Machine Learning (CE 40717)

Fall 2024

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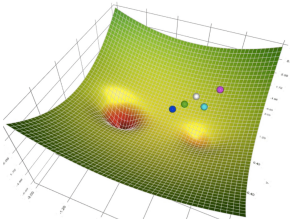
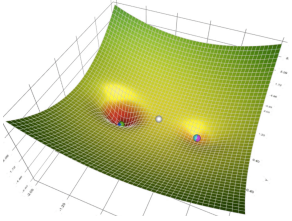
January 4, 2026

How to Update Weights?

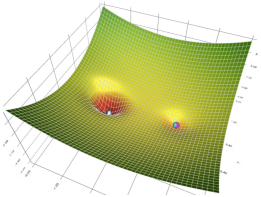
- Imagine training a large model like ChatGPT. It has billions of parameters that need to be adjusted.
- If we used **random search** to update these weights, it would take an astronomical number of trials to find good parameters.
- How to make training feasible at this massive scale?
- Image adapted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

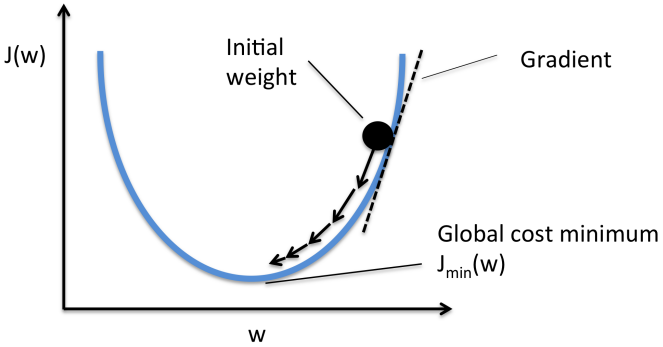
Options for Updating Weights:

- **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:

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

Where:

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

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:

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

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

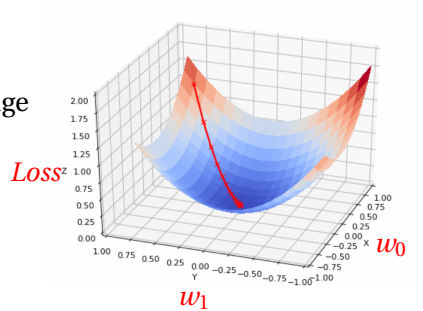
Gradient Descent: Formula and Process

Weight Update Formula:

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

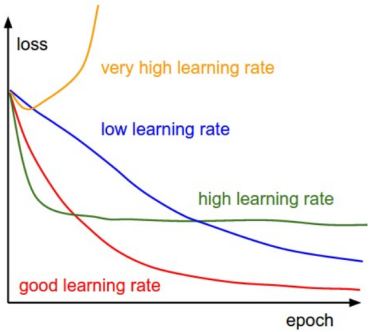
Steps in Gradient Descent:

- 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



Recap: Problem Setup

- Given the architecture of the network and training data $D = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(N)}, y^{(N)})\}$, we aim to minimize the total loss.

$$\hat{w} = \arg\min_{\mathbf{w}} E(\mathbf{w})$$

- To do so, we use the gradient descent method:

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

- How to calculate $\frac{\partial L}{\partial \mathbf{w}}$?

Finite Difference Method

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

- Change w_i by a small value ϵ.
- 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:

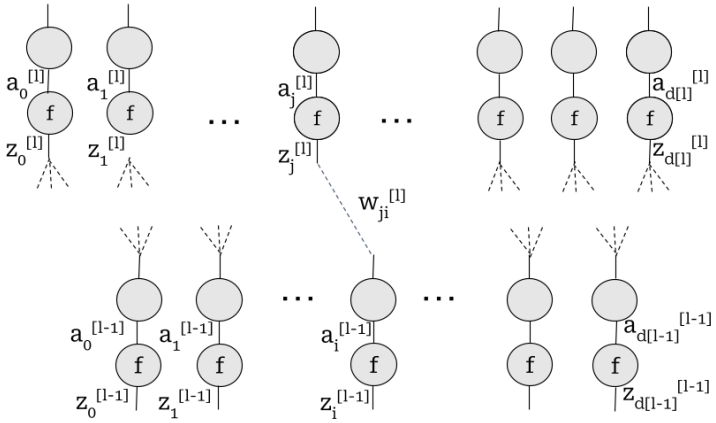
- Use the chain rule to compute all gradients in one backward pass.
- This method avoids changing each weight separately.

Advantages:

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

Notation Setup

The diagram below illustrates the l^{th} layer of a neural network.



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:

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

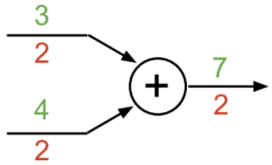
This means we multiply the gradient of the outer function by the gradient of the inner function.

Why Study Computational Gates?

