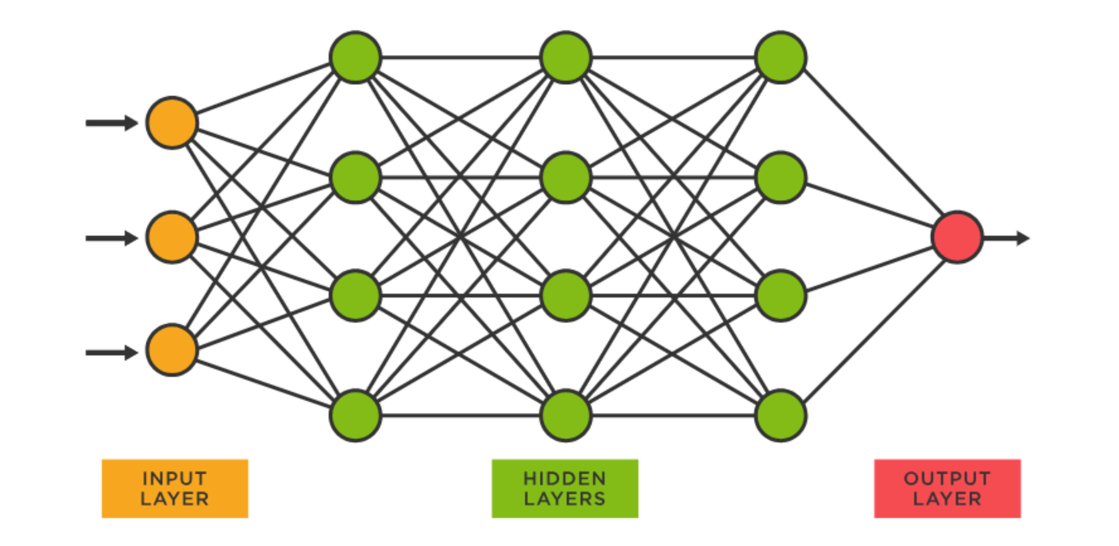
Lecture 9 (FNN)

Feedforward Neural Network

- Neural networks learns a mapping function $f: X \rightarrow Y$ from input features $X \in \mathbb{R}^n$ to output labels Y, where:
  - Classification: Y is discrete (e.g., $Y \in \{1,2,\cdots,k\}$).
  - Regression: Y is continuous (e.g., $Y \in \mathbb{R}$).
- Key components of a neural network:
  - Layers (Depth): define the number of layers. This include the input, hidden, and output layer.
  - Width (Number of neurons per layer): define the number of neurons per layers.
  - Activation function: This will add a layer of non-linearity to allow to model complex relationships
  - Loss function: Measures the difference between the predicted output and the actual target. (MSE [Regression], Cross-entropy [Classification])



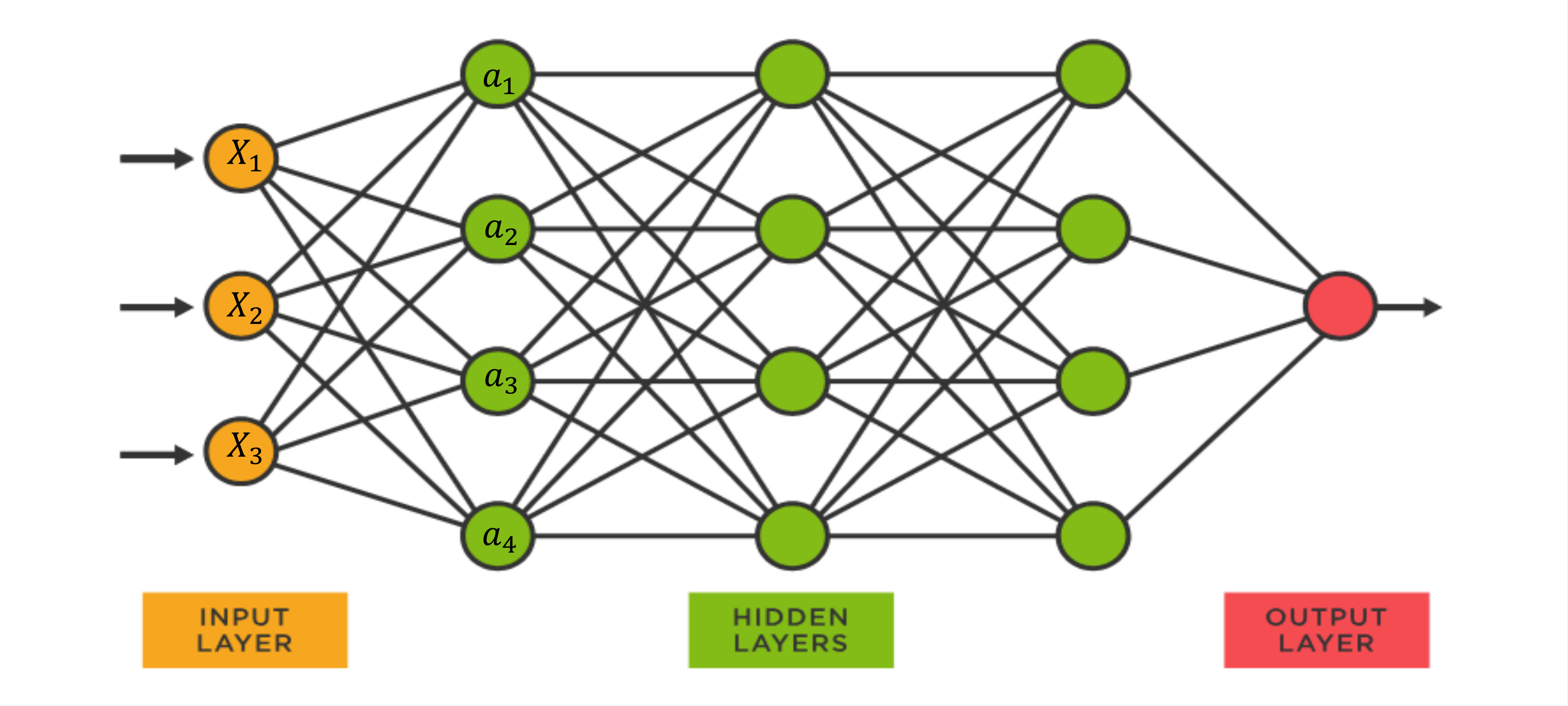
https://www.spotfire.com/glossary/what-is-a-neural-network

Feedforward Neural Network

- $a_1 = f(W_1 X + b_1)$

where $W_1 \in \mathbb{R}^{1\times 3}, X = \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix}, b_1 \in \mathbb{R}$

f is the activation function which could be a linear or a non-linear activation function. The non-linearity will give us the flexibility of modelling non-linear problems.



https://www.spotfire.com/glossary/what-is-a-neural-network

Feedforward Neural Network – Forward Propagation (Classification)

- $a_1 = f\left(W_1^{(1)}X + b_1\right) = \left(W_1^{(1)}X + b_1^{(1)}\right)$; f is a linear activation function.

where

$$W_1^{(1)} = [W_{11} \quad W_{21} \quad W_{31}] \in \mathbb{R}^{1\times 3}$$

$W_{ij}^{(k)}$ (i is the starting node and j is the ending node, and k is the layer)

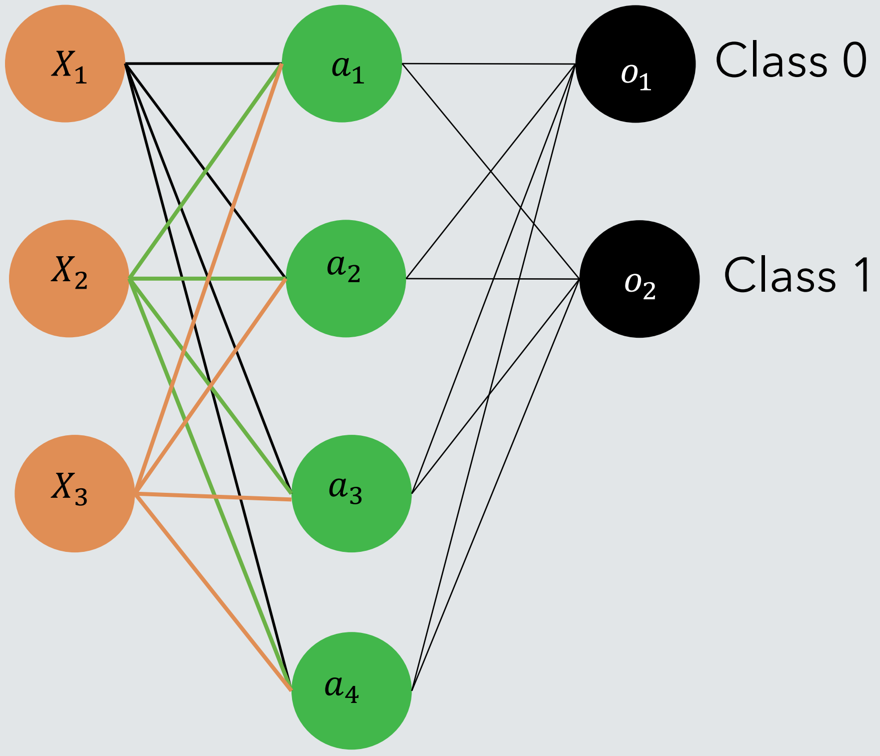
$$X = \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} \in \mathbb{R}^{3\times 1}; b_1^{(1)} \in \mathbb{R}$$

- $o_1 = f\left(W_1^{(2)}a + b_1^{(2)}\right) = f(\hat{o}_1) = \frac{e^{\hat{o}_1}}{e^{\hat{o}_1}+e^{\hat{o}_2}}$; f is a softmax function
- $o_2 = f\left(W_2^{(2)}a + b_2^{(2)}\right) = f(\hat{o}_2) = \frac{e^{\hat{o}_2}}{e^{\hat{o}_1}+e^{\hat{o}_2}}$; f is a softmax function

adds up to 1

- $l = -(y\log(o_2) + (1-y)\log(o_1))$; where y is the true label and $\hat{y}$ is the predicated label

loss



Feedforward Neural Network – Forward Propagation (Classification)

