STOCHASTIC VERSUS DETERMINISTIC UPDATE IN SIMULATED ANNEALING

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We propose an algorithm which has several of the characteristics of simulated annealing but whose updating rule is deterministic. The results of the comparison between the two algorithms indicate that the stochasticity of the Metropolis updating in the simulated annealing algorithm does not play a major role in the search of near-optimal minima.

Since simulated annealing was proposed in 1983 by Kirkpatrick et al. [1], it has been one of the most popular heuristic algorithms for finding near-optimal solutions of combinatorial optimization problems. Its popularity is mainly due to the generality of the algorithm. Simulated annealing has been successfully applied to an enormous variety of optimization problems, ranging from the classical traveling salesman problem [2,3] to learning in neural networks [4,5]. Consider the problem of minimizing the cost function $E(\{S\})$ where the set of variables $\{S\}$ describes a configuration of the problem. Starting with an arbitrary configuration $\{S\}$ one generates a new one $\{S'\}$ through some rearrangement which depends on the specific problem under analysis. In the iterative improvement strategy the new configuration is accepted, i.e. replaces the old one only if $\Delta E \equiv E' - E \leqslant 0$. A new rearrangement is then tried and the process is repeated until no further improvement is possible. Usually the algorithm gets trapped in a poor local minimum of the cost function. To escape from the local minima Kirkpatrick et al. [1] have employed a *stochastic* acceptance criterion, the Metropolis updating [6], which may accept a new configuration of higher cost than the previous one. The probability of acceptance of the new configuration is

$$P(\{S'\}) = \exp(-\Delta E/T), \quad \text{if } \Delta E > 0\,, \qquad = 1, \quad \text{otherwise}\,, \tag{1}$$

where T is a parameter which has the same role as the temperature in a thermodynamic system. For high T the configurations are equiprobable and the algorithm can visit practically all of them. By decreasing T one can reduce the number of accessible configurations until the algorithm freezes in a low-cost configuration. In analogy with the process of crystalization of a fluid, one expects that if the annealing process (Monte Carlo cooling) is realized slowly enough the algorithm will find a near-optimal solution. The annealing schedule is determined by the choice of the initial temperature T_i, the number of rearrangements attempted at each temperature $\mathcal{N}(T)$ and the geometrical ratio with which the temperature is decreased, α.

Although the choice of the Metropolis updating, eq. (1), has led to fruitful analogies between combinatorial optimization problems and disordered

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thermodynamic systems (spin-glasses) it is not clear whether the stochasticity of the updating rule, so essential to generate the Gibbs distribution at equilibrium, plays any important role in the search of near-optimal solutions. In fact, studying the mean-field equations for the site magnetization of an Ising spin-glass, Soukolis and co-workers [7,8] have observed that it is enough to follow the unique high-temperature state during the cooling process to find good minima. This result clearly emphasizes the role of the cooling process rather than the details of the updating rule.

In order to present a more straightforward support to the idea that the stochasticity of the updating rule is not essential to the good performance of simulated annealing we propose a *deterministic* updating rule which accepts rearrangements leading to higher cost configurations at high T and is reduced to the iterative improvement algorithm at $T=0$,

$$P(\{S'\})=0, \quad \text{if}\ \Delta E>T\,, \qquad =1, \quad \text{otherwise}\,. \tag{2}$$

Since it is the value of T which solely determines the acceptation of a rearrangement we refer to eq. (2) as *threshold* updating. In the following we compare the performance of this algorithm with the standard simulated annealing of eq. (1) in the optimization of two different NP-complete problems. The first is the Euclidean traveling salesman problem (TSP) which is stated as follows: given a list of N cities and the distances among them we have to find the tour or permutation P of the cities which minimizes the total length

$$E_{\text{TSP}}=\sum_{i=1}^{N} d_{P(i)P(i+1)}\,, \tag{3}$$

where $P(N+1)\equiv P(1)$ and $\mathbf{d}$ is the matrix of the Euclidean distances between the cities. We have studied the 30 city TSP depicted in fig. 1, where the coordinates of the cities were chosen randomly inside a square of side 10^4, and the Lin–Kernigham 318 city TSP [9,10] whose optimal tour is known. The second problem we study is the layout problem of Nugent et al. [11] which consists in the placement of 30 chips in a rectangular grid with 6×5 bins. Each chip is connected to the others by a variable number of wires specified by a symmetric matrix $\mathbf{c}$ whose