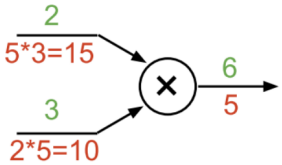
- These simple gates (add, multiply, copy, max) are the **fundamental building blocks** of all neural network computations.
- Any forward pass in a neural network can be decomposed into combinations of these basic operations.
- Understanding each gate's backward rule shows **how gradients flow** through a model during backpropagation.
- These gates illustrate how gradients are:
  - **Distributed** (add gate)
  - **Scaled** (multiply gate)
  - **Accumulated** (copy gate)
  - **Routed** (max gate)
- Mastering these rules builds intuition for **how learning happens**, why gradients change, and how models optimize their parameters.

Chain Rule for Important Gates

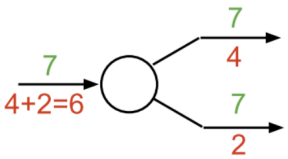
add gate: gradient distributor



mul gate: “swap multiplier”



copy gate: gradient adder



max gate: gradient router

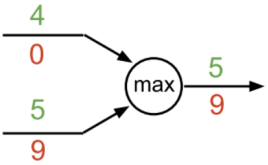
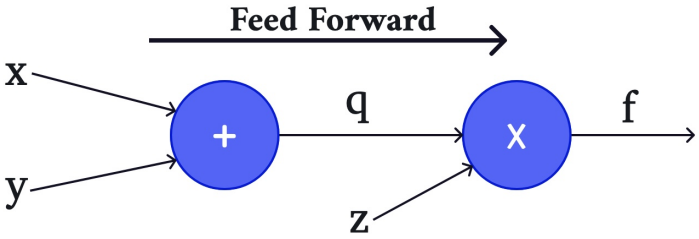


Figure adopted from Fei-Fei Li, Jiajun Wu, and Ruohan Gao, *CS231n*, Stanford, Fall 2022.

A Simple Example

Function:

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



A Simple Example: Forward Pass

Function:

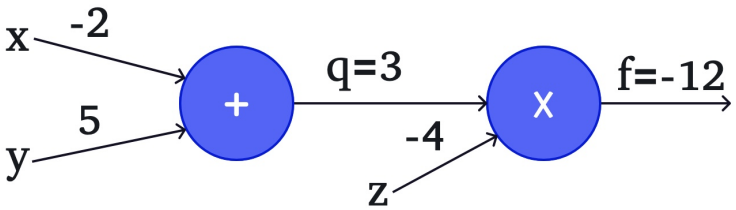
$$f(x, y, z) = (x + y)z$$

Example:

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

Steps:

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



Backpropagation: A Simple Example

Function:

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

Example:

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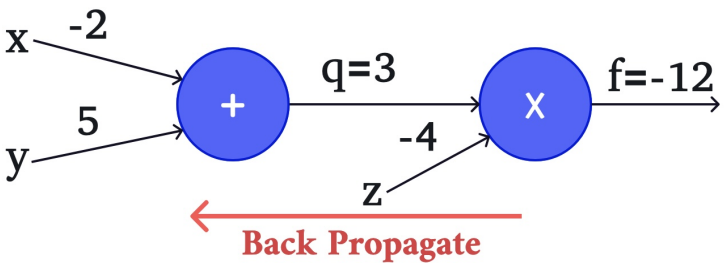


A Simple Example: Backpropagation

Function:

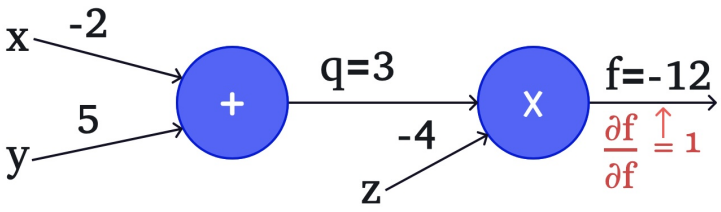
$$f(x, y, z) = (x + y)z$$

Example:

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

Step 1:

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



A Simple Example: Backpropagation

Function:

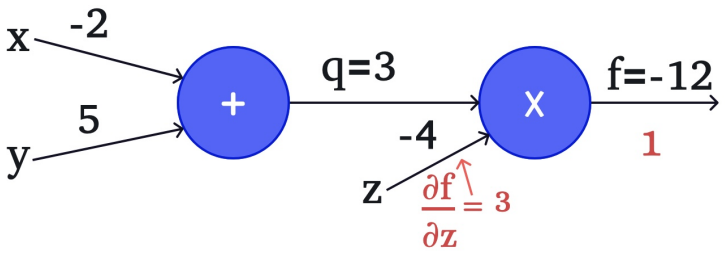
$$f(x, y, z) = (x + y)z$$

Example:

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

Step 2:

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



A Simple Example: Backpropagation

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Step 2:

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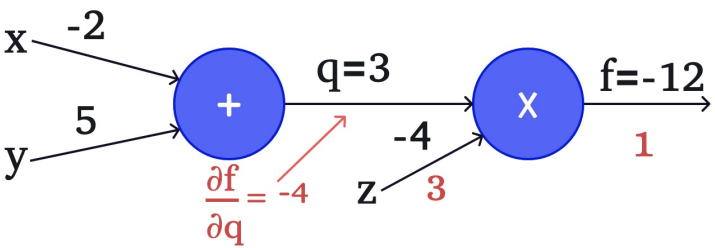
$$\frac{\partial f}{\partial q} = z = -4$$



