

A comparison of simulated annealing cooling strategies

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Received 4 August 1997, in final form 14 July 1998

Abstract. Using computer experiments on a simple three-state system and an NP-complete system of permanents we compare different proposed simulated annealing schedules in order to find the cooling strategy which has the least total entropy production during the annealing process for given initial and final states and fixed number of iterations. The schedules considered are constant thermodynamic speed, exponential, logarithmic, and linear cooling schedules. The constant thermodynamic speed schedule is shown to be the best. We are actually considering two different schedules with constant thermodynamic speed, the original one valid for near-equilibrium processes, and a version based on the natural timescale valid also at higher speeds. The latter one delivers better results, especially in case of fast cooling or when the system is far from equilibrium. Also with the lowest energy encountered during the entire optimization (the best-so-far-energy) as the indicator of merit, constant thermodynamic speed is superior. Finally, we have compared two different estimators of the relaxation time. One estimator is using the second largest eigenvalue of the thermalized form of the transition probability matrix and the other is using a simpler approximation for small deviations from equilibrium. These two different expressions only agree at high temperatures.

1. Introduction

The loss of available work is an important objective to be minimized for any process, especially in thermodynamics. It is equivalent to minimizing the total entropy production which is a measure of the degree of thermodynamic irreversibility or inefficiency of the process. The process, in this connection, may be either a physical process or a combinatorial process as simulated annealing [1, 19]. Simulated annealing [1] is based on an analogy to statistical mechanics. Having defined this analogy in section 2, a combinatorial problem can be viewed as a thermodynamic system and therefore all the equilibrium properties can be resolved by standard statistical mechanical methods.

Adopting constant thermodynamic speed annealing schedules has proven excellent at finding low-energy solutions to problems, justifying investigations of further improvements. Therefore the aim of this paper is to identify a cooling schedule which minimizes the total entropy production, and thus the inefficiency of the computation, for a given optimization. Traditionally simulated annealing is a quite time-consuming procedure, because care must be taken to proceed close to equilibrium so as not to be caught in highly local minima. We are comparing here annealing schedules applied at higher speeds.

Salamon *et al* [2] transferred optimality results from finite-time thermodynamics [3] to the context of simulated annealing and made the conjecture that constant thermodynamic

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speed is also the optimal annealing schedule. A consequence of their schedule is to keep the system and its driving reservoir close to equilibrium during the entire annealing process. Extensive use was made of thermodynamic properties in deriving this adaptive schedule.

Later, for a simple three-state system, Hoffmann and Salamon [4] have shown that a logarithmic cooling schedule is optimal in the asymptotic long-time regime. They have also shown that thermodynamic speed is not constant in this limit but decreases with time.

Andresen and Gordon [5] derived an improved lower bound on the entropy production for a finite-time process. Their derivation arrived at constant thermodynamic speed from first principles. They improved the original derivation [3] of the optimal schedule by not requiring the system to be close to equilibrium with the reservoir, i.e. they did not restrict the procedure to slow processes. They also showed that the rate of total entropy production is constant during the optimal annealing process when expressed in terms of the natural timescale of the system.

Considering the variety of annealing schedules proposed on abstract grounds, we decided to compare these different schedules, including the traditional exponential and linear cooling strategies, numerically on two representative problems using the best values for the free parameters. The results of this computer experiment show that the newest constant thermodynamic speed schedule [5] is producing the least entropy throughout the annealing process.

We start the paper with brief descriptions of the simulated annealing algorithm (section 2), the different annealing schedules (section 3), the entropy production expressions (section 4), and the two test systems (section 5). Results are presented and discussed in section 6.

2. Simulated annealing

Simulated annealing [1] solves combinatorial optimization problems by an analogy to statistical mechanics. Our aim is to minimize total entropy production during the process while reaching the lowest energy state, the ground state, in a given time.

Simulated annealing has been used in a large number of problems, including NP-hard† combinatorial problems. In combinatorial optimization problems the aim is developing efficient techniques for finding minimum (or maximum) values of a function with many degrees of freedom and many local minima.

States in thermodynamic usage correspond to solutions in the combinatorial optimization problem. Energy in thermodynamics is the cost function in simulated annealing. The ground state, change of state, and temperature in thermodynamics translate to the optimal solution, a neighbouring solution, and the control parameter in simulated annealing, respectively. Therefore, the abstract system can be described as if it were a thermal physical system for which the aim is to locate the ground state as the temperature is diminished.

