Adaptive Simulated Annealing for Maximum Temperature*

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Abstract – *It is difficult to determine the appropriate temperature parameters which control the acceptance probability in Simulated Annealing, which is a typical meta-heuristic method in the optimization methods. In this paper, we propose a new simulated annealing method that determines the maximum temperature adaptively. The proposed method is base on an important temperature where optimum solutions were sought effectively. The proposed method determines the maximum temperature by finding an upper limit of the important temperature in a heating process from the lowest temperature. Using this method, the total annealing steps can be decreased to half without making the accuracy of solution worse. We apply this method to some of the Traveling Salesman Problems and confirmed its effectiveness.*

Keywords: Modified Algorithm, Optimization, Simulated Annealing, Combinatorial Optimization, Adaptive Temperatures, Traveling Salesman Problems.

1 Introduction

Recently, heuristic search methods such as genetic algorithms (GA) and simulated annealing (SA) are becoming very important for solving complicated real-world problems[14]. Among various heuristic search methods, GA and SA are typical and widely-used optimization methods. However, GA and SA have different search mechanisms and therefore their effectiveness varies for different types of problems. The key features in GA are the evolution of a population of solutions and the crossover of solutions, while the key features in SA are the neighborhood search of a current solution and the probabilistic acceptance of a bad solution. Therefore, GA is suitable for the problems that have partial solutions, and SA is suitable for the problems that is hard to solve with GA. For example, SA is very popular for the search for the tertiary structures of protein[8].

It was Kirkpatrick et al. who first proposed simulated annealing, SA, as a method for solving combinatorial optimization problems[9]. It is reported that SA is very useful for several types of combinatorial optimization problems. However, the most remarkable disadvantages are that it needs a lot of time to find the optimum solution and it is very difficult to determine the proper cooling schedule[5].

For continuous optimization problems, reduced computation time can be realized by using sophisticated generating functions such as the very fast simulated re-annealing[6, 7], but we can not use such approaches for discrete optimization problems. For discrete optimization, the generation of a new solution is determined by defining the operation for changing the current solution. Therefore, we can control only the temperature schedule.

The most appropriate temperature schedule has the following characteristics: sufficiently high maximum temperature, sufficiently low minimum temperature, and sufficiently slow cooling[2, 10, 11]. However, this type of temperature schedule has one drawback, that is, a long computation time. There are three approaches to reduce the computation time. They are: 1) to decrease the maximum temperature, 2) to increase the minimum temperature, 3) to increase the cooling rate. Among those, the minimum temperature is generally determined by the acceptance ratio during the SA process, that is, the temperature is decreased until the system is 'freezed'. Therefore, the first and last approaches are promising. Klebsch et al. proposed a new method for estimating the maximum temperature by using equilibrium dynamics[15], and Romeo et al. proposed an efficient cooling method[4], but these methods use experimental parameters and some tuning of these parameters is necessary.

From this point of view, a new SA method with adaptive maximum temperature is proposed in this paper. In conventional SA, the maximum temperature is determined based on the acceptance ratio such that it should be more than 0.9 for all movements or it should be 0.5 for the worst movement [16]. However, this criterion is experimental, and the maximum temperature determined by such methods can be considered to be too high. The proposed method can yield the lowest maximum temperature for various combinatorial problems

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without experimental parameters.

2 Important Temperature Region

The most important characteristic of SA is the probabilistic acceptance of a bad solution. The probability of acceptance of a newly generated solution, P_{AC}, is as follows.

$$P_{AC} = \begin{cases} 1 & if \Delta E < 0 \\ \exp\left(-\frac{\Delta E}{T}\right) & otherwise \end{cases} \quad (1)$$

This type of criterion is called the Metropolis's Criterion[13], and ΔE is the change in the energy, T is the temperature.

