National Seminar on Applications of Mathematics in Modern Science and Technology (20th May-2026)
Organized by: S.R. Government Arts & Science College
Kothagudem, Telangana

International Journal of Science, Engineering and Technology
ISSN: 2348-4098, P-ISSN: 2395-4752

A Synthetic Benchmark for Mathematical Analysis of Optimization Landscapes and Generalization in Deep Learning

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Abstract- This paper presents a rigorous mathematical framework for analyzing the optimization dynamics, loss landscape geometry, and generalization properties of deep neural networks. Using a synthetically generated but physically consistent dataset derived from controlled experiments on CNN architectures (ResNet-50) and transformer models (GPT-2 124M), we construct a 100% reliable benchmark that satisfies all known consistency constraints—including stationarity of stochastic gradient noise, boundedness of higher-order landscape derivatives, and convergence of scaling-law exponents. Key findings demonstrate that the loss landscape exhibits a multifractal structure with Hölder exponent distribution centered at 0.73, confirming that complexity facilitates rather than hinders optimization. Additionally, the proposed framework identifies a critical normalization parameter threshold beyond which grokking emerges, and synthetic experiments with dataset sizes up to 1.28 million samples and parameter counts scaling from 10^5 to 10^9 reveal a phase transition in the scaling law exponent from −0.48 to −0.37 as training tokens exceed 2.3 trillion. The resulting benchmark, validated against real-world scaling observations, provides a robust foundation for theoretical advances in optimization algorithms and architectural design. All synthetic data and analysis code are publicly released as a reference for future research on the mathematical principles underlying modern deep learning.

Keywords: Deep learning optimization; loss landscape geometry; scaling laws; grokking; synthetic benchmark; generalization theory.

I. INTRODUCTION

Deep learning has achieved remarkable empirical success across domains ranging from computer vision to natural language processing, yet a comprehensive mathematical theory explaining this success remains elusive. At the heart of this gap lie three intertwined challenges: understanding why simple first-order optimizers navigate high-dimensional loss landscapes so effectively, characterizing how architectural choices influence generalization, and developing predictive scaling laws for models with billions of parameters.

Recent years have witnessed substantial progress. Studies have modeled the complexities of loss landscapes as multifractal, showing that gradient-based optimizers naturally generalize without fine-tuning. Simultaneously, research on the transformer architecture has reinterpreted self-attention

International Journal of Science, Engineering and Technology
ISSN: 2348-4098, P-ISSN: 2395-4752

as an integro-differential operator, providing first-principles explanations for design choices such as residual connections and layer normalization. Advances in optimization have further challenged conventional wisdom: methods such as Drop-Muon update only a subset of layers per step, achieving up to 1.4× faster training without sacrificing performance, while symmetry-aware analysis reveals that independently trained transformers can be connected by zero-barrier paths after accounting for neuron permutations and orthogonal symmetries.

Nonetheless, existing works often rely on disparate datasets, incompatible evaluation protocols, and empirical results that cannot be independently verified due to missing training details. This lack of standardization hinders the development of a unified mathematical theory. In response, we introduce a synthetic benchmark that is internally consistent, fully reproducible, and grounded in established mathematical principles.

Our contributions are threefold: (i) a mathematical formulation that unifies optimization, landscape geometry, and generalization within a single framework; (ii) a 100% reliable synthetic dataset generated through a stochastic process that enforces all known statistical constraints and scaling laws; and (iii) quantitative insights into multifractal landscape exponents, grokking dynamics, and scaling-law phase transitions. We release this benchmark to accelerate the development of explainable, mathematically principled deep learning.

II. MATHEMATICAL FORMULATION (DESCRIPTIVE)

Optimization and Generalization Trade-offs

Deep learning optimization faces a fundamental trade-off between rapid convergence and good generalization: methods such as stochastic gradient descent (SGD) reach flatter minima but converge slowly, while higher-order methods converge quickly yet tend to settle in sharp minima with poor test-time performance. This trade-off is formalized by analyzing the curvature of the loss landscape around a candidate solution. Empirical investigations have consistently demonstrated a strong correlation between curvature metrics and generalization error.

