

1 Introduction

In this paper I will be exploring the performance and trade-offs of four randomized optimization algorithms: randomized hill climbing, simulated annealing, genetic algorithms, and MIMIC against three problems. Later in the paper I will reexamine work I did previously in Assignment 1 and attempt to optimize the weights of a multi-layered perceptron using these same four algorithms. For the purposes of this assignment I used the `mlrose` library [1] which was publicly available. Note that I made some modifications to the library on my computer to be able to generate timing curves (and I do not know how to publish a Python package so I will include instructions for how to get my code in the Readme.)

2 Comparison of Randomized Optimization Algorithms

This section is dedicated to exploring a comparison of four randomized optimization algorithms against example problems which should highlight their relative strengths and weaknesses. The algorithms are randomized hill climbing, simulated annealing, genetic algorithms, and MIMIC. I will briefly introduce parameters I will be varying for each algorithm here and then we will compare their performance in each problems subsection below.

Randomized Hill Climbing

Randomized hill climbing is perhaps one of the more straightforward randomized optimization algorithms to understand. It begins in a random location in the search space and looks for random neighbors around that point for an optimal value defined by some fitness function. If it succeeds in finding such a point the algorithm terminates unless it is configured to restart from a random place elsewhere in the search space. The hope is that by randomly restarting we can prevent the algorithm from getting "stuck" in a local maximum and find a global maximum. The parameters I am varying are:

- `max_attempts` The number of attempts to find a neighbor with better fitness
- `max_iterations` The number of times to iterations to search (this will usually be lower than `max_attempts`)
- `restarts` The number of times to randomly restart the above search in a new location in a random location in the search space

Simulated Annealing

Simulated Annealing involves a randomized searching technique that involves dynamically constraining and relaxing the values that the algorithm will consider to be acceptable as

"better fit" by using a schedule to simulate "heating and cooling" or "better or worse fit." The theory is that by varying this schedule of heating and cooling that the algorithm will be able to avoid local maxima by eventually considering worse values as better outside of the space where the local maximum was in search of a possibly better global maximum.

- **max_attempts** The number of attempts to find a neighbor with better fitness
- **max_iterations** The number of times to iterations to search (this will usually be lower than **max_attempts**)
- **schedule** The decay schedule controls the temperature chance for each iteration of the SA algorithm. It can take on three values: Arithmetic, Geometric, and Exponential decay.
 - Arithmetic decay is modeled as $Temp(t) = T_0 - rt$ where T_0 is the initial temp and r is some value in (0,1) and represents the rate of arithmetic decay.
 - Geometric decay is modeled as $Temp(t) = T_0 - r^t$. We expect in this scenario the temperature to decrease much more rapidly.
 - Exponential decay is modeled as $Temp(t) = T_0 e^{-rt}$ This may look familiar as it is modeled similar to the continuously compounding interest rate formula and should decay the most quickly.

Genetic Algorithm

A genetic algorithm takes the concept biological evolution (particularly the concept of "survival of the fittest") and applies it to randomizes search. A grouping of randomly selected guesses is selected and the best ones are kept, and the worst fitting elements are replaced by random recombination of the elements of of the best performing guesses. In this way the algorithm hopes to find a global maximum or "most fit" population by always searching for better and better random recombinations of the the population. The parameters I am varying for this algorithm are:

- **max_attempts** The number of attempts to find a neighbor with better fitness
- **max_iterations** The number of times to iterations to search (this will usually be lower than **max_attempts**)
- **pop_size** The number of guesses (or population count) to retain at each iteration of the search
- **mutation_prob** The likelihood of an element in a vector to be randomly recombined if it is in a bad population. For example, if this value were 0.1 and the population is a grouping of 10 element vectors, then most likely 1 of the elements will be recombined if it is in the "worse performing" group at the end of a "generation" (iteration of the algorithm).

MIMIC

MIMIC expands on the concept of Genetic Algorithms combining the best of each generation and replacing the worst in the search with the concept of "memory" of previous generations through the use of probability distributions and information theory as modeled by Kullback-Libeler divergence. [2] Thus it should be able to converge much faster to an optimal solution than a genetic algorithm for the same problem. The parameters I will be varying for this algorithm are:

- **max_attempts** The number of attempts to find a neighbor with better fitness
- **max_iterations** The number of times to iterations to search (this will usually be lower than **max_attempts**)
- **pop_size** The number of guesses (or population count) to retain at each iteration of the search
- **keep_pct** The percentage of guesses to retain between each iteration of the algorithm.