In SA, a particular temperature region where the search can be performed very effectively exists [1]. It is called the important temperature region in this paper. In order to find the important temperature region, some traveling salesman problems (TSPs) are solved by a SA with constant temperature, where the neighbor is generated by using the 2-change method[12]. The temperature range is from 1E-6 to 1E+6, and the range is divided into 32 temperatures. The annealing steps are 3200n, where n is the number of the cities. Figure 1 shows the solutions to a TSP (ch150 in TSPLIB [3]) obtained by SA with constant temperatures. The results are the averages on 30 trials. At around the temperature of 10 the solution becomes the optimum, and such temperature is the important temperature for ch150 problem. Table 1 shows the important temperature regions, T_{imp}, of various TSPs, where the error ratio is the ratio of the difference between the solution obtained and the exact solution to the exact one. From this table, it is found that every TSP has its own important temperature region, and relatively good solutions can be obtained with this constant and important temperature.

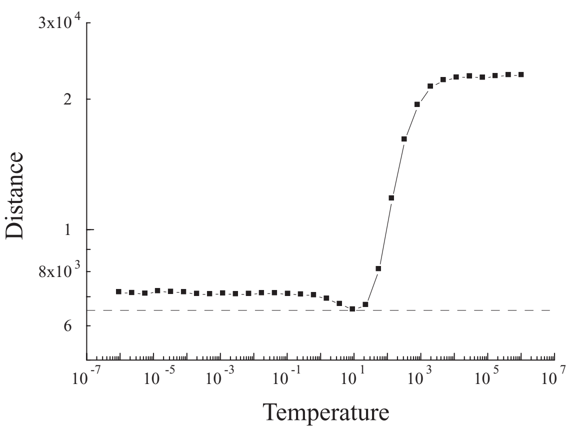

Figure 1: Effect of constant temperatures in SA

Table 1: Important temperature region

Problem	T_{imp}	Error ratio
a280	1.5～5	0.85
ch130	5～20	1.06
ch150	6～18	0.51
d198	4～20	0.36
eil51	1～4.5	0
gil262	1.2～3	1.26
kroA100	30～80	0.27
pr76	130～600	0.19
pr144	75～250	0.37
u159	60～150	0.74

In SA, the maximum temperature should be sufficiently high in order to escape local optima, but an excessively high maximum temperature wastes computational time. The relation between the important temperature region and the maximum temperature is investigated for some TSPs. The results are shown in Fig. 2, where the final tour distance of TSPs and the number of annealing steps are shown as the function of the maximum temperature. Each value is the average of 30 trials. The maximum temperatures are varied from 1E+6 to 1E-6 with 32 divisions. The shaded area represents the important temperature region of each TSP. The maximum temperature of 1E+6 is determined by the conventional method.

It is clearly found that the maximum temperature that is higher than the important temperature region provides good solutions, and the maximum temperature lower than the important temperature does not. Therefore, it can be concluded that the effective maximum temperature must be higher than the important temperature region and the lowest maximum temperature should be the upper bound of the important temperature region. If we can find this lowest maximum temperature before or at the beginning of searching an optimum, the number of annealing steps can be reduced to roughly half. That is, the maximum temperature determined by a conventional method is excessively high, and massive computation is consumed ineffectively.

3 SA with an adaptive maximum temperature

From the above result, the lowest maximum temperature is found to be the upper bound of the important temperature. However, each problem has its own important temperature regions, and a lot of experiments have to be performed to find them. Therefore, we have to find a characteristic movement of the solutions during the annealing. The histories of the solutions to some typical TSPs are investigated here. The temperature schedule is conventionally determined as follows.

