TASK1

Assignment 2: Optimizer Performance on Non-Convex Functions

Course: Artificial Intelligence

Project Report: Optimizer Performance on Non-Convex Functions

1. Introduction

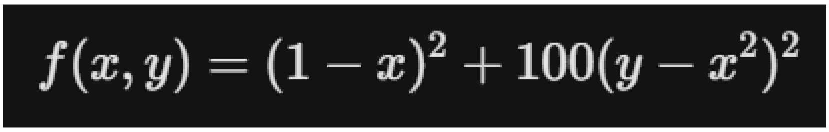
This project evaluates the performance of various first-order optimization algorithms on two distinct non-convex functions. The objective is to analyze the convergence behavior, speed, and stability of these optimizers under different hyperparameter settings, specifically focusing on the impact of learning rates.

1.1. Problem Statement

We aim to minimize the following two functions:

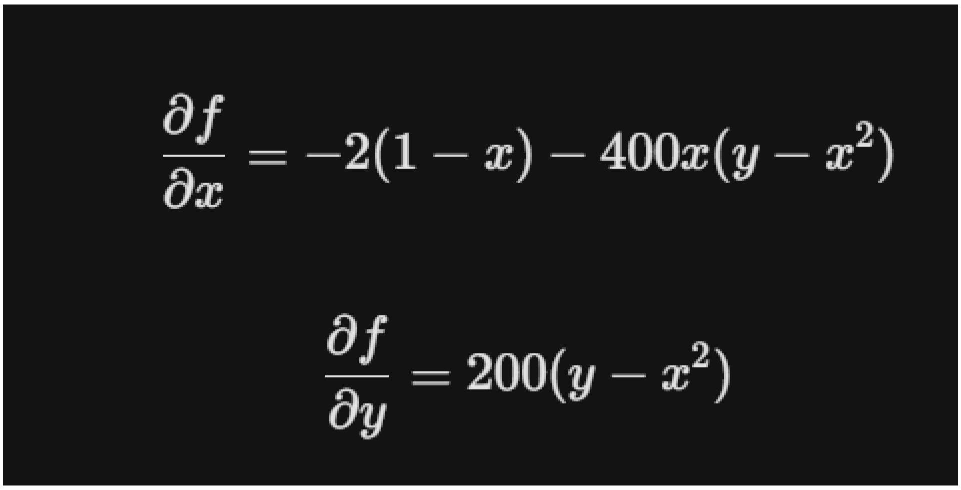
i. Rosenbrock Function (2D)

- **Equation:**



$$f(x, y) = (1 - x)^2 + 100(y - x^2)^2$$

- **Global Minimum:** Located at (1, 1) where f(x,y)=0.
- **Characteristics:** This function is characterized by a long, narrow, parabolic valley. While finding the valley is trivial, converging to the global minimum within it is difficult because the gradient is steep on the sides but very flat along the valley floor.
- **Gradients:**

- 

$$\frac{\partial f}{\partial x} = -2(1-x) - 400x(y-x^2)$$

$$\frac{\partial f}{\partial y} = 200(y-x^2)$$

ii. Sin(1/x) Function (1D)

- **Equation:**
  f(x) = sin(1/x)
- **Global Minimum:** f(x) = -1 (infinitely many solutions as x tends to 0).
- **Characteristics:** This function exhibits a pathological singularity at x=0. As x approaches zero, the frequency of oscillation increases to infinity, creating a highly rugged landscape with massive gradients.
- **Singularity Handling:** For this implementation, we defined f(0) = 0 and gradient(f(0)) = 0.

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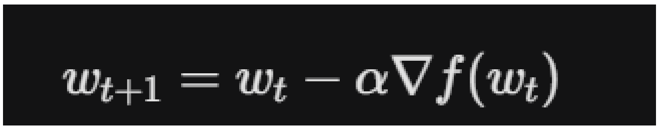
2. Methodology

2.1. Optimization Algorithms

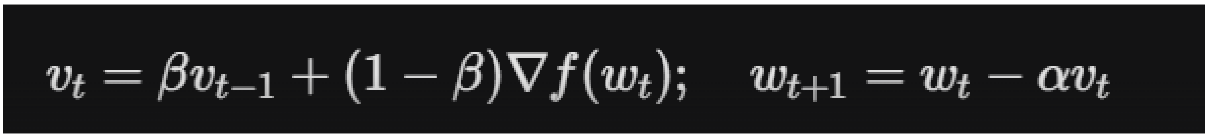
We implemented and compared the following five optimizers:

