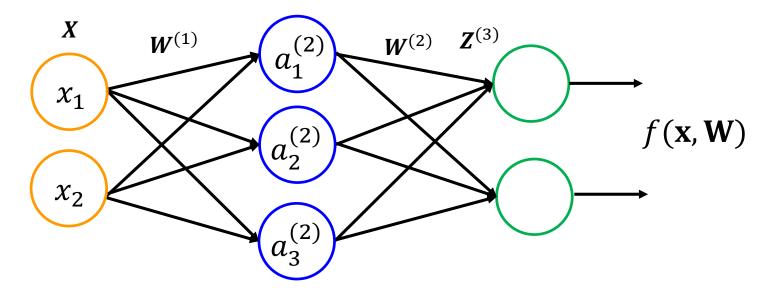


**Architectures** of the neural networks: patterns of connectivity between neurons.



# Multiple output units

Neural networks can also have multiple output units.



For example, in a medical diagnosis application, the vector **x** might give the input features of a patient, and the different outputs might indicate presence or absence of different diseases.



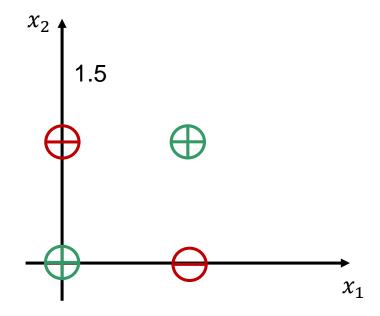
# Forward Propagation 3 Layer Neural Network Example



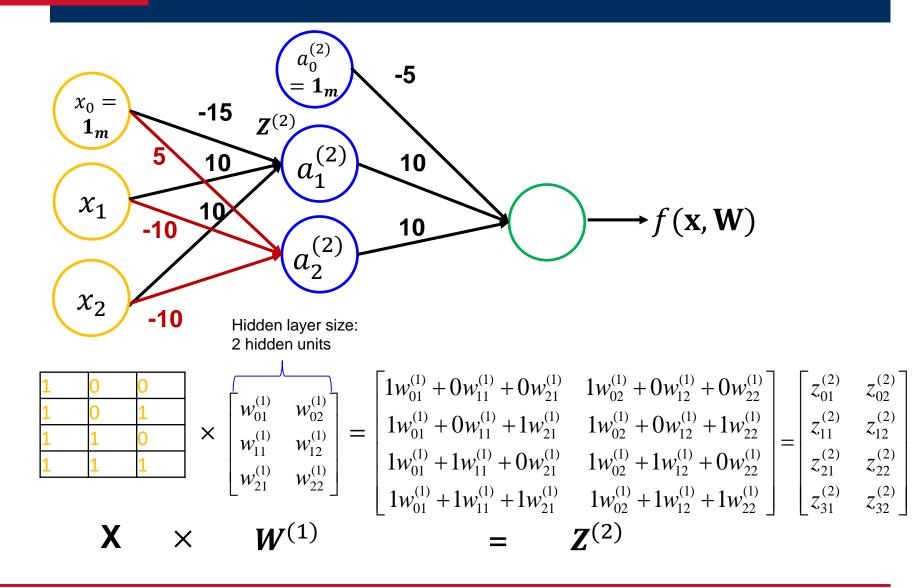
### **XNOR Function**

$x_1$	$x_2$	t
0	0	1
0	1	0
1	0	0
1	1	1

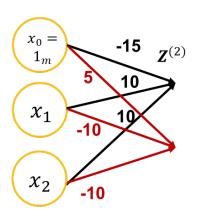
The problem is not linearly separable, or we cannot draw one decision boundary to separate the data







### Step 1



#### Suppose we have

$$\begin{bmatrix} w_{01}^{(1)} & w_{02}^{(1)} \\ w_{11}^{(1)} & w_{12}^{(1)} \\ w_{21}^{(1)} & w_{22}^{(1)} \end{bmatrix} = \begin{bmatrix} -15 & 5 \\ 10 & -10 \\ 10 & -10 \end{bmatrix}$$

$$\left\langle \begin{bmatrix} -15 & 5 \\ 10 & -10 \\ 10 & -10 \end{bmatrix} \right| =$$



#### Step 2

Threshold activation function with threshold at 0 is another common choice.

$$Z^{(2)}$$

$$a_1^{(2)}$$

$$a_2^{(2)}$$

$$\begin{bmatrix} z_{01}^{(2)} & z_{02}^{(2)} \\ z_{11}^{(2)} & z_{12}^{(2)} \\ z_{21}^{(2)} & z_{22}^{(2)} \\ z_{31}^{(2)} & z_{32}^{(2)} \end{bmatrix} = \begin{bmatrix} -15 & 5 \\ -5 & -5 \\ -5 & -5 \\ 5 & -15 \end{bmatrix}$$

