Project2 Report - Randomized Optimization

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***Abstract*—**Optimization is a common tool used in machine learning, and each problem has slightly different conditions which make optimization challenging. In complex problem spaces, global optimal values are challenging to find because there are often complex optimization surfaces. As a result, simple optimization methods may get stuck in a local peak instead of a global peak, requiring additional logic and randomization to escape and find a better solution. 4 randomized optimization methods are evaluated here: Random Hill Climbing, Simulated Annealing, Genetic Algorithm, and MIMIC.

1 RANDOMIZED OPTIMIZATION ALGORITHMS

Optimization frequently involves very complex problem spaces with many peaks and valleys on the optimization surface. As a result, reaching an optimal solution is not always easy. The simplest approach to the problem is a simple hill climbing algorithm. Start with randomized parameters in the problem space, and then move in the direction of positive gradient until a peak is reached. However, in complex problems, this is, more often than not, a local maximum, not the global maximum. In order to reach the global optimum, or at least a better local maximum, more of the problem space needs to be explored, which requires some amount of randomized exploration. The 4 optimization techniques explored in this project are Randomized Hill Climbing, Simulated Annealing, Genetic Algorithm, and MIMIC.

1.1 Random Hill Climbing

Random Hill Climbing is the simplest of the methods explored here. It involves a simple climbing algorithm, starting with random parameters and travering in the direction of positive gradient until a peak is reached, then it will restart at some new, random starting parameters. Once complete, the process is repeated, keeping the best of all parameters found. The idea here being that the randomized restarts allows the algorithm to move throughout the problem space and more likely escape local maxima.

This algorithm is very simple and very fast, and require little memory since each state is evaluated independent of history. The disadvantage is that it can take a very large number of restarts to explore a sufficient area in the problem space, and there is no guarantee that a global optimum is ever found.

1.2 Simulated Annealing

Simulated Annealing is a variation on hill climbing which allows for more exploration. The algorithm starts with a high temperature, which is essentially a probability of changing to a new random state. At each iteration, the algorithm finds a random state, decides based on the temperature if it will transition to that state, and if not, it will instead perform a basic hill climb at it's current state. Then at each step, the temperature will be reduced.

The concept here is that in the start, there is nothing known about the problem space, and very little to lose by randomly jumping to a new state. In doing so, much more of the problem space can be explored cheaply. As the algorithm continues, it should start narrowing in on an optimum, and reducing the temperature such that it is less likely to randomly jump out of the current state. This results in slowly settling in an a peak. It is generally able to explore much more of the problem space than Random Hill Climbing, but still needs to follow gradients to find the solution. This means it may not perform well when the problem space is non-differentiable, or if the global peak only touches a narrow portion of the problem space, making it very unlikely to randomly run into it.

1.3 Genetic Algorithm

Genetic Algorithm is a method inspired by DNA and natural selection. A population of states are created using random parameters, then evaluated according to the fitness function. On subsequent iterations, the previous states are weighted according to their fitness scores and then resampled, meaning higher scores are resampled more. During resampling, states are mixed together using crossover, creating 2 new states consiting of elements of both parents, similar to how DNA is shared during reproduction. To explore the space more, there may also be some "mutation" where a small number of features are changed randomly. The concept here is that the "parents" that scored the highest will produce the most "offspring", and those "offspring" will hopefully take the strengths of both parents. If they do, they will be resampled more, and if they don't, then they will "die off".

The advantage here is that features, and sometimes groups of features, are maintained throughout generations, and it does not rely on smooth objective functions or gradients. Since populations are made at random and created in bulk, it also very efficiently explores large parameters spaces and handles noisy and random functions well. The primary disadvantage is that iterations are much more expensive because it requires generating new populations and evaluating each state. As a result, unless there are features which can be easily captured through crossover, it might just be too slow to reach the optimal values.