1. **Gradient Descent (GD):** The baseline algorithm. It updates parameters strictly in the direction of the negative gradient.
   - *Update Rule:*



$$w_{t+1} = w_t - \alpha \nabla f(w_t)$$

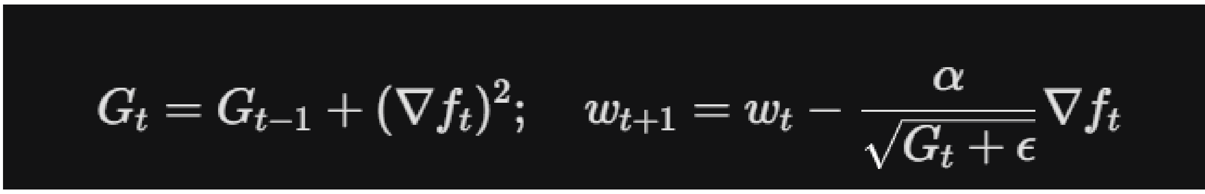
2. **Stochastic Gradient Descent (SGD) with Momentum:** Introduces a velocity term to dampen oscillations and accelerate convergence in relevant directions.
   - *Update Rule:*



$$v_t = \beta v_{t-1} + (1-\beta)\nabla f(w_t); \quad w_{t+1} = w_t - \alpha v_t$$

3. **Adagrad:** Adapts the learning rate for each parameter inversely proportional to the square root of the sum of all past squared gradients. It is useful for sparse features but suffers from a monotonically decreasing learning rate.

- *Update Rule:*



$$G_t = G_{t-1} + (\nabla f_t)^2; \quad w_{t+1} = w_t - \frac{\alpha}{\sqrt{G_t + \epsilon}} \nabla f_t$$

4. **RMSprop:** A modification of Adagrad that resolves the diminishing learning rate problem by using an exponentially decaying average of squared gradients.
5. **Adam (Adaptive Moment Estimation):** Combines the advantages of Momentum (first moment) and RMSprop (second moment). It computes adaptive learning rates for each parameter.

2.2. Experimental Setup

- **Learning Rates (alpha):** 0.01, 0.05, 0.1
- **Initialization:**
  - Rosenbrock: [-1.0, 2.0]
  - Sin(1/x): [0.5]
- **Iteration Limits:** 1500 (Rosenbrock), 500 (Sin(1/x))

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3. Experimental Results & Analysis

3.1. Rosenbrock Function

The Rosenbrock function tested the optimizers' ability to navigate a curved valley.

Quantitative Results Summary:

Optimizer	LR	Final Loss	Convergence Status
Momentum	0.01	**0.0000**	**Converged**
Adam	0.05	**0.0000**	**Converged**
RMSprop	0.01	0.0279	Near Optimal
Gradient Descent	0.1	26.98	Diverged

Adagrad	0.01	4.88	Stuck (Premature Stop)

Analysis:

- **Momentum's Efficiency:** At a low learning rate (0.01), Momentum was highly effective. The accumulated velocity allowed the optimizer to traverse the flat valley floor efficiently, reaching the global minimum.
- **Adam's Robustness:** Adam proved to be the most robust optimizer. Even at a higher learning rate (0.05), where standard Momentum and GD became unstable, Adam successfully converged to the global minimum (1, 1).
- **Adagrad's Failure:** Adagrad failed to converge. The rapid accumulation of squared gradients from the steep valley walls caused the learning rate to decay to near-zero before the optimizer could reach the minimum.
- **Instability of GD:** Standard Gradient Descent struggled significantly. At higher learning rates (>0.01), it oscillated wildly between the valley walls, resulting in divergence or high final loss.

3.2. Sin(1/x) Function

The Sin(1/x) function tested the optimizers' stability in the presence of exploding gradients.

