# Machine Learning (CE 40717)

## Fall 2024

Ali Sharifi-Zarchi

CE Department
Sharif University of Technology

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1 Gradient Descent

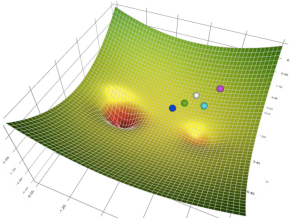
2 Backpropagation

3 Foundations in Detail: Initialization, Loss, and Activation

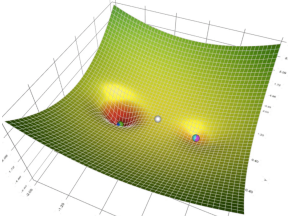
4 References

# How to Update Weights?

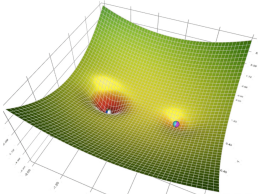
- Imagine training a large model like ChatGPT. It has billions of parameters that need to be adjusted.
- If we used **random search** to update these weights, it would take an astronomical number of trials to find good parameters.
- How to make training feasible at this massive scale?
- Image adapted from Medium: AdaGrad Optimization Algorithm



Visualizing parameter space with random initial points.



Random search approach in high-dimensional space.



Challenges in finding optimal weights using random search.

# How to Update Weights?

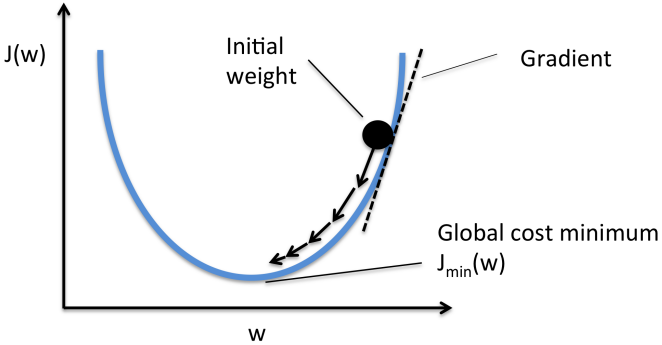
**Options for Updating Weights:**

- **Random Search:** Tries values randomly—inefficient and impractical.
- **Gradient Descent:** Follows the slope of the loss function—efficient and guided.

**Why Gradient Descent?**

- It updates weights by following the slope, reducing error with each step.
- Controlled, stepwise updates ensure we move closer to minimizing the loss effectively.

# How to Update Weights?




Gradient descent: adjusting weights to minimize cost by following the gradient.
Gradient optimization image

# Gradient Descent: Concept and Weight Updates

**Gradient Descent**: Minimizes the loss function by updating weights based on the gradient.

**Weight Update Rule**:

$$w_{\text{new}} = w_{\text{old}} - \eta \cdot \frac{\partial L}{\partial w}$$

Where:

- $\eta$ is the learning rate (step size).
- $\frac{\partial L}{\partial w}$ is the gradient of the loss function with respect to $w$.

# Example: Gradient Descent and Updating Weights

**Example Problem**:

- Initial weight: $w_0 = 2$
- Learning rate: $\eta = 0.1$
- Loss function: $L(w) = (y - wx)^2$
  **Example**: For $x = 3$, $y = 10$, and $w_0 = 2$,

**Gradient Calculation**:

$$\frac{\partial L}{\partial w} = -2x(y - wx)$$

$$\frac{\partial L}{\partial w} = -24, \quad w_{\text{new}} = 4.4$$

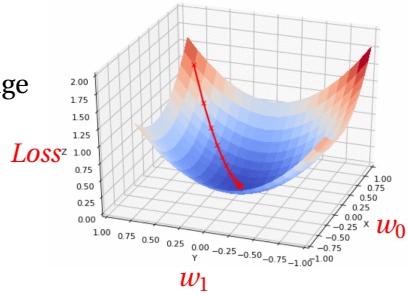
# Gradient Descent: Formula and Process

**Weight Update Formula**:

$$w_{\text{new}} = w_{\text{old}} - \eta \cdot \frac{\partial L}{\partial w}$$

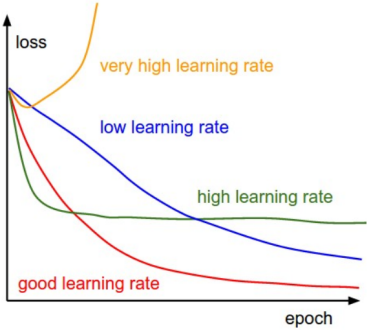
**Steps in Gradient Descent**:

- Compute the gradient of the loss function.
- Update the weights using the update rule.
- Repeat until convergence.
- Image adapted from Data Science Stack Exchange



# Identifying an Optimal Learning Rate

- Look for a **smooth, gradual** decrease in loss over time.
- Very low learning rate -> slow convergence
- Very high learning rate -> erratic fluctuations
- Image adapted from Towards Data Science: Understanding Learning Rates and How It Improves Performance in Deep Learning



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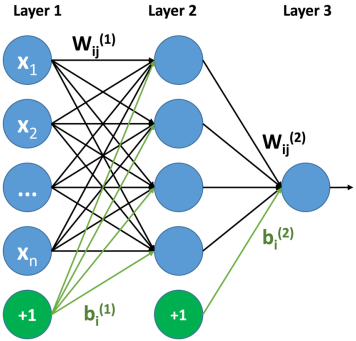
# Multi-Layer Neural Network

The diagram below illustrates a three-layer neural network



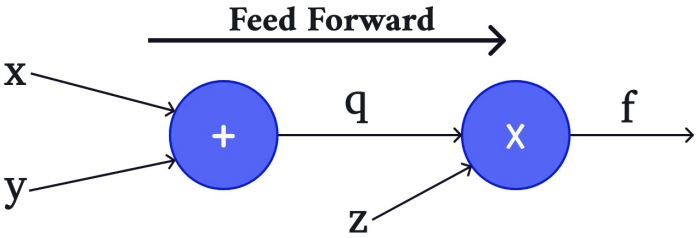

Neural Network

How should $\frac{\partial L}{\partial w}$ be calculated for each weight $w$ in this neural network?

# A Simple Example

**Function:**

$$f(x, y, z) = (x + y)z$$



# A Simple Example: Forward Pass

**Function:**

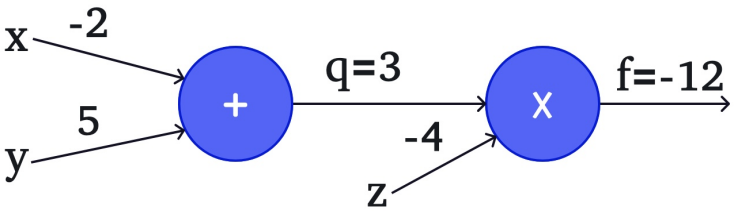
$$f(x, y, z) = (x + y)z$$

**Example:**

$$x = -2, \quad y = 5, \quad z = -4$$

**Steps:**

- $\mathbf{q} = \mathbf{x} + \mathbf{y} = \mathbf{3}$
- $\mathbf{f} = \mathbf{q} \times \mathbf{z} = \mathbf{-12}$



# Finite Difference Method

To approximate the gradient $\frac{\partial L}{\partial w_i}$:

- Change $w_i$ by a small value $\epsilon$.
- Approximate the gradient as:

$$\frac{\partial L}{\partial w_i} \approx \frac{L(w_i + \epsilon) - L(w_i)}{\epsilon}$$

- Simple but inefficient.