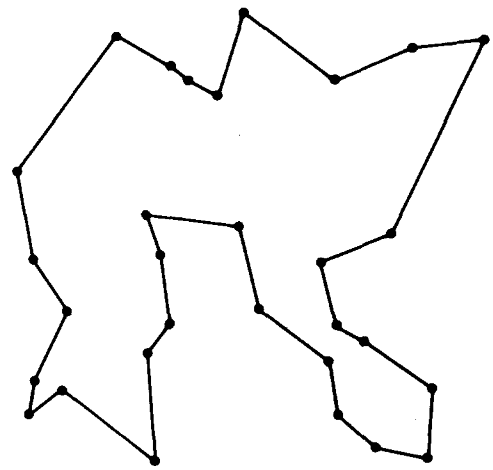

Fig. 1. The coordinates of the 30 cities were chosen randomly inside a square of side 10^4. The depicted tour is the best solution (48873) found by both algorithms.

elements are randomly chosen between 0 and 10. The goal is to minimize the total length of wires given by

$$E_{\text{NUG}}=\sum_{i,j=1}^{30} c_{ij}d_{P(i)P(j)}\,, \tag{4}$$

where P is again a permutation matrix and $\mathbf{d}$ is the matrix of the rectangular (Manhattan) distances between bins in the grid. Before presenting our results we describe our annealing schedule and rearrangement move.

Since the solutions of any matching problem can be presented by a permutation matrix, we choose a rearrangement move which interchanges two randomly chosen columns of the permutation matrix. In the context of the TSP, this move is known as *hyperswap* [12] and corresponds to the interchange of two cities, resulting in the deletion of four links and in the creation of another four. Hyperswap seems to be worse than the classical inversion of a substring (2 optimal move) [13] which changes two links and therefore breaks fewer links. We are aware of better moves for the TSP [14,15] but we have chosen hyperswap for its generality.

The choice of the initial temperature T_i is based on the following procedure. The ratio r between the number of accepted rearrangements with $\Delta E>0$ and the total number of attempted rearrangements with $\Delta E>0$ is measured for several temperatures. We pick

Table 1
The results for the 30 city TSP of fig. 1 for $\mathcal{N}=9\times10^2$ averaged over 10^3 initial tours, and for $\mathcal{N}=9\times10^3$ averaged over 10 initial tours. The numbers between parentheses indicate the number of times the algorithms reached the minimum length tours.

	Updating	Average length	Standard deviation	Minimum length
$\mathcal{N}=9\times10^2$	Metropolis	50817	1909	48873 (130)
	threshold	51589	2167	48873 (176)
$\mathcal{N}=9\times10^3$	Metropolis	49764	1084	48873 (3)
	threshold	48939	209	48873 (9)

T_i as the temperature where $r=0.1\pm0.01$. This procedure avoids wasting time in the high-temperature regime ($r\approx1$) where no important decisions are made. We have tried larger values of r but we have not observed any significative change in the final cost of the tours.

The geometrical ratio is fixed as $\alpha=0.99$ in all the simulations and the number of attempted rearrangements $\mathcal{N}(T)$ was chosen independent of T. The comparisons are made using the *same* annealing schedule in both algorithms.

The results for the 30 city TSP are presented on table 1 where $\mathcal{N}=9\times10^2$ and the average is realized over 10^3 different initial random tours. Table 1 also presents the results for $\mathcal{N}=9\times10^3$ and the average is over 10 initial random tours. As expected, not only the average tour length is improved when $\mathcal{N}$ increases but also the statistical fluctuations are greatly reduced since the algorithm loses the memory of the initial tour due to the large number of accepted rearrangements. These results show that within the statistical error the algorithms are equivalent though the threshold updating found the (supposed) optimal tour more times than the Metropolis.

