# CoE202 Fundamentals of Artificial intelligence <Big Data Analysis and Machine Learning>

#### Backpropagation in Neural Network

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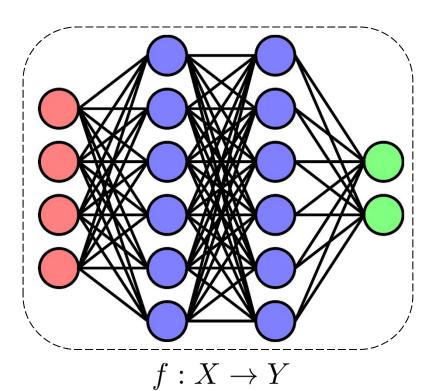




#### **Contents**

- Recap
  - Neural network
  - Single layer in a neural network
  - Activation function (Sigmoid & ReLU)
  - Universal approximation theorem
- Gradient descent for neural network
  - Forward propagation
  - Backward propagation

#### Revisit: The "Neural Network"



For a data set

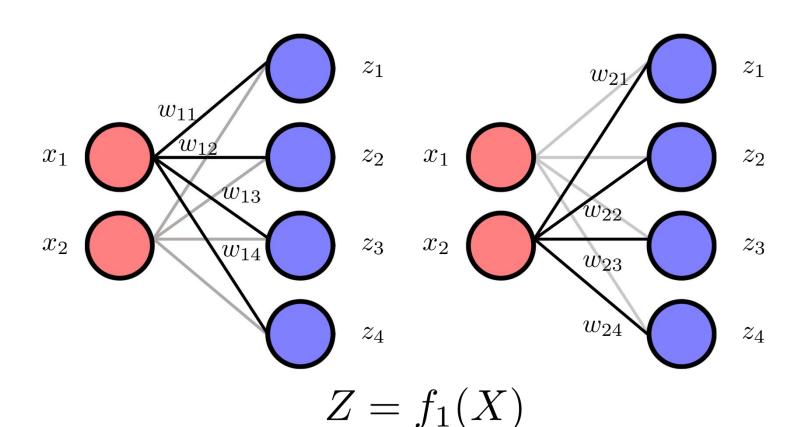
$$\mathcal{D} = \{ (\vec{x_1}, \vec{y_1}), (\vec{x_2}, \vec{y_2}), \cdots, (\vec{x_N}, \vec{y_N}) \}$$

Seeks a function  $f: X \to Y$ 

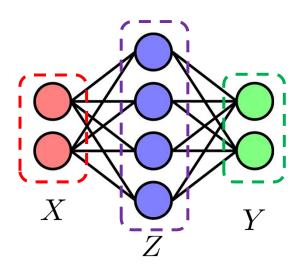
Such that a loss function

$$\mathcal{L}: X \times Y \to \mathcal{R}$$
 is minimized

# Revisit: single layer in a neural network



#### **Revisit: Activation function**



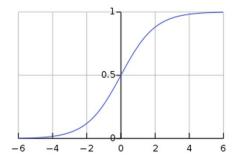
$$Y = f(X) = f_2(Z) = f_2(f_1(X))$$
  
 $Z = \mathbf{h}(W_{f_1}X) = f_1(X)$   
 $Y = \mathbf{h}(W_{f_2}Z) = f_2(Z)$ 

- h is called the activation function
- Single layer consists of a matrix multiplication & activation

## **Revisit: Activation function**

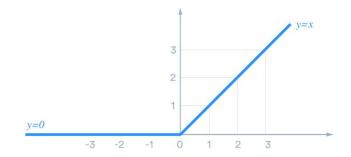
#### **Sigmoid function**

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



#### ReLU (rectified linear unit) function

$$\mathbf{R}(z) = max(z,0)$$



- These two functions are used often as the activation function
  - ReLU is the most popular choice these days
  - There are many other types of activation functions ...

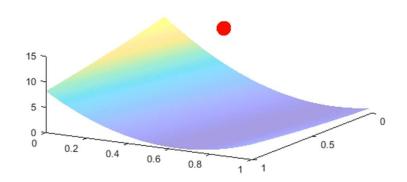
#### Revisit: Neural network as a function approximator

$$Y = f_W(X)$$

- Conceptually, for an (almost) arbitrary data set, we are using a neural network to model the relationship between the input and the output
- Universal approximation theorem, in a nutshell, states that any continuous function can be approximated by a neural network (with a sufficient number of neurons)
- Simply put, neural network is a good model for almost any supervised learning tasks (which is why neural network is so popular)