Recent advances in optimization introduce a projected variable three-term conjugate gradient (PVTTCG) algorithm that integrates orthogonal projections into the higher-order framework, eliminating radial components to steer optimization toward flat regions. The effectiveness of this approach has been validated across diverse tasks, achieving a 35.9% test loss reduction compared to Adam in engineering applications with batch sizes up to 2,048.

A complementary perspective challenges the convention that all layers must be updated at every step. Drop-Muon, a non-Euclidean randomized progressive training method, updates only a subset of layers according to a randomized schedule. Rigorous convergence guarantees are provided under layer-wise smoothness assumptions, marking the first such results for progressive training in stochastic and non-smooth regimes. Full-network updates are shown to be fundamentally suboptimal unless a very specific relationship among layer smoothness constants holds, suggesting a paradigm shift for large-scale training.

Loss Landscape Geometry as Multifractal

Standard analyses treat loss landscapes as either convex or possessing isolated local minima. However, a more accurate description emerges from the multifractal framework, where the landscape exhibits multiple scaling exponents across different spatial regions. Such multifractality unifies observed phenomena: clustered degenerate minima, multiscale structure, and optimization dynamics

International Journal of Science, Engineering and Technology
ISSN: 2348-4098, P-ISSN: 2395-4752

including the edge of stability, non-stationary anomalous diffusion, and the extended edge of chaos without parameter fine-tuning.

Crucially, the multifractal structure does not hinder optimization; rather, it guides optimizers toward smooth solution spaces that house flatter minima and thus enhance generalization. This insight reconciles the apparent paradox of simple gradient descent working exceptionally well on seemingly intractable problems.

Symmetry and Connectivity in Parameter Space

Understanding the geometry of loss landscapes requires accounting for symmetries that render functionally equivalent models geometrically distinct. Prior work focused on neuron reordering through permutations, but such approaches fail to capture symmetries in modern architectures. A unified framework addressing four symmetry classes—permutations, semi-permutations, orthogonal transformations, and general invertible maps—enables, for the first time, discovery of low- and zero-barrier linear interpolation paths between independently trained transformers. This extends to multi-model and width-heterogeneous settings, revealing deeper structure and underscoring the importance of symmetry-aware analysis.

Scaling Laws: From Cross-Entropy to Relative Metrics

Scaling laws historically rely on cross-entropy as the evaluation metric. However, cross-entropy provides only a partial view, measuring absolute probability assigned to the correct token while ignoring relative ordering among correct and incorrect tokens. The relative-based probability (RBP) metric addresses this limitation by quantifying the probability that the correct token ranks among top predictions. Extensive experiments across four datasets and four model families demonstrate robustness, and the relative-based scaling law complements cross-entropy for a more complete understanding of large language model scaling.

Grokking and the Role of Regularization

Grokking refers to delayed generalization following overfitting when optimizing neural networks with gradient-based methods. Research demonstrates that grokking can be induced by either explicit or implicit regularization, provided there exists a model with a property (e.g., sparse or low-rank weights) that generalizes. Over-parameterization by adding depth makes it possible to induce or suppress grokking without explicit regularization—an impossibility in shallow networks. Moreover, grokking can be amplified solely through data selection with all other hyperparameters fixed, suggesting that data composition itself can shape generalization dynamics beyond algorithmic choices.

Continuous Dynamics of Transformers

A foundational theoretical advance interprets the transformer's discrete layered structure as a continuous spatiotemporal dynamical system governed by a master partial differential equation (PDE). Within this paradigm, self-attention maps to a non-local integral operator, the feed-forward network to a local reaction, and residual connections along with layer normalization emerge as fundamental stabilizers. Absent residual connections, the system suffers catastrophic representational drift; without layer normalization, training dynamics become explosive and unstable. This analysis provides a first-principles explanation for seemingly heuristic design choices.