A Simple Example: Backpropagation

Function:

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

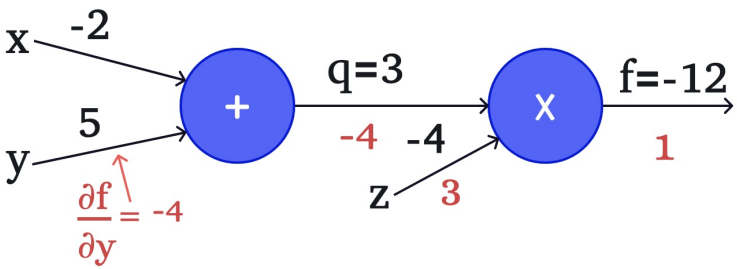
Example:

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

Step 3:

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

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



A Simple Example: Backpropagation

Function:

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

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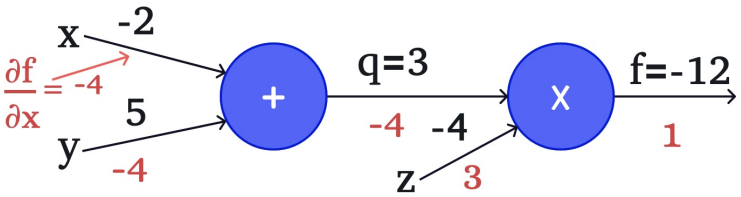

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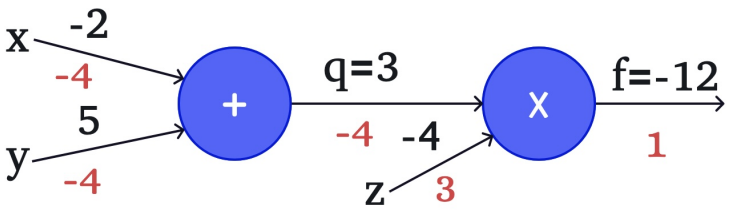


Step 1:

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

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

Example: One Neuron

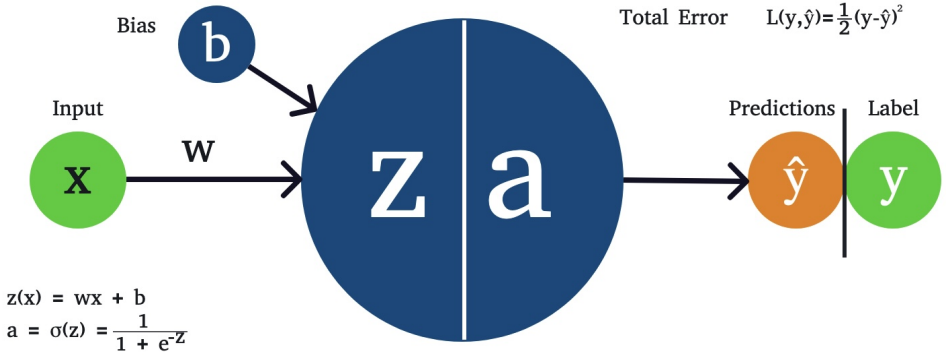
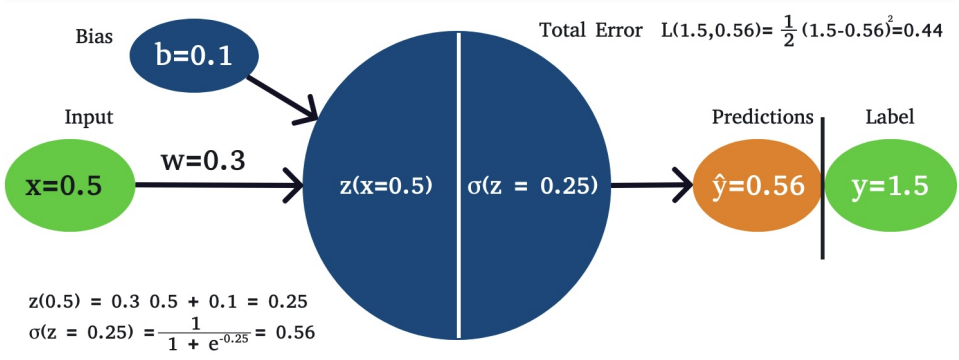
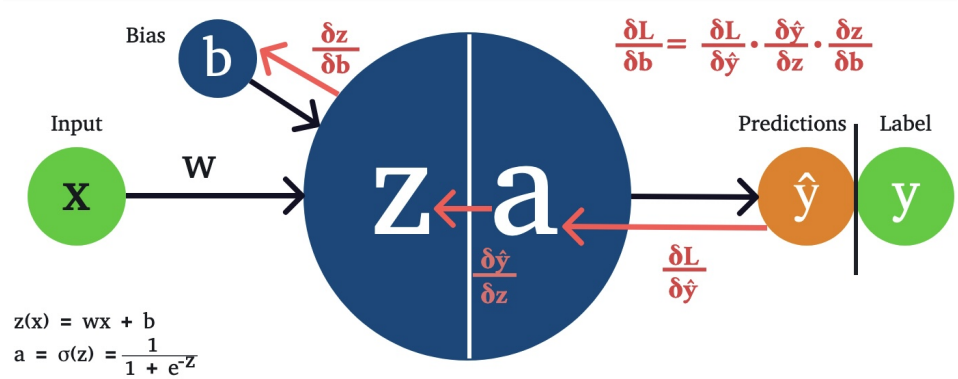


