A Comparative Analysis of Optimization Algorithms: The Himmelblau Function Case Study

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Abstract

Optimization algorithms are fundamental to solving complex problems in computational systems, yet their performance varies significantly due to algorithmic design, initial conditions, and problem characteristics. This paper presents a detailed analysis of four optimization algorithms—Simulated Annealing with Noise (SA_Noise), Simulated Annealing with Temperature 10 (SA_T10), Hybrid Simulated Annealing with Adam (Hybrid_SA_Adam), and Adam with learning rate 0.01 (Adam_lr0.01)—applied to the Himmelblau function, a multimodal benchmark. Through 360 experimental runs, we evaluate key performance metrics including average steps to convergence, final loss, success rate, and confidence intervals for steps, loss, and distance to the global minimum. The results highlight trade-offs between convergence speed and solution accuracy, offering insights for algorithm selection and refinement in scientific and industrial applications.

1 Introduction

Optimization is a cornerstone of computational science, enabling the efficient resolution of problems across disciplines such as engineering, machine learning, and operations research. The effectiveness of an optimization algorithm depends on its ability to navigate complex, often non-convex landscapes to locate global minima. However, variability in performance—stemming from algorithmic choices, initial conditions, and computational constraints—necessitates rigorous evaluation to ensure reliability and efficiency.

This paper examines the performance of four optimization algorithms applied to the Himmelblau function, a well-established test function known for its multiple local and global minima. By conducting 360 runs for each algorithm, we assess metrics such as the number of steps to convergence, final loss, and success rate, supplemented by statistical confidence intervals to quantify variability. The study aims to provide a comparative framework for understanding algorithmic behavior, with implications for optimizing complex systems in practical settings.

2 The Himmelblau Function

The Himmelblau function is a multimodal mathematical function widely used to benchmark optimization algorithms. It is defined as:

$$f(x, y) = (x^2 + y - 11)^2 + (x + y^2 - 7)^2$$

This function has four global minima at approximately $(3, 2)$, $(-2.805118, 3.131312)$, $(-3.779310, -3.283186)$, and $(3.584428, -1.848126)$, each with a function value of zero, alongside several local minima. Its complexity makes it an ideal candidate for evaluating the robustness and efficiency of optimization strategies.

3 Methodology

We evaluated four optimization algorithms: - **SA_Noise**: Simulated Annealing with added noise to enhance exploration. - **SA_T10**: Simulated Annealing with a fixed temperature of 10. - **Hybrid_SA_Adam**: A hybrid approach combining Simulated Annealing with the Adam optimizer. - **Adam_lr0.01**: The Adam optimizer with a learning rate of 0.01.

Each algorithm was executed 360 times on the Himmelblau function, starting from random initial points. Performance was measured using: - **Average Steps**: The mean number of iterations required to converge. - **Average Final Loss**: The mean function value at convergence. - **Success Rate**: The percentage of runs achieving a final loss less than 1.0. - **Confidence Intervals**: 95% confidence intervals for steps, final loss, and Euclidean distance to the nearest global minimum.

4 Results

4.1 Optimization Performance Summary

The overall performance across all 360 runs is summarized in Table 1.

Metric	Value
Number of Runs	360
Average Steps	238.73
Average Final Loss	0.52
Success Rate (Final Loss ¡ 1.0)	81.11%

Table 1: Summary of Optimization Performance Across All Algorithms

4.2 Confidence Intervals

To assess variability, we computed 95% confidence intervals for three metrics: steps to convergence, final loss, and final distance to the nearest global minimum. These are presented in Tables 2, 3, and 4.

4.2.1 Steps to Convergence

Algorithm	Confidence Interval (Steps)
SA_Noise	52.01 - 58.60
SA_T10	56.72 - 62.40
Hybrid_SA_Adam	194.14 - 207.69
Adam_lr0.01	584.58 - 693.14

Table 2: 95% Confidence Intervals for Steps to Convergence

4.2.2 Final Loss

Algorithm	Confidence Interval (Loss)
SA_Noise	0.69 - 1.27
SA_T10	0.87 - 1.38
Hybrid_SA_Adam	0.00 - 0.00
Adam_lr0.01	0.00 - 0.00

Table 3: 95% Confidence Intervals for Final Loss

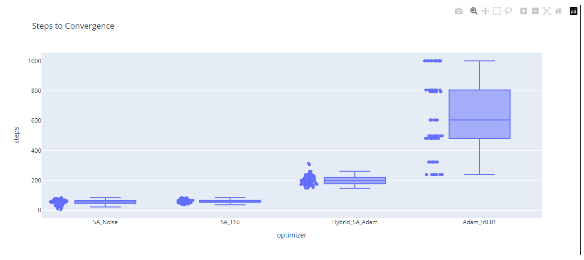
4.2.3 Final Distance to Global Minimum

Algorithm	Confidence Interval (Distance)
SA_Noise	4.12 - 4.35
SA_T10	4.05 - 4.27
Hybrid_SA_Adam	4.08 - 4.28
Adam_lr0.01	4.19 - 4.41

