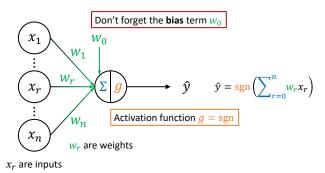
# Backprop

CS 3244 Machine Learning





### Perceptron



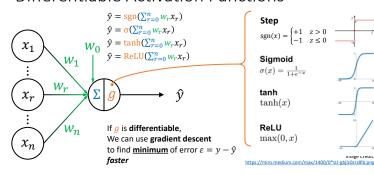
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### Perceptron Learning Algorithm

- 1. Initialize weights w
  - Could be all zero, or random small values
- 2. For each instance i with features  $x^{(i)}$ 
  - Classify  $\hat{y}^{(i)} = \operatorname{sgn}(\boldsymbol{w}^{\mathsf{T}}\boldsymbol{x}^{(i)})$
- 3. Select one misclassified instance
  - Update weights:  $w \leftarrow w + \eta (y \hat{y})x$
- 4. Iterate steps 2 to 3 until
  - Convergence (classification error < threshold), or
  - Maximum number of iterations

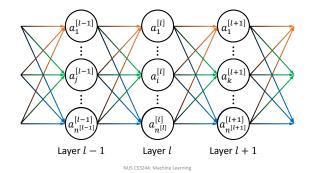
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### Differentiable Activation Functions



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### Multi-Layer Perceptron (Neural Network)



### Chain Rule

Consider composite function

$$g(x) = g\big(f(x)\big)$$

$$g=g(f), f=f(x)$$

$$g'(x) = \frac{dg}{dx} = \frac{dg}{df} \frac{df}{dx}$$

#### Intuition

Rate of change of g relative to x is the product of

- rates of change of g relative to f and
- rates of change of f relative to  $\boldsymbol{x}$

#### "If

- a car travels 2x fast as a bicycle and
- · the bicycle is 4x as fast as a walking man,

then the car travels  $2 \times 4 = 8$  times as fast as the man."

then the car travers 2 × 4 = 8 times as just as the man.

– George F. Simmons, Calculus with Analytic Geometry (1985)

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### Week 09B: Lecture Outline

- 1. Perceptron
- 2. Perceptron Learning Algorithm (PLA)
- 3. Activation Functions
- 4. Gradient Descent
- 5. Neural Networks
- Math Notation Primer
- 6. Backpropagation



## Math Primer



### Notation

n = Number of features in xm = Number of instances in dataset

• Scalar: not bolded, lower case

 $\chi$ 

• Vector: bolded, lower case

$$x = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$$

Matrix: bolded, upper case

$$\boldsymbol{X} = \begin{pmatrix} x_{11} & \cdots & x_{1m} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nm} \end{pmatrix}$$

### Functions with Vectors and Matrices

- Scalar-by-scalar:
  - y(x) = wx for scaling input
- Scalar-by-vector:

• 
$$y(x) = \mathbf{w} \cdot \mathbf{x} = \mathbf{w}^{\mathsf{T}} \mathbf{x} = \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = w_1 x_1 + w_2 x_2$$
 for weighted sum

Vector-by-vector:

• 
$$y(x) = wx = w {x_1 \choose x_2} = {wx_1 \choose wx_2}$$
 for scaled outputs (same weight)

• 
$$\sigma(z) = \frac{e^z}{1^T(1+e^z)}$$
 for softmax

### Functions with Vectors and Matrices

- Matrix-by-matrix:
  - Using Hadamard product of for element-wise multiplication

• 
$$\mathbf{y}(\mathbf{X}) = \mathbf{W} \circ \mathbf{X} = \begin{pmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{pmatrix} \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix} = \begin{pmatrix} w_{11}x_{11} & w_{12}x_{12} \\ w_{21}x_{21} & w_{22}x_{22} \end{pmatrix}$$

Using Convolution operator \* for element-wise multiplication then sum [W08b]

• 
$$Y(X) = W * X = \begin{pmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{pmatrix} \begin{pmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{pmatrix}$$

$$= \begin{pmatrix} w_{11}x_{11} + w_{12}x_{12} + w_{21}x_{21} + w_{22}x_{22} & w_{11}x_{12} + w_{12}x_{13} + w_{21}x_{22} + w_{22}x_{23} \\ w_{11}x_{21} + w_{12}x_{22} + w_{21}x_{31} + w_{22}x_{32} & w_{11}x_{22} + w_{12}x_{23} + w_{21}x_{32} + w_{22}x_{33} \end{pmatrix}$$

For computer vision filters (kernels)

1D Vectors, and 2D Matrices and ≥2D Tensors are for convenient notation of multiple similar calculations.