Image adapted from “Deep learning backpropagation” Web article

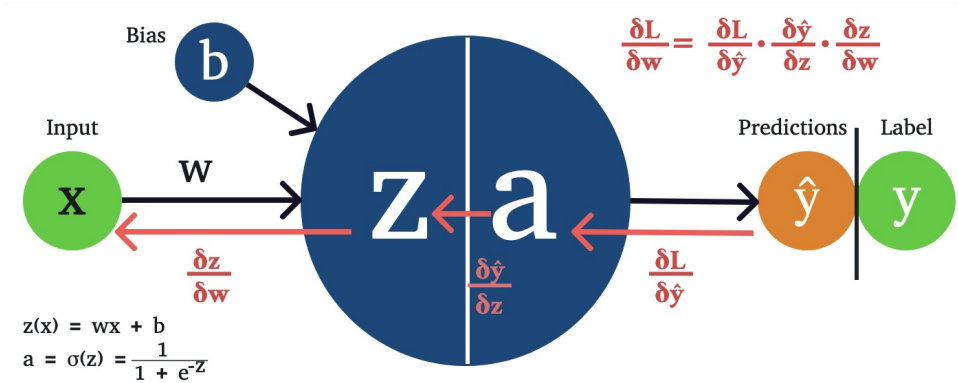
Forward Pass



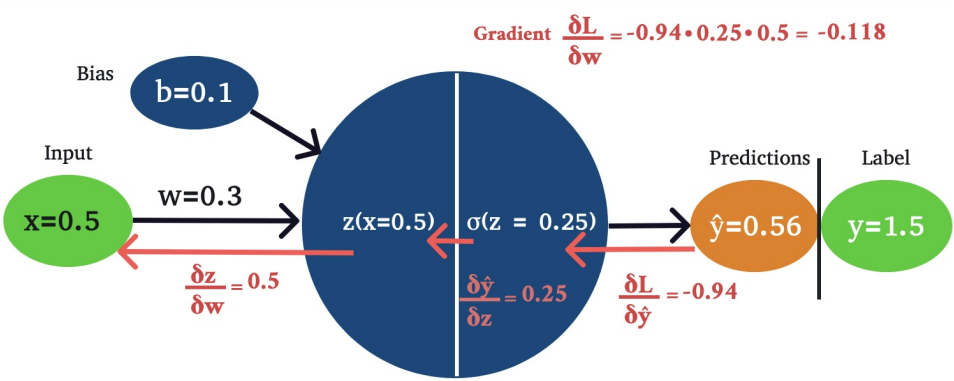
Backward Pass



Backward Pass



Backward Pass



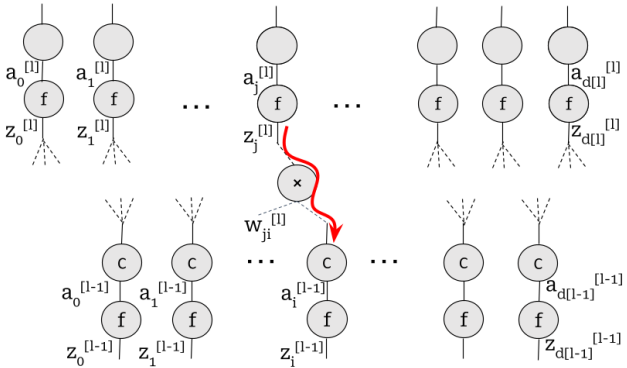
Backward Pass in the lth Layer

$$\frac{\partial L}{\partial w_{ji}^{[l]}} = \frac{\partial L}{\partial z_j^{[l]}} \frac{\partial z_j^{[l]}}{\partial w_{ji}^{[l]}} = \frac{\partial L}{\partial z_j^{[l]}} a_i^{[l-1]}$$