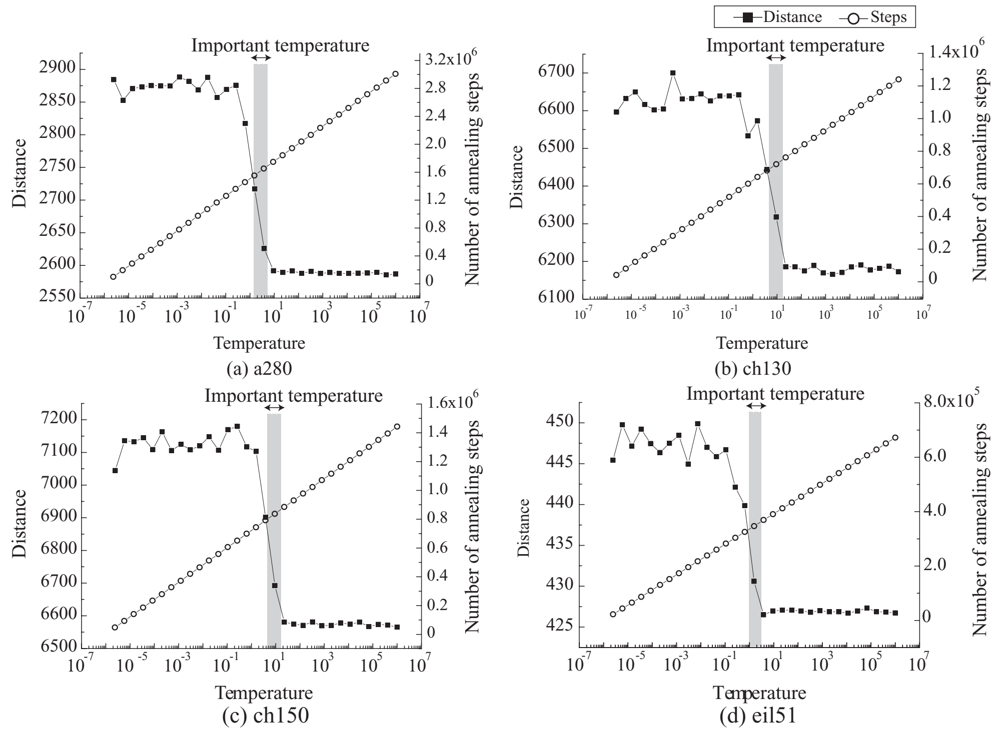

Figure 2: Relation between the accuracy of solutions, the number of annealing steps and the maximum temperature

- **Maximum temperature**:
  The temperature where the acceptance probability for the worst transition is 0.5.
- **Minimum temperature**:
  The temperature where the smallest bad transition is accepted once in the cooling interval.
- **Cooling interval**:
  20 times the number of cities in a TSP.
- **Termination condition**:
  160 times the cooling inteval.
- **Cooling rate**:
  Determined by 160 divisions of the range between the maximum and minimum temperatures, and therefore it differs from 0.93 to 0.96 depending the problems.

Figure 3 shows the typical history of the energy (tour distance) during conventional annealing for a TSP(kroA100), where the shaded area represents the important temperature region. All other results are similar to this result, and we cannot have no sign about the interaction of the history and the important temperature region.

Then, we conduct an experiment on SA with reversed temperature schedule, that is, heating, not cooling. Figure 4 shows a typical history of a solution to a TSP problem (KroA100), where the temperature increases from 1E-2 to 1E+3. At the beginning, the temperature

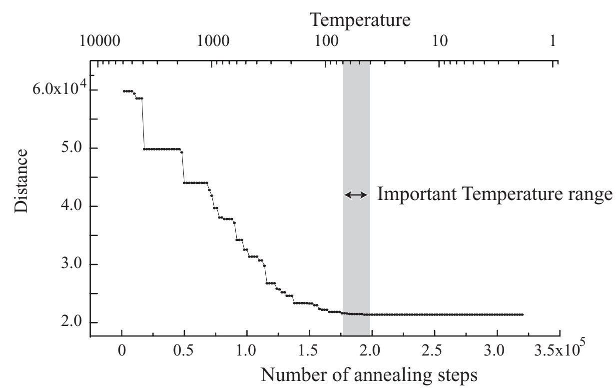

Figure 3: A typical history of the energy in solving a TSP(kroA100) with conventional SA

is very low and hill-climbing local search is performed, and a local minimum is obtained. And, as the temperature increases the solution remains at the local minimum, but the solution escapes the local minimum and it becomes better as the temperature enters the important temperature region. The solution becomes worse as the temperature increases beyond the important temperature region. Such characteristics can be seen in many other TSPs, and it is found that we can identify the upper bound of the important temperature region in this heating method.

