Abstract

We discuss a rejectionless global optimization technique which, while being technically similar to the recently introduced method of Extremal Optimization, still relies on a physical analogy with a thermalizing system. This method can be used at constant temperature or combined with annealing techniques, and is especially well suited for studying the low temperature relaxation of complex systems as glasses and spin glasses.

PACS: 02.60.Pn; 05.10.Ln; 75.10Nr

1 Introduction

The archetype of optimization approaches inspired by physics is arguably Simulated Annealing (SA) [1, 2]. In SA, putative solutions of the problem at hand are organized in an ‘energy landscape’ similar to the configuration space of a physical system. This landscape is searched for the global optimum using the Metropolis algorithm [3] while the temperature is slowly decreased during the simulation. The theoretical underpinning of SA is equilibrium statistical physics and the theory of Markov processes: at each temperature $T$, the Metropolis algorithm asymptotically samples the equilibrium Boltzmann distribution which, at $T = 0$, is supported on the set of ground states.

It is well known to practitioners of SA that maintaining thermalization at arbitrarily low temperatures is practically impossible in landscapes with
many local minima: The trajectories get trapped in subsets of configuration space (valleys or pockets) surrounding local minima, and most of the attempted moves are rejected. Thus, ergodicity is broken, and the final solution is just a ‘good’ local optimum, not the global optimum.

To mitigate the effects of ergodicity breaking one must make sure that many different valleys are thoroughly explored. Ways to do so is to employ ensemble methods [4] or use non-monotonic temperature schedules, as done in bouncing [5], thermal cycling [6], and tempering [7]. Another possibility is to select candidate moves from a broad distribution [8, 9], occasionally producing the ‘long jumps’ in configuration space which are needed to escape the neighborhood of a local minimum.

In this paper we discuss and test a ‘thermal’ Monte Carlo scheme, which we have chosen to call the Waiting Time Method or WTM. The WTM belongs to a family of rejectionless or ‘event driven’ algorithms [10] which developed from the so-called n-fold method introduced by Bortz et al. [11]. From an algorithmic point of view, the WTM is very close to a recent optimization method, Extremal Optimization (EO) [12, 13], notwithstanding the fact that the latter is inspired by the Bak-Sneppen model of biological evolution [14], rather than thermal annealing of a physical system.

Rejectionless methods can offer much improved performance, especially in simulations of glassy systems at low temperature. Yet, they do not seem to have gained widespread acceptance [15]. We hope that the present analysis will contribute to improve the situation.

As a prelude, we show the equivalence of the WTM with the Metropolis algorithm with regard to the equilibrium as well as to the dynamical (relaxation) properties. Secondly, we analyze the performance of the WTM and identify the temperature region where it is computationally advantageous to use it. Finally we compare the performance of Extremal Optimization with the WTM run at constant temperature and with the WTM in combination with the Geman-Geman annealing schedule [16, 17]. The numerical analyses all use a 3D Ising spin glass model with short range Gaussian interactions as a test problem.

2 The WTM algorithm

The WTM is well suited for problems where $N$ variables contribute to the cost function (energy) in an additive fashion. One such case is the short range Ising spin glass model: $N$ spins, $\sigma_i = \pm 1$ are placed on a cubic lattice, producing a total of $2^N$ configurations. Each configuration has $N$
neighbors, which correspond to the $N$ possible flips of a single spin. The energy of configuration $\alpha$ is given by

$$H = -\frac{1}{2} \sum_i \sigma_i^\alpha \sum_j J_{ij} \sigma_j^\alpha,$$

(1)

where the couplings $J_{ij}$ are independently drawn from a Gaussian distribution of unit variance and zero mean if $i$ and $j$ point to adjacent lattice sites. Otherwise $J_{ij} = 0$.

For any configuration $\alpha$, the WTM associates to each spin a stochastic variable $t_i$ which is the time at which this spin must flip, given that its local field $\sum_j J_{ij} \sigma_j$ stays put. A ‘global time’ value, which is initially set to zero, is stored in the variable $t_{\text{global}}$.

