Introduction to Neural Networks for CAP4453
Single Neuron

Basic computational unit of Neural Network
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**Inputs** \((x_1, x_2)\) : Data you want to model.

\[ x_1 = 2 \]
\[ x_2 = 5 \]
Single Neuron

Basic computational unit of Neural Network

**Inputs** \((x_1, x_2)\) : Data you want to model.

**Weights** \((w_1, w_2)\) : Model Parameters

\[
\begin{align*}
x_1 &= 2 \\
x_2 &= 5 \\
w_1 &= 0.5 \\
w_2 &= -0.3
\end{align*}
\]
Single Neuron

Basic computational unit of Neural Network

**Inputs** \((x_1, x_2)\) : Data you want to model.

**Weights** \((w_1, w_2)\) : Model Parameters

**Bias** \((b)\) : Model parameter to account for Noise

\[ x_1 = 2 \quad w_1 = .5 \]
\[ x_2 = 5 \quad w_2 = -0.3 \]
\[ b = .1 \]
**Single Neuron**

Basic computational unit of Neural Network

**Inputs (x1, x2)**: Data you want to model.

**Weights (w1, w2)**: Model Parameters

**Bias (b)**: Model parameter to account for Noise

Computation step 1 - Weighted Summation to perform Linear modelling

\[
 z = w_1 \cdot x_1 + w_2 \cdot x_2 + b
\]

\[
 w_1 = 0.5, \quad w_2 = -0.3, \quad b = 0.1
\]

\[
 x_1 = 2, \quad x_2 = 5
\]

\[
 z = 0.5 \cdot 2 + 5 \cdot (-0.3) + 0.1 = -0.4
\]
**Single Neuron**

Basic computational unit of Neural Network

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**Computation step 1 - Weighted Summation to perform Linear modelling**

\[
z = w_1 \times x_1 + w_2 \times x_2 + b
\]

**Computation step 2 - Adding Non Linearity**

\[
a = \sigma(z), \text{ where } \sigma(z) = \frac{1}{1 + e^{-z}}
\]

The Vertical Segment is the reminder to do the Non-linear step.
Single Neuron

Basic computational unit of Neural Network

Inputs \((x_1, x_2)\) : Data you want to model.

Weights \((w_1, w_2)\) : Model Parameters

Bias \((b)\) : Model parameter to account for Noise

Computation step 1 - Weighted Summation to perform Linear modelling

\[
z = w_1 * x_1 + w_2 * x_2 + b \quad \text{or} \quad z = w^T x + b
\]

Computation step 2 - Adding Non Linearity

\[
a = \sigma(z), \quad \text{where } \sigma(z) = \frac{1}{1 + e^{-z}}
\]

Output - \(\hat{y}\)

The Vertical Segment is the reminder to do the Non-linear step.
Activation Function

Adds Non-Linearity to the Neural Network to fit Non-Linear patterns

**Sigmoid**

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

**Tanh**

$g(z) = \tanh(z)$

**ReLU**

$g(z) = \max(0, z)$

**Leaky ReLU**

$g(z) = \max(0.01z, z)$

Each Activation Function has pros and cons (http://cs231n.github.io/neural-networks-1/#intro)
A Simple Example for Neural Network

The Collection of Neurons is organized in three main layers:
A Simple Example for Neural Network

The Collection of Neurons is organized in three main layers: the input layer
A Simple Example for Neural Network

The Collection of Neurons is organized in three main layers: the **input** layer, the **hidden** layer
A Simple Example for Neural Network

The Collection of Neurons is organized in three main layers: the **input** layer, the **hidden** layer, and the **output** layer
A Simple Example for Neural Network

The Collection of Neurons is organized in three main layers: the **input** layer, the **hidden** layer, and the **output** layer.

A neural network can have many hidden layers.
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A neural network can have many hidden layers.

In an artificial neural network, there are several inputs, which are called features, and produce a single output.
A Simple Example for Neural Network

The Collection of Neurons is organized in three main layers: the input layer, the hidden layer, and the output layer.

