

IT5005:

Multi-Layer Perceptrons

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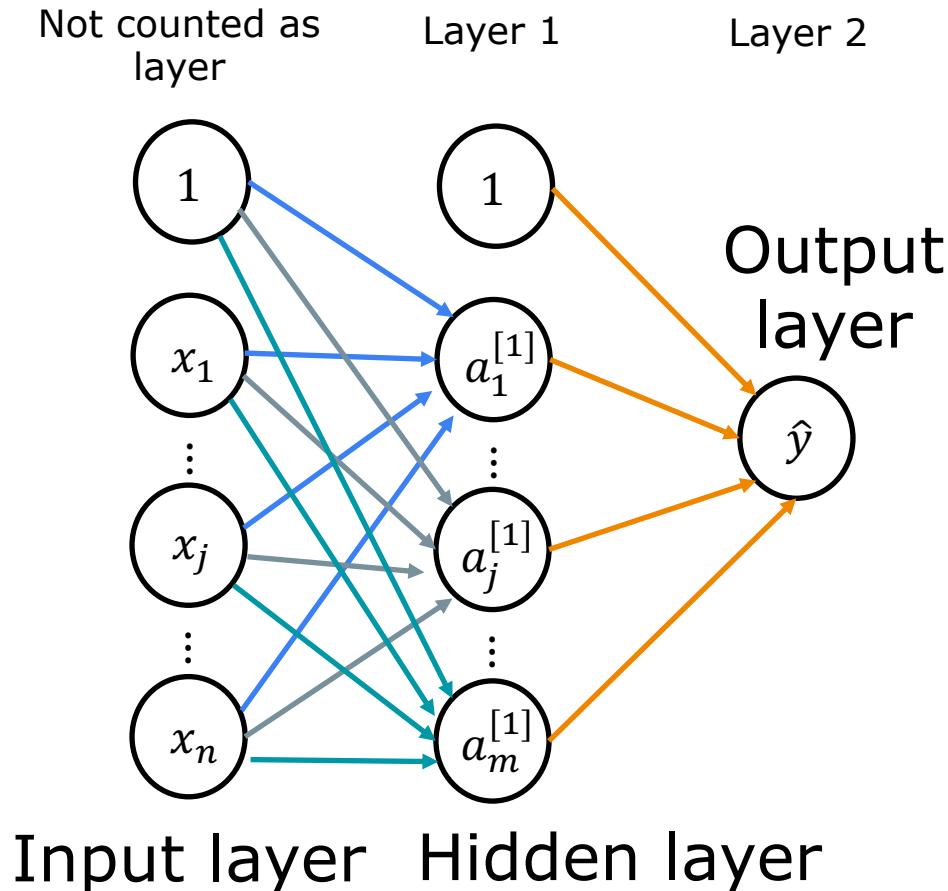
Slide Credit: Prof. Ben Leong
Revised for IT5005

Agenda

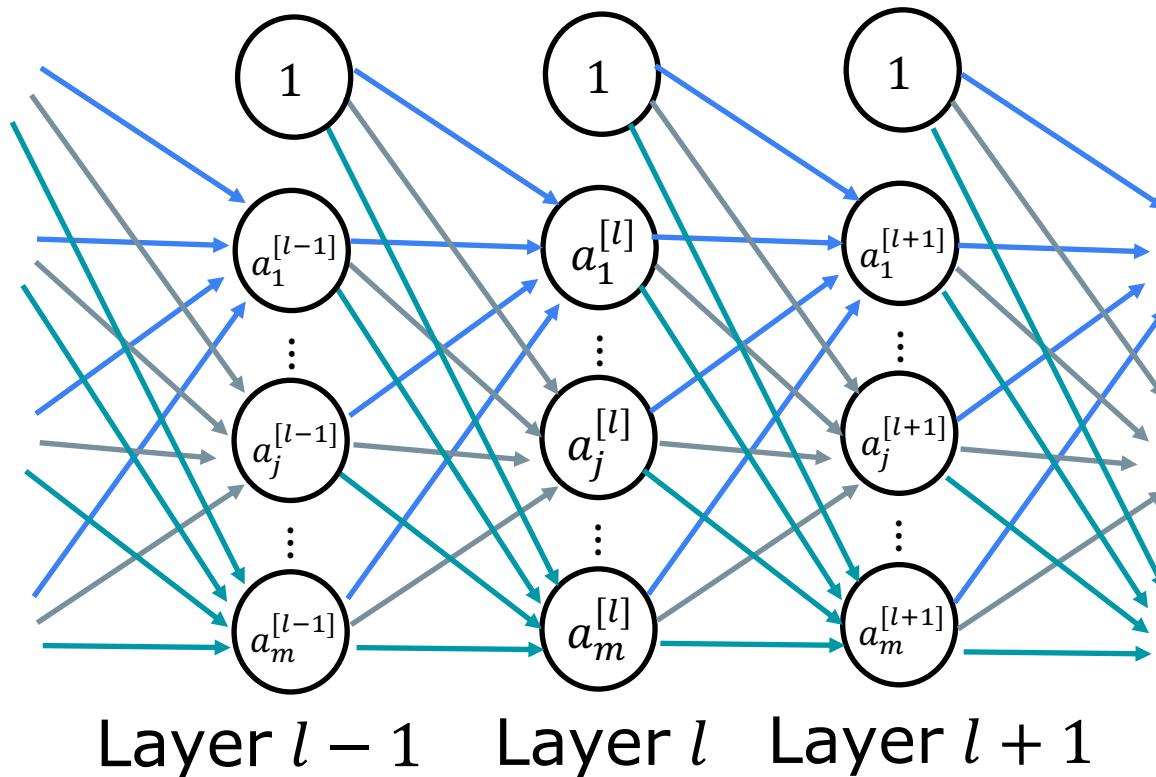
- Multilayer Perceptron
- Backpropagation

