Parallel Tempering Monte Carlo and Spin Glasses

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Bradley Dice

Abstract

A parallel tempering Monte Carlo sampling algorithm is applied to 3D Edwards-Anderson spin glasses. The simulation methods and outcomes are discussed as they pertain to the physics and symmetry breaking of spin glass systems.

Introduction

Monte Carlo methods are useful for integration via sampling: by taking many individual configurations from a configuration space and weighting them by their relative likelihood (often an exponential function of energy like $e^{-\beta E_i}$), values of interest may be obtained. In particular, this method is used with variants of the Ising model, important for understanding how spins align to form magnets. The typical Ising model is given by a Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

where i, j are pairs of neighboring sites on a lattice and $\sigma_i \sigma_j$ correspond to their spins (up or down). J is the coupling constant defining the strength of each pair's energetic contribution. However, if this model is extended to allow J to take a different value for each pair of neighbors on the lattice (that is, $J \rightarrow J_{i,j}$), then more complex results are possible. This is called the Edwards-Anderson model [1].

The Edwards-Anderson model produces spin glasses, disordered structures where the ground state is difficult to determine. Like a typical glass, the energy landscape has many local minima, because the system is frustrated, and simply reducing the temperature is not enough to relax the system to its ground state. Instead, to find the global minimum energy (ground state), one must sample a representative portion of configuration space. This can be tricky with traditional Monte Carlo methods and even methods like simulated annealing can struggle to find the true ground-state energy [1,2].

This paper introduces a technique called parallel tempering which is designed to optimize computations of this nature, enabling spin glass systems to be characterized with a variation of traditional Monte Carlo sampling. Past literature has written extensively about the utility of this method [1–5]. For this model, there will be many independent systems sampling the configuration space, each at a different temperature value kT. Simulations at low kT will get stuck in a local minimum, while simulations at high kT will explore more of the configuration space without necessarily relaxing to a local minimum. The parallel tempering algorithm is helpful because it will methodically swap the temperatures of the systems, so that all the systems can explore more of the configuration space in search of a global minimum.

Simulation Design and Samples

Traditional Ising model simulations use a fixed temperature and a coupling constant J does not change across the lattice. For the Edwards-Anderson model, the Hamiltonian is

$$H = -\sum_{\langle i,j \rangle} J_{i,j,d}\sigma_i\sigma_j$$

with parameters defined as in the introduction. Each neighboring pair shares a "bond" but the couplings $J_{i,j,d}$ are drawn from a normal distribution with mean 0 and standard deviation 1. The letter d explicitly signifies the direction of the coupling, i.e. 0 for a right neighbor along the x direction or 1 for a lower neighbor along the y direction. For a cubic lattice in D dimensions, the value of d ranges from 0 to $D-1$ inclusive and corresponds to the direction of the bond between i and j. The couplings are drawn at the beginning of the simulation and do not change as the simulation steps forward (each timestep is a "sweep," in Monte Carlo parlance). This means that sometimes neighbors will be more likely to align ($J_{i,j} > 0$ gives a negative contribution to the energy), and sometimes neighbors will be more likely to anti-align

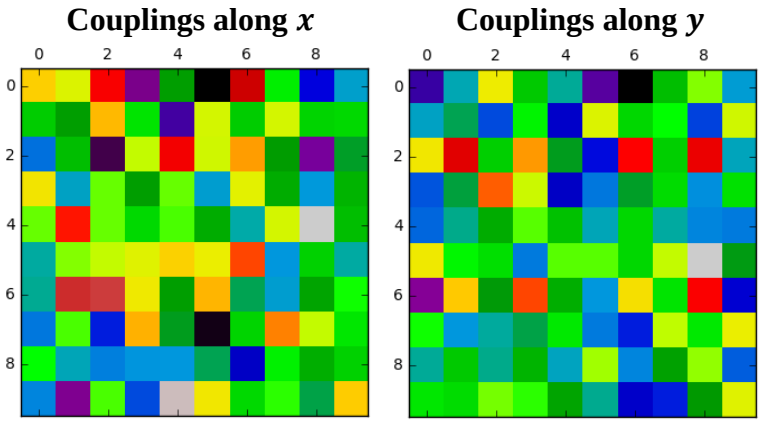

Figure 1 shows the normally-distributed strength of the couplings $J_{i,j,d}$ where each lattice point (i,j) has a coupling $J_{i,j,0}$ with its right neighbor and $J_{i,j,1}$ with its lower neighbor. The system has periodic boundaries. Black, purple, blue are negative, while orange, red, white are positive. Green is around 0 coupling strength.

