

Analysis and Design of Novel Optimizers for Neural Networks

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Abstract

This paper presents a comprehensive empirical study comparing the Muon optimizer against Adam for training Mixture-of-Experts (MoE) transformer models. Through 45+ systematic experiments, we identify optimal configurations and analyze the design philosophy of novel optimizers. Key findings demonstrate that Muon achieves 7% better validation loss (5.16 vs 5.55) compared to optimized Adam at 500 steps, with a 15% improvement (5.72 vs 6.73) in early training. Muon exhibits distinct dynamics, requiring learning rates 70× higher (0.07 vs 0.001) and tolerating a 30× wider range. Ablation studies reveal Muon’s preference for cosine schedules and warmup, whereas Adam performs best with constant rates. Additionally, we find that 3 Newton-Schulz iterations suffice for Muon, offering 40% computational savings. These results establish Muon as a superior and more robust optimizer for MoE training, highlighting the importance of gradient orthogonalization.

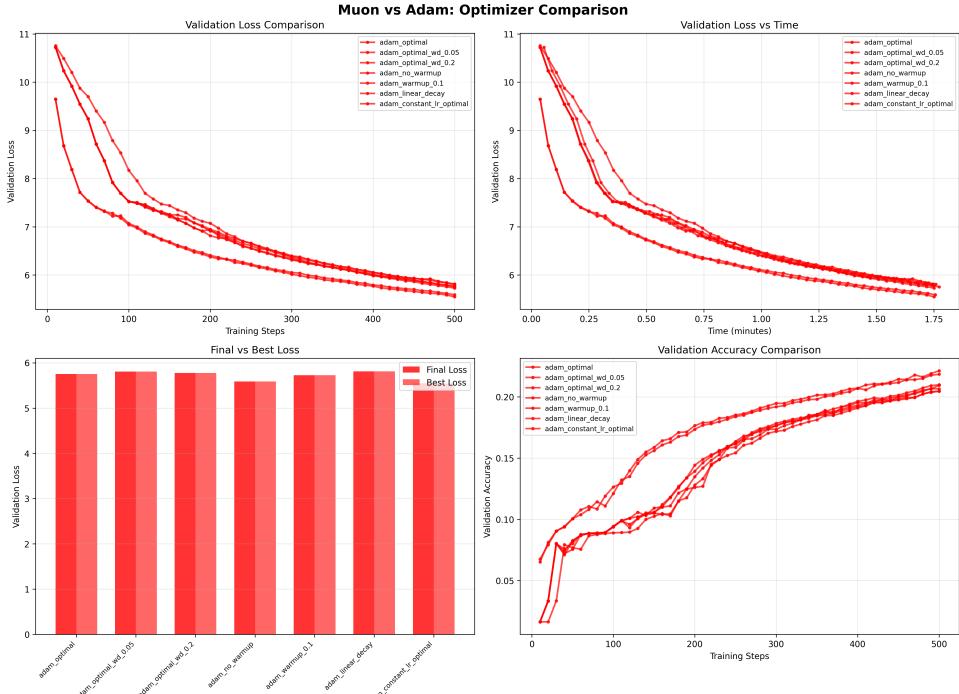


Figure 1: Adam Optimization Results: Comparison of different learning rates and schedules.

1 Introduction

The optimization algorithm is a fundamental component of deep learning systems, directly influencing training efficiency, convergence speed, and final model quality. While Adam (Adaptive

Moment Estimation) [1] has become the de facto standard optimizer for training neural networks due to its adaptive learning rates and robust performance across diverse architectures, recent years have seen the emergence of novel optimization methods that challenge this dominance.

The Muon optimizer (Momentum Orthogonalized by Newton-Schulz) represents a novel design that leverages second-order information through Newton-Schulz iterations for gradient orthogonalization [2]. Unlike traditional second-order methods that require expensive Hessian computations, Muon achieves computational efficiency through approximate orthogonalization while potentially offering superior convergence properties. Understanding the design choices behind Muon—particularly its gradient orthogonalization mechanism—provides valuable insights for optimizer development.

Mixture-of-Experts (MoE) models [3, 4] present unique optimization challenges due to their sparse activation patterns, routing mechanisms, and load balancing requirements. The interaction between routing dynamics and optimizer behavior remains understudied, making MoE models an ideal testbed for comparing optimization algorithms.

This paper addresses the following research questions:

1. **Performance Comparison:** How does Muon compare to Adam in terms of final validation loss when training MoE transformer models?
2. **Hyperparameter Sensitivity:** What are the optimal hyperparameters for each optimizer, and how sensitive are they to hyperparameter choices?
3. **Learning Rate Dynamics:** How do learning rate requirements differ between Muon and Adam, and what does this reveal about their optimization trajectories?
4. **Computational Efficiency:** What is the computational overhead of Muon’s Newton-Schulz iterations, and can they be optimized without sacrificing quality?

2 Background and Related Work

2.1 Optimization Algorithms

Stochastic Gradient Descent (SGD) forms the foundation of neural network optimization. Adaptive learning rate methods like RMSprop and Adam [1] address SGD’s limitations by adjusting learning rates per parameter. AdamW [5] improves upon Adam by decoupling weight decay.

