

685.621 Algorithms for Data Science

Neural Networks: Mathematical Foundations

Forward Propagation Mechanics

Neuron Equation

$$\widehat{y} = f\left(\sum_{i=1}^{n} w_i x_i + b\right)$$

Matrix Form 1-Layer Forward Propagation

$$Z = WX + b$$
$$A = \sigma(Z)$$

Single Node Forward Propagation

$$a^{[l+1]} = f(W^{[l]}a^{[l]} + b^{[l]})$$

Generalize for Multiple Layers

$$Z^{[l+1]} = W^{[l]}A^{[l]} + b^{[l]}$$
$$A^{[l]} = \sigma(Z^{[l]})$$



Loss Functions

Regression Problems

$$MSE = \frac{1}{m} \sum (y_i - \widehat{y}_i)^2$$

Classification Problems

$$CrossEntropy = \sum y \log(\hat{y})$$

- Loss functions quantify the difference between the network's predictions and the actual target values
- Mean Squared Error penalizes larger errors more heavily because of the square term.
- Cross Entropy penalizes incorrect class probabilities and rewards confident correct predictions (multi-class classification)
- During training, our goal is to minimize this loss, step by step, until our model generalizes well to new, unseen data



Backpropagation Algorithm

- Step 1: Compute output layer error
- Step 2: Compute gradients of weights and biases (output layer)
- Step 3: Propagate error backwards
- Step 4: Compute gradients of weights and biases (hidden layers)
- Step 5: Update parameters using learning rate

Output Layer Error

$$dZ^{[L]} = A^{[L]} - Y$$

Propagate Error Backwards

$$dZ^{[l]} = (W^{[l+1]})^T dZ^{[l+1]} \circ \sigma'(Z^{[l]})$$

Compute Gradients

$$dW^{[L]} = \frac{1}{m} dZ^{[L]} (A^{[L-1]})^T$$

Update Parameters

$$W^{[l]} = W^{[l]} - \eta dW^{[l]}$$



Gradient Descent Variants

- The gradient is a vector (or matrix) of partial derivatives.
- Backpropagation efficiently computes all these partial derivatives using the chain rule.
- Backpropagation isn't just computing "a gradient" — it computes the entire set of partial derivatives (the full gradient) for the entire network.
- Gradients guide how we update parameters to minimize loss

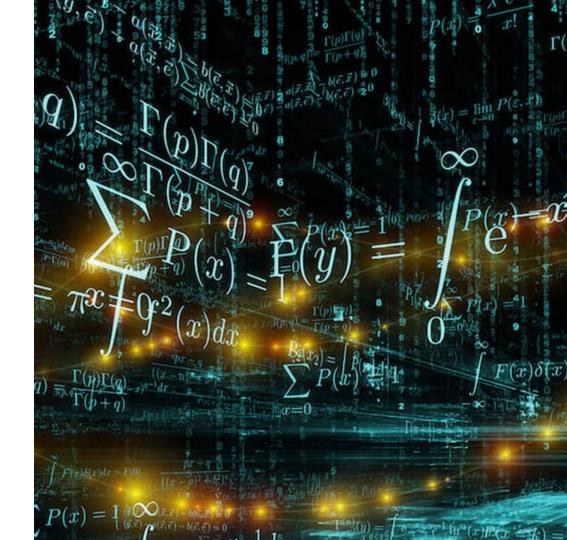
$$\nabla f = \left[\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \dots, \frac{\partial f}{\partial x_n}\right]$$

$$\nabla \mathcal{L} = [\frac{\partial \mathcal{L}}{\partial W_1}, \frac{\partial \mathcal{L}}{\partial W_2}, \dots, \frac{\partial \mathcal{L}}{\partial W_n}]$$



Computational Complexity

- Each architecture type has different training and testing complexity.
- Complexity mostly scaled with depth and width of the network.
- Deep architectures are powerful but come with cost and memory demands.





Hardware Acceleration for Training

- Graphics Processing Units (GPUs) have become the standard for accelerating deep learning workloads
- This has been a key enabler of modern AI advancements
- Although the cost of common GPUs has been going down the more advanced cards continue to be more expensive.

