# COMP 5630/6630:Machine Learning

Lecture 7: Neural Network, Backpropagation, MLP Demo

# Introduction to Neural Networks

#### Introduction to Neural Network

- The Perceptron algorithm for binary classification
  - How perceptron is different from logistic regression (LR)
  - Training steps a perceptron
  - Extending LR to multiclass LR
    - Extending perceptron to multilayer perceptron
- Forward Pass
  - Defining propagation equations
  - Defining loss function
- How to train
- Backward propagation

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#### The Perceptron: Supervised Binary Classifier

- Task: Predict whether an input image contains a cat (1) or not cat (0)
- Consider modifying the logistic regression method to "force" it to output values that are either 0 or 1 or exactly.
  - Change the definition of g to be the threshold function of logistic regression:

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

• Let  $h(x) = g(\theta^T x)$  as before but using this modified definition of g, and if we use the update rule

$$\theta_j := \theta_j + \alpha \left( y^{(i)} - h_{\theta}(x^{(i)}) \right) x_j^{(i)}$$

#### The Perceptron Algorithm: Difference w.r.t LR

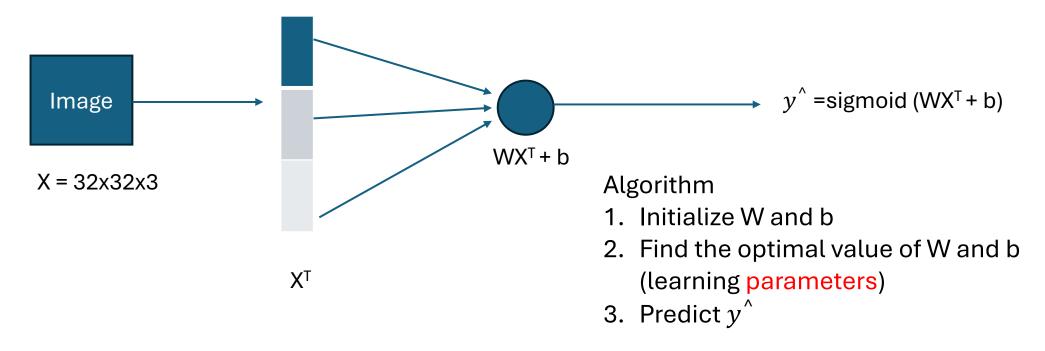
- In the 1960s, this "perceptron" was argued to be a rough model for how individual neurons in the brain work.
- Although the perceptron may be similar to the other algorithms we have seen, it is actually a very different type of algorithm than logistic regression.
  - The hypothesis in logistic regression provides a measure of uncertainty in the occurrence of a binary outcome based on a linear model.
  - The output from a *step function* can of course not be interpreted as any kind of probability.
  - Since a step function is *not differentiable*, it is not possible to train a perceptron using the same algorithms that are used for logistic regression.

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#### The Perceptron Algorithm: Training Idea

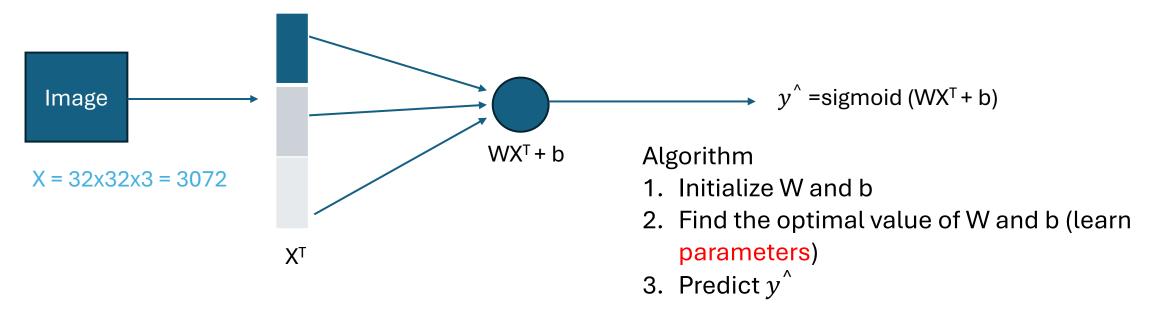
- Task: Predict whether an input image contains a cat (1) or not (0)
- Image representation from Lecture 2: Linear Classifier



How many parameters are in this model?