A system S of ‘walkers’ [16] explores the state space in a random but focused fashion in order to locate the ground state, or an approximation to it, in a given amount of time. The temperature is the control parameter which will take the system S through this change. In doing so the random search moves to a lower energy state with probability one but to a

† The name ‘NP’ stands for ‘nondeterministic polynomial time’. The class NP is the class of problems for which a given proposed solution for a given input can be verified by a polynomial-time algorithm. The class of NP-complete problems consists of the most difficult problems in NP, and no polynomial-time algorithm for solving the members of this class has been found so far [14]. This implies that existing algorithms require exponentially or faster increasing time as the size of the problem grows. If any single NP-complete problem can be solved in polynomial time, then all problems in the class NP can also be solved in polynomial time.

higher energy state only with probability

$$P = \exp(-\Delta E/kT) \quad (1)$$

where ΔE is the energy increase and T our control.

Lowering the temperature by itself is not a sufficient recipe for finding the ground state. In addition to this the system should not be allowed to become significantly out of equilibrium with its environment during the annealing. Otherwise it does not reach the global minimum energy state but will freeze into one of the great many higher energy local minima.

3. Annealing schedules

Most features in simulated annealing—state space, move class, cost function—are fixed by definition. The only feature which is variable during the calculation is the temperature. Therefore one of the most important features in simulated annealing is the choice of the annealing schedule, and many attempts have been made to derive or suggest good schedules.

Our annealing procedure involves first ‘melting’ the system at a high temperature, then repeatedly lowering the temperature by a constant factor α ($0 < \alpha < 1$), taking enough steps at each temperature to keep the system close to equilibrium, until the system approaches the ground state. This recipe results in an exponential schedule,

$$T(t) = T_0\alpha^t \quad (2)$$

where t , ‘time’ is the step count. This and a linear schedule

$$T(t) = T_0 - \eta t \quad (3)$$

have been used widely since they were introduced [1].

Of special theoretical importance is the logarithmic cooling scheme introduced by Geman and Geman [7],

$$T(t) = \frac{c}{\log(t+d)} \quad (4)$$

where d is usually set equal to one. As the only existence theorem, it has been proven that for c being greater than or equal to the largest energy barrier in the problem, this schedule will lead the system to the global minimum state in the limit of infinite time [8]. However, due to its asymptotically extremely slow temperature decrease, this schedule is utterly impractical. It simply undoes the exponential Boltzmann acceptance function in the algorithm and amounts to a random search in state space.

For a three-level system Hoffmann and Salamon [4] set up equations to derive an optimal schedule that minimizes the mean energy at a particular time. This optimum schedule did not follow a set of Boltzmann distributions but rather a turnpike solution,

$$T(t) \sim \frac{D-1}{\log t}. \quad (5)$$

All of the above schedules are predetermined, i.e. they are fixed before the calculation starts and are not influenced by its progress. In contrast finite-time thermodynamic optimization [3] suggests an analogous adaptive optimal schedule based on constant thermodynamic speed, v_s [20]. The speed v_s is defined on thermodynamic state space

with $-D^2S$ as the metric [9]. The schedule leading to least overall dissipation (entropy production) is [10]

$$\frac{dT}{dt} = \frac{-v_s T}{\epsilon \sqrt{C}} \quad (6)$$

where C is the heat capacity, and ϵ is the relaxation time of the system, both of which may depend on T . In the derivation [10] it is assumed that either v_s is a small quantity or $C(T)$ and $\epsilon(T)$ are slowly varying. This adaptive schedule was later improved [5] so that it can be used for systems far from equilibrium:

$$\frac{dT}{dt} = \frac{-v_s T}{\epsilon \sqrt{C} \sqrt{1 + \frac{\Theta(T)\epsilon(dT/dt)}{T} + \dots}} \quad (7)$$

where

$$\Theta(T) = 1 + \frac{T}{2C} \frac{\partial C}{\partial T}. \quad (8)$$

The original derivation [10], equation (6) contains only the dominant term of equation (7).

4. Entropy production

Entropy is a measure of disorder present in a system. The second law of thermodynamics states that any isolated process cannot reduce the entropy of the universe (system plus environment), $\Delta S^u \geq 0$. The corresponding loss of available work is connected through

$$-\Delta A = T_e \Delta S^u \quad (9)$$

where T_e is the temperature of the environment. Since the entropy production depends on the path taken to go from one equilibrium state to another, we attempt to find that path which produces the least entropy.

The entropy production rates for the different annealing schedules used here are derived from the basic equation

$$dS^u = \Delta Y \cdot dX \quad (10)$$

where ΔY is the vector of intensity differences between the system and the environment, and dX is the corresponding vector of flow of extensity from the environment to the system. The procedure is outlined in [5]. By introducing the respective temperature schedules, equations (2)–(7), we arrive at the expressions listed below.