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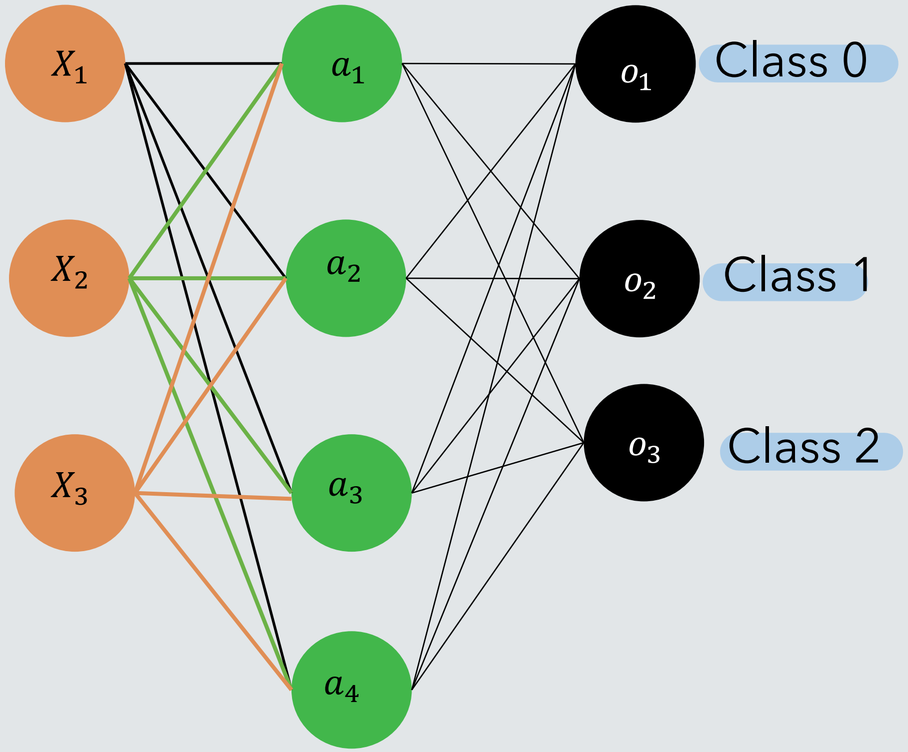
- $o_3 = f\left(W_2^{(2)}a + b_3^{(2)}\right) = f(\hat{o}_3) = \frac{e^{\hat{o}_3}}{e^{\hat{o}_1}+e^{\hat{o}_2}+e^{\hat{o}_3}}$; f is a softmax function
- $l = -\sum_{i=1}^{3} p_i \log(o_i)$; where p_i is the true distribution and o_i is the predicated distribution

↓ cross-entropy loss



Feedforward Neural Network – Forward Propagation (Regression)

- $a_1 = f\left(W_1^{(1)}X + b_1\right) = \left(W_1^{(1)}X + b_1^{(1)}\right)$; f is a linear activation function.

where

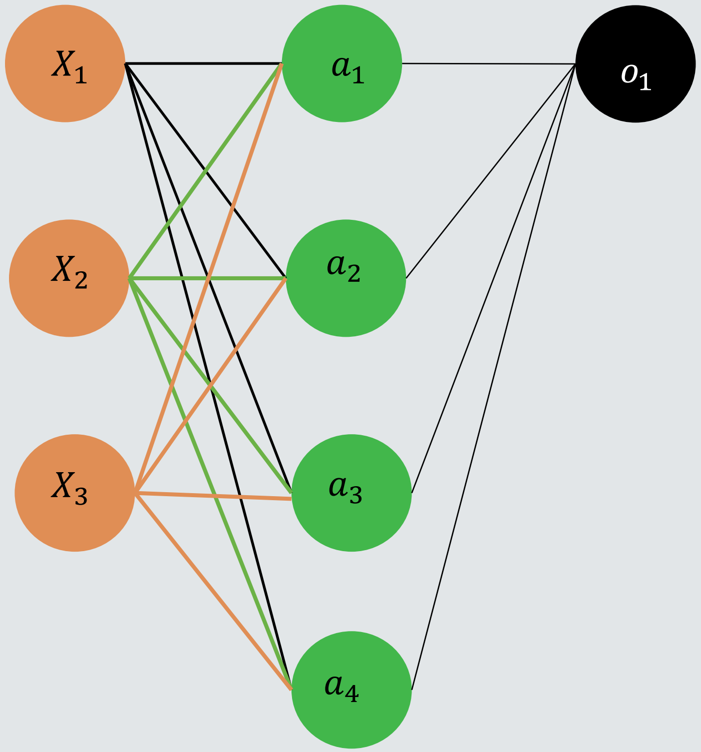
$$W_1^{(1)} = [W_{11} \quad W_{21} \quad W_{31}] \in \mathbb{R}^{1\times3}$$

$W_{ij}^{(k)}$ (i is the starting node and j is the ending node, and k is the layer)

$$X = \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} \in \mathbb{R}^{3\times1}; b_1^{(1)} \in \mathbb{R}$$

- $o_1 = f\left(W_1^{(2)}a + b_1^{(2)}\right) = W_1^{(2)}a + b_1^{(2)}$; f is a linear function
- $l = (y - o_1)^2$ (SE); where y is the true value and o_1 is the predicated value

squared error



Feedforward Neural Network – Forward Propagation (Regression)

- $a_1 = f\left(W_1^{(1)}X + b_1\right) = \left(W_1^{(1)}X + b_1^{(1)}\right)$; f is a linear activation function.

where

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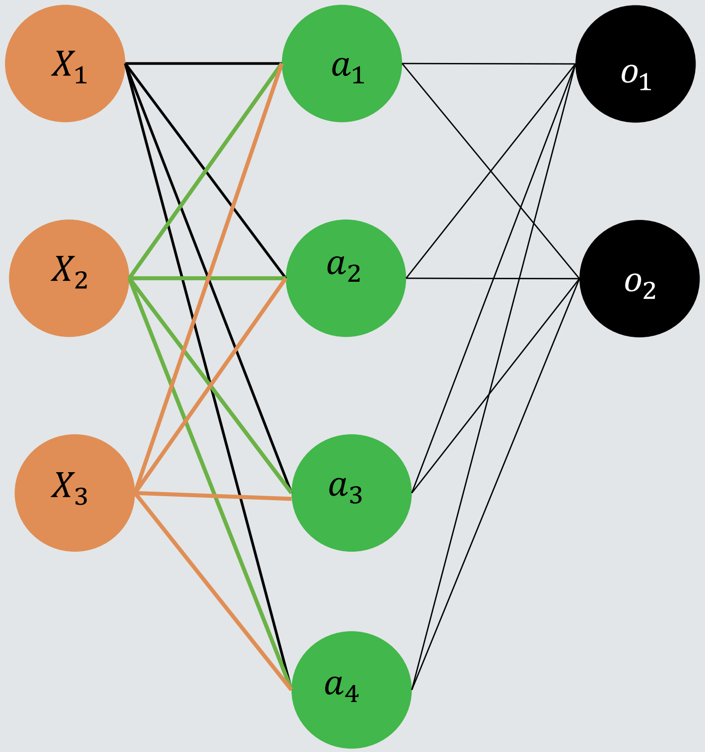
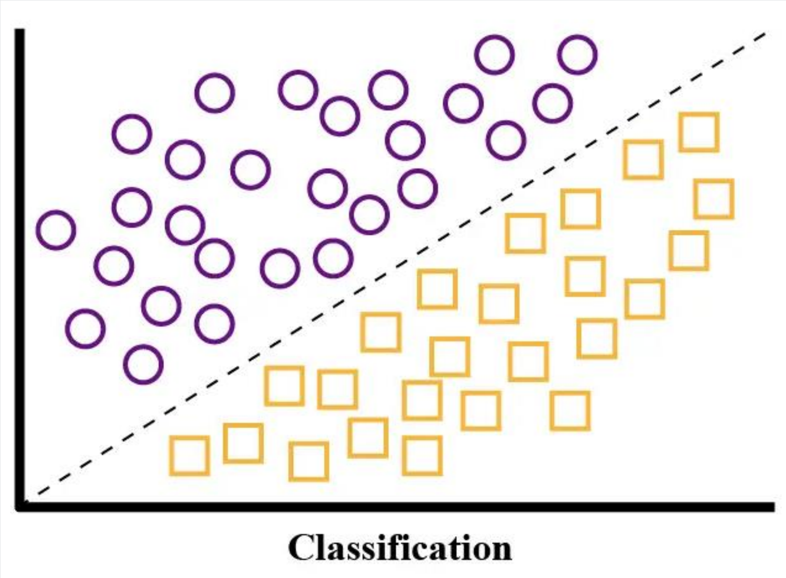
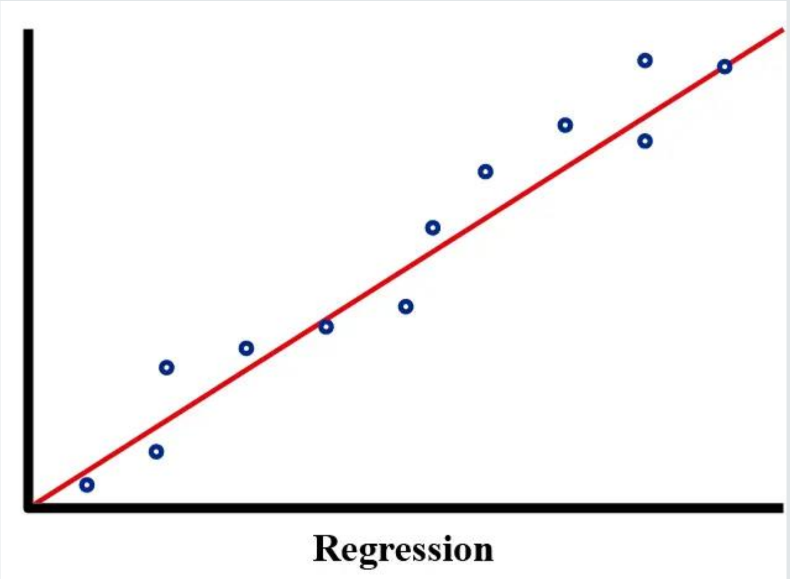
- $o_1 = f\left(W_1^{(2)}a + b_1^{(2)}\right) = W_1^{(2)}a + b_1^{(2)}$; f is a linear function
- $o_2 = f\left(W_2^{(2)}a + b_2^{(2)}\right) = W_2^{(2)}a + b_2^{(2)}$; f is a linear function
- $l = \frac{1}{2}[(y_1 - o_1)^2 + (y_2 - o_2)^2]$ (MSE); where y_1, y_2 is the true value and o_1, o_2 is the predicted value