1.4 MIMIC

MIMIC (De Bonet, Isbell, and Viola, 1997) (Mutual-Information-Maximizing Input Clustering) is an algorithm which uses probability densities and information learned from previous iterations to improve on the solution. Random candidate solutions uniformly dispersed throughout the problem space are chosen to generate a probability density function. Each iteration of the algorithm then adds new parameters to improve this function, and then only points above a certain threshold are maintained. Successive iterations then refine that probability function, and raise the threshold.

The greatest strengths of this algorithm are that it is able to cover a large portion of the problem space in relatively few iterations. It also encapsulated structured information very well, so it performs well when structure and relationships between parameters is significant. The biggest downside is that it is very expensive, and takes much longer to run than other optimization techniques discussed.

2 PROBLEMS

In order to demonstrate the strengths and weaknesses of different optimization techniques, there must be problems to solve or optimize. To fit the criteria for this project, the problems must have some fitness function to maximize, and they must be over discrete-valued parameters. Continuous valued parameters are possible with some algorithms and will be discussed more in the neural network section.

2.1 Problem Descriptions

2.1.1 *Problem 1 - Four Peaks*

The Four Peaks problem consists of counting the number leading ones (the head) and trailing zeros (the tail), and selecting the max value between the two. If both of those counts are above some threshold, there is also an additional n points added to the fitness score, where n is the total number of parameters in the problem. This results in 2 local maxima when there are large head or tail counts, and 2 global maxima when the bonus is applied, hence the name, Four Peaks.

2.1.2 *Problem 2 - Flip Flop*

The Flip Flip problem consists of counting each pair of consecutive bits in an array that "flip flop". In other words, a point is added to the fitness score for each index, i, in an array where $x_i \neq x_{i+1}$.

2.1.3 *Problem 3 - Traveling Salesperson*

Traveling Salesperson is really a class of optimization problems that revolve around optimizing routes. In the simplest sense, and the one which is used for this project, it consists of a list of points in 2D space. The problem is to determine the shortest route which visits each point exactly once and returns back to the starting point at the end. The Traveling Salesperson problem is different from the previous two problems because it is a minimization problem instead of a maximization. The goal is to minimize the travel distance, so to interpret this as a fitness function, the fitness score would just be the negative of the distance.

2.2 Results

2.3 Four Peaks

2.3.1 *Theory and Prediction*

The Four Peaks problem is a simple situation which exploits the weaknesses of climbing algorithms and strengths of techniques which don't require gradients to improve. Since there is a discontinuity in the function when the bonus is applied, gradient-based algorithms would need to luck into finding the region. Because of this, I predicted that Genetic Algorithm and MIMIC would outperform both random hill climbing and simulated annealing.