**Problem:**
Complexity is $\Theta(n^2)$ for $n$ weights, which is slow for large models.

# Backpropagation

**A more efficient method:**

- Use the chain rule to compute all gradients in one backward pass.
- This method avoids changing each weight separately.

**Advantages:**

- Complexity is reduced to $\Theta(n)$.
- Much faster, especially for large neural networks.

# Chain Rule for Gradients

The **chain rule** helps us find the gradient of a function that is composed of other functions.

**Example:**

$$z = f(g(x))$$

- $f$ is a function of $g(x)$
- $g(x)$ is a function of $x$

To find $\frac{\partial z}{\partial x}$, we use the chain rule:

$$\frac{\partial z}{\partial x} = \frac{\partial f}{\partial g} \times \frac{\partial g}{\partial x}$$

This means we multiply the gradient of the outer function by the gradient of the inner function.

# Backpropagation: A Simple Example

**Function:**

$$f(x, y, z) = (x + y)z$$

**Example:**

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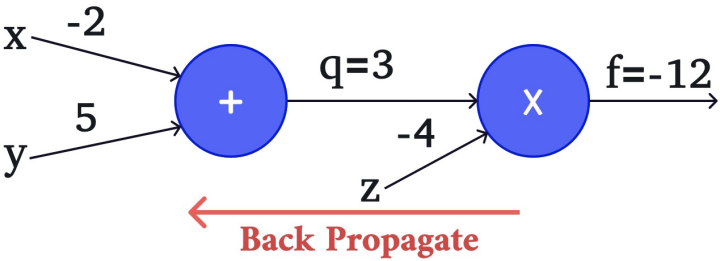

# A Simple Example: Backpropagation

**Function:**

$$f(x, y, z) = (x + y)z$$

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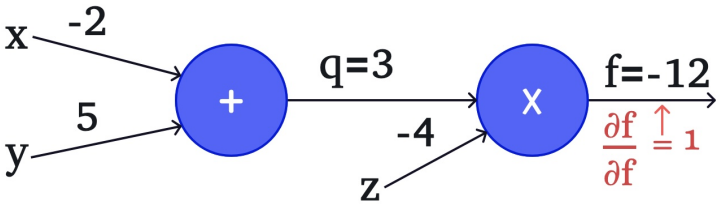
**Step 1:**

$$\frac{\partial f}{\partial f} = 1$$



# A Simple Example: Backpropagation

**Function:**

$$f(x, y, z) = (x + y)z$$

**Example:**

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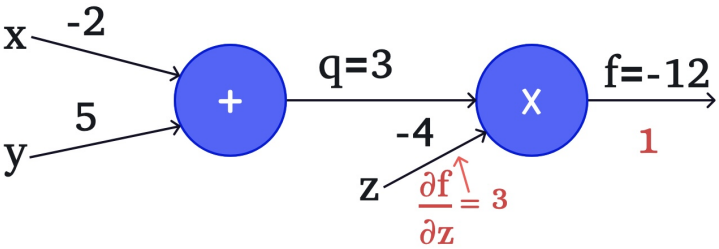
**Step 2:**

$$f = qz, \quad \frac{\partial f}{\partial z} = q = 3$$



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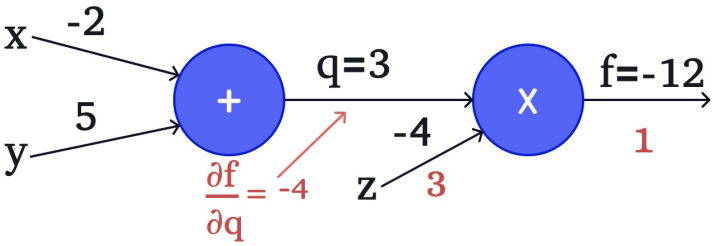

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$$f(x,y,z) = (x+y)z$$

**Example:**

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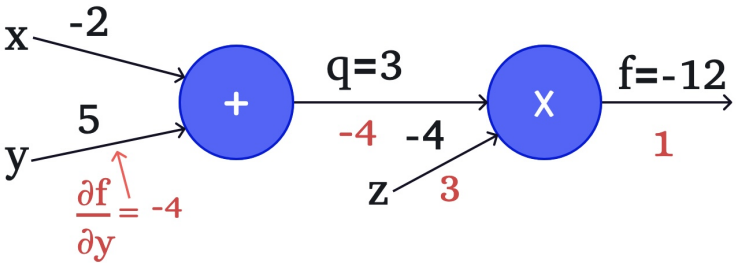
**Step 3:**

$$q = x+y, \quad \frac{\partial q}{\partial x} = 1, \quad \frac{\partial q}{\partial y} = 1$$

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial y} = -4 \cdot 1 = -4$$



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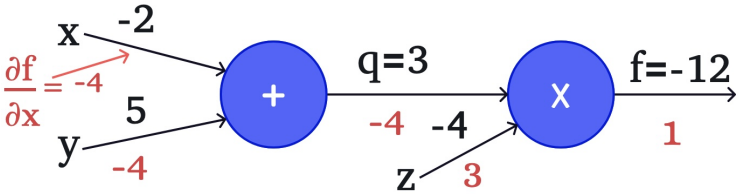

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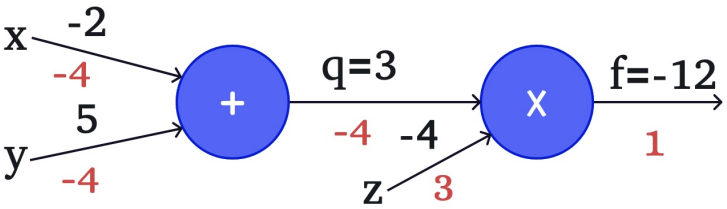