Linear cooling schedule equation (3):

$$\frac{dS^u}{dt} = \frac{\epsilon C \eta^2}{T^2} \left(1 - \frac{\epsilon \Theta(T) \eta}{T} + \dots \right). \quad (11)$$

Exponential cooling schedule equation (2):

$$\frac{dS^u}{dt} = \frac{\epsilon C}{\omega^2} \left(1 + \frac{\Theta(T)\epsilon}{\omega} + \dots \right) \quad (12)$$

with

$$\omega = \frac{-\tau}{\ln(T(t)/T_0)} \quad (13)$$

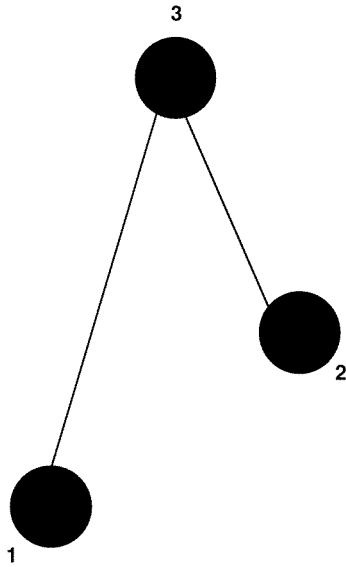


Figure 1. The simple three-state system.

where τ is the total number of steps during the annealing, T_0 is the start temperature, and t is the time or step count.

Logarithmic cooling schedule equation (4):

$$\frac{dS''}{dt} = \frac{\epsilon CT^2}{c^2(t+d)^2} \left(1 - \frac{\Theta(T)\epsilon T}{(t+d)c} + \dots \right). \quad (14)$$

Constant thermodynamic speed equation (8) [5]:

$$\frac{dS''}{dt} = \frac{\epsilon C}{T^2} \left(\frac{dT}{dt} \right)^2 \left(1 + \frac{\Theta(T)\epsilon}{T} \frac{dT}{dt} + \dots \right). \quad (15)$$

5. The systems

In this paper we study two previously defined systems. A very simple and small system and an NP-hard problem. Both are chosen not for their own sake but as examples of two extreme computational situations. It should be pointed out that these systems are non-stochastic in nature which means that the statistical component of the calculations is only in the annealing procedure itself, not in the system definition as would for example have been the case for a spin glass or a travelling salesman problem (TSP).

The simple system is a four-state system which is reduced to a three-state system by lumping [4], figure 1. Lumping means combining all the states of a given energy into a single level in order to reduce the size of the problem [16]. The state space has states with energies 0, 1, and 3. There is one local ($E = 1$) and one global ($E = 0$) minimum [4]. The system is set up in such a way that there is no direct connection between $E(1) = 0$ and $E(2) = 1$ in one time step, but the move can be done in two steps by going through $E(3) = 3$. Being very small, this system does not satisfy the expectations of simulated annealing of a large state space and is thus at the low end of complexity of systems studied.

The second example involves computing the permanent of an $n \times n$ (0,1)-matrix A , i.e. a square matrix with entries either zero or one. This computation is chosen as an example of a large NP-hard problem [11–14] and is thus a typical difficult simulated annealing problem.

