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Optimization by multicanonical annealing and the traveling salesman problem

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We propose a powerful and general simulated annealing method to study combinatorial optimization problems. It combines the multicanonical method, which samples directly the microcanonical entropy of the system, with an elaborate but straightforward annealing scheme. The information about the local entropy obtained during short Monte Carlo simulations is fully utilized for optimization in an iterative fashion. We present results of an extensive investigation of the traveling salesman problem in a unit square. We estimate the optimal length in the limit of a large number of cities.

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Many optimization problems that arise in various areas of science and engineering are hard to solve: Many of them belong to the NP-complete class, where the number of computing steps required to solve the problem increases faster than any power of the size of the system. One of the well-known classic examples is the traveling salesman problem (TSP), which consists of finding the shortest tour connecting N cities [1]. The TSP is widely believed to require computing time which grows exponentially with N. Perhaps the most impressive achievement in the TSP has been obtained by the branch-and-cut algorithm which has found *proven* optimal solutions in reasonable amounts of time for up to $N=2392$ [2]. In practice, however, near-optimal solutions are usually satisfactory, and it is more desirable to obtain such approximate solutions rather quickly than to find the true optimal solution. Therefore many studies have been concentrated on heuristic methods, which find near-optimal solutions in polynomial time [1]. The Lin-Kernighan (LK) algorithm [3] is known to be the best among these methods.

A decade ago some common features between optimization problems and disordered spin systems were recognized, leading to the application of the simulated annealing (SA) method [4]. This method is based on Monte Carlo (MC) simulations, which have been very successful in studying various statistical systems [5]. The method also leads to analytical studies via statistical mechanics [6] as well as other approaches such as algorithms based on neural networks [7–9], genetic algorithms [10,11], and simulated tunneling [12]. In reality, the SA may be outperformed by the best heuristic (deterministic) algorithms for a specific optimization problem. For example, it has been claimed that the iterative LK algorithm finds better solutions of the TSP [13]. Nevertheless, the SA is far superior to the heuristic algorithms in its *simplicity* and *versatility*. Owing to this character, the SA has been applied not only to the canonical optimization problems such as graph partitioning, graph matching, and the TSP [4,14,15], but also to various optimization problems [16,17]. It is thus desirable to improve the SA so that it is *both efficient and versatile* by considering more efficient algorithms and annealing schemes. Conventional importance sampling [18] may fail to access all the possible near-optimal configurations if there exist many barriers among them; this is believed to be the case for hard optimization problems such as the TSP.

Recently, significant progress has been achieved in the search for more efficient MC sampling algorithms. Valleau and co-workers [19] introduced umbrella sampling to successfully investigate the Lennard-Jones system over a wide range of temperatures and densities. Berg and Neuhaus [20] introduced the multicanonical method (MM) to study systems with strong first-order transitions and demonstrated its efficiency. A method related to the MM has also been proposed by Hüller [21]. Berg and Celik [22] further applied the MM to study thermodynamic properties as well as ground-state properties of the two-dimensional Edward-Anderson spin-glass model, indicating the relevance of the MM for disordered systems. Marinari and Parisi [23] proposed simulated tempering as an optimization scheme. Berg also proposed a random-cost approach [24].

In this paper we present a powerful and general SA method based on the MM [22]. In particular, we follow the notation of Ref. [25]. The MM allows one to sample the density of states $\Omega(E)$ directly by imposing the appropriate detailed balance condition. One can show [25] the sampling distribution of E to be independent of E, if the ratio of the transition probability W is chosen as

$$\frac{W(x\rightarrow x')}{W(x'\rightarrow x)}=\exp\{-[S(E(x'))-S(E(x))]\}, \qquad (1)$$

where the entropy $S(E)$ is defined as $S(E)=\ln\Omega(E)$ [26]. The framework of the current optimization method is based on the feedback of information about the *local entropy* as described in the following schematic procedure: (i) Assume the system is in a particular local minimum A. (ii) Obtain

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new information on the local entropy S near A via a short MC sampling to update the old value of S. (iii) Modify the transition probability of the MC move according to the new S so with a high probability the system is driven out of A and falls into a new local minimum A'. (iv) Iterate the three steps until a chosen convergence criterion is met.