Note that:

$$z_j^{[l]} = \sum_{i=0}^{d[l-1]} w_{ji}^{[l]} a_i^{[l-1]}$$

$$a_i^{[l]} = f(z_i^{[l]})$$

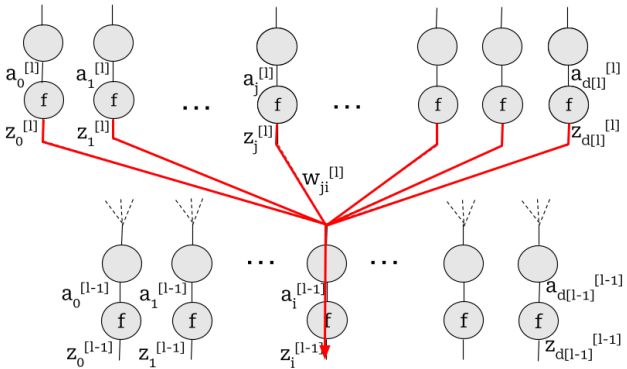


Backward Pass in the lth Layer

Now we need to calculate $\frac{\partial L}{\partial z_j^{[l]}}$

$$\frac{\partial L}{\partial z_i^{[l-1]}} = \frac{\partial L}{\partial a_i^{[l-1]}} \frac{\partial a_i^{[l-1]}}{\partial z_i^{[l-1]}}$$

$$= \frac{\partial a_i^{[l-1]}}{\partial z_i^{[l-1]}} \sum_{j=0}^{d[l]} w_{ji}^{[l]} \frac{\partial L}{\partial z_j^{[l]}}$$



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.

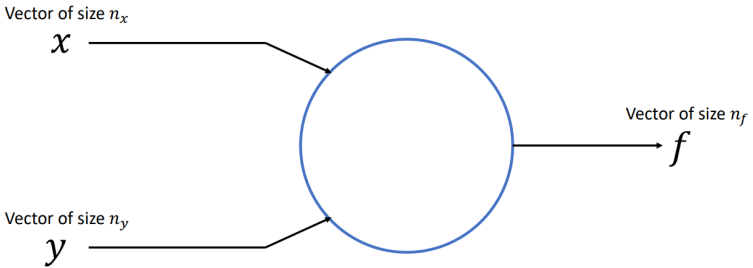
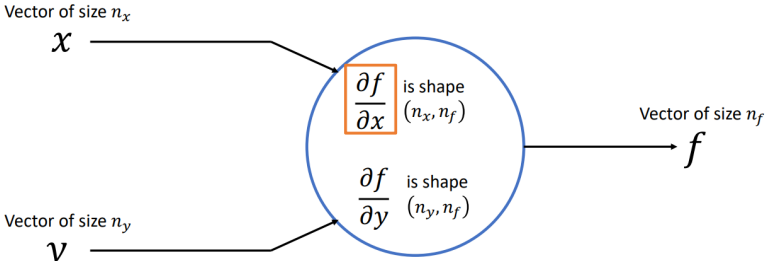


Image adapted from Elec502 vectorized backpropagation slides

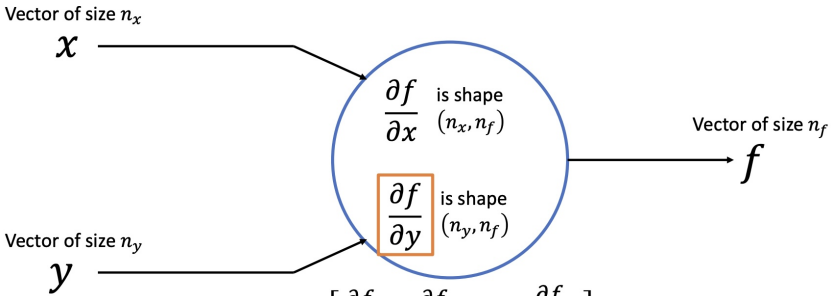
Vectorized Backpropagation

Local Derivatives are Jacobian Matrices



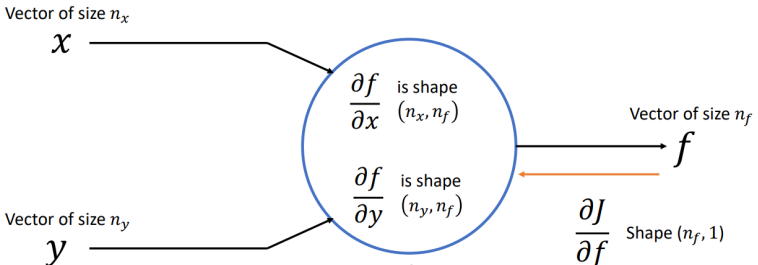
$$\frac{\partial f}{\partial x} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_2}{\partial x_1} & \cdots & \frac{\partial f_{n_f}}{\partial x_1} \\ \frac{\partial f_1}{\partial x_2} & \frac{\partial f_2}{\partial x_2} & & \frac{\partial f_{n_f}}{\partial x_2} \\ \vdots & & \ddots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

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

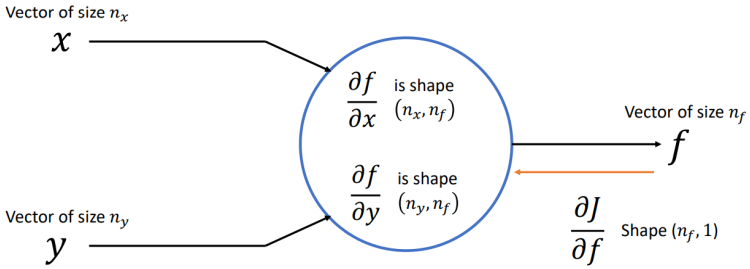


$$\frac{\partial J}{\partial f} = \begin{bmatrix} \frac{\partial J}{\partial f_1} \\ \frac{\partial J}{\partial f_2} \\ \vdots \\ \frac{\partial J}{\partial f_{n_f}} \end{bmatrix}$$