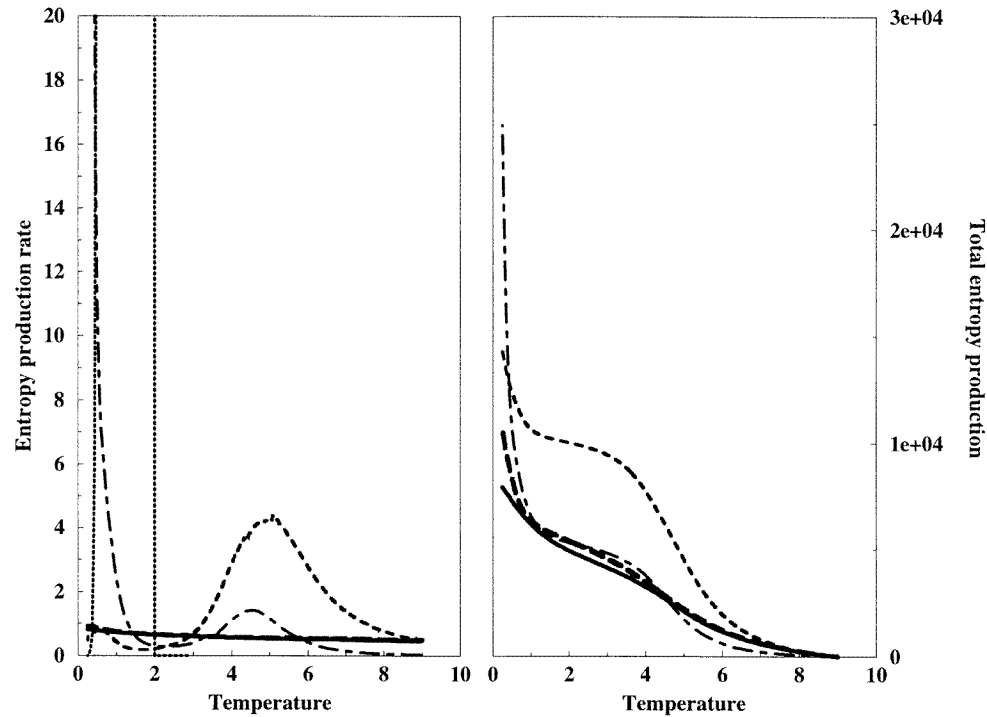


Figure 2. The entropy production rate and the total accumulated entropy production for a slow cooling of the permanent system using 13 673 integration steps. — TDS2, --- TDS1, - - - exponential, ····· logarithmic, and — · — linear cooling. TDS2 and TDS1 are almost the same, in both graphs. The logarithmic curve is not visible in the right graph because the overall entropy production for logarithmic cooling is around 10^9 .

Simulated annealing has been used to sample the possible values of the permanent of fully irreducible $(0,1)$ -matrices. Interest in permanents is based on the fact that they are ‘complete’ for the class $\#P$ of enumeration problems, which is as hard as counting the number of accepting computations of any non-deterministic polynomial time Turing machine [11]. It is worth noting that this problem is NP-hard due to the complexity of the individual function evaluation (calculation of the permanent), not because of an exponentially large number of function evaluations. Thus we are facing a ‘doubly’ hard problem.

The permanent of a matrix A is defined as

$$\text{Per}(A) = \sum_{\sigma} \prod_{i=1}^n A_{i\sigma(i)} \quad (16)$$

where σ runs over all permutations of $1, \dots, n$. We have made use of graph theory to define the move class since there is a one-to-one correspondence between directed graphs and $(0,1)$ -matrices. However, these details are not important for the present comparison but they are explained in [15]. Specifically, we search for the largest permanent values of eight-dimensional directed graphs. This results in a 14×14 A -matrix and energies in the range $[-129, -9]$, as we define the energy $E = -\text{Per}(A)$.

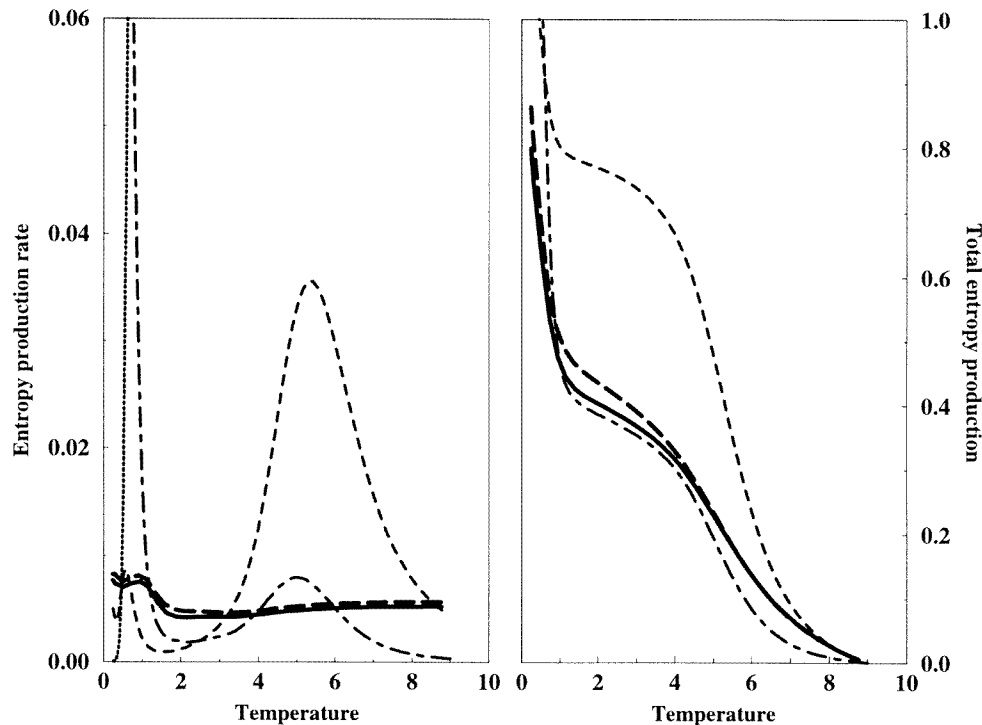


Figure 3. The entropy production rate and the total accumulated entropy production for a fast cooling of the permanent system using 141 integration steps. — TDS2, --- TDS1, exponential, - · - · - logarithmic, and - - - linear cooling. At this cooling rate the difference between the TDS2 and TDS1 curves is clear in both graphs.