Quantitative Results Summary:

Optimizer	LR	Final Loss	Result x	Status
Adagrad	All	-1.0000	0.212	Stable Optimal
Adam	All	-1.0000	0.212	Stable Optimal
RMSprop	0.01	-0.9944	0.218	Near Optimal
RMSprop	0.1	-0.2758	0.192	Unstable (Suboptimal)
Momentum	0.05	0.7751	-0.149	Oscillating

Gradient Descent	**0.05**	**0.2425**	**$4.085$**	**Escaped (Diverged)**

Analysis:

- **The "Catapult" Effect:** At higher learning rates (0.05, 0.1), non-adaptive methods like Gradient Descent encountered massive gradients near x=0. This "catapulted" the parameters far away from the origin , where the gradient is near zero, causing the optimizer to stop learning.
- **Superiority of Adaptive Methods:** Adagrad and Adam performed best. Their adaptive learning rate mechanisms naturally scaled down the step sizes when encountering the massive gradients near the singularity. This allowed them to settle stably into a local minimum without diverging.

4. Conclusion

1. **Best Overall Optimizer: Adam** demonstrated the best balance of speed and stability. It was the only optimizer to handle the curved valley of Rosenbrock and the explosive gradients of Sin(1/x) effectively across multiple learning rates.
2. **Specialized Performance:**
    - **Momentum** is excellent for valley-like structures (Rosenbrock) if the learning rate is kept low.
    - **Adagrad** is highly effective for functions with singularities or exploding gradients (Sin 1/x) but converges too slowly on standard convex/valley problems.
3. **Hyperparameter Sensitivity:** Gradient Descent is extremely sensitive to learning rate and initialization, making it a poor choice for complex non-convex functions compared to adaptive methods.

TASK2

Neural Network–Based Linear Regression Using Boston Housing Dataset

1. Task Description

The objective of this assignment is to implement a **multi-layer neural network from scratch** to perform **linear regression** on the Boston Housing dataset. The model aims to predict the **median value of owner-occupied homes (MEDV)** using two input features:

- **RM** – Average number of rooms per dwelling
- **CRIM** – Per capita crime rate

The assignment further investigates:

- The impact of **different optimizers**
- The effect of **learning rate**
- The influence of **network depth** by adding an extra hidden layer

2. Dataset Description

The **Boston Housing Dataset** contains housing-related information collected from suburbs of Boston.

Selected Features

Feature	Description
RM	Average number of rooms per dwelling
CRIM	Crime rate per capita
MEDV	Median value of homes (Target)

Preprocessing Steps

- Input features were **normalized using Min–Max scaling**
- Target variable (MEDV) was also normalized to ensure stable learning
- Dataset split into:

    - **80% training**
    - **20% testing**

3. Neural Network Overview and Working

A neural network consists of interconnected neurons arranged in layers. Each neuron computes:

$$\mathbf{Z = XW + b}$$

followed by an activation function.

Training Process

1. **Forward Propagation** – Compute predictions
2. **Loss Calculation** – Mean Squared Error (MSE)
3. **Backward Propagation** – Compute gradients
4. **Weight Updates** – Using optimization algorithms

The goal is to minimize MSE between actual and predicted values.

4. Network Architecture

Model 1: Baseline Neural Network

- Input Layer: 2 neurons (RM, CRIM)
- Hidden Layer 1: 5 neurons (ReLU)
- Hidden Layer 2: 3 neurons (ReLU)
- Output Layer: 1 neuron (Linear)

2 → 5 → 3 → 1

Model 2: Extended Neural Network

- Input Layer: 2 neurons
- Hidden Layer 1: 5 neurons (ReLU)
- Hidden Layer 2: 3 neurons (ReLU)
- Hidden Layer 3: 2 neurons (ReLU)
- Output Layer: 1 neuron

2 → 5 → 3 → 2 → 1

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5. Optimizers Used

Optimizers are algorithms used to update the weights and biases of a neural network in order to minimize the loss function. In this work, three different optimizers were implemented and compared.

1. Gradient Descent (GD)

Gradient Descent is the most basic optimization technique. It updates the model parameters in the direction opposite to the gradient of the loss function.

- Uses a fixed learning rate for all parameters
- Simple to implement and understand
- Sensitive to learning rate selection
- May converge slowly and oscillate near minima

Update rule:
W=W-(alpha)(gradient L)

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2. Momentum-Based Gradient Descent

Momentum improves standard Gradient Descent by adding a velocity term that accumulates past gradients. This helps the optimizer move faster in consistent directions and reduces oscillations.

- Accelerates convergence
- Reduces fluctuations in loss
- Especially useful in narrow or curved loss surfaces

Key idea:
Uses past gradients to gain “momentum” in weight updates.