Let $\Delta_i$ be the energy change associated with the flip of $\sigma_i$. Flipping times $t_i$ are initially assigned as

$$t_i = -\tau_i \log X_i,$$

(2)

where the $X_i$ are independent stochastic variables with a uniform distribution in the unit interval. Thus, each $t_i$ has an exponential probability distribution with average waiting time given by

$$\tau_i = \max(1, \exp(\Delta_i/T)).$$

(3)

After the initialization has been completed, the WTM iterates the following three steps:

1. Flip the spin $\sigma_m$ having the lowest flipping time.
2. Update the global time: $t_{\text{global}} = t_m$.
3. Generate from an exponential distribution with average $\tau_i$ fresh waiting times $\delta_i$ for the spin $\sigma_m$ and its lattice neighbors (e.g. six other spins in a cubic lattice). The waiting times are added to the global time in order to obtain the updated flipping times: $t_i = t_{\text{global}} + \delta_i$.

In order to identify the next move, one needs to search (and update) a database of size $N$ storing the current flipping time of each degree of freedom as well as pointers to the $z$ degrees of freedom interacting with it. Ordering in a balanced tree (a heap), with the shortest flipping time placed at the root node, requires a computational effort for the search and update procedure of order $\log N$. Since the number of updates per spin flip is equal to $z + 1$, the computational overhead per spin flip is $(z + 1) \log N$, independent of the temperature $T$.

\footnote{We will often leave the dependence on $\alpha$ understood.}
3 Theoretical considerations

For completeness, we discuss below a few basic statistical properties of the WTM. The main results are derived analytically and then checked numerically for illustration purposes. We also briefly describe Extremal Optimization, which is used in the performance comparison of the next section.

**Equilibrium distribution for the WTM**

It is simple to establish that the WTM fulfills *detailed balance* [10]. Consider two configurations, \( \alpha \) and \( \beta_k \), the latter obtained from the former by flipping spin \( k \). Given that spin \( k \) is the next spin to flip, the probability that the system remains in state \( \alpha \) for at least a time \( t \) is (by construction)

\[
q_k(t) = \exp(-t/\tau_k).
\]  

(4)

The rate \( R_{\beta_k,\alpha} \) of probability flow from \( \alpha \) to \( \beta_k \) is then

\[
R_{\beta_k,\alpha} = \frac{1}{\tau_k} = \min(1, \exp(-\Delta_k/T)).
\]  

(5)

Detailed balance follows since \( R_{\beta_k,\alpha}/R_{\alpha,\beta_k} = \exp(-\Delta_k/T) = P_{eq}(\beta_k)/P_{eq}(\alpha) \), where \( P_{eq}(\alpha) \) is the probability of visiting configuration \( \alpha \) in equilibrium. As a consequence thereof [18], the stationary distribution of the WTM is the Boltzmann distribution over the states of the system, as in the case of the Metropolis algorithm.

**Metropolis and WTM dynamics**

Since detailed balance is fulfilled, the WTM has the same equilibrium (Boltzmann) distribution as the Metropolis algorithm. To an excellent approximation, there is also a *dynamical* equivalence, in the sense that the transition probabilities from one state to another are very nearly the same in the two schemes. This equivalence simplifies a performance comparison considerably, since one only needs to compare the computer times spent on average to achieve a flip.

\(^{2}\)If a number of waiting times \( \tau_i \), which all equal one, happens to enter the heap in close succession, the WTM has a bias towards flipping the corresponding spins in the same order as the \( \tau_i \) are submitted. This feature hardly has any practical consequences and is neglected in the formulae.
The WTM remains in a state $\alpha$ for a time at least equal to $t$ with a ‘survival’ probability given by

$$Q^W_\alpha(t) = \prod_{k=1}^N \exp(-t/\tau_k) = \exp(-t \sum_{k=1}^N \tau_k^{-1}).$$  \hspace{1cm} (6)$$

The probability that spin $k$ be the first to flip is

$$p^W_k = \int_0^\infty \tau_k^{-1} Q^W_\alpha(t) dt = \frac{\tau_k^{-1}}{\sum_j \tau_j^{-1}}.$$  \hspace{1cm} (7)$$