6. Results

6.1. Experimental comparison of schedules

As mentioned in section 5, we have considered two different problems. The simple three-state system was defined in [4] while the NP-hard problem of permanents was used to show the power of simulated annealing in [15].

For a given initial state, a fixed number of iterations, and the same initial and final temperatures we have numerically compared the above mentioned schedules, i.e. exponential cooling equation (2), linear cooling equation (3), logarithmic cooling equation (4), simple constant thermodynamic speed cooling (using only the first term in a power expansion away from equilibrium) equation (6), and improved constant thermodynamic speed (taking into account the second term as well) equation (7). To distinguish between the two constant thermodynamic speed schedules we will call the former TDS1 and the latter TDS2. We have also taken both c and d in equation (4) to be parameters in order to satisfy the common boundary conditions. Initially we let the system ‘simmer’ at infinite temperature until it equilibrates before starting the actual annealing. The stop temperature is set low enough to reach the ground state(s) in a fast cooling.

In figures 2–4 we compare the results for the permanent problem. While working with this system and making different runs with different start and stop temperatures, we learned that if the system starts to anneal with $T = 9$, it may reach the ground state at around

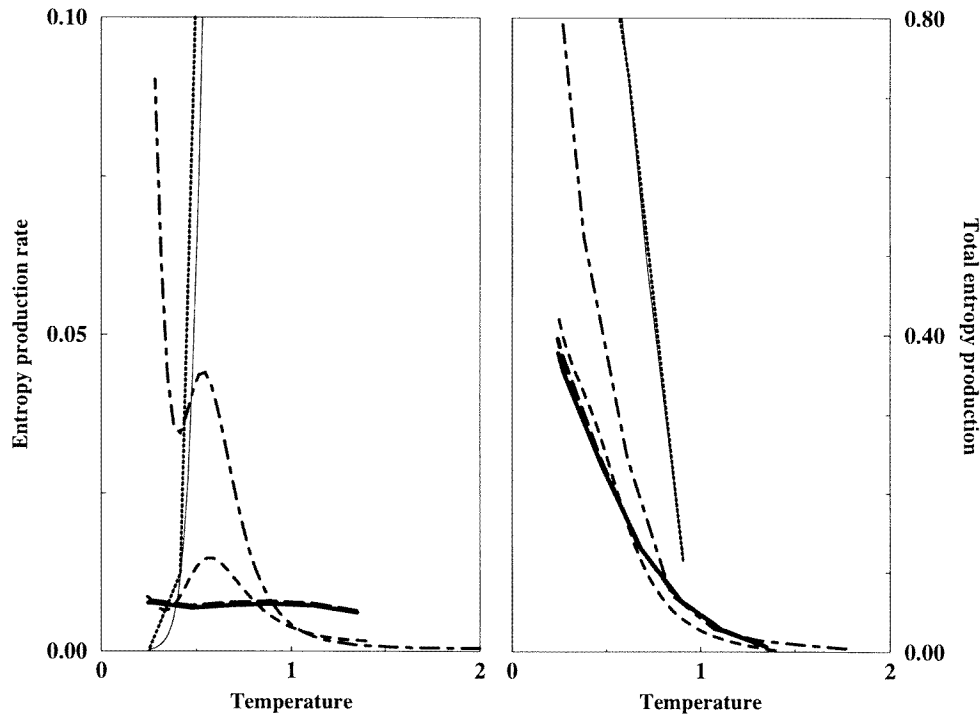


Figure 4. The entropy production rate and total accumulated entropy production for a yet faster cooling of the permanent system using only 53 integration steps. — TDS2, --- TDS1, - · - · - exponential, ····· logarithmic, and - · - · - linear and — HS-logarithmic cooling.

$T = 0.25$ with a fairly slow cooling rate without wasting much computer time. Those two temperatures have therefore been adopted as the common start and stop temperatures for all runs. We have made several runs with different cooling rates.