## Weighted Sum

### **Summation Series** = Scalar

$$\sum_{r=0}^{n} w_n x_r$$

$$w_1 x_1 + \dots + w_r x_r + \dots + w_n x_n$$

### **Vector Dot Product** = Scalar

$$\boldsymbol{w} \cdot \boldsymbol{x} = \begin{pmatrix} w_1 \\ \vdots \\ w_r \\ \vdots \\ w_n \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ \vdots \\ x_r \\ \vdots \\ x_n \end{pmatrix}$$

### **Transposed Vector Multiplication** = Scalar

$$\mathbf{w}^{\mathsf{T}}\mathbf{x} = (w_1 \quad \cdots \quad w_r \quad \cdots \quad w_n) \begin{pmatrix} x_1 \\ \vdots \\ x_r \\ \vdots \\ x_n \end{pmatrix}$$

### **Transposed Matrix Multiplication** = Vector

$$\boldsymbol{W}^{\mathsf{T}}\boldsymbol{x} = \begin{pmatrix} w_{11} & \cdots & w_{1r} & \cdots & w_{1n} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ w_{r1} & \cdots & w_{rr} & \cdots & w_{rn} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ w_{n1} & \cdots & w_{nr} & \cdots & w_{nn} \end{pmatrix}^{\mathsf{T}} \begin{pmatrix} x_1 \\ \vdots \\ x_r \\ \vdots \\ x_n \end{pmatrix}$$

### Gradient

- Derivative: d
  - $\frac{dy}{dx}$  is the derivative of y relative to x
- Partial derivative:  $\partial$ 
  - $\frac{\partial y}{\partial x_1}$  is the derivative of y relative to  $x_1$
  - But y also depends on other variables (e.g.,  $x_2$  so, we can also calculate  $\frac{\partial y}{\partial x_2}$ )
- Gradient: ∇
  - To calculate the derivative relative to all  $x_1$  and  $x_2$  together
  - $\nabla y(x)$  is the gradient of y relative to all variables  $x = (x_1, ..., x_n)^T$

Vector in denominator means
Derivative for each variable is
put in separate, corresponding

$$\nabla y(\mathbf{x}) = \frac{dy}{d\mathbf{x}} = \begin{pmatrix} \frac{\partial y}{\partial x_1} \\ \vdots \\ \frac{\partial y}{\partial x_n} \end{pmatrix} = \begin{pmatrix} \frac{\partial y}{\partial x_1} & \cdots & \frac{\partial y}{\partial x_n} \end{pmatrix}^{\mathsf{T}}$$

variable days unimes Cartesian coordinates (linear, orthogonal)

### Matrix Calculus

Scalar-by-Vector (1D Vector)

$$\frac{dy}{dx} = \begin{pmatrix} \frac{\partial y}{\partial x_1} \\ \vdots \\ \frac{\partial y}{\partial x_n} \end{pmatrix}$$

Vector-by-Vector (2D Matrix) – not in exam

$$\frac{d\mathbf{y}}{d\mathbf{x}} = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_N}{\partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_1}{\partial x_n} & \cdots & \frac{\partial y_N}{\partial x_n} \end{pmatrix}$$

n =Number of features in x

m = Number of instances in dataset

N = Number of y prediction tasks

Scalar-by-Matrix (2D Matrix)

$$\frac{dy}{dX} = \begin{pmatrix} \frac{\partial y}{\partial x_{11}} & \cdots & \frac{\partial y}{\partial x_{1m}} \\ \vdots & \ddots & \vdots \\ \frac{\partial y}{\partial x_{n1}} & \cdots & \frac{\partial y}{\partial x_{nm}} \end{pmatrix}$$

Vector-by-Matrix (3D Tensor) – not in exam

$$\frac{d\mathbf{y}}{d\mathbf{X}} = \begin{pmatrix} \frac{\partial y_1}{\partial x_{11}} & \cdots & \frac{\partial y_1}{\partial x_{1m}} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_1}{\partial x_{n1}} & \cdots & \frac{\partial y_1}{\partial x_{nm}} \end{pmatrix} \quad \cdot \quad \begin{pmatrix} \frac{\partial y_N}{\partial x_{11}} & \cdots & \frac{\partial y_N}{\partial x_{1m}} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_N}{\partial x_{n1}} & \cdots & \frac{\partial y_N}{\partial x_{nm}} \end{pmatrix}$$

Along 3<sup>rd</sup> dimension

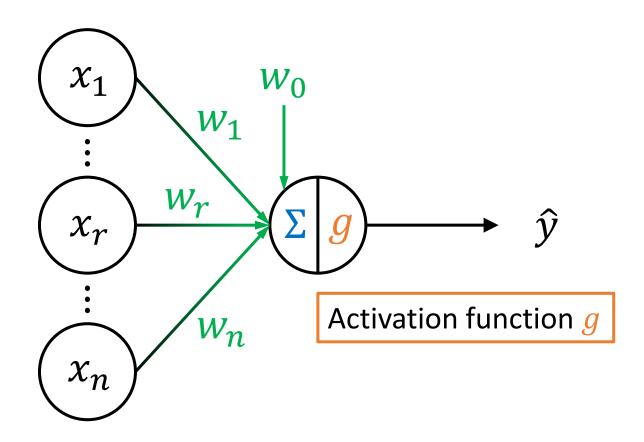
This math informs what matrix **shapes** you need to implement