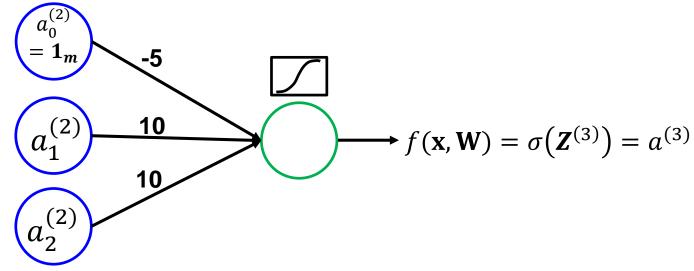
Apply activation function for EACH element of the matrix

$$a^{(2)} = \sigma(\mathbf{Z}^{(2)}) = \begin{bmatrix} \approx 0 & \approx 1 \\ \approx 0 & \approx 0 \\ \approx 0 & \approx 0 \\ \approx 1 & \approx 0 \end{bmatrix}$$

4 by 2 matrix

#### **Step 3&4**

Add the bias unit



Suppose:

$$a^{(2)} = \sigma(\mathbf{Z}^{(2)}) = \begin{bmatrix} 1 & \approx 0 & \approx 1 \\ 1 & \approx 0 & \approx 0 \\ 1 & \approx 0 & \approx 0 \\ 1 & \approx 1 & \approx 0 \end{bmatrix} \quad \mathbf{W}^{(2)} = \begin{bmatrix} w_{01}^{(2)} \\ w_{11}^{(2)} \\ w_{21}^{(2)} \end{bmatrix} = \begin{bmatrix} -5 \\ 10 \\ 10 \end{bmatrix} \qquad \mathbf{Z}^{(3)} = a^{(2)} \mathbf{W}^{(2)}$$

$$4 \times (2+1)$$
  $(2+1) \times 1$   $4 \times 1$ 



$$a^{(2)} = \begin{bmatrix} 1 & \approx 0 & \approx 1 \\ 1 & \approx 0 & \approx 0 \\ 1 & \approx 0 & \approx 0 \\ 1 & \approx 1 & \approx 0 \end{bmatrix}$$

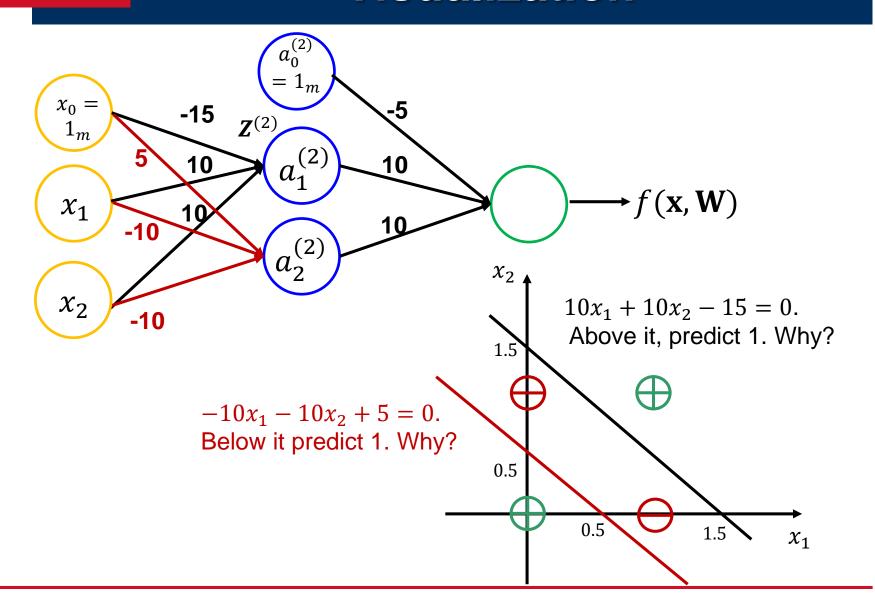
$$a^{(2)} = \begin{vmatrix} 1 & \approx 0 & \approx 1 \\ 1 & \approx 0 & \approx 0 \\ 1 & \approx 0 & \approx 0 \\ 1 & \approx 1 & \approx 0 \end{vmatrix} \qquad \mathbf{W}^{(2)} = \begin{vmatrix} w_{01}^{(2)} \\ w_{11}^{(2)} \\ w_{21}^{(2)} \end{vmatrix} = \begin{bmatrix} -5 \\ 10 \\ 10 \end{bmatrix}$$

$$\mathbf{Z}^{(3)} = a^{(2)}\mathbf{W}^{(2)} = \begin{bmatrix} \approx 5 \\ \approx -5 \\ \approx -5 \\ \approx 5 \end{bmatrix} \qquad f(\mathbf{x}, \mathbf{W}) = a^{(3)} = \sigma(\mathbf{Z}^{(3)}) = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix} \qquad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Try to use threshold activation function with threshold at 0.



#### Visualization



#### **Derivative Exercise**

- Self study/review on derivative summation rule
- Self study/review derivative chain rule
- Calculate the derivative of the following sigmoid function

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

$$\sigma'(z) = ?$$