#### The Perceptron Algorithm

- Task: Predict whether an input image contains a cat (1) or not cat (0)
- Image representation from Lecture 2: Linear Classifier



How many parameters are in this model?

$$W = 1x 3072, X^{T} = 3072x 1, b = 1$$
  
Parameters = 3072 + 1

### Vocabulary of Neural Network

- Neuron = linear + activation
  - In our example
    - Linear= WX<sup>T</sup> + b
    - Activation= sigmoid on the linear output

- Model: architecture + parameter
  - In our example
    - Model = logistic regression
    - Parameter = 3073

# Vocabulary of Neural Network: Activation **Functions**

- Neuron = linear + activation (non-linear)
- The  $z_i$  is a linear component, corresponds to outputs of inputs from previous layer
  - or input layer of network
- Each activation  $a_i$  transforms  $z_i$  using differentiable nonlinear activation functions
- Three examples of activation functions:

  - 1. Logistic sigmoid 2. Hyperbolic tangent

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

$$tanh(a) = \frac{e^a - e^{-a}}{e^a + e^{-a}}$$

$$f(x) = \max(0, x)$$

• Some functions: step, softplus  $\log(1+e^x)$ ), leak RELU, softmax

$$\frac{\exp(a_{_k})}{\sum_{_j} \exp(a_{_j})}$$

# Activation Functions: Examples

• Task: Predict the age of the animal of the image

What changes will you make in the previous network and why?

## Activation Functions: Examples

- Task: Predict the age of the animal of the image
  - What changes will you make in the previous network?
  - Sigmoid activation function will not be a valid choice
    - ReLU: the age is non-negative
    - The identity or linear activation function

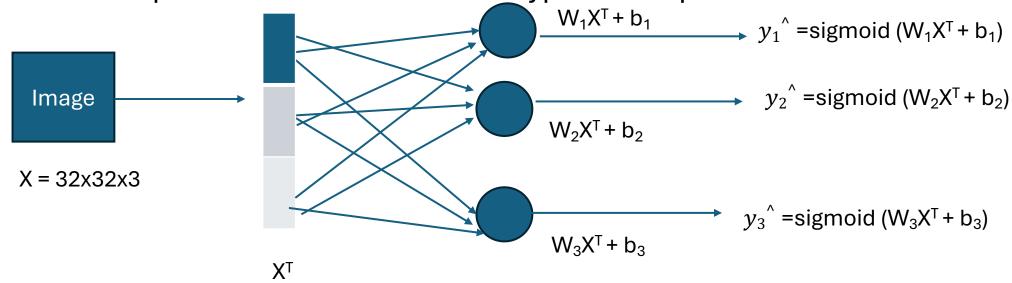
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# Multiclass Logistic Regression & Neural Network

Task: Predict whether an input image contains a cat/sheep/dog. *Image may contain multiple types of animals*.

Extend the previous network for three types of outputs



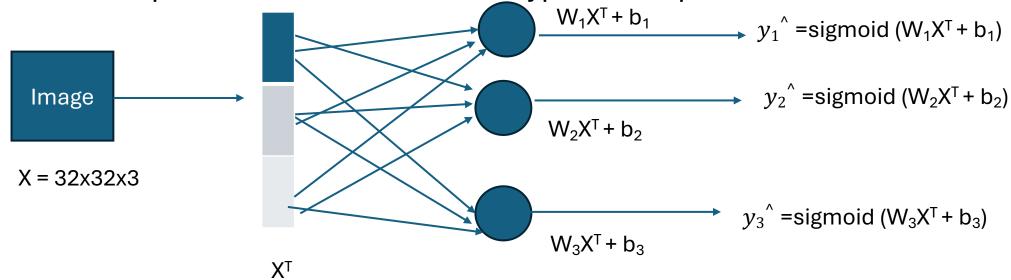
Assignment 1 question answer hint

How many parameters are in this model? Can this network classify if an image contains BOTH cat and dog?

## Multiclass Logistic Regression & Neural Network

Task: Predict whether an input image contains a cat/sheep/dog. *Image may contain multiple types of animals*.

