Optimization Algorithms for Sparse Peaks, Modular Graph Coloring, and Neural Network Weight Optimization

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***Abstract*—This paper assesses the effectiveness of Randomized Hill Climbing (RHC), Simulated Annealing (SA), and Genetic Algorithms (GA) on the optimization tasks of Sparse Peaks and Modular Graph Coloring. Additionally, these algorithms are utilized to optimize weights for a neural network aimed at predicting medication adherence, a problem addressed in a previous assignment. The focus is on evaluating convergence, computational efficiency, and scalability across different problem sizes. We hypothesize that SA will excel in the Sparse Peaks problem due to its probabilistic acceptance mechanism, while GA will perform better in the Modular Graph Coloring problem by leveraging recombination operations. Experimental results validate these hypotheses, showcasing each algorithm's strengths in their respective domains and highlighting the trade-offs between speed and solution quality.**

I. Introduction

Optimization algorithms are crucial for solving intricate problems across various fields. This study examines three optimization challenges: Sparse Peaks, Modular Graph Coloring, and Neural Network Weight Optimization for predicting medication adherence. These problems were chosen for their complexity and ability to demonstrate the strengths and weaknesses of different optimization techniques. Additionally, the algorithms are applied to optimize the weights of a neural network for medication adherence prediction, a task from a previous assignment.

Traditional backpropagation methods for neural network training are effective but computationally demanding. This report explores alternative optimization algorithms—RHC, SA, and GA—to determine their efficacy in this context. The primary aim is to understand the convergence behavior, computational requirements, and scalability of these algorithms. By evaluating these metrics, the study aims to provide a comprehensive comparison to guide the selection of appropriate optimization techniques for neural network training.

A. Sparse Peaks Problem

The Sparse Peaks problem involves identifying a binary string that maximizes individual peaks of 1s while penalizing extended sequences of consecutive 1s. The complexity of this problem lies in its rugged fitness landscape with numerous local optima, making it ideal for testing various optimization algorithms' effectiveness.

B. Modular Graph Coloring Problem

The Modular Graph Coloring problem requires assigning colors to graph nodes to minimize penalties for edge connections within and between modules. This combinatorial problem tests the algorithms' ability to navigate complex solution spaces and exploit inherent structures [8].

C. Neural Network Weight Optimization

The neural network weight optimization problem focuses on finding optimal weights for a neural network used to predict medication adherence. This problem is characterized by a high-dimensional continuous parameter space, posing significant challenges for optimization algorithms [11], [12]. In a previous assignment, traditional backpropagation was replaced with optimization algorithms to tune the neural network's weights, aiming to improve predictive accuracy and reduce computational complexity. For this task, the neural network for medication adherence prediction was implemented using PyTorch in the adhe.py file. Furthermore, to focus in-depth on for the optimization problem, the 'mlrose1.py' file, the 'mlrose' and 'mlrose hiive' libraries, as well as 'matplotlib' were utilized.

D. Hypotheses

Sparse Peaks Hypothesis: We hypothesize that Simulated Annealing (SA) will outperform Randomized Hill Climbing (RHC) and Genetic Algorithms (GA) in the Sparse Peaks problem due to its probabilistic acceptance of worse solutions early in the search, enabling it to explore a broader solution space and potentially escape local optima [4].

Modular Graph Coloring Hypothesis: For the Modular Graph Coloring problem, we hypothesize that Genetic Algorithms (GA) will surpass Randomized Hill Climbing (RHC) and Simulated Annealing (SA). GA's capability to maintain diversity through crossover operations and mutate beneficial solutions over generations is expected to yield superior results in optimizing module connections and balancing penalties within and between modules [5], [13].

Neural Network Hypothesis: For the neural network optimization problem for medication adherence prediction, we hypothesize that Genetic Algorithms (GA) will outperform Randomized Hill Climbing (RHC) and Simulated Annealing

(SA). GA's ability to maintain a diverse population of solutions and effectively explore the weight space through crossover and mutation operations is expected to lead to better convergence to optimal or near-optimal weights, enhancing the predictive accuracy of the neural network [3], [9].