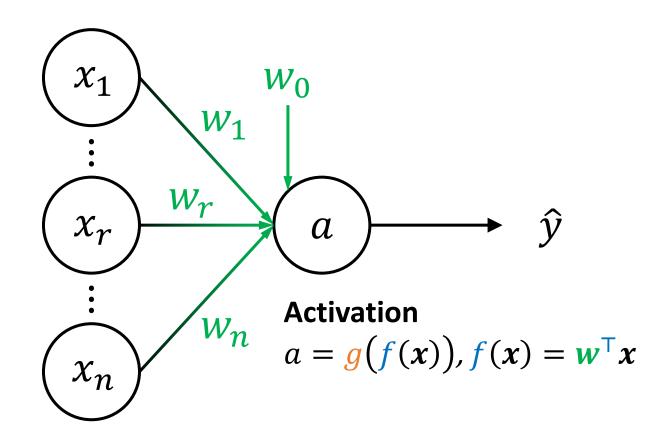
# Neural Network (recap)



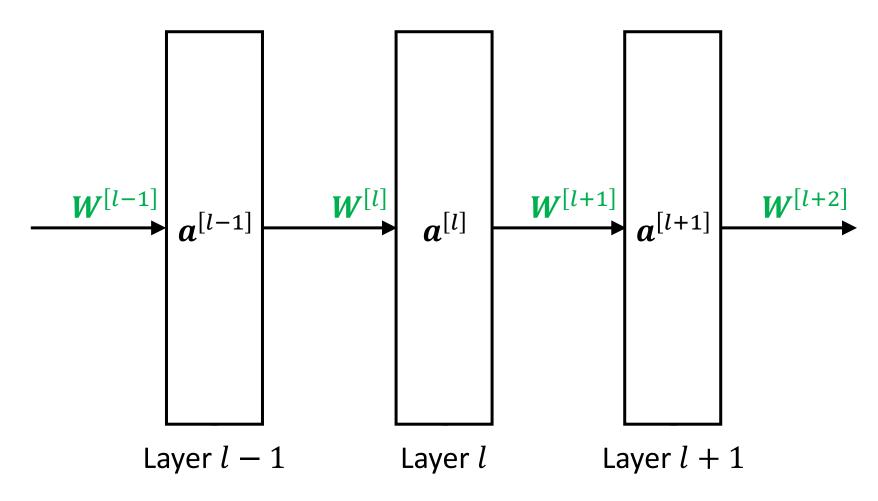
## Single-Layer Perceptron



## Single-Layer Perceptron



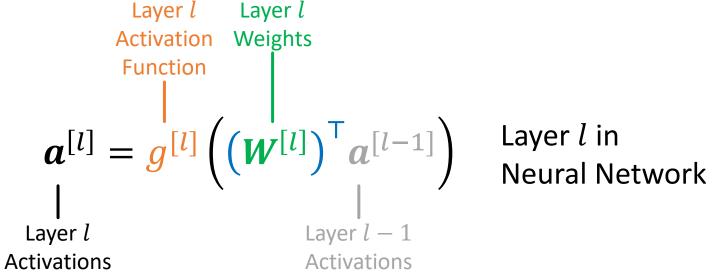
## Neural Network



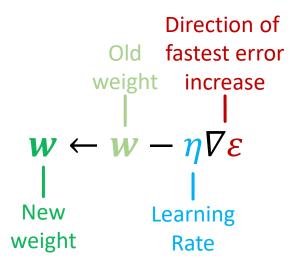
## Layer Activation

$$a = g(f(x)), f(x) = \mathbf{w}^{\mathsf{T}} x$$

Single-Layer Perceptron



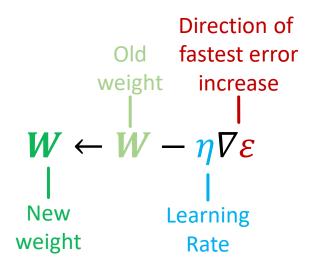
### Gradient Descent Weight Update (Single Neuron)



### Gradient of error

$$abla_{\varepsilon} = \frac{d\varepsilon}{dw} = \begin{pmatrix} \partial \varepsilon / \partial w_1 \\ \vdots \\ \partial \varepsilon / \partial w_r \\ \vdots \\ \partial \varepsilon / \partial w_n \end{pmatrix}$$

## Gradient Descent Weight Update (Neural Network)



$$\frac{d\varepsilon}{d\mathbf{W}^{[l]}} = \frac{d\varepsilon}{d\hat{y}} \left( \frac{\bar{d}\hat{y}}{d\mathbf{W}^{[l]}} \right)$$

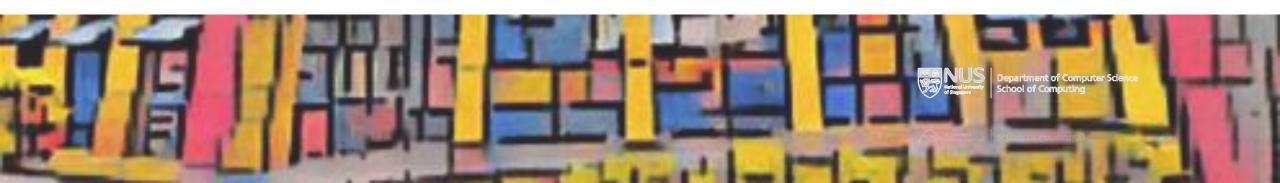
### Gradient of error

$$\nabla \varepsilon = \frac{d\varepsilon}{dW} = \begin{pmatrix} \partial \varepsilon / \partial W^{[1]} \\ \vdots \\ \partial \varepsilon / \partial W^{[l]} \\ \vdots \\ \partial \varepsilon / \partial W^{[L]} \end{pmatrix}$$