This optimization method, which we call *multicanonical annealing*, is applied here to the classic traveling salesman problem. It turns out to be very efficient, yielding better approximate solutions more quickly than conventional SA. We consider the classic Euclidean problem of N cities randomly distributed inside a unit square for N up to 40 000. The minimal tour length $l_m(N)$ was shown [27] to scale as $l_m(N)=\alpha\sqrt{N}$ in the large-N limit. However, there has not been much progress on the estimate of $\alpha(N)\equiv l_m(N)/\sqrt{N}$ for a given N, not to mention the estimate of the limiting value $\alpha(N\rightarrow\infty)$. First, one has to find an "optimal" tour length $l_m(N)$ for a given random configuration of N cities. Then the variation of $l_m(N)$ due to the randomness of the configurations needs to be carefully studied. A commonly cited value of $\alpha(N\rightarrow\infty)$ is 0.749 [27]. In much of the literature [1,11,14], 0.749 has been considered to be the "optimal" solution for all N, with which solutions obtained have been compared. Recently, Krauth and Mèzard used the cavity method to obtain $\alpha(N\rightarrow\infty)=0.7251$ for a different version of the TSP, where the symmetric distance matrix is distributed uniformly between 0 and 1 [6(b)]. A special case of that problem was then argued to be mapped onto the current problem. We find that $\alpha(N\rightarrow\infty)$ from our numerical study agrees reasonably well with 0.7251, and rules out the value 0.749.

In conventional SA, directed cooling is achieved by slowly lowering the temperature coupled to the function l to be minimized. Here, we place a hard wall potential on the other end of the annealing direction, rejecting all attempts beyond the wall. We define l_{max} as the location of the wall, and l_{min} as the optimal l obtained thus far in our annealing process. Annealing is achieved by reducing the value of l_{max} (moving the wall in the annealing direction) as a better value of l_{min} is obtained. This allows one to control the size of the sampling interval. If the interval chosen is too small, then ergodicity can be questioned in the MC procedure when one is interested in finding the equilibrium properties of the system. For the purpose of annealing, however, it does not matter as long as one can anneal the system efficiently. For problems like the TSP, ergodicity is neither satisfied in the conventional MC procedure, nor in the MM due to the complicated frustration at low temperatures. We choose the size of the sampling interval to be fixed and large enough to allow important fluctuations throughout the annealing process, whereas the corresponding interval for conventional SA becomes smaller as the temperature is lowered (it eventually vanishes at zero temperature).

In general, we do not know the value of the entropy S. In fact, obtaining the global S is equivalent to solving the problem. Nevertheless, it is rather easy to approximate S locally by Eq. (2) below [25]. We treat the intercity distance as a real number while the total tour length l is discretized to define histogram $H(l)$ and entropy $S(l)$. We describe the overall algorithm as follows.

(1) Start with an arbitrary tour configuration. In the case of the TSP, we have been able to use the configuration from the exhaustive two-bond optimization [28], which on average has about a 5% longer length than the final result. For conventional SA, the starting configuration is of longer length. This advantage is due to the point that in the MM the ergodicity problem can be alleviated to some extent by helping the system escape quickly from local minima by Eq. (2) below. We set l_{max} to be between 1% and 10% longer than the result from 2-opt heuristics. The precise value of l_{max} is not important as long as it is large enough. Initially the entropy $S(l)$ is set to be a constant for all properly discretized lengths l. Observing that the distance between neighboring cities scales as $1/\sqrt{N}$, we multiply the tour length by $10\sqrt{N}$ and set it to an integer. We have also made a lookup table, which lists the 20 nearest cities for each city.

(2) Use the 2-bond move, which reverses the sequence of cities for a chosen segment, in order to obtain trial tours. Suppose that the current tour is given by $(c_1,c_2,\ldots,c_N)$. For a randomly selected city c_i, we choose a city c_j, one of the 20 nearest cities of c_i excluding the adjacent cities in the path (i.e., $j\neq i\pm1$). We consider a 2-bond move which replaces the two bonds (c_i,c_{i+1}) and (c_j,c_{j+1}) by (c_i,c_j) and (c_{i+1},c_{j+1}). We use the heat-bath MC algorithm by considering all 20 neighbors from the lookup table. The new tour of length l is chosen out of these trial tours and the current tour with the probability proportional to $\exp[-S(l)]$. If the new length is larger than l_{max}, the new tour is rejected (due to the hard wall potential).