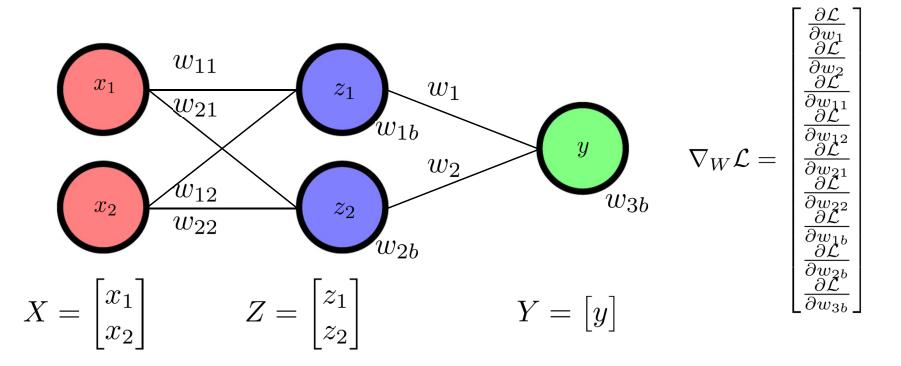
## **Revisit: Gradient Descent**

$$\theta^{(k+1)} = \theta^{(k)} - \gamma \nabla \mathcal{L}(\theta^{(k)})$$



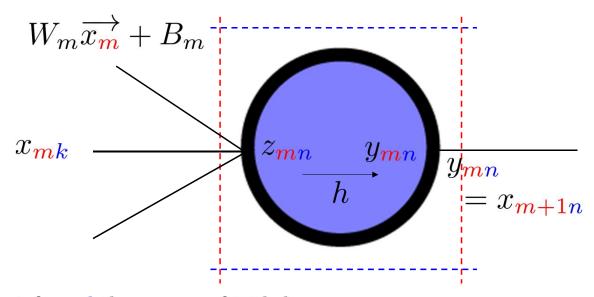
- Gradient descent is an iterative algorithm for finding a local minimum of a differentiable function
- It requires only the gradient value at one point at each iteration step (does not require closed-form gradient function)

# We need gradient!



This notation is not good for gradient calculation ...