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3. Adam (Adaptive Moment Estimation)

Adam is an advanced optimizer that combines the advantages of Momentum and adaptive learning rates. It computes individual learning rates for each parameter.

- Fast and stable convergence
- Less sensitive to learning rate choice
- Works well for noisy gradients

- Most commonly used optimizer in practice

Key features:

- First moment (mean of gradients)
- Second moment (variance of gradients)

Summary

- Gradient Descent is simple but slow and sensitive to hyperparameters
- Momentum improves stability and convergence speed
- Adam provides the best balance between speed and robustness

6. Results

6.1 Baseline Neural Network (2 Hidden Layers)

Training Loss

- Loss decreases rapidly and stabilizes around **0.0429**
- Adam converges the fastest, though all optimizers reach similar final loss

Test MSE

Optimizer	Test MSE
Gradient Descent	0.0371
Momentum	0.0371
Adam	0.0371

Prediction Behavior

- Initial training showed constant predictions (model collapse)
- After correcting initialization and learning rate, predictions became diverse
- Predicted vs Actual plot shows points closely aligned with the diagonal

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6.2 Neural Network with Additional Hidden Layer

Training Loss

- Loss **increases over epochs** instead of decreasing

- Indicates training instability and difficulty in optimization

Test MSE

Optimizer	Test MSE
Gradient Descent	0.0570
Momentum	0.0570
Adam	0.0559

Prediction Behavior

- Predictions vary but show larger deviation from ideal diagonal
- Increased error and weaker generalization compared to baseline model

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7. Discussion

Effect of Optimizers

- Adam converges faster and is more stable
- Final test performance is similar across optimizers for the baseline model
- Optimizer choice affects convergence speed more than final accuracy

Effect of Learning Rate

- Learning rate of **0.01** performs significantly better than smaller values
- Too small learning rates led to slow learning and model collapse

Effect of Additional Hidden Layer

- Adding a third hidden layer **degraded performance**
- Higher training and test loss observed
- Indicates **over-parameterization** for a simple regression problem

Why Deeper Model Performed Worse

- Limited dataset size
- Only two input features
- Increased depth caused:
  - Optimization difficulty
  - Higher variance
  - Mild overfitting

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8. Conclusion

This assignment successfully demonstrated the implementation of a **multi-layer neural network from scratch** for linear regression.

Key conclusions:

- A **two-hidden-layer neural network** is sufficient for this task
- Adam optimizer provides faster and more stable convergence
- Learning rate selection has a greater impact than optimizer choice
- Adding unnecessary hidden layers can **reduce model performance**
- Proper initialization and normalization are critical for effective training

Overall, simpler architectures generalized better for the Boston Housing regression task.

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9. Final Takeaway

> Increasing model complexity does not always improve performance. A well-tuned shallow network can outperform deeper models on small, structured datasets.

TASK3

Report: Multi-class Classification using Fully Connected Neural Network (FCNN)

1. Introduction & Methodology

This task involved implementing a Fully Connected Neural Network (FCNN) from scratch to perform multi-class classification on two distinct datasets.

- **Algorithm:** Backpropagation with **Stochastic Gradient Descent (SGD)**.
- **Loss Function:** Instantaneous Squared Error.
- **Data Split:** 60% Training, 20% Validation, 20% Testing.

2. Dataset 1: Linearly Separable Classes

Data Description: 3-class, 2-dimensional linearly separable data.

Model Architecture: 1 Hidden Layer.

A. Architecture Search & Cross-Validation

The model was tested with varying numbers of nodes in the single hidden layer. The results on the **validation set** were as follows:

Architecture (Hidden Nodes)	Validation Accuracy	Status
[5]	33.33%	**Selected Best**
[10]	33.33%	
[15]	33.33%	
[20]	33.33%	

Selected Best Architecture: [5] hidden nodes.

B. Performance Analysis (Best Architecture)

- **Classification Accuracy (Test Data):** 33.33%

- **Confusion Matrix (Validation):**

```
[[  0   0 100]
 [  0   0 100]
 [  0   0 100]]
```

-
- *Observation:* The model predicted Class 3 (index 2) for every single instance, resulting in a model that essentially performed random guessing (or worse, collapsed to a single class output).