(3) Repeat step (2) for M MC sweeps (MCS's) while obtaining a histogram of the distribution of l from the MN events. Typically we have used $M=25$.

(4) The new estimate of $S(l)$ is now given by

$$S(l)=\begin{cases} S(l) & \text{for } H(l)=0, \\ S(l)+\ln H(l) & \text{otherwise,} \end{cases} \tag{2}$$

where $H(l)$ is the (unnormalized) histogram of the sampling and $S(l)$ on the right hand side of Eq. (2) is the old value of $S(l)$. If l_{min} is the minimum tour length obtained so far, then for $S(l)$ with $l<l_{min}$, $S(l)$ is obtained by linear extrapolation with the slope $[S(l_{max})-S(l_{min})]/(l_{max}-l_{min})$. This procedure expedites the movement of the system in the desired direction. If we choose a steeper slope, the rate of updating l_{min} increases in the early stage, but the final result of the minimum tour length appears to be of relatively poorer quality than that obtained with a shallower slope. This effect, along with that of the size of the interval, may be compared to the fast and slow cooling rates in conventional SA.

(5) The new l_{max} is chosen so that l_{min} and l_{max} form a new interval with a fixed difference of $5\sqrt{N}$. If the length l_c of the current tour is longer than the new l_{max}, the latter is set equal to l_c.

This defines one iteration. With the new estimate of $S(l)$ and l_{max} one repeats the iteration (2)–(5) until it fails to find a better tour for 20 consecutive iterations. Here the number 20 is completely arbitrary, and a more elaborate annealing schedule should improve the results. It is interesting to observe that Eq. (2) makes the local minimum flat and helps the system to escape out of it. The current annealing scheme is

TABLE I. Performance of the multicanonical annealing for the TSP with N cities in a unit square. n is the number of independent random configurations. σ corresponds to the one standard deviation of the mean $\alpha(N)$.

N	n	$\alpha(N)=l/\sqrt{N}$	σ	MCS
50	1300	0.8075	0.0010	1100
64	900	0.7968	0.0010	1300
81	700	0.7886	0.0010	1400
100	600	0.7802	0.0009	1500
121	500	0.7754	0.0009	1700
144	400	0.7704	0.0010	1800
200	300	0.7639	0.0009	1900
256	200	0.7594	0.0010	2100
400	120	0.7515	0.0010	2500
900	80	0.7418	0.0007	3300
1600	50	0.7362	0.0007	4700
2500	25	0.7331	0.0008	5400
10 000	8	0.7278	0.0007	8600
40 000	4	0.7239	0.0004	22 000

based on the learning process by the feedback of information on the local entropy in Eq. (2).

In Table I, we summarize the performance of the multicanonical annealing method, which is mainly due to the elaborate but straightforward annealing strategy of (i)–(iv) with the cooling scheme as explained above. Note that only 22 000 total MCS's have been used for $N=40\,000$. It is important to obtain information about the entropy of the current local minimum quickly, so that the system can easily escape from it. This is based on the fact that the systems under consideration are not ergodic, especially near ground states. Since there exist many tours with comparable lengths which do not belong to the same local minimum, it is necessary to update the information about the local entropy very frequently.

Figure 1 shows the annealed configuration for $N=10\,000$ with a tour of length $l=72.56$. In Fig. 2 we plot $\alpha(N)\equiv l/\sqrt{N}$ as a function of $1/\sqrt{N}$, assuming $l(N)=\alpha\sqrt{N}+\beta$ [27], where $\alpha\equiv\alpha(N\to\infty)$. We find a good straight line fit with $\alpha=0.7211(3)$ and $\beta=0.604(5)$. Our

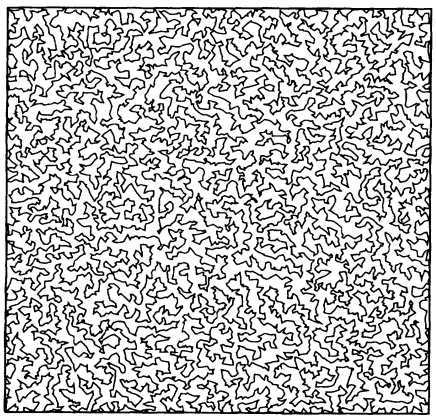

FIG. 1. Annealed tour for $N=10\,000$ with $l=72.56$.