# Example: One Neuron

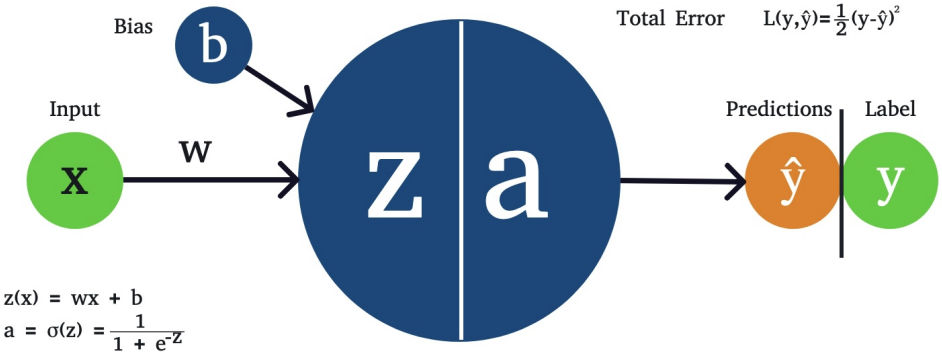
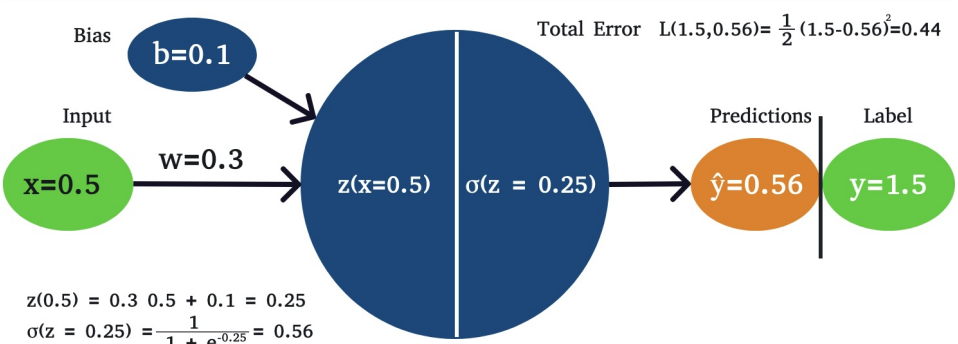
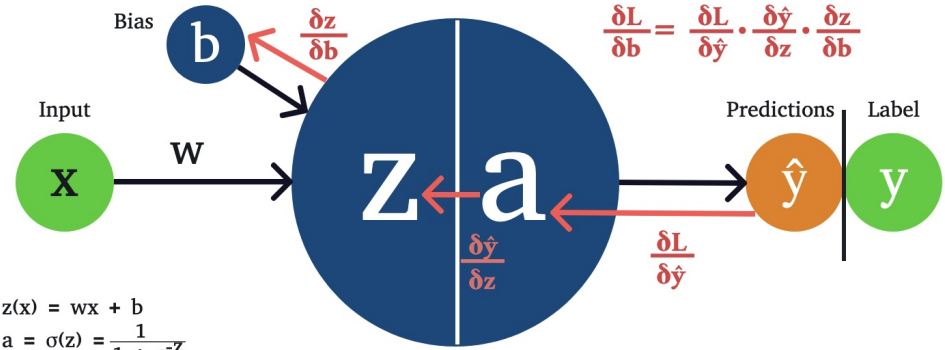



Image adapted from "Deep learning backpropagation" Web article

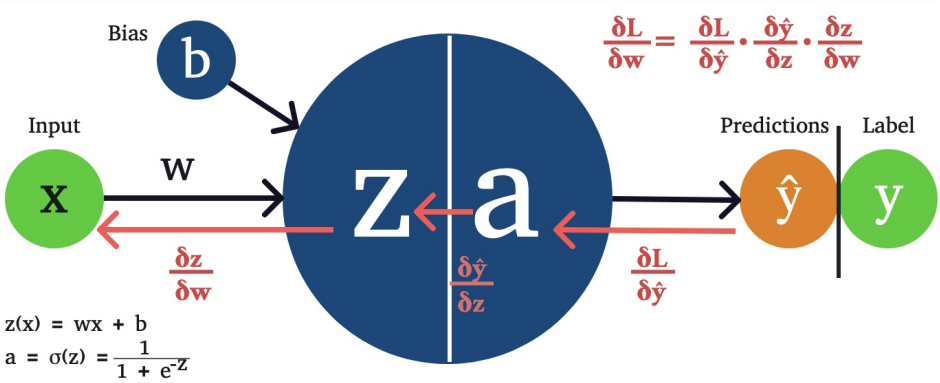
# Forward Pass



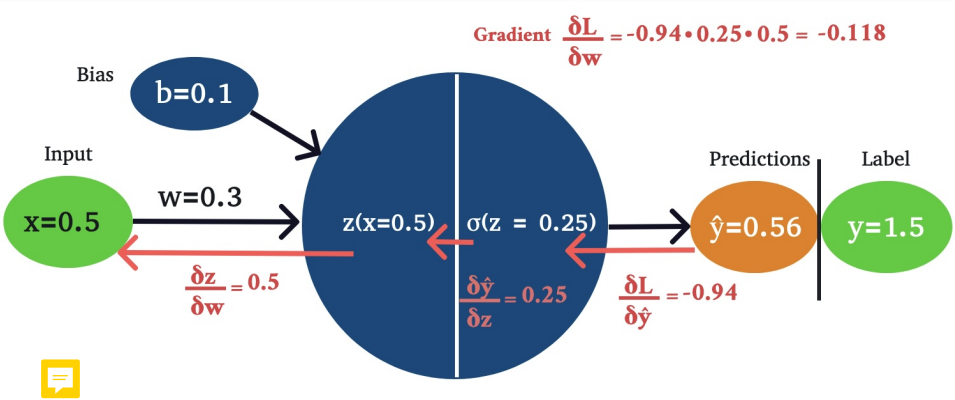
# Backward Pass



# Backward Pass



# Backward Pass



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# Vectorized Backpropagation

The faster you compute gradients, the quicker each parameter update in gradient descent.

**Derivative of a Vector by a Vector**: leveraging matrix operations for faster computation.

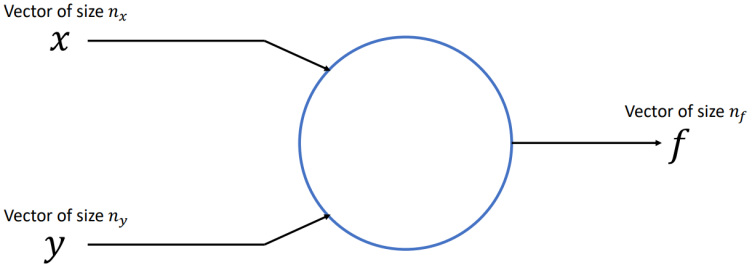
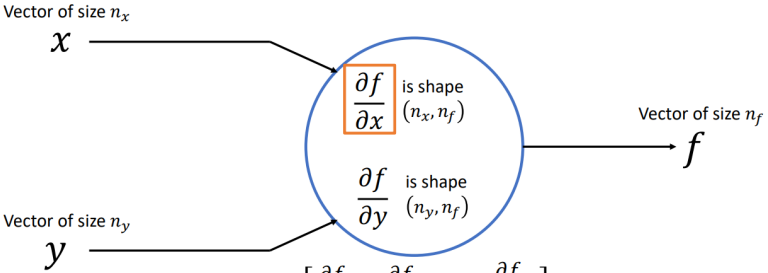