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

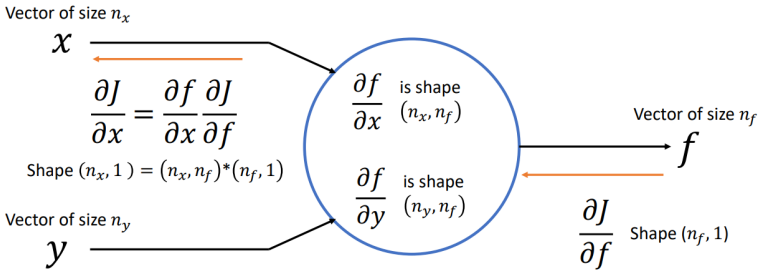
i.e. How does each output f_i affect the Cost

Vectorized Backpropagation



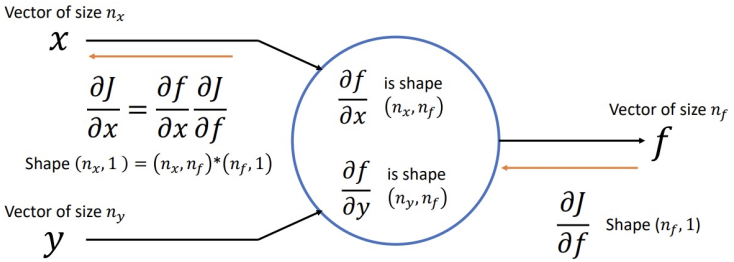
Apply chain rule like before!

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

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

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

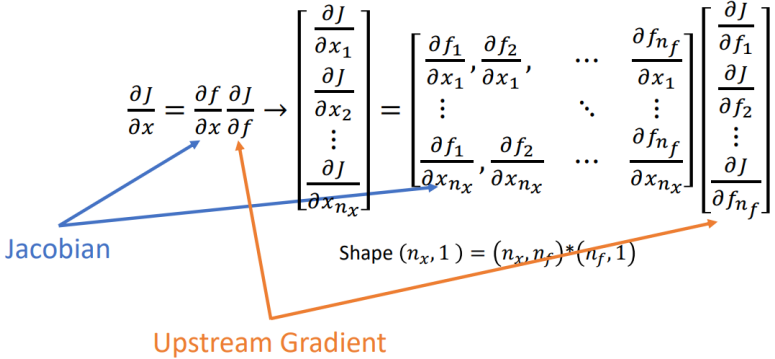
Chain Rule – Matrix-Vector Multiply

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

Jacobian

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

Chain Rule – Matrix-Vector Multiply



Chain Rule – Matrix-Vector Multiply

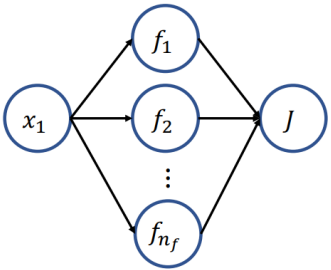
$$\frac{\partial J}{\partial x} = \frac{\partial f}{\partial x}\frac{\partial J}{\partial f} \rightarrow \begin{bmatrix} \frac{\partial J}{\partial x_1} \\ \frac{\partial J}{\partial x_2} \\ \vdots \\ \frac{\partial J}{\partial x_{n_x}} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1},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

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

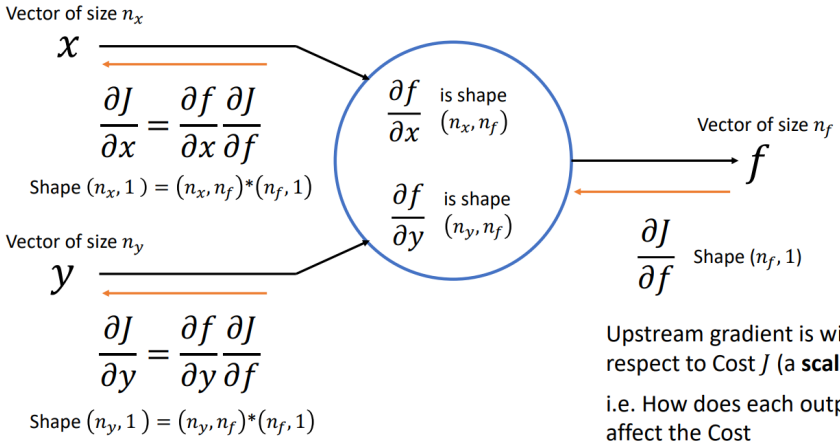
$$\frac{\partial J}{\partial x} = \frac{\partial f}{\partial x}\frac{\partial J}{\partial f} \rightarrow \begin{bmatrix} \frac{\partial J}{\partial x_1} \\ \frac{\partial J}{\partial x_2} \\ \vdots \\ \frac{\partial J}{\partial x_{n_x}} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1},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