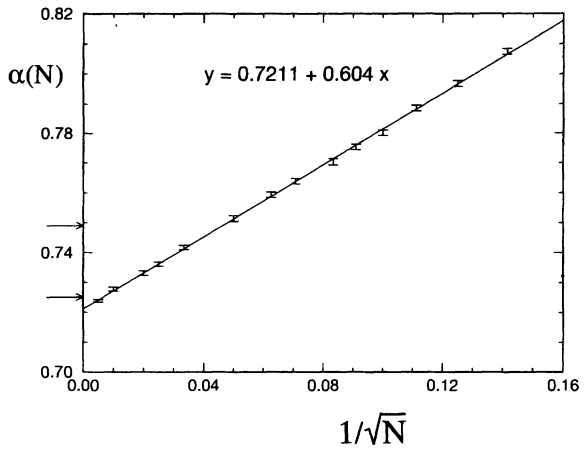

FIG. 2. $\alpha(N)$ vs $1/\sqrt{N}$. Arrows indicate the commonly cited value 0.749 in Ref. [27] and the predicted value 0.7251 in Ref. [6(b)]. Even though 0.7251 is in fair agreement with our estimate 0.7211, the exact value should be somewhat smaller than 0.7211 since this work provides only an upper bound.

value for $\alpha=0.7211(3)$ is slightly smaller than 0.7251 by Krauth and Mèzard [6(b)]. The commonly cited value $\alpha(N)=0.749$ is neither accurate nor appropriate since $\alpha(N)$ depends on N. We have performed a systematic finite-size scaling analysis [29] for the TSP. The variance of the true optimal l is expected not to scale with N [27]. The empirical variance from Table I, $[\Delta l(N)]^2=Nn\sigma^2\sim 0.05(1)$, is indeed independent of N.

Although our data serve only as an upper bound for the TSP in a unit square, the results are overwhelmingly better than existing large scale TSP studies [9,14] using the conventional SA method. It should also be noted that the direct approach by the conventional SA method takes too long to obtain reasonable results for the large scale TSP, and some tricks such as the divide-and-conquer strategy are often used [1,14]. This strategy divides the cities into a set of subregions, and solutions are obtained by combining the solutions of subregions. The only source we have been able to find for comparison with our results is Ref. [14], where the tour length $l=76.3$ was obtained for $N=10\,000$ by dividing the data into 4096 subdivisions. Our average result $l=72.8$ is shorter than $l=76.3$ by almost the perimeter of the unit square. We also find that the computer time used is quite small compared to the conventional SA method [8,9,11]. For $N>2500$, we had to compute the intercity distances each time due to the limited memory. Notwithstanding this restriction, our results for $N=10\,000$ took about 7 CPU hours on a single IBM 340h workstation, which corresponds to 8600 MCS's.

Even though our results represent a major improvement over those obtained using the conventional SA approach, there are also other ingenious approaches based on heuristics. For the same realization of $N=31\,623$, with 20 000 MCS's we found a tour of $\alpha(N)=0.723$, which is only slightly better than the average result of the LK heuristics by Johnson; the latter took about 67 s in a large-memory workstation. Using the iterative LK procedure, Johnson has obtained a tour of $\alpha(N)=0.716$ with 16 h of CPU time. Even

so, we believe that our annealing method is very powerful, not only due to its versatility but also its efficiency. There are numerous ways that one could improve our results, for example by optimizing the annealing schedule or, more importantly, by developing more efficient moves than the 2-bond move we used. Most importantly, our annealing method has wide applicability, since it can be applied to any optimization problem to which the conventional SA method is applicable. Our approach is certainly more general than a particular heuristic algorithm such as the iterative LK algorithm. It should be very interesting to see our annealing method applied to various optimization problems with more complicated cost functions and to compare the results with those from problem-specific heuristics.

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