Extend the previous network for three types of outputs



Assignment 1 question answer hint

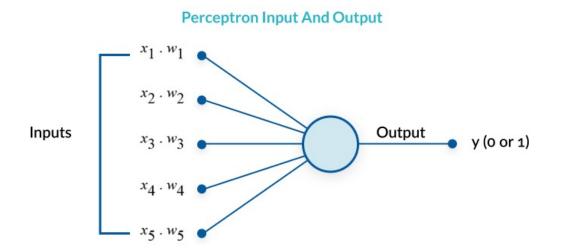
How many parameters are in this model? = 3 x prev. model Can this network classify if an image contains BOTH cat and dog? YES. As each neuron is independent

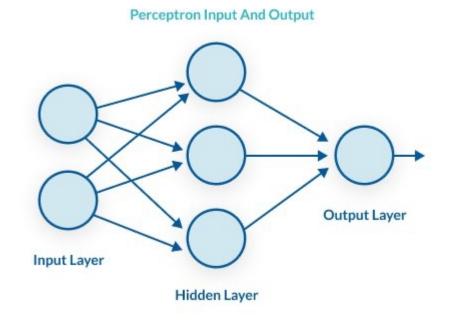
#### **Activation Function Selection**

- Determined by the nature of the data and the assumed distribution of the target variables
- For standard regression problems the activation function is the identity function so that  $y_k = a_k$ 
  - (e.g. predicting the age of the animal in an input image)
- For multiple binary classification problems, each output unit activation is transformed using a logistic sigmoid function so that  $y_k = \sigma(a_k)$ 
  - (e.g. predicting whether an input image contains a cat/sheep/dog. Image may contain multiple types of animals)
- For multiclass problems, a softmax activation function of the form:

$$\frac{\exp(a_{_k})}{\sum_{_j} \exp(a_{_j})}$$

# Perceptron vs Multilayer Perceptron (MLP)

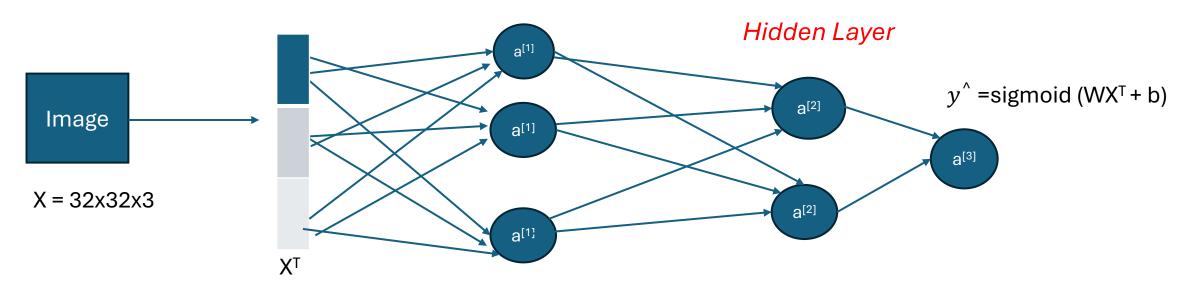




Why do we need more layers?

## Multilayer Perceptron

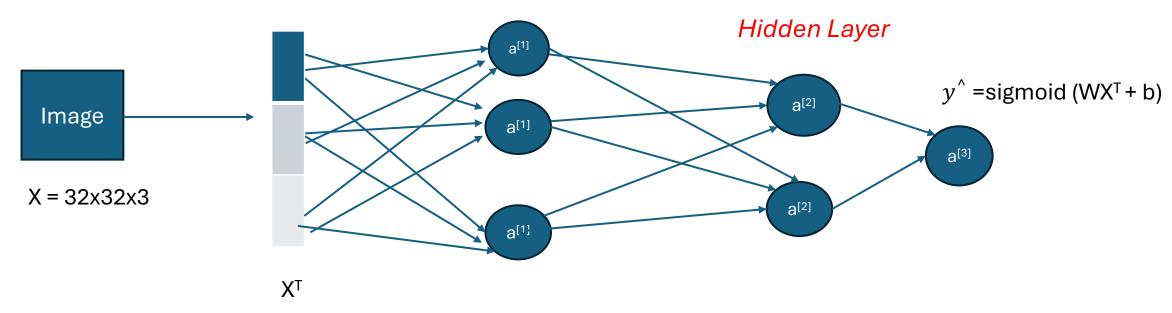
Task: Predict whether an input image contains a cat or not