$$\frac{d\boldsymbol{\varepsilon}}{d\boldsymbol{W}^{[l]}} = \begin{pmatrix} \frac{\partial \boldsymbol{\varepsilon}}{\partial w_{11}^{[l]}} & \cdots & \frac{\partial \boldsymbol{\varepsilon}}{\partial w_{1m}^{[l]}} \\ \vdots & \ddots & \vdots \\ \frac{\partial \boldsymbol{\varepsilon}}{\partial w_{n1}^{[l]}} & \cdots & \frac{\partial \boldsymbol{\varepsilon}}{\partial w_{nm}^{[l]}} \end{pmatrix}$$



# Gradient Descent for Neural Networks Backpropagation



## Backpropagation

Backpropagation efficiently computes the gradient by

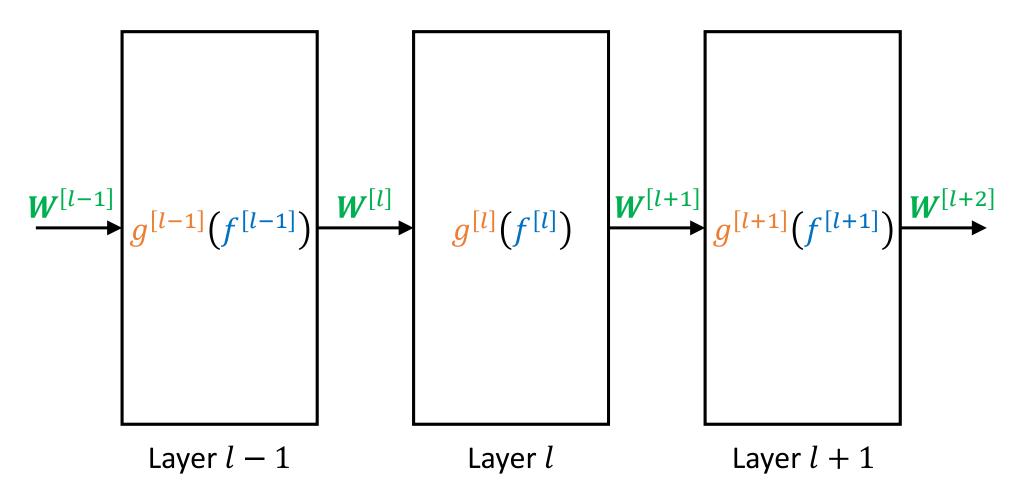
- Avoiding duplicate calculations
- Not computing unnecessary intermediate values,
- Computing the gradient of each layer

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

$$\frac{d\hat{y}}{d\boldsymbol{W}^{[l]}} = \boldsymbol{a}^{[l-1]} (\boldsymbol{\delta}^{[l]})^{\mathsf{T}} \qquad \boldsymbol{\delta}^{[l]} = \left(\frac{d\boldsymbol{g}^{[l]}}{d\boldsymbol{f}^{[l]}}\right) (\boldsymbol{W}^{[l+1]} \boldsymbol{\delta}^{[l+1]})$$

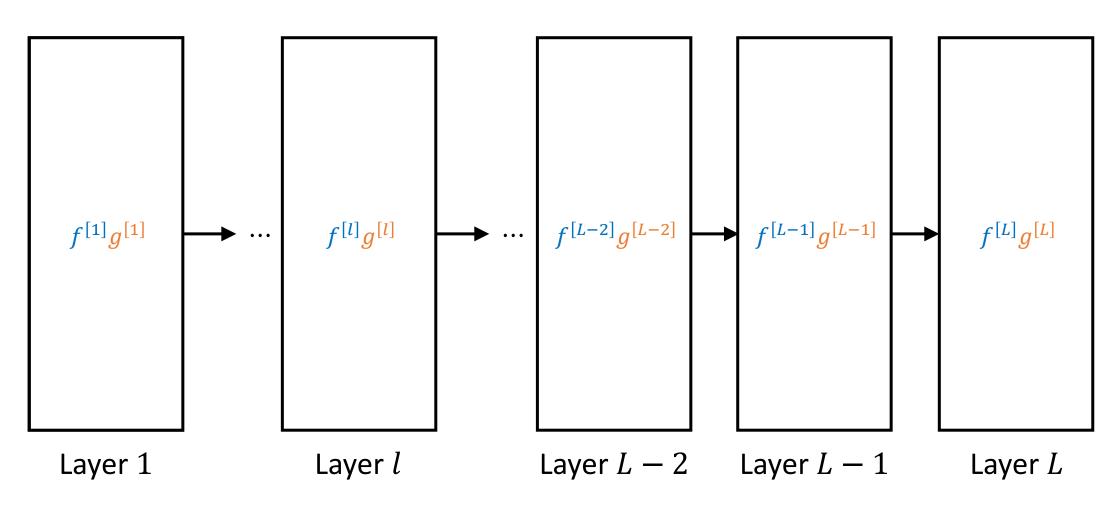
Adapted from: <a href="https://en.wikipedia.org/wiki/Backpropagation">https://en.wikipedia.org/wiki/Backpropagation</a>

