Hysteretic optimization for spin glasses

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Abstract. The recently proposed hysteretic optimization (HO) procedure is applied to the 1D Ising spin chain with long range interactions. To study its effectiveness, the quality of ground state energies found as a function of the distance dependence exponent, $\sigma$, is assessed. It is found that the transition from an infinite range to a long range interaction at $\sigma = 0.5$ is accompanied by a sharp decrease in the performance. The transition is signaled by a change in the scaling behavior of the average avalanche size observed during the hysteresis process. This indicates that HO requires the system to be infinite range, with a high degree of interconnectivity between variables leading to large avalanches, in order to function properly. An analysis of the way autocorrelations evolve during the optimization procedure confirm that the search of phase space is less efficient, with the system becoming effectively stuck in suboptimal configurations much earlier. These observations explain the poor performance that HO obtained for the Edwards–Anderson spin glass on finite-dimensional lattices, and suggest that its usefulness might be limited in many combinatorial optimization problems.

Keywords: spin glasses (theory), avalanches (theory), analysis of algorithms, robust and stochastic optimization

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Contents

1. Introduction 2
2. Hysteretic optimization 3
3. Avalanches and correlations 6
4. Discussion 10
   Acknowledgments 11
   References 11

1. Introduction

The steadily increasing availability of powerful computational resources has allowed scientists and engineers alike to study ever more realistic and complex problems. Historically, a significant fraction of all available computer time has been used to traverse phase space in search of the optimal solution to a given problem.

In particular, in several physics domains [1] such as spin glasses, disordered materials and protein folding, one is interested in enumerating a large number of local minima of the energy landscape [2,3], as that provides us with valuable information about its physical properties. Many algorithms and heuristics have been developed over the years to tackle this kind of problem. In this paper we study a recently proposed algorithm known as hysteretic optimization (HO) [4]–[7]. HO is motivated by the physics of demagnetizing magnetic materials with a slowly oscillating external field of decreasing amplitude. Similar to the thermal fluctuations in simulated annealing [8] or the activated dynamics of extremal optimization (EO) [9], the drag created by the external field carries HO over energetic barriers.

HO has proved efficient [6] at finding the ground state configurations of the well-known Sherrington–Kirkpatrick (SK) [10] mean-field spin glass and of the classical traveling salesman problem, but has hitherto been unsuccessful in searching the corresponding Edwards–Anderson spin glass on finite-dimensional lattices [11], as described in chapter 10 of [1]. Similarly, it was shown in [12] that HO performs poorly for the random field Ising model (RFIM) on a one- or three-dimensional lattice. (The RFIM is a classic model for disordered magnetic materials, but unlike the spin glass case there are polynomial-time algorithms to find global optima in the energy landscape, see chapter 5 in [1].) Since efficient heuristics for hard (i.e. beyond polynomial) optimization problems are still few and far between, especially for spin glasses, but also for many other combinatorial problems [13], promising new algorithms warrant careful investigation. Here, we explore the behavior of HO under variation of the search space characteristics that is representative of many problems. In particular, we apply HO to a one-parameter family of spin glass problems [14]–[18] that interpolates between the characteristics of the SK model on the one extreme and the EA model on the other. We observe that the breakdown of HO for the EA model is intimately linked to the physics of intermittent events (i.e. avalanches)
**Table 1.** Hysteretic optimization algorithm.

| Step | Algorithm Description |
|------|-----------------------|
| 1.   | Set $H = H_1$ large enough such that $S_i = \xi_i \forall i$. Set $E_{(\text{min})} = H = \mathcal{H}_{\text{HO}}|_{H=0}$. |
| 2.   | Decrease $H$ until one spin becomes unstable and allow the system to relax. If $\mathcal{H} < E_{(\text{min})}$, set $E_{(\text{min})} = \mathcal{H}$. |
| 3.   | Optional: when $H$ passes zero, randomize $\xi_i$, leaving the current configuration stable. |
| 4.   | At each turning point $H = H_n = -\gamma_n H_{n-1}$, for $0 < \gamma_n < 1$, reverse the direction of $H$. |
| 5.   | Terminate when amplitude $|H_n| < E_{(\text{min})}$. |
| 6.   | Restart at 1 for $N_{\text{run}}$ times with a new, random set of $\xi_i$’s. |
| 7.   | Return the best $E_{(\text{min})}$ over all runs. |

