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N-City Traveling Salesman Problem: Optimization by Simulated Annealings

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The problem of finding the shortest closed path connecting N randomly chosen points is one of the classic Np-complete problems. We show that the length of tour depends logarithmically on the cooling rate Q in a simulated Monte Carlo anneal. We speculate that this is a general property of all Np-complete problems.

Key WORDS: Optimization; simulated annealing Monte Carlo.

Recently there has been great interest in combinatorial optimization using Monte Carlo (MC) simulated annealing[1] based on the Metropolis[2] algorithm from statistical physics. For problems with many constraints, simple algorithms based on iterative approaches are often not effective in finding the lowest energy state.[3] However, by making an analogy between statistical mechanics and combinatorial optimization, Kirkpatrick *et al*[1] found that by starting at high temperature[3] and cooling slowly, significant improvement over standard optimization techniques was obtained for the N-city traveling salesman problem,[1,3] the min-cut partitioning problem,[1] and global wiring.[4] The method has since been used for a wide variety of problems, including image analysis,[5] least square fitting of many unknowns,[6] and spin-glass ground states.[7]

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[3] For the traveling salesman problem the energy of a state is equivalent to the tour length. The lowest energy state is therefore the optimum tour length. Temperature is introduced as in statistical mechanics. Raising the temperature introduces disorder, thereby allowing the system to go over energy barriers.

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While it is clear that the MC method will always find the lowest energy for a finite system given enough computer time, little is known about how the final state depends on the actual annealing schedule. Most theoretical effort has concentrated on finding the optimal annealing schedule for a fixed number of Monte Carlo steps. While some progress in this direction has been made, much less attention has been paid to the dependence of this final ground state on the total number of Monte Carlo steps. Grest *et al.*[7] examined the dependence on the cooling rate of the lowest energy state for several spin glass models. In this note, we present results for a similar study of the shortest tour length as a function of cooling rate Q for the N-city traveling salesman problem, since it is one of the classic optimization problems. This problem belongs to the general class of *Np*-complete problems,[8] for which the amount of computer time to find the lowest energy state grows faster than any power law with N, the size of the system. For this reason, it has been speculated[7] that for all *Np*-complete problems, finding the lowest energy state should depend logarithmicaly on Q. In fact, we believe that a necessary condition for a problem to be *Np*-complete is that the dependence on the cooling rate to find the lowest energy state should be no faster than logarithmic. This is consistent with the results found by Grest *et al.*[7] for several spin glass models and in agreement with a theoretical analysis by Huse and Fisher.[9] While the logarithmic dependence on the cooling rate may or may not be a sufficient condition to prove a problem is *Np*-complete, it is probably a necessary condition.

Following Kirkpatrick,[3] we carried a MC simulated annealing study of the N-city traveling salesman problem in which the objective is to find the shortest closed route which that connects all N cities. The sequence of city coordinates is randomly distributed on a unit square, with the distance from s_i to s_j denoted as d_{ij} and $d_{ij} = d_{ji}$. This distance is calculated using the Euclidean metric.[10] An $N \times N$ distance matrix D is specified as $D = (d_{ij})$. Each tour through N cities is represented by γ of the set P_n of all permutations $\{1, 2, ..., N\}$. We define

$$L_{\gamma,D} = \text{total distance} = \sum_i D_{i,\gamma(i)}$$

The problem is to find $\tilde{\gamma}$ such that

$$L_{\tilde{\gamma},D} = \min_{\gamma \in P_n} L_{\gamma,D}$$

Our initial configuration is obtained using a greedy strategy, in which we start from a city chosen at random and go to the nearest city. From there the tour continues to the nearest unvisited city. After all cities are visited,

the loop is completed by returning to the starting city. Because of the long steps taken near the end, the tour length is about 20% above its optimal value. This state is then disordered further by beginning our simulations at a temperature high enough that the length of the tour increases to a value greater than 2. This is done using a Monte Carlo procedure in which a change in route is accepted with probability 1 with $\Delta l \leqslant 0$ and $\exp(-\Delta l/t)$ if $\Delta l > 0$. The initial temperature is $t = 1.2$, in scaled units, $T = t\sqrt{N}$. The length is normalized by $l = L/\sqrt{N}$. Our basic rearrangement strategy is a two city or "2-opt" replacement.[3] This operation is one in which two cities chosen at random exchange their positions in the order of the tour. The cities between these two are then traversed in the opposite direction. This operation has the effect of "flipping" the subsection with respect to the entire tour. One MC step is defined as N attempted rearrangements, chosen at random. Here we study $N = 100$ and 400.

Previous work on this problem has shown the merits of the simulated annealing algorithm.[1,3,10,12] Rather than employ the cooling schedule adopted by Kirkpatrick,[3] $T_{i+1} = AT_i$, where $A \approx 0.9$, we use a linear cooling schedule in which after a number of steps m, the temperature is reduced by an amount $\Delta T\,(<0)$. We define the cooling rate $Q \equiv -\Delta T/m$. We have also carried out simulations using the exponential cooling scheme[3] and find similar results, as described below. ΔT is chosen small enough that the final results depend only on Q and not ΔT and m seperately. At least seven cooling rates were chosen for each N and the results for l versus $-1/(\ln Q)$ are shown in Fig. 1. In Table I we present the numerical values for the data points and the number M of configurations averaged. For each random placement of the N cities, we did only one cooling run. It was necessary to average over many city configurations to reduce the standard of deviation

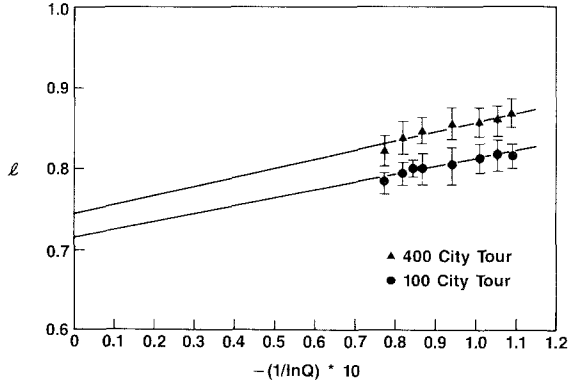

Fig. 1. Normalized tour length l versus $-1/(\ln Q)$ for $N = 100$ and 400.