# Let's change our notation

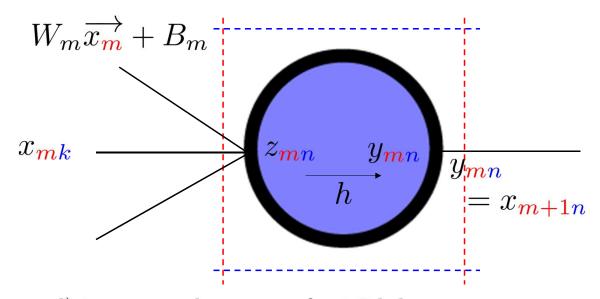


 $x_{mk}$ : input from kth neuron of mth layer

 $\overrightarrow{x_m}$ : input from mth layer as a vector

 $W_m$  and  $B_m$ : weight parameters

# Let's change our notation

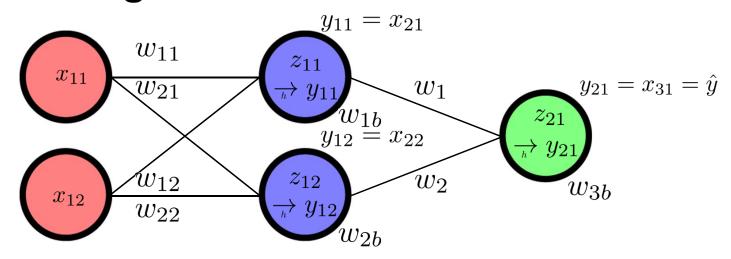


 $z_{mn}$ : (summed) input to nth neuron of m+1th layer

 $y_{mn}$ : output from nth neuron of m+1th layer

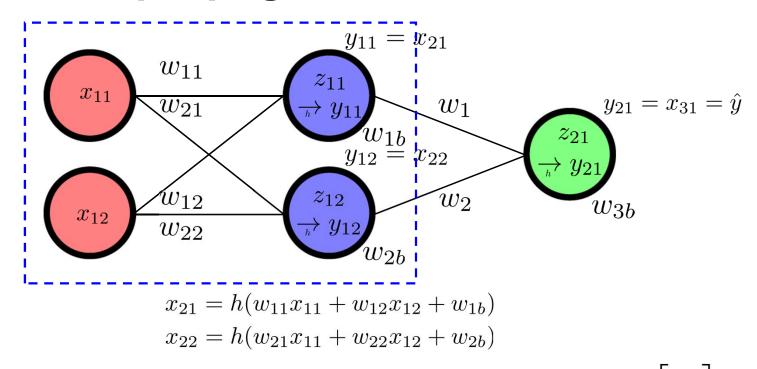
 $W_m$  and  $B_m$ : weight parameters

## Let's change our notation



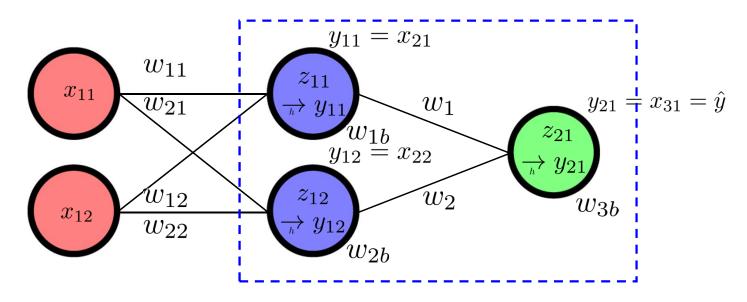
$$z_{11} = w_{11}x_{11} + w_{12}x_{12} + w_{1b}$$
$$x_{21} = y_{11} = h(z_{11}) = h(w_{11}x_{11} + w_{12}x_{12} + w_{1b})$$

# Forward propagation



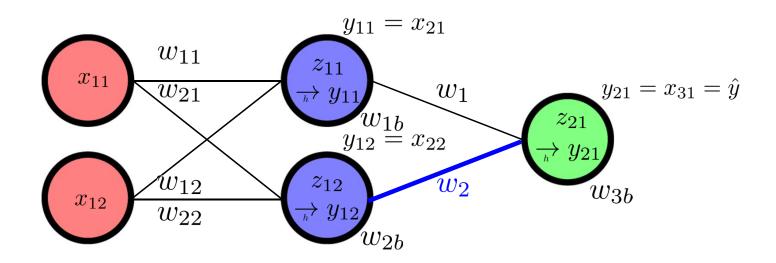
$$\begin{bmatrix} x_{21} \\ x_{22} \end{bmatrix} = h(\begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{bmatrix} \begin{bmatrix} x_{11} \\ x_{12} \end{bmatrix} + \begin{bmatrix} w_{1b} \\ w_{2b} \end{bmatrix}) = h(\begin{bmatrix} w_{11} & w_{12} & \mathbf{w_{1b}} \\ w_{21} & w_{22} & \mathbf{w_{2b}} \end{bmatrix} \begin{bmatrix} x_{11} \\ x_{12} \\ 1 \end{bmatrix})$$

# Forward propagation

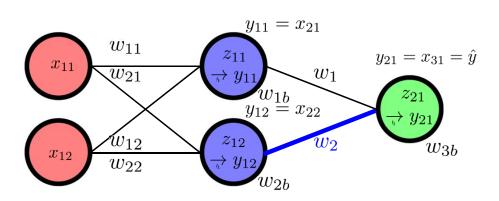


$$\hat{y} = x_{31} = h(w_1 x_{21} + w_2 x_{22} + w_{3b})$$

$$\hat{y} = x_{31} = h(\begin{bmatrix} w_1 & w_2 \end{bmatrix} \begin{bmatrix} x_{21} \\ x_{22} \end{bmatrix} + w_{3b}) = h(\begin{bmatrix} w_1 & w_2 & \mathbf{w_{3b}} \end{bmatrix} \begin{bmatrix} x_{21} \\ x_{22} \\ 1 \end{bmatrix})$$



$$\frac{\partial \mathcal{L}}{\partial w_2} = \frac{\partial \mathcal{L}}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial w_2} = \frac{\partial \mathcal{L}}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z_{21}} \frac{\partial z_{21}}{\partial w_2} = \frac{\partial \mathcal{L}}{\partial y_{21}} \frac{\partial y_{21}}{\partial z_{21}} \frac{\partial z_{21}}{\partial w_2}$$