## Forward Propagation



## Forward Propagation (Reverse Polish Notation)

$$(x^{[0]}, \mathbf{W}^{[1]}) f^{[1]} g^{[1]} \cdots f^{[l]} g^{[l]} \cdots f^{[L-2]} g^{[L-2]} f^{[L-1]} g^{[L-1]} f^{[L]} g^{[L]} = \hat{y}$$



## Forward Propagation (Reverse Polish Notation)

$$(x^{[0]}, \mathbf{W}^{[1]}) f^{[1]} g^{[1]} \cdots f^{[l]} g^{[l]} \cdots f^{[L-2]} g^{[L-2]} f^{[L-1]} g^{[L-1]} f^{[L]} g^{[L]} = \hat{y}$$

$$(a^{[L-1]}, W^{[L]})f^{[L]}g^{[L]} = \hat{y}$$

$$(a^{[L-2]}, \mathbf{W}^{[L-1]})f^{[L-1]}g^{[L-1]}f^{[L]}g^{[L]} = \hat{y}$$

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

## Gradients of Layer Weights (Backwards)

$$(x^{[0]}, \boldsymbol{W^{[1]}}) f^{[1]} g^{[1]} \cdots f^{[l]} g^{[l]} \cdots f^{[L-2]} g^{[L-2]} f^{[L-1]} g^{[L-1]} f^{[L]} g^{[L]} = \hat{y}$$

$$(a^{[L-1]}, \mathbf{W}^{[L]}) f^{[L]} g^{[L]} = \hat{y}$$

$$\frac{df^{[L]}}{d\mathbf{W}^{[L]}} \frac{dg^{[L]}}{df^{[L]}} = \frac{\partial \hat{y}}{\partial \mathbf{W}^{[L]}}$$

$$(a^{[L-2]}, \mathbf{W}^{[L-1]}) f^{[L-1]} g^{[L-1]} f^{[L]} g^{[L]} = \hat{y}$$

$$\frac{df^{[L-1]}}{d\mathbf{W}^{[L-1]}} \frac{dg^{[L-1]}}{df^{[L-1]}} \frac{df^{[L]}}{df^{[L]}} = \frac{\partial \hat{y}}{\partial \mathbf{W}^{[L-1]}}$$

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

$$\frac{df^{[L-2]}}{dW^{[L-2]}} \frac{dg^{[L-2]}}{df^{[L-2]}} \frac{df^{[L-1]}}{df^{[L-1]}} \frac{df^{[L]}}{df^{[L-1]}} \frac{dg^{[L]}}{df^{[L]}} = \frac{\partial \hat{y}}{\partial W^{[L-2]}}$$

## Gradients of Layer Weights (Backwards)

$$(x^{[0]}, \boldsymbol{W^{[1]}}) f^{[1]} g^{[1]} \cdots f^{[l]} g^{[l]} \cdots f^{[L-2]} g^{[L-2]} f^{[L-1]} g^{[L-1]} f^{[L]} g^{[L]} = \hat{y}$$

$$(a^{[L-1]}, W^{[L]})f^{[L]}g^{[L]} = \hat{y}$$

$$\frac{df^{[L]}}{dW^{[L]}}\delta^{[L]} = \frac{\partial \hat{y}}{\partial W^{[L]}}$$

$$(a^{[L-2]}, W^{[L-1]}) f^{[L-1]} g^{[L-1]} f^{[L]} g^{[L]} = \hat{y}$$

$$\frac{df^{[L-1]}}{dW^{[L-1]}} \delta^{[L-1]} = \frac{\partial \hat{y}}{\partial W^{[L-1]}}$$

## Recursive Gradients of Layer Weights

$$\frac{\partial \hat{y}}{\partial W^{[l]}} = \frac{df^{[l]}}{dW^{[l]}} \frac{dg^{[l]}}{df^{[l]}} \frac{dg^{[l+1]}}{dg^{[l]}} \cdots \frac{df^{[l]}}{dg^{[l-1]}} \frac{dg^{[l]}}{df^{[l]}}$$

$$\frac{\partial \hat{y}}{\partial W^{[l]}} = \frac{df^{[l]}}{dW^{[l]}} \frac{dg^{[l]}}{df^{[l]}} \frac{df^{[l+1]}}{dg^{[l]}} \delta^{[l+1]}$$