Neural Network
= Multi-layer Perceptron

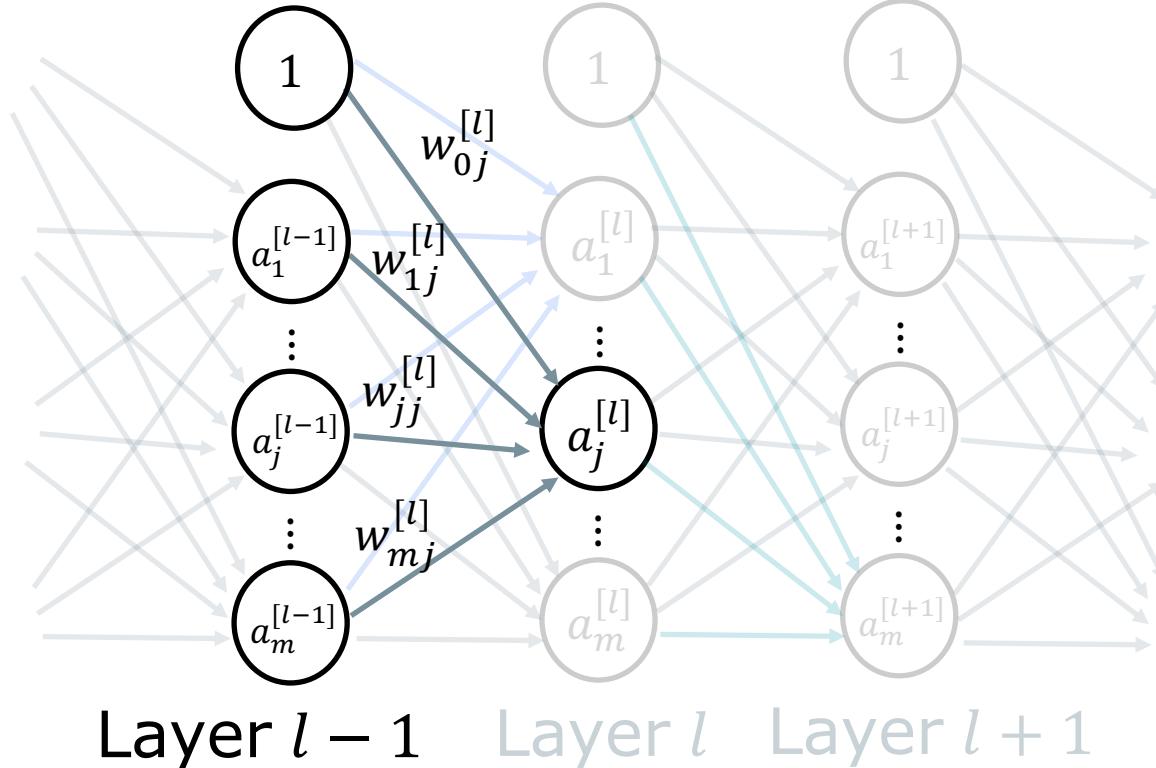
2-layer Perceptron



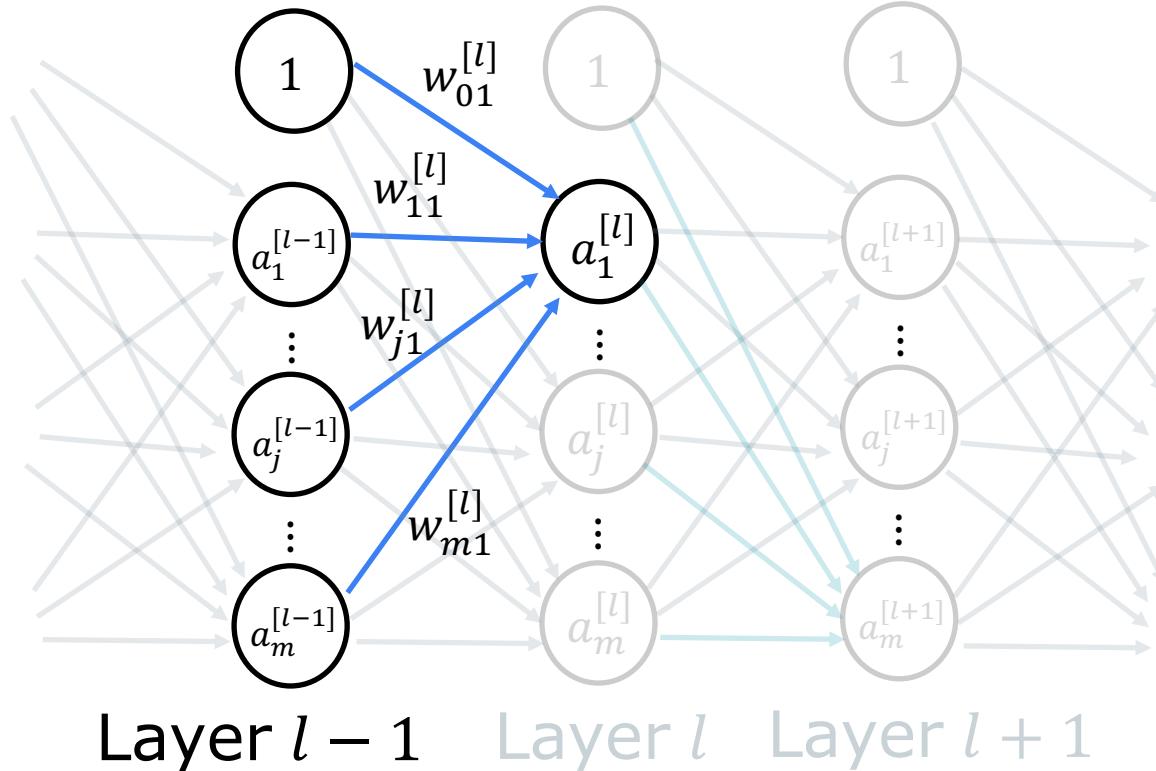
Multi-layer Perceptron



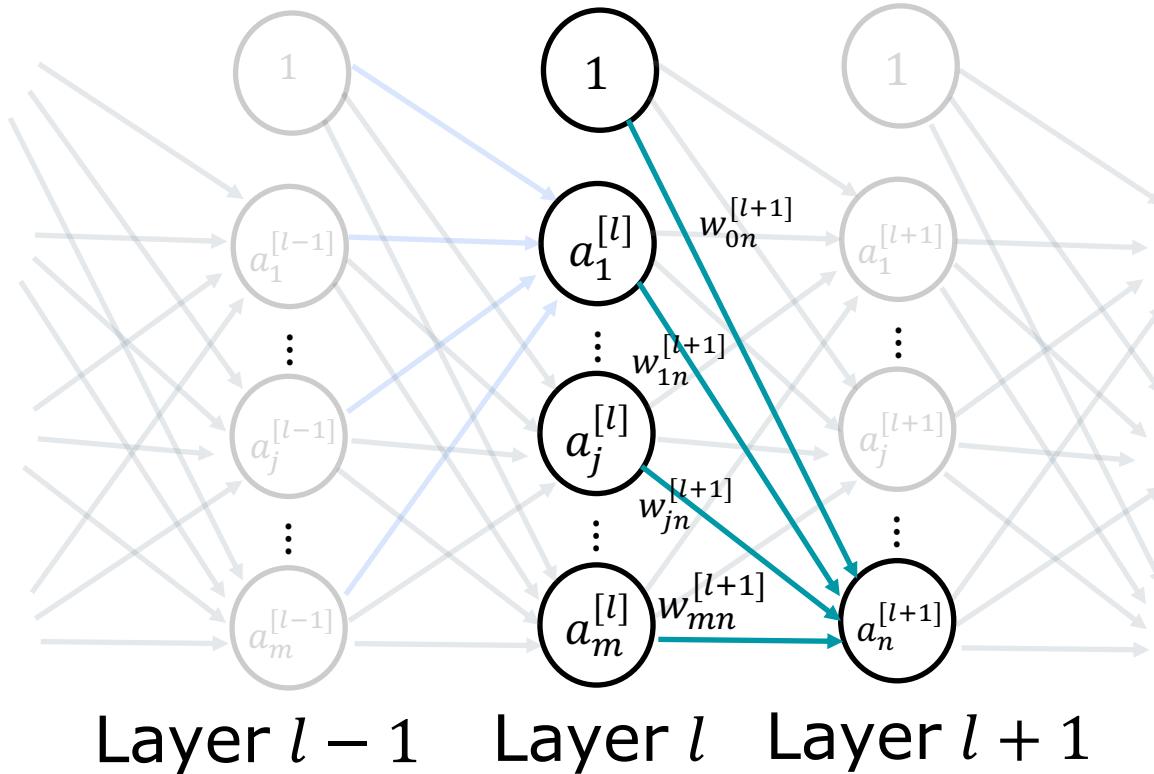
Multi-layer Neural Network



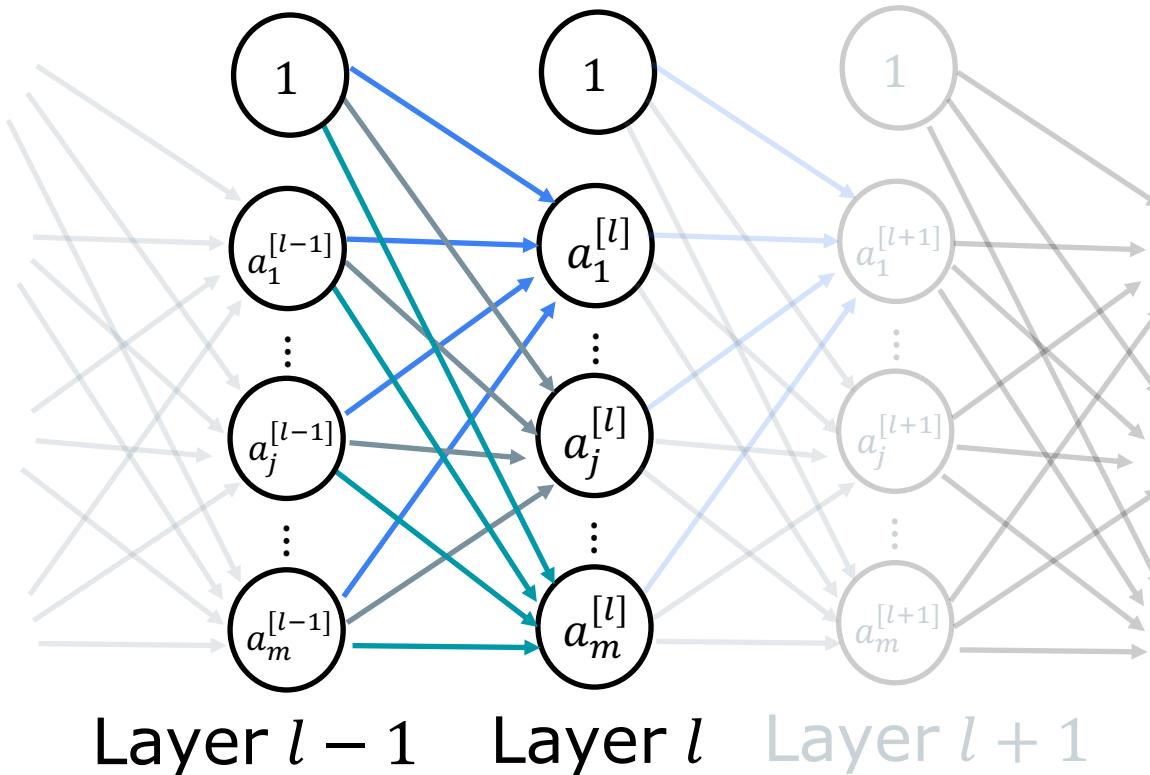
Multi-layer Neural Network



Multi-layer Neural Network



Multi-layer Perceptron



Layer Activation

$$a = \textcolor{brown}{g}(\textcolor{blue}{f}(x)), \textcolor{blue}{f}(x) = \textcolor{green}{w} \cdot x$$

Single-Layer
Perceptron

$$a^{[l]} = \textcolor{brown}{g}^{[l]} \left((\textcolor{green}{W}^{[l]})^\top \textcolor{black}{a}^{[l-1]} \right)$$

Diagram illustrating the computation of layer activations:

- Layer l Activation Function:** $\textcolor{brown}{g}^{[l]}$ (highlighted in orange)
- Layer l Weights:** $(\textcolor{green}{W}^{[l]})^\top$ (highlighted in green)
- Layer l Activations:** $a^{[l]}$ (highlighted in black)
- Layer $l - 1$ Activations:** $\textcolor{black}{a}^{[l-1]}$ (highlighted in black)

Annotations with vertical lines pointing to specific parts of the equation:

- A vertical line points from the label "Layer l Activation Function" to the term $\textcolor{brown}{g}^{[l]}$.
- A vertical line points from the label "Layer l Weights" to the term $(\textcolor{green}{W}^{[l]})^\top$.
- A vertical line points from the label "Layer l Activations" to the term $a^{[l]}$.
- A vertical line points from the label "Layer $l - 1$ Activations" to the term $\textcolor{black}{a}^{[l-1]}$.

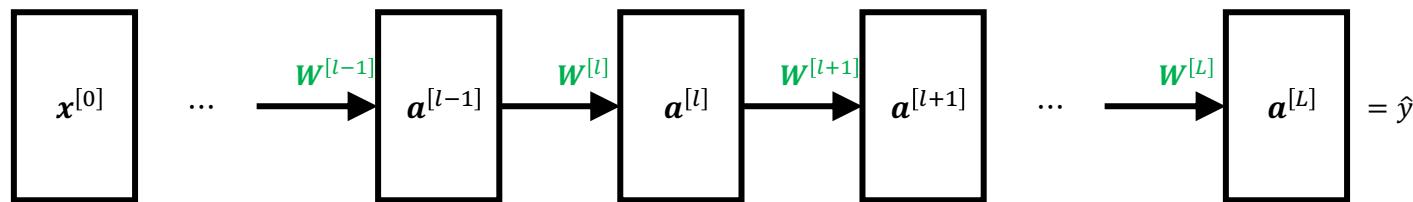
Text on the right side of the equation:

Layer l in Neural Network

Forward Propagation

$$\mathbf{a}^{[l]} \equiv g^{[l]}(\mathbf{f}^{[l]}), \quad \mathbf{f}^{[l]} \equiv (\mathbf{W}^{[l]})^\top \mathbf{a}^{[l-1]}$$

$$g^{[1]}(\mathbf{f}^{[1]}(\mathbf{x}^{[0]})) = \mathbf{a}^{[1]} \quad g^{[l]}(\mathbf{f}^{[l]}(\mathbf{a}^{[l-1]})) = \mathbf{a}^{[l]} \quad g^{[L]}(\mathbf{f}^{[L]}(\mathbf{a}^{[L-1]})) = \mathbf{a}^{[L]}$$

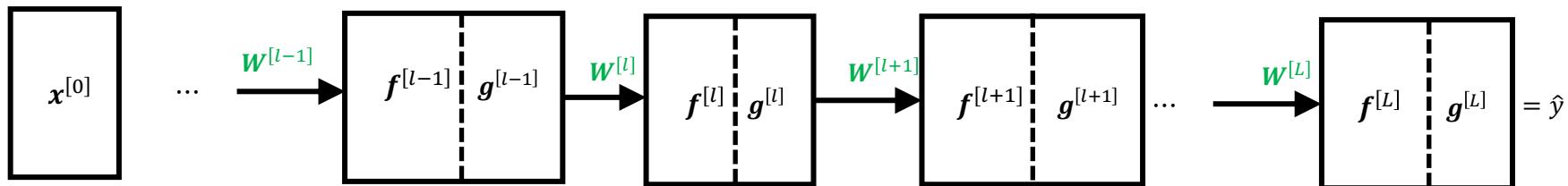


$$\hat{y}(\mathbf{x}) = g^{[L]}(\mathbf{f}^{[L]}(g^{[L-1]}(\dots(g^{[l]}(\mathbf{f}^{[l]}(g^{[l-1]}(\dots(g^{[1]}(\mathbf{f}^{[1]}(\mathbf{x}^{[0]})))))))))))$$

Forward Propagation

$$\mathbf{a}^{[l]} \equiv g^{[l]}(\mathbf{f}^{[l]}), \quad \mathbf{f}^{[l]} \equiv (\mathbf{W}^{[l]})^\top \mathbf{a}^{[l-1]}$$

$$g^{[1]}(\mathbf{f}^{[1]}(\mathbf{x}^{[0]})) = \mathbf{a}^{[1]} \quad g^{[l]}(\mathbf{f}^{[l]}(\mathbf{a}^{[l-1]})) = \mathbf{a}^{[l]} \quad g^{[L]}(\mathbf{f}^{[L]}(\mathbf{a}^{[L-1]})) = \mathbf{a}^{[L]}$$

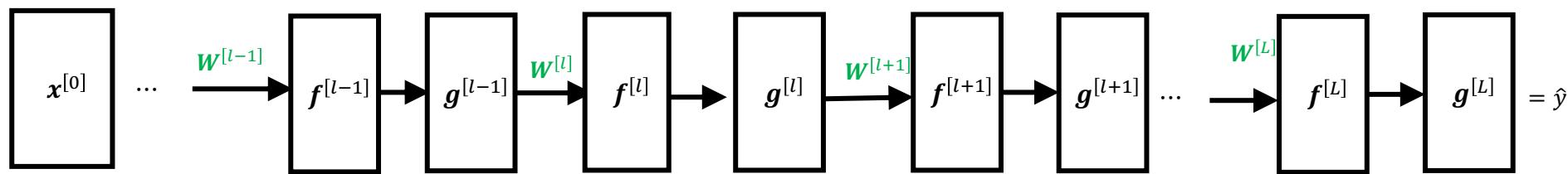


$$\hat{y}(\mathbf{x}) = g^{[L]}(\mathbf{f}^{[L]}(g^{[L-1]}(\dots(g^{[l]}(\mathbf{f}^{[l]}(g^{[l-1]}(\dots(g^{[1]}(\mathbf{f}^{[1]}(\mathbf{x}^{[0]})))))))))))$$

Forward Propagation

$$\mathbf{a}^{[l]} \equiv g^{[l]}(f^{[l]}), \quad f^{[l]} \equiv (\mathbf{W}^{[l]})^\top \mathbf{a}^{[l-1]}$$

$$g^{[1]}(f^{[1]}(\mathbf{x}^{[0]})) = \mathbf{a}^{[1]} \quad g^{[l]}(f^{[l]}(\mathbf{a}^{[l-1]})) = \mathbf{a}^{[l]} \quad g^{[L]}(f^{[L]}(\mathbf{a}^{[L-1]})) = \mathbf{a}^{[L]}$$



$$\hat{y}(\mathbf{x}) = g^{[L]}(f^{[L]}(g^{[L-1]}(\dots(g^{[l]}(f^{[l]}(g^{[l-1]}(\dots(g^{[1]}(f^{[1]}(\mathbf{x}^{[0]}))))))))))$$

How do we
compute the
weights $W^{[l]}$?