In the Metropolis algorithm, the transition probability $P(\beta_k, \alpha)$ from a configuration $\alpha$ to one of its $N$ neighbors $\beta_k$ is

$$P(\beta_k, \alpha) = \frac{1}{N} \min(1, \exp(-\Delta_k/T)).$$  \hspace{1cm} (8)$$

Hence, the probability that spin $k$ be the first to flip is

$$p^M_k = \frac{P(\beta_k, \alpha)}{\sum_j P(\beta_j, \alpha)}.$$  \hspace{1cm} (9)$$

Since Eq. (7) is identical to Eq. (8), the WTM and the Metropolis method generate the same Markov chain of spin flips.

We also note that the intrinsic (or ‘physical’) time of the WTM approximately corresponds to the number of MC steps in the Metropolis algorithm. The latter leaves state $\alpha$ unchanged for at least $t$ MC steps with the probability

$$Q^M_\alpha(t) = \left(1 - \sum_{k=1}^N P(\beta_k, \alpha)\right)^t.$$  \hspace{1cm} (10)$$

If $\alpha$ is a local minimum all the $\Delta_k$ are positive and the sum in Eq. (10) is close to zero for small $T$. A similar conclusion applies to configurations close to a local minimum, which is where the algorithm will spend most of the computer time in a multi-minima landscape at low $T$. In this situation one easily obtains

$$Q^M_\alpha(t) \approx \exp[-t \sum_{k=1}^N \min(1, \exp(-\Delta_k/T))].$$  \hspace{1cm} (11)$$

Hence, using the usual Monte Carlo step as time unit makes Eq. (6) and (11) identical. Note however that Eq. (11) is an approximation while Eq. (6) is exact.
Figure 1: The normalized density of states $P(\varepsilon)$ for a Gaussian Ising spin glass with $N = 8^3$ spins is sampled through $10^6$ MC steps. The Metropolis algorithm and two variants of the WTM, which are based upon Eq. (3) and Eq. (12), respectively, were utilized to obtain the data. See the main text for further details.

Fig. 1 shows, for different temperatures, the density of states of the spin glass problem sampled with the WTM (dashed lines), the Metropolis algorithm (dotted lines) and finally the WTM with a different choice of rates, (henceforth "choice b") given in Eq. (12) and discussed below. In all cases we used $10^6$ MC steps: At $T = 1.2$ and $T = 1.0$ this suffices to equilibrate the system (the discrepancies barely visible at high energies are more pronounced for smaller systems (not shown) and are likely to stem from a finite size effect). At $T = 0.8$ the WTM and Metropolis are still indistinguishable. The incipient lack of equilibration transpires from the fact that the data sampled by the WTM with choice b of rates now visibly differs from the other two sets at high energies. This difference is enhanced at $T = 0.6$, while at $T = 0.4$ the trajectories become trapped in different local minima and the three methods strongly differ due to insufficient statistics.

Other choices of the average waiting time

Within all possible choices of rates fulfilling detailed balance, Eq. (3) stands out as the one which, besides producing the desired equilibrium distribution, also guarantees dynamical equivalence with the Metropolis algorithm.
In systems like spin glasses, where the relaxation is dominated by partial
equilibrations in configuration space traps, one nevertheless expects the dy-
namics to be insensitive to the precise choice of rates. To check this, we
considered the choice
\[ \tau_i = \exp(\Delta_i/2T), \]
whose appeal mainly lies in the fact that the same expression for \( \tau_i \) applies
regardless of the sign of \( \Delta_i \).

In Fig. 2 we compare the densities of states sampled at \( T = 0.8 \) by
the WTM with rates chosen according to Eq. 12 and Eq. 5. The latter
choice is, we recall, equivalent to the Metropolis scheme. The data shown
are averages over 10000 very short runs. All these runs started from the
same initial state, with energy per spin \( \varepsilon = -1.6200 \), and lasted 100 MC
steps, which is not even remotely sufficient for equilibration purposes. As
anticipated, the densities of states sampled by the two methods are quite
similar, even at very short time times.