Image adapted from Elec502 vectorized backpropagation slides

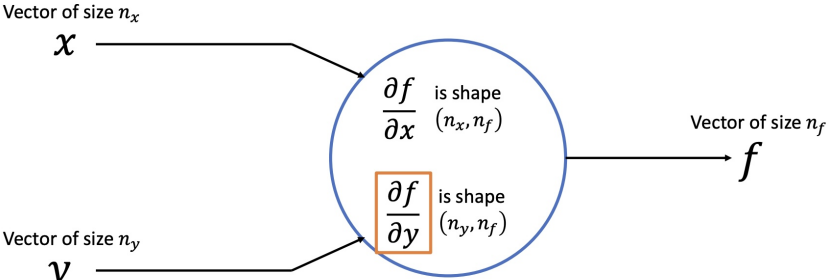
# Vectorized Backpropagation

## Local Derivatives are Jacobian Matrices



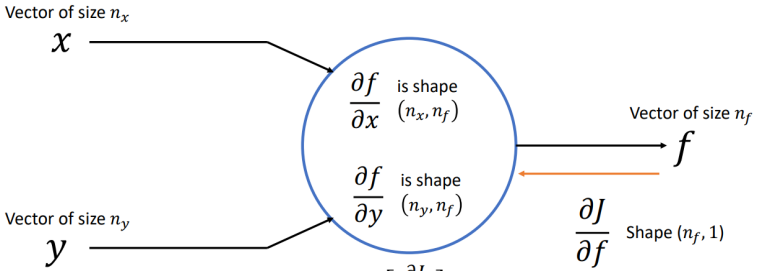

$$\frac{\partial f}{\partial x} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_2}{\partial x_1} & \cdots & \frac{\partial f_{n_f}}{\partial x_1} \\ \frac{\partial f_1}{\partial x_2} & \frac{\partial f_2}{\partial x_2} & & \frac{\partial f_{n_f}}{\partial x_2} \\ \vdots & & \ddots & \vdots \\ \frac{\partial f_1}{\partial x_{n_x}} & \frac{\partial f_2}{\partial x_{n_x}} & \cdots & \frac{\partial f_{n_f}}{\partial x_{n_x}} \end{bmatrix}$$

# Vectorized Backpropagation




$$\frac{\partial f}{\partial y} = \begin{bmatrix} \frac{\partial f_1}{\partial y_1} & \frac{\partial f_2}{\partial y_1} & \cdots & \frac{\partial f_{n_f}}{\partial y_1} \\ \frac{\partial f_1}{\partial y_2} & \frac{\partial f_2}{\partial y_2} & & \frac{\partial f_{n_f}}{\partial y_2} \\ \vdots & & \ddots & \vdots \\ \frac{\partial f_1}{\partial y_{n_y}} & \frac{\partial f_2}{\partial y_{n_y}} & \cdots & \frac{\partial f_{n_f}}{\partial y_{n_y}} \end{bmatrix}$$

# Vectorized Backpropagation

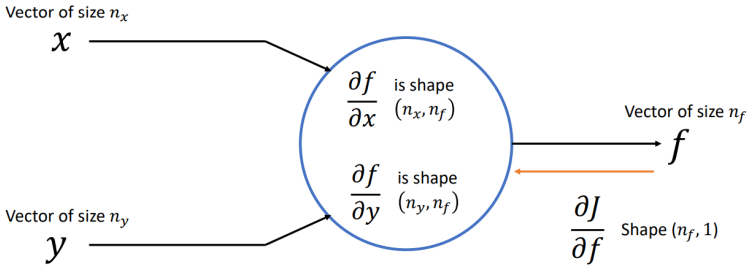



$$\frac{\partial J}{\partial f} = \begin{bmatrix} \frac{\partial J}{\partial f_1} \\ \frac{\partial J}{\partial f_2} \\ \vdots \\ \frac{\partial J}{\partial f_{n_f}} \end{bmatrix}$$

Upstream gradient is with respect to Cost $J$ (a **scalar**)

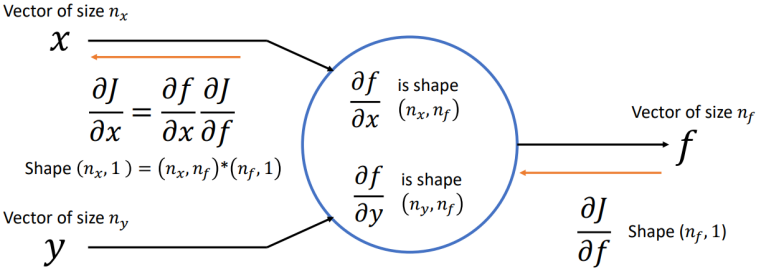
i.e. How does each output $f_i$ affect the Cost

# Vectorized Backpropagation



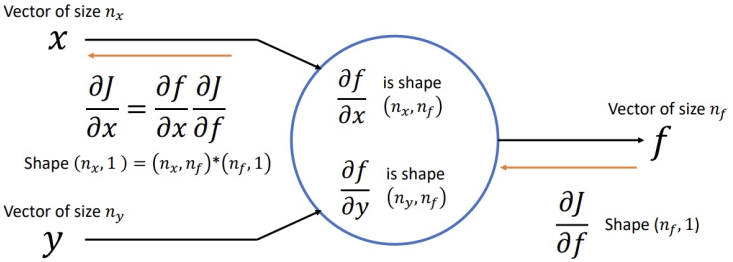

Apply chain rule like before!

# Vectorized Backpropagation




Applying the chain rule involves matrix-vector multiplication

# Vectorized Backpropagation




$$\frac{\partial J}{\partial x} = \frac{\partial f}{\partial x}\frac{\partial J}{\partial f} \rightarrow \begin{bmatrix} \frac{\partial J}{\partial x_1} \\ \frac{\partial J}{\partial x_2} \\ \vdots \\ \frac{\partial J}{\partial x_{n_x}} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1}, & \frac{\partial f_2}{\partial x_1}, & \cdots & \frac{\partial f_{n_f}}{\partial x_1} \\ \vdots & & \ddots & \vdots \\ \frac{\partial f_1}{\partial x_{n_x}}, & \frac{\partial f_2}{\partial x_{n_x}} & \cdots & \frac{\partial f_{n_f}}{\partial x_{n_x}} \end{bmatrix} \begin{bmatrix} \frac{\partial J}{\partial f_1} \\ \frac{\partial J}{\partial f_2} \\ \vdots \\ \frac{\partial J}{\partial f_{n_f}} \end{bmatrix}$$

# Chain Rule – Matrix-Vector Multiply

$$\frac{\partial J}{\partial x} = \frac{\partial f}{\partial x}\frac{\partial J}{\partial f} \rightarrow \begin{bmatrix} \frac{\partial J}{\partial x_1} \\ \frac{\partial J}{\partial x_2} \\ \vdots \\ \frac{\partial J}{\partial x_{n_x}} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1}, \frac{\partial f_2}{\partial x_1}, & \cdots & \frac{\partial f_{n_f}}{\partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_1}{\partial x_{n_x}}, \frac{\partial f_2}{\partial x_{n_x}} & \cdots & \frac{\partial f_{n_f}}{\partial x_{n_x}} \end{bmatrix} \begin{bmatrix} \frac{\partial J}{\partial f_1} \\ \frac{\partial J}{\partial f_2} \\ \vdots \\ \frac{\partial J}{\partial f_{n_f}} \end{bmatrix}$$

$$\text{Shape } (n_x, 1) = (n_x, n_f) * (n_f, 1)$$

# Chain Rule – Matrix-Vector Multiply

$$\frac{\partial J}{\partial x} = \frac{\partial f}{\partial x}\frac{\partial J}{\partial f} \rightarrow \begin{bmatrix} \frac{\partial J}{\partial x_1} \\ \frac{\partial J}{\partial x_2} \\ \vdots \\ \frac{\partial J}{\partial x_{n_x}} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1}, \frac{\partial f_2}{\partial x_1}, & \cdots & \frac{\partial f_{n_f}}{\partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_1}{\partial x_{n_x}}, \frac{\partial f_2}{\partial x_{n_x}} & \cdots & \frac{\partial f_{n_f}}{\partial x_{n_x}} \end{bmatrix} \begin{bmatrix} \frac{\partial J}{\partial f_1} \\ \frac{\partial J}{\partial f_2} \\ \vdots \\ \frac{\partial J}{\partial f_{n_f}} \end{bmatrix}$$