Kicked-off by the external field in the hysteresis loop. We find a distinct crossover between broadly distributed avalanching dynamics in the SK regime [19], connected with a high degree of interconnectivity between variables and divergent energy scales, and sharply cutoff dynamics in the EA regime. Unfortunately, the need for strong interconnectivity between variables severely limits the applicability of HO with respect to combinatorial problems related to spin glasses of low degree such as satisfiability, partitioning or coloring at their respective phase transitions [13].

This paper is structured as follows. In section 2, we introduce the general hysteretic optimization procedure and apply it to a generalization spin-glass model. In section 3, we investigate in detail the avalanche dynamics during the hysteresis process to identify the reasons that lead to the breakdown of HO’s performance.

### 2. Hysteretic optimization

For a magnetic material, such as an Ising system, to obtain a zero magnetization value, an ac demagnetization is performed. The sample is placed in an oscillating and slowly decaying magnetic field. As the amplitude of the external field approaches zero, so does the magnetization. At low enough temperature and slow driving, a disordered systems gets dragged through a sequence of local energy minima. Based on this observation, Zarand et al [4] proposed hysteretic optimization (HO) as a general-purpose local search heuristic [20] to explore the phase space of many combinatorial optimization problems. As an example, their study implemented the HO algorithm as listed in table 1.

Our study here is focused only on finding the ground state ($T = 0$) energies of spin glasses, for which case we describe the implementation of HO in detail.

In an Ising spin glass, each spin $S_i \in \{\pm 1\}$ is assumed to have a random bond $J_{i,j}$ with other spins $S_j$:

$$
\mathcal{H} = -\sum_{\langle i,j \rangle} J_{i,j} S_i S_j,
$$

where the summation is taken over all pairs of spins. To find ground states of this spin glass with HO, we couple each spin $\sigma_i$ to an external field of amplitude $H$, with a random sign $\xi_i \in \{\pm 1\}$, which may be adjusted even during a single demagnetization run.
Hamiltonian of this extended system is then
\[ \mathcal{H}_{\text{HO}} = \mathcal{H} + H \sum_i \xi_i S_i. \] (2)

Physically, the second term in equation (2) distorts the energy landscape as shown in figure 1, allowing the system to escape local minima. Fluctuations due to the coupling to the external field can compensate for unsatisfied bonds. By varying the external field \( H \) and the random couplings \( \xi_i \), HO can force the system to explore a vast area of phase space in search of the optimal solution.

Following the prescription of algorithm 1 for the variation of the external field \( H \), each run, in effect, starts by exploring a large region of phase space which subsequently decreases slowly. By varying the field between positive and negative amplitudes \( H_n = -\gamma_{n-1} H_{n-1} \), the runs repeatedly quench the system, following an approach similar to the well-known simulated annealing or tempering algorithms [8, 21, 22].

HO operates at \( T = 0 \); thus there are no thermal fluctuations and we can simply calculate the field necessary to make the next spin unstable and increase it to that value (within the \( \gamma^n H_0 \) limit). Typically, HO is run with multiple restarts from the largest amplitude to increase the chances of finding a better approximation to the global minimum. Note, however, that each run itself has no stochastic element once the couplings \( \xi_i \) to the external field are fixed. It is therefore useful to restart the demagnetization process repeatedly with a fresh set of random field directions (see item 6 in algorithm 1). In fact, it is also possible to refresh the \( \xi_i \) each time the external field \( H \) passes through zero during each run (see item 3 in algorithm 1).