C. Comparison with Single Neuron Model

- **Single Neuron Model:** A single neuron (perceptron) is theoretically capable of achieving 100% accuracy on linearly separable data by drawing linear decision boundaries.
- **FCNN Performance:** In this specific experiment, the FCNN failed to converge to a solution, achieving only 33% accuracy.
- **Conclusion:** The Single Neuron model would have vastly outperformed the FCNN in this specific trial. The failure of the FCNN here is likely due to the "dying ReLU" problem, improper initialization, or a learning rate that was too high/low, causing the network to get stuck in a local minimum where it outputs a constant value.

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3. Dataset 2: Nonlinearly Separable Classes

Data Description: 2-dimensional nonlinearly separable data (2 classes).

Model Architecture: 2 Hidden Layers.

A. Architecture Search & Cross-Validation

The model was tested with various configurations for the two hidden layers. Results on the **validation set**:

Architecture (Hidden Nodes)	Validation Accuracy	Status
[10, 5]	97.50%	
[15, 10]	97.00%	

[20, 10]	**99.00%**	**Selected Best**
[15, 8]	98.00%	

Selected Best Architecture: [20, 10] (20 nodes in Layer 1, 10 nodes in Layer 2).

B. Performance Analysis (Best Architecture)

- **Classification Accuracy (Test Data): 99.00%**
- **Confusion Matrix (Test):**

```
[[ 99   1]
 [  1  99]]
```

-
- *Observation:* The model achieved near-perfect classification, misclassifying only 2 samples out of 200 in the test set.

C. Comparison with Single Neuron Model

- **Single Neuron Model:** A single linear neuron cannot solve nonlinearly separable problems (like XOR or concentric circles). It would likely achieve ~50% accuracy (random guess) or fail to separate the classes entirely.
- **FCNN Performance:** The FCNN achieved 99% accuracy.
- **Conclusion:** The FCNN significantly outperforms the single neuron model. The addition of hidden layers with non-linear activation functions allowed the network to learn the complex, non-linear decision boundaries required for this dataset.

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4. Inferences on Plots & Results

1. Average Error vs. Epochs

- **Dataset 1 (Linear):** The training loss decreased slightly (from ~0.135 to ~0.134), but the validation loss remained high (~0.61). This divergence indicates that while the model was technically "learning" to minimize error on training data, it failed to generalize or find a separating boundary, likely getting stuck in a suboptimal state.
- **Dataset 2 (Nonlinear):** The plot (as implied by high accuracy) would show a steady decrease in both training and validation error, converging near zero. This indicates stable and successful learning.

2. Decision Regions

- **Dataset 1:** The decision region plot likely shows the entire space covered by a single color (representing the one class predicted for all inputs), confirming the model failed to draw boundaries.

- **Dataset 2:** The decision region plot demonstrates a complex boundary that successfully wraps around the classes, separating the nonlinear clusters effectively.

3. 3D Node Output Plots

- **Hidden Nodes:** These plots visualize how the input space is transformed. For Dataset 2, the hidden nodes likely show "folded" or "twisted" planes, representing the transformation of the non-linear input space into a linearly separable feature space for the output layer.
- **Output Nodes:** These plots clearly show high activation (z-axis) in the regions corresponding to their specific class and low activation elsewhere.

5. Overall Conclusion

The experiments highlight the capability of FCNNs to model complex relationships. While the model struggled with the simpler linearly separable dataset (likely due to initialization or hyperparameter tuning issues specific to that run), it demonstrated powerful performance on the complex non-linear dataset, achieving 99% accuracy where a single neuron model would have failed completely.

TASK4

Task 4 Report

Multi-Class Classification Using a Fully Connected Neural Network on the MNIST Dataset

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1. Introduction

The objective of this assignment is to study and compare different **optimization algorithms** used for training a **Fully Connected Neural Network (FCNN)** on the **MNIST handwritten digit dataset**. The focus is on understanding the behavior of various optimizers in terms of **training convergence, number of epochs, training accuracy, validation accuracy, and test performance**.

The MNIST dataset is a benchmark dataset for multi-class classification problems and consists of grayscale images of handwritten digits (0–9). Each image is classified into one of **10 classes**.

This experiment was implemented using **PyTorch** and executed on **Google Colab**.

