ML ORANGE PROBLEM

Project Title: Week 6: Artificial Neural Networks (ORANGE PROBLEM)

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Course: UE23CS352A: Machine Learning

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1. Introduction

The primary objective of this laboratory exercise is to implement a neural network from scratch for function approximation, without reliance on high-level frameworks such as TensorFlow or PyTorch. This hands-on approach provides a foundational understanding of the core mechanics of neural networks.

Key tasks involved generating a synthetic dataset based on a unique student identifier, implementing the fundamental components of a neural network (activation functions, loss calculation, forward and backward propagation), training the model using gradient descent, and conducting a systematic analysis of hyperparameter tuning to observe its impact on model performance.

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2. Dataset Description

A synthetic dataset was generated based on the student SRN (PES2UG23CS195). The specific characteristics of this dataset are as follows:

- **Polynomial Type:** The assigned function is a **Quadratic** polynomial.
- **Governing Equation:** The ground truth function is defined by the equation:

y=1.42x2+3.49x+8.52

- **Sample Size:** The dataset contains **100,000 samples**. This was split into a training set of 80,000 samples (80%) and a testing set of 20,000 samples (20%).
- **Features:** The dataset consists of a single input feature, x, and a single output target, y.
- **Noise Level:** Gaussian noise with a standard deviation (N0) of **2.08** was added to the output variable y to simulate real-world data imperfections.
- **Standardization:** Both the input (x) and output (y) features were standardized using StandardScaler to have a mean of zero and a standard deviation of one, which is a crucial preprocessing step for optimizing neural network training.

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3. Methodology

A feedforward neural network was implemented from scratch to approximate the generated polynomial function. The core components and architecture are detailed below:

- **Network Architecture:** The model utilizes a multi-layer perceptron (MLP) with one input layer, two hidden layers, and one output layer.
  - **Baseline Architecture: 1-96-96-1** (1 input neuron, 96 neurons in the first hidden layer, 96 in the second, and 1 output neuron).
  - **Experiment 4 Architecture: 1-64-64-1** was used to study the impact of network capacity.
- **Weight Initialization: Xavier Initialization** was employed to set the initial weights of the network, which helps prevent vanishing or exploding gradients during training. Biases were initialized to zero.
- **Activation Function:** The **Rectified Linear Unit (ReLU)** function was used for both hidden layers to introduce non-linearity, allowing the model to learn complex patterns. The output layer used a linear activation function (i.e., no activation) suitable for regression tasks.
- **Loss Function:** The **Mean Squared Error (MSE)** was used to quantify the difference between the model's predictions and the true target values.

- **Optimization:** The network's weights and biases were updated iteratively using **Batch Gradient Descent**. The entire training dataset was processed in each epoch to compute the gradient of the loss function with respect to each parameter.
- **Training Procedure:** The model was trained for a specified number of epochs with an early stopping mechanism. Training was halted if the test loss did not improve for a set number of consecutive epochs (patience), ensuring the model with the best generalization performance was retained.

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4. Results and Analysis

Five distinct experiments were conducted: a baseline model followed by four experiments where hyperparameters were systematically varied to analyze their effect on performance.

Results Summary Table

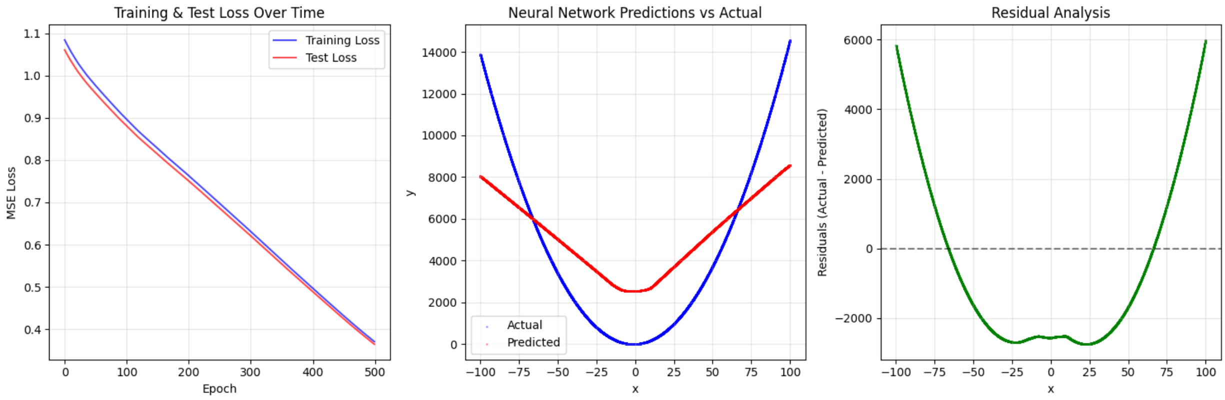
The performance of each experimental run is summarized below. The optimizer remained Batch Gradient Descent and the activation function was ReLU for all experiments.