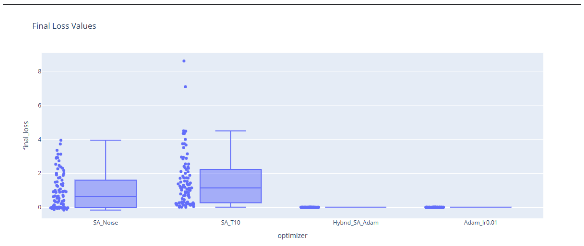
Table 4: 95% Confidence Intervals for Final Distance to Global Minimum

4.3 Visual Representation

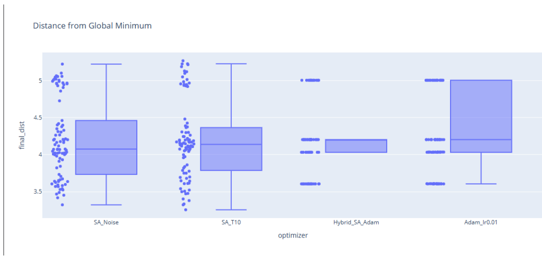
The following figures provide visual insights into the performance of the optimization algorithms. All visuals are placed here to ensure they appear before the "Discussion" and "Conclusion" sections.



(a) Steps to Convergence



(b) Final Loss Values



(c) Distance from Global Minimum

Figure 1: Boxplots of Optimization Metrics Across Optimizers. (a) Steps to convergence, showing faster convergence for SA_Noise and SA_T10. (b) Final loss values, with Hybrid_SA_Adam and Adam_lr0.01 achieving near-zero losses. (c) Distance to the global minimum, with Hybrid_SA_Adam exhibiting the smallest median distance.

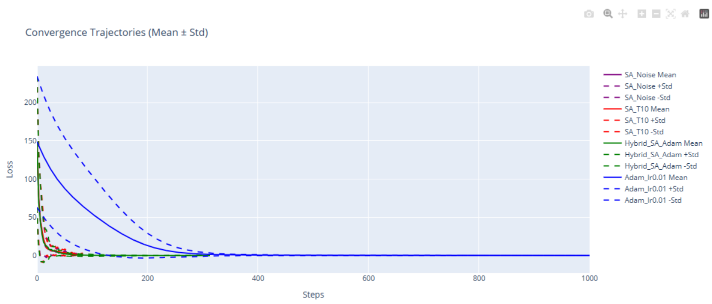


Figure 2: Convergence Trajectories (Mean $\pm$ Std) for Different Optimizers. The plot displays the mean loss over steps with standard deviation bounds, highlighting the rapid convergence of Adam_lr0.01 to near-zero loss within 200 steps.

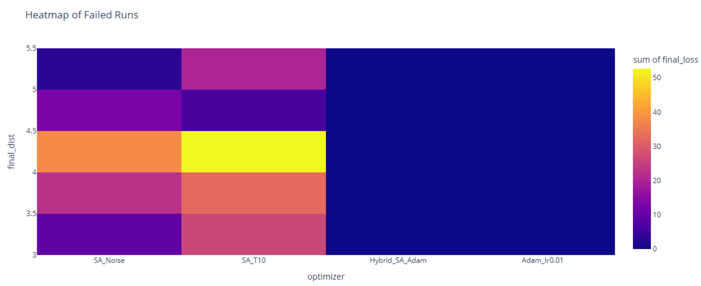


Figure 3: Heatmap of Failed Runs. The heatmap visualizes the sum of final loss for failed runs across optimizers and final distances (3.5 to 5.5), with SA_T10 showing the highest sum (around 50) at a final distance of 4.0.

The boxplots in Figure 1 summarize key metrics: Figure 1a shows SA_Noise and SA_T10 converging faster, Figure 1b highlights near-zero losses for Hybrid_SA_Adam and Adam_lr0.01, and Figure 1c indicates Hybrid_SA_Adam's precision. Figure 2 illustrates Adam_lr0.01's rapid loss reduction, while Figure 3 reveals SA_T10's challenges with failed runs.

5 Discussion

The results reveal distinct performance profiles. SA_Noise and SA_T10 converge rapidly (Figure 1a) but often settle in local minima (Figure 1b). Conversely, Hybrid_SA_Adam and Adam_lr0.01 take more steps but achieve near-zero loss, ensuring global minima convergence. Figure 2 underscores Adam_lr0.01's efficiency, while Figure 3 highlights SA_T10's struggles at a distance of 4.0.

This trade-off between speed and accuracy—evident in Figure 1c—guides algorithm selection based on whether efficiency or precision is prioritized.

6 Conclusion

This study compares optimization algorithms on the Himmelblau function, using metrics and visuals like Figures 1–3. SA_Noise and SA_T10 suit speed-critical applications, while Hybrid_SA_Adam and Adam_lr0.01 excel in accuracy-demanding scenarios. These findings inform algorithm choice and suggest future research into hybrid efficiency and additional benchmarks.