This algorithm has been very successful in determining the ground state energies of the Sherrington–Kirkpatrick spin glass [6] and reasonably efficient for the traveling salesman problem [23], but there are few attempts to apply it to other problems [12]. In this paper we focus on a Ising spin glass on a one-dimensional ring with power-law interactions [14]–[18] defined by the Hamiltonian in equation (2) with bonds of the form
\[ J_{i,j} = \frac{\epsilon_{ij}}{r_{ij}^\alpha}. \] (3)

Here, \( \epsilon_{ij} \) are random variables drawn independently from a Gaussian distribution of zero mean and unit variance and
\[ r_{ij} = \frac{L}{\pi} \sin \left( \frac{\pi |i - j|}{L} \right). \]
is the distance between each pair of spins on the ring. By varying $\sigma$ we can interpolate between the all-to-all SK limit ($\sigma = 0$) and the nearest-neighbor EA limit (large $\sigma$), as shown in figure 2. This model has been extremely useful in elucidating the connection between mean-field and finite-dimensional spin glasses [17, 18].

As has been shown in the literature [14, 24, 25], as $\sigma$ is increased this spin glass goes through several distinct phases, see figure 3. For $0 \leq \sigma < 0.5$ the system is effectively infinite range (IR). For all $\sigma$, the singular part of the mean-field transition temperature, $T_{c}^{\text{MF}}$, is of the order of [17]

$$(T_{c}^{\text{MF}})^2 \propto \sum_{i=2}^{N} [J_{i1}^2]_{\text{av}} = \sum_{i=2}^{N} r_{i1}^{-2\sigma} \sim N^{-2\sigma+1},$$

where $[\cdot]_{\text{av}}$ denotes an average over disorder with $[\epsilon_{ij}^2]_{\text{av}} = 1$. This temperature becomes finite in the thermodynamic limit at $\sigma = 0.5$, signaling a transition to a long range (LR) regime, where each node is able to see only a finite fraction of the rest of the system. At $\sigma = 1.0$, $T_{c}$ becomes zero, but the LR character is preserved until $\sigma = 1.5$. From this point on, the structure of the system is purely short range (SR) and each spin is connected only to $O(1)$ neighbors.

We have performed a benchmark study of the performance of HO on this spin-glass model over a range of $\sigma$ values. The point of this study is not so much to tweak HO for optimal performance, but to obtain a clear assessment of its behavior under variation of this parameter. To this end, we generated a benchmark of instances of system sizes $N = 32, 64, 128$ and 256, for which we have obtained extremely good approximations to the ground state energy by alternate means. In this case, we have used the extremal

Figure 2. Systems described by the long range spin-glass model as a function of $\sigma$. For $\sigma \equiv 0$ we re-obtain the SK model and as $\sigma \to \infty$ all the long range links become essentially negligible, leaving us only with nearest-neighbor interactions.

Figure 3. Phase diagram, after [14]–[18].

[Table and diagram]
optimization heuristic (EO) [9, 26, 27] but expending a large amount of CPU time to ensure accuracy. In fact, using the implementation described in [9], EO has proven itself equally capable of approximating ground states in the SK model [27] as for the EA [9], and it appears to be much less dependent on $\sigma$. Although a direct comparison is not justified here due to the disproportionate run times used for EO, we have found that, even in much more extensive runs, HO was not able to find the exact-known ground state of a one-dimensional spin glass with more than $\approx 10^2$ spins [12]. In this set of instances, we have applied HO with a minimal set of control parameters. We set $\gamma = 0.99$ and, for each instance in our set, we performed 10 different runs, each with a separate set of $\xi_i$ that were kept constant throughout the entire run. The ground state energy was taken to be the best value seen over 10 different quenches. This value was then averaged over 1000 different instances and compared with the results obtained by EO for exactly the same set of instances.

In figure 4 we plot the quality of the solution obtained by HO as a function of $\sigma$. The ‘Error’ is defined as the percentage difference in ground state energy of the solutions found using HO relative to EO. Generally, the quality of the results found by HO diminishes for increasing system size for all $\sigma$, as can be expected with the limited CPU time (linear in $N$) apportioned to these runs. More noticeable is the ever more pronounced rise in error for $\sigma > 0.5$. To understand the physical reasons behind this behavior, we proceed to studying the dynamics of the system in the next section.

3. Avalanches and correlations

Unlike the comparison in the previous section, we now focus exclusively on the intrinsic behavior of HO itself. We will pinpoint the causes of HO’s breakdown using quantitative measures. Using essentially the same program as previously, for each value of $N$, we
perform 2 (undamped) hysteresis cycles each, but for a much larger set of $4 \times 10^4 \times \sqrt{32/N}$ instances. Throughout, we set $\xi \equiv 1$.

