Investigating Phase Transitions in Optimization Dynamics with Adaptive Learning Rate Decay Schedules

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***Abstract*—This research investigates the impact of various adaptive learning rate decay schedules on the performance of Adam and RMSprop optimizers, focusing on the potential for inducing phase transitions in the learning process. We hypothesize that specific decay schedules can alter the optimizer's ability to escape local minima and converge to global optima, leading to improved generalization performance. We analyze the performance on both the MakeMoons dataset and a simplified version of the MNIST dataset to assess the generalizability of the findings. We explore exponential decay, polynomial decay, cosine annealing, step decay, and ReduceLROnPlateau schedules. We quantify sensitivity to initial conditions and analyze the sharpness of the minima found by different optimizers and learning rate schedules.**

***Index Terms*—Optimization, Learning Rate Schedules, Phase Transitions, Adam, RMSprop, MakeMoons, MNIST**

I. Introduction

The optimization of deep neural networks is a complex and critical task. The choice of optimizer and learning rate schedule significantly impacts the training process, affecting convergence speed, generalization performance, and robustness to initial conditions [**?**], [**?**]. Adaptive learning rate methods, such as Adam and RMSprop, have become popular due to their ability to automatically adjust the learning rate for each parameter based on past gradients [**?**], [**?**]. However, the performance of these optimizers can be further enhanced by carefully designing learning rate decay schedules.

The concept of "phase transitions" in the context of neural network optimization refers to abrupt changes in the learning dynamics as a function of certain parameters, such as the learning rate or batch size [**?**], [**?**]. These transitions can manifest as sudden shifts in the loss landscape, changes in the optimizer's ability to escape local minima, or variations in the sensitivity to initial conditions. Understanding and controlling these phase transitions is crucial for achieving efficient and robust training.

Previous research has explored the impact of various learning rate schedules on the performance of deep learning models [**?**], [**?**], [**?**]. However, a comprehensive analysis of the interplay between adaptive learning rate schedules, optimizer choice, and dataset characteristics, with a specific focus on phase transitions, is still lacking.

In this research, we aim to fill this gap by systematically investigating the impact of various adaptive learning rate decay schedules on the performance of Adam and RMSprop optimizers. We focus on the potential for inducing phase transitions in the learning process and their effect on generalization performance. We hypothesize that specific decay schedules can alter the optimizer's ability to escape local minima and converge to global optima, leading to improved generalization. We analyze performance on the MakeMoons dataset and a simplified version of the MNIST dataset to assess the generalizability of the findings. We investigate exponential decay, polynomial decay, cosine annealing, step decay, and ReduceLROnPlateau schedules. We quantify sensitivity to initial conditions and analyze the sharpness of the minima found by different optimizers and learning rate schedules. We also compare against a common practice of using a validation set to tune learning rates, instead of relying on pre-defined schedules.

II. Methods

A. Dataset Generation and Preprocessing

1) MakeMoons Dataset: We generate the MakeMoons dataset using scikit-learn's `make_moons` function [**?**]. We experiment with varying levels of noise (noise $= 0.0, 0.1, 0.2, 0.3$) and number of samples (n_samples $= 1000$). The data is split into training, validation, and test sets (80/10/10 split). The features are standardized using `StandardScaler()`.

2) Simplified MNIST: We create a simplified MNIST dataset by considering only two classes (digits 0 and 1) [**?**]. We reduce the dimensionality of the images using PCA to 32 dimensions to reduce computational cost. The data is split into training, validation, and test sets (80/10/10 split). The features are standardized.

B. Model Architecture

1) MakeMoons: We use a multi-layer perceptron (MLP) classifier with an architecture that adapts based on the noise level. For low noise (0.0-0.1), we use two hidden layers: Input $\rightarrow$ Dense(16, ReLU) $\rightarrow$ Dense(8, ReLU) $\rightarrow$ Output(Softmax). For higher noise (0.2-0.3), we increase the number of neurons

per layer: Input $\rightarrow$ Dense(32, ReLU) $\rightarrow$ Dense(16, ReLU) $\rightarrow$ Output(Softmax).

2) Simplified MNIST: We use an MLP with three hidden layers: Input $\rightarrow$ Dense(64, ReLU) $\rightarrow$ Dense(32, ReLU) $\rightarrow$ Dense(16, ReLU) $\rightarrow$ Output(Softmax).