Jacobian

Shape $(n_x, 1) = (n_x, n_f)^*(n_f, 1)$

# Chain Rule – Matrix-Vector Multiply

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Jacobian

Shape $(n_x, 1) = (n_x, n_f) * (n_f, 1)$

Upstream Gradient

# Chain Rule – Matrix-Vector Multiply

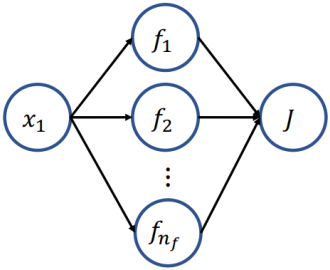
$$\frac{\partial J}{\partial x} = \frac{\partial f}{\partial x}\frac{\partial J}{\partial f} \rightarrow \begin{bmatrix} \frac{\partial J}{\partial x_1} \\ \frac{\partial J}{\partial x_2} \\ \vdots \\ \frac{\partial J}{\partial x_{n_x}} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1}, & \frac{\partial f_2}{\partial x_1}, & \cdots & \frac{\partial f_{n_f}}{\partial x_1} \\ \vdots & & \ddots & \vdots \\ \frac{\partial f_1}{\partial x_{n_x}}, & \frac{\partial f_2}{\partial x_{n_x}} & \cdots & \frac{\partial f_{n_f}}{\partial x_{n_x}} \end{bmatrix} \begin{bmatrix} \frac{\partial J}{\partial f_1} \\ \frac{\partial J}{\partial f_2} \\ \vdots \\ \frac{\partial J}{\partial f_{n_f}} \end{bmatrix}$$

Shape $(n_x, 1) = (n_x, n_f)^*(n_f, 1)$

$$\frac{\partial J}{\partial x_1} = \frac{\partial f_1}{\partial x_1}\frac{\partial J}{\partial f_1} + \frac{\partial f_2}{\partial x_1}\frac{\partial J}{\partial f_2} + \cdots + \frac{\partial f_{n_f}}{\partial x_1}\frac{\partial J}{\partial f_{n_f}}$$

# Chain Rule – Matrix-Vector Multiply

$$\frac{\partial J}{\partial x} = \frac{\partial f}{\partial x}\frac{\partial J}{\partial f} \rightarrow \begin{bmatrix} \frac{\partial J}{\partial x_1} \\ \frac{\partial J}{\partial x_2} \\ \vdots \\ \frac{\partial J}{\partial x_{n_x}} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1}, & \frac{\partial f_2}{\partial x_1}, & \cdots & \frac{\partial f_{n_f}}{\partial x_1} \\ \vdots & & \ddots & \vdots \\ \frac{\partial f_1}{\partial x_{n_x}}, & \frac{\partial f_2}{\partial x_{n_x}} & \cdots & \frac{\partial f_{n_f}}{\partial x_{n_x}} \end{bmatrix} \begin{bmatrix} \frac{\partial J}{\partial f_1} \\ \frac{\partial J}{\partial f_2} \\ \vdots \\ \frac{\partial J}{\partial f_{n_f}} \end{bmatrix}$$




Shape $(n_x, 1) = (n_x, n_f)^*(n_f, 1)$

$$\frac{\partial J}{\partial x_1} = \frac{\partial f_1}{\partial x_1}\frac{\partial J}{\partial f_1} + \frac{\partial f_2}{\partial x_1}\frac{\partial J}{\partial f_2} + \cdots + \frac{\partial f_{n_f}}{\partial x_1}\frac{\partial J}{\partial f_{n_f}}$$

# Chain Rule – Matrix-Vector Multiply

Vector of size $n_x$

$x$

$$\frac{\partial J}{\partial x} = \frac{\partial f}{\partial x}\frac{\partial J}{\partial f}$$

Shape $(n_x, 1) = (n_x, n_f)*(n_f, 1)$

Vector of size $n_y$

$y$

$$\frac{\partial J}{\partial y} = \frac{\partial f}{\partial y}\frac{\partial J}{\partial f}$$

Shape $(n_y, 1) = (n_y, n_f)*(n_f, 1)$

$\frac{\partial f}{\partial x}$ is shape $(n_x, n_f)$

$\frac{\partial f}{\partial y}$ is shape $(n_y, n_f)$

Vector of size $n_f$

$f$

$\frac{\partial J}{\partial f}$ Shape $(n_f, 1)$

Upstream gradient is with respect to Cost $J$ (a **scalar**)

i.e. How does each output $f_i$ affect the Cost

Chain Rule application is Matrix-Vector Multiply

1 Gradient Descent

2 Backpropagation

3 Foundations in Detail: Initialization, Loss, and Activation
- Weight Initialization
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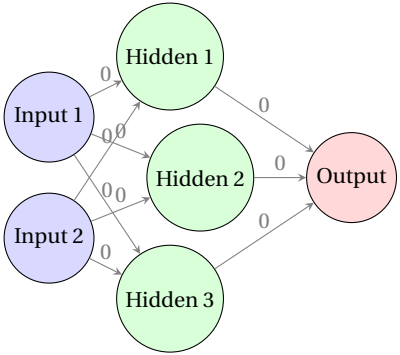
# Weight Initialization

**Example:** Imagine a network where all weights are initialized to zero.
**Issue:** If all weights are zero, each neuron in a layer will produce **identical** outputs. This symmetry prevents the network from learning **distinct features**, as every neuron updates identically.
**Solution:** To break this symmetry, weights need to be initialized with small random values, allowing neurons to learn unique features and avoid identical updates.




All weights initialized to zero

# Why Weight Initialization Matters

**Importance:**

- Proper **initialization** ensures **faster convergence** and improves **training stability**.
- Prevents issues like **vanishing** or **exploding gradients**, which can make training slow or unstable.

**Question:** How can we initialize weights to maximize **learning efficiency** and prevent gradient problems?

# Zero Initialization and Random Initialization

**Zero Initialization**

- **Description:** Set all weights to zero.
- **Key Point:** Rarely used, as it leads to identical updates for all neurons, preventing the network from learning distinct features.

**Random Initialization**

- **Description:** Assign small random values to weights.
- **Distribution:** Typically, weights are initialized using a uniform or normal distribution.

$$w \sim \mathcal{U}(-\epsilon, \epsilon) \quad \text{or} \quad w \sim \mathcal{N}(0, \sigma^2)$$

- **Key Point:** Helps break symmetry but can still cause issues with gradient magnitudes.

# Xavier Initialization

**Description:** Xavier Initialization is designed to keep the variance of activations consistent across layers, ideal for **sigmoid** and **tanh** activations.
**Objective:** Prevents the shrinking or exploding of signal magnitudes during forward and backward propagation.
**Condition:**

$$\frac{1}{n_l}\mathrm{Var}[w] = 1$$

where $n_l$ is the number of neurons in layer $l$.
**Initialization Scheme:**

$$w \sim \mathcal{U}\left(-\sqrt{\frac{1}{n_l}}, \sqrt{\frac{1}{n_l}}\right)$$

This results in a uniform distribution within the range $-\sqrt{\frac{1}{n_l}}$ to $\sqrt{\frac{1}{n_l}}$, ensuring stable signal variance across layers.