- The first layer processes the input.
- The two neuron in the hidden layer may identify two different features of a cat, such as eye color or size of the head. We don't know how the layers operate (thus called hidden layer).
- Assumption: given enough data and adding more layers, the network can accurately identify the image

# Multilayer Perceptron

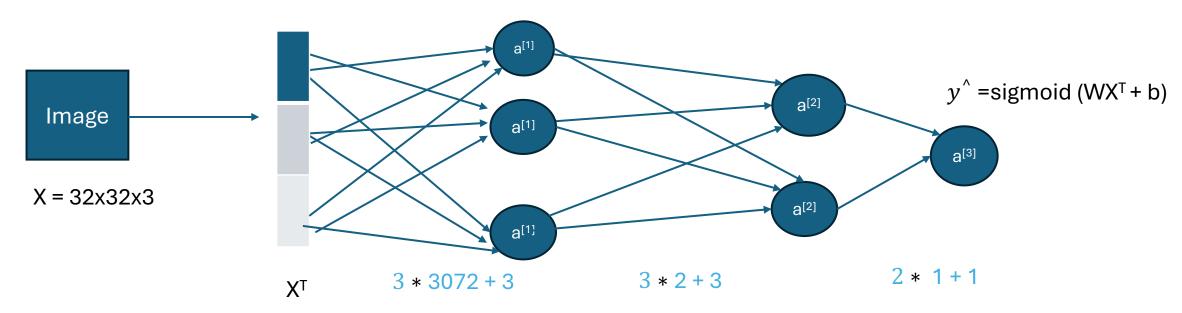
Task: Predict whether an input image contains a cat or not



How many parameters are in this model?

## Multilayer Perceptron

Task: Predict whether an input image contains a cat or not



How many parameters are in this model?

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#### **Notations and Forward Pass**

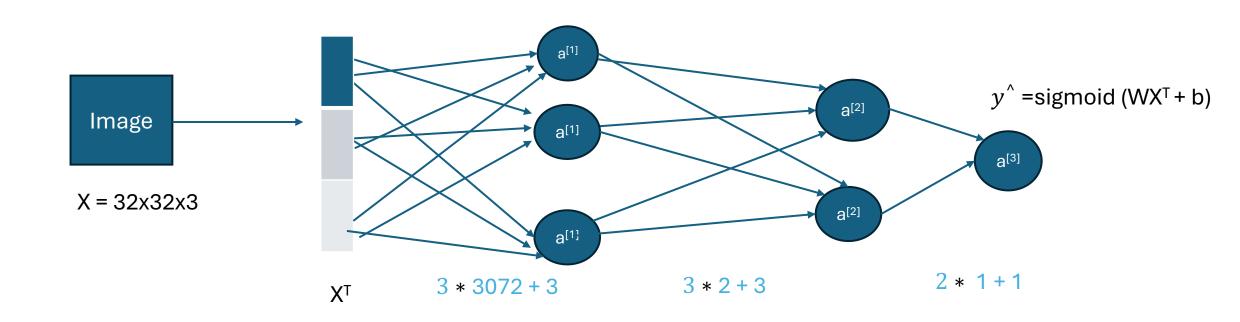
• Output of a layer l is given by  $z^{[\ell]} = W^{[\ell]} a^{[\ell-1]} + b^{[\ell]}$ 

• Where W^I is the weights of the layer, b^I is the bias and a^I is the activation  $a^{[\ell]}=g^{[\ell]}(z^{[\ell]})$ 

• Neuron = linear  $(z^{[l]})$ + activation  $(a^{[l]})$ 

#### Task: How to Train this MLP Network

Task: Predict whether an input image contains a cat or not



## Steps: How to Train this MLP Network

- Forward Pass
  - Defining propagation equations
  - Defining loss function
- How to train
  - Gradient Descent
  - Backward propagation

## **Defining Propagation Equations**

- X = [n x f]
- b = [n x1]