**Extremal Optimization**

The WTM is in many respects algorithmically similar to Extremal Opti-
mization [12, 13]. We have, unsuccessfully, tried to map the two meth-
ods onto each other, and we also failed to produce an analytical descrip-
tion of the stationary distribution belonging to EO. In short, with optimal
choice of parameters for optimization, \( P_{\text{EO}}(\varepsilon) \) is significantly broader than
\( P_{\text{WTM}}(\varepsilon) \) [19].

The quality of the contribution to the overall cost from a degree of free-
dom is considered in EO as a fitness measure. The actual way in which
the fitness is assigned is not rigidly specified, but reflects one’s intuition and
knowledge of the problem at hand. In our case, we use the local energy contribution $-\sigma_i \sum_j J_{ij} \sigma_j$ as the fitness $f_i$ of $\sigma_i$, in accordance with [20].

The following steps are then iterated:

1. Rank the spins according to their fitness, and pick a spin with rank $n$ with probability $p \propto n^{-\gamma}$. The exponent $\gamma$ is a free parameter which can be tuned for a given class of problems but which is not changed dynamically during the runs.

2. Flip the chosen spin and calculate the ensuing change in the fitness of its neighbors.

If $\gamma$ is very large, the least fit spin is chosen every time, and EO resembles the Bak-Sneppen model of evolution [14].

The major difference between EO and WTM is that only the rank (relative magnitude) of the energy changes is important in the former method, while the absolute magnitudes are important in the latter. Secondly, EO chooses its next move probabilistically from a deterministic ranking of the $f_i$. By way of contrast, the WTM chooses the next move deterministically from a list of waiting times produced by a stochastic algorithm. Thirdly, the ranking procedure in EO utilizes the current energy contribution, while the WTM looks ahead and generates the waiting times according to the projected energy change.

4 Tests and results

This section presents the salient features of the WTM algorithm, found by simulations of the 3D Gaussian spin glass model with $N$ spins. We do not attempt a complete characterization, which would be tedious for those not interested in the particular model used. Likewise, the physical aspects of low temperature relaxation in spin glasses will be discussed elsewhere [21].

Acceptance rates and intrinsic WTM time

The ‘intrinsic’ or physical time elapsed in a WTM simulation determines the amount of configuration space explored and how close the system is to thermal equilibrium. Its linear relation to the number of Monte Carlo steps is displayed in the left panel of Fig. 3 for three different temperatures and a number of systems sizes. There is no discernible $N$ dependence, except at the lowest temperature, where the smallest systems, $N = 5^3$ and $7^3$, are seen to follow slightly steeper lines (longer times) [21].
Figure 3: The left panel shows the elapsed intrinsic time in the WTM as a function of the number of updates measured in MC steps. Results for three different temperatures and a number of system sizes are displayed. The right panel shows the acceptance rate, i.e., the ratio of the number of flips to the number of attempted flips, for the Metropolis algorithm, with the box marking the temperature region $T < 1.3$ where the WTM is faster.

The right panel of Fig. 3 shows, for three different system sizes, the empirical temperature dependence of the acceptance rate $a(T)$ of the Metropolis algorithm, i.e., the ratio of the number of flips to the number of attempted flips. Again, the size dependence is negligible.

The slopes in the left panel are, for each temperature, nearly equal to the reciprocal acceptance rate $1/a(T)$ obtained from the right panel. This confirms the correspondence between the WTM time $t$ and the number of MC steps discussed in Section 3.

**Tuning of parameters**

In ergodic systems, and in particular in finite systems, the best-so-far energy per spin $\varepsilon_{\text{bsf}}(t)$ seen in a simulation of length $t$ must approach the ground state energy as $t \to \infty$, regardless of the temperature. Nonetheless, for realistic values of $t$ and all but the smallest systems, the ground state energy is never reached and one can meaningfully study the parameter dependence
of a suitably averaged the best-so-far energy $\langle \varepsilon_{bsf}(t) \rangle$.