Let's assume that we are using binary cross entropy loss

$$\mathcal{L} = -(y \log \hat{y} + (1 - y) \log(1 - \hat{y}))$$

and we are using the sigmoid function as our activation function *h* 

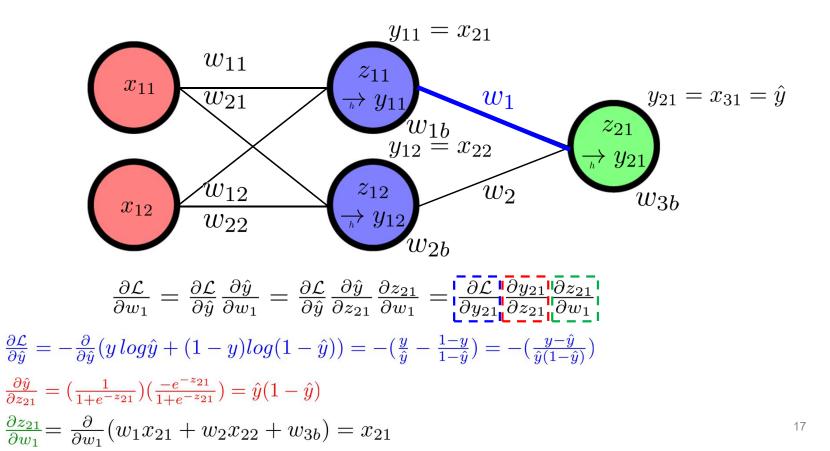
$$h(x) = \frac{1}{1 + e^{-x}}$$

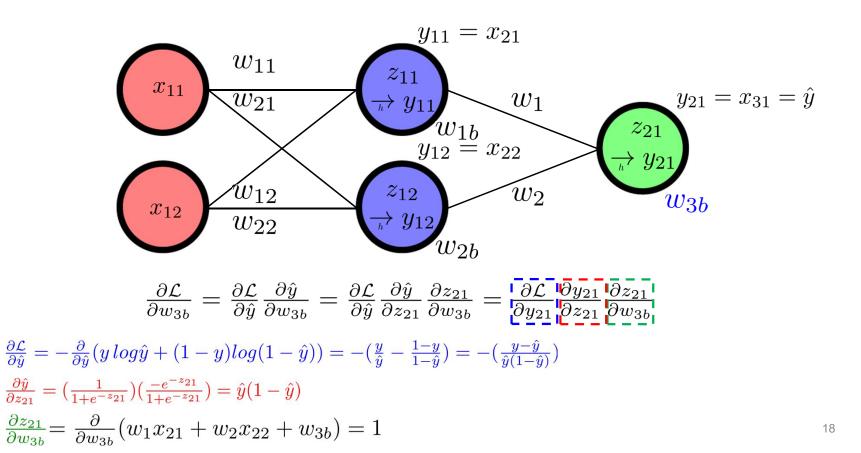
$$\frac{\partial \mathcal{L}}{\partial w_2} = \frac{\partial \mathcal{L}}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial w_2} = \frac{\partial \mathcal{L}}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z_{21}} \frac{\partial z_{21}}{\partial w_2}$$

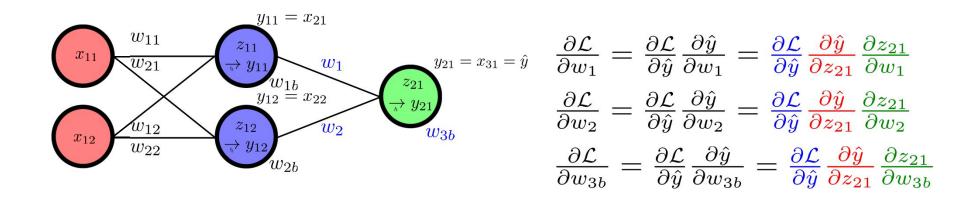
$$\frac{\partial \mathcal{L}}{\partial \hat{y}} = -\frac{\partial}{\partial \hat{y}} (y \log \hat{y} + (1 - y) \log (1 - \hat{y})) = -(\frac{y}{\hat{y}} - \frac{1 - y}{1 - \hat{y}}) = -(\frac{y - \hat{y}}{\hat{y}(1 - \hat{y})})$$

$$\frac{\partial \hat{y}}{\partial z_{21}} = \left(\frac{1}{1 + e^{-z_{21}}}\right) \left(\frac{-e^{-z_{21}}}{1 + e^{-z_{21}}}\right) = \hat{y}(1 - \hat{y})$$

$$\frac{\partial z_{21}}{\partial w_2} = \frac{\partial}{\partial w_2} (w_1 x_{21} + w_2 x_{22} + w_{3b}) = x_{22}$$



