Unbiased generation of metastable states for 2D Ising spin glasses

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1 Introduction

We consider the problem of estimating the number of local minima in spin glass models with a regular lattice structure. This is done by generating a search tree which contains the local minima in its leaves and then estimating the search tree leaf size by Knuth's method. It turns out that there are exponential number of local minima such that equation $y = e^{\alpha N}$ holds, where N is the number of spins and y is the number of local minima. Values of α are calculated for different lattices.

Additionally this paper contains some analysis on the energy distribution of the local minima for the lattice systems described above. Typical energy value for a local minimum is estimated. Although this would also be easy to do by other means, the alogrithm used could probably be extended to sample other local minima than the typical ones as well.

1.1 Definitions

Spin glass lattice is a regular structure where the edges of the lattice represent the interactions between spins while the nodes represent the spins. In this paper hexagonal (honeycomb) lattice and square lattice are considered.

If two spins interact with each other the energy contribution of the interaction is either negative or positive depending whether the edge is satisfied or not. Red edge corresponds to the positive contribution (unsatisfied) and green edge to the negative contribution (satisfied). Therefore the energy of the system is directly related to the difference between the amount of these edges.

Local minimum is a state where no spin can be flipped to obtain a better energy state. Flipping a spin always changes the colors of the leaving edges, so a local minimum is a state where no node contains more neighboring red edges than green edges. Local minima are also called metastable states.

Ground state of the system is the lowest-energy state. In terms of energy a more optimal solution can not be found from a given system. Ground states are also called global minima.

2 Method

Let N be the number of spins in our lattice and let J be a symmetrical $N \times N$ adjacency matrix, which contains cells J_{ij} that represent the interactions between the spins i and j. $J_{ij} = 1$ for ferromagnetical interactions and $J_{ij} = -1$ for antiferromagnetical interactions. With these definitions the Hamiltonian of the spin glass model is

$$H(\sigma) = -\frac{1}{2} \sum_{ij}^{N} J_{ij} \sigma_i \sigma_j \tag{1}$$

where σ represents the current state. σ_i is $+1$ if spin i points upwards and -1 if it points downwards. One can present J as a graph, where nodes are the spins and edges are the interactions.

If an edge is satisfied, $J_{ij} \sigma_i \sigma_j = -1$ and we denote these edges with green color. Else, the edge is not satisfied and we denote those edges with red color. From the edge coloring it is then easy to calculate the Hamiltonian. Let M be the number of edges in the graph. Then

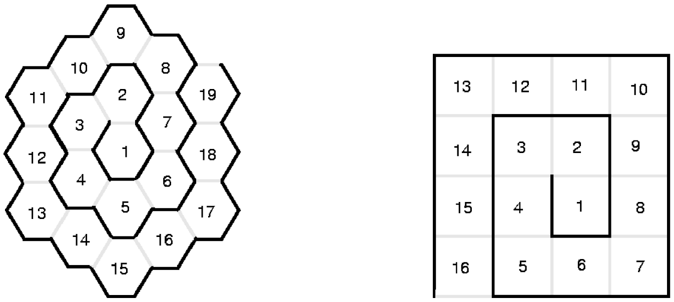
$$H(\sigma) = H_0 + 2H_+ = -\frac{1}{2} \sum_{ij}^{N} |a_{ij}| + 2H_+ = -M + 2H_+ \tag{2}$$

where H_+ is the number of red edges in the graph and H_0 is the Hamiltonian in case all of the edges are green.

Our definition for the local minima is somewhat troublesome, because if a node has equally many red edges as green edges then flipping the spin does not change energy at all even though the configuration changes. Therefore we mostly consider the honeycomb lattice as an example, because there most of the nodes have three neighbors and thus the problem does not appear.

We are searching for the local minima and so we want to color our graph in such a way that the coloring represents a local minimum. During the process we must take frustration into account. This basically means that if any cycle in the graph cotains an odd number of negative edges then it must contain an odd number of red edges as well. Otherwise the coloring is not valid. Additionally we want to make sure that no two red edges are adjacent to each other, because then it is not a local minimum in the honeycomb system.