2.1 One Max Problem; highlights advantages of MIMIC

The One Max Problem is a fitness function that seeks to maximize a vector v such that:

$$\sum_{i=0}^{n-1} v_i \quad (1)$$

is a maximum, where v_i is the i th component of vector v with length n . This is a relatively easy optimization problem to understand and it illustrates the effectiveness of MIMIC and Genetic Algorithms quite nicely from an efficiency standpoint. The best values found for each algorithm were as follows:

Algorithm	Parameters	Value
RHC	Max Iterations, Max Attempts, Restarts	40, 40, 0
SA	Max Iterations, Max Attempts, Decay Schedule	180, 180, Exponential
GA	Max Iterations, Max Attempts, Pop Size, Mutation Prob	10,10,0.1,100
MIMIC	Max Iterations, Max Attempts, Pop Size, Keep %	10,10,0.1,300

As you can see, MIMIC converged to the correct optimal value within 10 iterations of the function making it a very powerful algorithm for this particular problem type.

Figures 1 and 2 illustrate how quickly MIMIC converged and that it took less wall clock time to do so than Genetic Algorithms (a similar class of algorithm.) This result

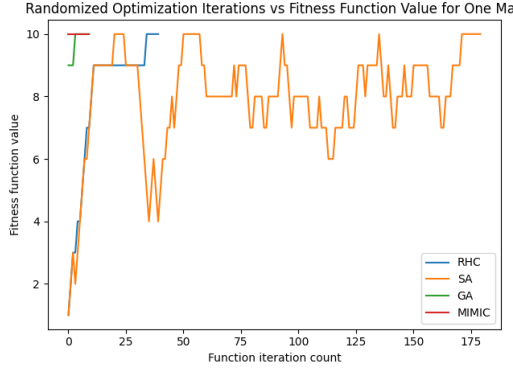


Figure 1: Function value by iteration count

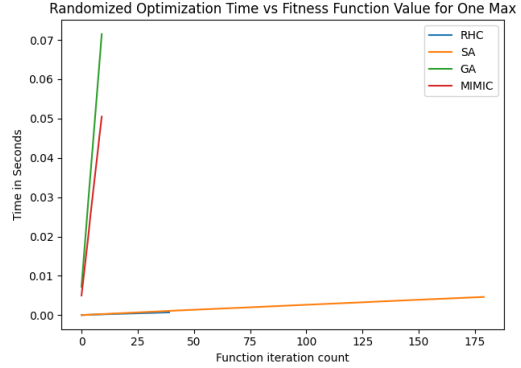


Figure 2: Total time by iteration count

is most likely due to the fact that while MIMIC requires time to calculate probability density functions, by using this to improve its guess each time it saw the most dramatic improvement between iterations. By contrast Simulated Annealing took over 175 iterations to converge to the the correct value.

2.2 8 Queens Problem; highlights advantages of Simulated Annealing

The eight queens problem is a specific implementation of the n-queens optimization problem. [3] It poses an $n \times n$ board like in chess where n queens need to be placed such that a minimum number of queens could "attack" each other (diagonally, horizontally, or vertically.) So the space to search is a collection of vectors of 8 elements where each element is an integer between 0 and 7 and represents where the queen is on that column of the chess board.

2.3 Traveling Salesman; highlights advantages of Genetic Algorithms

3 Neural Network Weight Optimization

References

- [1] G Hayes. mlrose: Machine Learning, Randomized Optimization and SEarch package for Python. <https://github.com/gkhayes/mlrose>, 2019. Accessed: 20 September 2020.
- [2] Paul Viola Jeremy De Bonet, Charles Isbell Jr. Mimic: Finding optima by estimating probability densities. <https://www.cc.gatech.edu/~isbell/papers/isbell-mimic-nips-1997.pdf>, 1997.

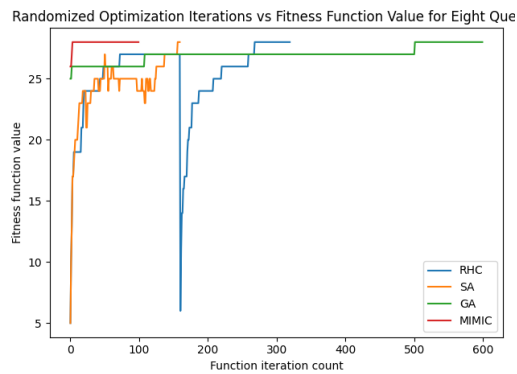


Figure 3: Interpolation for Data 1

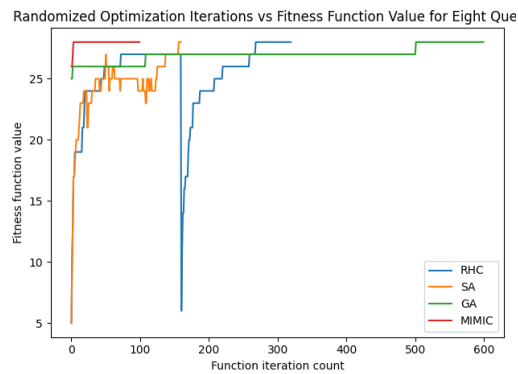


Figure 4: Interpolation for Data 2

- [3] S. Russell and P Norvig. Artificial intelligence: A modern approach, 3rd edition. Prentice Hall, New Jersey, USA., 2010.