A guided Monte Carlo method for optimization problems

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We introduce a new Monte Carlo method by incorporating a guided distribution function to the conventional Monte Carlo method. In this way, the efficiency of Monte Carlo methods is drastically improved. To further speed up the algorithm, we include two more ingredients into the algorithm. First, we freeze the sub-patterns that have high probability of appearance during the search for optimal solution, resulting in a reduction of the phase space of the problem, a concept inspired by the renormalization group equation method in statistical physics. Second, we perform the simulation at a temperature which is within the optimal temperature range of the optimization search in our algorithm. We use this algorithm to search for the optimal path of the traveling salesman problem and the ground state energy of the Anderson-Edwards spin glass model and demonstrate that its performance is comparable with more elaborate and heuristic methods.

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Optimization problems arise in areas of science, engineering and other fields. Many of them are NP hard problems, in the sense that the number of computing steps required to solve the problem increases faster than any power of the size of the system. The traveling salesman problem (TSP) [1], the spin glass problem [2] and the Lennard-Jones microcluster problem [3] are some of the examples belonging to this class. Over the years, people have developed heuristic methods that can allow one to possibly obtain optimal solutions in some optimization problems, e.g. the TSP. However, these methods are usually specially designed for the problem that one is seeking to solve. In many cases, these heuristic methods will either not be applicable or will take a much longer time to locate the optimal solution of the problem. In many practical situations, it is more desirable to obtain a near-optimal solution quickly than to find the true optimal solution of the problem. Furthermore, it is also preferable to have an algorithm that is simple to use and general enough to treat various optimization problems.

Since its introduction about half a century ago, the Monte Carlo (MC) method [4] has been widely used to treat optimization problems. Despite its simplicity and versatility, it is known that Monte Carlo method cannot usually give one an acceptable solution since it can easily get trapped in local minima of the problem. In the past decades, people have developed new algorithms based on the original Monte Carlo method. Simulated Annealing (SA) [5] is one of the algorithms that originates from the Monte Carlo method. Because of its simplicity and versatility, SA has been employed to study various statistical systems with success. Despite its improvement over the original Monte Carlo method, SA also suffers from a similar problem, that the algorithm can easily get trapped in local minima. Progress has been made to improve SA and Monte Carlo methods further by developing more efficient MC sampling algorithms. More recent developments include algorithms such as the multicanonical method [6] and simulated tempering [7]. All the above mentioned algorithms are meant to give a more efficient MC sampling over the original method.

In this paper, we introduce a new algorithm by incorporating the Monte Carlo method with a guided distribution function. The advantage of this new algorithm is that it is very simple to use and is generally suitable for most optimization problems, whether they involve continuous or discrete parameter spaces. The essentials of this algorithm is from both biology and theoretical physics. In the following, we will give the main ingredients of this algorithm and apply it to two problems, namely, the traveling salesman problem and the spin glass problem (SGP). The task of the TSP is to find a route through a given set of N cities. The spin glass model we are testing here is the three-dimensional Edwards-Anderson Ising spin glass model [8] in which Ising spins (Si = ±1) are placed on a three dimensional lattice and there are nearest neighbor interaction only. The corresponding Hamiltonian for this model is

\[ H = - \sum_{<i,j>} J_{ij} \sigma_i \sigma_j , \]

where in our simulation, the \( J_{ij} \) takes on values \( \pm J \) randomly and \( \sigma_i, \sigma_j \) can take values +1 or -1. The task here is to find the spin values which minimizes \( H \). As it turns out, its performance in these two tests is comparable to the more elaborate methods and it can obtain near-optimal solutions rather quickly.

A new substance in this algorithm is the addition of a guided distribution function to the original Monte Carlo method. This introduction of the guided distribution function is motivated from biology. Similar to the subject of evolutionary programming [9], this guided distribution function is based on the cooperative effort of individuals. To begin with, we have a population of \( M \) randomly
generated solutions. We let each of them evolve independently and according to the conventional Monte Carlo rules, i.e. we accept a new solution over its old solution when the new solution is better fit than the old solution. If a new solution is less fit than the old solution, we pick the new solution over the old solution with respect to a Boltzmann factor. At this point, it is equivalent to $M$ independent runs of the Monte Carlo method. In each of the $M$ individual runs, we keep record of its best fit solution while the individual solution is evolving.