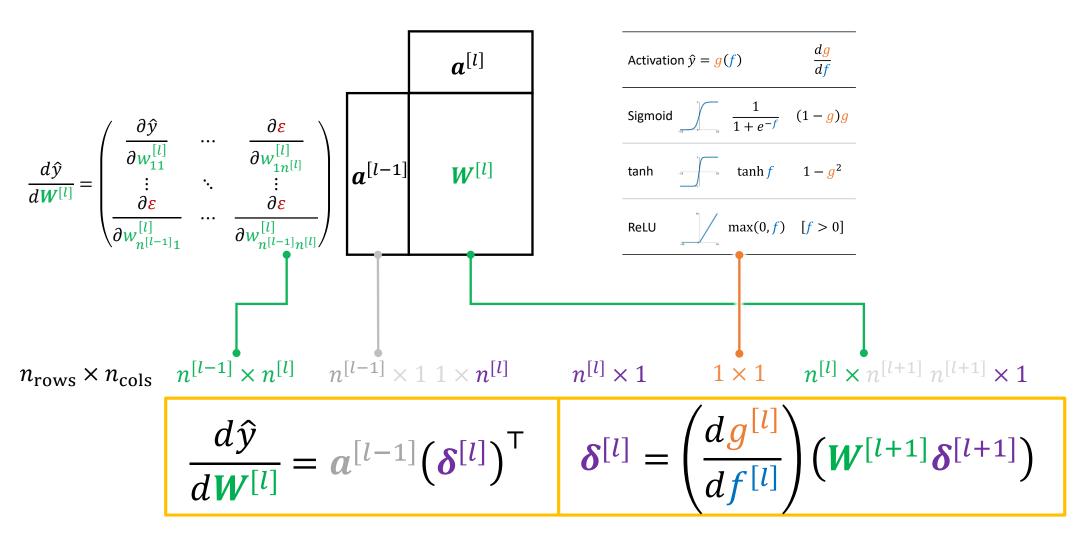
$$\frac{\partial \hat{y}}{\partial W^{[l]}} = \frac{df^{[l]}}{dW^{[l]}} \delta^{[l]}$$

$$\frac{df^{[l]}}{dW^{[l]}} = \frac{d\left(\left(W^{[l]}\right)^{\mathsf{T}} a^{[l-1]}\right)}{dW^{[l]}} = a^{[l-1]} \delta^{[l]} \frac{df^{[l+1]}}{dg^{[l]}} \delta^{[l+1]}$$

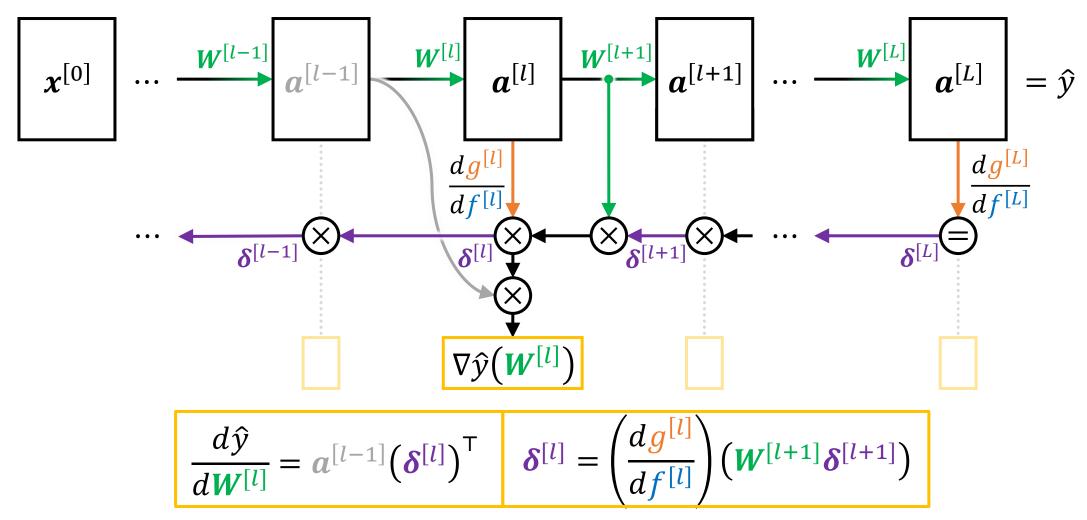
$$\frac{df^{[l+1]}}{dg^{[l]}} = \frac{df^{[l+1]}}{da^{[l]}} = W^{[l+1]}$$

$$\frac{\partial \hat{y}}{\partial W^{[l]}} = a^{[l-1]} \delta^{[l]} \delta^{[l]} = \frac{dg^{[l]}}{df^{[l]}} W^{[l+1]} \delta^{[l+1]}$$
Recursive

### Matrix multiplication to match shape (not in exam)



## **Backward Propagation**





## Backpropagation

Backpropagation efficiently computes the gradient by

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

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

$$\frac{d\hat{y}}{d\boldsymbol{W}^{[l]}} = \boldsymbol{a}^{[l-1]} (\boldsymbol{\delta}^{[l]})^{\mathsf{T}} \qquad \boldsymbol{\delta}^{[l]} = \left(\frac{d\boldsymbol{g}^{[l]}}{d\boldsymbol{f}^{[l]}}\right) (\boldsymbol{W}^{[l+1]} \boldsymbol{\delta}^{[l+1]})$$