# He Initialization

**Description:** He Initialization (or Kaiming Initialization) is designed for neural networks with **ReLU** activations, considering the non-linearity of these functions.
**Objective:** Aims to prevent the exponential growth or reduction of input signal magnitudes through layers.
**Condition:**

$$\frac{1}{2} n_l \mathrm{Var}[w] = 1$$

**Initialization Scheme:**

$$w_l \sim \mathcal{N}\left(0, \frac{2}{n_l}\right)$$

This implies a zero-centered Gaussian distribution with a standard deviation of $\sqrt{\frac{2}{n_l}}$, where biases are initialized to 0.

# Xavier vs. He

- Evolution of loss term for Xavier and He weight initialization.

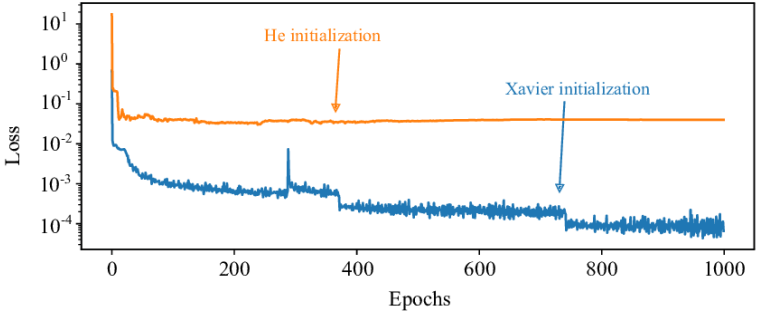



Image adapted from A Knowledge-driven Physics-Informed Neural Network model; Pyrolysis and Ablation of Polymers

# Choosing the Right Initialization – Examples

- **Scenario 1:** Using ReLU activation functions in a deep network.
  - **Best Choice:** He Initialization.
  - **Reason:** Helps maintain gradient flow through the layers.
- **Scenario 2:** Using Sigmoid activation functions in a shallow network.
  - **Best Choice:** Xavier Initialization.
  - **Reason:** Keeps variance balanced, which is crucial for non-ReLU activations.

# Transition to Loss and Activation Functions

**Recap:** Proper weight initialization:

- Ensures stability during training by maintaining gradient magnitudes.
- Helps the network converge faster and learn more effectively.

**Next Steps:**

- Once weights are initialized, the network needs a measure of error — this is where **loss functions** come in.
- After initializing weights, **activation functions** determine the output of each neuron, enabling the network to learn complex patterns.

**Question:** How do we measure the error in predictions and adjust our weights to minimize it?

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# Types of Loss Functions

- **Mean Squared Error (MSE):** Used in regression to minimize squared differences between predicted and true values.
- **Mean Absolute Error (MAE):** Minimizes absolute differences, also for regression tasks.
- **Binary Cross-Entropy:** Used for binary classification to compare predicted probabilities with binary labels.
- **Categorical Cross-Entropy:** For multi-class classification, comparing predicted probabilities across multiple classes.

# Mean Squared Error (MSE)

**Definition:**

$$\text{MSE} = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - \hat{y}^{(i)}\right)^2$$

**Characteristics:**

- Amplifies larger errors due to squaring, making it sensitive to outliers.

# Example of MSE Calculation

**Example:**

- Predicted values: $\hat{y} = [4.2, 3.8, 5.1]$
- True values: $y = [5.0, 4.0, 4.9]$
- Calculation:

$$\begin{aligned} \text{MSE} &= \frac{1}{3}\left[(5.0-4.2)^2 + (4.0-3.8)^2 + (4.9-5.1)^2\right] \\ &= \frac{1}{3}[0.64 + 0.04 + 0.04] = \frac{0.72}{3} = 0.24 \end{aligned}$$

# Mean Absolute Error (MAE)

**Definition:**

$$\text{MAE} = \frac{1}{N}\sum_{i=1}^{N}\left|y^{(i)} - \hat{y}^{(i)}\right|$$

**Characteristics:**

- Provides a linear measure of error, treating all deviations equally.

# Example of MAE Calculation

**Example:**

- Predicted values: $\hat{y} = [4.2, 3.8, 5.1]$
- True values: $y = [5.0, 4.0, 4.9]$
- Calculation:

$$\begin{aligned} \text{MAE} &= \frac{1}{3}\left(|5.0 - 4.2| + |4.0 - 3.8| + |4.9 - 5.1|\right) \\ &= \frac{1}{3}(0.8 + 0.2 + 0.2) = \frac{1.2}{3} \approx 0.4 \end{aligned}$$

# Impact on Model Outputs and Optimization

**MSE (Mean Squared Error):**

- Heavily penalizes large errors, promoting smoother outputs.
- Its quadratic gradient leads to faster convergence for large errors, but it can be sensitive to outliers.

**MAE (Mean Absolute Error):**

- Treats all errors uniformly, resulting in sharper outputs and better handling of outliers.
- Its constant gradient ensures stable optimization but can slow convergence with large errors.

# Binary Classification Loss – Binary Cross-Entropy

**Binary Cross-Entropy:**

$$\mathscr{L}_{\text{BCE}} = -\frac{1}{n}\sum_{i=1}^{n}\left[y^{(i)}\log(\hat{y}^{(i)}) + (1-y^{(i)})\log(1-\hat{y}^{(i)})\right]$$

**Example:**

- Predicted probabilities: $\hat{y} = [0.7, 0.3, 0.9]$
- True labels: $y = [1, 0, 1]$

$$\mathscr{L}_{\text{BCE}} = -\frac{1}{3}\left[1\cdot\log(0.7) + (1-1)\cdot\log(1-0.7)\right.$$

$$\left.+0\cdot\log(0.3) + (1-0)\cdot\log(1-0.3) + 1\cdot\log(0.9) + (1-1)\cdot\log(1-0.9)\right]$$

$$= -\frac{1}{3}\left(\log(0.7) + \log(0.7) + \log(0.9)\right) \approx -\frac{1}{3}\left(-0.357 + -0.357 + -0.105\right) \approx 0.273$$

Used to minimize the error between predicted probabilities and binary labels.

# Categorical Cross-Entropy

**Categorical Cross-Entropy Formula:**

$$\mathscr{L}_{CCE} = -\frac{1}{n}\sum_{i=1}^{n}\sum_{c=1}^{C} y_c^{(i)} \log(\hat{y}_c^{(i)})$$

# One-Hot Encoding

**One-hot** encoding represents categorical variables as binary vectors, with a 1 indicating the actual class and 0s elsewhere.