After a certain number of Monte Carlo steps, a distribution function of the $M$ best fit Monte Carlo solutions will be recorded. Let us use the TSP as an example. After we perform a preset number of Monte Carlo steps, each of the $M$ independent runs has its own best fit solution, or path. In each of these paths, we record the links between any two cities. There are a total of $N$ links in each path and a total of $MN$ links of the $M$ best fit solutions. One has now a distribution function of the probability of appearance among all possible links that connects any two cities. This completes our first layer of Monte Carlo simulation. In our discussion, a layer of simulation always means a set of $M$ individual Monte Carlo runs for a preset Monte Carlo steps plus the evaluation of the distribution function that we just mentioned. The distribution function that we obtain here will be used as a guided distribution function in the next layer of Monte Carlo simulation of $M$ individual runs.

In the next layer of Monte Carlo simulation, a set of $M$ individual Monte Carlo runs is again performed. An important point here is that we also start with $M$ randomly generated solutions at the beginning of the simulation in this layer. There is however one more criterion here—that we pick the links which appear less frequent in the guided distribution function and try to change them into links with a higher probability of appearance. In practice, we pick one of the two cities that are connected with a less probable link and connect it to a city where this new link appears more often in the guided distribution function. The new solution will be compared with the old one to decide whether we keep or discard it according to the conventional Monte Carlo method. The idea behind this is simple. The more (less) often that a certain link appears among the $M$ best fit solutions, the more (less) likely that it would (not) appear in the optimal solution. One would then let a given solution evolve into solutions with links of high probability of appearance while avoiding links of low probability of appearance. The Monte Carlo method still allows enough fluctuation to search for optimal, or near-optimal solutions. After a preset number of Monte Carlo steps is performed, a new guided distribution function will again be obtained for the next layer simulation. In principle, the more Monte Carlo steps one performs in each layer, and the more layers of simulations one has, the better will be the result.

Two more ingredients can be added into this new algorithm. The first is the elimination of irrelevant degrees of freedom. Again taking the TSP as an example. There are a total of $\frac{N(N-1)}{2}$ possible links among the $N$ cities. Some of them have a higher probability of appearing in the best fit solutions while others have very low probability. We can eliminate some of the links by freezing a link between two cities that exceeds a certain probability of appearance in the guided distribution function. In practice, after the guided distribution function in a layer is obtained, one freezes links which have a high probability say, 0.8 of appearance before one performs the next layer simulation. In this way, one reduces the available degrees of freedom in the system in the next layer, thus speeds up the search process. This idea is inspired by the renormalization group equation method in statistical physics and is similar in spirit to a recent work [10] which has proposed to treat optimization problems using the idea of renormalization in statistical physics. By freezing high probability links, one can obtain near-optimal solutions within a much faster CPU time. One can unfreeze the frozen links during the simulation to avoid missing the optimal solution.

The last ingredient that we include in this algorithm is from an observation in a recent work [11]. It was [11] observed that the average first passage time to reach the global optimum of an optimization problem in Monte Carlo simulation was a U-shape temperature dependent curve. At the optimal temperature, the average first passage time to find the global optimal will be the shortest. This means that for the optimization problem one has, it is best to perform simulation at the optimal temperature so that one can locate the optimal, or near-optimal solution in the fastest CPU time possible. The reason for the appearance of such an optimal temperature can be understood as follows. At a given temperature, the system tends to stay in states near the equilibrium value determined by that particular temperature rather than going to the global optimum. As the system relaxes toward this equilibrium value, it would fluctuate around this equilibrium value. The Gaussian like fluctuation would then carry the system from its equilibrium value to the global optimum as long as there are no insurmountable barriers between them. When the simulation is performed at high temperatures, there are too many paths available and it would take the system too long to locate the path that would reach the global optimum. As the temperature lowers, the number of available paths are reduced. When the temperature further decreases, the potential barriers and traps make the system more difficult to move out of the local optima. There is therefore an optimal temperature at which the two factors balance each other and the system approaches the global optimum with the shortest time.