2.3.2 *Performance*

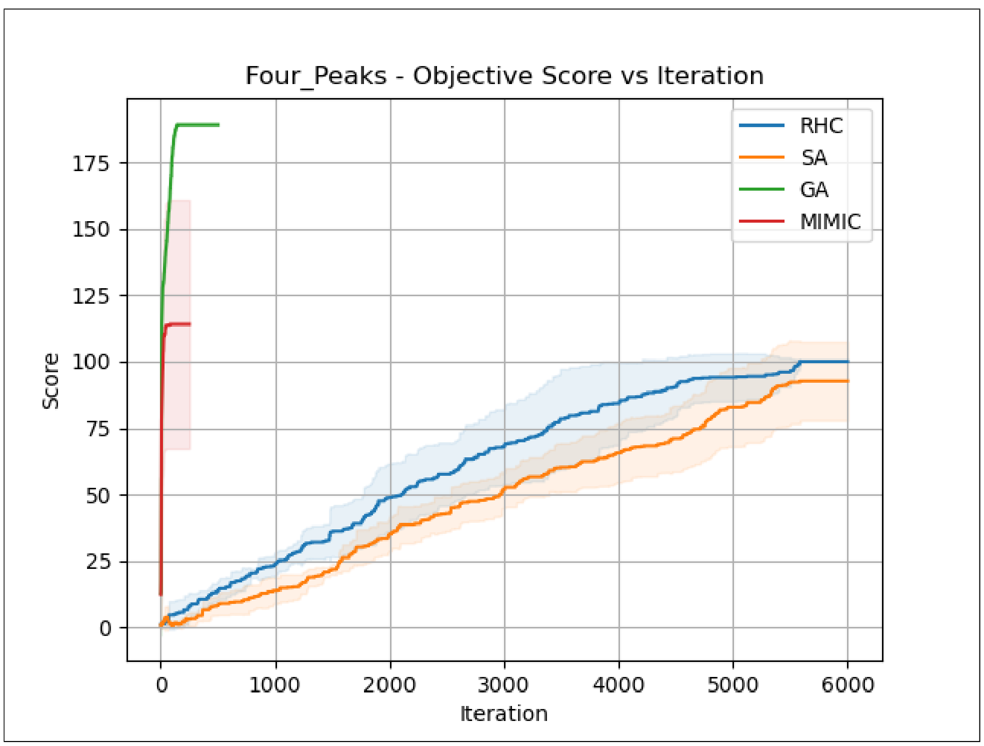
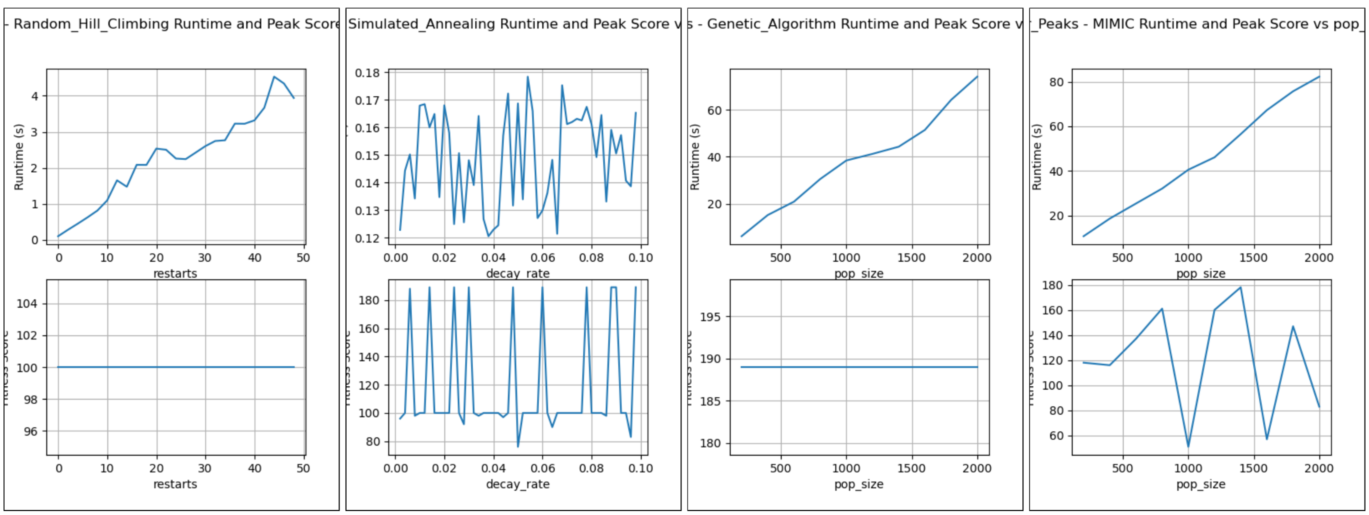


Figure 1—Performance comparison for the Four Peaks problem. Lines represent the average score over each iteration when using different random state seeds. Shaded areas are the standard deviation.

Algorithm	Final Score	Average Runtime	Avg Time to Peak
Random Hill Climb	100	0.865s	0.618s
Simulated Annealing	100	0.147s	0.133s
Genetic Algorithm	189.0	32.992s	8.791s
MIMIC	162.0	40.976s	7.673s

As predicted, both random hill climbing and simulated annealing both settled in on suboptimal solutions, and genetic algorithm found the optimal fairly easily. Even though Simulated Annealing and Hill Climbing were orders of magnitude faster, it doesn't make much difference when the global optimals are never found. They could have run forever and never reached it. Throughout testing, there were some occasions when they got lucky, but most of the time, they settled on local maxima.