In applying the WTM to the spin glass problem, we averaged over many runs with the same length and different $J_{ij}$. We observed a clear temperature dependence of the resulting $\langle \varepsilon_{bsf} \rangle$ and defined an ‘optimal’ parameter $T_{\text{opt}}$ as the temperature minimizing $\langle \varepsilon_{bsf} \rangle$ after $10^3 N$ spin flips. Empirically, this $T_{\text{opt}}$ is independent of the runtime through several orders of magnitude \cite{13}. It is however dependent on the system size in the following way: For $N = 5^3, 6^3, 8^3, 10^3$ and $12^3$, we find $T_{\text{opt}} = 1.0, 0.9, 0.7, 0.65$ and 0.6, respectively.

While we cannot make any theoretical statements regarding EO, the behavior with respect to $\langle \varepsilon_{bsf} \rangle$ is very much the same, with $\gamma$ in lieu of $T$. However, running EO on the same systems as above showed a much weaker $N$ dependence: though $d\gamma_{\text{opt}}/dN < 0$ is observed, $\gamma = 1.1$ produces good results for $N \leq 12^3$. Compared to the temperature in the WTM, $\gamma_{\text{opt}}$ is insensitive to changes in the system size.

Runtime considerations

A ball park figure for the temperature $T_b$ where the WTM is faster than Metropolis can be obtained by noticing that the generation of waiting times, see Eq. (2), is the most time consuming part of the algorithm. For each performed spin flip the WTM generates $z + 1 = 7$ new waiting times, while Metropolis requires $1/a(T)$ attempted spin flip operations on average. Equating the two expressions yields $a(T_b) \simeq 1/7 \approx 0.15$ and $T_b \approx 1.5$. The actually measured value of $T_b$ is indicated by the lower corner of the box in Fig. 3 and equals $\approx 1.3$. This is somewhat lower than the estimate, likely because we neglected the computational cost of order $(z + 1) \log N$, confirmed in Fig. 4, which is needed in the search and update procedure. From Fig. 3 we see that at $T = 0.5$ the WTM is approximately three times as fast as standard Metropolis. A closer examination of $a(T)$ reveals that at $T \simeq 0.25$ and $T \simeq 0.035$ the WTM is 10 and 100 times faster, respectively, if both methods are to produce the same number of spin flips.

Performance comparisons

We have compared the WTM with an annealing version and with EO. The result is shown in Fig. 5. In the annealing case we have used the Geman-Geman logarithmic schedule $T(t) = T_0/(1 + \log(1 + t))$. We observed the reasonable fact that $\langle \varepsilon_{bsf} \rangle$ is minimized when the initial temperature $T_0$ is chosen so that the final temperature is slightly below $T_{\text{opt}}$ in the WTM.

The WTM is seen to be inferior to EO in terms of spin flips needed to
reach the same value of $\langle \varepsilon_{\text{bsf}} \rangle$. However, when implementing EO ad literam\textsuperscript{3}, at equal runtime EO and the WTM produce similar results for $N = 10^3$, i.e. they reach approximately the same $\langle \varepsilon_{\text{bsf}} \rangle$. For larger systems EO is slower than the WTM\textsuperscript{19}.

When applied to an annealing schedule like Geman-Geman, the WTM is seen to perform better than EO, since varying the temperature in the WTM does not change the runtime notably. We note in passing that while the Geman-Geman schedule is usually dismissed as unrealistically slow, it performs quite satisfactorily in connection with WTM.

5 Summary and conclusions

The WTM belongs to a family of rejectionless algorithms related to the $n$-fold way of Ref.\textsuperscript{11}. These algorithms asymptotically sample the Boltzmann distribution and are mathematically equivalent to the ubiquitous Metropolis algorithm. Compared to Metropolis, they also require a computational and implementation overhead. However they are considerably

\textsuperscript{3}which is usually not done\textsuperscript{12, 13}, since an exact ordering is costly and an approximate ordering is assumed to work just as well.
faster at low temperatures, especially in systems with short range interactions. The n-fold way, in particular, is efficient if $n$ is small, i.e. if the possible values of the $\Delta_k$ belong to a small, discrete set. The WTM method does not suffer from the same limitation, and is therefore especially well suited for low $T$ simulations of the dynamics of disordered and glassy systems.