Recap: Gradient Descent

1. Decide on some loss function \mathcal{E} , which is general some function of $\hat{y} - y$

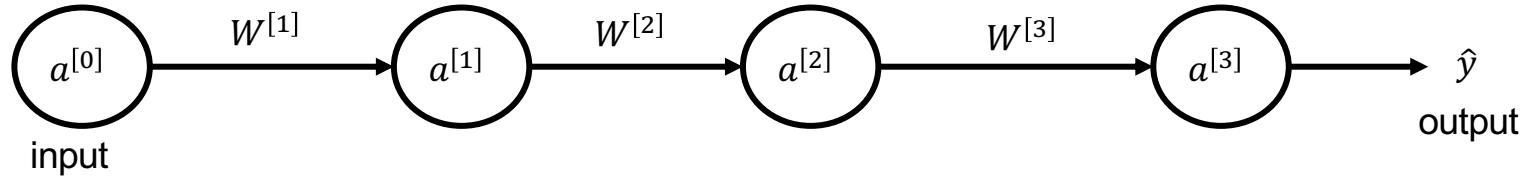
2. Compute $\frac{\partial \mathcal{E}}{\partial \mathbf{w}}$

3. Iterate until convergence:

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \frac{\partial \mathcal{E}}{\partial \mathbf{w}}$$

Backpropagation

Backpropagation: Scalar Example

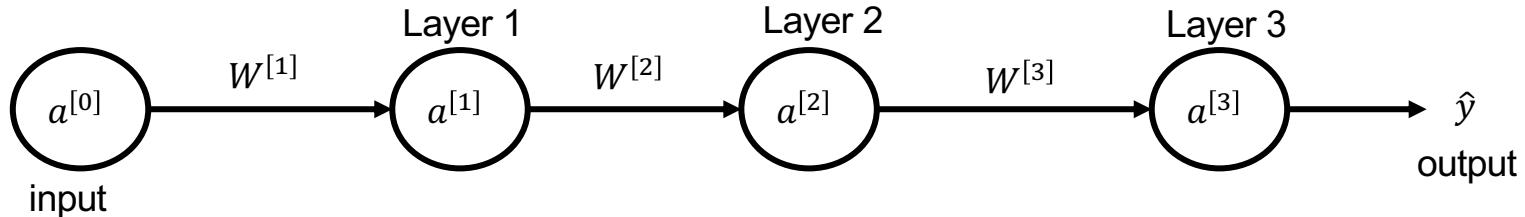


A three-layer NN with single perceptron in each layer

scalar variables

Back Propagation: Scalar Example

A three-layer NN with single perceptron in each layer (scalar variables)



$$\hat{y} = a^{[3]} = g^{[3]} \left(f^{[3]} \left(g^{[2]} \left(f^{[2]} \left(g^{[1]} \left(f^{[1]}(a^{[0]}) \right) \right) \right) \right) \right)$$

$a^{[l]}$: Output of perceptron at l -th layer

$f^{[l]}$: Input of perceptron at l -th layer

$W^{[l]}$: Weights of l -th layer

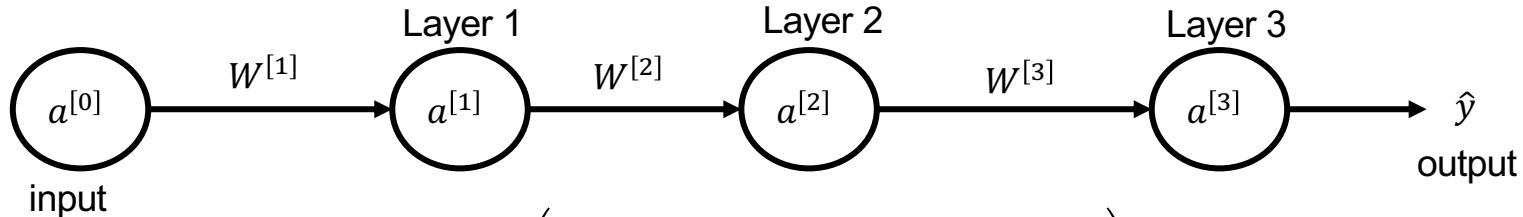
Input Layers : Layer 0

Hidden Layers : Layer 1 and Layer 2

Output Layer : Layer 3

Back Propagation: Scalar Example

A three-layer NN with single perceptron in each layer (scalar variables)



$$\hat{y} = a^{[3]} = g^{[3]} \left(f^{[3]} \left(g^{[2]} \left(f^{[2]} \left(g^{[1]} \left(f^{[1]}(a^{[0]}) \right) \right) \right) \right) \right)$$

$$\begin{aligned}\hat{y} &= a^{[3]} \\ a^{[3]} &= g^{[3]}(f^{[3]}) \\ a^{[2]} &= g^{[2]}(f^{[2]}) \\ a^{[1]} &= g^{[1]}(f^{[1]}) \\ a^{[0]} &= x\end{aligned}$$

$$\begin{aligned}f^{[3]} &= W^{[3]} a^{[2]} \\ f^{[2]} &= W^{[2]} a^{[1]} \\ f^{[1]} &= W^{[1]} a^{[0]}\end{aligned}$$

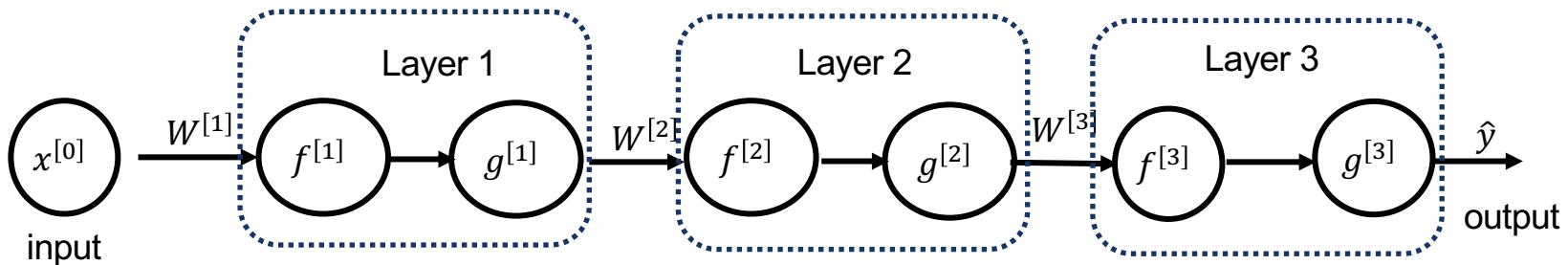
Loss function: MSE

$$\varepsilon = \frac{1}{2}(\hat{y} - y)^2$$

$$W^{[i]} := W^{[i]} - \eta \frac{\partial \varepsilon}{\partial W^{[i]}}$$

Back Propagation: Scalar Example

A three-layer NN with single perceptron in each layer (scalar variables)



$$\hat{y} = a^{[3]} = g^{[3]} \left(f^{[3]} \left(g^{[2]} \left(f^{[2]} \left(g^{[1]} \left(f^{[1]}(a^{[0]}) \right) \right) \right) \right) \right)$$

$$\begin{aligned}\hat{y} &= a^{[3]} \\ a^{[3]} &= g^{[3]}(f^{[3]}) \\ a^{[2]} &= g^{[2]}(f^{[2]}) \\ a^{[1]} &= g^{[1]}(f^{[1]}) \\ a^{[0]} &= x\end{aligned}$$

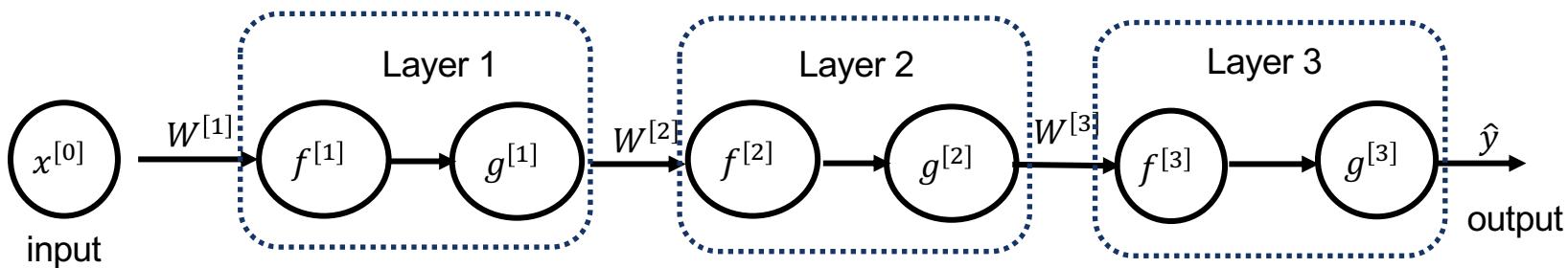
$$\begin{aligned}f^{[3]} &= W^{[3]} a^{[2]} \\ f^{[2]} &= W^{[2]} a^{[1]} \\ f^{[1]} &= W^{[1]} a^{[0]}\end{aligned}$$

Loss function: MSE

$$\varepsilon = \frac{1}{2} (\hat{y} - y)^2$$

$$W^{[i]} := W^{[i]} - \eta \frac{\partial \varepsilon}{\partial W^{[i]}}$$

$$\mathcal{E} = \frac{1}{2}(\hat{y} - y)^2 \quad \frac{\partial \mathcal{E}}{\partial W^{[l]}} = (\hat{y} - y) \frac{\partial \hat{y}}{\partial W^{[l]}}$$



$$\frac{\partial \hat{y}}{\partial W^{[3]}} = \frac{\partial g^{[3]}}{\partial W^{[3]}} = \frac{\partial g^{[3]}}{\partial f^{[3]}} \frac{\partial f^{[3]}}{\partial W^{[3]}}$$

$$\begin{aligned}\hat{y} &= a^{[3]} \\ a^{[3]} &= g^{[3]}(f^{[3]}) \\ a^{[2]} &= g^{[2]}(f^{[2]}) \\ a^{[1]} &= g^{[1]}(f^{[1]})\end{aligned}$$

Store this value and reuse for gradients w.r.t $W^{[1]}$ and $W^{[2]}$

$$f^{[3]} = W^{[3]} a^{[2]}$$

$$\rightarrow \frac{\partial f^{[3]}}{\partial W^{[3]}} = a^{[2]}$$

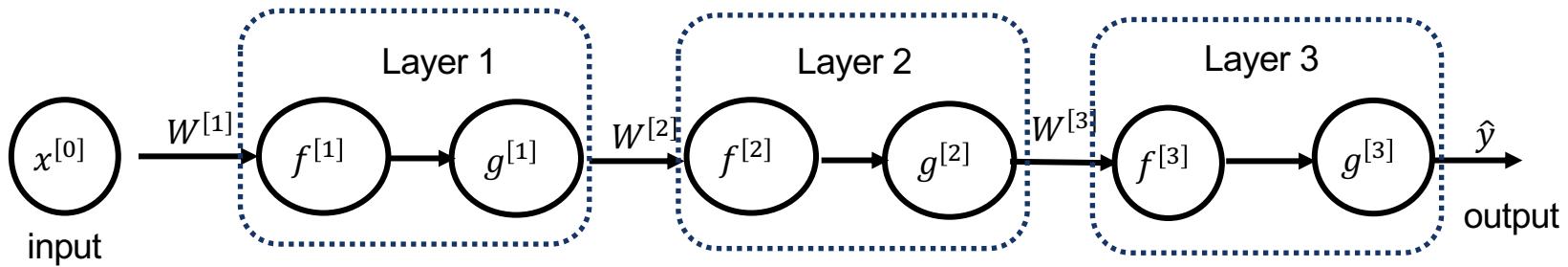
$$\rightarrow \frac{\partial \hat{y}}{\partial W^{[3]}} = \delta^{[3]} a^{[2]} \quad \text{where } \delta^{[3]} = \frac{\partial g^{[3]}}{\partial f^{[3]}}$$

$$\begin{aligned}f^{[3]} &= W^{[3]} a^{[2]} \\ f^{[2]} &= W^{[2]} a^{[1]} \\ f^{[1]} &= W^{[1]} a^{[0]}\end{aligned}$$

$$\delta^{[l]} = \frac{\partial g^{[l]}}{\partial f^{[l]}}$$

$$\mathcal{E} = \frac{1}{2}(\hat{y} - y)^2$$

$$\frac{\partial \mathcal{E}}{\partial W^{[l]}} = (\hat{y} - y) \frac{\partial \hat{y}}{\partial W^{[l]}}$$