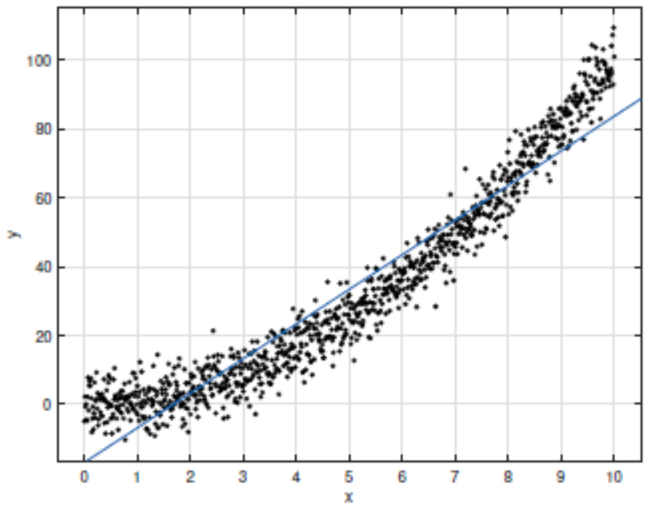
Feedforward Neural Network

- These linear activation functions will allow us to model and capture linear relationships as shown below but it fails in the case of non-linear relationships.

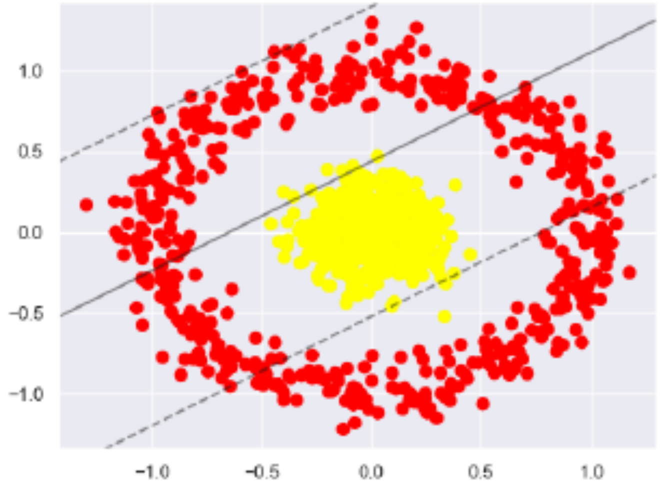




Feedforward Neural Network



(a) Linear Regression on non-linear data



(b) Linear svm on non-linearly separable data

Therefore, we need non-linear activation functions

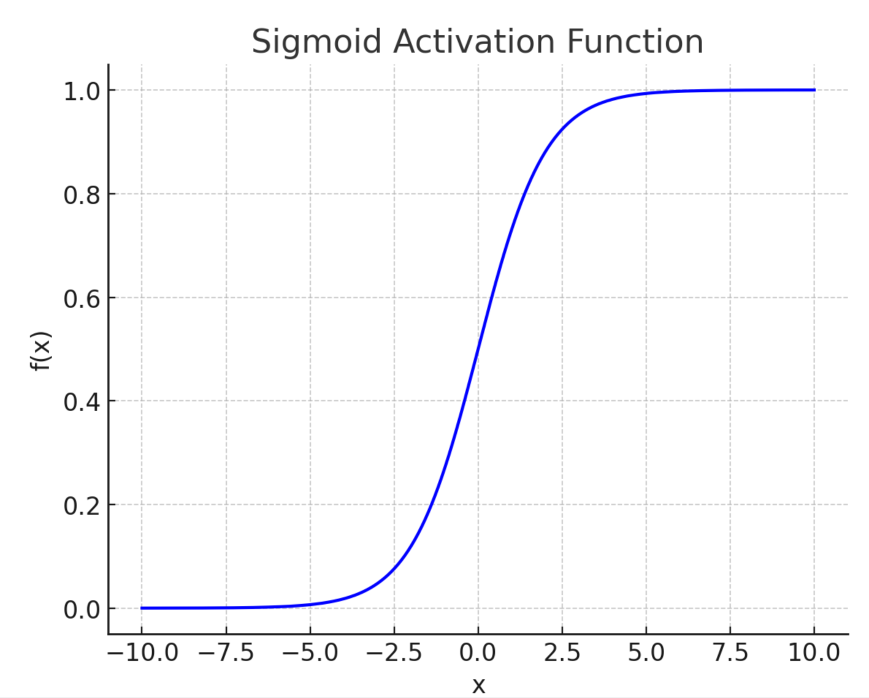
Feedforward Neural Network – Activation Functions

- Activation functions introduce non-linearity into neural networks, enabling them to approximate complex functions. Each function has unique characteristics that impact the network's performance, convergence, and generalization. Below are common activation functions used in neural networks.

Feedforward Neural Network – Activation Functions

- Sigmoid function

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



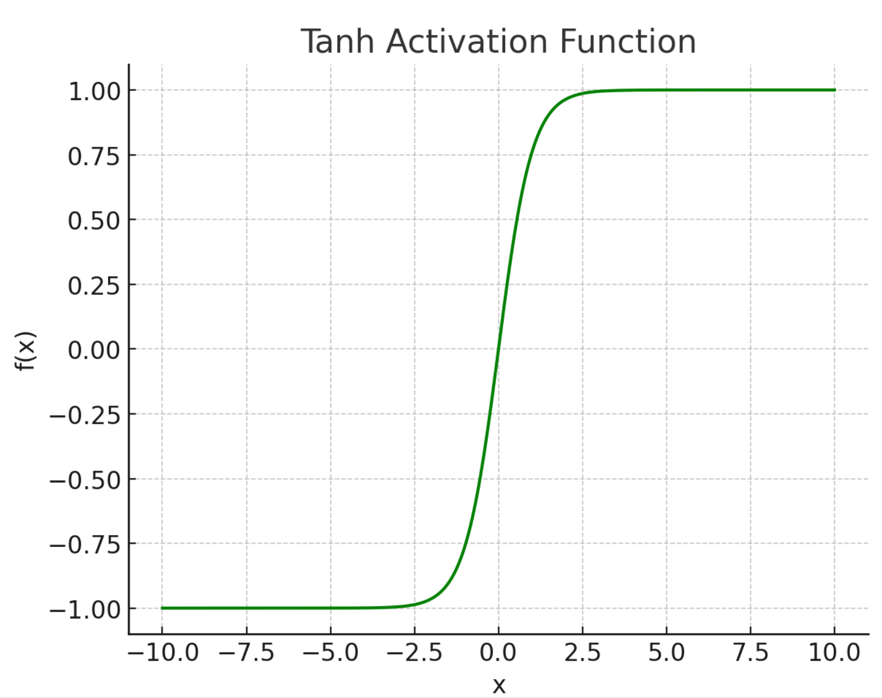
- **Advantages**:
  - *Smooth gradient, useful for binary classification.*
  - *Output values between 0 and 1, which can represent probabilities.*

- **Disadvantages:**
  - *Vanishing gradient problem for large or small inputs, slowing down training.*

Feedforward Neural Network – Activation Functions

- Tanh function

$$f(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$



- **Advantages**:
  - *Zero-centered output, which helps faster convergence*
  - *Larger gradients compared to sigmoid, reducing vanishing gradient*

- **Disadvantages:**
  - *Still suffers from the vanishing gradient problem, especially in deep networks.*

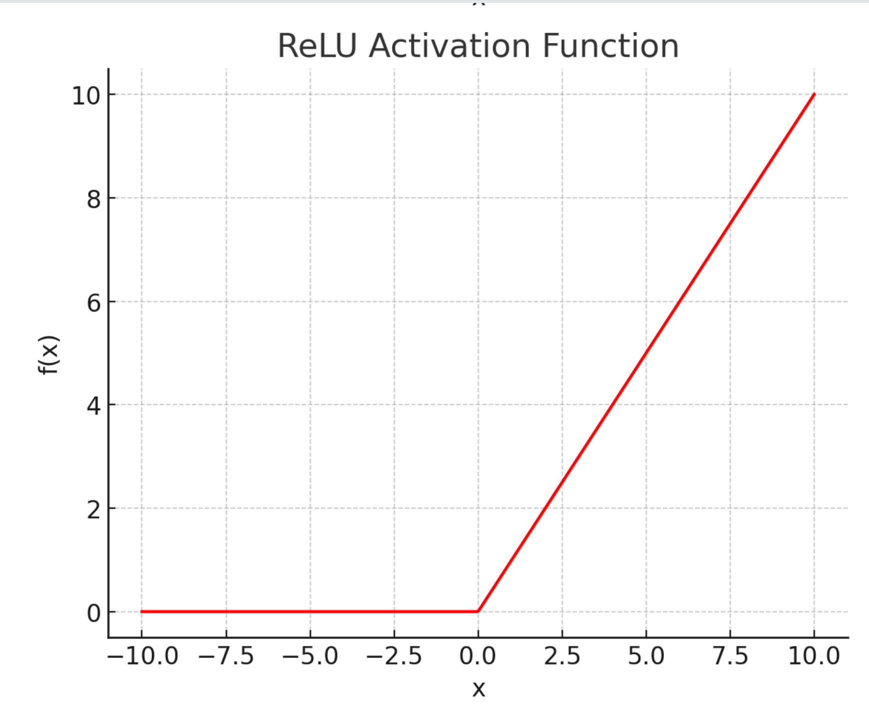
more layers

Feedforward Neural Network – Activation Functions

- Relu function

$$\boxed{f(x) = \max(0, x)}$$

- **Advantages**:
  - Solves vanishing gradient problem for positive values
- **Disadvantages:**
  - *Dead neurons issue, where certain neurons always output zero and stop learning.*
  - *Can cause gradient explosion in certain cases.*



