Distribution of metastable states of spin glasses

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Distribution of metastable states of spin glasses

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Abstract. The complex behavior of systems like spin glasses, proteins or neural networks is typically explained in terms of a rugged energy or fitness landscape. Within the high-dimensional conformation space of these systems one finds features like barriers, saddle points, and metastable states whose number – at least in the case of spin glasses – grows exponentially with the size of the system. We propose a novel Monte Carlo sampling algorithm that employs an ensemble of short Markovian chains in order to visit all metastable states with equal probability. We apply this algorithm in order to measure the number of metastable states for the two-dimensional and the three-dimensional Edwards-Anderson model and compare with theoretical predictions.

1. Introduction

Although the Edwards-Anderson [1] spin-glass model has been the subject of interest for several decades, many question are still unanswered. When it comes to numerical investigations of the low-temperature phase, it seems today that the prevalently used algorithms like parallel tempering [2] are at times inadequate. Even the employment of special purpose computers has not been as successful as hoped. While it must be said that Monte Carlo simulations might be a priori of limited use due to the supposed NP-hardness of the problem, we believe that more advanced algorithms can still make a difference.

The complex behavior of the Edwards-Anderson model is the result of a rough energy landscape. A huge number of local minima (metastable states) with basins of attraction of varying sizes separated by high energy barriers hamper the investigation of the state space by means of random walks. Albeit being promising objects of investigation, metastable states of spin glasses have so far attracted interest mostly in the form of analytical studies, e.g., Ref. [3]. Numerically, they have been accessed by means of exact enumeration [4, 5, 6] or random quenches [7] with the drawback that the former can only be used for very small systems while the latter cannot provide an unbiased sampling. In a recent study we introduced a dynamic greedy algorithm [8] which can very efficiently sample low-energy metastable states of larger systems directly. However, for this technique the distribution is not uniform; each metastable state is occupied with a probability proportional to the size of the respective basin of attraction. With the intent to create a process with good efficiency and uniformly distributed metastable states we propose a new algorithm [9] which uses an ensemble of short Monte Carlo trajectories to sample the metastable states directly. We apply this algorithm in order to measure the number of metastable states.

2. Model and metastability

We consider the Edwards-Anderson model

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} s_i s_j, \qquad s_i \in \{-1, 1\}, \tag{1}$$

where pairs $\langle ij \rangle$ indicate that the spins s_i and s_j are adjacent in a quadratic or simple cubic lattice. The strength of interaction is given by the bonds J_{ij} which are randomly drawn from a Gaussian distribution:

$$P(J_{ij}) = \frac{1}{\sqrt{2\pi J^2}} e^{-J_{ij}^2/2J^2}. \tag{2}$$

Alternatively, the Hamiltonian can be written as

$$\mathcal{H} = \frac{1}{2} \sum_k e_k = E, \tag{3}$$

where e_k denotes single-site energies, i.e., the sum of all terms to which an individual spin s_k contributes,

$$e_k = -\sum_{\langle ij \rangle} J_{ij} s_i s_j (\delta_{ik} + \delta_{jk}). \tag{4}$$

The division by two in (3) becomes necessary since all terms are counted twice, $J_{1,2} s_1 s_2$ for instance is a summand in e_1 and in e_2. For a single spin flip

$$\mathbf{S} = (s_1, \ldots, s_{k-1}, s_k, s_{k+1}, \ldots, s_N) \to \mathbf{S}' = (s_1, \ldots, s_{k-1}, -s_k, s_{k+1}, \ldots, s_N), \tag{5}$$

one finds that

$$e_k \to e_k' = -e_k \tag{6}$$

and

$$\mathcal{H}(\mathbf{S}') - \mathcal{H}(\mathbf{S}) = -2e_k. \tag{7}$$

Therefore, if $e_k < 0$ for all k, every possible single spin flip causes an increase in energy. Such spin configurations are called metastable or single-flip stable, sometimes they are also referred to as inherent structures.