For slow cooling in figure 2 the constant thermodynamic speed schedules TDS1 and TDS2 result in an almost constant rate of entropy production as analytically derived for an optimal linear process in [17]. The exponential cooling schedule, on the other hand, yields an entropy production rate peaking at intermediate temperatures thus indicating a large discrepancy between system and reservoir in this region. There is a second but smaller peak at low temperatures. The entropy production rate using the logarithmic annealing schedule starts out at the higher temperatures about 10 orders of magnitude above the others and then decreases sharply at the lower temperatures. The linear cooling schedule has a low entropy production rate at the beginning (high temperatures) which then grows rapidly at lower temperatures. The overall entropy production is very low when the system is cooling slowly, whereas a fast cooling produces a larger amount of entropy.

Figure 3 shows the results from a faster cooling annealing, i.e. fewer steps have been taken and thus the system was further from equilibrium. The superiority of TDS2 over TDS1 in producing less entropy is now more evident, as expected for a faster process. Linear, exponential, and logarithmic schedules result in higher entropy productions. And once again the total entropy production with logarithmic cooling is so high that the curve cannot be seen in the range of figure 3(b).

Applying the logarithmic schedule in the manner of [4]—which from now on we will

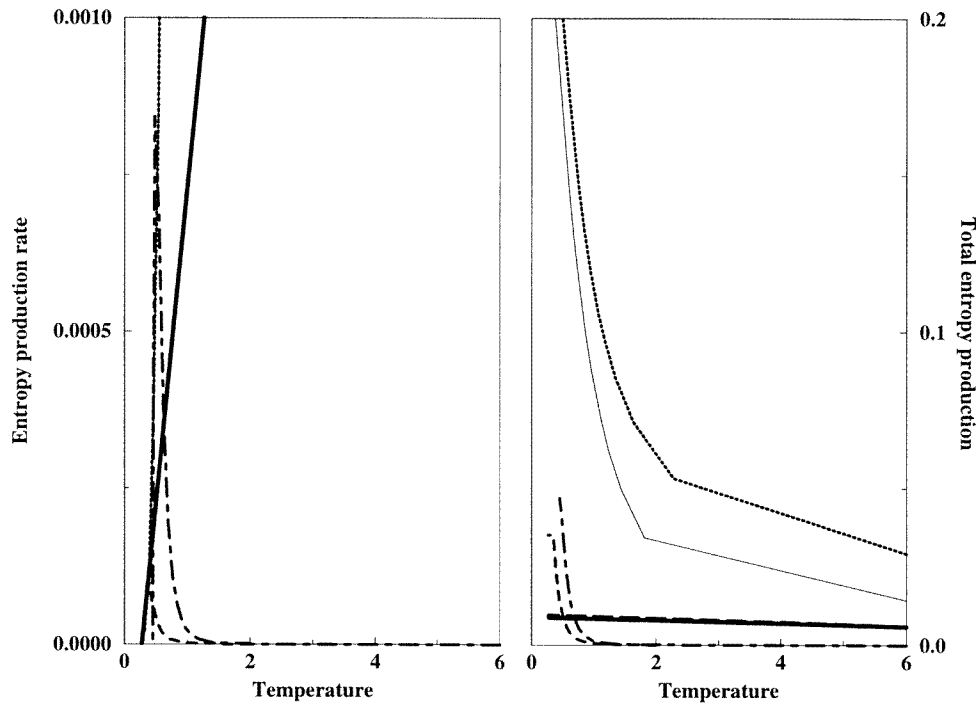


Figure 5. The entropy production rate and total accumulated entropy production for the simple three-state system using 1468 integration steps. — TDS2, --- TDS1, - - - exponential, logarithmic, - · - linear and — HS-logarithmic cooling.

call HS-logarithmic—using the highest energy barrier for c and setting $d = 1$ fixes the temperature interval. In the next figure, figure 4, we reduce the start temperature to 2 in order to permit a comparison between this schedule and the other schedules. The interesting point is that there is very little difference between the behaviour of the system using logarithmic cooling, i.e. considering c and d as parameters, and HS-logarithmic. The entropy production rates and the total productions are almost identical for these two schedules, and much higher than for the other cooling schedules. TDS2 has the least total entropy production. Another point worth mentioning is that at this high speed the exponential entropy production rate is less than the linear one.

Figure 5 shows the entropy production rate of our five different schedules for the simple three-state system. Clearly the logarithmic cooling schedule is performing the worst and the TDS2 schedule is giving the best result. There is not much difference between the general behaviour of this simple system and the NP-hard permanents.