- First layer:  $W_1$ , bias =  $b_1$
- Second layer:  $W_2$ , bias =  $b_2$
- Third layer:  $W_3$ , bias =  $b_3$

#### The Forward Pass

- Output of layer 1:  $z^{[1]}=W^{[1]}x+b^{[1]}$   $a^{[1]}=g(z^{[1]}); \qquad a^{[1]}=activation function$
- Output of layer 2:  $z^{[2]} = W^{[2]} a^{[1]} + b^{[2]}$  $a^{[2]} = g(z^{[2]});$   $a^{[2]} = activation function$
- Output of layer 3:  $z^{[3]} = W^{[3]} a^{[2]} + b^{[3]}$  $a^{[3]} = g(z^{[3]});$   $a^{[3]} = activation function$
- Output of neural network:  $y^{\circ} = a^{[3]}$

## Defining the Loss

Task: Binary classification

Loss: binary cross entropy or log loss

• L = 
$$-[(1-y)\log(1-y^{'}) + y.\log y^{'}]$$

#### How to Train this MLP Network?

Gradient Descent + Backpropagation!

What is Backpropagation

 Backprop or Backpropagation is a way to train multilayer neural networks using gradients

#### **Gradient Descent**

• 1. Provide random value for weight and biases

- 2. Update weights by gradient descent of the ith layer
  - Wi = wi  $\alpha \frac{\partial L}{\partial w_i}$  bi = bi  $\alpha \frac{\partial L}{\partial b_i}$

Repeat until convergence

#### **Gradient Descent**

• We have three weight matrices, Wi, i = 1, 2, 3.

 We need to compute loss and update weights for each weight matrix

• Wi = wi - 
$$\alpha \frac{\partial L}{\partial w_i}$$

What will be the ordering of updating the weight matrices? Justify your answer.

# Gradient Descent and Backpropagation

- We have three weight matrices, Wi, i = 1, 2, 3.
- We need to compute loss and update weights for each weight matrix
- Wi = wi  $\alpha \frac{\partial L}{\partial w_i}$
- What will be the ordering of updating the weight matrices? Justify your answer
  - $W_3$ ,  $W_2$ ,  $W_1$ . The loss, L is computed from the output and the last layer of the network,  $W_3$ . So, it is straightforward to compute.
  - The relationship between L and  $W_1$  is not straightforward to compute
  - This is called backpropagation, as it calculates gradients backwards through the network

# $dL/dW_3$

• 
$$\frac{\partial L}{\partial w_3} = \frac{\partial}{\partial w_3} [-[(1-y)\log(1-y^*) + y.\log y^*]]$$

# dL/dW<sub>3</sub>

# dL/dW<sub>3</sub>

• 
$$\frac{\partial L}{\partial w_3} = \left[\frac{y^{\wedge}(1-y)-y(1-y^{\wedge})}{y^{\wedge}(1-y^{\wedge})}\right] \frac{\partial y^{\wedge}}{\partial w_3}$$

$$= \left[\frac{y^{\wedge}-yy^{\wedge}-y+yy^{\wedge}}{y^{\wedge}(1-y^{\wedge})}\right] \frac{\partial y^{\wedge}}{\partial w_3}$$

$$= \left[\frac{y^{\wedge}-y}{y^{\wedge}(1-y^{\wedge})}\right] \frac{\partial y^{\wedge}}{\partial w_3}$$

We will compute  $\frac{\partial y}{\partial w_3}$  and then put its value to  $\frac{\partial L}{\partial w_3}$ 

# dL/dW<sub>3</sub>

• 
$$\frac{\partial y}{\partial w_3}$$
 =  $\frac{\partial a_3}{\partial w_3}$  =  $\frac{\partial g(z_3)}{\partial w_3}$ 

If g is a sigmoid function,  $g'(z_3) = g(z_3)(1 - g(z_3))$ 

$$\frac{\partial L}{\partial w_3} = \left[\frac{(y^{\hat{}} - y)}{y^{\hat{}} (1 - y^{\hat{}})}\right] y^{\hat{}} (1 - y^{\hat{}}) a_2 \quad [\text{Replacing value of } \frac{\partial y^{\hat{}}}{\partial w_3}]$$

$$\frac{\partial L}{\partial w_3} = (y^{\hat{}} - y) a_2$$

$$\frac{\partial L}{\partial w_3} = (a^{[3]} - y) a_2^{\mathsf{T}} \text{ (vectoral solution)}$$

### dL/db<sub>3</sub>

Similar derivation

$$\frac{\partial L}{\partial b_3} = (a^{[3]} - y)$$

• We need to use the chain rule from calculus.