Feedforward Neural Network – Activation Functions

- Add something about 0/1 function and the difficultity of optimization

Feedforward Neural Network – Forward Propagation (Classification)

- $a_1 = f\left(W_1^{(1)}X + b_1\right) = \begin{cases} \max\left(0, W_1^{(1)}X + b_1\right); f \text{ } is \text{ } a \text{ } relu \text{ } function \\ \frac{1}{1+e^{-W_1^{(1)}X+b_1}}; f \text{ } is \text{ } a \text{ } sigmoid \text{ } function \\ \frac{e^{W_1^{(1)}X+b_1} - e^{-W_1^{(1)}X+b_1}}{e^{W_1^{(1)}X+b_1} + e^{-W_1^{(1)}X+b_1}}; f \text{ } is \text{ } a \tanh function \end{cases}$

where

$$W_1^{(1)} = [W_{11} \quad W_{21} \quad W_{31}] \in \mathbb{R}^{1\times 3}$$

$$W_{ij}^{(k)} (\text{i is the starting node and j is the ending node, and k is the layer})$$

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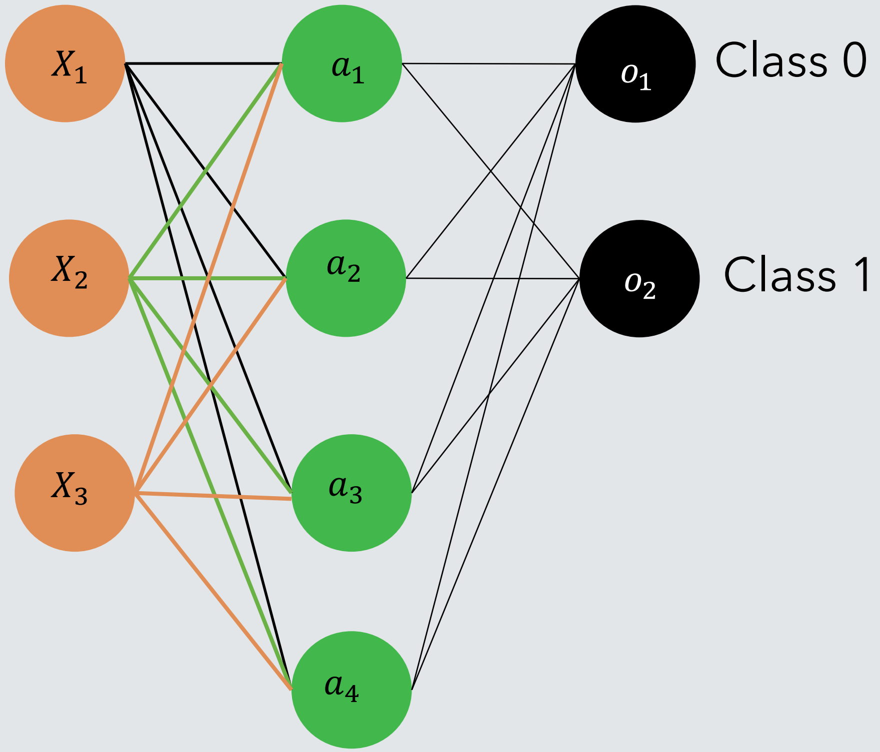
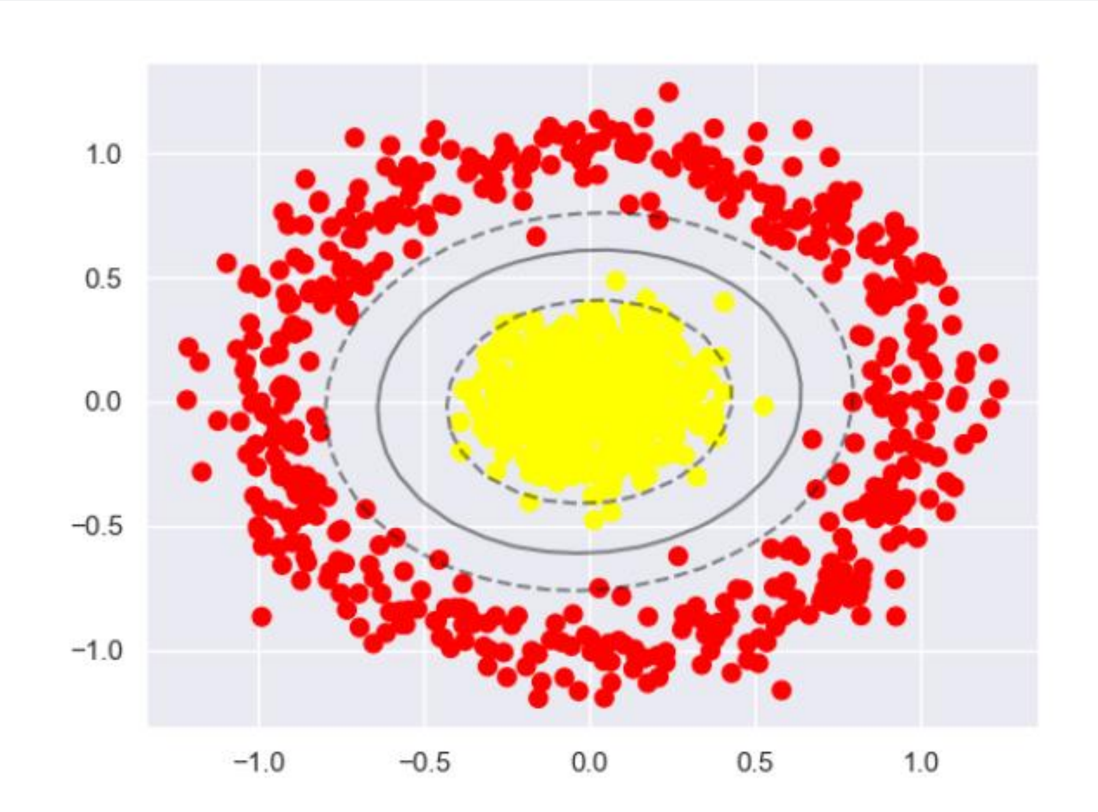
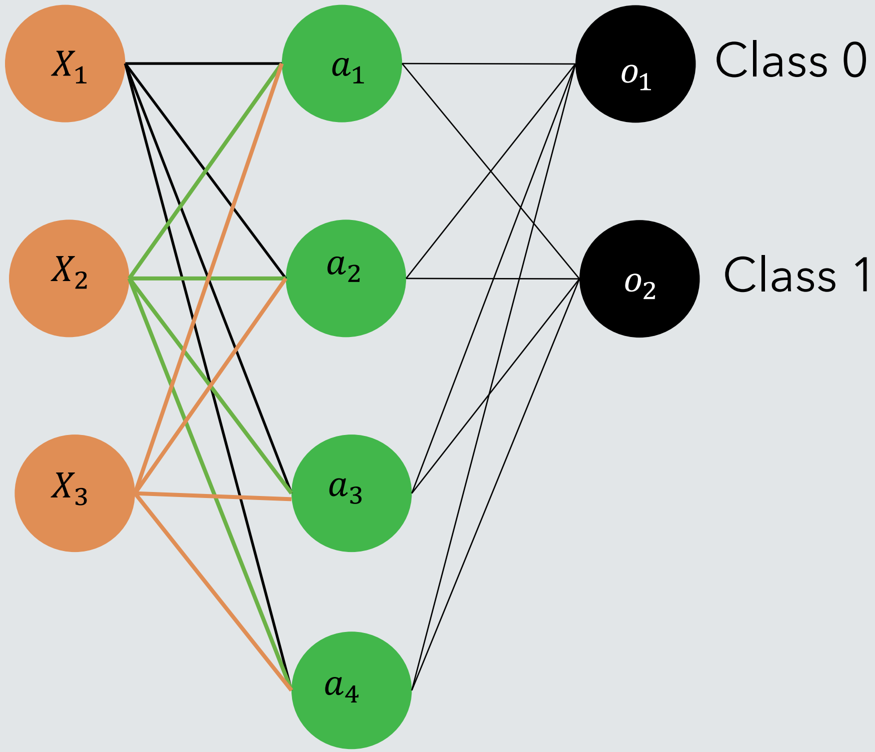
- $l = -(y\log(o_2) + (1-y)\log(o_1))$; where y is the true label and $\hat{y}$ is the predicated label



Feedforward Neural Network – Forward Propagation (Classification)





Feedforward Neural Network

Wait!

How do we calculate all of the weights and biases of the neural network?