The proposed method, which is called the Adaptive SA for Maximum Temperature (ASA/MaxT) is based

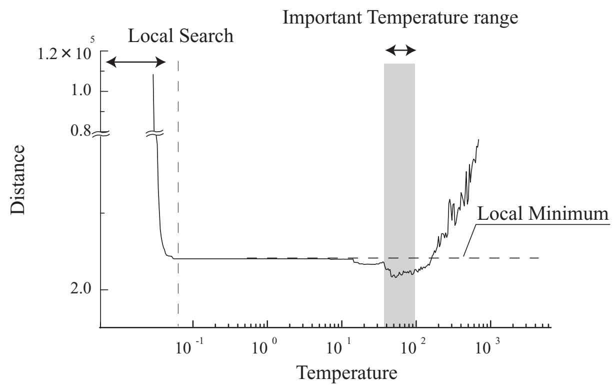

Figure 4: A typical history of the energy in solving a TSP(kroA100) with a reversed temperature schedule in SA

on this method. At first, the temperature is the lowest, and it is increased until the preliminary maximum temperature determined by a conventional method. The histories of the energy can be classified into three types as shown in Fig. 5, where the histories move from left to right. At T=0, the local hill-climbing search is performed and a local minimum is obtained. After that, the temperature is increased to the maximum temperature. During this process, the energy decreases below the local minimum once (Type 1) or more than once (Type 2), or the energy do not decrease (Type3), and the energy increases as the temperature increases. The actual maximum temperature is determined as the temperature where the energy finally increases across the local minimum, as shown in this figure (Types 1 and 2). When the actual maximum temperature is found, a conventional SA is carried out with this maximum temperature. The heating rate is 10 times as fast as the cooling rate, and therefore, the total computation time can be reduced considerably. If the energy history during the heating has no decrease blow the local minimum as shown as Type 3 in Fig. 5, this local minimum is the global minimum, and the optimum solution has been obtained already. In this case, a conventional SA is not necessary. Some easy problems show such behavior, and the probabilistic hill climbing provides the global optimum.

This method is called the Adaptive Simulated Annealing for Maximum Temperature (ASA/MaxT), and this method determines the effective maximum temperature in SA adaptively. There is no parameter in the method, and therefore the method can be considered to be easy to use for many combinatorial problems.

4 Experimental results and discussions

The effectiveness of the proposed method, ASA/MaxT, is verified with numerical experiments for

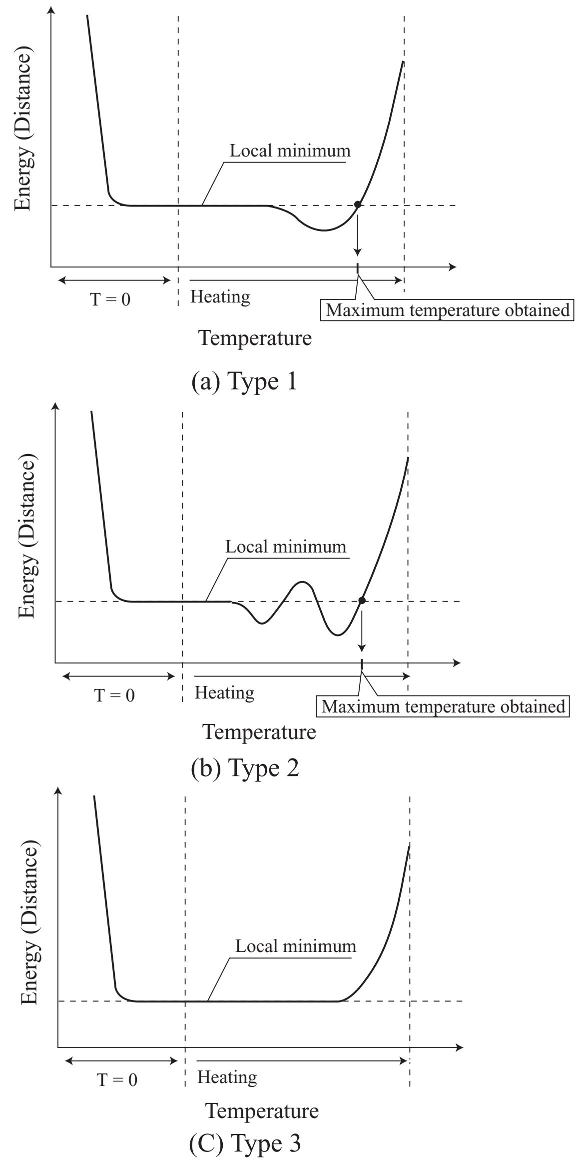

Figure 5: Tipical history of the energy for the heating process

typical ten TSPs. The parameters used are the same as shown in section 3.