A comparison of the total entropy productions in figures 2–5 indicates that quite generally TDS2 results in the least entropy production and the logarithmic annealing schedule the highest entropy production. Linear and exponential display the same overall behaviour, while TDS1 is similar to TDS2 but slightly higher, increasing with speed. All comparisons of the total entropy production among the different schedules are of course done using the same number of annealing steps.

An independent way to check the performance of an optimization method is to follow the best-so-far-energy (BSFE) seen after a certain number of iterations [18]. $BSFE(t)$ is the lowest energy value seen up to iteration t . After all, one does run the annealing in

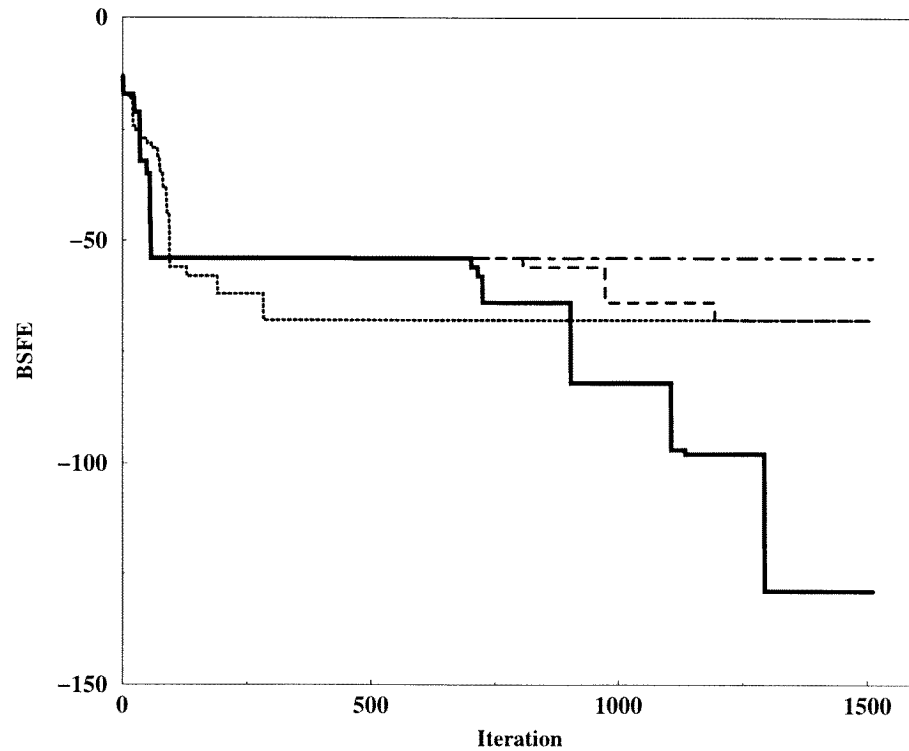


Figure 6. The BSFE as the annealing progresses for the permanent system using 1510 integration steps. — TDS2, --- TDS1, - - - exponential, ····· logarithmic, — · — linear cooling. TDS2 and TDS1 curves are identical. The global minimum is -129 .

order to find the global minimum. Figure 6 shows the BSFE as a function of iteration number for the five different schedules used on the permanent problem. It is obvious how superior TDS2 and TDS1 are as the annealing progresses. They have found the lowest BSFE almost all the time along the annealing compared to other schedules, except that in a short interval the logarithmic schedule is doing better. The logarithmic schedule is almost like a quenching, at the early stage of the run it rapidly gives good results only to get caught in a local minimum. TDS2 and TDS1 display similar behaviour initially but they successfully overcome the energy barriers and eventually reach the global minimum. Linear and exponential cooling perform poorly, and the final BSFE seen with these and the logarithmic cooling are much higher than the global minimum.

In summary, TDS2 is superior to all the other annealing methods in the sense of consistently having the least entropy production. Also the BSFE curves show that this method is better than the other schedules in reaching the lowest energies within a finite time. This conclusion is of course not surprising since the constant thermodynamic speed schedules were developed analytically to be the optimal ones for a given duration. However, this has not been verified experimentally previously which also means that we have had no quantitative indication of how inferior the other schedules are. Figures 2–6 provide this information for two systems which are representative of a very simple and a very hard calculation.