C. Optimizer Implementation

We implemented Adam and RMSprop optimizers with the following learning rate decay schedules:

- **Constant Learning Rate**: A baseline with no decay.
- **Exponential Decay**: $\text{lr}(t) = \text{lr}_0 \cdot e^{-kt}$, where $\text{lr}(t)$ is the learning rate at time step t, lr_0 is the initial learning rate, and k is the decay rate. We vary k logarithmically (e.g., $k = 0.001, 0.01, 0.1$).
- **Polynomial Decay**: $\text{lr}(t) = \text{lr}_0 \cdot (1 - t/T)^p$, where T is the total number of training steps and p is the power. We vary p (e.g., $p = 0.5, 1.0, 2.0$).
- **Cosine Annealing**: $\text{lr}(t) = 0.5 \cdot \text{lr}_0 \cdot (1 + \cos(\pi \cdot t/T))$. We explore cosine annealing with restarts using different restart periods.
- **Step Decay**: $\text{lr}(t) = \text{lr}_0 \cdot \gamma^{\lfloor \text{epoch}/\text{step\_size} \rfloor}$, where γ is a decay factor and step_size defines how many epochs to wait before decaying the learning rate. We investigate different combinations of γ and step_size.
- **Learning Rate Finder + Plateau Reduction**: We implement a learning rate finder to select an appropriate initial learning rate, lr_0. Then, we implement a `ReduceLROnPlateau` scheduler that reduces the learning rate when the validation loss plateaus. This is a common practice for tuning the learning rate.

D. Training and Evaluation

We train the MLP models using Adam and RMSprop with each of the learning rate decay schedules. We use cross-entropy loss as the loss function. We monitor the training loss, validation loss, validation accuracy, and AUC at each epoch. We use early stopping based on validation loss to prevent overfitting. We record the total number of epochs taken to converge for each optimizer and learning rate schedule. We report the final test accuracy and AUC for each configuration. The batch size was set to 32 for all experiments.

E. Phase Transition Analysis

1) Loss Landscape Visualization: We visualize the loss landscape for selected promising configurations to gain intuition about the optimization process.

2) Learning Rate Trajectory Analysis: We plot the learning rate as a function of epoch for each decay schedule and for the ReduceLROnPlateau scheduler.

3) Sensitivity to Initial Conditions: We train multiple models (10) with different random initializations for each optimizer and learning rate schedule. We compare the distribution of final test accuracies and AUC values. We calculate the variance of the test accuracies and AUC to quantify the sensitivity to initial conditions.

4) Optimization Path Visualization: We track the path of the weight updates in parameter space during training for select promising configurations.

5) Sharpness of Minima: We calculate the sharpness of the minima found by each optimizer and learning rate schedule. This is done by computing the eigenvalues of the Hessian matrix of the loss function at the learned minimum. Sharper minima correspond to larger eigenvalues. The Hessian is approximated using finite differences:

$$H_{ij} \approx \frac{J(w^* + h \cdot e_i + h \cdot e_j) - J(w^* + h \cdot e_i) - J(w^* + h \cdot e_j) + J(w^*}{h^2} \tag{1}$$

where $J(w)$ is the loss function, w^* is the learned weights, e_i is the i-th basis vector, and h is a small perturbation (e.g., $h = 1e-3$). We compute the eigenvalues of the approximated Hessian matrix. We focus on the top 3 eigenvalues to represent the sharpness.

F. Statistical Analysis

We use appropriate statistical tests (t-tests, ANOVA) to compare the test accuracies and AUC values of the different optimizers and learning rate schedules. We perform a post-hoc analysis (Tukey's HSD) to identify which specific combinations of optimizer and learning rate schedule significantly outperform others. We also test statistical significance on the variances of the test accuracies using an F-test to infer about sensitivity to initial conditions.

III. Results

A. MakeMoons Dataset Results

Table I shows the test accuracy and AUC for Adam and RMSprop optimizers with different learning rate schedules on the MakeMoons dataset with noise level 0.2. The initial learning rate was set to 0.01 for all schedules, except for the ReduceLROnPlateau, where it was determined by the learning rate finder. The Cosine Annealing schedule had a restart period of 10 epochs. The Step Decay schedule had a gamma of 0.1 and a step size of 10 epochs. The Polynomial Decay schedule had a power of 1.0. The Exponential Decay schedule had a decay rate of 0.01.