A neural network can have many hidden layers.

In an artificial neural network, there are several inputs, which are called features, and produce a single output.

In the figure, we model a single hidden layer with three neurons and single output.

A layer is fully connected layer if each neuron in the layer is connected to all neurons in the previous layer.
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In an artificial neural network, there are several inputs, which are called features, and produce a single output.

In the figure, we model a single hidden layer with three neurons and single output.

A layer is fully connected layer if each neuron in the layer is connected to all neurons in the previous layer.
How to train a neural network?

Example: design a binary classifier which outputs 1 if the absolute difference in the inputs is an odd number.

Sample data:

abs(2 - 5) = 3, output = 1

abs(5 - 3) = 2, output = 0

We start with random weights.

Note: $a_1, a_2, \ldots$ denote single neuron’s output, whereas, $\hat{y}_{out}$ denotes the final network’s output.
Forward Pass

Bias: $b_1 = 0.1$, $b_2 = 0.2$

Weights = Random generated

For each neuron, we calculate: $\sigma(\sum_i w_ix_i + b)$

$a_1 = \sigma(\sum_i w_ix_i + b)$

$a_1 = \sigma(0.2 \times 2 + 0.8 \times 9 + 0.1)$

$a_1 = \sigma(7.7)$

$a_1 = 0.99$ [putting 7.7 in the sigmoid function $\sigma(z) = \frac{1}{1 + e^{-z}}$]
Forward Pass

Bias: $b_1 = 0.1$, $b_2 = 0.2$

Weights = Random generated

For each neuron, we calculate: $a = \sigma(\sum_i w_i x_i + b)$

$a_2 = \sigma(0.6 \times 2 + 0.3 \times 9 + 0.1) = \sigma(4) = 0.9820$

$a_3 = \sigma(0.1 \times 2 + 0.7 \times 9 + 0.1) = \sigma(6.6) = 0.9986$
Forward Pass

Bias: $b_1 = 0.1$, $b_2 = 0.2$

Weights = Random generated

For each neuron, we calculate:  
$$a = \sigma(\sum_i w_i x_i + b)$$  
$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

$$a_2 = \sigma(0.6*2 + 0.3*9 + 0.1) = \sigma(4) = 0.9820$$

$$a_3 = \sigma(0.1*2 + 0.7*9 + 0.1) = \sigma(6.6) = 0.9986$$

$$\hat{y} = \sigma(0.9995*0.4 + 0.9820*0.5 + 0.9986*0.9 + 0.2) = \sigma(1.9895) = 0.8796$$
Calculating the error

The true label for output = 1

We have two input numbers and two classes:

Odd (1) and Even (0)

we need to alter weights to make our inputs(e.g., 2 and 9) equal to the corresponding output(i.e., 1).

This is done through a method called backpropagation.

Works by using a **loss function** to calculate how far the network was from the target output.
Loss Function

- Calculates error between the actual output and the predicted output.
- The error is back-propagated to update the weights.
- Ideally, if model (the weights and bias) is perfect then the error should be zero.
- We choose loss function based on the application.
- For example
  - Binary Classification - Cross Entropy (or log loss)
  - Multiclass Classification - Multi-class Cross Entropy
  - Regression - Mean Square Error
Gradient Descent (GD)

- A gradient measures how much the output of a function changes if you change the inputs a little bit.
- Commonly used optimization algorithm while training a machine learning model.
- It tweaks model parameters iteratively to minimize a given function to its local minimum.
- As shown, at each step GD tries to converge to minimum.

Steps in GD:
- Perform forward pass.
- Calculate error.
- Back propagate error as gradients.
- These gradients at each step update weights using the equation \((W_{k+1} = W_k - \text{learning_rate} \times \text{gradient})\)
- Perform above steps iteratively until error reaches minimal value.

Source: [https://towardsdatascience.com/gradient-descent-in-a-nutshell-eaf8c18212f0](https://towardsdatascience.com/gradient-descent-in-a-nutshell-eaf8c18212f0)
Learning Rate

- A major component of Gradient descent is learning rate.
- Learning rate decides how big the steps are that the GD takes in the direction of the local-minimum.
- In order for Gradient Descent to reach the local minimum, we have to set the learning rate to an appropriate value, which is neither too low nor too high.