Feedforward Neural Network – Backpropagation (Regression)

- $a_1 = \left(W_1^{(1)} X + b_1^{(1)}\right)$

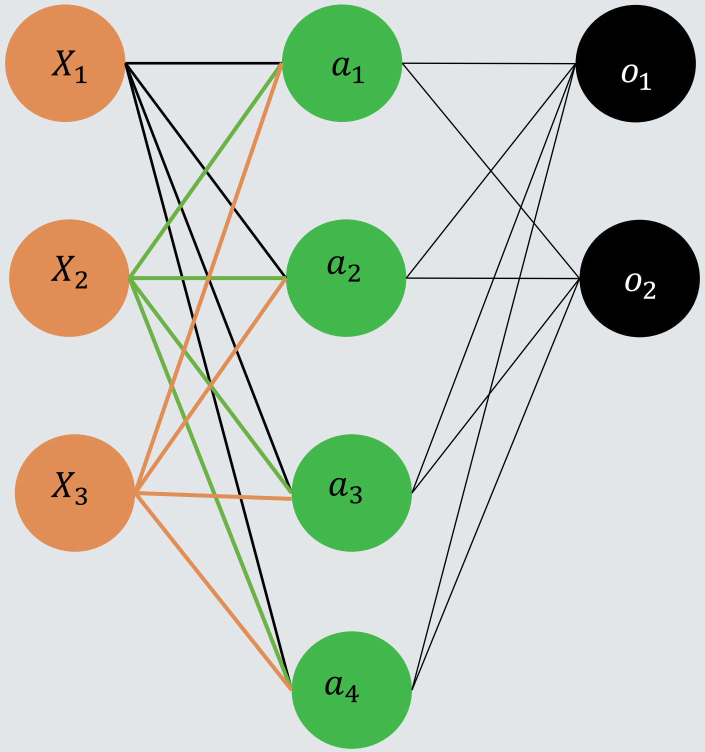
$$W_1^{(1)} = \begin{bmatrix} W_{11}^{(1)} & W_{21}^{(1)} & W_{31}^{(1)} \end{bmatrix} \in \mathbb{R}^{1\times 3}$$

$$X = \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} \in \mathbb{R}^{3\times 1};\ b_1^{(1)} \in \mathbb{R}$$

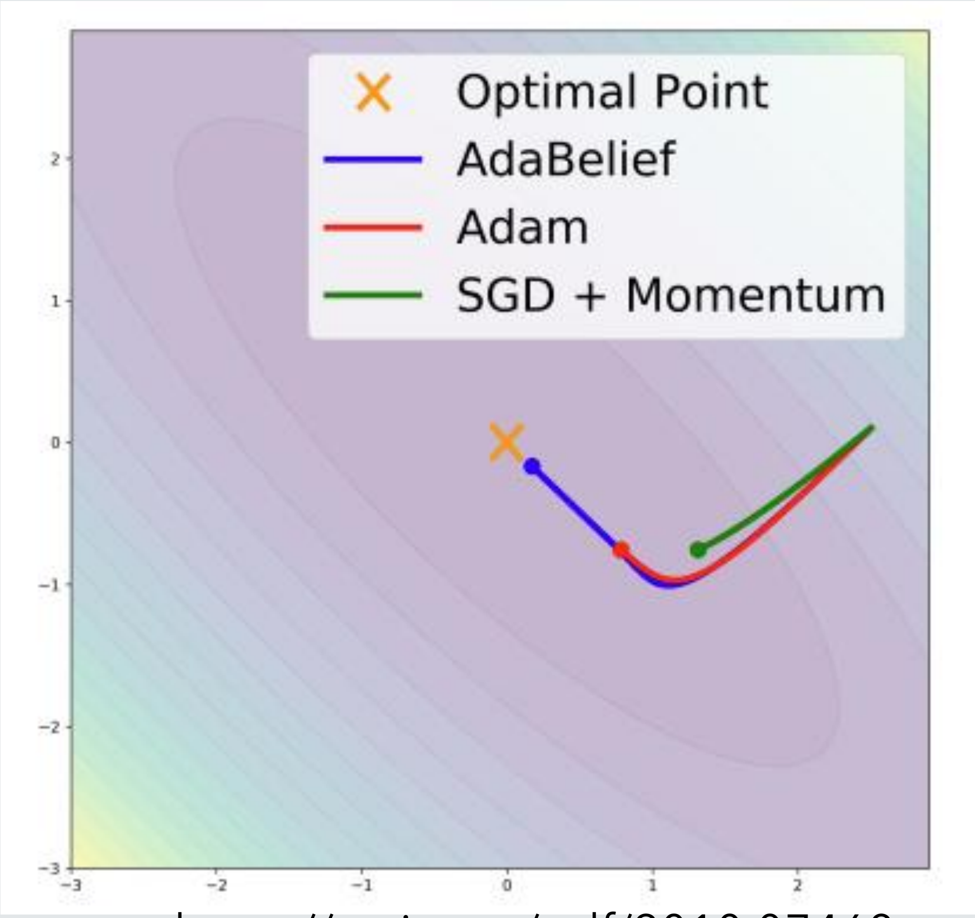
- $o_1 = W_1^{(2)} a + b_1^{(2)};\ o_2 = W_2^{(2)} a + b_2^{(2)}$
- $l = \frac{1}{2}[(y_1 - o_1)^2 + (y_2 - o_2)^2]$
- How to update the weights and biases?

$$\min_{W_{11}^{(1)}, W_{21}^{(1)}, W_{31}^{(1)}, W_{12}^{(1)}, W_{22}^{(1)}, W_{32}^{(1)}, W_{13}^{(1)}, W_{23}^{(1)}, W_{33}^{(1)}, W_{11}^{(2)}, W_{21}^{(2)}, \ldots} l$$

- There are several optimizier that will be used:
- Stochastic Gradient Descent
- SGD with momentum
- Adam



Feedforward Neural Network – Backpropagation (Regression)



https://arxiv.org/pdf/2010.07468

Feedforward Neural Network – Backpropagation (Regression)

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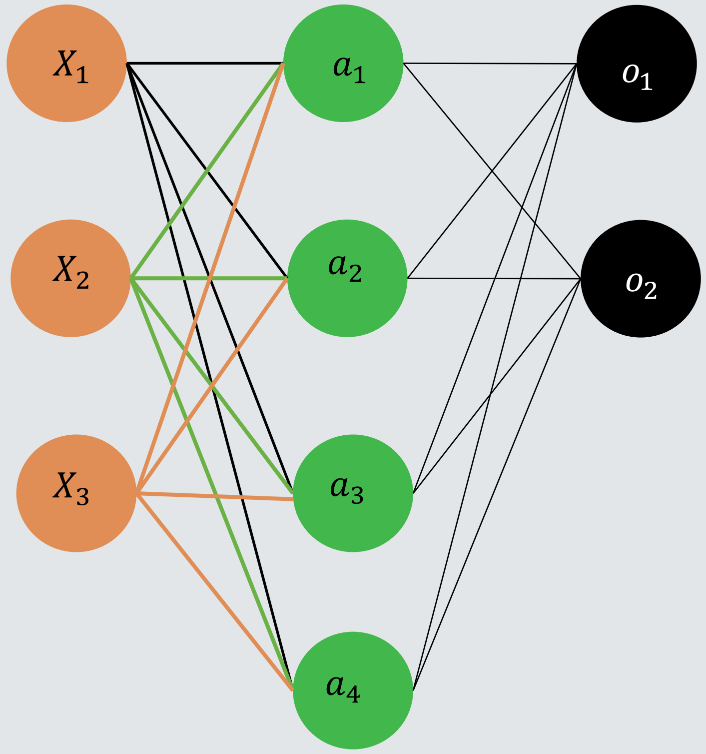
- $o_1 = W_1^{(2)} a + b_1^{(2)};\, o_2 = W_2^{(2)} a + b_2^{(2)}$
- $l = \frac{1}{2}[(y_1 - o_1)^2 + (y_2 - o_2)^2]$ → MSE
- $W_{11}^{(2)} = W_{11}^{(2)} - \eta \frac{\partial l}{\partial W_{11}^{(2)}} = W_{11}^{(2)} - \eta \frac{\partial o_1}{\partial W_{11}^{(2)}} \frac{\partial l}{\partial o_1}$

$$= W_{11}^{(2)} - \eta \frac{\partial o_1}{\partial W_{11}^{(2)}} \frac{\partial}{\partial o_1} \left(\frac{1}{2}[(y_1 - o_1)^2 + (y_2 - o_2)^2]\right)$$

$$= W_{11}^{(2)} - \eta \frac{\partial}{\partial W_{11}^{(2)}} \left[W_{11}^{(2)} a_1 + W_{21}^{(2)} a_2 + W_{31}^{(2)} a_3 + W_{41}^{(2)} a_4\right] (-(y_1 - o_1)) = W_{11}^{(2)} - \eta a_1$$



The same procedure will be done for all of the weights and biases in the neural network.