(1) The Traveling Salesman Problem (TSP)

Since we have already used the TSP as an example to explain the implementation of our algorithm above, we do not need to repeat the essential steps here but instead only state the parameters we used and give some comments at the end. In the simulation, we used $M = 50$
in all the TSP cases that we tested. We performed 150 Monte Carlo steps in each layer at a temperature that is near the optimal temperature in each of the cases which we give in Table I. We have tested five cases from the TSP databank [12]: d198, lin318, pcb442, rat783 and fl1577. These cases are selected from the set of sample problem instances as listed in [1]. We have performed 100 trial runs in each case and computed the average value of the best solutions obtained in each of the 100 trial runs. We also kept record of the best solution among the 100 trial runs and list them in Table I. We used 6 layers for the first three cases and 8 layers for the last two cases respectively. To make our discussion simple, we only consider 2-opt moves in our algorithm. Other moves can be considered but is not our main emphasis here.

Table I. Tests on 5 cases from TSPLIB. $T$ is the temperature used for the Monte Carlo simulation, $RQ(\%)$ is the relative quality of the average length of the best paths obtained for the 100 trial runs with respect to the optimal solutions given in TSPLIB. $Best$ is the shortest path length obtained in the 100 trial runs using the present algorithm and $Op$ is the optimal solution given in TSPLIB.

| Case   | $T$  | $RQ$  | Best  | Op   |
|--------|------|-------|-------|------|
| d198   | 10.0 | 0.0155% | 15780 | 15780 |
| lin318 | 37.5 | 0.30%  | 42029 | 42029 |
| pcb442 | 27.5 | 0.67%  | 50798 | 50778 |
| rat783 | 4.0  | 0.68%  | 8819  | 8806  |
| fl1577 | 2.75 | 0.88%  | 22273 | 22249 |

As can be seen in Table I, the algorithm can locate the optimal paths in the two cases with fewest cities, i.e. d198 and lin318 while it can obtain near-optimal solutions for the other three cases within the number of Monte Carlo steps we preset. In general, the more the individual Monte Carlo runs, i.e. the larger the $M$, and the more the Monte Carlo steps and layers one uses, the better will be the solution obtained. For example, in the case of d198, 23 out of 100 trial runs found the optimal solution when we perform 150 Monte Carlo steps in each layer. When we increased the Monte Carlo steps in each layer to 200, the average value of the best runs would now be only 0.00906% above the optimal solution with 41 out of 100 trial runs found the optimal solution. As a comparison, we have performed a simulation on the d198 case using the conventional Monte Carlo method, for 100 trial runs with 45,000 Monte Carlo steps per run. The number of Monte Carlo steps here is equivalent to the number of $M$ (50 here) times the number of layers (6 in the case of d198) times the 150 Monte Carlo steps in each layer. The average value for the best solution of the 100 trial runs is 1.07% above the optimal value and the best solution is 15843. A further increase of Monte Carlo steps to $10^3$ improves the average value slightly to 0.90% above the optimal value. This shows the superiority of the present algorithm over the conventional Monte Carlo method.

It is perhaps worth mentioning that locating the optimal or near-optimal temperature should help one perform simulations in the case of random TSP in a two-dimensional unit square or something similar. As an example, we have obtained an average optimal temperature around 0.02 over 10 configurations of the random TSP with 100 cities, when 100 Monte Carlo steps are performed in each layer of a 6 layer simulation. The optimal temperature range is however affected by the number of Monte Carlo steps and the moves (we use 2opt moves here). A rescaling of the optimal temperature range with respect to the system size, i.e. the number of cities, is also needed.

(2) The Spin Glass Problem (SGP)

Spin glasses have been a subject in statistical physics that is under intensive study. The simplest spin glass model is the Edwards-Anderson model and its Hamiltonian has been given in the above. There are exact methods available [13] for such spin glass models in two-dimensions but are not effective in three-dimensions. Estimates of the ground state energy are available for the three dimensional case [14,15] in the literature for lattice sizes up to $L = 12$ and could be used for comparison. Our task here is to use the present algorithm to estimate the ground state energy of the three-dimensional Anderson-Edwards model within a reasonable amount of CPU time. Employing our algorithm to this model is straightforward. To begin with, we have a set of $M$ randomly generated spin configuration for an $L \times L \times L$ lattice with randomly assigned $\pm J$ couplings. We again let each of the configurations evolve for a preset Monte Carlo steps and record the $M$ best solutions from the $M$ individual runs. These $M$ best solutions are then used to construct the guided distribution function. Similar to the TSP, we freeze a sub-spin configuration pattern on this three-dimensional lattice if it exceeds a certain preset probability. In this way, we reduce the spin degrees of freedom after each layer of simulation. We again randomly generate $M$ spin configurations at the beginning of each new layer. There is one thing one needs to keep in mind in constructing the guided distribution function of the spin glass problem. When all the spins on the three-dimensional lattice changes sign, the energy of the system does not change. Therefore, one needs to fix one of the spins to take on the same value for all the $M$ best solutions when one constructs the guided distribution function. For example, we can set the spin value of the $(0,0,0)$ site of the $L \times L \times L$ lattice to be 1. If a particular best solution has a value -1 for this site, then all the spins have to flip sign in this best solution before one records its spin configuration.