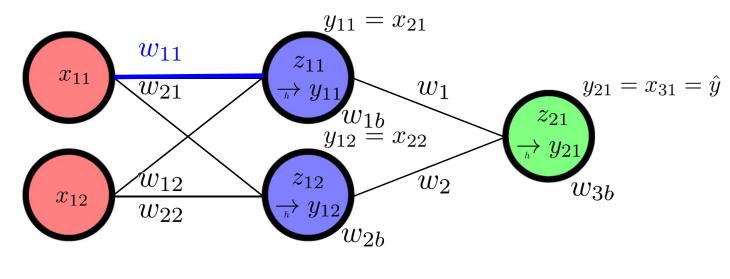




$$\frac{\partial z_{21}}{\partial w_1} = \frac{\partial}{\partial w_1} (w_1 x_{21} + w_2 x_{22} + w_{3b}) = x_{21}$$

$$\frac{\partial z_{21}}{\partial w_2} = \frac{\partial}{\partial w_2} (w_1 x_{21} + w_2 x_{22} + w_{3b}) = x_{22}$$

$$\frac{\partial z_{21}}{\partial w_{3b}} = \frac{\partial}{\partial w_{3b}} (w_1 x_{21} + w_2 x_{22} + w_{3b}) = 1$$

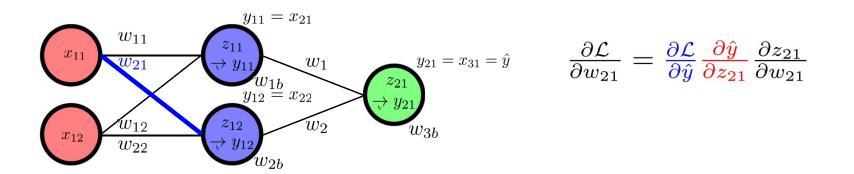


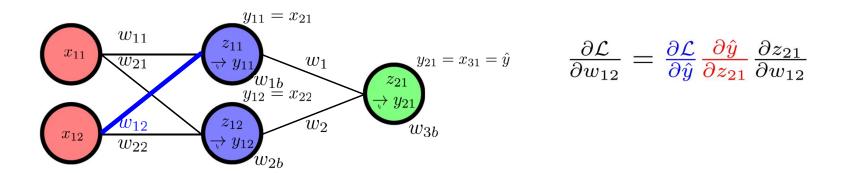
$$\frac{\partial \mathcal{L}}{\partial w_{11}} = \frac{\partial \mathcal{L}}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z_{21}} \frac{\partial z_{21}}{\partial w_{11}} = \frac{\partial \mathcal{L}}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z_{21}} \frac{\partial z_{21}}{\partial y_{11}} \frac{\partial y_{11}}{\partial z_{11}} \frac{\partial z_{11}}{\partial w_{11}}$$

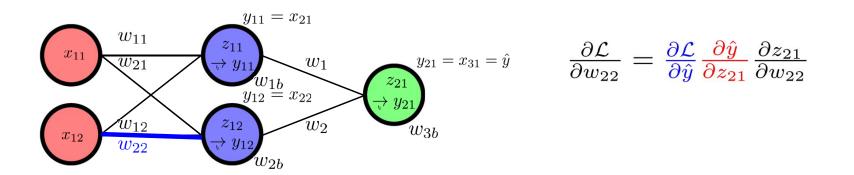
$$\frac{\partial z_{21}}{\partial y_{11}} = \frac{\partial}{\partial y_{11}} (w_1 x_{21} + w_2 x_{22} + w_{3b}) = w_1$$

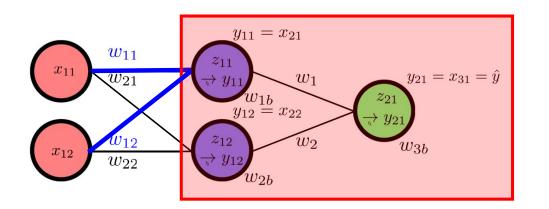
$$\frac{\partial y_{11}}{\partial z_{11}} = y_{11}(1 - y_{11})$$

$$\frac{\partial z_{11}}{\partial w_{11}} = \frac{\partial}{\partial w_{11}} (w_{11}x_{11} + w_{12}x_{12} + w_{1b}) = x_{11}$$





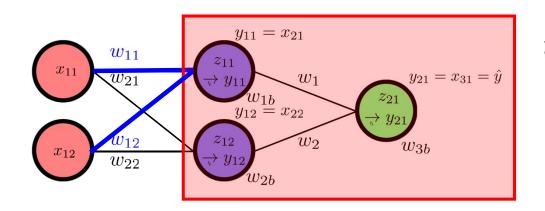




$$\frac{\partial \mathcal{L}}{\partial w_{11}} = \frac{\partial \mathcal{L}}{\partial x_{21}} \frac{\partial x_{21}}{\partial w_{11}}$$

$$\frac{\partial \mathcal{L}}{\partial w_{12}} = \frac{\partial \mathcal{L}}{\partial x_{21}} \frac{\partial x_{21}}{\partial w_{12}}$$