From Layer 3

Store this value and reuse for gradients w.r.t \$W^{[1]}

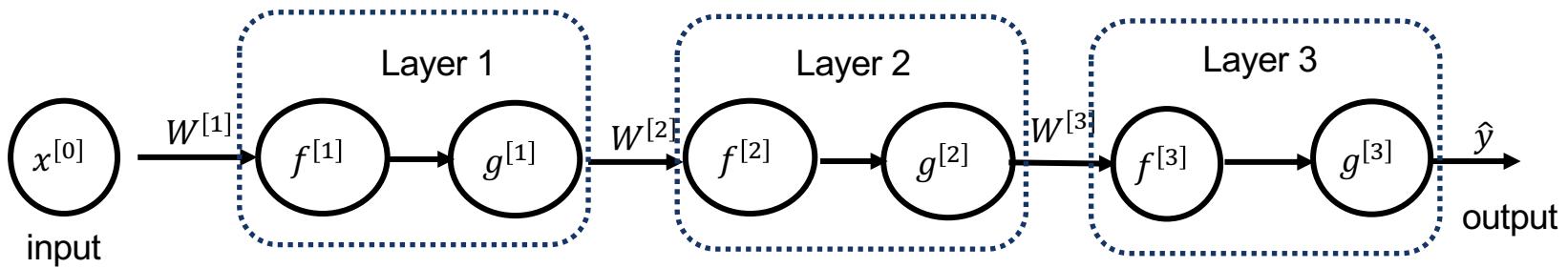
$$\begin{aligned}\frac{\partial \hat{y}}{\partial W^{[2]}} &= \frac{\partial g^{[3]}}{\partial W^{[2]}} = \underbrace{\frac{\partial g^{[3]}}{\partial f^{[3]}}}_{\delta^{[3]}} \underbrace{\frac{\partial f^{[3]}}{\partial g^{[2]}}}_{W^{[3]}} \underbrace{\frac{\partial g^{[2]}}{\partial f^{[2]}}}_{\frac{\partial g^{[2]}}{\partial f^{[2]}}} \underbrace{\frac{\partial f^{[2]}}{\partial W^{[2]}}}_{a^{[1]}} \\ &= \delta^{[3]} W^{[3]} \frac{\partial g^{[2]}}{\partial f^{[2]}} a^{[1]}\end{aligned}$$

$\frac{\partial \hat{y}}{\partial W^{[2]}} = \delta^{[2]} a^{[1]}$ where $\delta^{[2]} = \frac{\partial g^{[3]}}{\partial f^{[2]}} = \delta^{[3]} W^{[3]} \frac{\partial g^{[2]}}{\partial f^{[2]}}$

$\hat{y} = a^{[3]}$
 $a^{[3]} = g^{[3]}(f^{[3]})$
 $a^{[2]} = g^{[2]}(f^{[2]})$
 $a^{[1]} = g^{[1]}(f^{[1]})$

$f^{[3]} = W^{[3]} a^{[2]}$
 $f^{[2]} = W^{[2]} a^{[1]}$
 $f^{[1]} = W^{[1]} a^{[0]}$

$$\mathcal{E} = \frac{1}{2}(\hat{y} - y)^2 \quad \frac{\partial \mathcal{E}}{\partial W^{[l]}} = (\hat{y} - y) \frac{\partial \hat{y}}{\partial W^{[l]}}$$



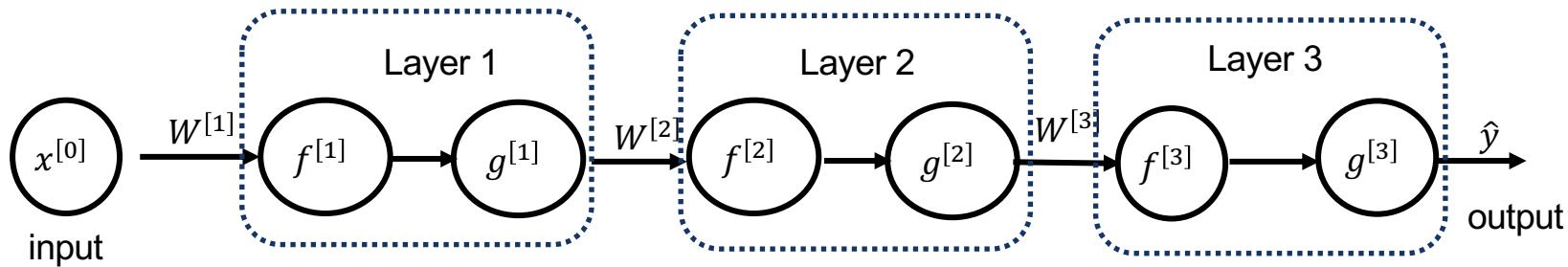
$\frac{\partial \hat{y}}{\partial W^{[1]}} = \frac{\partial g^{[3]}}{\partial W^{[1]}} = \underbrace{\frac{\partial g^{[3]}}{\partial f^{[3]}} \frac{\partial f^{[3]}}{\partial g^{[2]}} \frac{\partial g^{[2]}}{\partial f^{[2]}}}_{\frac{\partial g^{[3]}}{\partial f^{[2]}} \text{ from layer 2}} \underbrace{\frac{\partial f^{[2]}}{\partial g^{[1]}} \frac{\partial g^{[1]}}{\partial f^{[1]}} \frac{\partial f^{[1]}}{\partial W^{[1]}}}_{\frac{\partial g^{[3]}}{\partial f^{[1]}}} = \delta^{[2]} W^{[2]} \frac{\partial g^{[1]}}{\partial f^{[1]}} a^{[0]}$

$$\frac{\partial \hat{y}}{\partial W^{[1]}} = \delta^{[1]} a^{[0]}, \quad \text{where } \delta^{[1]} = \delta^{[2]} W^{[2]} \frac{\partial g^{[1]}}{\partial f^{[1]}}$$

$$\begin{aligned}\hat{y} &= a^{[3]} \\ a^{[3]} &= g^{[3]}(f^{[3]}) \\ a^{[2]} &= g^{[2]}(f^{[2]}) \\ a^{[1]} &= g^{[1]}(f^{[1]})\end{aligned}$$

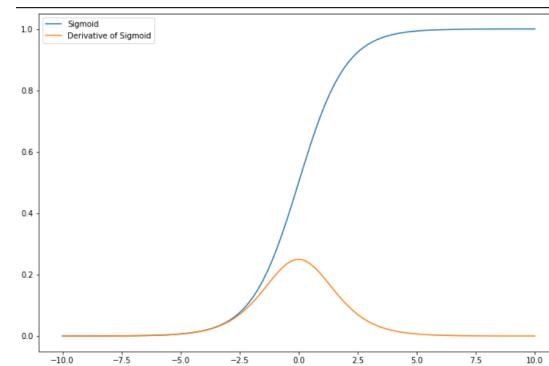
$$\begin{aligned}f^{[3]} &= W^{[3]} a^{[2]} \\ f^{[2]} &= W^{[2]} a^{[1]} \\ f^{[1]} &= W^{[1]} a^{[0]}\end{aligned}$$

Vanishing Gradient Problem



$$\frac{\partial \hat{y}}{\partial W^{[1]}} = \frac{\partial g^{[3]}}{\partial W^{[1]}} = \frac{\partial g^{[3]}}{\partial f^{[3]}} \frac{\partial f^{[3]}}{\partial g^{[2]}} \frac{\partial g^{[2]}}{\partial f^{[2]}} \frac{\partial f^{[2]}}{\partial g^{[1]}} \frac{\partial g^{[1]}}{\partial f^{[1]}} \frac{\partial f^{[1]}}{\partial W^{[1]}}$$

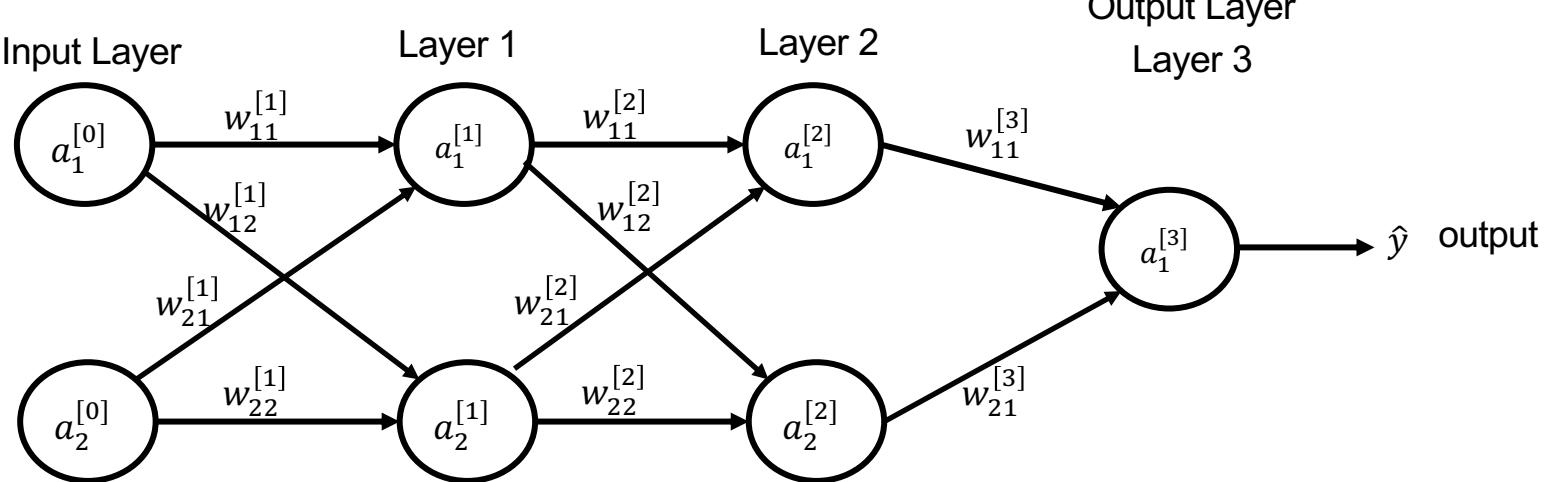
< 0.25 for Sigmoid



The gradients approach zero as number of layers increase
Zero gradients mean, no update to the weights