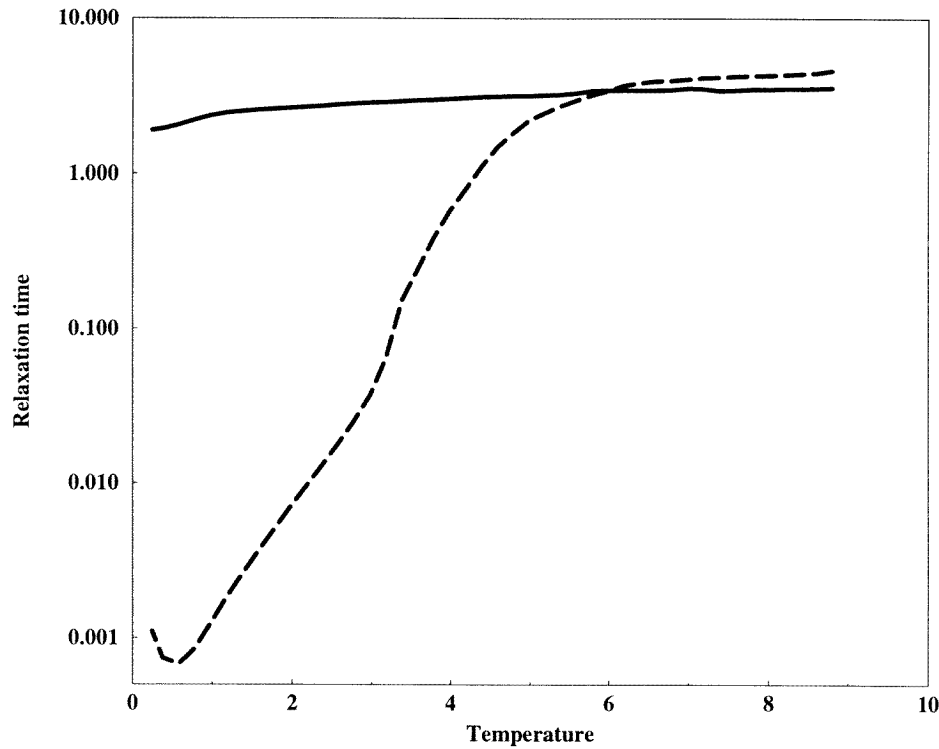


Figure 7. The relaxation time ϵ for the permanent system computed in two different ways as described in section 6.2 at very low speed using 13 673 integration steps. — using the second largest eigenvalue equation (17), and - - - using the approximation equation (19). The two relaxation calculations agree at high temperatures but at lower temperatures the approximate value drops sharply.

6.2. Relaxation time

A technique has been introduced by Andresen *et al* [16] for the estimation of average energy, heat capacity, and relaxation time, needed in equations (6)–(8), for an ensemble system as the annealing calculation progresses. While the system is annealing, one collects information about all attempted moves from any state to any other state. This information is gathered in a matrix Q . We can normalize this Q -matrix column by column and turn it into a good estimate of the real transition probability matrix P from where the partition function and thus all related thermodynamic quantities may be derived through the traditional methods of statistical mechanics.

We are using this method in the present work to estimate the average energy and the heat capacity. As for relaxation time, we use the second largest eigenvalue of the G matrix, λ_2 , to find the exact value for the final approach to equilibrium,

$$\epsilon = \frac{-1}{\ln \lambda_2} \quad (17)$$

where G is the thermalized form of the P matrix [16]:

$$G_{ji} = P_{ji} \exp\left(-\frac{E_j - E_i}{T}\right). \quad (18)$$

The largest eigenvalue of G , $\lambda_1 = 1$, corresponds to equilibrium itself.

In [2, 10, 16] an estimate of ϵ has been provided for thermal, near-equilibrium relaxation:

$$\epsilon(T) \approx \frac{T^2 C(T)}{\sum_i g_i \sum_{j>i} (E_j - E_i)^2 G_{ji}} \quad (19)$$

where g_i is the equilibrium distribution at temperature T .

The authors called this the ‘Boltzmann–Boltzmann’ relaxation time, because it is based on a Boltzmann distribution relaxing to a nearby Boltzmann distribution at temperature T . They claim that this simpler expression is reasonable since the system does not depart much from equilibrium during slow annealing [2].

We have compared these two estimators of the relaxation time, equations (17) and (19). Figure 7 is the result of a very slow cooling from a high temperature of the permanent problem. As can be seen, the two expressions agree at high temperatures while at lower temperatures ϵ computed using the approximation equation (19) drops sharply. This difference between the two ways of computing relaxation time appears for all annealing schedules used in this work, at all cooling rates, and for both systems. The reason is that equation (19) is a statement of local equilibration which at low temperatures is blind to other areas of state space separated by large barriers, whereas equation (17) by construction is global. As the size and complexity of the system increases, the difference becomes more pronounced, and the global relaxation time may eventually diverge.

Acknowledgments

YN wishes to thank the Ørsted Laboratory, University of Copenhagen for their support and hospitality. This paper has been supported by the Danish Natural Science Research Council under contract no 9502152.

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