Why?

- We need to use the chain rule from calculus.
- Why?
  - There is no direct relationship between the weights W<sub>2</sub> and the loss L.
  - We cannot differentiate a variable by another if there is no direct relationship
    - Else it would be 0
    - Not true if the variable/function is composite

$$\frac{\partial L}{\partial w_2} = \frac{\partial L}{\partial a_3} \cdot \frac{\partial a_3}{?} \cdot \frac{?}{\partial w_2}$$

We know  $a^{[3]} = g(z^{[3]})$ .

Putting this value to make differentiable w.r.t. z<sup>[3]</sup>

$$\frac{\partial L}{\partial w_2} = \frac{\partial L}{\partial a_3} \cdot \frac{\partial a_3}{\partial z_3} \cdot \frac{\partial z_3}{?} \cdot \frac{?}{\partial w_2}$$

- $z^{[3]} = W^{[3]} a^{[2]} + b^{[3]}$
- $z^{[3]}$  is dependent on  $a^{[2]}$ . So, we add  $\frac{\partial z_3}{\partial a_2}$  to make the component differentiable w.r.t.  $a^{[2]}$

• 
$$\frac{\partial L}{\partial w_2} = \frac{\partial L}{\partial a_3} \cdot \frac{\partial a_3}{\partial z_3} \cdot \frac{\partial z_3}{\partial a_2} \cdot \frac{\partial a_2}{\partial a_2} \cdot \frac{?}{\partial w_2}$$

$$\mathbf{a}^{[2]} = \mathbf{g}(\mathbf{z}^{[2]});$$

$$\frac{\partial L}{\partial w_2} = \frac{\partial L}{\partial a_3} \cdot \frac{\partial a_3}{\partial z_3} \cdot \frac{\partial z_3}{\partial a_2} \cdot \frac{\partial a_2}{\partial z_2} \cdot \frac{\partial z_2}{\partial z_2} \cdot \frac{\partial z_2}{\partial w_2}$$

$$z^{[2]}=W^{[2]}a^{[1]}+b^{[2]}$$
. So the  $\frac{\partial L}{\partial w_2}$  becomes

$$\frac{\partial L}{\partial w_2} = \frac{\partial L}{\partial a_3} \cdot \frac{\partial a_3}{\partial z_3} \cdot \frac{\partial z_3}{\partial a_2} \cdot \frac{\partial a_2}{\partial z_2} \cdot \frac{\partial z_2}{\partial w_2}$$



We already know this value

$$\frac{\partial L}{\partial w_2} = \frac{\partial L}{\partial a_3} \cdot \frac{\partial a_3}{\partial z_3} \cdot \frac{\partial z_3}{\partial a_2} \cdot \frac{\partial a_2}{\partial z_2} \cdot \frac{\partial z_2}{\partial w_2}$$

Rewrite 
$$\frac{\partial L}{\partial w_3} = \frac{\partial L}{\partial a_3} \cdot \frac{\partial a_3}{\partial z_3} \cdot \frac{\partial z_3}{\partial w_3}$$

### Recap: dL/dW<sub>3</sub>

$$\bullet \frac{\partial y^{\wedge}}{\partial w_3} = \frac{\partial a_3}{\partial w_3} = \frac{\partial g(z_3)}{\partial w_3}$$

If g is a sigmoid function,  $g'(z_3) = g(z_3)(1 - g(z_3))$ 

$$\frac{\partial g(z_3)}{\partial w_3} = g(z_3)(1 - g(z_3)) \frac{\partial z_3}{\partial w_3}$$

$$= a_3(1 - a_3) \frac{\partial}{\partial w_3}(w_3 a_2 + b_3)$$

$$= a_3(1 - a_3) a_2$$

$$= y(1 - y^{\hat{}}) a_2$$
Thus,  $\frac{\partial z_3}{\partial w_3} = a_2$ 

$$= y(1 - y^{\hat{}}) a_2$$

$$\frac{\partial L}{\partial w_2} = \frac{\partial L}{\partial a_3} \cdot \frac{\partial a_3}{\partial z_3} \cdot \frac{\partial z_3}{\partial a_2} \cdot \frac{\partial a_2}{\partial z_2} \cdot \frac{\partial z_2}{\partial w_2}$$