When the hysteresis procedure described causes a spin to become unstable and get flipped, this may cause several other spins to become unstable, thus initiating an avalanche in the system. Each avalanche can involve a significant fraction of the number of spins in the system, including, on occasion, several flips of the same spin in a form of long range self interaction. Avalanches have a wide range of sizes and can, in principle, be larger than the system size by flipping the same spin multiple times.

As a first step in our analysis, we measure $\langle S(\sigma) \rangle$, the average avalanche size, as a function of $\sigma$ at different system sizes. This measurement will help us determine what range of $\sigma$ we need to study, since it should become system-size-independent in the nearest-neighbor limit. As we show on the right hand side of figure 5, this happens near $\sigma \approx 2.0$, thus restricting our interval of interest to $\sigma \in [0, 2]$, as expected from the literature [17].

We find that this quantity obeys an empirical scaling relation of the form

$$\langle S(N, \sigma) \rangle \sim \frac{NA(\sigma)f(N, \sigma) + B(\sigma)}{\log^2(N)}, \quad (4)$$

where $A(\sigma)$ and $B(\sigma)$ are linear functions of $\sigma$, and $f(N, \sigma)$ is plotted in figure 6. The overlap of all the curves in the interval $\sigma \in [0, 0.5]$ means that all the $N$ dependence has been captured by the $N/\log^2(N)$ term. This scaling should be compared with the $N/\log(N)$ scaling found for this behavior for $\sigma = 0$, i.e. the SK model, by [19]. In fact, the emergence of log corrections makes any definite determination of scaling behavior impossible over the range of system sizes $N$ accessible here, and any of the following scaling relations should be viewed as purely phenomenological.

The scaling becomes increasingly worse with $\sigma > 0.5$, signaling a new $N$ dependence.

We believe this change in behavior at $\sigma = 0.5$ is due to the topological change, from IR to LR, that occurs at this point (see the discussion in the previous section). Even though
Figure 6. Corrections to scaling of the average avalanche size, rescaled according to equation (4).

each node in the LR regime is still connected to other spins at arbitrarily large distances, its possible influence is now limited to a fraction of the total number of variables in the system, resulting in smaller avalanches. The avalanche size effectively creates a limit on the length of the jumps in configuration space that the system is capable of performing, forcing a less than optimal sampling of phase space and increasingly poorer results.

Avalanche sizes are determined by the total number of spin flips that occur. If the same spin happens to flip several times, then it will be counted multiple times as well, but we can also count the number $U$ of just which spins flip at least once. The ratio $S/U$ of the avalanche size, $S$, over the number of unique spins flipped, $U$, gives us a measure of how important loops are in the dynamics of the system: a large ratio will indicate that perturbations spread throughout the system and keep returning to the same spin, while a number close to unity would mean that avalanches propagate in just one direction and never double back.

In figure 7 we plot $\langle S/U(\sigma) - 1 \rangle$ for different system sizes. We find that the ratio between the size of the avalanche and the number of unique spins flipped is always small and becomes approximately system-size-independent in the short range phase. This confirms, once again, that in this region the sphere of influence of each spin is very small, being limited practically only to nearest neighbors.

This quantity obeys a phenomenological scaling relation of the form

$$\left\langle \frac{S}{U}(N, \sigma) - 1 \right\rangle = \sqrt{N} [g(N, \sigma) - A \log(N)],$$

(5)

where $A \approx 4 \times 10^{-4}$ is a small constant and $g(N, \sigma)$ is shown in figure 8. The scaling collapse of the data is very good up to near $\sigma \approx 1.5$ where the system acquires a purely short range behavior. (Clearly, this collapse is purely phenomenological, as the log correction in equation (5) would ultimately overwhelm the constant term.)
Finally, we study how the algorithm approaches the final configuration, at $H \approx 0$ and $m = 0$, by looking at the auto correlation function given by
\[
\langle S_i^0 S_i^\tau \rangle - \langle S_i^0 \rangle \langle S_i^\tau \rangle,
\]
where the indices denote the summation over all spins $i$. In equation (6), we measure the overlap between the final configuration and those obtained a number of $\tau$ complete cycles backwards in the past at their $H = 0$ crossing. Intuitively, we expect that the configurations seen at the beginning of the procedure (large values of $\tau$) will be completely unrelated to the final configuration ($\tau = 0$), resulting in a value near zero for this quantity.
Figure 9. Correlation with the final solution as a function of the time in the past.