For calculation of  $\frac{\partial \mathcal{L}}{\partial w_{11}}$  and  $\frac{\partial \mathcal{L}}{\partial w_{12}}$  we just need to know  $\frac{\partial \mathcal{L}}{\partial x_{21}}$  about the latter part of the network

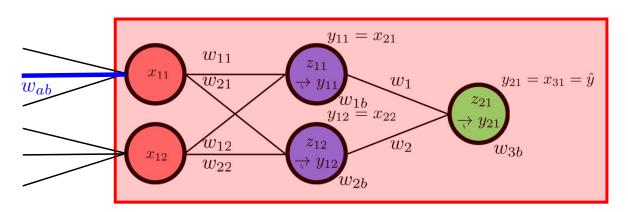


$$\frac{\partial \mathcal{L}}{\partial w_{11}} = \frac{\partial \mathcal{L}}{\partial x_{21}} \frac{\partial x_{21}}{\partial w_{11}} \qquad \frac{\partial \mathcal{L}}{\partial w_{12}} = \frac{\partial \mathcal{L}}{\partial x_{21}} \frac{\partial x_{21}}{\partial w_{12}}$$

For calculation of  $\frac{\partial \mathcal{L}}{\partial w_{11}}$  and  $\frac{\partial \mathcal{L}}{\partial w_{12}}$  we just need to know  $\frac{\partial \mathcal{L}}{\partial x_{21}}$  about the latter part of the network

$$\frac{\partial \mathcal{L}}{\partial x_{21}} = \frac{\partial \mathcal{L}}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z_{21}} \frac{\partial z_{21}}{\partial x_{21}}$$

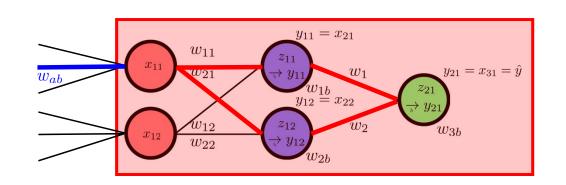
$$\frac{\partial z_{21}}{\partial x_{21}} = \frac{\partial z_{21}}{\partial y_{11}} = \frac{\partial}{\partial y_{11}} (w_1 x_{21} + w_2 x_{22} + w_{3b}) = w_1$$



$$y_{21} = x_{31} = \hat{y}$$
  $\frac{\partial \mathcal{L}}{\partial w_{ab}} = \frac{\partial \mathcal{L}}{\partial x_{11}} \frac{\partial x_{11}}{\partial w_{ab}}$ 

For calculation of  $\frac{\partial \mathcal{L}}{\partial w_{ab}}$ 

we just need to know  $\frac{\partial \mathcal{L}}{\partial x_{11}}$  about the latter part of the network



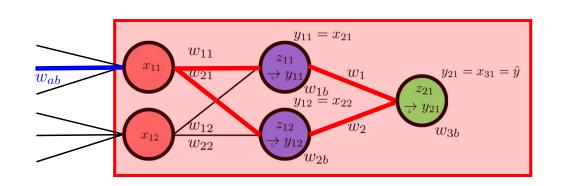
$$\frac{\partial \mathcal{L}}{\partial w_{ab}} = \frac{\partial \mathcal{L}}{\partial x_{11}} \frac{\partial x_{11}}{\partial w_{ab}}$$

For calculation of  $\frac{\partial \mathcal{L}}{\partial w_{ab}}$  we just need to know  $\frac{\partial \mathcal{L}}{\partial x_{11}}$  about the latter part of the network

$$\frac{\partial \mathcal{L}}{\partial x_{11}} = \frac{\partial \mathcal{L}}{\partial x_{21}} \frac{\partial x_{21}}{\partial x_{11}} + \frac{\partial \mathcal{L}}{\partial x_{22}} \frac{\partial x_{22}}{\partial x_{11}}$$

$$= \frac{\partial \mathcal{L}}{\partial x_{21}} \frac{\partial x_{21}}{\partial x_{21}} \frac{\partial x_{21}}{\partial x_{11}} + \frac{\partial \mathcal{L}}{\partial x_{22}} \frac{\partial x_{22}}{\partial x_{22}} \frac{\partial x_{22}}{\partial x_{212}} \frac{\partial x_{22}}{\partial x_{11}}$$

We have these terms from backpropagation (from the latter layer)