Our tests on a spin glass system show that Simulated Annealing with Geman-Geman type of schedule is slightly faster Extremal Optimization, a recent addition to the arsenal of optimization tools. This indicates that ‘thermal’ schemes remain a viable approach to global optimization.

6 Acknowledgement

We would like to thank Stefan Boettcher for kindly sharing his work and ideas with us. P.S. thanks the participants of the 1999 Telluride Workshop on Energy Landscapes for valuable input and Statens Naturvidenskabelige Forskningsråd for financial support.
References

[1] S. Kirkpatrick, C.D. Gelatt Jr., and M. P. Vecchi. Optimization by simulated annealing. *Science*, 220:671–680, 1983.

[2] V. Černý. Thermodynamical approach to the traveling salesman problem: An efficient simulation algorithm. *Journal of Optimization Theory and its Applications*, 45:41–55, 1985.

[3] Nicholas Metropolis, Arianna W. Rosenbluth, Marshall N. Rosenbluth, Augusta H. Teller, and Edward Teller. Equation of State Calculations by Fast Computing Machines. *Journal of Chemical Physics*, 21:1087–1092, 1953.

[4] George Ruppeiner, Jacob Mørch Pedersen, and Peter Salamon. Ensemble approach to simulated annealing. *Journal de Physique I*, 1:455–470, 1991.

[5] J. Schneider, I. Morgenstern, and J. M. Singer. Bouncing towards the optimum - improving the results of Monte Carlo optimization algorithms. *Physical Review E*, 58:5085–5095, 1998.

[6] A. Möbius, A. Neklioudov, A. Díaz-Sánchez, K. H. Hoffmann, A. Fachat, and M. Schreiber. Optimization by Thermal Cycling. *Physical Review Letters*, 79:4297–4301, 1997.

[7] Enzo Marinari, Georgio Parisi, and Juan J. Ruiz-Lorenzo. Phase structure of the three-dimensional Edwards-Anderson spin glass. *Physical Review B*, pages 14852–14863, 1998.

[8] Harold Szu and Ralph Hartley. Fast simulated annealing. *Physics Letters A*, 122:157, 1987.

[9] Constantino Tsallis and Daniel A. Stariolo. Generalized simulated annealing. *Physica A*, 233:395–406, 1996.

[10] K. Binder. *Monte Carlo Methods in Statistical Physics*. Springer-Verlag, 1979.

[11] A. B. Bortz, M. H. Kalos, and J. L. Lebowitz. A new algorithm for Monte Carlo simulation of Ising spin systems. *Journal of Computational Physics*, 17:10–18, 1975.
[12] Stefan Boettcher and Allon Percus. Nature’s way of optimizing. *Artificial intelligence*, 119:275–286, 2000.

[13] Stefan Boettcher. Extremal optimization of graph partitioning at the percolation threshold. *J. Phys. A*, 32:5201–5211, 2000.

[14] Per Bak and Kim Sneppen. Punctuated equilibrium and criticality in a simple model of evolution. *Physical Review Letters*, 71:4083–4086, 1993.

[15] David P. Landau and Kurt Binder. *A Guide to Monte Carlo Simulations in Statistical Physics*. Cambridge University Press, 2000.

[16] S. Geman and D. Geman. Stochastic Relaxation, Gibbs Distributions, and the Bayesian Restoration of Images. In *Proc. Sixth IEEE Pattern Analysis and Machine Intelligence*, pages 721–741, 1984.

[17] B. Hajek. Cooling Schedules for Optimal Annealing. *Mathematics of Operations Research*, 13:311–329, 1988.

[18] N. G. Van Kampen. *Stochastic Processes in Physics and Chemistry*. North Holland, 1992.

[19] Jesper Dall. Searching complex state spaces with extremal optimization and other stochastic techniques. *Master Thesis*, 2000.

[20] Stefan Boettcher and Allon G. Percus. Optimization with extremal dynamics. *Physical Review Letters*, 86:5211–5214, 2001.

[21] Jesper Dall and Paolo Sibani. In preparation.