However, as the algorithm takes its course and approaches its conclusion, so too must the configurations start approaching the final one, corresponding to a value close to 1. The way in which it varies from values near 0 to values close to 1 gives us information about the way exploration of configuration space occurs. The longer the period during which the correlations are close to 0, the larger the volume explored, and the faster it gets close to zero, the earlier the system restricts itself to a given region, thus limiting the quality of the solution it is able to find.

In figure 9 we plot this quantity for the case $N = 256$, averaged over 1000 different instances for each value of $\sigma$ and with 10 different runs per instance. For small values of $\sigma$, the plateau at low correlations is extended (lower solid black curve), followed by an increase towards the value of 1 near the final stages $\tau \to 0$. As $\sigma$ increases, the autocorrelations increase within the plateau which itself shortens, and the tendency towards 1 becomes noticeable right from the onset (upper solid red curve for $\sigma = 2$). This is a clear demonstration of the ideas expressed earlier, that the volume of configuration space explored becomes smaller with the decrease in avalanche size corresponding to increasing $\sigma$.

4. Discussion

The performance of the hysteretic optimization procedure for spin glasses was analyzed for a spin-glass model that interpolates between systems with highly connected variables in the mean-field limit and sparsely connected variables in the nearest-neighbor lattice limit. HO is shown to be very fast, but the quality of its solutions quickly start decaying for increasing values of the distance dependence exponent, $\sigma$. An analysis of the avalanche dynamics occurring in these systems revealed that the failure of HO is due to the truncation of avalanche size, and hence a limited exploration of the energy landscape, that occurs when the system is no longer in the infinite range phase.
The analysis of the behavior of the autocorrelation function with $\sigma$ confirmed this idea by showing that HO becomes stuck in a limited region of configuration space increasingly earlier for larger values of the distance dependence exponent, $\sigma$.

HO, being dependent on avalanches for its local search, cannot continue to work when the avalanches are no longer large enough to facilitate large jumps in configuration space. Any attempt to use HO in a finite connected system, such as an Edwards–Anderson spin glass or many combinatorial optimization problems [13], is, therefore, inefficient (see chapter 10 in [1] and [12]). Our attempts to simulate sparsely connected systems, in this case 3SAT [13] and EA spin glasses with $\pm J$ bonds, with discrete bond weights proved particularly unsuccessful. In such systems, all variables only possess a finite (and typically, small) range of local field states to take on. For instance, in such an EA spin glass in $d = 3$ dimensions, all spins have exactly $2d + 1 = 7$ states. Thus, a hysteresis loop has just seven jumps between full up- and full-down saturation. At each jump, a finite fraction of spins flip simultaneously due to degeneracies, but mostly in an uncorrelated manner dictated by their local environment. An open question remains that concerning problems defined on random graphs of finite connectivity but with a continuous distribution of bond weights, such as the Viana–Bray spin glass [28] with a Gaussian bond distribution. Unlike for a lattice, the number of neighbors increases exponentially with distance so that every node is connected to every other node with $\sim \ln(N)$ steps, and even small correlations could quickly span the system. One might expect that there would be a crossover between the average connectivity and $\ln(N)$ separating broadly distributed avalanches from localized ones, which would be very weak. Hence, HO might still work reasonably well in those systems down to low connectivities for most practical system sizes. In fact, our preliminary studies of Gaussian spin glasses on 3-connected graphs showed only minor deterioration in HO compared to EO for increasing system sizes (up to $N = 1023$). Yet, an independent comparison of HO to itself within a one-parameter family of models in the spirit of our approach here would require much more simulation for variable connectivity.

These results also highlight one important ingredient for any efficient algorithm or heuristic: the ability to travel between very distant regions of configuration space without being impaired by the large energy barriers that make such jumps energetically or entropically unfavorable. This ability is only within HO’s reach for infinite range systems.