2.3.3 *Parameter Variation*



(a) (b) (c) (d)

Figure 2—Four Peaks Parameter tuning for (a) RHC using number of random restarts, and (b) Simulated Annealing using rate of decay (c) GA using population size, and (d) MIMIC using population size

Iterating over a number of random restarts for the RHC algorithm shows expected results. There is basically a linear increase in runtime as restarts are increased, and it still doesn't help the end score. Hypothetically, with enough restarts, it would eventually find it, but that would be expensive.

Simulated Annealing doesn't fair much better. Changing the decay rate changes how quickly the algorithm settles on a solution. It shouldn't affect the runtime unless it finds a solution faster. Interestingly, there are a handful of configurations that are able to find the global optimal solution, but it seems to be mostly related to randomness, as there is no real trend.

Genetic Algorithm performs exceptionally well regardless of the population size. Since this is a relatively simple objective, that isn't too surprising. It also makes sense that runtime would scale linearly with increasing population.

MIMIC runtime scales linearly with population as well, but behaves strangely when it comes to the fitness score. Honestly, I can't really make sense of why there is no pattern. I would have expected fitness to improve with larger population since it would be able to gain more information about the probability densities and explore more of the problem space.

2.4 Flip Flop

2.4.1 *Theory and Prediction*

The Flip Flop problem is an interesting case because structure and relationships are important, which means that GA and MIMIC are likely to perform well, but it could still be captures using a gradient to some extent. Since what is most important is the relationship between parameters, and spacial information is relevant, I predict that MIMIC will perform the best, followed by GA, SA, then Random Hill climbing in last. MIMIC is especially good at capturing structure and relationship, and GA does this well too, but SA and RHC are not designed for this. The reason why I predict that SA will still perform relatively well is because it is designed to search the problem space more, so it is more likely to "accidentally" jump into a better solution.