3. Algorithm

Often, metastable states are obtained by starting with a random configuration and applying some sort of energy minimization process, e.g., rapid cooling (quench). However, this way different minima are found with different probability based on the size of their basins of attraction. In order to sample all metastable stats uniformly, a method of energy minimization is needed which finds all metastable states with the same probability. As it turns out, this can be achieved by means of a random minimization: Starting with some spin configuration $\mathbf{S}$ a spin with positive energy is chosen randomly and is flipped. This is repeated until no spins with positive energy remain and a metastable configuration ρ is reached. Formally, we introduce a function

$$\mu(\mathbf{S}, \{\xi\}) = \rho, \tag{8}$$

which takes $\mathbf{S}$ and a set of random numbers $\{\xi\}$ uniformly distributed in $(0, 1]$ as arguments, performs the random minimization using $\{\xi\}$ to perform the selections, and returns a metastable state. If n_i^{p} is the number of spins with positive energy of the configurations $\sigma_0, \sigma_1, \ldots, \sigma_f$ that are assumed during the minimization starting with n_0^{p} for $\mathbf{S} \equiv \sigma_0$ and ending with n_f^{p} for $\rho \equiv \sigma_f$

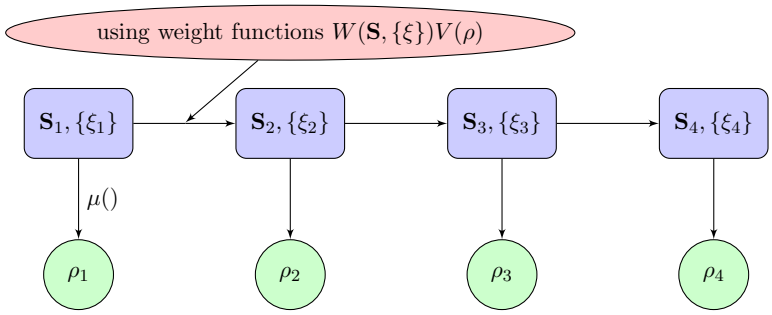

Figure 1. A schematic depiction of the algorithm's basic elements.

and if in the same way n_i^{n} is the number of spins with negative energy it can be shown [9] that if the ensemble of combined states $\mathbf{S},\{\xi\}$ is biased according to the weight function

$$W(\mathbf{S},\{\xi\}) = \frac{\prod_{i=0}^{f-1} n_i^{\mathrm{p}}}{\prod_{i=1}^{f} n_i^{\mathrm{n}}} \tag{9}$$

the derived ensemble of metastable states ρ is uniformly distributed. This means that if an importance sampling method in the space of spin configurations and random numbers is performed with the Metropolis-Hastings acceptance criterion:

$$p_{\mathrm{acc}}\left((\mathbf{S},\{\xi\}) \to (\mathbf{T},\{\tau\})\right) = \min\left(1, \frac{W(\mathbf{T},\{\tau\})}{W(\mathbf{S},\{\xi\})}\right), \tag{10}$$

the algorithm at the same time performs a simple sampling walk in the space of metastable states. In order to perform importance sampling in the space of metastable states it is now possible to apply another weight function that takes the metastable states as arguments:

$$V(\rho) = V(\mu(\mathbf{S},\{\xi\})). \tag{11}$$

In practice just as in standard Monte Carlo simulations, these weights will only depend on a single observable of ρ, e.g., the energy:

$$V_{\mathrm{Boltzmann}}(\rho) = e^{-\beta\mathcal{H}(\rho)}. \tag{12}$$

The basic concept is laid out in figure 1.