Feedforward Neural Network – Forward Propagation (Regression)

- $a_1 = f\left(W_1^{(1)}X + b_1\right) = \begin{cases} \max\left(0, W_1^{(1)}X + b_1\right); f \text{ is a relu function} \\ \frac{1}{1+e^{-W_1^{(1)}X+b_1}}; f \text{ is a sigmoid function} \\ \frac{e^{W_1^{(1)}X+b_1} - e^{-W_1^{(1)}X+b_1}}{e^{W_1^{(1)}X+b_1} + e^{-W_1^{(1)}X+b_1}}; f \text{ is a tanh function} \end{cases}$

where

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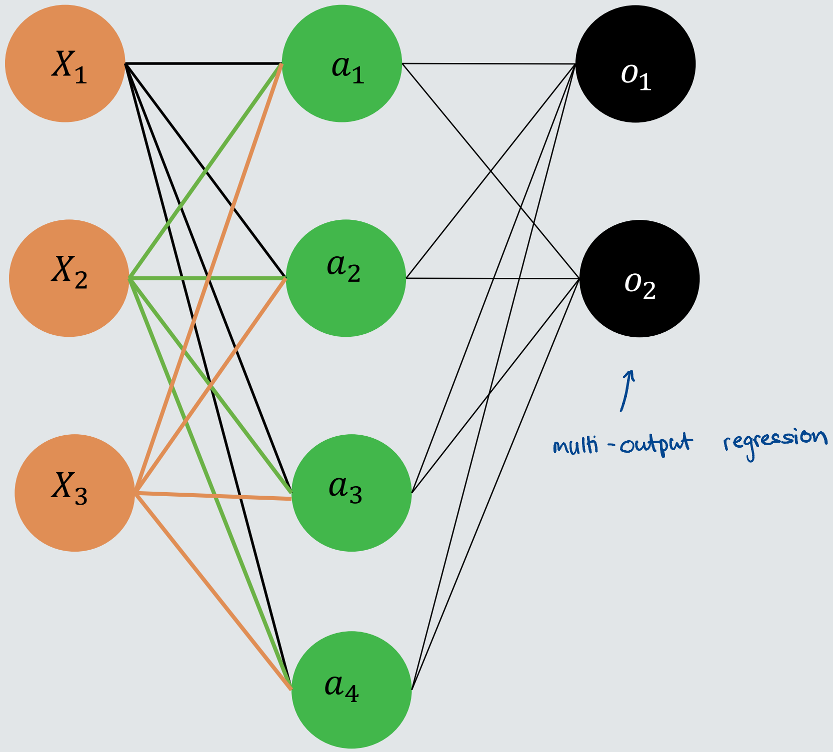
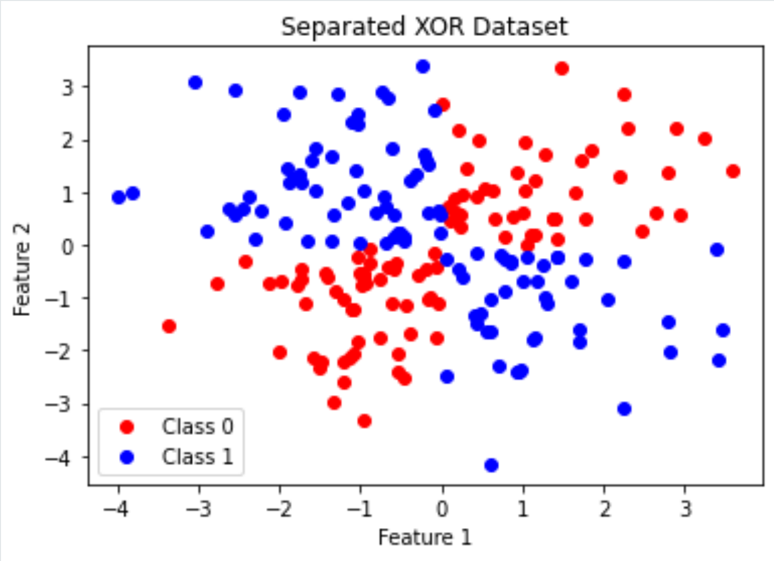
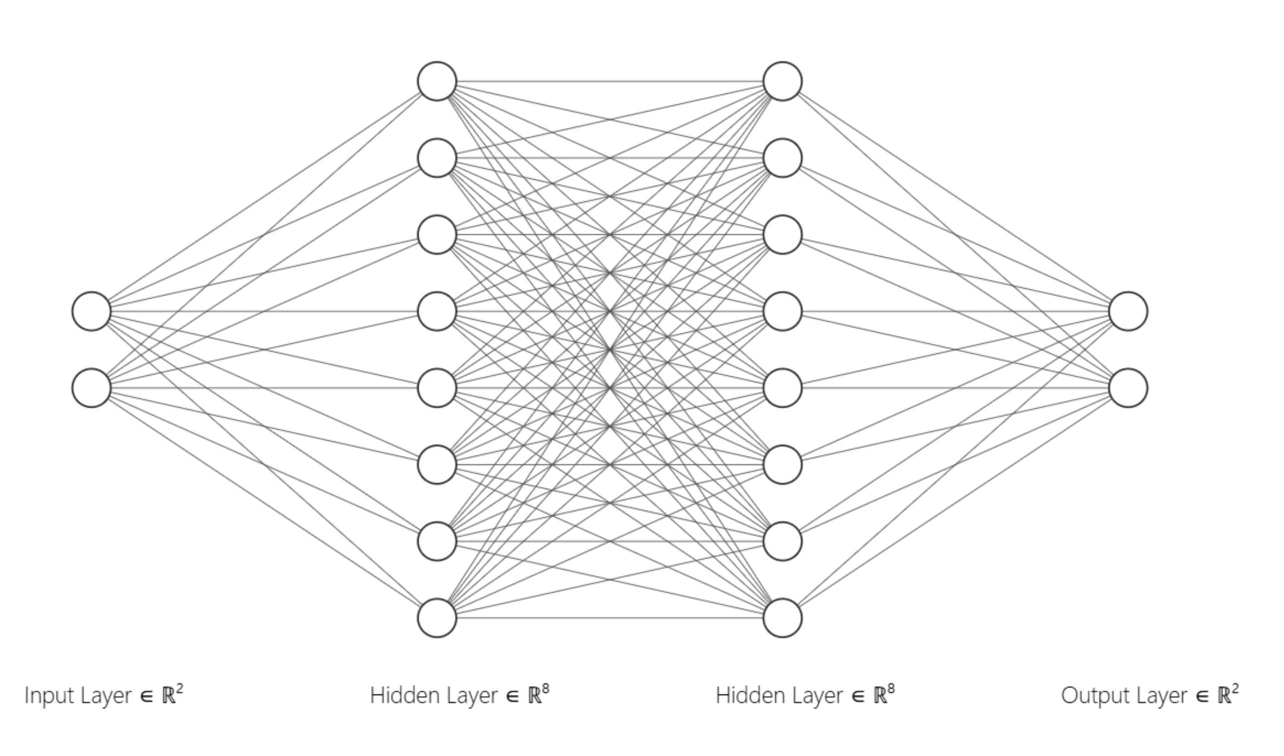
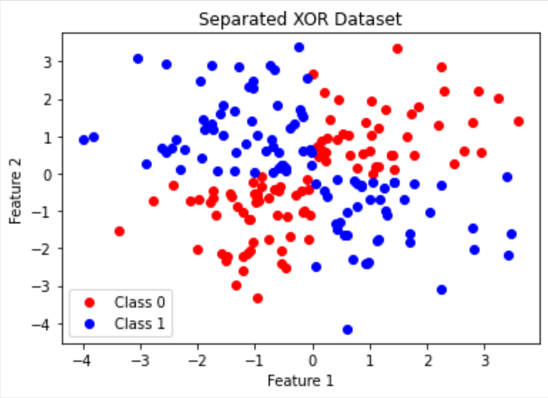