2.4.2 *Performance*

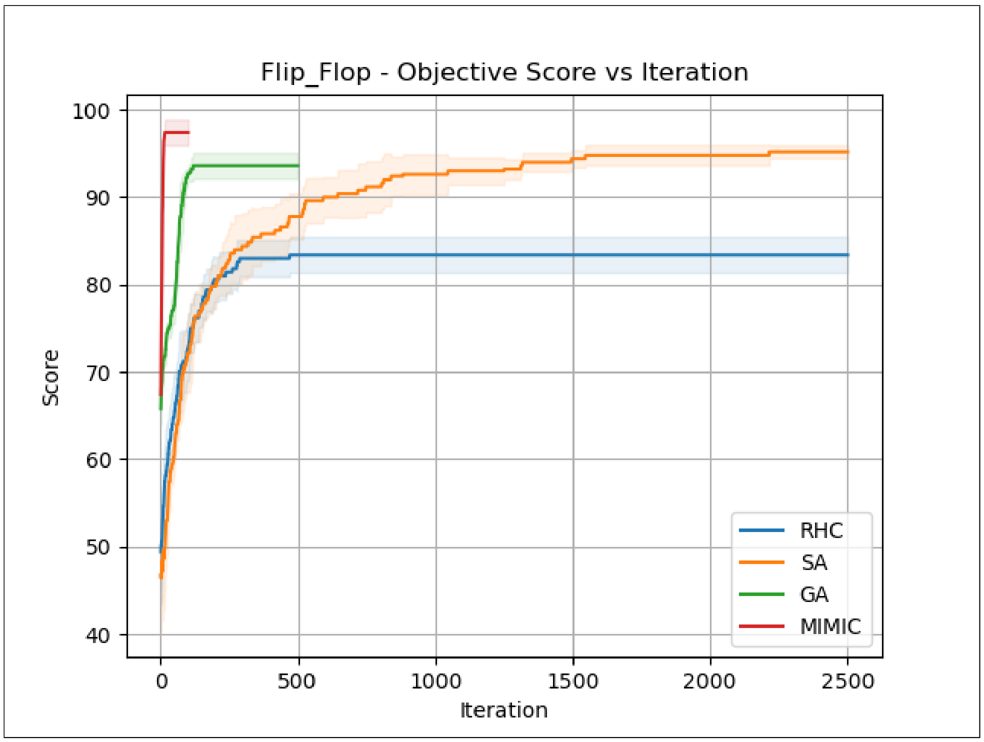
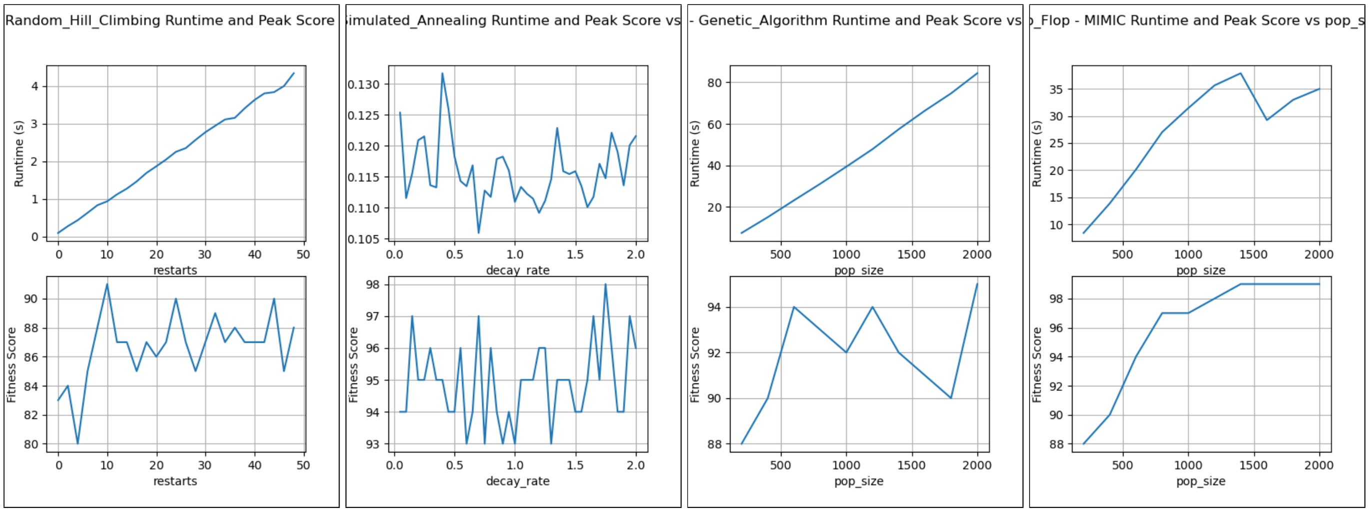


Figure 3—Performance comparison for the Flip Flop problem. Lines represent the average score over each iteration when using different random state seeds. Shaded areas are the standard deviation.

Algorithm	Final Score	Average Runtime	Avg Time to Peak
Random Hill Climb	87	0.446s	0.051s
Simulated Annealing	96	0.121s	0.069s
Genetic Algorithm	95	39.87s	7.93s
MIMIC	99	17.43s	2.336s

Most of this is as predicted. MIMIC scores the best, but is also the slowest, and RHC is fast but does not perform well. The surprise here is how well Simulated Annealing has done. It has performed just barely better than GA, but much faster. Once again, it performs orders of magnitude faster than GA or MIMIC, and actually performs nearly just as well. Really the only algorithm not suited for this problem is RHC.



(a) (b) (c) (d)

Figure 4—Flip Flop Parameter tuning for (a) RHC using number of random restarts, and (b) Simulated Annealing using rate of decay (c) GA using population size, and (d) MIMIC using population size

2.4.3 *Parameter Variation*

Since random hill climbing requires luck to perform well in this situation, it's no surprise that increased restarts generally improve the fitness score, but it still plateaus since there is not a strong gradient to follow.