Rewrite 
$$\frac{\partial L}{\partial w_3} = \frac{\partial L}{\partial a_3} \cdot \frac{\partial a_3}{\partial z_3} \cdot \frac{\partial z_3}{\partial w_3}$$

We know 
$$\frac{\partial L}{\partial w_3} = (a^{[3]} - y) a_2 T$$

Thus, 
$$\frac{\partial L}{\partial w_3} = \frac{\partial L}{\partial a_3} \cdot \frac{\partial a_3}{\partial z_3} \cdot \frac{\partial z_3}{\partial w_3} = (a^{[3]} - y) a_2^T$$

[See the final form of 
$$\frac{\partial L}{\partial w_3}$$
]

Because 
$$\frac{\partial z_3}{\partial w_3} = a_2$$
, so  $\frac{\partial L}{\partial a_3} \cdot \frac{\partial a_3}{\partial z_3} = = (a^{[3]} - y)$ 

$$\frac{\partial L}{\partial w_2} = \frac{\partial L}{\partial a_3} \cdot \frac{\partial a_3}{\partial z_3} \cdot \frac{\partial z_3}{\partial a_2} \cdot \frac{\partial a_2}{\partial z_2} \cdot \frac{\partial z_2}{\partial w_2}$$

Thus,

$$\frac{\partial L}{\partial w_2} = (a_3 - y) \cdot \frac{\partial z_3}{\partial a_2} \cdot \frac{\partial a_2}{\partial z_2} \cdot \frac{\partial z_2}{\partial w_2}$$
$$= (a_3 - y) \cdot w_3 \cdot g'(z_2) \cdot a_1$$

$$z^{[2]} = W^{[2]} a^{[1]} + b^{[2]}$$

$$\frac{\partial z_2}{\partial w_2} = a_1$$

$$a^{[2]} = g(z^{[2]})$$

$$\frac{\partial a_2}{\partial z_2} = g'(z^{[2]})$$

$$z_3 = W^{[3]} a^{[2]} + b^{[3]}$$

$$\frac{\partial z_3}{\partial a_2} = W_3$$

$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial a_3} \cdot \frac{\partial a_3}{\partial z_3} \cdot \frac{\partial z_3}{\partial a_2} \cdot \frac{\partial a_2}{\partial z_2} \cdot \frac{\partial a_2}{\partial a_1} \cdot \frac{\partial z_2}{\partial z_1} \cdot \frac{\partial a_1}{\partial z_1} \cdot \frac{\partial z_1}{\partial w_1}$$
[Chain rule of derivative]

= 
$$(a_3 - y)$$
.  $w_3 . g'(z_2)$ .  $w_2 . g'(z_1).x$ 

$$\frac{\partial L}{\partial b_1}$$
 = (a<sub>3</sub>-y). w<sub>3.</sub> g'(z<sub>2</sub>). w<sub>2</sub>.g'(z<sub>1</sub>)

# Improving the Neural Network

### Improving the Neural Network

- Initialization
  - Normalization
  - Mitigating vanishing and exploding gradient
- Optimization

### Initialization

- Normalization
- Mitigating vanishing and exploding gradient
- Optimization

### Normalizing Input

 Normalizing can help improve the speed and accuracy of the machine learning model.