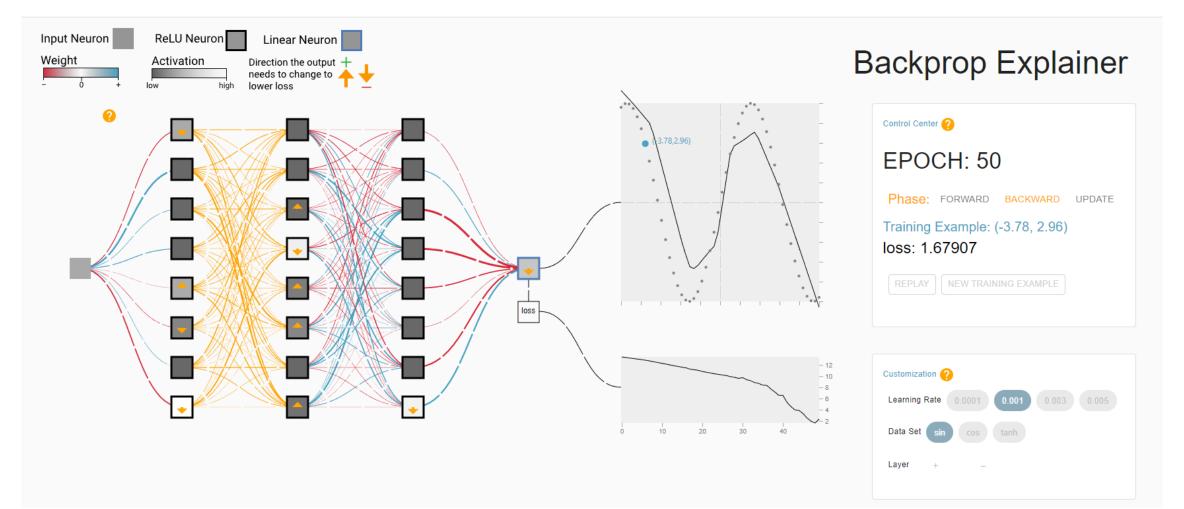
Adapted from: <a href="https://en.wikipedia.org/wiki/Backpropagation">https://en.wikipedia.org/wiki/Backpropagation</a>

### Backprop Explainer Quick Start

### https://xnought.github.io/backprop-explainer/

- 1. Press to start training
- 2. Then press CLICK TO ANIMATE EPOCH # to see forward propagation, backward propagation, and update animation at the epoch #
- 3. To go back to fitting mode click operations of the state of the sta

Click on 60 to reveal extra descriptions



### Insert Web Page

This app allows you to insert secure web pages starting with https:// into the slide deck. Non-secure web pages are not supported for security reasons.

Please enter the URL below.

https://

xnought.github.io/backprop-explainer/

Note: Many popular websites allow secure access. Please click on the preview button to ensure the web page is accessible.

## Practice Backprop during tutorial

CS3244, Solution to Tutorial 07—Perceptrons and Neural Networks

1

National University of Singapore School of Computing CS3244: Machine Learning Solution to Tutorial 07

### Perceptrons and Neural Networks

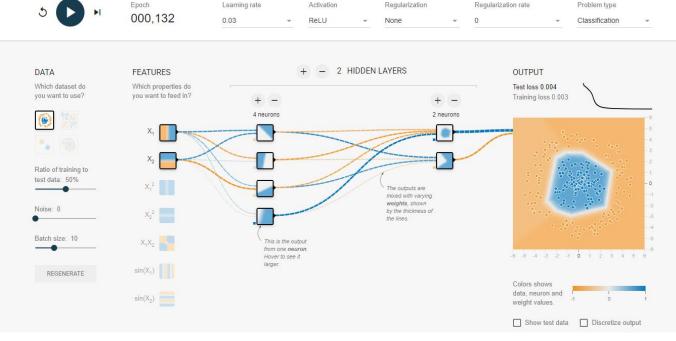
Colab Notebook: Perceptrons and Neural Networks

1. Backpropagation algorithm. In this question, we're going to use a neural network with a

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### Resources for self-study

- What is backpropagation really doing?, Backpropagation calculus 3Blue1Brown
- A worked example of backpropagation Alexander Schiendorfer
- TensorFlow Playground



## Auto Differentiation for Backprop

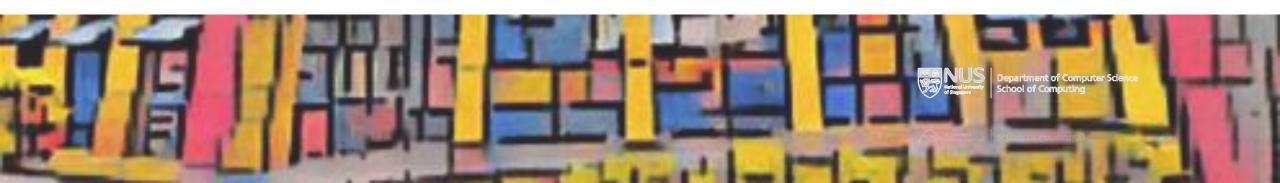
- Even with backprop, implementing the gradients is tedious
- Deep learning APIs have automated differentiation.
  - Tensor Flow <u>autodiff</u>
  - PyTorch <u>autograd</u>
  - Implement derivatives of many common functions
  - You just need to implement your layers and neurons; API will handle gradients