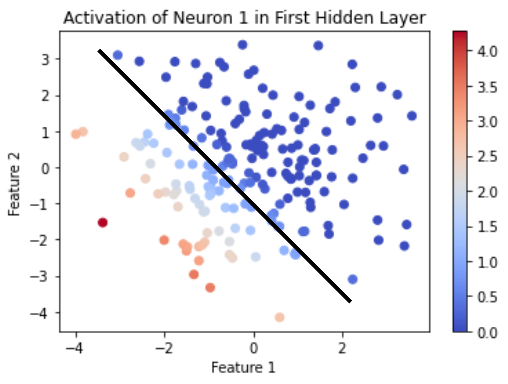
Feedforward Neural Network

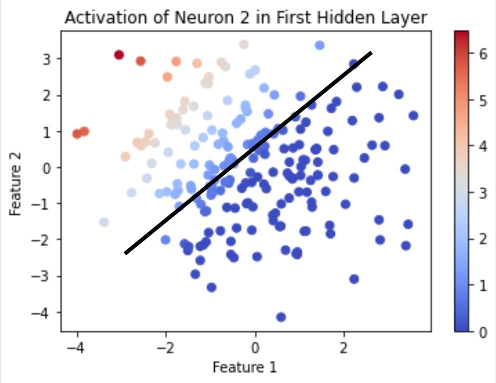


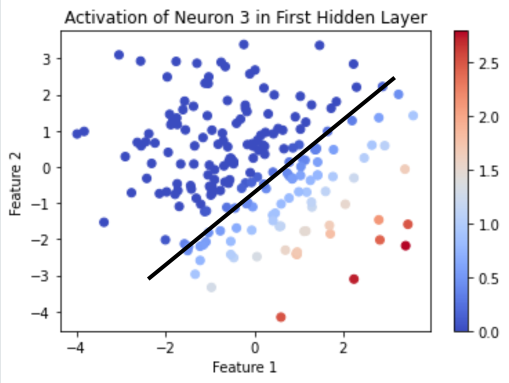


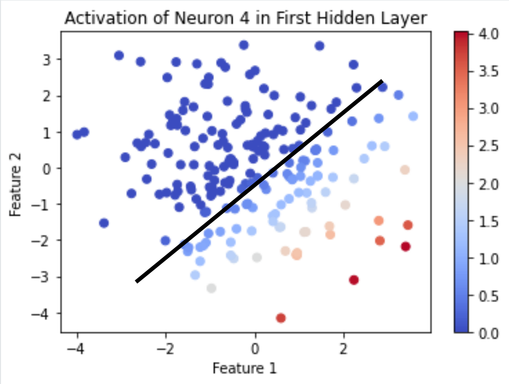
Feedforward Neural Network

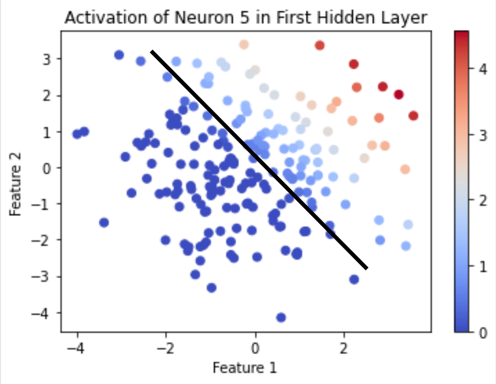


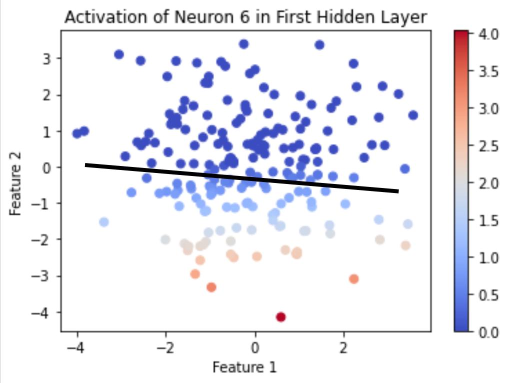


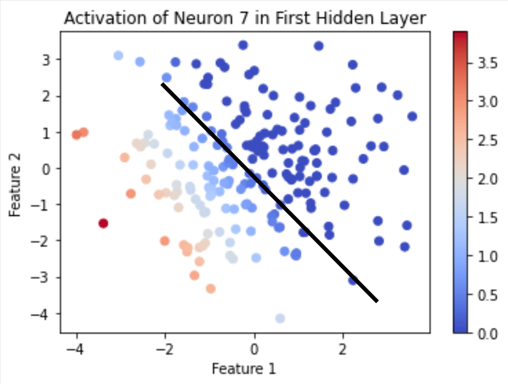


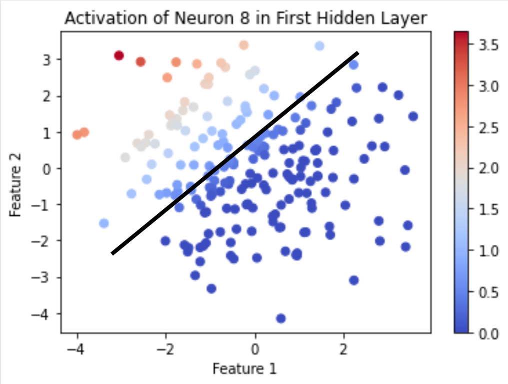


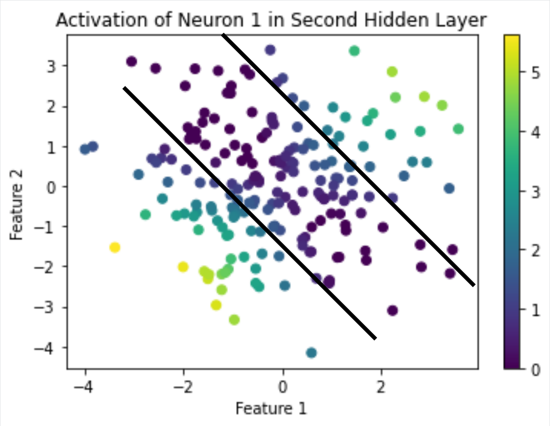


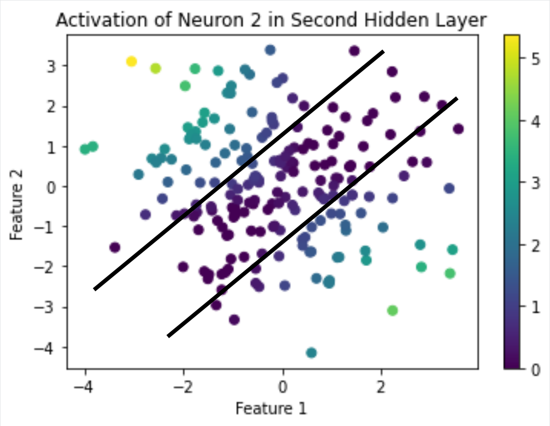


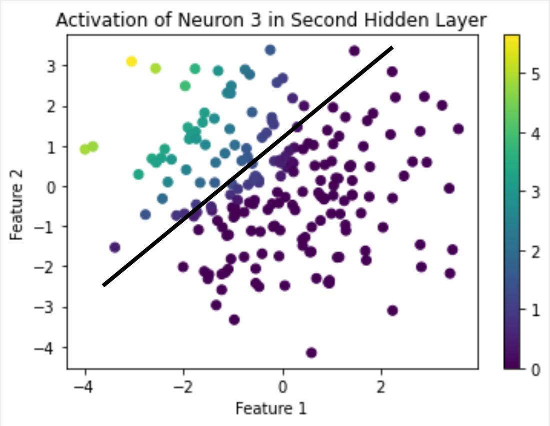


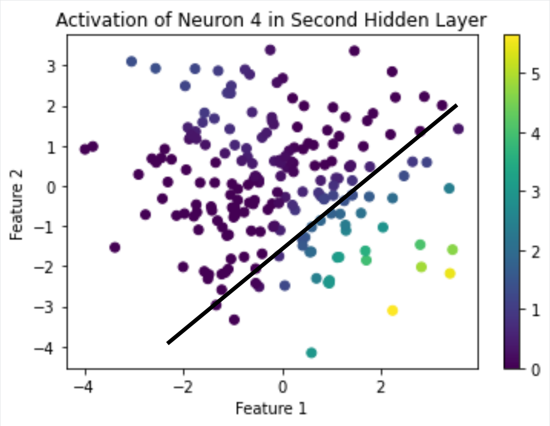


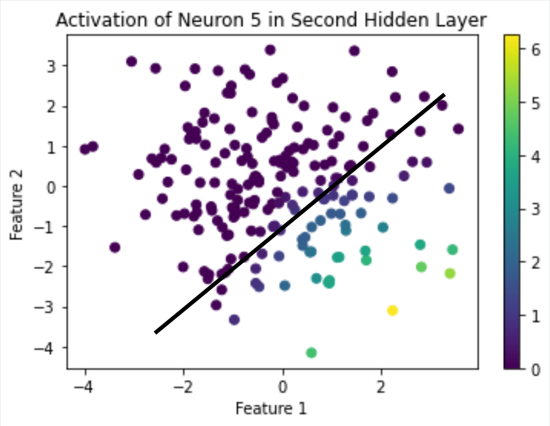


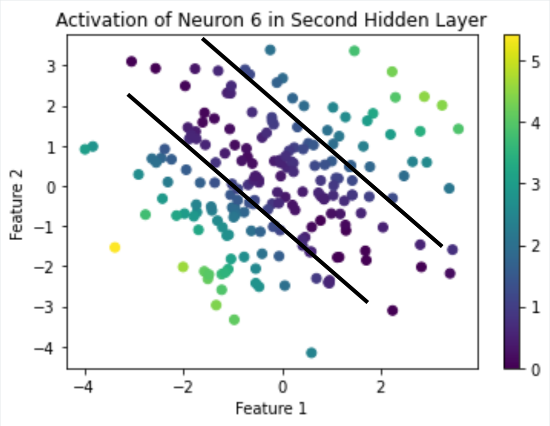

Activation of Neuron 1 in Second Hidden Layer
Feature 1
Feature 2

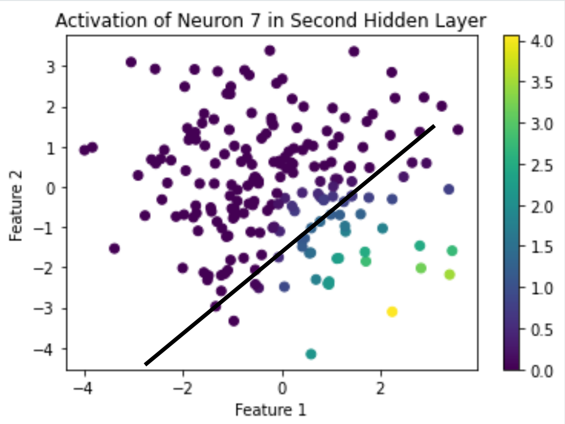

Activation of Neuron 2 in Second Hidden Layer
Feature 1
Feature 2

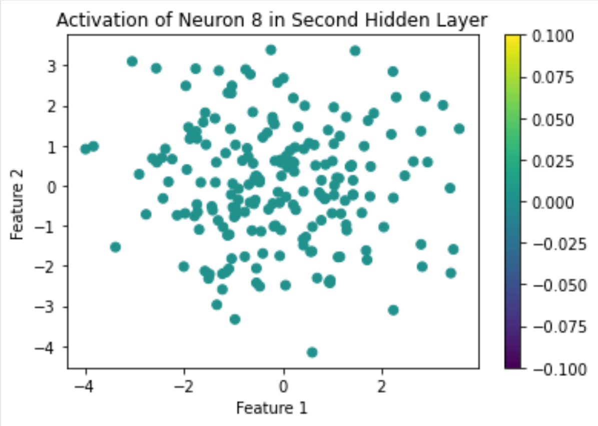

Activation of Neuron 3 in Second Hidden Layer
Feature 1
Feature 2


Activation of Neuron 4 in Second Hidden Layer
Feature 1
Feature 2

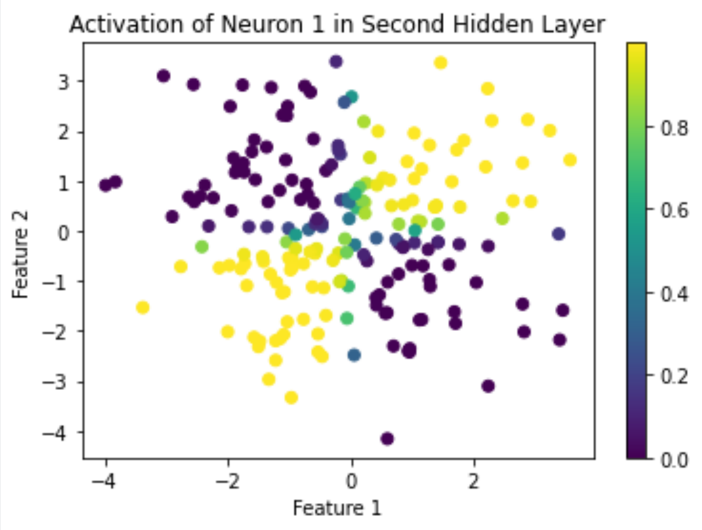

Activation of Neuron 5 in Second Hidden Layer
Feature 1
Feature 2

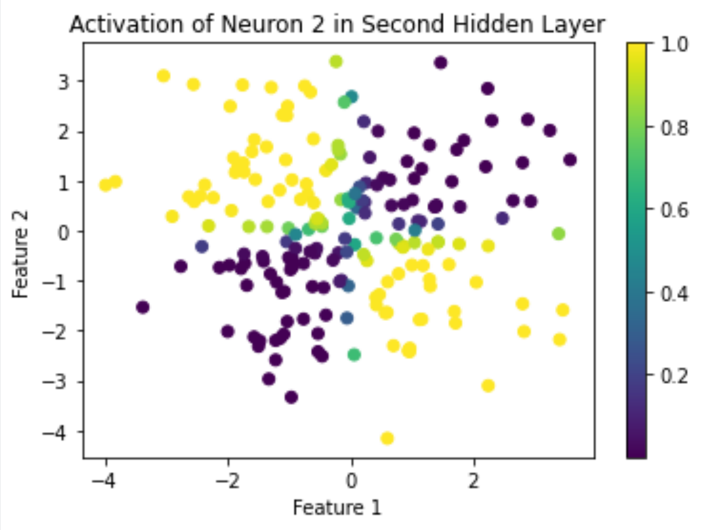

Activation of Neuron 6 in Second Hidden Layer
Feature 1
Feature 2

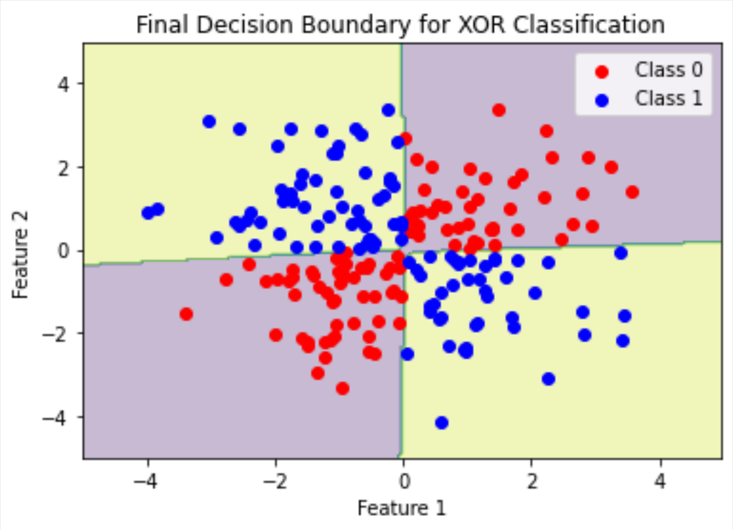

Activation of Neuron 7 in Second Hidden Layer
Feature 1
Feature 2


Activation of Neuron 8 in Second Hidden Layer
Feature 1
Feature 2

Feedforward Neural Network







Feedforward Neural Network – Weight Initialization

- Random Initialization: weights are random initialization, typically from a uniform or normal distribution. The issue with this initialization that it can leaf to large or small gradients that can cause slow convergence or divergence.