- Performed on input features before feeding them into a NN
- Ensures features are in same scale
- Ensure all features contribute equally
- Neural networks perform better with smaller values (0-1), easier to train

### Normalizing Input

#### • Z-score

- For each feature type
  - convert each value into its corresponding z-score by subtracting mean from every value and dividing by standard deviation of all values (mean normalization)

#### Min-max normalization

- For each feature type
  - divide each entry by maximum possible value (min-max scaling)

- Initialization
  - Normalization
  - Mitigating vanishing and exploding gradient
- Optimization

### Recap: The Forward Pass

- Output of layer 1:  $z^{[1]} = W^{[1]}x + b^{[1]}$  $a^{[1]} = g(z^{[1]});$   $a^{[1]} = activation function$
- Output of layer 2:  $z^{[2]} = W^{[2]} a^{[1]} + b^{[2]}$  $a^{[2]} = g(z^{[2]});$   $a^{[2]} = activation function$
- Output of layer 3:  $z^{[3]} = W^{[3]} a^{[2]} + b^{[3]}$  $a^{[3]} = g(z^{[3]});$   $a^{[3]} = activation function$
- Output of neural network:  $y^{-} = a^{[3]}$

### Vanishing and Exploding Gradient

• [From forward pass equations, replace a<sup>[l]</sup> values gradually]

• 
$$y^{^{^{^{^{^{^{^{3}}}}}}} = w^{[3]} w^{[2]} w^{[1]} x + ...$$

 Weight matrices are initialized randomly and updated in the training process

How does the initialization of weight matrices impact the output?

### Vanishing Gradient

• 
$$y^{}$$
 =  $a^{[3]}$  =  $W^{[3]}W^{[2]}W^{[1]}x$ 

• Assume all weight matrices, W<sup>[L]</sup> are initialized with a value little below than the identity matrix

$$\cdot \begin{bmatrix} 0.5 & 0 \\ 0 & 0.5 \end{bmatrix}^L$$

Multiplicative value of the resulting weight matrix will be very small,  $y^{\wedge}$  will be close to zero (or vanish)

### **Exploding Gradient**

• 
$$y^{}$$
 =  $a^{[3]}$  =  $W^{[3]}W^{[2]}W^{[1]}x$ 

 Assume all weight matrices, W<sup>[L]</sup> are initialized with a value little higher than the identity matrix

$$\cdot \begin{bmatrix} 1.5 & 0 \\ 0 & 1.5 \end{bmatrix}^L$$

Multiplicative value of the resulting weight matrix will be very big,  $y^{\wedge}$  will explode

### Solution to Vanishing and Exploding Gradients

- Initialize weight matrices will values ~ 1.
- In practice,

W<sup>[l]</sup> = np.random.randn(shape)\*nsqrt( $\frac{1}{n^{l-1}}$ )

Number of inputs, n, coming to layer l

- Initialize weight of the layer with the number of inputs coming to the layer
- Works well for sigmoid activation function
- ReLU
- W<sup>[l]</sup> = np.random.randn(shape)\*nsqrt( $\frac{2}{n^{l-1}}$ )

- Initialization
  - Normalization
  - Mitigating vanishing and exploding gradient
- Optimization

### Optimization

- Batch Gradient descent
  - Updates gradient using the entire dataset

- Stochastic Descent
  - Updates gradient for each training example
  - As updates frequently, may stuck in local minima

- Trade-off between these two: mini-batch gradient descent
- Why do we need mini-batch gradient descent?

### **Optimization: Limitations**

- If we have a lot of training example, say 1 million images
  - Batch gradient descent will take a long time to compute gradient once
  - Stochastic gradient descent will update frequently
- A trade-off solution
  - Update gradients, may be batches of 10,000 examples
  - That will give an approximate direction of gradient

## Mini-Batch Gradient Descent: Definition, Advantages, and Disadvantages

• Mini-batch gradient descent splits the training dataset into small batches that are used to calculate ML model error and update gradients.

#### Advantages

- Update frequency is higher than batch gradient descent, allowing faster convergence in large dataset
- Avoids local minima.
- Gradient updates are computationally efficient than stochastic gradient descent.

#### Disadvantages

- Requires an additional hyperparameter tuning: "batch size" for the learning algorithm.
- Error information need to be accumulated across mini-batches of training examples like batch gradient descent.

## Colab Demo: MLP

- https://proceedings.mlr.press/v133/wang21a/wang21a.pdf
- https://2025.msrconf.org/track/msr-2025-mining-challenge
- <a href="https://2024.msrconf.org/track/msr-2024-mining-challenge?#Call-for-Mining-Challenge-Papers-">https://2024.msrconf.org/track/msr-2024-mining-challenge?#Call-for-Mining-Challenge-Papers-</a>

## Task: Digit Classification on the MNIST Dataset