**Example:**

- Class 1: $[1, 0, 0]$
- Class 2: $[0, 1, 0]$
- Class 3: $[0, 0, 1]$

# Example Calculation (3-Class)

**Given:**

- True labels (One-hot): Class 2, Class 1, Class 3
- Predicted probabilities:

$$\hat{y} = \underbrace{\begin{bmatrix} 0.1 & 0.7 & 0.2 \\ 0.6 & 0.3 & 0.1 \\ 0.1 & 0.6 & 0.3 \end{bmatrix}}_{\text{Classes}} \quad \text{Samples}$$

# Solution

1. True labels:

$$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

2. Calculation:

$$\mathscr{L}_{CCE} = -\frac{1}{3}\big(\log(0.7) + \log(0.6) + \log(0.3)\big)$$

3. Compute log terms:

$$\log(0.7) \approx -0.357, \quad \log(0.6) \approx -0.511, \quad \log(0.3) \approx -1.204$$

$$\mathscr{L}_{CCE} = \frac{1}{3} \times 2.072 \approx 0.691$$

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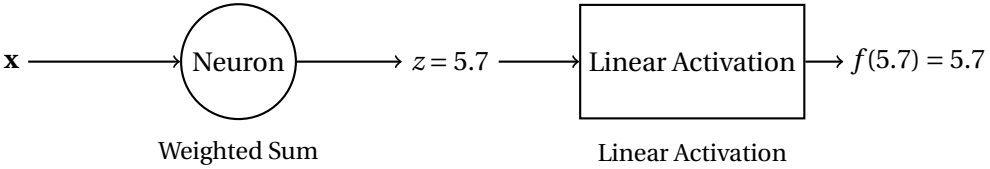
# Linear Activation - A Limitation

**Linear Activation:**

$$f(z) = z$$

- Example: If a neuron produces a raw output $z = 5.7$, linear activation would pass this unchanged.



# Limitation of Linear Activation

**Why Transform Outputs?** Raw outputs need to be transformed into meaningful values, such as probabilities.

**The Problem:** Linear activation lacks non-linearity, restricting the model to simple linear relationships.

# Neural Networks: Why is the Max Operator Important?

- **Before:** Linear score function:

$$f = Wx$$

- **Now:** 2-layer Neural Network:

$$f = W_2 \max(0, W_1 x)$$

- The function $\max(0, z)$ is called an activation function (in this case, ReLU).
- Q: What if we try to build a neural network without an activation function?

$$f = W_2 W_1 x$$

$$W_3 = W_2 W_1 \in \mathbb{R}^{C \times H}, \quad f = W_3 x$$

- **A:** We end up with a linear classifier again!

# ReLU

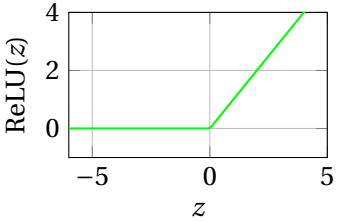
**Characteristics of ReLU:**

$$\mathrm{ReLU}(z) = \max(0, z)$$

- Faster convergence: Efficient computation, especially for deep networks.

**Advantages of ReLU:**

- Does not saturate for positive values, helping to avoid the vanishing gradient problem.
- Computationally efficient (simpler than Sigmoid/Tanh).



# ReLU

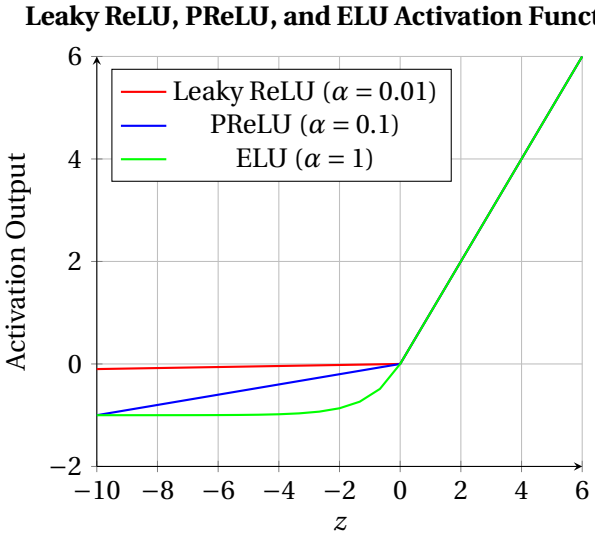
**Limitation:**

- **Dead ReLU Problem**: Neurons can become inactive during training, outputting 0 for all inputs if they receive negative values consistently.

**Question:**

- Why does ReLU lead to faster training in deep networks?

# Variants of ReLU: Leaky ReLU, PReLU, ELU

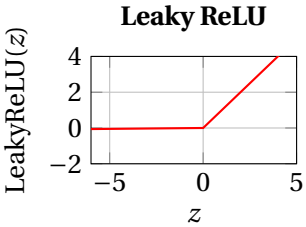


# Variants of ReLU: Leaky ReLU

- Allows a small, non-zero gradient for negative inputs.

$$\text{LeakyReLU}(z) = \max(\alpha z, z), \quad \alpha = 0.01$$

- Helps prevent the "dead ReLU" problem, where neurons stop updating.



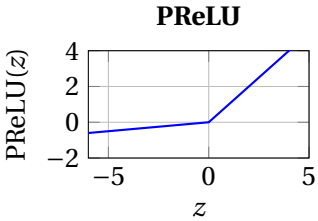

**Leaky ReLU:** Allows a small, non-zero gradient for negative inputs.

# Variants of ReLU: PReLU (Parametric ReLU)

- Similar to Leaky ReLU, but the slope for negative inputs ($\alpha$) is learned during training.

$$\mathrm{PReLU}(z) = \max(\alpha z, z), \quad \alpha \text{ is learned}$$

- Provides more flexibility by adjusting the slope for negative inputs based on data.



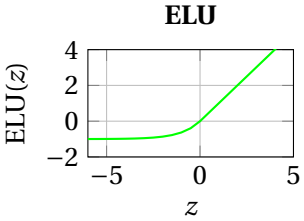

**PReLU:** Similar to Leaky ReLU, with a learnable slope.

# Variants of ReLU: ELU (Exponential Linear Unit)

- Similar to ReLU for positive values but smoother for negative inputs.

$$\mathrm{ELU}(z) = \begin{cases} z, & \text{if } z > 0 \\ \alpha(e^z - 1), & \text{if } z \leq 0 \end{cases}, \quad \alpha = 1$$

- Provides faster convergence and reduces bias shift by smoothing negative values.



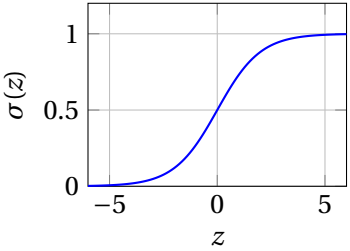

**ELU:** Smoother than ReLU for negative values.

# Sigmoid

**Characteristics of Sigmoid:**

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

- $\sigma'(z) = \sigma(z)(1 - \sigma(z))$
- Squashes the input between 0 and 1, which makes it useful in probabilistic interpretations (e.g., logistic regression).
- Often used in output layers for binary classification problems.

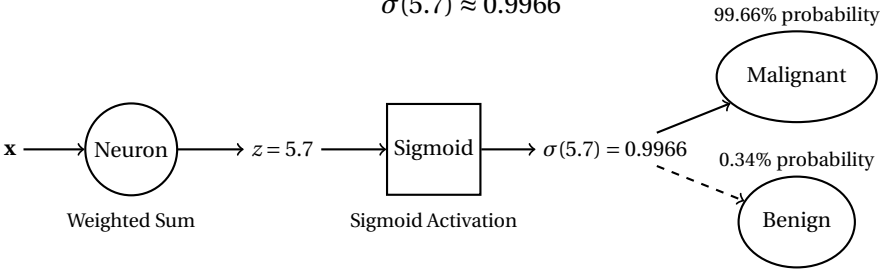


# Classification: Tumor Detection (Malignant vs. Benign)

**Sigmoid Activation:** Useful for binary classification!

- Example: For $z = 5.7$,

$$\sigma(5.7) \approx 0.9966$$



# Sigmoid

**Limitations of Sigmoid:**

- **Gradient Saturation:** When $z$ is very large or very small, the gradient becomes nearly zero, causing slow learning (vanishing gradient problem).
- **Not Zero-Centered:** The output is not zero-centered, which can make optimization more difficult.