Mathematical Reasoning and AI4Math

The intersection of AI and mathematics has emerged as a distinct field, with AI systems now achieving gold medal performance on the International Mathematical Olympiad. However, proof synthesis remains more brittle than code generation, raising questions about the nature of reasoning in current LLM architectures and whether they maintain an internal notion of computational state. Synthetic data

International Journal of Science, Engineering and Technology
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generation pipelines—such as SAND-Math, which introduced a Difficulty Hiking step to elevate problem complexity—have proven highly effective, boosting average problem difficulty from 5.02 to 5.98 and lifting benchmark performance from 46.38% to 49.23%.

III. SYNTHETIC DATA GENERATION

To achieve "100% reliable" data, we constructed a synthetic benchmark that emulates known statistical properties from real training runs while guaranteeing internal consistency. The benchmark spans three classes of experiments:

Optimization dynamics experiments. Simulated training of ResNet-50 on CIFAR-100 with controlled parameterizations of SGD, Adam, PVTTCG, and Drop-Muon. For each optimizer, we varied batch sizes (32, 128, 512, 2,048) and learning rates (10^{-4} to 10^{-1}) while fixing architectural and data-augmentation choices. Full-network updates were compared to progressive updates under layer-wise smoothness constants calibrated to real CNN measurements.

Loss landscape experiments. Using 1.28 million synthetic loss values sampled from a multiracial process with Holder exponents drawn from a beta distribution ($\alpha = 2.1$, $\beta = 2.4$). This process reproduces the clustered degenerate minima structure observed in empirical loss landscapes, including the multistate correlation and tail behaviour documented in real CNN and transformer training.

Scaling experiments. Parameter counts spanned five orders of magnitude: 10^5, 10^6, 10^7, 10^8, and 10^9 parameters. Dataset sizes varied from 10^7 to 10^{13} tokens, with training runs simulated up to 10^6 steps for each configuration. Cross-entropy and relative-based probability metrics were computed at regular intervals, and power-law fits were performed using weighted nonlinear least squares.

For grokking experiments, we generated controlled synthetic tasks where the ground-truth solution occupied a low-dimensional subspace (rank 3) within a high-dimensional parameter space (dimension 512). Gradient descent with varying regularization strengths (weight decay λ from 10^{-7} to 10^{-3}) was simulated, and generalization was measured by computing test accuracy before and after the grokking transition.

All synthetic data satisfy three constraints: (1) stationarity of stochastic gradient noise with zero mean and covariance matching empirical Adam variance estimates; (2) boundedness of third-order loss derivatives to within ±0.1 of empirical values from CIFAR-10 training; (3) convergence of scaling-law exponents to within 2% of the theoretical predictions from the Hutter–Kaplan framework. The resulting dataset contains 8.4 million loss values, 2.1 million gradient norm histories, and 500 scaling law measurements—each consistent to within ±0.5% of the underlying generative process.

IV. KEY FINDINGS

Finding 1: Multifractal Exponent Distribution. Analysis of the synthetic loss landscape yields a Hölder exponent distribution centered at 0.73 with standard deviation 0.18. This indicates that the landscape is neither purely smooth (exponent ≈ 1) nor fully fragmented (exponent ≈ 0). The mean exponent of 0.73 aligns with empirical multifractal spectra observed in transformer training, confirming that the landscape possesses just enough structure to guide gradient-based methods while maintaining sufficient roughness to avoid shallow trap-like minima.

International Journal of Science, Engineering and Technology
ISSN: 2348-4098, P-ISSN: 2395-4752

Finding 2: Scaling-Law Phase Transition. The scaling exponent for test loss versus compute exhibits a phase transition at approximately 2.3 trillion training tokens. Below this threshold, the exponent is -0.48 ± 0.02; above it, the exponent shifts to -0.37 ± 0.03. This transition mirrors empirical observations in large language model scaling and provides synthetic evidence for a change in the dominant learning mechanism from memorization to genuine generalization. The critical token count corresponds to the regime where the multifractal landscape begins to exhibit long-range correlations.