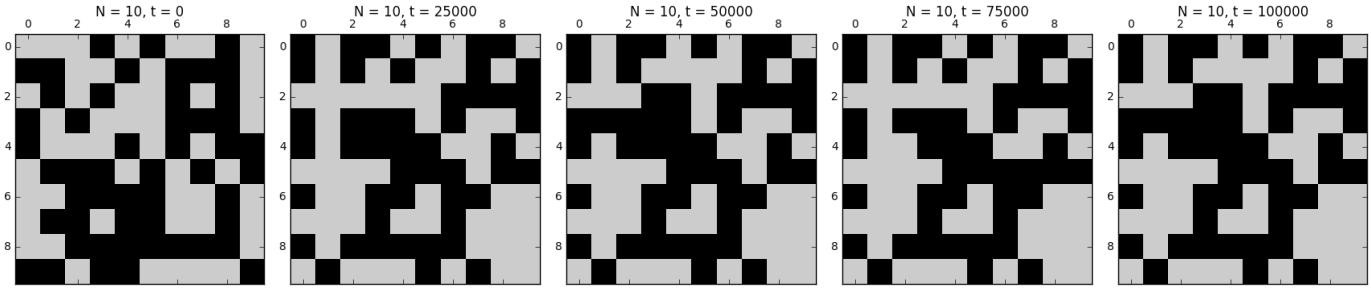

Figure 2 shows a 10×10 2D spin glass simulated at $kT = 0.5$ with the couplings previously shown in Figure 1, after intervals of 25,000 sweeps (individual spin flips). The structure at $t = 0$ is initialized with random spins, but all subsequent structures are very similar to one another.

($J_{i,j} < 0$ gives a positive contribution to the energy). An example set of couplings is shown in Figure 1.

A sample spin glass is simulated in two dimensions, with a 10×10 lattice and periodic boundaries. The results are shown in Figure 2. For this sample, the temperature has been fixed at $kT = 0.5$.

Measuring the average energy as a function of kT gives the graphs shown in Figure 3. This is used to verify that the system is indeed frustrated, and to emphasize its different behavior from the Ising model simulation code from which this was adapted.

Finally, the key components of parallel tempering are introduced. A total of N_T different temperatures will be simulated simultaneously [3]. Pairs of systems with adjacent temperatures will swap after N_{sweep} steps with probability $A = \min\{1, e^{\Delta\beta\Delta E}\} = \min\{1, e^{(\beta_i-\beta_j)(E_i-E_j)}\}$ [2].

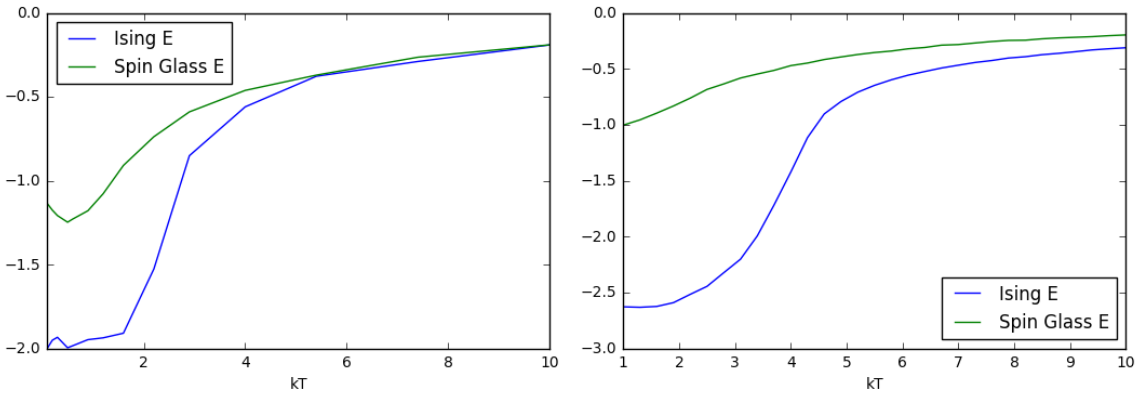

Figure 3 shows average energy as a function of temperature for a 24×24 2D lattice at left, and a 20×20×20 3D lattice at right. At high temperature, the Ising model and spin glass behave similarly, but at low temperature, the frustrated nature of the spin glass and its lack of a sharp transition become apparent. The 2D simulation shows some artifacts from insufficient thermalization at very low temperatures. This same lack of thermalization for kT below 0.20 occurs in the literature [3].

Importantly, the systems much continue to obey detailed balance. Two replicate systems (replicas) of each set of coupling constants are simulated, so there are two separate "ladders" of temperatures swapping, both of which contain one of each replica. The reason that these replicas are used is a bit complicated, but there is a fundamental "replica symmetry" broken by spin glasses because of their complicated energy landscape. This is described excellently in G. Parisi's Dirac Medal talk [6]. The replicas swap temperatures independently.