### 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

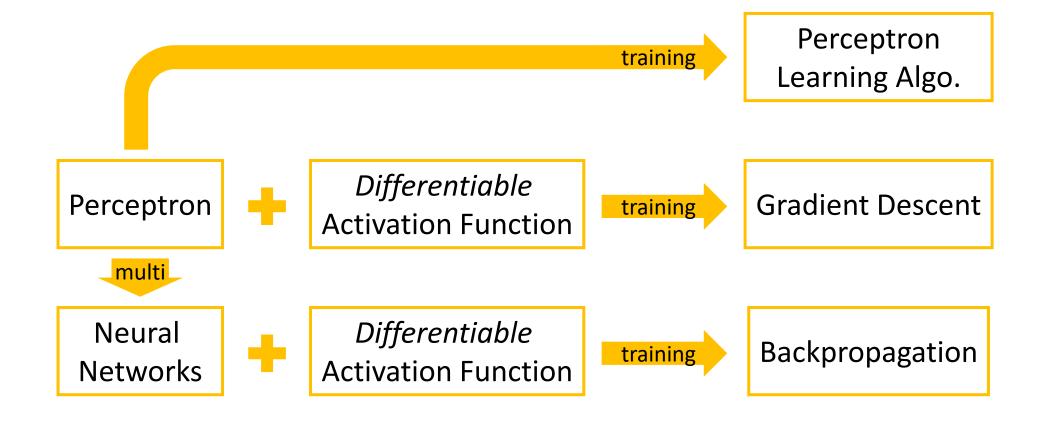


## Wrapping Up

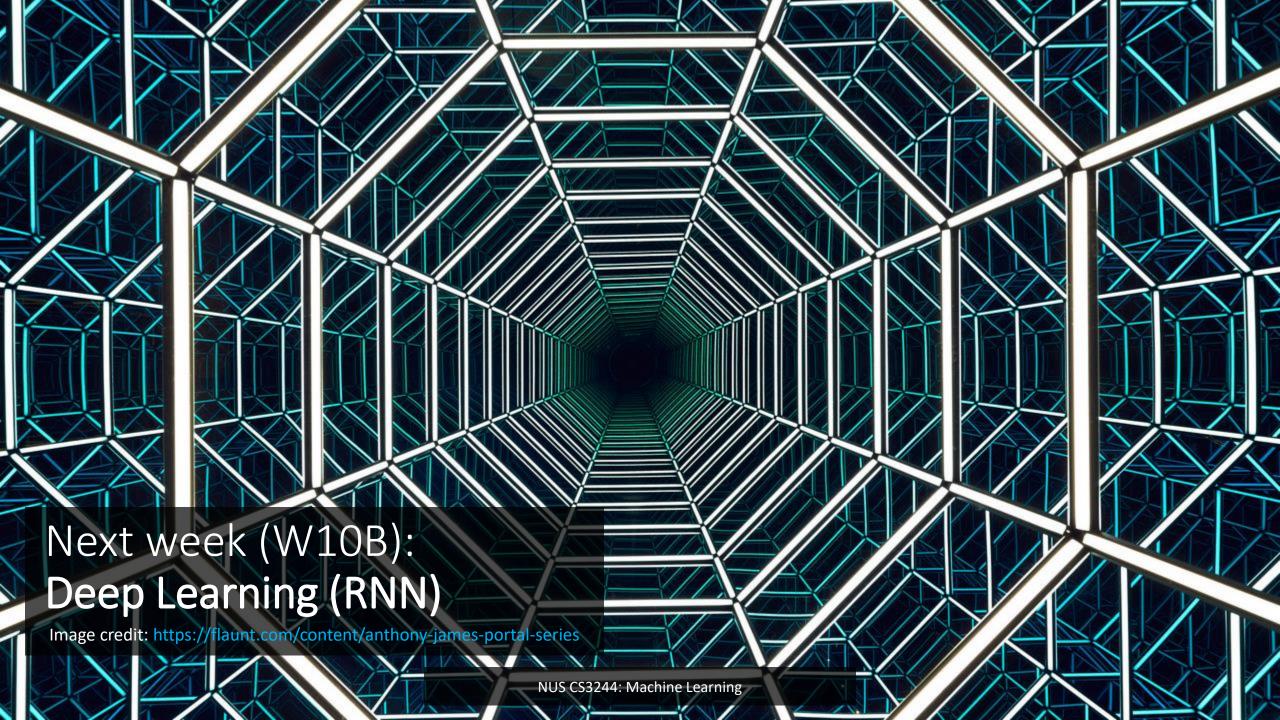




### What did we learn?







## W10 Pre-Lecture Task (due before next Mon)

### Watch

Who Invented A.I.? - The Pioneers of Our Future by ColdFusion

### Play

- https://distill.pub/2018/building-blocks/
  - Don't worry about reading the whole article

### **Discuss**

- 1. <u>Identify</u> what is strange, funny, or erroneous in the deep learning model in Building-Blocks
- 2. <u>Take a screenshot</u> of the issue and share with your tutorial mates
- 3. Try to explain why the model was behaving as identified
- 3. Post a 2-3 sentence description to the topic in your tutorial group: #tg-xx