4. Number of metastable states

As a basic application of the algorithm we measure the number of metastable states. Since the system performs a random walk in the space of metastable states, this corresponds to measuring the volume of the accessible state space. Such a measurement is a somewhat unusual task since for most Monte Carlo simulations the number of possible states or the volume of the state space is known beforehand. It is for instance trivial that there are 2^N states (spin configurations) in the Ising model. Mathematically the number of states can be obtained by integrating a distribution like the density of states as function of energy. However, for this purpose the distribution in question has to be normalized properly. It is for that reason advisable to chose a quantity that

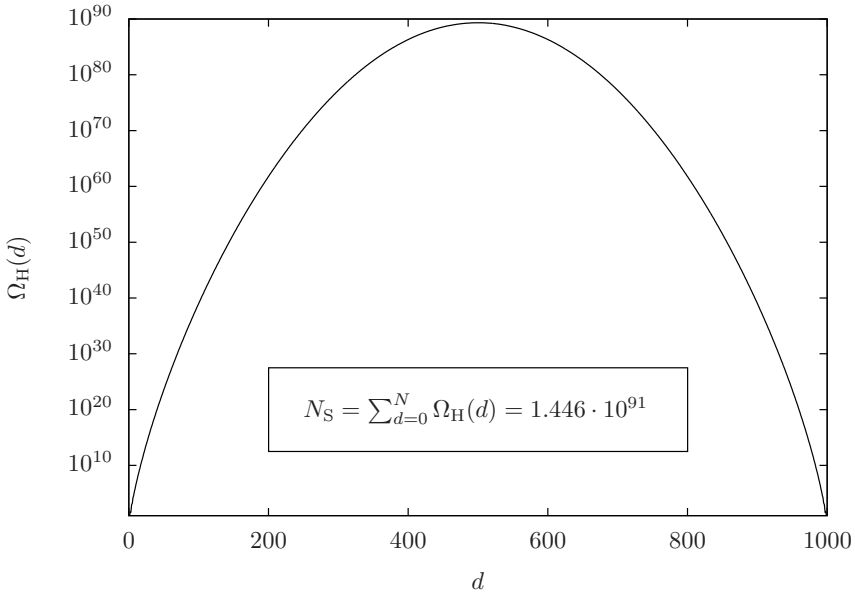

Figure 2. Distribution of metastable states as function of the Hamming distance to a reference configuration for a single $10 \times 10 \times 10$ – sample.

facilitates normalization. We chose the Hamming distance to an arbitrary reference metastable state ρ_{ref}:

$$D_{\mathrm{H}}(\mathbf{S}) = \sum_i (1 - \delta_{S_i, \rho_{\mathrm{ref},i}}), \tag{13}$$

since we know that for the distribution

$$\Omega_{\mathrm{H}}(d) = \sum_{\rho} \delta_{D_{\mathrm{H}}(\rho), d} \quad , \tag{14}$$

where the sum goes over all metastable states and δ is the Kronecker symbol, it is $\Omega_{\mathrm{H}}(0) = \Omega_{\mathrm{H}}(N) = 1$, i.e., there is exactly one state equal to ρ_{ref} and exactly one state where all N spins are inverted.

In our simulation we used a flat-histogram method. We set

$$V(\rho) \equiv \tilde{V}(D_{\mathrm{H}}(\rho)) \approx \Omega_{\mathrm{H}}(D_{\mathrm{H}}(\rho))^{-1} \tag{15}$$

and determined $\tilde{V}$ using the Wang-Landau [10] algorithm. Subsequently, in an extended production run we measured $\Omega_{\mathrm{H}}(d)$ and calculated the number of metastable states

$$N_{\mathrm{S}} = \sum_{d=0}^{N} \Omega_{\mathrm{H}}(d) \tag{16}$$

for 1000 samples of the two-dimensional ($L = 32$) and the three-dimensional ($L = 10$) Edwards-Anderson model. For a single 3d sample the data are shown in figure 2. The histograms of the logarithm of the number of metastable states for these 1000 samples are displayed in figure 3. Some properties are listed in table 1, with the minute values for skewness and with kurtosis close to 3, we conclude that as expected the logarithmic numbers of metastable states follow a Gaussian distribution.