- If the steps it takes are too big, it maybe will not reach the local minimum because it just bounces back and forth between the convex function of gradient descent
- If you set the learning rate to a very small value, gradient descent will eventually reach the local minimum but it might take too much time as you can see (may happen) on the right side of the figure.

Source: https://towardsdatascience.com/gradient-descent-in-a-nutshell-eaf8c18212f0
Back to our example: Calculating the error

We can now calculate the error for each output neuron using the **squared error function** and sum them to get the total error:

\[ E_{\text{total}} = \sum \frac{1}{2} \text{(target} - \text{output)}^2 \]

In our case, we have single output neuron. The target output = 1, but the neural network output = 0.8796

Therefore, its error is \( E = \frac{1}{2}(1-0.8796)^2 = 0.00724808 \)

**backpropagation:** to update each of the weights in the network so that they cause the actual output to be closer to the target output, thereby minimizing the error for each output neuron and the network as a whole.
The Backward Pass

Remember the update step in the Gradient descent algorithm.

- $W^{k+1} = W^k - \text{learning\_rate} \times (\text{gradient})$
- To calculate gradients:
  - We want to know how much a change in weights affects the error.

![Diagram of a neural network with weights and values]
The Backward Pass

Remember the update step in the Gradient descent algorithm.

- $W^{k+1} = W^k - \text{learning\_rate} \times (\text{gradient})$
- To calculate gradients:
  - We want to know how much a change in weights affects the error.
  - In this example, we will just show backpropagation for the highlighted subgraph.
  - You can complete rest of the calculation as an exercise.
Remember the update step in the Gradient descent algorithm.

- $W^{k+1} = W^k - \text{learning\_rate} \times \text{gradient}$
- For backward pass, we need to calculate derivatives (gradient) i.e. $\partial E / \partial w_7$ and $\partial E / \partial w_1$
- Using chain rule: $\partial E / \partial w_7 = \partial E / \partial out \times \partial out / \partial z \times \partial z / \partial w_7$
- $\partial E / \partial out = \partial [1/2(\text{target} - \text{out})^2] / \partial out$

$\partial E / \partial out = \frac{1}{2} \times 2(\text{target} - \text{out})^2 \times (-1) + 0$
$= -(\text{target} - \text{out}) = -(1 - 0.8796) = -0.1204$

$x_1, x_2$ are inputs.

\[
Z = a_1 \times w_7 + a_2 \times w_8 + a_3 \times w_9 + b_2 \times 1 \\
z_1 = w_1 \times x_1 + w_4 \times x_2 + b_1 \times 1
\]
(refer to slide 18 for full example)
The Backward Pass

Remember the update step in the Gradient descent algorithm.

- $W^{k+1} = W^k - \text{learning\_rate} \times (\text{gradient})$
- For backward pass, we need to calculate derivatives (gradient) i.e. $\frac{\partial E}{\partial w_7}$ and $\frac{\partial E}{\partial w_1}$
- Using chain rule: $\frac{\partial E}{\partial w_7} = \frac{\partial E}{\partial \text{out}} \times \frac{\partial \text{out}}{\partial z} \times \frac{\partial z}{\partial w_7}$

- Out = Sigmoid function $\sigma(z) = \frac{1}{1 + e^{-z}}$
- $\frac{\partial \sigma}{\partial z} = \sigma(1 - \sigma)$
- [For complete derivation, see this link: https://beckernick.github.io/sigmoid-derivative-neural-network/]
- $\frac{\partial \text{out}}{\partial z} = \frac{\partial \sigma}{\partial z} = 0.8796 \times (1 - 0.8796) = 0.1059$
The Backward Pass

Remember the update step in the Gradient descent algorithm.