A way to do the coloring is to choose a feasible spanning tree from the graph. If we only color the edges of the tree then the rest of the edges are determined because of the frustration. This way we will obtain a valid state, but during the progress we must keep in mind to choose coloring in such a way that we actually do obtain the local minima. To be able to do this, the spanning tree is selected in a clever way such that it is a spiral shaped path from center to the edges, which is demonstrated in Figure 1. This kind of construction allows us to take care of the frustration in a local way. The path constructs a cycle and then moves on to the next cycle and so on. By gathering only local information we are able to know whether it is possible to obtain a local minimum or not when choosing a coloring for an edge.



(a) Hex lattice

(b) Square lattice

Figure 1: Construction order of the different lattices

The next step is to enumerate the spanning path and to generate a binary search tree. If we color an edge with green color then we choose left branch in the binary tree and if we choose red color then we choose the right branch. By using a spiral shaped spanning path we can then cut uninteresting branches to reduce tree size in such a way that result is a tree with the local minima in its leaves.

Figure 2 demonstrates the search tree idea. It contains a search tree for a graph C_6 with an odd number of negative edges, thus valid colorings are ones with an odd number of red edges. Valid colorings for local minima are then visible from the picture. Dash lines represent red edges and normal lines represent green edges.

By estimating the number of leaves of the search tree using Knuth's method [3] we can find out the relationship between the number of spins and

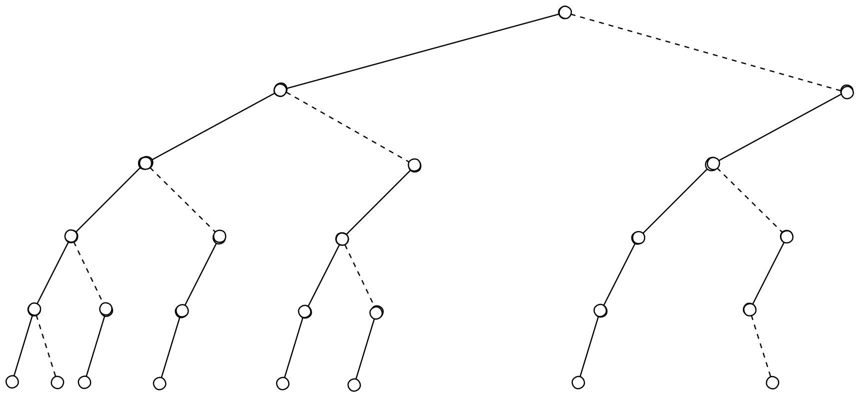


Figure 2: The search tree for a graph with one hex

the number of local minima. The principle of the method is quite simple. Each time the search tree branches pick a random branch and multiply the existing size estimate by two. When the algorithm has reached a leaf we have obtained one estimate for the number of the leaves. If the process is repeated enough times this algorithm will guarantee us an unbiased estimate. Formally the method can be described with equation $N = 1 + b_1 + b_1 b_2 + ...$, where N is the size of the tree and b_i is the branching rate at depth i when descending randomly in the tree. If our spanning path length is j then $b_1 b_2 ... b_j$ is an estimate for the number of leaves. Let the number of iterations for the leaf number approximation be I.

Also, by using Knuth's method recursively, it is possible to construct an algorithm which returns each of the local minima, or actually the coloring instructions to obtain the minimum, with equal probability. Basically the principle of this algorithm is to randomly descend in the search tree, but at each branching point, the leaf number of both branches is estimated and the probing is continued with a fixed probability. If the leaf number of left branch is a and the leaf number of right branch is b then the left branch is chosen with probability $\frac{a}{a+b}$. The number of red edges in the descending route is calculated to obtain the energy value of the local minimum. Also, the edges which are not part of the spanning path must be taken into account in the calculation, but their color is determined by the spanning path colors. This method is used to find out the energy distribution and the average energy of a local minimum.