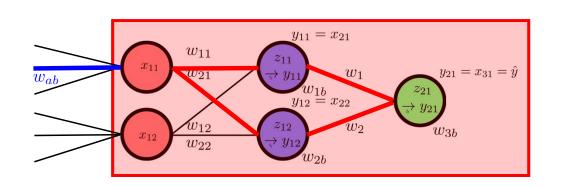
$$\frac{\partial \mathcal{L}}{\partial w_{ab}} = \frac{\partial \mathcal{L}}{\partial x_{11}} \frac{\partial x_{11}}{\partial w_{ab}}$$

For calculation of  $\frac{\partial \mathcal{L}}{\partial w_{ab}}$  we just need to know  $\frac{\partial \mathcal{L}}{\partial x_{11}}$  about the latter part of the network

$$\frac{\partial \mathcal{L}}{\partial x_{11}} = \frac{\partial \mathcal{L}}{\partial x_{21}} \frac{\partial x_{21}}{\partial x_{11}} + \frac{\partial \mathcal{L}}{\partial x_{22}} \frac{\partial x_{22}}{\partial x_{11}}$$

$$= \frac{\partial \mathcal{L}}{\partial x_{21}} \frac{\partial x_{21}}{\partial z_{11}} \frac{\partial z_{11}}{\partial x_{11}} + \frac{\partial \mathcal{L}}{\partial x_{22}} \frac{\partial x_{22}}{\partial z_{12}} \frac{\partial z_{12}}{\partial x_{11}}$$

These are just differentiation of Sigmoid function



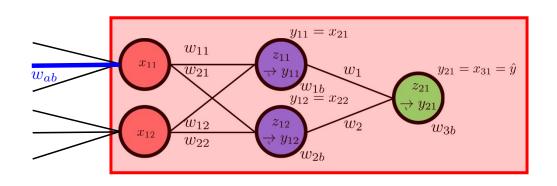
$$\frac{\partial \mathcal{L}}{\partial w_{ab}} = \frac{\partial \mathcal{L}}{\partial x_{11}} \frac{\partial x_{11}}{\partial w_{ab}}$$

For calculation of  $\frac{\partial \mathcal{L}}{\partial w_{ab}}$  we just need to know  $\frac{\partial \mathcal{L}}{\partial x_{11}}$  about the latter part of the network

$$\frac{\partial \mathcal{L}}{\partial x_{11}} = \frac{\partial \mathcal{L}}{\partial x_{21}} \frac{\partial x_{21}}{\partial x_{11}} + \frac{\partial \mathcal{L}}{\partial x_{22}} \frac{\partial x_{22}}{\partial x_{11}}$$

$$= \frac{\partial \mathcal{L}}{\partial x_{21}} \frac{\partial x_{21}}{\partial z_{11}} \frac{\partial z_{11}}{\partial x_{11}} + \frac{\partial \mathcal{L}}{\partial x_{22}} \frac{\partial x_{22}}{\partial z_{12}} \frac{\partial z_{12}}{\partial x_{11}}$$

These are just w<sub>11</sub> and w<sub>21</sub>



$$\frac{\partial \mathcal{L}}{\partial x_{11}} = \frac{\partial \mathcal{L}}{\partial x_{21}} \frac{\partial x_{21}}{\partial x_{11}} + \frac{\partial \mathcal{L}}{\partial x_{22}} \frac{\partial x_{22}}{\partial x_{11}}$$

$$= \frac{\partial \mathcal{L}}{\partial x_{21}} \frac{\partial x_{21}}{\partial z_{11}} w_{11} + \frac{\partial \mathcal{L}}{\partial x_{22}} \frac{\partial x_{22}}{\partial z_{12}} w_{21}$$

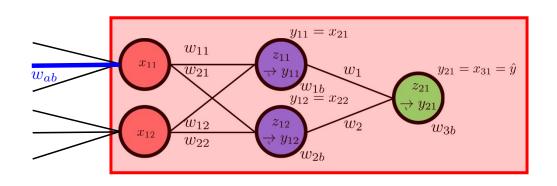
$$\frac{\partial \mathcal{L}}{\partial x_{12}} = \frac{\partial \mathcal{L}}{\partial x_{21}} \frac{\partial x_{21}}{\partial x_{12}} + \frac{\partial \mathcal{L}}{\partial x_{22}} \frac{\partial x_{22}}{\partial x_{12}}$$

$$= \frac{\partial \mathcal{L}}{\partial x_{21}} \frac{\partial x_{21}}{\partial z_{11}} w_{12} + \frac{\partial \mathcal{L}}{\partial x_{22}} \frac{\partial x_{22}}{\partial z_{12}} w_{22}$$

$$\begin{bmatrix} \frac{\partial \mathcal{L}}{\partial x_{11}} \\ \frac{\partial \mathcal{L}}{\partial x_{12}} \end{bmatrix} = \begin{bmatrix} w_{11} & w_{21} \\ w_{12} & w_{22} \end{bmatrix} \begin{bmatrix} \frac{\partial \mathcal{L}}{\partial x_{21}} & \frac{\partial x_{21}}{\partial z_{11}} \\ \frac{\partial \mathcal{L}}{\partial x_{22}} & \frac{\partial x_{22}}{\partial z_{12}} \end{bmatrix}$$