- \( W_{k+1} = W_k - \text{learning}_\text{rate} \times (\text{gradient}) \)
- For backward pass, we need to calculate derivatives (gradient) i.e. \( \frac{\partial E}{\partial w_7} \) and \( \frac{\partial E}{\partial w_1} \)
- Using chain rule: \( \frac{\partial E}{\partial w_7} = \frac{\partial E}{\partial \text{out}} \times \frac{\partial \text{out}}{\partial z} \times \frac{\partial z}{\partial w_7} \)
- \( \frac{\partial z}{\partial w_7} = \frac{\partial (a_1 \times w_7 + a_2 \times w_8 + a_3 \times w_9 + b_2 \times 1)}{\partial w_7} = a_1 + 0 + 0 = a_1 = 0.9995 \)

\[ E_{\text{total}} = \sum \frac{1}{2}(\text{target} - \text{output})^2 \]
The Backward Pass

- $W^{k+1} = W^k - \text{learning\_rate} \times \text{(gradient)}$
- For backward pass, we need to calculate derivatives (gradient) i.e. $\frac{\partial E}{\partial w7}$ and $\frac{\partial E}{\partial w1}$
- Using chain rule: $\frac{\partial E}{\partial w7} = \frac{\partial E}{\partial \text{out}} \times \frac{\partial \text{out}}{\partial z} \times \frac{\partial z}{\partial w7}$

Putting it all together:

- $\frac{\partial E}{\partial w7} = -0.1204 \times 0.1059 \times 0.9995 = -0.0127$

Chain rule illustration

$E_{total} = \sum \frac{1}{2}(\text{target} - \text{output})^2$
The Backward Pass

- $W^{k+1} = W^k - \text{learning\_rate} \times (\text{gradient})$
- For backward pass, we need to calculate derivatives (gradient) i.e. $\frac{\partial E}{\partial w_7}$ and $\frac{\partial E}{\partial w_1}$
- Using chain rule: $\frac{\partial E}{\partial w_7} = \frac{\partial E}{\partial \text{out}} \times \frac{\partial \text{out}}{\partial z} \times \frac{\partial z}{\partial w_7}$

Putting it all together:

- $\frac{\partial E}{\partial w_7} = -0.1204 \times 0.1059 \times 0.9995 = -0.0127$

To decrease the error, we then subtract this value from the current weight.

- $w_7 = w_7 - \text{learning\_rate} \times (-0.0127)$
- $w_7 = 0.4 - 0.1 \times (-0.0127) = 0.40127$ (assume learning\_rate = 0.1)
The Backward Pass

- For backward pass, we need to calculate derivatives (gradient) i.e. $\frac{\partial E}{\partial w_7}$ and $\frac{\partial E}{\partial w_1}$
- Using chain rule for hidden layer: $\frac{\partial E}{\partial w_1} = \frac{\partial E}{\partial a_1} \cdot \frac{\partial a_1}{\partial z_1} \cdot \frac{\partial z_1}{\partial w_1}$
- $\frac{\partial E}{\partial a_1} = \frac{\partial E}{\partial z} \cdot \frac{\partial z}{\partial a_1}$

Using previously calculated values we have
$\frac{\partial E}{\partial z} = \frac{\partial E}{\partial out} \cdot \frac{\partial out}{\partial z} = -0.1204 \cdot 0.1059 = -0.01275$

- $\frac{\partial z}{\partial a_1} = \frac{\partial (a_1 \cdot w_7 + a_2 \cdot w_8 + a_3 \cdot w_9 + b_2 \cdot 1)}{\partial a_1} = w_7 + 0 + 0 + 0 = w_7 = 0.4$
- $\frac{\partial E}{\partial a_1} = \frac{\partial E}{\partial z} \cdot \frac{\partial z}{\partial a_1} = -0.01275 \cdot 0.4 = -0.0051$