Just as with the last problem, Simulated Annealing is not affected much by the decay rate, at least not to where an obvious trend can be observed. There might a weak trend toward increasing fitness with increasing decay rate, but not enough to put much stock into it.

Genetic Algorithm improves with larger population, but it's a weak relationship since there are still dips. It is still surprising that it is weaker than the SA regardless of population. But just as before, larger population slows it down even more.

MIMIC is the only algorithm in this problem that has a very clear and obvious trend. As population size increases, so does the final accuracy. This is not surprising since it allows the algorithm to gain more information about the probability densities, and therefore make better predictions.

2.5 Traveling Salesperson

2.5.1 *Theory and Prediction*

The TSP (Traveling Salesperson Problem) involves iterating over many different paths in a large problem space. Because of the complexity of the problem, there are likely to be many local optimal solutions. Since there is a blend of a smooth objective function and significant structural or relational information, I predicted that MIMIC and GA will both reach more optimal solutions, but SA and RHC will reach suboptimal, but still very good solutions much faster.

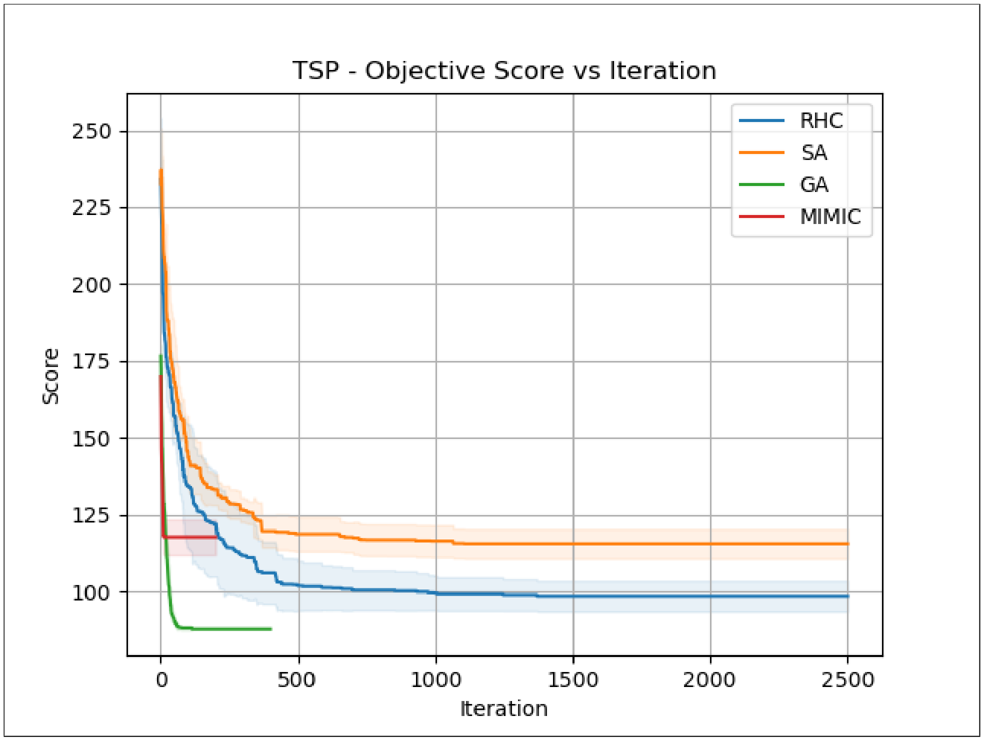


Figure 5—Performance comparison for the Traveling Salesperson problem. Lines represent the average score over each iteration when using different random state seeds. Shaded areas are the standard deviation.