Back Propagation: Vector Example

A three-layer NN with two perceptrons in hidden layers

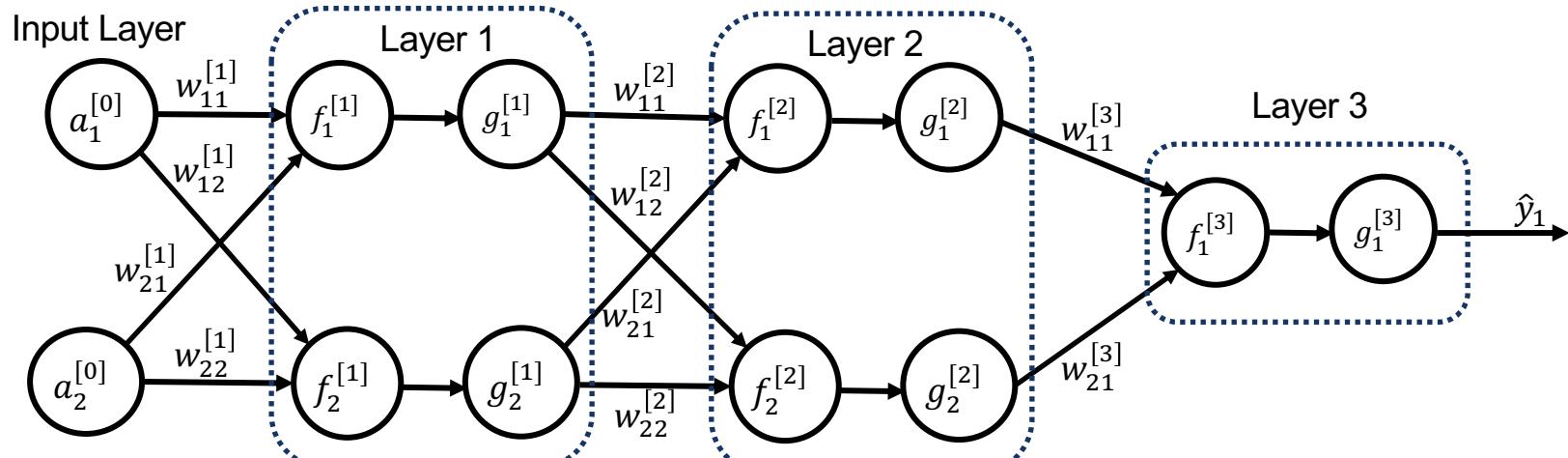


$$\hat{y} = \mathbf{a}^{[3]} = \mathbf{g}^{[3]} \left(\mathbf{f}^{[3]} \left(\mathbf{g}^{[2]} \left(\mathbf{f}^{[2]} \left(\mathbf{g}^{[1]} \left(\mathbf{f}^{[1]}(W^{[1]}, \mathbf{a}^{[0]}) \right) \right) \right) \right) \right)$$

$$W^{[l]} = \begin{bmatrix} w_{11}^{[1]} & w_{12}^{[1]} \\ w_{21}^{[1]} & w_{22}^{[1]} \end{bmatrix} \quad \mathbf{a}^{[l]} = \begin{bmatrix} a_1^{[l]} \\ a_2^{[l]} \end{bmatrix} \quad \mathbf{f}^{[l]} = \begin{bmatrix} f_1^{[l]} \\ f_2^{[l]} \end{bmatrix} \quad \mathbf{g}^{[l]} = \begin{bmatrix} g_1^{[l]} \\ g_2^{[l]} \end{bmatrix} \quad \hat{y} = a_1^{[3]}$$

- $\mathbf{a}^{[l]}$: Output of perceptron at l -th layer
- $\mathbf{f}^{[l]}$: Input of perceptron at l -th layer
- $\mathbf{g}^{[l]}$: Activation at l -th layer
- $W^{[l]}$: Weights of l -th layer
- Input Layers** : Layer 0
- Hidden Layers** : Layer 1 and Layer 2
- Output Layer** : Layer 3

Back Propagation: Vector Example



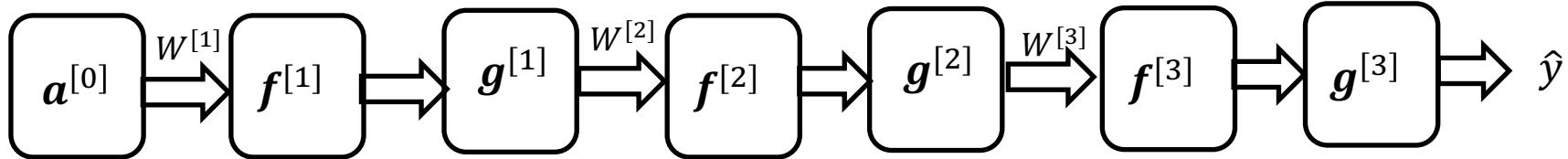
$$\mathbf{a}^{[l]} \equiv \mathbf{g}^{[l]}(\mathbf{f}^{[l]})$$

$$\hat{y} = \mathbf{a}^{[3]} = \mathbf{g}^{[3]} \left(\mathbf{f}^{[3]} \left(\mathbf{g}^{[2]} \left(\mathbf{f}^{[2]} \left(\mathbf{g}^{[1]} \left(\mathbf{f}^{[1]}(W^{[1]}, \mathbf{a}^{[0]}) \right) \right) \right) \right) \right)$$

$$\mathbf{f}^{[l]} \equiv (\mathbf{W}^{[l]})^\top \mathbf{a}^{[l-1]}$$

$$W^{[l]} = \begin{bmatrix} w_{11}^{[l]} & w_{12}^{[l]} \\ w_{21}^{[l]} & w_{22}^{[l]} \end{bmatrix} \quad \mathbf{a}^{[l]} = \begin{bmatrix} a_1^{[l]} \\ a_2^{[l]} \end{bmatrix} \quad \mathbf{f}^{[l]} = \begin{bmatrix} f_1^{[l]} \\ f_2^{[l]} \end{bmatrix} \quad \mathbf{g}^{[l]} = \begin{bmatrix} g_1^{[l]} \\ g_2^{[l]} \end{bmatrix} \quad \mathbf{f}^{[3]} = [f_1^{[3]}] \quad \mathbf{g}^{[3]} = [g_1^{[3]}]$$

Back Propagation: Vector Example



$$\begin{aligned}\hat{y} &= \mathbf{a}^{[3]} = \mathbf{g}^{[3]} \left(\mathbf{f}^{[3]} \left(\mathbf{g}^{[2]} \left(\mathbf{f}^{[2]} \left(\mathbf{g}^{[1]} \left(\mathbf{f}^{[1]}(\mathbf{a}^{[0]}) \right) \right) \right) \right) \right) \\ &= g_1^{[3]} \left(f_1^{[3]}(\mathbf{g}^{[2]}) \right)\end{aligned}$$

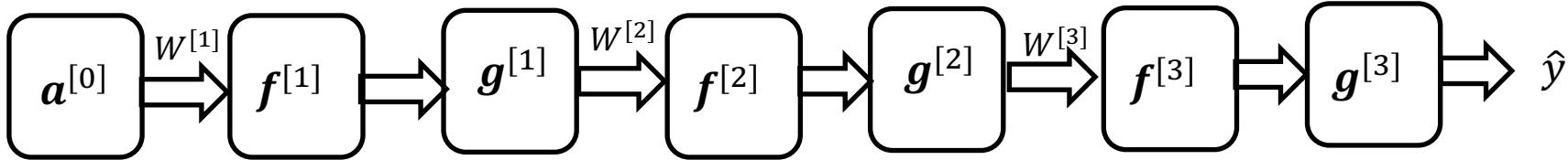
Refer slide 8 of "MatrixCalculus_January2025.pdf" for the proof

$$\begin{aligned}\hat{y}'(W^{[3]}) &= \frac{\partial \mathbf{g}^{[3]}}{\partial W^{[3]}} = \frac{\partial f_1^{[3]}}{\partial W^{[3]}} \frac{\partial g_1^{[3]}}{\partial f_1^{[3]}} = \mathbf{a}^{[2]} \left(\frac{\partial g_1^{[3]}}{\partial f_1^{[3]}} \right)^T \\ &= \mathbf{a}^{[2]} (\delta^{[3]})^T\end{aligned}$$

$$f_1^{[3]}(\mathbf{g}^{[2]}) = (W^{[3]})^\top \mathbf{a}^{[2]}$$

$$\delta^{[3]} = \frac{\partial g_1^{[3]}}{\partial f_1^{[3]}}$$

Back Propagation: Vector Example



$$\begin{aligned}\hat{y} &= a^{[3]} = \mathbf{g}^{[3]} \left(\mathbf{f}^{[3]} \left(\mathbf{g}^{[2]} \left(\mathbf{f}^{[2]} \left(\mathbf{g}^{[1]} \left(\mathbf{f}^{[1]}(a^{[0]}) \right) \right) \right) \right) \right) \\ &= g_1^{[3]} \left(f_1^{[3]} \left(\mathbf{g}^{[2]} \left(\mathbf{f}^{[2]}(\mathbf{g}^{[1]}) \right) \right) \right)\end{aligned}$$

Refer slide 8 of
“MatrixCalculus_January2025.pdf” for
the proof

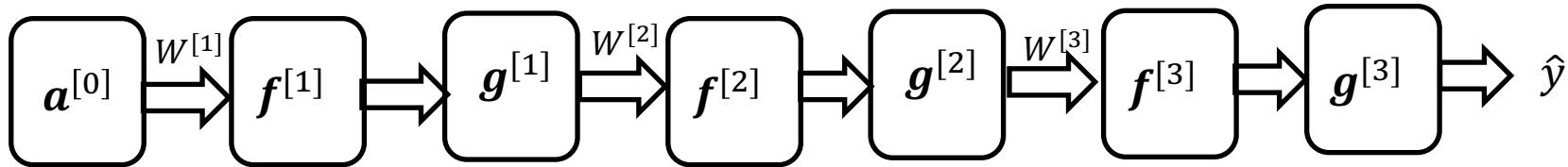
$$\begin{aligned}\hat{y}'(W^{[2]}) &= \frac{\partial g_1^{[3]}}{\partial W^{[2]}} = \frac{\partial f^{[2]}}{\partial W^{[2]}} \frac{\partial g_1^{[3]}}{\partial f^{[2]}} = \mathbf{a}^{[1]} \left(\frac{\partial g_1^{[3]}}{\partial f^{[2]}} \right)^T \\ &= \mathbf{a}^{[1]} \left(\frac{\partial g^{[2]}}{\partial f^{[2]}} \frac{\partial f_1^{[3]}}{\partial g^{[2]}} \frac{\partial g_1^{[3]}}{\partial f_1^{[3]}} \right)^T \\ &= \mathbf{a}^{[1]} \left(\frac{\partial g^{[2]}}{\partial f^{[2]}} \frac{\partial f_1^{[3]}}{\partial g^{[2]}} \delta^{[3]} \right)^T \\ &= \mathbf{a}^{[1]} (\boldsymbol{\delta}^{[2]})^T\end{aligned}$$

$$f^{[2]}(\mathbf{g}^{[1]}) = (W^{[2]})^T \mathbf{a}^{[1]}$$

$$\boldsymbol{\delta}^{[3]} = \frac{\partial g_1^{[3]}}{\partial f_1^{[3]}}$$

$$\begin{aligned}\boldsymbol{\delta}^{[2]} &= \frac{\partial g_1^{[3]}}{\partial f^{[2]}} \\ &= \frac{\partial g^{[2]}}{\partial f^{[2]}} \frac{\partial f_1^{[3]}}{\partial g^{[2]}} \boldsymbol{\delta}^{[3]}\end{aligned}$$

Back Propagation: Vector Example



$$\hat{y} = a^{[3]} = g_1^{[3]} \left(f_1^{[3]} \left(g^{[2]} \left(f^{[2]} \left(g^{[1]} \left(f^{[1]}(a^{[0]}) \right) \right) \right) \right) \right)$$