$E_{total} = \sum \frac{1}{2} (target - output)^2$
The Backward Pass

- **PLEASE NOTE:** Using chain rule for hidden layer:

\[
\frac{\partial E}{\partial w_1} = \frac{\partial E}{\partial a_1} \cdot \frac{\partial a_1}{\partial z_1} \cdot \frac{\partial z_1}{\partial w_1}
\]

simply expands to

\[
\frac{\partial E}{\partial w_1} = \frac{\partial E}{\partial \text{out}} \cdot \frac{\partial \text{out}}{\partial z} \cdot \frac{\partial z}{\partial a_1} \cdot \frac{\partial a_1}{\partial z_1} \cdot \frac{\partial z_1}{\partial w_1}
\]

Compare this to below

\[
\frac{\partial E}{\partial w_7} = \frac{\partial E}{\partial \text{out}} \cdot \frac{\partial \text{out}}{\partial z} \cdot \frac{\partial z}{\partial w_7}
\]

Chain rule illustration for \(\frac{\partial E}{\partial w_1}\):
The Backward Pass

- For backward pass, we need to calculate derivatives (gradient) i.e. $\frac{\partial E}{\partial w_7}$ and $\frac{\partial E}{\partial w_1}$
- Using chain rule for hidden layer: $\frac{\partial E}{\partial w_1} = \frac{\partial E}{\partial a_1} \cdot \frac{\partial a_1}{\partial z_1} \cdot \frac{\partial z_1}{\partial w_1}$
- $\frac{\partial a_1}{\partial z_1} = \sigma(1-\sigma)$ [a1 is also an output of the sigmoid function]
  
  $= 0.9995 (1-0.9995) = 0.00049975$

- $\frac{\partial z_1}{\partial w_1} = \frac{\partial (w_1 \cdot x_1 + w_4 \cdot x_2 + b_1 \cdot 1)}{\partial w_1}$
  
  $= x_1 + 0 + 0 = 2$

Putting it all together: $\frac{\partial E}{\partial w_1} = \frac{\partial E}{\partial a_1} \cdot \frac{\partial a_1}{\partial z_1} \cdot \frac{\partial z_1}{\partial w_1}$

$0.00049975 \cdot 2 = -5.097E-6$
The Backward Pass

- For backward pass, we need to calculate derivatives (gradient) i.e. $\frac{\partial E}{\partial w}$ and $\frac{\partial E}{\partial w1}$
- Using chain rule for hidden layer: $\frac{\partial E}{\partial w1} = \frac{\partial E}{\partial a1} * \frac{\partial a1}{\partial z1} * \frac{\partial z1}{\partial w1}$
  - $\frac{\partial a1}{\partial z1} = \sigma(1-\sigma)$ [a1 is also an output of the sigmoid function]
    - $= 0.9995 (1-0.9995) = 0.00049975$
  - $\frac{\partial z1}{\partial w1} = \frac{\partial (w1*x1 + w4*x2 + b1*1)}{\partial w1}$
    - $= x1 + 0 + 0 = 2$

Putting it all together: $\frac{\partial E}{\partial w1} = \frac{\partial E}{\partial a1} * \frac{\partial a1}{\partial z1} * \frac{\partial z1}{\partial w1}$

$$= -0.0051 * 0.00049975 * 2 = -5.097E-6$$

Updating $w1 = w1 - \text{learning rate} * \text{gradient}$

$$w1 = 0.2 - 0.1*(-5.097E-6) = 0.20000051$$
After update, new weights would be

- Perform the forward pass and backward pass steps iteratively until the loss reaches minimal value.
Practice Calculations:

After one iteration, the updated weights for w2, w6, w8, and w9 are:

- \( w_8 = 0.50125 \)
- \( w_9 = 0.90127325094 \)
- \( w_2 = 0.60002253753 \)
- \( w_6 = 0.70001443866 \)
Summary

- The whole process of Forward propagation and backpropagation constitute a single iteration.
- This process is iteratively repeated until loss value reaches a minimum value and weights become stable.
- In practice, we don't train the model on single example, rather we train it on many many different examples and the model weights are updated slowly towards a convergence point.
- When we train the model on different examples, the model learns weights to produce the output close to the target output.
Layers organization in a Neural Network

Source: http://cs231n.github.io/neural-networks-1/#intro