Table 2 shows the comparison of the accuracy of the solutions obtained by ASA/MaxT and the conventional SA, where the exact optimum solutions are known for all these TSPs, and the error ratio can be defined. All the experimental values are calculated from 30 trials. From this table, it is found that the accuracy of the proposed method is almost the same as a conventional SA. On the other hand, the number of the total annealing steps are considerably decreased with the proposed method. Figure 6 shows the comparison of the necessary annealing steps for obtaining solutions with the accuracy being below 1%. It should be noted that the number of the annealing steps in ASA/MaxT includes the annealing

Table 2: Comparison of the accuracy of the solutions obtained by ASA/MaxT and a conventional SA

	Error ratio (%)					
	Best (%)		Ave. (%)		Worst (%)	
Problems	SA	ASA/MaxT	SA	ASA/MaxT	SA	ASA/MaxT
a280	0	0	0.24	0.54	1.2	2.17
ch130	0	0.08	1.06	1.26	2.47	2.39
ch150	0	0.06	0.72	0.86	2.27	2.48
d198	0.07	0.1	0.34	0.55	1.05	3.36
eil51	0	0	0.13	0.17	0.47	0.7
gil262	0.17	0.13	0.96	1.12	2.57	2.06
kroA100	0	0	0.64	1.05	1.72	5.46
pr76	0	0	0.54	0.61	1.32	1.08
pr144	0	0	0.52	0.37	1.53	1.41
u159	0	0	0.65	1	1.52	7.02

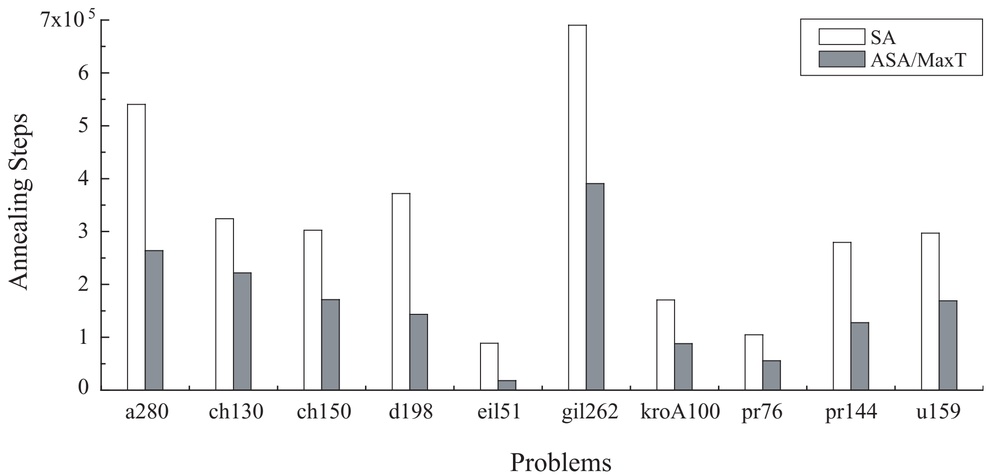

Figure 6: Comparison of the number of the total annealing steps in ASA/MaxT and a conventional SA

steps during heating process. It can be seen from this figure, the numbers of the required annealing steps for a prescribed accuracy of the solutions are about the half of those in conventional SA , and it can be recognized that the proposed method provides doubled speedups.

5 Conclusions

In solving dicrete optimization problems with SA, there exists the important temperature region, and the reduction in the number of the annealing steps can be realized when the maximum temperature is set to the upper bound of the important temperature region. The region can be found by a heating process from very low temperature in SA. The proposed method, the Adaptive SA for Maximum Temperature (ASA/MaxT), is based on this mechanism and it provides considerable speedup in SA.

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