Refer slide 8 of “MatrixCalculus.pdf”
for the proof

$$\hat{y}'(\mathbf{W}^{[1]}) = \frac{\partial g^{[3]}}{\partial \mathbf{W}^{[1]}} = \frac{\partial f^{[1]}}{\partial \mathbf{W}^{[1]}} \frac{\partial g^{[3]}}{\partial \mathbf{f}^{[1]}} = \mathbf{a}^{[0]} \left(\frac{\partial g^{[3]}}{\partial \mathbf{f}^{[1]}} \right)^T$$

$$f^{[1]}(\mathbf{a}^{[0]}) = (\mathbf{W}^{[1]})^T \mathbf{a}^{[0]}$$

$$= \mathbf{a}^{[0]} \left(\frac{\partial g^{[1]}}{\partial \mathbf{f}^{[1]}} \frac{\partial \mathbf{f}^{[2]}}{\partial g^{[1]}} \frac{\partial g^{[2]}}{\partial \mathbf{f}^{[2]}} \frac{\partial f_1^{[3]}}{\partial g^{[2]}} \frac{\partial g_1^{[3]}}{\partial f_1^{[3]}} \right)^T$$

$$\delta^{[3]} = \frac{\partial g_1^{[3]}}{\partial f_1^{[3]}}$$

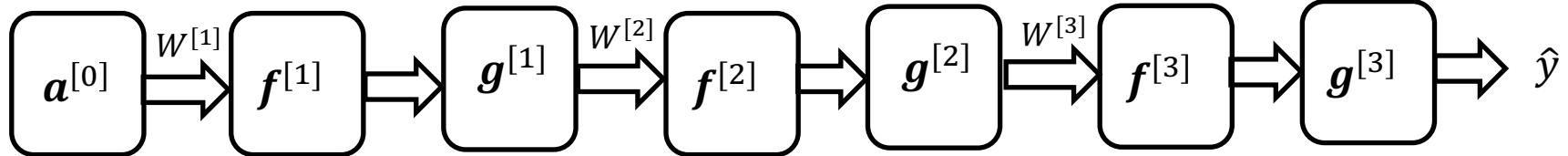
$$= \mathbf{a}^{[0]} \left(\frac{\partial g^{[2]}}{\partial \mathbf{f}^{[1]}} \frac{\partial f^{[3]}}{\partial g^{[2]}} \boldsymbol{\delta}^{[2]} \right)^T$$

$$\boldsymbol{\delta}^{[2]} = \frac{\partial g^{[2]}}{\partial \mathbf{f}^{[2]}} \frac{\partial f_1^{[3]}}{\partial g^{[2]}} \delta^{[3]}$$

$$= \mathbf{a}^{[0]} (\boldsymbol{\delta}^{[1]})^T$$

$$\boldsymbol{\delta}^{[1]} = \frac{\partial g^{[2]}}{\partial \mathbf{f}^{[1]}} \frac{\partial f_1^{[3]}}{\partial g^{[2]}} \delta^{[2]}$$

Back Propagation: Vector Example



$$\hat{y} = a^{[3]} = \mathbf{g}^{[3]} \left(\mathbf{f}^{[3]} \left(\mathbf{g}^{[2]} \left(\mathbf{f}^{[2]} \left(\mathbf{g}^{[1]} \left(\mathbf{f}^{[1]}(a^{[0]}) \right) \right) \right) \right) \right)$$

Derivatives	Recursion
$\hat{y}'(W^{[3]}) = \mathbf{a}^{[2]}(\boldsymbol{\delta}^{[3]})^T$	$\boldsymbol{\delta}^{[3]} = \frac{\partial g_1^{[3]}}{\partial f_1^{[3]}}$
$\hat{y}'(W^{[2]}) = \mathbf{a}^{[1]}(\boldsymbol{\delta}^{[2]})^T$	$\boldsymbol{\delta}^{[2]} = \frac{\partial \mathbf{g}^{[2]}}{\partial \mathbf{f}^{[2]}} \frac{\partial f_1^{[3]}}{\partial \mathbf{g}^{[2]}} \boldsymbol{\delta}^{[3]}$
$\hat{y}'(W^{[1]}) = \mathbf{a}^{[0]}(\boldsymbol{\delta}^{[1]})^T$	$\boldsymbol{\delta}^{[1]} = \frac{\partial \mathbf{g}^{[1]}}{\partial \mathbf{f}^{[1]}} \frac{\partial f_1^{[2]}}{\partial \mathbf{g}^{[1]}} \boldsymbol{\delta}^{[2]}$

$$\mathbf{a}^{[l]} \equiv \mathbf{g}^{[l]}(\mathbf{f}^{[l]})$$

$$\mathbf{f}^{[l]} \equiv (W^{[l]})^T \mathbf{a}^{[l-1]}$$

$$\boldsymbol{\delta}^{[l]} = \frac{\partial \mathbf{g}^{[l]}}{\partial \mathbf{f}^{[l]}}$$

$\frac{\partial \mathbf{g}^{[l]}}{\partial \mathbf{f}^{[l]}}$: Diagonal Matrix

Generalizing to the L -layer MLP

$$\hat{y}(\mathbf{x}) = g^{[L]}(f^{[L]}(g^{[L-1]}(\dots(g^{[l]}(f^{[l]}(g^{[l-1]}(\dots(g^{[1]}(f^{[1]}(\mathbf{x}^{[0]})\))))))))))$$

Gradient relative to $\mathbf{W}^{[l]}$

$$\hat{y}'(\mathbf{W}^{[l]}) = \frac{\partial \hat{y}}{\partial \mathbf{W}^{[l]}} = \frac{\partial g^{[L]}}{\partial \mathbf{W}^{[l]}} = \frac{\partial f^{[l]}}{\partial \mathbf{W}^{[l]}} \frac{\partial g^{[L]}}{\partial f^{[l]}} = \mathbf{a}^{[l-1]} (\boldsymbol{\delta}^{[l]})^T$$

$$\mathbf{a}^{[l]} = g^{[l]}(\mathbf{f}^{[l]})$$

$$\mathbf{f}^{[l]} = (\mathbf{W}^{[l]})^T \mathbf{a}^{[l-1]}$$

$$\boldsymbol{\delta}^{[l]} = \frac{\partial g^{[L]}}{\partial \mathbf{f}^{[l]}} = \frac{\partial g^{[l]}}{\partial \mathbf{f}^{[l]}} \frac{\partial \mathbf{f}^{[l+1]}}{\partial g^{[l]}} \frac{\partial g^{[L]}}{\partial \mathbf{f}^{[l+1]}}$$

$$\frac{\partial g^{[l]}}{\partial \mathbf{f}^{[l]}} = g'^{[l]}(\mathbf{f}^{[l]})$$

$$\frac{\partial \mathbf{f}^{[l+1]}}{\partial g^{[l]}} = \frac{\partial \mathbf{f}^{[l+1]}}{\partial \mathbf{a}^{[l]}} = \mathbf{W}^{[l+1]}$$

$$\frac{\partial g^{[L]}}{\partial \mathbf{f}^{[l+1]}} = \boldsymbol{\delta}^{[l+1]}$$

$$\hat{y}'(\mathbf{W}^{[l]}) = \mathbf{a}^{[l-1]} (\boldsymbol{\delta}^{[l]})^T$$

$$\boldsymbol{\delta}^{[l]} = g'^{[l]}(\mathbf{f}^{[l]}) \mathbf{W}^{[l+1]} \boldsymbol{\delta}^{[l+1]}$$

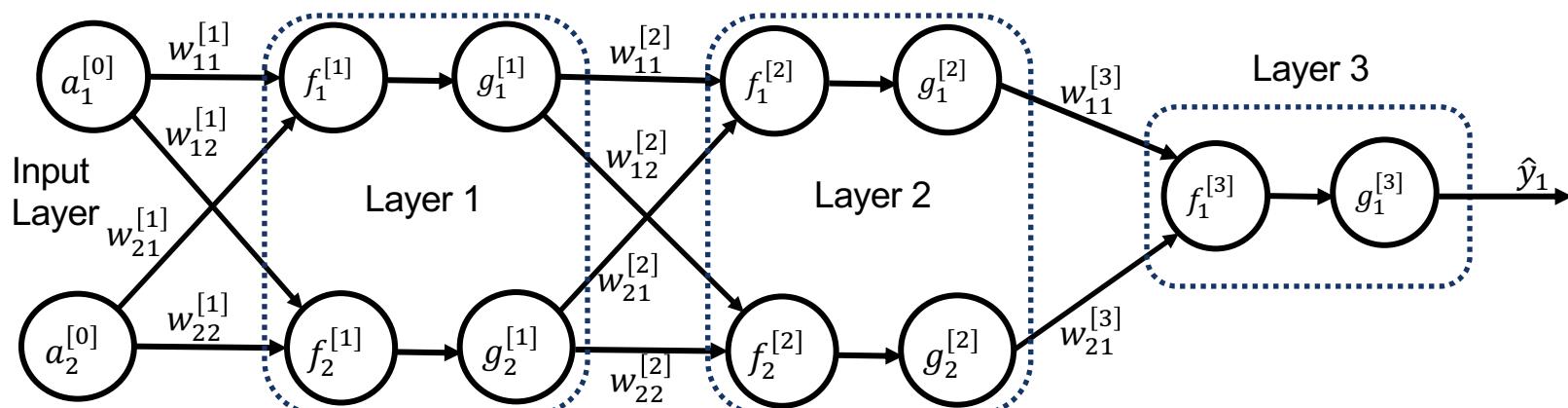
Recursion

A Closer Look at $\delta^{[l]}$:

$$\delta^{[l]} = g'^{[l]}(f^{[l]}) \underbrace{W^{[l+1]} \delta^{[l+1]}}_{\substack{n^{[l]} \times n^{[l+1]} \\ n^{[l+1]} \times 1 \\ \text{Diagonal Matrix}}} \quad n^{[l]} \times 1$$

$n^{[l]}$: # of perceptrons in l -th layer

$$n^{[l]} = 2, \forall l$$



$$g'^{[l]}(f^{[l]}) = \frac{\partial g^{[l]}(f^{[l]})}{\partial f^{[l]}} = \begin{bmatrix} \frac{\partial g_1^{[l]}(f_1^{[l]})}{\partial f_1^{[l]}} & \frac{\partial g_2^{[l]}(f_2^{[l]})}{\partial f_1^{[l]}} \\ \frac{\partial g_1^{[l]}(f_1^{[l]})}{\partial f_2^{[l]}} & \frac{\partial g_2^{[l]}(f_2^{[l]})}{\partial f_2^{[l]}} \end{bmatrix} = \begin{bmatrix} \frac{\partial g_1^{[l]}(f_1^{[l]})}{\partial f_1^{[l]}} & 0 \\ 0 & \frac{\partial g_2^{[l]}(f_2^{[l]})}{\partial f_2^{[l]}} \end{bmatrix} = diag \left(\begin{bmatrix} \frac{\partial g_1^{[l]}(f_1^{[l]})}{\partial f_1^{[l]}} \\ \frac{\partial g_2^{[l]}(f_2^{[l]})}{\partial f_2^{[l]}} \end{bmatrix} \right) \quad g^{[l]} = \begin{bmatrix} g_1^{[l]} \\ g_2^{[l]} \end{bmatrix} \quad f^{[l]} = \begin{bmatrix} f_1^{[l]} \\ f_2^{[l]} \end{bmatrix}$$

Exploiting Diagonal Matrix

- Product of a diagonal matrix and a vector is equivalent to Hadamard product of diagonal elements of the matrix and vector