Analysis Methods

Two quantities can be used to correlate the replicas [3]. First, the spin overlap

$$q = \frac{1}{N}\sum_{i=1}^{N} \sigma_i^{(1)}\sigma_i^{(2)}$$

where we have N total sites on the cubic lattice, and (1) and (2) are replicas with the same coupling constants. Second, we define the link overlap

$$q_l = \frac{1}{N_b}\sum_{\langle i,j\rangle} \sigma_i^{(1)}\sigma_j^{(1)}\sigma_i^{(2)}\sigma_j^{(2)}$$

where N_b is the number of bonds. For a D-dimensional system, each site on a cubic lattice has $2D$ neighbors. Since each bond is shared twice, this means that the number of bonds is ND [3].

The link overlap is particularly of interest for characterizing the similarity of replicas. The system energy is invariant under swapping the sign of all the spins (since we have no magnetic field term in the Hamiltonian, like in some Ising variants). Therefore, it is more important to know how neighboring spins compare in terms of "aligned" or "anti-aligned" instead of in terms of "both up/down" or "one down/up, one up/down." The link overlap accounts for this, while the spin overlap does not. It should be expected that high temperatures will have small link overlaps, since

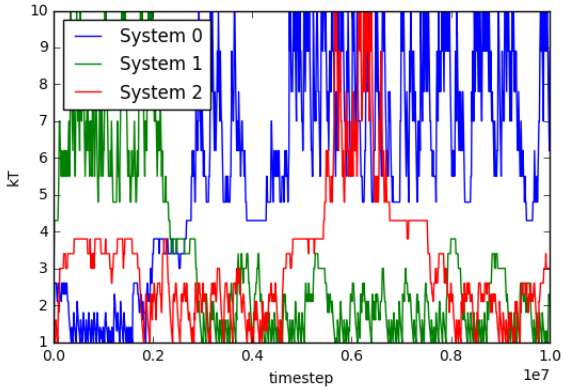

Figure 4 shows three systems sampling 10^7 steps and potentially swapping temperatures every 10^4 steps. There were 21 temperatures in this range, from $kT = 0.1$ to $kT = 20$. The temperatures were geometrically spaced (same ratio between steps). This suggestion was given in the literature, since adaptive temperature methods are not used [4].

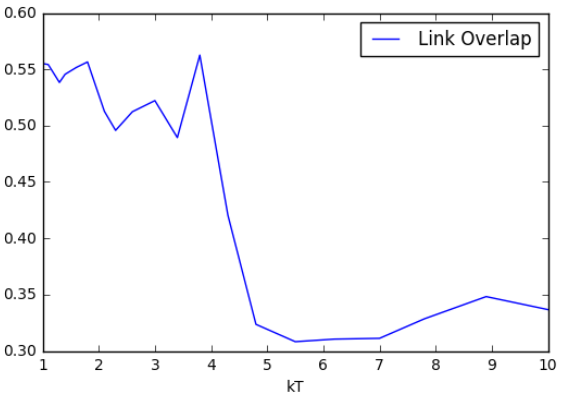

Figure 5 shows an overview of the link overlap, which generally behaves as expected – more overlap at lower temperatures, where the configurations have more in common, driven by energetic relaxations. At high temperatures, there is less overlap because thermal fluctuations are large. These simulations were run for 8×8×8 3D grids with 21 temperatures ranging from $kT = 0.1$ *to* $kT = 20$*. Each simulation ran for* 10^7 *steps and had a chance of swapping temperatures every* 10^4 *steps. To achieve good statistics, many more samples would be required.*

independent thermal fluctuations in each replica should decorrelate them. Similarly, low temperatures should show large link overlaps on average (overlaps are smaller when the replicas find different local energy minima).

Results and Discussion

The parallel tempering method is extremely useful because it makes problems of this kind much more tractable. Due to the complex nature of spin glasses, achieving results comparable to the literature would have taken significantly more time and more samples than were simulated for this exploration of parallel tempering Monte Carlo methods. Additionally, choosing the optimal set of parameters is a nontrivial exercise. Optimal strategies have been studied extensively but disagreements persist in the literature over the best parameters/heuristics to choose [4,5]. In particular, adaptive temperatures are considered an acceptable solution by some authors, with temperatures shifting to create a fixed acceptance rate around 23%, though others disagree with the optimality of this solution [4].

When a sample goes from the lowest temperature to the highest temperature and back, it has completed a “round trip.” One important measurement to make is the round-trip time τ [4]. For the parallel tempering method to be most efficient, this time should be minimized. Figure 4 shows that System 2 completes a full round-trip, but neither of the other two systems shown complete a round trip in the number of steps simulated for that figure. Finally, Figure 5 shows that the link overlaps follow the general trend previously predicted: high overlap at low temperature and low overlap at high temperature.

In summary, the parallel tempering method enables sampling across complex energy landscapes in glassy and similar systems. Not limited to spin glasses, parallel tempering has been successfully applied to simulate biomolecules like cyclic peptides, Lennard-Jones fluids, polymers, zeolites, and more [2,5]. This work has shown a model system for parallel tempering,

a 3D Edwards-Anderson spin glass, and establishes a basic understanding of how the many parameters and heuristics may be used to analyze and optimize the model for spin glasses.

Works Cited

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