Table I. Average Optimum Tour for Given Q through N Cities for M Configurations and Least Square Fit to the Results[a]

	Q	$\bar{l}$	DEV[b]	M
$N=400$	1×10^{-4}	0.86519	0.01723	25
(intercept	7.5×10^{-5}	0.85901	0.02014	30
$=0.7455$,	5×10^{-5}	0.85451	0.02201	30
$\chi^2=0.9517$)	2.5×10^{-5}	0.85330	0.02108	30
	1×10^{-5}	0.84642	0.01924	20
	5×10^{-6}	0.8379	0.02241	20
	2.5×10^{-6}	0.82103	0.02121	20
$N=100$	1×10^{-4}	0.81473	0.01730	30
(intercept	7.5×10^{-5}	0.81725	0.01930	30
$=0.7145$;	5×10^{-5}	0.81263	0.01657	30
$\chi^2=0.9517$)	2.5×10^{-5}	0.80615	0.02482	30
	1×10^{-5}	0.80104	0.01882	20
	7.5×10^{-6}	0.80092	0.01050	20
	5×10^{-6}	0.79628	0.01231	30
	2.5×10^{-6}	0.78331	0.01210	20

[a] χ^2 is the correlation coefficient.
[b] $\text{DEV}=\sum_{i=1}^{M}(|l_i-\bar{l}|/M)$.

in l. This averaging is necessary even when carrying out exact enumeration of the optimal tour. We find that reasonable values for standard of deviation can be obtained for M between 20 and 30. We also tried to fit our results to a power law dependence Q^x, where x varied from 0.3 to 0.05. The correlation coefficient was found to be monotonically increasing with decreasing x. This lends support to our belief that the underlying relation between l and Q is indeed logarithmic. When the logarithmic relation l versus $-1/(\ln Q)$ was tried, the data fit to a correlation coefficient of 0.95, and the intercepts of the graphs (0.7455 and 0.7145) were very close to the minimum length reported: 0.749 for $N=400$[10] and 0.7169 for $N=100$.[12] We compared our results using a linear cooling rate to that using the exponential cooling scheme $T_{i+1}=AT_i$ by determining an average cooling rate. The final length l using this cooling schedule falls on the curves represented by the data. In a test case of $Q\approx5\times10^{-6}$, the length l was 0.8647 for the linear cooling and 0.9110 for the exponential scheme, where the total number of MC steps was 250,000 for each. A comparison of these two cooling schemes is shown in Fig. 2.

For problems in which the final energy and not the configuration is important, this analysis can give a considerable saving on computational time. A few points can be plotted, and then the relation extrapolated to the

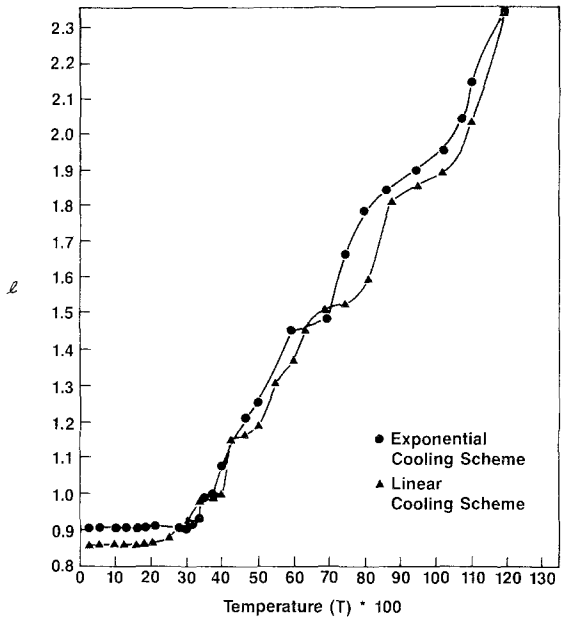

Fig. 2. Cooling curves for an exponential and a linear cooling schedule for $Q \approx 5 \times 10^{-6}$.

intercept for $Q \to 0$ to obtain the value of the lowest energy. However, as is most often the case, the final configuration is needed, and an estimate of the relative computational expense to yield a given energy or configurational improvement can easily be assesed. Thus, a study of the cooling rate dependence can give a measure of the balance between computational expense and exactness of solution.

In conclusion, we have examined a prototypical *Np*-complete problem using the Monte Carlo annealing technique. In agreement with the earlier studies of Grest *et al.*[7] for five model spin glasses, we find that for *Np*-complete problems, the lowest energy or optimal state is assessable using MC simulated annealing as $-1/\ln Q$. Our results also agree with an analytic analysis due to Huse and Fisher.[9] For problems that are complex but not *Np*-complete, the cooling rate dependence may be more rapid, as found for two two-dimensional spin-glass models.[7]

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