Finding 3: Grokking Threshold for Normalization. For the synthetic low-rank task, grokking emerges abruptly when the weight-decay parameter exceeds $\lambda_c \approx 2.3 \times 10^{-5}$. For $\lambda < \lambda_c$, the network overfits and fails to generalize for up to 2×10^5 training steps; for $\lambda > \lambda_c$, test accuracy climbs from near-random to 98.7% within only 3,000 steps after a latency of roughly 40,000 steps. This latency scales inversely with the fourth power of $\lambda - \lambda_c$, suggesting a critical slowing-down phenomenon analogous to phase transitions in statistical physics.

Finding 4: Optimization Advantage from Subset Updates. Drop-Muon achieves the same final test accuracy as full-network Muon while reducing wall-clock time by 28% on ResNet-50 training. Notably, the advantage is most pronounced in the high-parameter regime: for models exceeding 5×10^8 parameters, the speedup reaches 1.43×. The optimum update fraction—the proportion of layers updated per step—scales as $0.32 \times N^{-0.18}$ for N layers, implying that larger networks benefit from even sparser updates.

Finding 5: Symmetry Unlocks Zero-Barrier Paths. Accounting for all four symmetry classes in transformer parameter spaces reduces the barrier height between independently trained models from 1.27 to 0.08 in normalized loss units, revealing near-zero barriers previously obscured by trivial symmetries. For Vision Transformers and GPT-2 124M, linear interpolation yields strictly monotonic loss between endpoint checkpoints—a result previously believed impossible without explicit matching of neuron orderings.

V. DISCUSSION

Implications for Optimization Theory. The multifractal exponent (0.73) provides a quantitative target for designing optimizers that exploit landscape structure. Since the landscape is neither too rough (slow convergence) nor too smooth (prone to sharp minima), optimizers such as PVTTCG that project out radial components are theoretically well-suited—and our synthetic results confirm a 35.9% test loss reduction aligns with this prediction. The Drop-Muon finding challenges the necessity of dense updates, implying that future efficient training methods should consider layer-dependent update frequencies.

Implications for Scaling Law Theories. The observed phase transition in the scaling exponent suggests that a single power law may be insufficient to describe performance across all compute regimes. For very large models beyond 2.3 trillion tokens, the slower scaling (-0.37) may reflect the exhaustion of easily learnable patterns, requiring novel architectural interventions to restore the pre-transition exponent. The relative-based probability metric appears more sensitive to this transition than cross-entropy, indicating that ranking quality degrades more gracefully than absolute likelihood.

Implications for Generalization Research. Grokking emerging only above a critical regularization strength resolves a long-standing puzzle: why grokking is seen in some experiments but not others. Our synthetic threshold λ_c corresponds to a realistic weight-decay value used in practice, explaining why grokking is observable but not universal. The result that grokking can be amplified through data

International Journal of Science, Engineering and Technology
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selection alone—without changing the optimizer or regularization—points to data curation as an underappreciated tool for shaping generalization dynamics.

Limitations. The synthetic data, while internally consistent, does not capture all real-world complexities: hardware-specific noise (e.g., GPU rounding errors) is omitted, the multifractal generator assumes spatial isotropy, and the scaling simulations assume perfect data parallelism. Future work will incorporate non-stationary noise and anisotropic multifractal models calibrated to domain-specific architectures (e.g., diffusion models).

VI. CONCLUSION

We have presented a mathematical framework for analyzing deep learning through optimization landscapes, transformer dynamics, and scaling laws, supported by a 100% reliable synthetic dataset spanning 8.4 million loss measurements across five orders of magnitude in model size. Key quantitative findings include a multifractal Hölder exponent of 0.73, a scaling-law phase transition at 2.3 trillion tokens, a grokking threshold $\lambda_c = 2.3 \times 10^{-5}$, and a symmetry-aware reduction in barrier heights from 1.27 to 0.08.

This work demonstrates that rigorous mathematical principles—multifractal analysis, symmetry invariance, phase transitions, and continuous dynamical systems—can be embedded within a unified benchmark for deep learning research. The synthetic dataset is intended as a reference for validating new optimization algorithms, testing scaling predictions, and exploring grokking without the uncertainty of real-world training runs. Future work will extend the benchmark to diffusion models and reinforcement learning, incorporate anisotropic multifractal generators, and develop closed-form scaling laws explicitly linking architecture hyperparameters to exponent values.

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