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

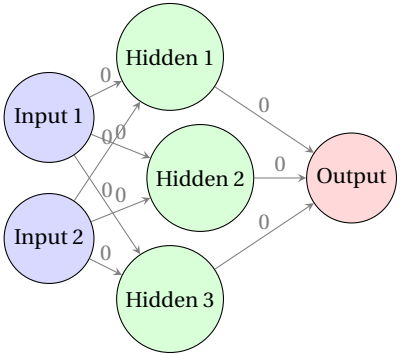
$$\frac{\partial J}{\partial x_1} = \frac{\partial f_1}{\partial x_1}\frac{\partial J}{\partial f_1} + \frac{\partial f_2}{\partial x_1}\frac{\partial J}{\partial f_2} + \cdots + \frac{\partial f_{n_f}}{\partial x_1}\frac{\partial J}{\partial f_{n_f}}$$

Chain Rule – Matrix-Vector Multiply



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:

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

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.

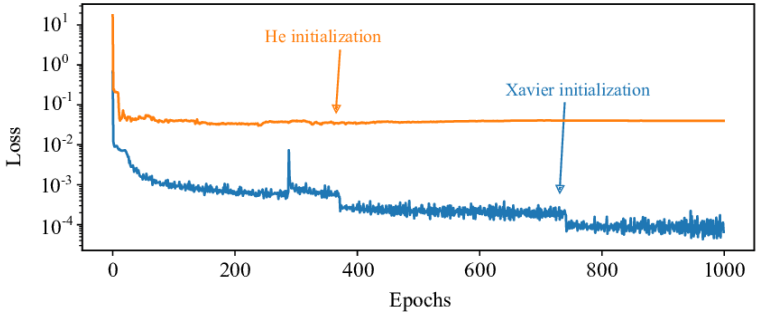


Image adapted from A Knowledge-driven Physics-Informed Neural Network model; Pyrolysis and Ablation of Polymers

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?

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:

$$\text{MSE} = \frac{1}{3}\left[(5.0-4.2)^2 + (4.0-3.8)^2 + (4.9-5.1)^2\right]$$

$$= \frac{1}{3}\left[0.64 + 0.04 + 0.04\right] = \frac{0.72}{3} = 0.24$$

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:

$$\text{MAE} = \frac{1}{3}\left(|5.0 - 4.2| + |4.0 - 3.8| + |4.9 - 5.1|\right)$$

$$= \frac{1}{3}(0.8 + 0.2 + 0.2) = \frac{1.2}{3} \approx 0.4$$

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: $y = [1, 0, 1]$

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

$$+0\cdot\log(0.3) + (1-0)\cdot\log(1-0.3) + 1\cdot\log(0.9) + (1-1)\cdot\log(1-0.9)\big]$$

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

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:

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

3. Compute log terms:

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

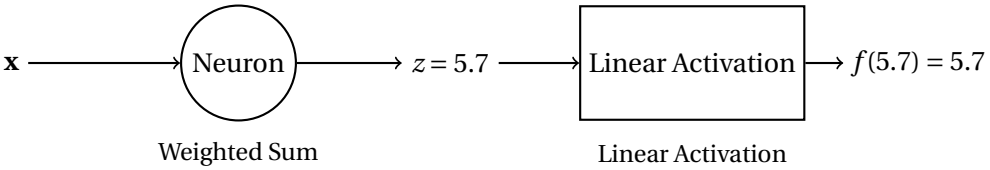
$$\mathscr{L}_{CCE} = \frac{1}{3} \times 2.072 \approx 0.691$$

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

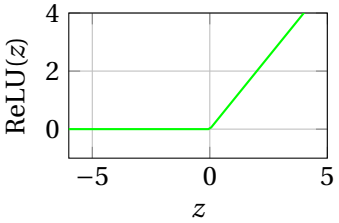
Characteristics of ReLU:

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

- 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

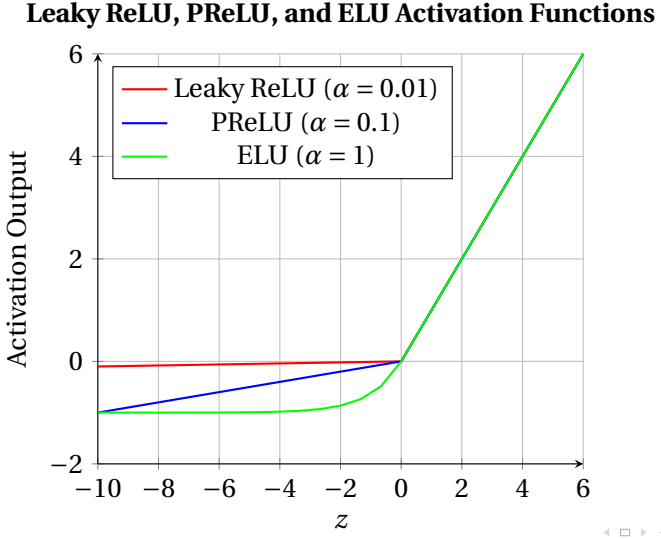
Limitation:

- **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

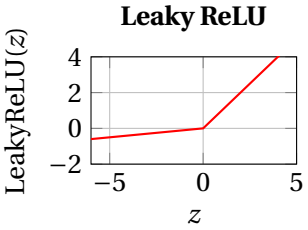


Variants of ReLU: Leaky ReLU

- 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.