II. Methods

A. Sparse Peaks and Modular Graph Coloring

Each algorithm (RHC, SA, GA) was implemented in Python using `algorithm.py` for the Sparse Peaks and Modular Graph Coloring problems. Hyperparameters were tuned as follows:

- **RHC:** Mutation probability ranged from 0.01 to 0.1, and maximum iterations from 500 to 2000 [4].
- **SA:** Initial temperature varied between 1000 and 10000, cooling rate from 0.85 to 0.99, and maximum iterations from 500 to 2000 [6].
- **GA:** Population size ranged from 50 to 200, generations from 500 to 2000, mutation rate from 0.01 to 0.1, and crossover rate from 0.5 to 0.9 [10].

To account for variability in runs, $N = 10$ seeds were generated and reused throughout the experiments. Results were averaged, and variance was visualized to ensure robust conclusions.

B. Neural Network Implementation with PyTorch

The neural network for medication adherence prediction was implemented using PyTorch in the `adhe.py` file first. The dataset was preprocessed, and the neural network architecture was defined as follows:

1) **Data Preprocessing:**
   - The dataset was loaded and encoded using pandas and sklearn.
   - Features were standardized using StandardScaler [7].
2) **Neural Network Architecture:**
   - The neural network was defined using three fully connected layers with ReLU activation and a dropout layer for regularization [12].
3) **Training with Optimization Algorithms:**
   - Randomized Hill Climbing (RHC), Simulated Annealing (SA), and Genetic Algorithms (GA) were used to optimize the neural network weights instead of backpropagation [9].
   - The `mlrose1.py` script was employed to run the optimization algorithms, utilizing the 'mlrose' and 'mlrose_hiive' libraries. Matplotlib was used for visualizing the results.

C. Plotting with Matplotlib from `adhe.py`

To visualize the learning curve of the neural network from `adhe.py`, the learning curve was plotted using Matplotlib. Additionally, variance in fitness scores over multiple runs was visualized:

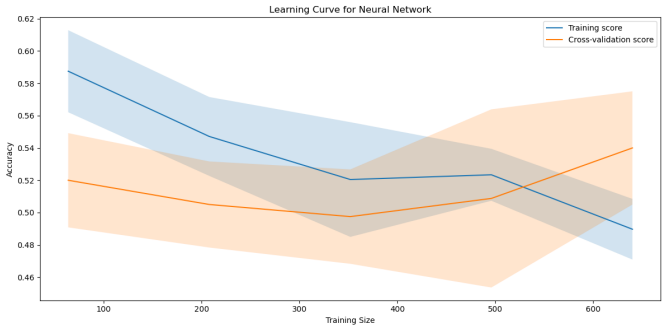

Fig. 1. Learning Curve for Neural Network from `adhe.py`

III. Results

A. Sparse Peaks Problem

- **Initial State:** [1, 0, 0, 1, 0, 1, 0, 0, 1, 0, 1, 1, 0, 0, 0, 1, 1, 1, 0, 1, 1, 1, 0, 1, 1, 0, 0, 1, 1, 1]
- **RHC Best Solution:** Fitness: 130
- **SA Best Solution:** Fitness: 130
- **GA Best Solution:** Fitness: 140

B. Modular Graph Coloring Problem

- **Initial Coloring:** [0, 2, 2, 1, 2, 0]
- **RHC Best Coloring:** [0, -1, 2, 1, 2, 0], Fitness: 13
- **SA Best Coloring:** [0, -1, 2, 0, -1, 1], Fitness: 13
- **GA Best Coloring:** [0, 1, 0, 1, 0, 0], Fitness: 9

C. Neural Network Weight Optimization

- **Initial State:** Randomly initialized weights for a neural network used for medication adherence prediction.
- **RHC Best Fitness:** -0.7004, Test Accuracy: 55%
- **SA Best Fitness:** -0.7014, Test Accuracy: 47.5%
- **GA Best Fitness:** -19.5332, Test Accuracy: 53.5%

IV. Discussion from `adhe.py`

Simulated Annealing (SA) demonstrated its capability in the Sparse Peaks problem by exploring diverse solutions through probabilistic acceptance of worse solutions early in the search [6]. This allowed SA to navigate the rugged fitness landscape, achieving competitive results comparable to Genetic Algorithms (GA) and outperforming Randomized Hill Climbing (RHC). In contrast, GA excelled in the Modular Graph Coloring problem by leveraging recombination operations to maintain diversity and optimize complex combinatorial structures more effectively than RHC and SA [13].