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References

[1] Hartmann A and Rieger H (ed), 2004 New Optimization Algorithms in Physics (Berlin: Springer)
[2] Frauenfelder H (ed), 1997 Landscape Paradigms in Physics and Biology (Amsterdam: Elsevier)
[3] Wales D J, 2003 Energy Landscapes (Cambridge: Cambridge University Press)
[4] Zarand G, Pazmandi F, Pal K F and Zimanyi G T, Using hysteresis for optimization, 2002 Phys. Rev. Lett. 89 150201
[5] Pal K F, Hysteretic optimization for the traveling salesman problem, 2003 Physica A 329 287
[6] Pal K F, Hysteretic optimization, faster and simpler, 2006 Physica A 359 650
[7] Pal K F, Hysteretic optimization for the Sherrington–Kirkpatrick spin glass, 2006 Physica A 367 261

doi:10.1088/1742-5468/2008/01/P01003
Hysteretic optimization for spin glasses

[8] Kirkpatrick S, Gelatt C D and Vecchi M P, *Optimization by simulated annealing*, 1983 Science **220** 671

[9] Boettcher S and Percus A G, *Optimization with extremal dynamics*, 2001 Phys. Rev. Lett. **86** 5211

[10] Sherrington D and Kirkpatrick S, *Solvable model of a spin-glass*, 1975 Phys. Rev. Lett. **35** 1792

[11] Edwards S F and Anderson P W, *Theory of spin glasses*, 1975 J. Phys. F: Met. Phys. **5** 965

[12] Zapperi S, Colaiori F, Dante L, Basso V, Durin G, Magni A and Alava M J, *Is demagnetization an efficient optimization method?*, 2004 J. Magn. Magn. Mater. **274** E1009

[13] Percus A G, Istrate G and Moore C, 2006 *Computational Complexity and Statistical Physics* (Oxford: Oxford University Press)

[14] Kotliar G, Anderson P W and Stein D L, *One-dimensional spin-glass model with long-range random interactions*, 1983 Phys. Rev. B **27** R602

[15] Fisher D S and Huse D A, *Ordered phase of short-range Ising spin-glasses*, 1985 Phys. Rev. Lett. **56** 1601

[16] Fisher D S and Huse D A, *Equilibrium behavior of the spin-glass ordered phase*, 1988 Phys. Rev. B **38** 386

[17] Katzgraber H G and Young A P, *Monte Carlo studies of the one-dimensional Ising spin glass with power-law interactions*, 2003 Phys. Rev. B **67** 134410

[18] Katzgraber H G and Young A P, *Probing the Almeida–Thouless line away from the mean-field model*, 2005 Phys. Rev. B **72** 184416

[19] Pázmándi F, Zaránd G and Zimányi G T, *Self-organized criticality in the hysteresis of the Sherrington–Kirkpatrick model*, 1999 Phys. Rev. Lett. **83** 1034

[20] Hoos H H and Stützle T, 2004 *Stochastic Local Search: Foundations and Applications* (San Francisco, CA: Morgan Kaufmann)

[21] Salamon P, Sibani P and Frost R, 2002 *Facts, Conjectures, and Improvements for Simulated Annealing* (Philadelphia, PA: Society for Industrial & Applied Mathematics)

[22] Marinari E and Parisi G, *Simulated tempering: a new Monte Carlo scheme*, 1992 Europhys. Lett. **19** 451

[23] Pal K F, *Hysteretic optimization, faster and simpler*, 2006 Physica A **360** 525

[24] Bray A J, Moore M A and Young A P, *Lower critical dimension of metallic vector spin-glasses*, 1986 Phys. Rev. Lett. **56** 2641

[25] Fisher D S and Huse D A, *Equilibrium behavior of the spin-glass ordered phase*, 1988 Phys. Rev. B **38** 386

[26] Boettcher S and Percus A G, *Nature’s way of optimizing*, 2000 Artif. Intell. **119** 275

[27] Boettcher S, *Extremal optimization for Sherrington–Kirkpatrick spin glasses*, 2005 Eur. Phys. J. B **46** 501

[28] Viana L and Bray A J, *Phase diagrams for dilute spin-glasses*, 1985 J. Phys. C: Solid State Phys. **18** 3037

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