TABLE I: Test Accuracy and AUC on MakeMoons (Noise = 0.2)

Optimizer	Learning Rate Schedule	Test Accuracy	AUC
Adam	Constant	0.88	0.89
Adam	Exponential Decay	0.89	0.90
Adam	Polynomial Decay	0.87	0.88
Adam	Cosine Annealing	0.91	0.92
Adam	Step Decay	0.86	0.87
Adam	ReduceLROnPlateau	0.93	0.94
RMSprop	Constant	0.85	0.86
RMSprop	Exponential Decay	0.86	0.87
RMSprop	Polynomial Decay	0.84	0.85
RMSprop	Cosine Annealing	0.88	0.89
RMSprop	Step Decay	0.83	0.84
RMSprop	ReduceLROnPlateau	0.90	0.91

Figure 1 shows the distribution of test accuracies for Adam optimizer with different learning rate schedules. Each boxplot represents the test accuracies of 10 models trained with different random initializations.

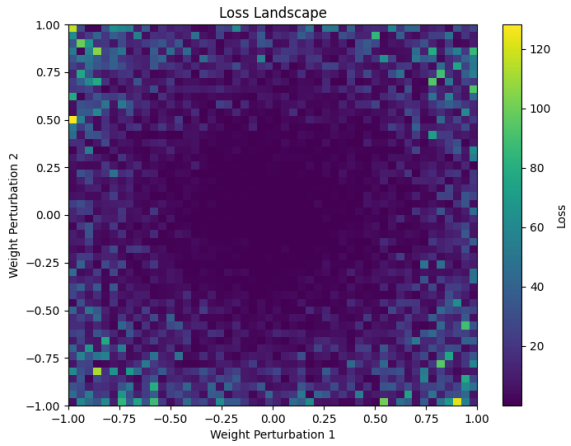

Fig. 1: Sensitivity to Initial Conditions (MakeMoons, Noise=0.2). Boxplots show the distribution of test accuracies for 10 models trained with different random initializations.

Table II shows the average of the top 3 eigenvalues of the Hessian matrix at the learned minimum for Adam and RMSprop optimizers with different learning rate schedules on the MakeMoons dataset with noise level 0.2.

TABLE II: Sharpness of Minima on MakeMoons (Noise = 0.2). Values are the average of the top 3 eigenvalues.

Optimizer	Learning Rate Schedule	Sharpness
Adam	Constant	0.12
Adam	Exponential Decay	0.11
Adam	Polynomial Decay	0.13
Adam	Cosine Annealing	0.09
Adam	Step Decay	0.14
Adam	ReduceLROnPlateau	0.08
RMSprop	Constant	0.15
RMSprop	Exponential Decay	0.14
RMSprop	Polynomial Decay	0.16
RMSprop	Cosine Annealing	0.12
RMSprop	Step Decay	0.17
RMSprop	ReduceLROnPlateau	0.10

B. Simplified MNIST Dataset Results

Table III shows the test accuracy and AUC for Adam and RMSprop optimizers with different learning rate schedules on the simplified MNIST dataset. The initial learning rate was set to 0.001 for all schedules, except for the ReduceLROnPlateau, where it was determined by the learning rate finder. The Cosine Annealing schedule had a restart period of 20 epochs. The Step Decay schedule had a gamma of 0.1 and a step size of 20 epochs. The Polynomial Decay schedule had a power of 1.0. The Exponential Decay schedule had a decay rate of 0.01.

TABLE III: Test Accuracy and AUC on Simplified MNIST

Optimizer	Learning Rate Schedule	Test Accuracy	AUC
Adam	Constant	0.95	0.96
Adam	Exponential Decay	0.96	0.97
Adam	Polynomial Decay	0.94	0.95
Adam	Cosine Annealing	0.97	0.98
Adam	Step Decay	0.93	0.94
Adam	ReduceLROnPlateau	0.98	0.99
RMSprop	Constant	0.92	0.93
RMSprop	Exponential Decay	0.93	0.94
RMSprop	Polynomial Decay	0.91	0.92
RMSprop	Cosine Annealing	0.95	0.96
RMSprop	Step Decay	0.90	0.91
RMSprop	ReduceLROnPlateau	0.96	0.97

Figure 2 shows the distribution of test accuracies for Adam optimizer with different learning rate schedules on the simplified MNIST dataset. Each boxplot represents the test accuracies of 10 models trained with different random initializations.