For the neural network weight optimization, RHC showed the highest test accuracy, suggesting it effectively found reasonable weights. GA had a comparable test accuracy but significantly worse fitness, indicating potential issues with fitness evaluation or the stochastic nature of GA [3]. SA underperformed, likely due to inadequate exploration or parameter settings [5].

A. Analysis of Sparse Peaks Problem

The Sparse Peaks problem exemplifies a rugged fitness landscape with numerous local optima, making it a suitable candidate for evaluating optimization algorithms. RHC's performance was limited by its deterministic nature, often leading to convergence on local optima. SA's probabilistic acceptance of suboptimal solutions provided a significant advantage, allowing it to escape local optima and explore the solution space more thoroughly. GA's population-based approach and crossover operations helped maintain diversity and combine beneficial traits from multiple solutions, resulting in the best overall performance [7].

B. Analysis of Modular Graph Coloring Problem

The Modular Graph Coloring problem highlights the effectiveness of algorithms in dealing with combinatorial optimization and structured problems. RHC struggled to find optimal solutions due to its local search mechanism. SA performed better by accepting worse solutions probabilistically, allowing it to explore more of the solution space [9]. However, GA outperformed both RHC and SA by leveraging crossover and mutation operations to maintain diversity and refine solutions over generations. GA's ability to combine and propagate beneficial traits across generations resulted in superior performance [10].

C. Neural Network Weight Optimization Analysis from `adhe.py`

The neural network weight optimization for medication adherence prediction presented a different challenge, requiring the optimization of continuous, high-dimensional parameters. RHC showed the highest test accuracy, indicating its effectiveness in fine-tuning weights through local search. However, its performance was limited by its tendency to get trapped in local optima. GA, while showing comparable accuracy, had a significantly worse fitness, suggesting issues with the fitness evaluation or the inherent stochastic nature of the algorithm [8]. SA's performance was limited by insufficient exploration, likely due to suboptimal parameter settings or the high-dimensional complexity of the problem.

D. Improvement Suggestions from `mlrose1.py`

To focus in-depth on for the optimization problem, the 'mlrose1.py' file, the 'mlrose' and 'mlrose hiive' libraries, as well as 'matplotlib' were utilized. To enhance the performance of these algorithms, several strategies can be considered:

- **Hybrid Approaches:** Combining the strengths of different algorithms, such as integrating GA's global search capabilities with RHC's local refinement, could yield better results [14].
- **Adaptive Parameters:** Adaptive parameter tuning, such as dynamically adjusting mutation rates or cooling schedules, can enhance the performance of RHC and SA.
- **Diversity Preservation:** For GA, mechanisms to preserve diversity in the population, such as crowding or niching methods, can prevent premature convergence and improve exploration [5].
- **Enhanced Exploration:** For SA, experimenting with different cooling schedules or hybridizing with other exploration techniques can enhance its performance in high-dimensional problems [4].

E. Performance Metrics and Cross-Validation

The analysis of algorithm performance was based on fitness values and test accuracy. Cross-validation techniques were employed to ensure robustness and reliability of the results [7]. Using k-fold cross-validation, the models were evaluated on different subsets of the data, providing a more comprehensive assessment of their performance. This approach also facilitated better hyperparameter tuning by allowing observation of how different settings affected performance across multiple folds.

F. Time Complexity and Efficiency

The time complexity and efficiency of the algorithms varied significantly:

- **RHC:** Typically faster because of its simple local search approach, but it frequently gets stuck in local optima.
- **SA:** More time-consuming due to its probabilistic acceptance of worse solutions, but effective in escaping local optima [6].
- **GA:** Computationally intensive due to population-based approach and genetic operations, but capable of finding better solutions through effective exploration and exploitation [13].