This would be just  $x_{21}(1-x_{21})$  if we are using Sigmoid as our activation

# Forward propagation vs. Backpropagation



#### Forward propagation

$$\begin{bmatrix} x_{21} \\ x_{22} \end{bmatrix} = h(\begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{bmatrix} \begin{bmatrix} x_{11} \\ x_{12} \end{bmatrix} + \begin{bmatrix} w_{1b} \\ w_{2b} \end{bmatrix})$$
 Backpropagation Transpose!

$$\begin{bmatrix} \frac{\partial \mathcal{L}}{\partial x_{11}} \\ \frac{\partial \mathcal{L}}{\partial x_{12}} \end{bmatrix} = \begin{bmatrix} w_{11} & w_{21} \\ w_{12} & w_{22} \end{bmatrix} \begin{bmatrix} \frac{\partial \mathcal{L}}{\partial x_{21}} \frac{\partial x_{21}}{\partial z_{11}} \\ \frac{\partial \mathcal{L}}{\partial x_{22}} \frac{\partial x_{22}}{\partial z_{12}} \end{bmatrix}$$

# Forward propagation vs. Backpropagation

#### Forward propagation

$$\begin{bmatrix} x_{21} \\ x_{22} \end{bmatrix} = h(\begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{bmatrix} \begin{bmatrix} x_{11} \\ x_{12} \end{bmatrix} + \begin{bmatrix} w_{1b} \\ w_{2b} \end{bmatrix}) \qquad \begin{bmatrix} \frac{\partial \mathcal{L}}{\partial x_{11}} \\ \frac{\partial \mathcal{L}}{\partial x_{12}} \end{bmatrix} = \begin{bmatrix} w_{11} & w_{21} \\ w_{12} & w_{22} \end{bmatrix} \begin{bmatrix} \frac{\partial \mathcal{L}}{\partial x_{21}} \frac{\partial x_{21}}{\partial x_{22}} \\ \frac{\partial \mathcal{L}}{\partial x_{22}} \frac{\partial x_{22}}{\partial x_{22}} \end{bmatrix}$$

- 1. Output (ŷ) can be obtained by **repeating** single layer forward propagation
- 2. For single layer forward propagation
  - 1. We take input from the previous layer
  - 2. Multiply with weight matrix
  - 3. Add bias terms
  - 4. Apply activation function

#### Backpropagation

$$\begin{bmatrix} \frac{\partial \mathcal{L}}{\partial x_{11}} \\ \frac{\partial \mathcal{L}}{\partial x_{12}} \end{bmatrix} = \begin{bmatrix} w_{11} & w_{21} \\ w_{12} & w_{22} \end{bmatrix} \begin{bmatrix} \frac{\partial \mathcal{L}}{\partial x_{21}} \frac{\partial x_{21}}{\partial z_{11}} \\ \frac{\partial \mathcal{L}}{\partial x_{22}} \frac{\partial x_{22}}{\partial z_{12}} \end{bmatrix}$$

- 1. Output (dL/dx, dL/dw) can be obtained by repeating single layer backpropagation
- 2. For single layer backpropagation
  - 1. We take dL/dx from the latter layer
  - 2. Element-wise multiplication with the partial derivative of activation function
  - 3. Multiply with the transpose of weight matrix

# **Summary**

- We can use gradient descent to train a neural network
- Gradient descent requires calculation of gradient
- We can calculate gradient (partial derivatives) using chain rule
- Gradient in a neural network can be efficiently computed by "reusing" terms
  - Backpropagation allows us to do this!

#### References

- Lecture notes
  - MIT 6.036 Intro to Machine Learning (Chapter 8)
    - https://www.mit.edu/~lindrew/6.036.pdf
  - CC229 lecture note
    - http://cs229.stanford.edu/notes-spring2019/cs229-notes-deep\_learning.pdf
    - http://cs229.stanford.edu/notes-spring2019/backprop.pdf
- Website
  - CS231n course website: <a href="https://cs231n.github.io/">https://cs231n.github.io/</a>