2.5.2 *Performance*

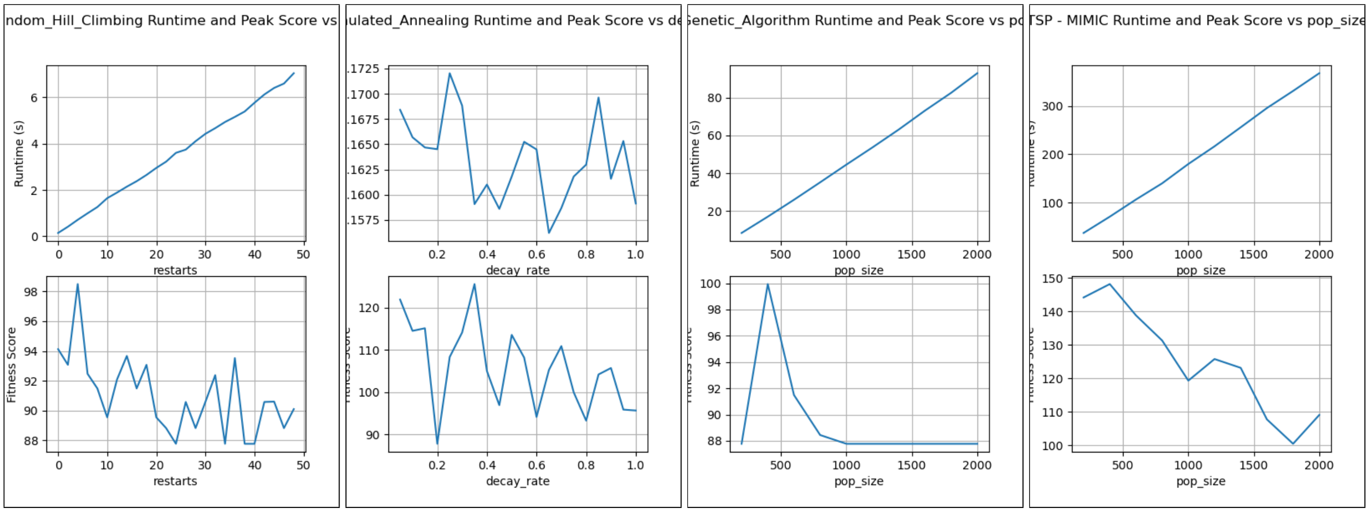
Algorithm	Final Score	Average Runtime	Avg Time to Peak
Random Hill Climb	102.2	1.121s	2.80e-4s
Simulated Annealing	120.8	0.263s	1.43e-4s
Genetic Algorithm	87.8	57.4s	0.115s
MIMIC	133.2	238s	0.952s

TSP definitely has the most surprising results compared to what I predicted. Basically the only thing I was correct about is that GA would be most accurate but slow, and SA/RHC would both be fast but suboptimal. However, I don't understand what happened to MIMIC and why it performed so poorly, nor do I understand why RHC was better than SA. Both of the gradient based algorithms are subject to chance regarding whether they would reach a global optimal, or something near the same value. They were much more likely to quickly settle on a local minimum, but I cant think of any reason why RHC would settle on a better solution than SA, since SA is more likely to explore more of the problem space. It could be related to tuning, but otherwise, it doesn't make much sense.

2.5.3 *Parameter Variation*

Even though RHC compared to other algorithms was surprising, the parameter tuning was not. It has the same linear increase in runtime, and gets closer to optimal with more restarts.

Simulated Annealing is apparently very sensitive to how the TSP problem is designed. In this configuration used, setting the decay rate to 0.4 would have resulted in a much better solution, but no real trend otherwise. It seems that having a rate too low doesn't allow it to converge, and too high means it converges too soon. It's also likely that the optimal decay rate would change based on the parameters of the TSP.



(a) (b) (c) (d)

Figure 6—TSP Parameter tuning for (a) RHC using number of random restarts, and (b) Simulated Annealing using rate of decay (c) GA using population size, and (d) MIMIC using population size

Genetic Algorithm behaved exactly as expected. Since it can explore the problem space very well, it reaches an optimal solution with higher population. It is particularly well suited to this kind of problem.

MIMIC is similar to GA in that higher population increases end accuracy, but I'm still surprised that it was not able to reach an optimal solution, even at a pop size of 2000.