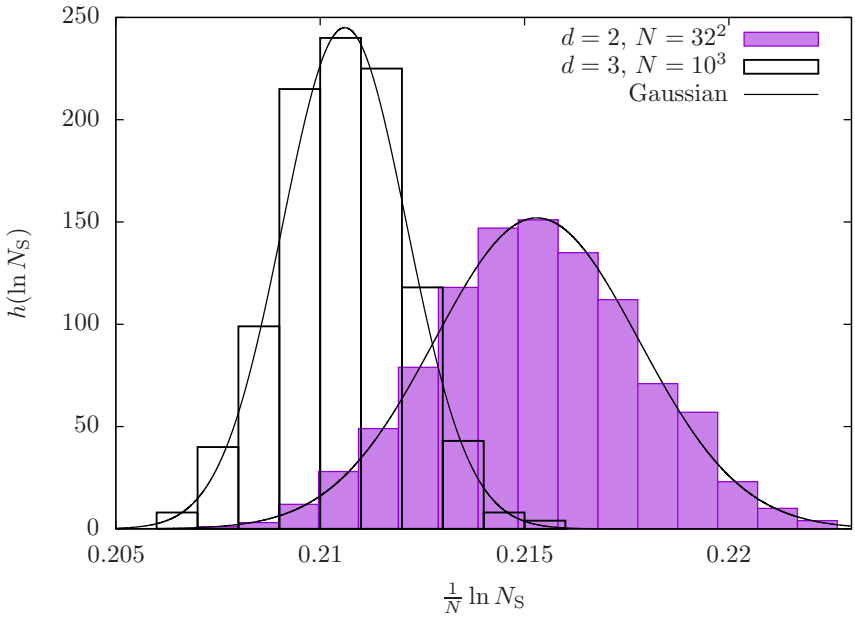

Figure 3. Histogram of the logarithm of the number of minima for 1000 disorder realizations (samples). The curves represent Gaussian distributions possessing the mean values and the standard deviations from table 1.

Table 1. Properties of the distribution of the normalized logarithmic number of minima $\frac{1}{N}\ln(N_S)$.

	2d	3d
mean	0.2153(1)	0.21060(5)
std. deviation	0.0025(1)	0.00152(3)
skewness	0.004(7)	0.05(8)
kurtosis	2.8(1)	2.9(2)

In an earlier study Waclaw and Burda [6] have used an analytic approximation in order to calculate the (non-logarithmic) averages. We compare with our results in table 2. While we observe a very good agreement in two dimensions, there is a slight mismatch for the three-dimensional case. At this point we can not judge whether this is a finite-size effect or a result of the approximation in Ref. [6]. In the third line in table 2 we estimate the mean values exploiting the properties of lognormal distributions. If $\ln(N_S)$ is Gaussian distributed it follows that

$$\ln\langle N_S\rangle = \langle \ln N_S\rangle + \frac{1}{2}\sigma^2_{\ln N_S}, \tag{17}$$

where σ_ξ is the standard deviation of the variable ξ. It follows that

$$\frac{\ln\langle N_S\rangle}{N} = \left\langle \frac{1}{N}\ln N_S \right\rangle + \frac{N}{2}\sigma^2_{\frac{1}{N}\ln N_S} \quad . \tag{18}$$

5. Conclusion

We have introduced a novel method that allows to specifically sample the metastable states of the Edwards-Anderson model. We have applied the algorithm in order to measure the number of metastable states in two and three dimensions. The results agree well with earlier analytic approximations by Waclaw and Burda.

Table 2. Comparison of estimates for $\ln\langle N_S\rangle/N$.

	2d	3d
Waclaw and Burda [6]	0.21808(2)	0.21125(1)
this study	0.2182(2)	0.2118(1)
from parameters in table 1	0.2185	0.21176

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