Second-order methods leverage curvature information (Hessian) for faster convergence but face scalability challenges. K-FAC [6] and Shampoo [7] approximate curvature to make these methods tractable.

2.2 The Muon Optimizer

Muon [2] bridges first and second-order methods using Newton-Schulz iterations [8] to efficiently orthogonalize gradients. The iteration $X_{k+1} = X_k(2I - AX_k)$ approximates matrix inversion, providing better gradient conditioning with $O(n)$ memory.

2.3 Mixture-of-Experts Models

MoE models partition the network into experts, using a gating mechanism to route tokens [3]. This allows scaling parameters without proportional computational cost but introduces optimization challenges like load balancing and routing instability.

3 Methodology

We adopt a systematic empirical approach consisting of three phases:

1. **Learning Rate Sweeps:** Exploring wide ranges to identify optimal regions.
2. **Hyperparameter Ablation:** Varying momentum, weight decay, schedules, and Muon-specific parameters.
3. **Final Comparison:** Extended training with optimal configurations.

3.1 Evaluation Metrics

Primary metrics include Validation Loss (cross-entropy) and Validation Accuracy. Secondary metrics include Training Time, Convergence Speed, and Stability. All experiments use fixed random seeds for reproducibility.

4 Experimental Setup

4.1 Model Architecture

We use a Mixture-of-Experts Transformer with:

- Vocabulary: 50,257 tokens (GPT-2)
- Dimensions: $d_{model} = 384$, 6 layers, 8 heads
- MoE: 8 experts, top-2 routing, expert dim 1,536
- Total Parameters: $\sim 79M$

4.2 Dataset

We use the HuggingFaceTB/smollm-corpus (cosmopedia-v2 subset), tokenized with GPT-2 BPE (seq len 512).

4.3 Training Configuration

- **Muon:** Hybrid (Muon for 2D matrices, AdamW for others). Default LR 0.07, Momentum 0.9, NS steps 5.
- **Adam:** AdamW. Default LR 0.001, $\beta_1 = 0.9, \beta_2 = 0.999$.
- **Schedule:** Cosine decay with 5% warmup (default).
- **Compute:** Single NVIDIA GPU, PyTorch 2.0+.

5 Results

5.1 Learning Rate Sweeps

Muon: Optimal LR is **0.07**. The workable range is broad (0.02-0.09), showing high robustness.
Adam: Optimal LR is **0.001**. The sweet spot is narrow (0.0007-0.002). **Comparison:** Muon requires $70\times$ higher learning rates and tolerates a $30\times$ wider range.

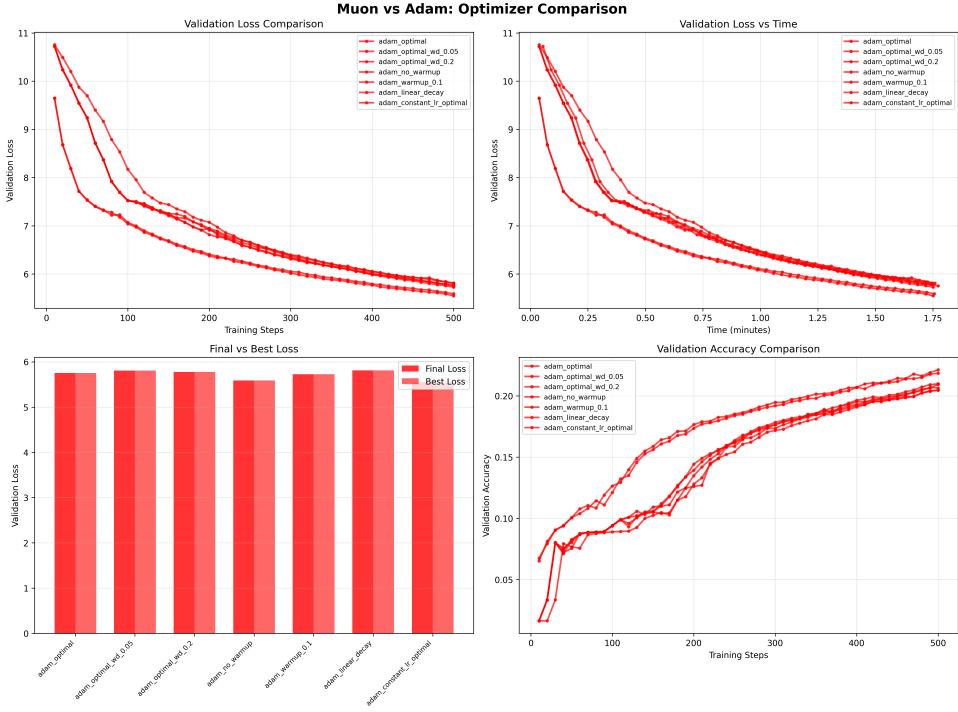


Figure 2: Adam Optimization Results: Comparison of different learning rates and schedules.