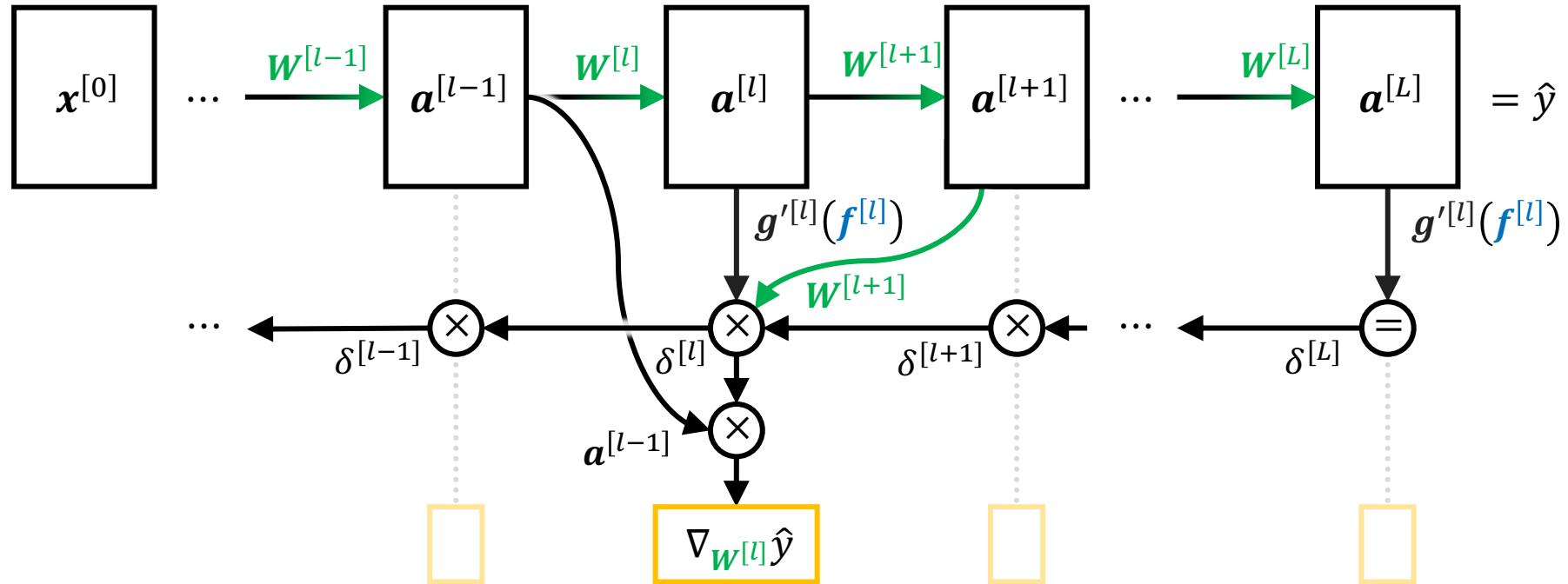
Hadamard Product: elementwise multiplication

$$\begin{bmatrix} x & 0 & 0 \\ 0 & y & 0 \\ 0 & 0 & z \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} xa \\ yb \\ zc \end{bmatrix} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} \circ \begin{bmatrix} a \\ b \\ c \end{bmatrix}$$

$$\delta^{[l]} = g'^{[l]}(f^{[l]}) \underbrace{W^{[l+1]}}_{\substack{n^{[l]} \times n^{[l]} \\ \text{Diagonal Matrix}}} \underbrace{\delta^{[l+1]}}_{n^{[l]} \times 1} \quad \longrightarrow \quad \delta^{[l]} = g'^{[l]}(f^{[l]}) \circ \underbrace{W^{[l+1]}}_{\substack{n^{[l]} \times 1 \\ \text{Vector with} \\ \text{Diagonal Elements}}} \underbrace{\delta^{[l+1]}}_{n^{[l]} \times 1}$$

Hadamard Product: Elementwise multiplication of matrices

Backward Propagation

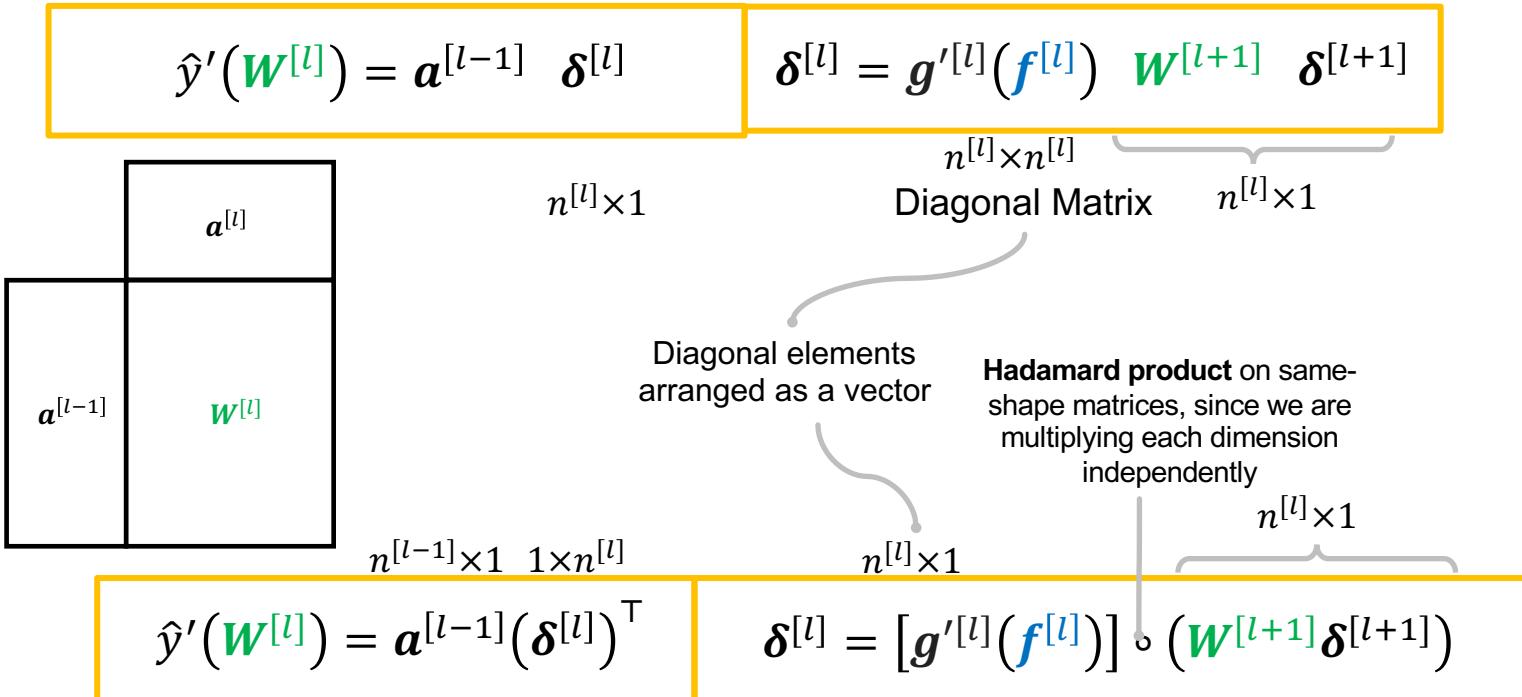


$$\hat{y}'(\mathbf{W}^{[l]}) = \mathbf{a}^{[l-1]} (\boldsymbol{\delta}^{[l]})^\top$$

$$\boldsymbol{\delta}^{[l]} = [g'^{[l]}(\mathbf{f}^{[l]})] \circ (\mathbf{W}^{[l+1]} \boldsymbol{\delta}^{[l+1]})$$

Matrix multiplication

nRows×nCols $n^{[l-1]} \times n^{[l]}$ $n^{[l-1]} \times 1$ $n^{[l]} \times 1$ $n^{[l]} \times n^{[l+1]}$ $n^{[l+1]} \times 1$



Gradients in MLP: Intuition

$$\hat{y}(\mathbf{x}) = g^{[L]}(f^{[L]}(g^{[L-1]}(\dots(g^{[l]}(f^{[l]}(g^{[l-1]}(\dots(g^{[1]}(f^{[1]}(\mathbf{x}^{[0]})))))))))))$$

$$\hat{y}'(\mathbf{W}^{[l]}) = \mathbf{a}^{[l-1]} (\boldsymbol{\delta}^{[l]})^T$$

$$\frac{\partial g^{[L]}}{\partial f^{[l]}} = \boldsymbol{\delta}^{[l]}$$

$\boldsymbol{\delta}^{[l]}$ indicates how much the output (error) of the NN will change in response to small changes in the weighted sum of inputs to the neurons at the l -th layer

$$\boldsymbol{\delta}^{[l]} = g'^{[l]}(f^{[l]}) \mathbf{W}^{[l+1]} \boldsymbol{\delta}^{[l+1]}$$

Recursion

$$\frac{\partial g^{[l]}}{\partial f^{[l]}} = g'^{[l]}(f^{[l]})$$

local gradient

Indicates how much output of a neuron changes in response to a change in weighted sum of its inputs

$$\frac{\partial f^{[l+1]}}{\partial g^{[l]}} \frac{\partial g^{[l]}}{\partial f^{[l+1]}} = W^{[l+1]} \boldsymbol{\delta}^{[l+1]}$$

Backpropagated Error Signal

This product represents the error signal from the next layer ($l + 1$) propagated backward through the weights $W^{[l+1]}$ to l -th layer

Back propagation

Backpropagation **efficiently** computes the gradient by

- Avoiding **duplicate** calculations
- Not computing **unnecessary intermediate values**,
- Computing the gradient of **each layer**

In particular, the gradient of the weighted input of each layer is calculated from back $[l + 1]$ to front $[l]$:

$$\hat{y}'(\mathbf{W}^{[l]}) = \mathbf{a}^{[l-1]}(\boldsymbol{\delta}^{[l]})^\top$$

$$\boldsymbol{\delta}^{[l]} = [g'^{[l]}(f^{[l]})] \circ (\mathbf{W}^{[l+1]} \boldsymbol{\delta}^{[l+1]})$$

Tensors

A Tensor is a multi-dimensional “matrix” containing elements of a single data type

- 0-D Tensor $X \Rightarrow$ scalar
- 1-D Tensor $X[i] \Rightarrow$ vector
- 2-D Tensor $X[i, j] \Rightarrow$ matrix
- 3-D Tensor $X[i, j, k]$

Tensors

- Similar to numpy arrays
<https://rickwierenga.com/blog/machine%20learning/numpy-vs-pytorch-linalg.html>
- Hardware wise, tensors can be loaded onto CUDA enabled GPUs for faster computations,
- Software wise, tensors keep track of additional information (Computational Graph) in order to compute the gradients.

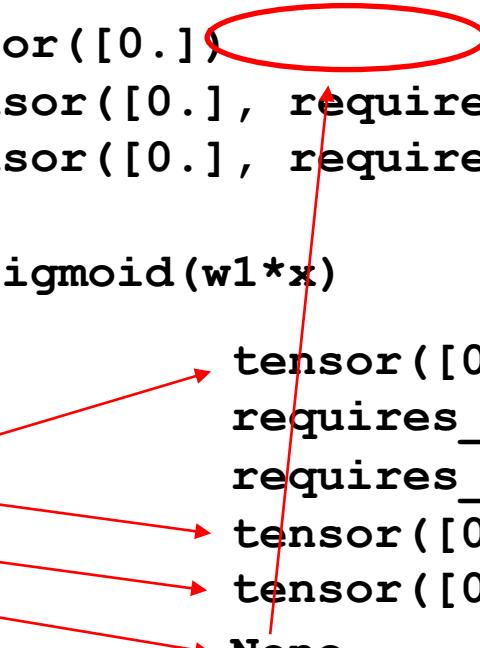
Implementation in PyTorch

```
import torch # Import PyTorch

x = torch.tensor([0.])  
w1 = torch.tensor([0.], requires_grad=True)  
w2 = torch.tensor([0.], requires_grad=True)

y = w2*torch.sigmoid(w1*x)
y.backward()

print(x,w1,w2)           tensor([0.]) tensor([0.],  
print(w1.grad)           requires_grad=True) tensor([0.],  
print(w2.grad)           requires_grad=True)  
print(x.grad)            tensor([0.])  
None
```



How do we know that PyTorch is doing the right thing?

```
epsilon = 0.001
```

```
def y2(w1,w2,x):
```

```
    def sigmoid(x):
```

```
        return 1/(1+math.exp(-x))
```

```
    return w2*sigmoid(w1*x)
```

```
def gradient_w1(w1,w2,x):
```

```
    return (y2(w1+epsilon,w2,x) - \  
           y2(w1-epsilon,w2,x)) / (2*epsilon)
```

$$\hat{y} = w_2 \sigma(w_1 x)$$

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

$$\frac{\partial \hat{y}}{\partial w_i} \approx \frac{\hat{y}(w_i + \varepsilon) - \hat{y}(w_i - \varepsilon)}{2\varepsilon}$$

How do we know that PyTorch is doing the right thing?

```
def gradient_w2(w1,w2,x):  
    return (y2(w1,w2+epsilon,x) - \  
            y2(w1,w2-epsilon,x)) / (2*epsilon)
```

```
print(gradient_w1(0,0,x)) → 0.0  
print(gradient_w2(0,0,x)) → 0.5
```

What happened
to the loss
function ε ?