Experiment	Learning Rate	Architecture	Max Epochs	Patience	Final Training Loss	Final Test Loss	R^2 Score	Observations
Baseline	0.003	1-96-96-1	500	10	0.370694	0.364594	0.6285	Moderate performance; slow convergence. The model captures the general trend but lacks precision.
Exp. 1	0.01	1-96-96-1	500	10	0.022361	0.021992	0.9776	Best Performance. The higher learning rate led to significantly faster convergence and a much better fit.

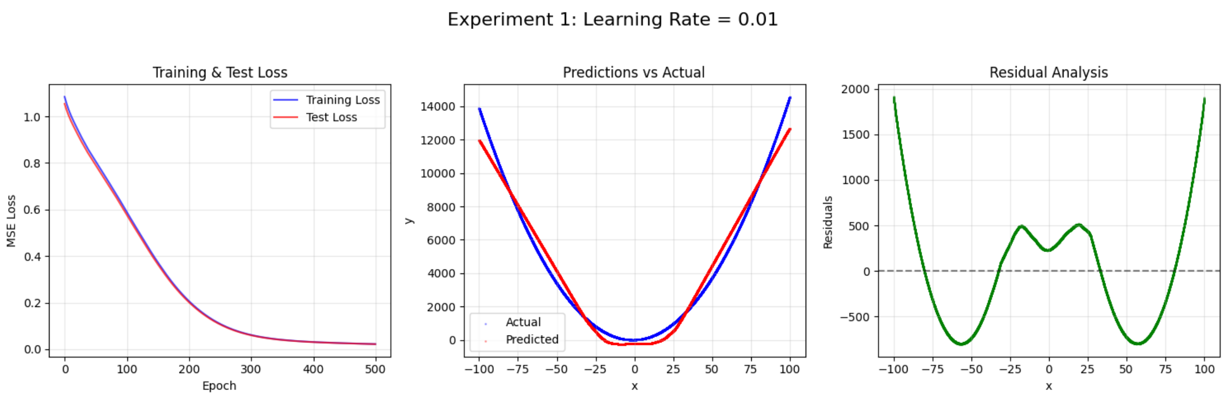
Exp. 2	0.0005	1-96-96-1	500	10	0.921649	0.906451	0.0764	Poor performance. The learning rate was too low, resulting in extremely slow learning and underfitting.
Exp. 3	0.003	1-96-96-1	1000	20	0.060735	0.0597	0.9392	Excellent performance. Shows that the baseline model was undertrained and benefited from more epochs.
Exp. 4	0.003	1-64-64-1	500	10	0.202243	0.19909	0.7971	Good performance, outperforming the baseline but less effective than the higher LR or more epochs.

OUTPUT SCREENSHOTS:

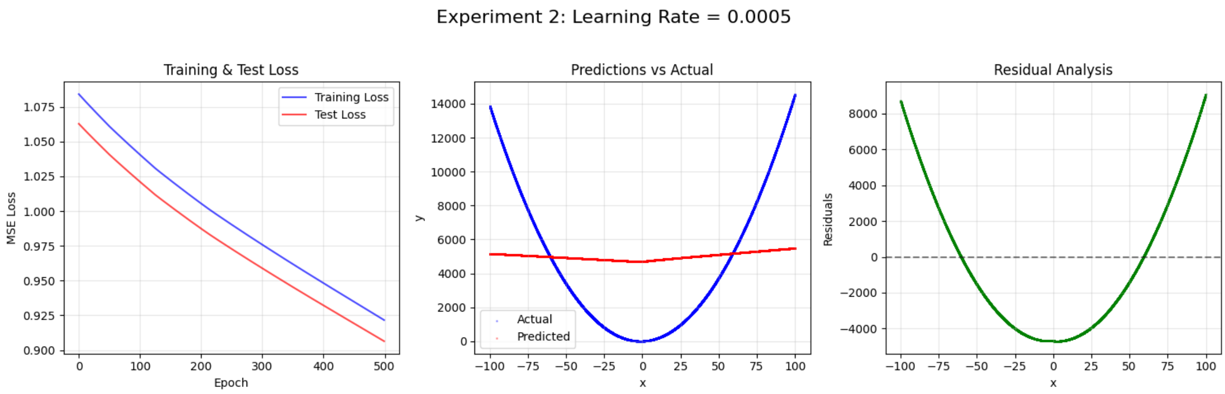
BASE-LINE:



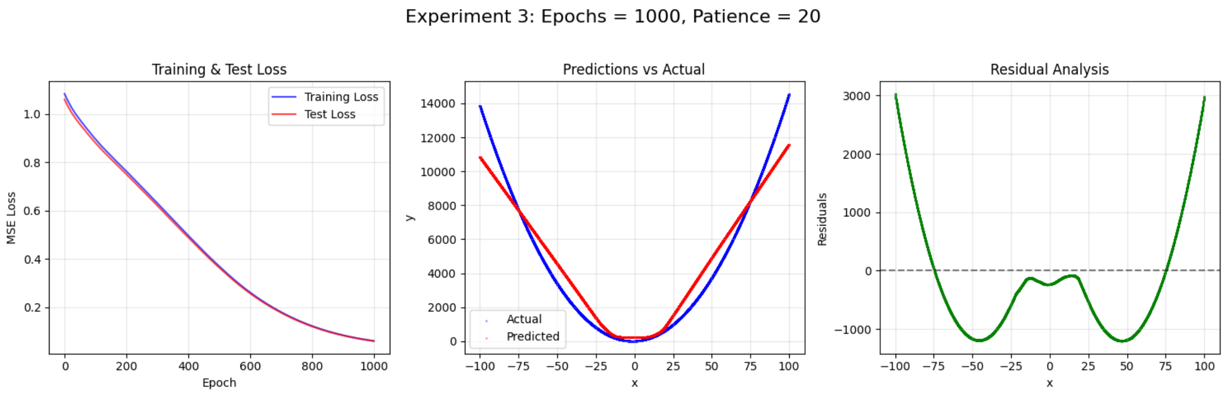
EXPERIMENT-1:



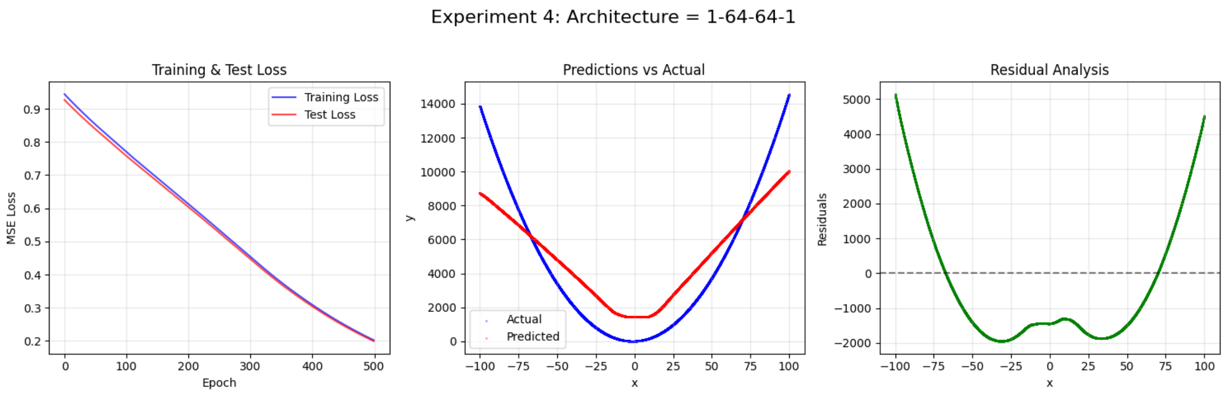
EXPERIMENT-2:



EXPERIMENT-3:



EXPERIMENT-4:



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5. Conclusion

This investigation successfully demonstrated the end-to-end implementation of a neural network for function approximation. The pivotal role of hyperparameter tuning was underscored through systematic experimentation.

The key findings are:

- The **learning rate** was the most impactful hyperparameter. A rate of **0.01** (Experiment 1) provided the optimal balance, leading to rapid convergence and the highest R^2 score (0.9776). A rate that was too low (0.0005) resulted in severe underfitting.
- The **number of epochs** was also critical. The baseline model was undertrained, and extending the training duration (Experiment 3) significantly enhanced performance, achieving an R^2 of 0.9392.

- **Network architecture** had a noticeable but less pronounced effect compared to other hyperparameters. The larger 1-96-96-1 network slightly outperformed the 1-64-64-1 architecture, suggesting its higher capacity was beneficial for this dataset.