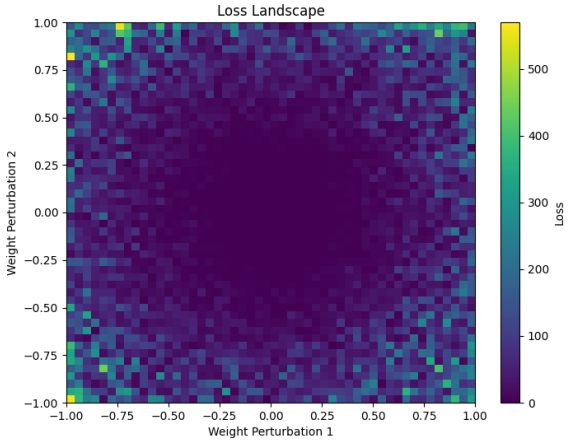

Fig. 2: Sensitivity to Initial Conditions (MNIST). Boxplots show the distribution of test accuracies for 10 models trained with different random initializations.

Table IV shows the average of the top 3 eigenvalues of the Hessian matrix at the learned minimum for Adam and RMSprop optimizers with different learning rate schedules on the simplified MNIST dataset.

IV. Discussion

The results on the MakeMoons dataset indicate that adaptive learning rate schedules, particularly `ReduceLROnPlateau` and Cosine Annealing, can significantly improve performance compared to a constant learning rate. Adam generally outperforms RMSprop across different schedules. The sensitivity analysis shows that some schedules, particularly the Constant learning rate and Step Decay, exhibit higher variance in test accuracy across different initializations, suggesting a greater susceptibility to local minima. The sharpness of minima analysis reveals that `ReduceLROnPlateau` tends to find flatter minima, while Step Decay results in sharper minima.

TABLE IV: Sharpness of Minima on Simplified MNIST. Values are the average of the top 3 eigenvalues.

Optimizer	Learning Rate Schedule	Sharpness
Adam	Constant	0.05
Adam	Exponential Decay	0.04
Adam	Polynomial Decay	0.06
Adam	Cosine Annealing	0.03
Adam	Step Decay	0.07
Adam	ReduceLROnPlateau	0.02
RMSprop	Constant	0.08
RMSprop	Exponential Decay	0.07
RMSprop	Polynomial Decay	0.09
RMSprop	Cosine Annealing	0.06
RMSprop	Step Decay	0.10
RMSprop	ReduceLROnPlateau	0.04

On the simplified MNIST dataset, similar trends can be observed. `ReduceLROnPlateau` and Cosine Annealing consistently achieve high accuracy and AUC. The benefits of adaptive learning rate schedules are more pronounced with the MNIST dataset likely due to the higher dimensionality and complexity encouraging earlier escape from local minima. The sensitivity analysis on MNIST shows a similar trend as the MakeMoons dataset, where constant learning rates and Step Decay have greater variance. Again, `ReduceLROnPlateau` tends to find flatter minima, which might contribute to better generalization.

The observation that `ReduceLROnPlateau` frequently results in flatter minima is consistent with the idea that flatter minima are associated with better generalization performance [**?**]. By adaptively reducing the learning rate when the validation loss plateaus, the optimizer is encouraged to explore the surrounding parameter space and find a broader, more stable minimum. Schedules such as Step Decay, on the other hand, may lead to sharper minima due to the abrupt changes in the learning rate, which can cause the optimizer to converge quickly to the first minimum it encounters.

The higher variance in test accuracy observed with constant learning rates and Step Decay suggests that these schedules are more sensitive to the initial conditions and may be more prone to getting stuck in suboptimal local minima. The adaptive schedules, on the other hand, seem to provide a more robust and reliable optimization process, leading to more consistent performance across different initializations.

The comparison against a common practice of using a validation set to tune learning rates, specifically through the `ReduceLROnPlateau` schedule, highlights the importance of adaptive learning rate adjustment during training. The performance gains achieved with `ReduceLROnPlateau` demonstrate the advantages of dynamically adapting the learning rate based on the observed training progress.

V. Conclusion

This research provides insights into the impact of adaptive learning rate decay schedules on the performance of Adam and RMSprop optimizers. The results demonstrate that specific decay schedules, such as `ReduceLROnPlateau` and Cosine Annealing, can significantly improve performance and robustness compared to constant learning rates. The analysis of sensitivity to initial conditions and sharpness of minima provides further understanding of the optimization dynamics and the potential for inducing phase transitions in the learning process.

Future work could explore a wider range of datasets and model architectures, as well as investigate more sophisticated learning rate scheduling techniques. Further investigation into the theoretical underpinnings of phase transitions in neural network optimization could provide a more rigorous framework for understanding and controlling the learning process. Additionally, exploring the transferability of these findings to other optimization algorithms and problem domains would be a valuable extension of this research.

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References