To better compare these algorithms we show in figs. 2 and 3 the dependence on the temperature of the tour length (E_{TSP}) and of the ratio of acceptance (r), respectively. These figures seem to corroborate the mean-field scenario (at least for low T) with the threshold updating always close to the bottom of a minimum (it has the lowest average cost) while the Metropolis jumps to nearby minima (it accepts more rearrangements) resulting in an average cost which is higher than if it just remained close to the bottom of one of the minima.

In fig. 4 we plot the size of the typical variations of the tour length,

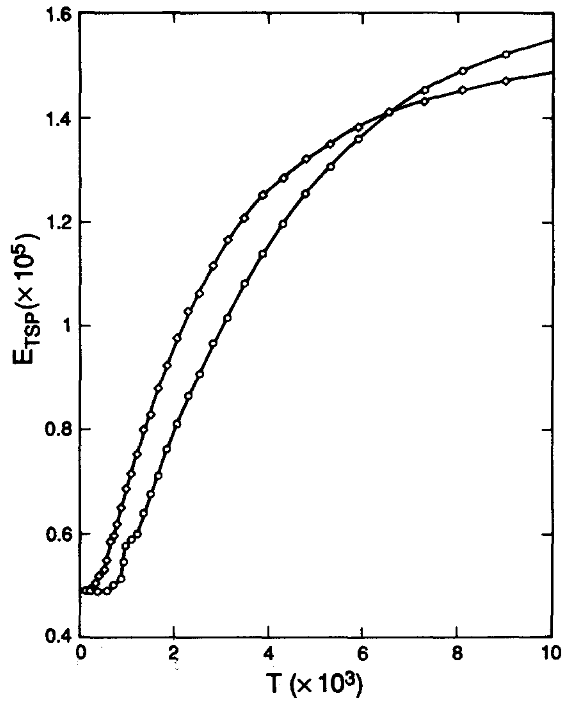

Fig. 2. The average tour length E_{TSP} as a function of the temperature T for the Metropolis updating (◇) and for the threshold updating (○). The data are from the 30 city TSP.

$$C=\frac{\langle E^2_{TSP}\rangle_T-\langle E_{TSP}\rangle^2_T}{T^2} \quad (5)$$

as a function of T for the threshold updating. In contrast to the Metropolis updating, the signaling of ordering occurs through jumps instead of peaks in the "specific heat". We think that these jumps are related to the existence of clusters in the configuration (tour) space of the TSP. For instance, consider two clusters C_1 and C_2, each one containing a large number of tours. If there exists only one way for the al-

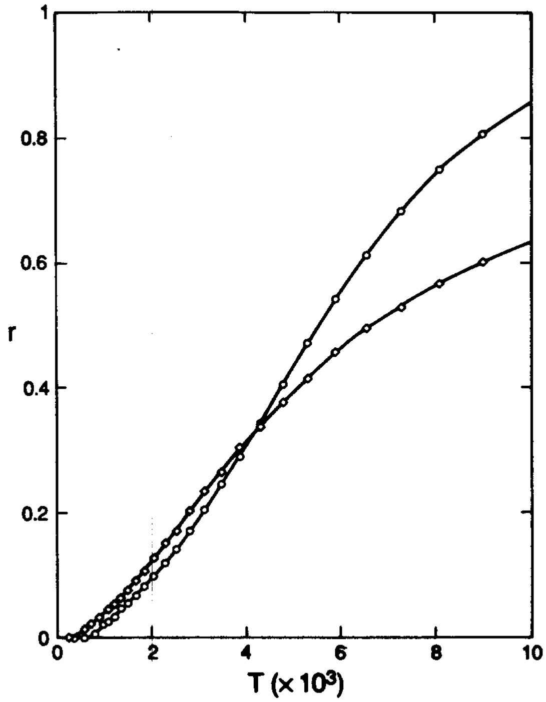

Fig. 3. The average ratio of acceptance r as a function of T measured in the 30 city TSP for the Metropolis updating (◇) and for the threshold updating (○).