Key insight:

$\frac{\partial \varepsilon}{\partial w_i} = \frac{\partial \varepsilon}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial w_i}$ so once we have all the $\frac{\partial \hat{y}}{\partial w_i}$'s, we can compute any $\frac{\partial \varepsilon}{\partial w}$ for use with gradient descent

Recap: Gradient Descent

1. Decide on some loss function \mathcal{E} , which is general some function of $\hat{y} - y$

2. Compute $\frac{\partial \mathcal{E}}{\partial \mathbf{w}}$

3. Iterate until convergence:

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \frac{\partial \mathcal{E}}{\partial \mathbf{w}} = \frac{\partial \mathcal{E}}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \mathbf{w}}$$

Auto Differentiation for Backprop

- Even with backprop, implementing the gradients is tedious
- Deep learning APIs have automated differentiation.
 - Tensor Flow autodiff
 - PyTorch autograd
 - Implement derivatives of many common functions
 - You just need to implement your layers and neurons; API will handle gradients

Caution

- If you want to implement **custom functions/layers** (not simple weighted sum)
 - They need to be **differentiable** to be able to calculate their **gradients**
 - Otherwise, backprop **cannot update** weights accurately

So how do we go
about training a
Neural Network?

Let's train a NN for $y = x^2$

```
import torch.nn as nn

class MultilayerPerceptron(nn.Module): # 3 layers, with 2
hidden layers of the same size

    def __init__(self, input_size, hidden_size):
        # Call to the __init__ function of the super class
        super(MultilayerPerceptron, self).__init__()

        # Bookkeeping: Saving the initialization parameters
        self.input_size = input_size
        self.hidden_size = hidden_size
```

Let's train a NN for $y = x^2$

```
# Defining of our layers
self.linear = nn.Linear(self.input_size, \
                      self.hidden_size)
self.linear2 = nn.Linear(self.hidden_size, \
                      self.hidden_size)
self.linear3 = nn.Linear(self.hidden_size, 1)
self.relu = nn.ReLU()

def forward(self, x):
    linear = self.linear(x)      Auto-randomized weights. w/o this, all
                                the neurons in the same layer will
                                "learn" the same function/update to the
                                same value.
    linear2 = self.linear2(self.relu(linear))
    linear3 = self.linear3(self.relu(linear2))
    return linear3
```

What's in the model?

```
[('linear.weight',
  Parameter containing:
  tensor([[-8.4808e-01],
         [-1.6513e+00],
         [ 7.3262e-04],
         [ 1.2931e+00],
         [-1.2794e+00],
         [ 6.2609e-01],
         [ 1.0877e+00],
         [ 1.0415e+00]], requires_grad=True)),
 ('linear.bias',
  Parameter containing:
  tensor([-7.2229, -4.7316, -1.6215, -2.8653, -1.5121, -0.3011, -1.2276, -7.6588],
        requires_grad=True)),
 ('linear2.weight',
  Parameter containing:
  tensor([[ 4.6861, -0.4884,  0.3506, -0.3301,  0.3303, -0.5205, -0.5355,  6.3255],
         [-0.5538, -0.5617, -0.3647, -0.1368, -0.5342, -0.7102, -0.8007, -0.3282],
         [ 0.5950,  1.6070, -0.1568,  1.1529,  0.0298,  0.0076,  0.4839,  0.9624],
         [ 0.6179,  1.8320, -0.2905,  1.0212, -0.4870, -0.1435,  0.5969,  0.6689],
         [ 0.3527,  1.6112,  0.0848,  1.5503, -0.8342,  0.3396,  0.8760,  0.8615],
         [-0.5923, -0.6296, -0.6366, -0.4786, -0.5051, -0.5808, -0.8134, -0.6187],
         [ 1.6187,  1.2003,  0.0634,  0.7204,  2.4347,  1.3357,  1.4979,  1.7267],
         [ 1.5565,  1.7537, -0.1973,  1.4202,  0.1672, -0.0336,  0.6651,  0.6998]], requires_grad=True)),  
.....
```

What's in the model?

```
.....  
('linear2.bias',  
 Parameter containing:  
 tensor([-1.3254, -0.6541, -5.4646, -6.0203, -4.0982, -0.4350,  0.0093, -6.5684],  
       requires_grad=True)),  
('linear3.weight',  
 Parameter containing:  
 tensor([[0.7400, 0.4930, 0.6233, 0.5519, 0.7737, 0.4144, 1.4362, 0.9378]],  
       requires_grad=True)),  
('linear3.bias',  
 Parameter containing:  
 tensor([0.5673], requires_grad=True))]
```

Let's generate the training data

```
# Create the y data
x = 5*torch.randn(100, 1)
# Add some noise to our goal y to generate our x
# We want out model to predict our original data, albeit
the noise
y = torch.square(x) + torch.randn_like(x)
```

$$x^2$$

100 samples of Normally distributed random numbers with mean 0 and variance 1



Same size vector with Normally distributed random numbers with mean 0 and variance 1

Simulate $y = x^2$ with white noise

Set up for training

```
import torch.optim as optim

# Instantiate the model
model = MultilayerPerceptron(1,8)

# Define the optimizer
adam = optim.Adam(model.parameters(), lr=1e-1)

# Define loss using a predefined loss function
loss_function = nn.MSELoss()

# Calculate how our model is doing now
y_pred = model(x)
```

Training Loop

```
n_epoch = 10000
for epoch in range(n_epoch):
    # Set the gradients to 0
    adam.zero_grad()

    # Get the model predictions
    y_pred = model(x)

    # Get the loss
    loss = loss_function(y_pred, y)

    # Print stats
    if epoch%1000==0:
        print(f"Epoch {epoch}: traing loss: {loss}")

    # Compute the gradients
    loss.backward() Backpropagation

    # Take a step to optimize the weights
    adam.step()
```

Let's see how well we do!

```
x2 = 5*torch.randn(5, 1)
print(x2.tolist())
```

```
y2 = torch.square(x2)
print(y2.tolist())
```

```
y_pred = model(x2)
print(y_pred.tolist())
```

Ground truth with
no noise

```
[[5.367788791656494], [0.8833026885986328], [-0.6179562211036682],
[4.864236831665039], [5.316009998321533]]
[[28.813156127929688], [0.7802236676216125], [0.3818698823451996],
[23.660799026489258], [28.25996208190918]]
[[29.595108032226562], [0.8340979814529419], [0.5545129179954529],
[23.755483627319336], [28.972129821777344]]
```

Install PyTorch and
try out the examples
in this lecture

https://web.stanford.edu/class/cs224n/materials/CS224N_PyTorch_Tutorial.html

Why did we use 8x8 with ReLU?

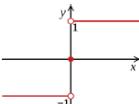
Stack Overflow
suggested! ☺

Neural Network for $\hat{y} = |x - 1|$

Which activation function(s)?

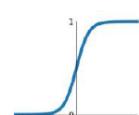
Step

$$\text{sgn}(x) = \begin{cases} +1 & z > 0 \\ -1 & z \leq 0 \end{cases}$$



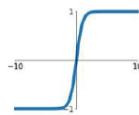
Sigmoid

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



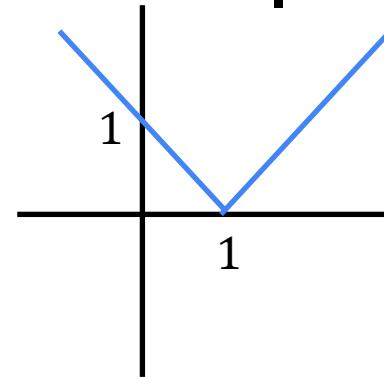
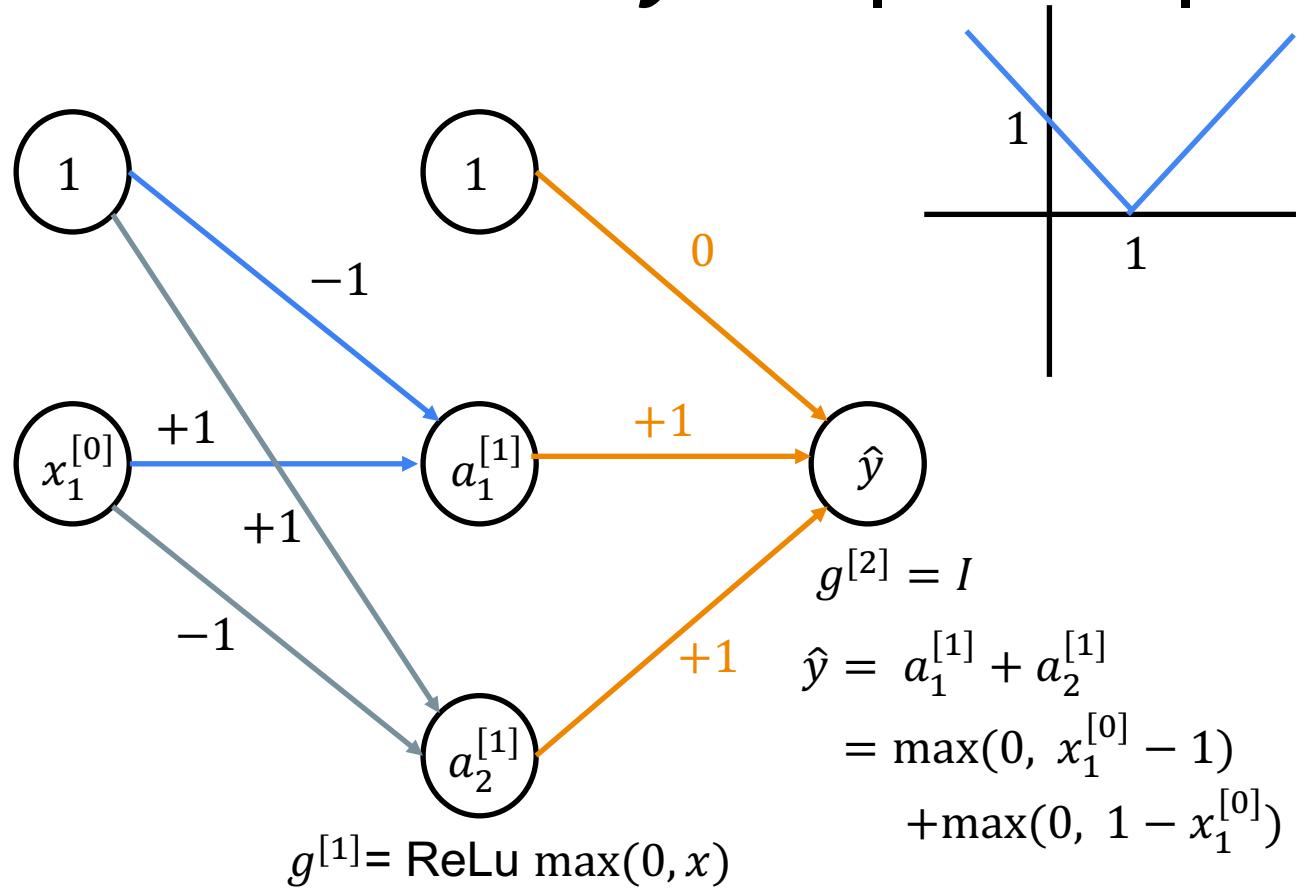
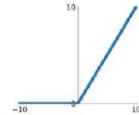
tanh

$$\tanh(x)$$



ReLU

$$\max(0, x)$$



Use PyTorch to
train a network for

$$\hat{y} = |x - 1|$$

<https://playground.tensorflow.org/>

Epoch 000,000 Learning rate 0.03 Activation Tanh Regularization None Regularization rate 0 Problem type Classification

DATA
Which dataset do you want to use?

Ratio of training to test data: 50%
Noise: 0
Batch size: 10

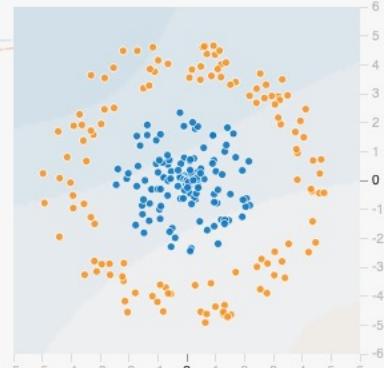
FEATURES
Which properties do you want to feed in?
X¹ X² X¹² X²² X^{1X2} sin(X¹)

2 HIDDEN LAYERS
+ - 4 neurons + - 2 neurons

The outputs are mixed with varying weights, shown by the thickness of the lines.

This is the output from one neuron. Hover to see it larger.

OUTPUT
Test loss 0.503
Training loss 0.505



Summary

- Back Propagation
- Intro to Pytorch
- Training Neural Network
using Gradient Descent