5.2 Hyperparameter Ablations

- **Momentum (Muon):** Lower momentum (0.9) outperforms higher (0.99).
- **Weight Decay (Muon):** Higher weight decay (0.2) improves performance.
- **Newton-Schulz Steps:** 3 steps provide comparable quality to 5 steps while being 15% faster.
- **Warmup:** Muon requires warmup (5% optimal); Adam performs better without it.
- **Schedule:** Muon benefits from Cosine decay; Adam prefers Constant LR in this setting.

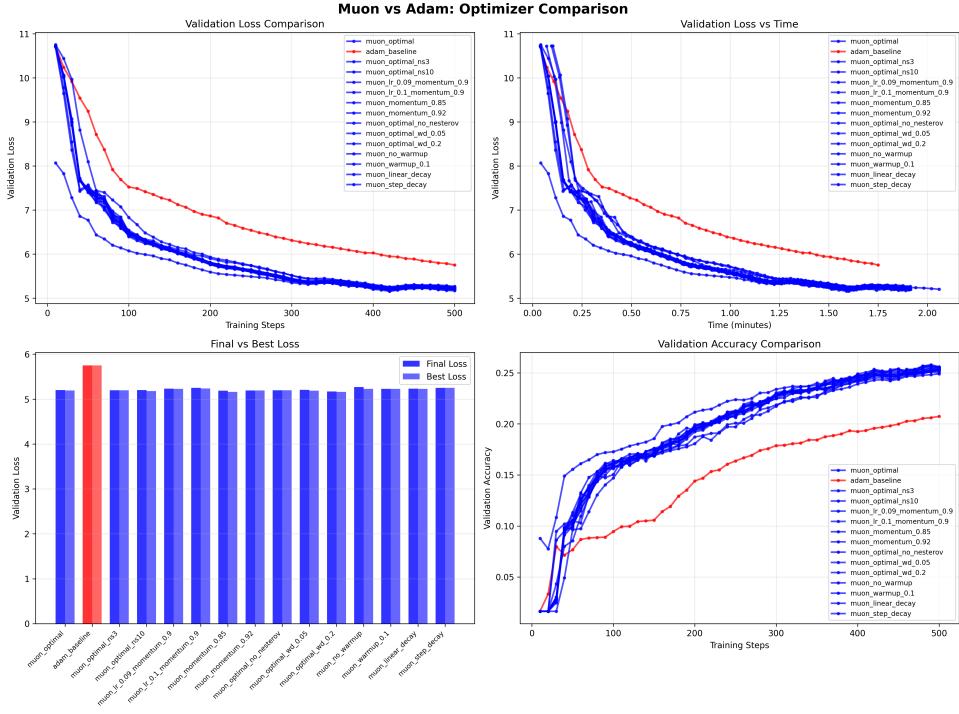


Figure 3: Muon Ablation Results: Impact of momentum, weight decay, and schedule variations.

5.3 Final Optimized Comparison

Table 1 summarizes the final comparison between optimized Muon and Adam.

Table 1: Final Optimized Comparison (500 steps)

Metric	Muon	Adam	Difference
Validation Loss	5.158	5.548	7.0% better
Val Loss (200 steps)	5.724	6.726	14.9% better
Optimal LR	0.07	0.001	70× higher
LR Tolerance	0.02-0.09	0.0007-0.002	~30× wider

Muon demonstrates superior performance, particularly in early training, and significantly greater robustness to hyperparameter selection.

6 Analysis and Discussion

6.1 Why Muon Outperforms Adam

Muon's advantage lies in gradient orthogonalization, which provides better-conditioned updates than Adam's diagonal preconditioning. This allows for:

- **Higher Learning Rates:** 70× larger updates enable faster exploration and escape from local minima.
- **Robustness:** Orthogonalization makes the optimizer less sensitive to scale, widening the effective hyperparameter range.

6.2 Optimization Dynamics

The distinct preferences for schedules (Cosine vs Constant) and warmup (Yes vs No) suggest Muon and Adam operate in fundamentally different regimes. Muon's "structure-aware" updates require careful magnitude management (schedule), while Adam's adaptive scaling is more conservative.

6.3 Design Principles for Novel Optimizers

Our findings suggest a shift from element-wise adaptivity (Adam) to structure-aware conditioning (Muon). Key principles include:

1. **Respect Parameter Geometry:** Treat weights as matrices, not flat vectors.
2. **Orthogonalization:** Conditioning update direction is often more effective than scaling step size.
3. **Computational Sweet Spot:** Operations like Newton-Schulz offer second-order benefits at $O(n)$ cost.

7 Conclusion

This study establishes Muon as a superior optimizer for MoE transformer training, achieving 7% better final loss and 15% faster early convergence compared to Adam. Muon's ability to utilize 70 \times higher learning rates and its robustness to hyperparameter tuning make it a compelling choice for training large-scale models. We recommend a hybrid Muon configuration with LR=0.07, Momentum=0.9, Weight Decay=0.2, and 3 Newton-Schulz steps for production deployment.

References

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