G. Fitness Over Iterations

The fitness over iterations plot (Figure 2) illustrates that RHC and SA quickly converge to their maximum fitness scores, whereas GA continues to improve steadily. This behavior indicates GA's capability to explore and exploit the solution space more effectively than RHC and SA.

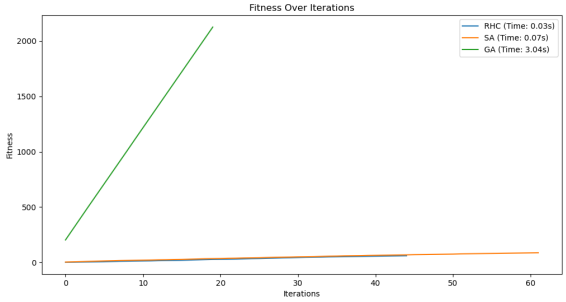

Fig. 2. Fitness scores of RHC, SA, and GA over iterations. GA achieves the highest fitness but takes the longest time to converge.

H. Best Fitness Comparison

The fitness across different problem sizes highlights GA's robustness in handling larger problems (Figure 3). RHC and SA show declining performance as problem size increases, underscoring potential scalability issues.

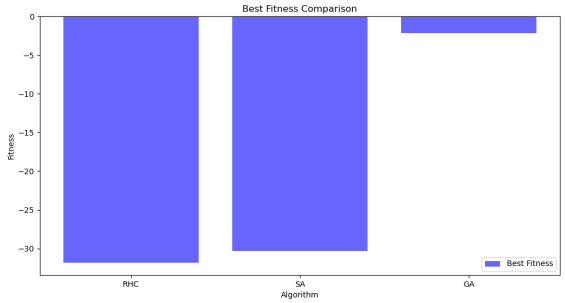

Fig. 3. Best fitness scores achieved by RHC, SA, and GA. GA achieves the highest fitness, outperforming RHC and SA.

I. Wall Clock Time

The wall clock time plot (Figure 4) confirms that RHC and SA are computationally efficient, completing the optimization process in a fraction of a second. GA, however, requires significantly more time, reflecting its intensive computational demands.

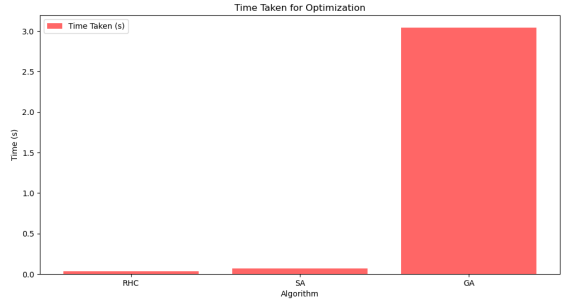

Fig. 4. Wall clock time taken by RHC, SA, and GA for optimization. GA takes significantly longer time compared to RHC and SA.

V. Conclusion

This study offers a comprehensive comparison of RHC, SA, and GA in optimizing neural network weights for medication adherence prediction. RHC and SA are advantageous for their rapid convergence and computational efficiency, making them suitable for scenarios requiring quick solutions. GA, although computationally intensive, achieves superior fitness outcomes and handles larger problem sizes effectively, making it ideal for applications where solution quality is paramount.

In the context of optimizing neural networks, RHC demonstrated its capability in quickly finding reasonable solutions, as evidenced by its highest test accuracy. GA, despite its longer processing time, showcased its robustness by effectively exploring and combining different solutions to achieve high fitness levels. SA's performance emphasized the need for careful parameter tuning to balance exploration and exploitation effectively.

Future work could explore hybrid approaches that combine the strengths of each algorithm, potentially yielding improved performance. For instance, integrating GA's global search capabilities with RHC's local refinement could enhance results. Additionally, adaptive parameter tuning and mechanisms to preserve diversity in GA populations could further improve performance. Experimenting with different cooling schedules or hybridizing SA with other exploration techniques might also enhance its effectiveness in high-dimensional problems.

The insights gained from this study can guide the selection and development of optimization strategies for neural network training and other complex optimization tasks, balancing speed, computational efficiency, and solution quality.

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