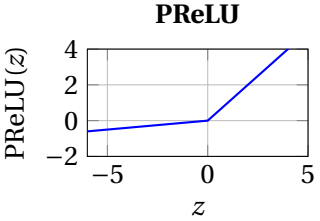
Leaky ReLU: Allows a small, non-zero gradient for negative inputs.

Variants of ReLU: PReLU (Parametric ReLU)

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

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

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



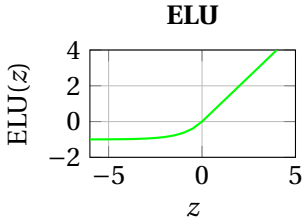
PReLU: Similar to Leaky ReLU, with a learnable slope.

Variants of ReLU: ELU (Exponential Linear Unit)

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

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

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



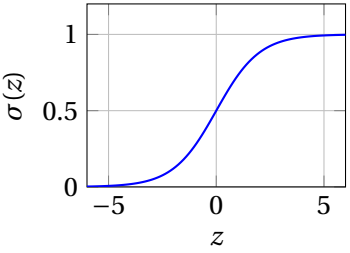
ELU: Smoother than ReLU for negative values.

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.

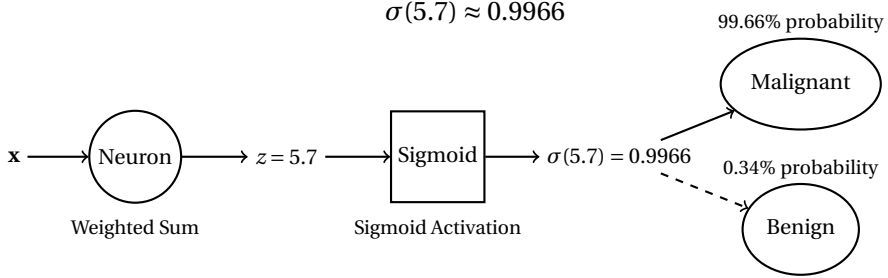


Classification: Tumor Detection (Malignant vs. Benign)

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)

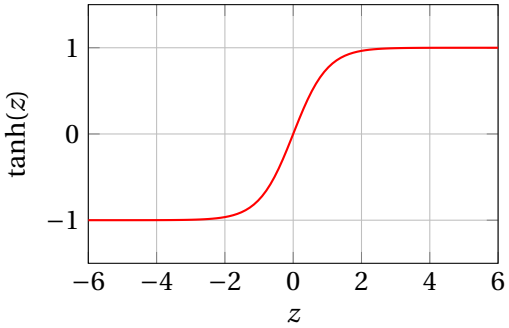
Advantages of Tanh:

- **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).

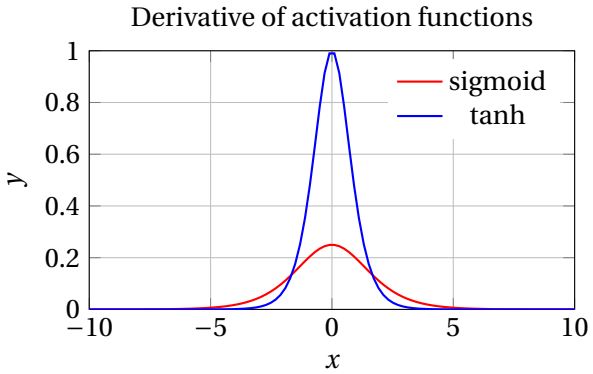
Tanh (Hyperbolic Tangent)



Question:

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

Comparison: Sigmoid vs Tanh

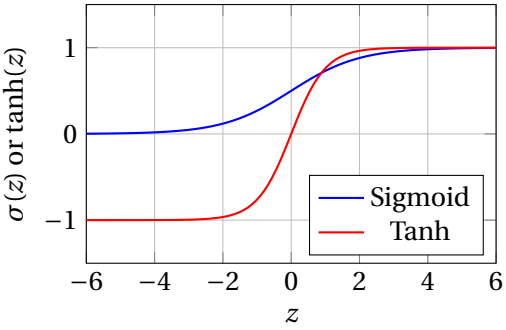


- The derivative of the Tanh function has a much steeper slope at $x = 0$, meaning it provides a larger gradient for backpropagation compared to the Sigmoid function.

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.

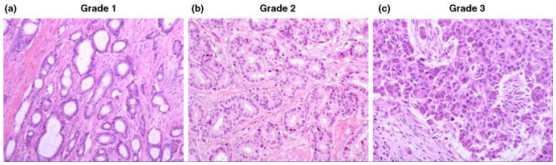


Problem: Multi-Class Tumor Classification

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.

Contributions

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

Any Questions?