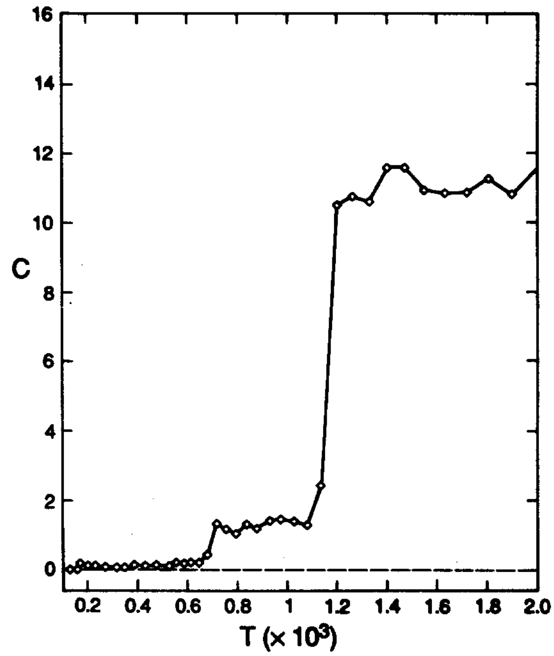

Fig. 4. "Specific heat" of the threshold updating as a function of T. Data from the 30 city TSP.

gorithm to access any tour in C_2 from C_1 and it involves the acceptance of a rearrangement with $\Delta E_{12}>0$ then for $T\leqslant\Delta E_{12}$, where the algorithm cannot accept such a rearrangement, there will be a sudden reduction in the number of accessible tours producing the observed jumps in C.

Now we consider the 318 city TSP. The length of the optimal tour is 41345. Our results, averaged over 20 initial random tours, are presented in table 2 for $\mathcal{N}=9540$ and for $\mathcal{N}=318\times10^2$. The minimum lengths were found only once and are, respectively, 35% and 21% higher than the optimal. Unfortunately we have not found any results in the literature of simulated annealing studying this instance of the TSP to compare the effects of different sets of moves and different annealing schedules. Again, the algorithms proved to be equivalent within the statistical error and the threshold updating found a better minimum than the Metropolis.

The results for the layout problem are presented in table 3 for $\mathcal{N}=9\times10^2$ and the average is over 10^2 initial random configurations. This problem is as computationally expensive as the 318 city TSP due to the double summation in eq. (4). Our average

Table 2
The results for the 318 city TSP averaged over 20 initial tours for $\mathcal{N}=9540$ and $\mathcal{N}=318\times10^2$. The optimal tour length is 41345.

	Updating	Average length	Standard deviation	Minimum length
$\mathcal{N}=9540$	Metropolis	60700	2513	56921
	threshold	60000	2702	55341
$\mathcal{N}=318\times10^2$	Metropolis	54205	1609	52390
	threshold	54308	1739	49412

Table 3
The results for the 30 chip layout problem for $\mathcal{N}=9\times10^2$ averaged over 10^2 initial configurations.

	Updating	Average	Standard deviation	Minimum
$\mathcal{N}=9\times10^2$	Metropolis	6158	22	6124 (5)
	threshold	6171	30	6124 (2)

E_{NUG} compares favourably with the best result of Nugent et al., $E_{NUG}=6186$ [11]. The performance of the algorithms seems to be equivalent although, for this problem, the Metropolis reached the (supposed) lowest cost configuration more times than the threshold updating.

Finally we remark that the threshold updating is faster than the Metropolis because it does not need the generation of a random number and the evaluation of the exponential in eq. (1), although the gain in speed is considerably reduced in those problems where the computation of the energy change is the main time consuming step. The analytical study of the threshold updating promises to be much harder than the studies carried out for the Metropolis updating [16], since the former algorithm does not satisfy the detailed balance.

Summarizing, our results indicate that the stochasticity of the updating rule in the simulated annealing algorithm *does not* play a major role in the search of near-optimal minima. It seems to us that the smoothening of the cost function landscape at high temperature and the gradual definition of the minima during the cooling process are the fundamental ingredients for the success of simulated annealing.

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