In our simulation, we have used $M = 15$. We have carried out simulations for $L$ ranging from 4 to 12 and the result is given in Table II. Since our purpose here is to obtain the ground state energy of the model, we
will instead perform several runs for each spin configurations and pick the lowest energy as its ground state. The number of layers and the number of Monte Carlo steps in each layer that we used will also depend on $L$. For example, for $L=6$, we used 2 layers with 150 Monte Carlo steps in each layer and 5 trial runs for each randomly assigned coupling configuration we generated. In the case of $L=8$, we used 6 layers with 200 Monte Carlo steps in each layer and 10 trial runs for each randomly assigned coupling configuration before we take the best solution as the ground state energy for that particular spin configuration. The number of Monte Carlo steps and layers for different $L$ are given in Table II.

In the simulation of the spin glass model, we have observed that unlike the case of the TSP, the temperature range in the Boltzmann factor that is most efficient to locate the ground state or near ground state energy is between $T=J$ and $T=1.1J$ for all the $L$ that we tested and we have used $T=1.05J$ for all our simulation of the spin glass model. That the optimal temperature range is not sensitive to the lattice size here is probably related to the fact that one only considers the nearest neighbor interaction in the model.

As shown in Table II, the ground state energy that we obtained by using our algorithm is comparable with the present estimate of the ground state energy of the model by using other methods. If more layers, Monte Carlo steps and trial runs are used, the result will be improved.

In this paper, we have introduced a new algorithm by incorporating a guided distribution function into the conventional Monte Carlo method. This new algorithm is both biologically and physically motivated. By evolving a population of $M$ solutions and record their best individual solutions in each layer, we are relying on the cooperative effort of the population, similar to many evolutionary algorithms such as genetic algorithms[16]. Reducing the computational phase space by eliminating irrelevant degrees of freedom of the problem as we continue our layer by layer simulation is similar to the renormalization group equation method in statistical physics. Together with the use of an optimal temperature in Monte Carlo simulation for optimization problems, which results in a speed up of optimum search processes, it proves to be a powerful new algorithm. It takes about 24 seconds and 9 seconds of a Pentium II 450 MHz CPU time to perform a trial run of the d198 of the TSP and $L=8$ of the SGP.

Tests of our algorithm in the TSP and SGP are promising. Incorporating heuristic methods into this algorithm will certainly improve the efficiency and power of its optimum search. This algorithm is very general and can be applied to many optimization problems including discrete optimization problems we tested here and optimization problems with continuous parameters. The present algorithm has been applied to the Lennard-Jones microcluster problem and can reproduce all the known ground state energy for the system sizes that the algorithm has so far tested [17]. We believe that this algorithm should be a simple and general enough algorithm that can obtain optimal or near-optimal solutions within a reasonable CPU time for optimization problems.

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**Table II. Tests on $L \times L \times L$ SG instances.** $m$ is the number of randomly assigned $\pm J$ ($J=1$ here) cases, $MC$ is the number of Monte Carlo steps in each layer and $E$ is the average ground state energy of the $M$ spin configurations. We have set $J=1$ in our simulation. We also include here the results from Ref[14,15] for comparison.

| $L$  | $m$  | $MC$ | $E$          | Ref[14]  | Ref[15] |
|------|------|------|--------------|----------|---------|
| 4    | 200000 | 50   | -1.73750(13) | -1.73749(8) | -1.7370(9) |
| 6    | 50000  | 150  | -1.77128(12) | -1.77130(12) | -1.7723(7) |
| 8    | 4000   | 200  | -1.77910(28) | -1.77991(22) | -1.7802(5) |
| 10   | 400    | 400  | -1.7831(8)   | -1.78339(27) | -1.7840(4) |
| 12   | 40     | 600  | -1.7847(14)  | -1.78407(121) | -1.7851(4) |

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