  Advantages: Allows neurons to learn different features

  Disadvantages: Without further scaling, it can lead to large or small gradients, causing small convergence or divergence.

- He Initialization: specifically designed for Relu activation

$$W \sim Normal\left(0, \sqrt{\frac{2}{n_{in}}}\right)$$

  Ensures that the variance of the weights does not shrink or explode.

- Xavier Initialization: or layer l, weights are initialized with a uniform or normal distribution scaled by

$$W \sim Uniform\left(-\frac{\sqrt{6}}{\sqrt{n_{in}+n_{out}}}, \frac{\sqrt{6}}{\sqrt{n_{in}+n_{out}}}\right)$$

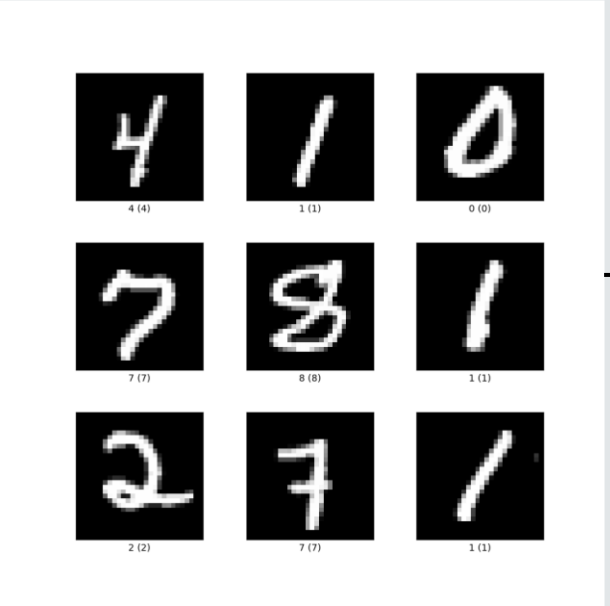
where n_{in} and n_{out} are the number of input and output units in the layer.

  Balances the variance across layers, making it suitable for sigmoid and tanh activations.

Feedforward Neural Network – Wider vs Deeper

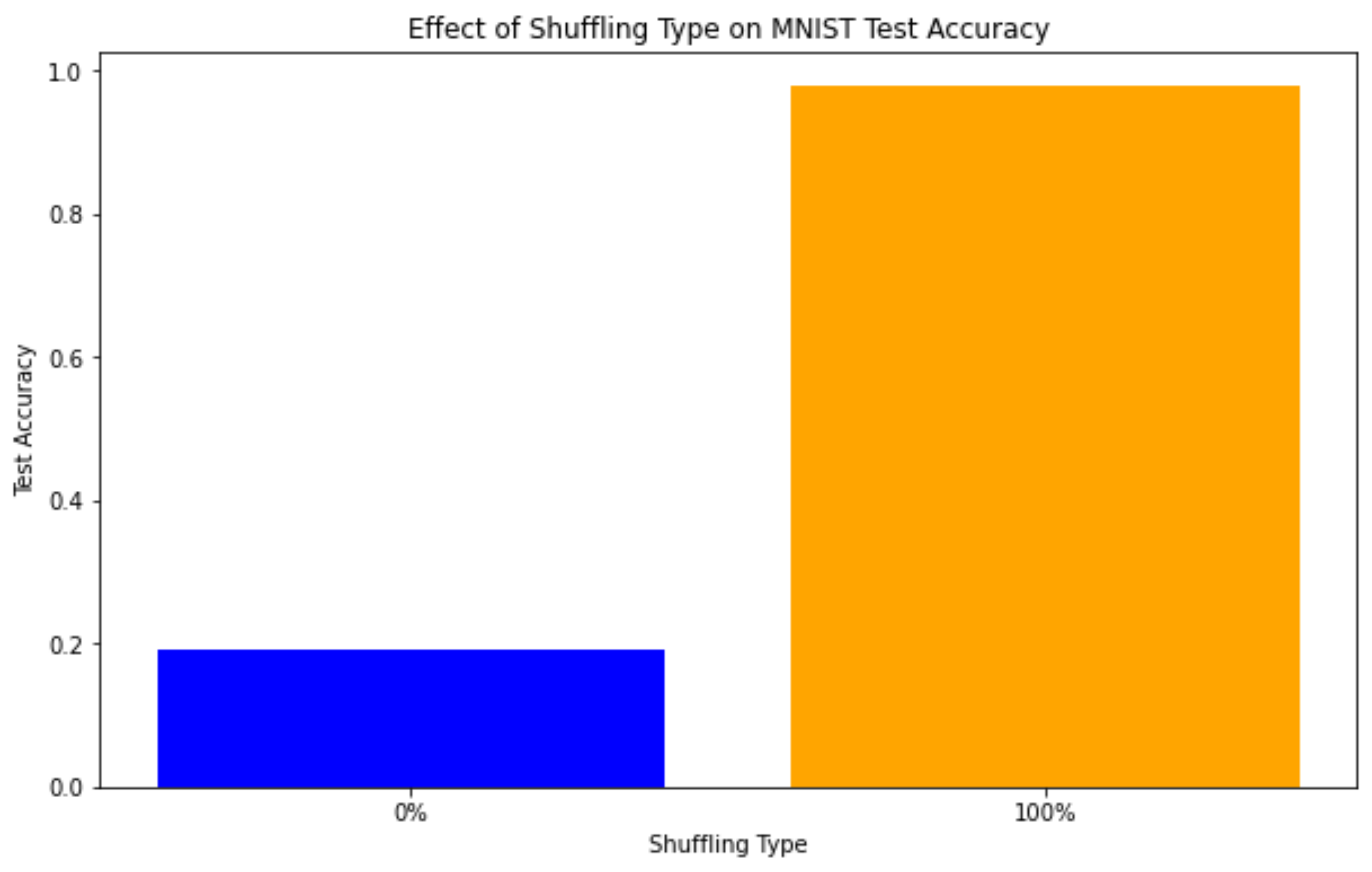
- **Are there functions that can be expressed by wide and shallow neural networks, that cannot be approximated by any narrow neural network, unless its depth is very large?**
- (Correct) On the other hand, if the answer is negative, then depth generally plays a more significant role than width for the expressive power of neural networks. [Proven in https://proceedings.mlr.press/v178/vardi22a/vardi22a.pdf]
- (Wrong) If the answer is positive, then width and depth, in principle, play an incomparable role in the expressive power of neural networks, as sometimes depth can be more significant, and sometimes width.

Feedforward Neural Network – MNIST



Neural Network

Feedforward Neural Network – MNIST



Feedforward Neural Network – MNIST