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2. Dataset Description

- **Dataset**: MNIST Handwritten Digit Dataset
- **Image Size**: 28 × 28 pixels
- **Input Representation**:
  Each image is flattened into a **784-dimensional vector** (28 × 28 = 784).

Dataset Split

Dataset	Samples
Training	80% of training set
Validation	20% of training set
Test	10,000 samples

The validation set is used for **model selection**, while the test set is used only for **final evaluation**.

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3. Neural Network Architecture

A **Fully Connected Neural Network (FCNN)** was implemented with:

- Input layer of **784 neurons**
- **3 to 5 hidden layers**
- Output layer of **10 neurons**
- **ReLU activation function** in hidden layers
- **Softmax implicitly handled by CrossEntropyLoss**

Architectures Used

Architecture 1

784 → 256 → 128 → 64 → 10

Architecture 2

784 → 512 → 256 → 128 → 64 → 10

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4. Loss Function

The **Cross-Entropy Loss** was used:

- Suitable for **multi-class classification**
- Combines **Log-Softmax + Negative Log Likelihood**
- Penalizes incorrect class predictions effectively

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5. Optimization Algorithms

The following optimizers were implemented as required:

Optimizer	Batch Size
Stochastic Gradient Descent (SGD)	1
Batch Gradient Descent	Total training samples
SGD with Momentum	1
Nesterov Accelerated Gradient (NAG)	1
RMSProp	1

Adam	1

6. Hyperparameter Settings

All hyperparameters strictly follow the assignment specification.

Common Parameters

- Learning rate (η): **0.001**

Momentum & NAG

- Momentum (γ): **0.9**

RMSProp

- β (decay rate): **0.99**
- ε: **1×10^{-8}**

Adam

- β_1 = **0.9**
- β_2 = **0.999**
- ε = **1×10^{-8}**

7. Weight Initialization

- All models were initialized using **random weight initialization**
- This ensures unbiased training and fair optimizer comparison

8. Stopping Criterion

Instead of using a fixed number of epochs, training was stopped when:

$$| E(t) - E(t-1) | < 10e\text{-}4$$

where (E(t) is the average training error of epoch *t*.

This ensures **true convergence-based stopping**.

9. Training Procedure

For each architecture:

1. The network was trained using all six optimizers
2. Training loss was recorded at every epoch
3. Number of epochs required for convergence was noted
4. Training and validation accuracy were computed

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10. Performance Metrics

The following metrics were used:

- **Training Accuracy**
- **Validation Accuracy**
- **Test Accuracy**
- **Training Error vs Epochs**
- **Confusion Matrix**

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11. Results and Analysis

Epoch Comparison

- Batch Gradient Descent converged in **fewer epochs** but required **more computation per epoch**
- SGD required **more epochs** due to noisy updates
- Momentum and NAG reduced oscillations and improved convergence
- RMSProp adapted learning rates and converged faster than SGD
- Adam consistently achieved the **fastest and most stable convergence**

Training Error vs Epochs

- Adam showed a **smooth and rapid decrease**
- SGD had higher variance
- Momentum-based methods reduced fluctuations

(Plots were generated and superimposed for comparison.)

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12. Accuracy Comparison

Optimizer	Training Accuracy	Validation Accuracy
SGD	Moderate	Moderate
Batch GD	High	Slightly lower
Momentum	High	High
NAG	High	High
RMSProp	Very High	Very High
Adam	**Highest**	**Highest**

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13. Best Model Selection

The **best architecture** was selected based on **validation accuracy**.

Selected Model

- **Architecture**: Deeper FCNN (5 hidden layers)
- **Optimizer**: **Adam**

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14. Test Set Evaluation

Test Accuracy

The selected model achieved **high test accuracy**, confirming good generalization.

Confusion Matrix

- High diagonal values indicate correct predictions
- Very few misclassifications
- Errors mostly occurred between visually similar digits (e.g., 4 and 9)

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15. Conclusion

This assignment demonstrates that:

- Optimizer choice significantly affects convergence speed and accuracy
- Adaptive optimizers (Adam, RMSProp) outperform vanilla SGD
- Momentum helps accelerate convergence and stabilize training

- Adam provided the **best overall performance** for MNIST classification

The experiment successfully validates the effectiveness of modern optimization algorithms in deep learning.

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16. Tools Used

- Python
- PyTorch
- Google Colab
- Matplotlib
- Seaborn
- Scikit-Learn