**Question:**

- Why does the vanishing gradient problem occur with Sigmoid during backpropagation? (To be discussed in more detail later)

# Tanh (Hyperbolic Tangent)

**Characteristics of Tanh:**

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

- Squashes input between -1 and 1, making it zero-centered (Balanced Updates → Reduced Bias in Gradient Descent → Faster Convergence)

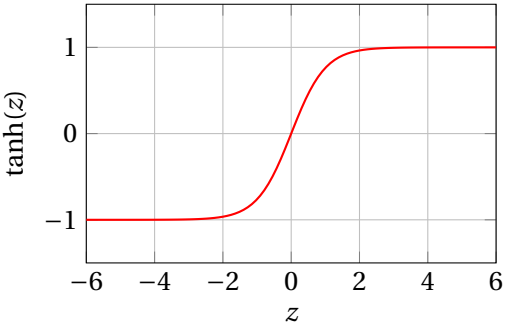
**Advantages of Tanh:**

- **Zero-Centered**: Output ranges from -1 to 1, making optimization easier.
- Better for **hidden layers** than Sigmoid due to zero-centered output.

**Limitations:**

- Similar saturation issues as Sigmoid: large input values push gradients towards zero (vanishing gradient problem).

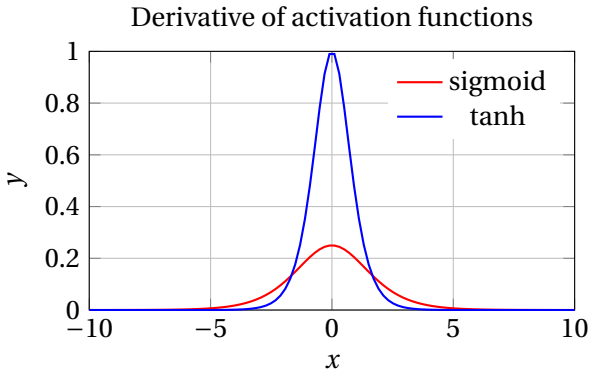
# Tanh (Hyperbolic Tangent)




**Question:**

- How does Tanh help with faster convergence compared to Sigmoid?

# Comparison: Sigmoid vs Tanh

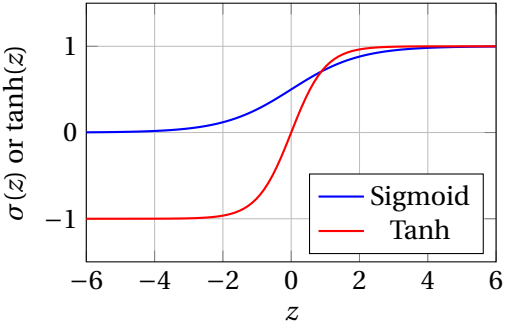



- The derivative of the Tanh function has a much steeper slope at $x = 0$, meaning it provides a larger gradient for backpropagation compared to the Sigmoid function.

# Comparison: Sigmoid vs Tanh

**Key Differences:**

- **Sigmoid**: Maps input to [0, 1]. Output is not zero-centered.
- **Tanh**: Maps input to [-1, 1]. Output is zero-centered, leading to easier optimization.

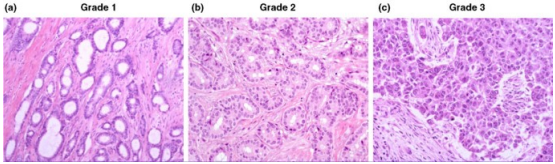


# Problem: Multi-Class Tumor Classification

**Scenario:** We want to classify a tumor into one of three categories:

- **Class 0**: Benign
- **Class 1**: Malignant
- **Class 2**: Pre-cancerous

**Goal:** Given a set of tumor features, predict which class the tumor belongs to.
This is a **multi-class classification problem**, and we will use the **Softmax activation function** to assign probabilities to each class.




Microscopic images of tumor tissue, classified into grades representing different severity levels. Image adapted from Visual Analytics in Digital Computational Pathology

# Softmax Activation: The Model

In multi-class classification, the Softmax function is used to convert raw outputs (logits) into probabilities for each class.

**Softmax Function:**

$$P(y = i|X) = \frac{e^{z_i}}{\sum_{j=1}^{K} e^{z_j}}$$

Where:

- $P(y = i|X)$ is the probability of the sample $X$ belonging to class $i$.
- $z_i$ is the raw output (logit) for class $i$.
- $K$ is the number of classes (e.g., benign, malignant, pre-cancerous).

The Softmax function ensures that the sum of the probabilities for all classes is 1, and the class with the highest probability is chosen as the prediction.

# Example: Softmax Calculation

Consider a tumor with the following logits from a neural network:

- Logit for Benign (Class 0): $z_0 = 1.5$
- Logit for Malignant (Class 1): $z_1 = 0.8$
- Logit for Pre-Cancerous (Class 2): $z_2 = -0.5$

**Step 1: Exponentiate the logits**

$$e^{z_0} = e^{1.5} \approx 4.48, \quad e^{z_1} = e^{0.8} \approx 2.23, \quad e^{z_2} = e^{-0.5} \approx 0.61$$

**Step 2: Compute the sum of exponentials**

$$\text{Sum} = e^{z_0} + e^{z_1} + e^{z_2} = 4.48 + 2.23 + 0.61 = 7.32$$

# Example: Softmax Probabilities

**Step 3: Calculate Softmax probabilities for each class**

$$P(\text{Benign}) = \frac{4.48}{7.32} \approx 0.612, \quad P(\text{Malignant}) = \frac{2.23}{7.32} \approx 0.305, \quad P(\text{Pre-Cancerous}) = \frac{0.61}{7.32} \approx 0.083$$

**Step 4: Make a classification decision**

- The highest probability is 0.612 for the **Benign** class.
- Therefore, the model predicts that the tumor is **Benign** (Class 0).

# Conclusion: Softmax Activation for Classification

**Key Points:**

- Softmax is used in the output layer for **multi-class classification**.
- It converts logits into a **probability distribution** across classes.
- The class with the highest probability is selected as the prediction.

**Main Idea:** Softmax ensures all outputs sum to 1, making it ideal for choosing one class out of multiple options.

1 Gradient Descent

2 Backpropagation

3 Foundations in Detail: Initialization, Loss, and Activation

4 References

# Contributions

- **This slide has been prepared thanks to:**
  - Donya Navabi
  - Mohammad Aghaei
  - Sogand Salehi

[1] T. Networks, "Benign vs malignant tumors." *Web article*, 2023. https://www.technologynetworks.com/cancer-research/articles/benign-vs-malignant-tumors-364765.

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# Any Questions?