3 RANDOMIZED OPTIMIZATION IN NEURAL NETWORKS

3.1 Summary

Neural Networks are an example of a machine learning model in which optimization is required. They require optimizing the weight values for each node in the network to maximize the accuracy of the model. This is another form of a fitness function, because it is an equation where parameters are being tuned to maximize some output. In the case of Neural Networks, this is normally done using backpropagation, which is similar to hill climbing, although there are some other heuristics and techniques which help prevent it from getting stuck in local optima.

Since neural networks meet the requirements of a fitness function, the same randomized optimization algorithms can be used to optimize the weights. The main difference between this and the previous problems is that neural network weights are continuous where the previous problems were all discrete. As a result, MIMIC could not be used because it requires the parameters to be discrete.

3.2 Results

For testing out these optimizers on a neural network, I have implemented a standard neural network using back-propagation, as well as one using Random Hill Climbing, Simulated Annealing, and Genetic Algorithm. To test them out, I'm using the water quality dataset (adityakadiwal,) from the Supervised Learning project.

Algorithm	Accuracy	Avg Train Time	Avg Query Time
Backpropagation	66.25%	0.7882s	2.062e-3s
Random Hill Climb	39.95%	103.4s	3.0523-4s
Simulated Annealing	60.05%	20.76s	2.241e-4s
Genetic Algorithm	60.30%	218.0s	3.207e-4s

It comes as no surprise that backpropagation resulted in the best method all around considering it is the industry standard for training neural networks. It is an optimization algorithm that is designed for this use case. That being said, the others still performed relatively well.

RHS was clearly the weakest of all of the options, which is not at all surprising. Neural network weight optimization is a continuous problem space, so it following gradients works very well, but it is usually also a very complex surface, which means there are many local maxima and minima, and a simple hill climbing approach doesn't work very well. Additionally, it doesn't even take advantage of the ability to stop training once no more improvement is made because it will just have to repeat. So some attempts may be more efficient, but others will have to run their course. As a result, it ended up being quite a bit slower than other algorithms as well.

Simulated Annealing seems to work very well, but it's still slower than backpropagation, however, that may be heavily influenced by the implementation. I attempted to set the backpropagation and SA nets to terminate early if the loss function did not continue to improve, but it did not seem to be working. As a result, the backpropagation version only required 328 iterations, while the SA version had to use the full 5000. Just doing a proportional adjustment (scaling 5000 iterations down to 328) would put SA at 1.36s for training time, which is not much more that backpropagation. I obviously can't just assume that it would require the name number of iterations, but it is worth noting that if I could have configured it to terminate early, it likely would have been much closer since the time per iteration was only a little bit higher. Either way, it still fell a little bit short when it comes to accuracy as well.

The Genetic Algorithm was once again very effective when it came to accuracy, but much slower. I'm a little bit surprised that it performed just as well as SA because it is a smooth, continuous problem space. Because of that, I assumed that a gradient based algorith such as SA would perform better than GA, but it seems that it is a complex enough space that GA is able to do more exploration and capture some relational information to help it find good solutions. It is clearly too slow for it to be an effective optimizer for Neural Networks, but it was able to get a good accuracy in the end.

4 CONCLUSION

Randomized optimization is a complex and challenging problem for machine learning. There are many different kinds of problems, each of which have their own complexities and pitfalls, making it impossible to find a sinlge solution for everything. It is no surprise that there are many different algorithms, each with their strengths and weaknesses.

Gradient based solutions such as Random Hill Climbing and Simulated Annealing perform very well on problems where there is a natural gradient, and contains a continuous problem space. They are also very fast, so if a local optimal value is good enough, as is the case sometimes, then they are very effictive at finding them.

Genetic Algorithm and MIMIC are much slower, but capture different information that is easily lost by gradient-based algorithms. There is less left up to chance since they do not need to rely on their current space as much, and instead branch out through crossover and mutation. In situations where a true, global optimal is needed, and some extra time can be spend finding it, they are very effective.

5 REFERENCES

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