3 Experimental results

3.1 The number of local minima as a function of N

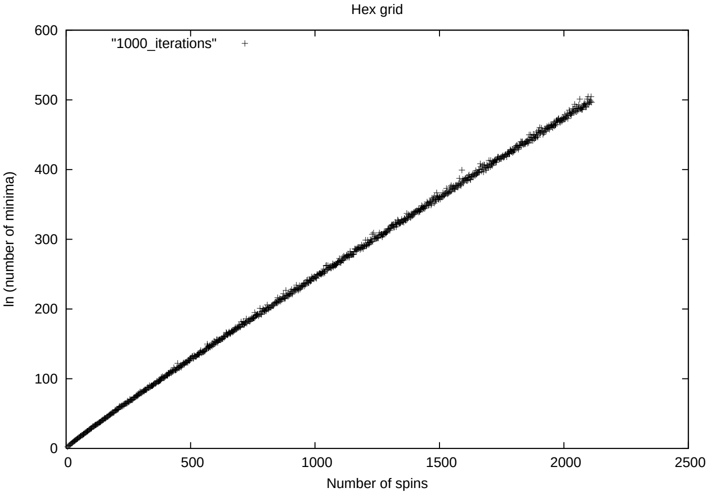


Figure 3: Logarithm of the number of local minima as a function of the number of spins in hex lattice; $I = 1000$

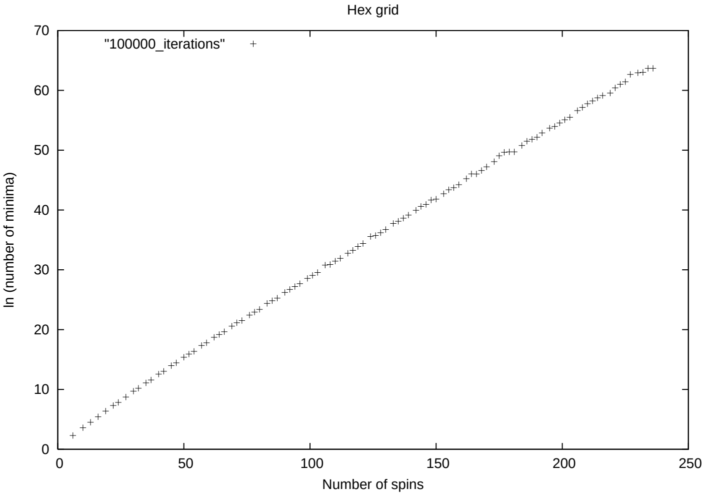


Figure 4: Logarithm of the number of local minima as a function of the number of spins in hex lattice; $I = 100000$

Figure 3 shows us results with very large N and Figure 4 shows us quite accurate results with relatively small N for a hex lattice. If the whole data was used the slope of the linear estimate from the data of Figure 3 would be 0.2335 and the slope of Figure 4 would be 0.2659. But because the effects of the borders are quite significant with small N, more accurate results can be obtained by using only the later half of the data. With this method the corresponding values would be 0.2283 and 0.2587. Therefore it seems obvious that we must use large N in order to obtain a reliable asymptotic approximation for the slope rather than just performing lots of iterations.

Assuming N is the number of spins in the grid and the estimate for the number of local minima is y. Then

$$y = e^{\alpha N} \tag{3}$$

where $\alpha \approx 0.22$ for an infinite hex lattice.

3.2 The energy distribution as a function of N

To find out about the energy distribution of these lattices as a function of N we will have to use Knuth's method recursively as it was introduced in the previous section. Our hypothesis was that as the number of spins increases, the values of H_+/N (H_+ defined in (2)) concentrate on some constant value. The accuracy of the recursive use of Knuth's method depends on the balance of the search tree. With totally unbalanced trees the algorithm is likely to descend to some minimum more often than to another unless the number of iterations used in the size estimation before each branching is increased. And with more balanced trees it is possible to get decent results even with a small number of iterations.

It is assumed that the search trees of these lattices are quite balanced and therefore we have used just one iteration per branch when choosing the descending route with the recursive algorithm. According to a couple of test runs the results did not significantly change when the number of iterations was increased, but computing time required increased dramatically.

Figure 5 and Figure 6 show us the energy distribution of the local minima of the hex lattice with a differing number of spins.

With the ferromagnetic hex lattice model we obtained a result which indicates that most of the descents to the local minima tend to end up to a state, whose energy per spin value is between -0.85 and -0.70 as can be seen in Figure 5. Similarly a typical local minimum in a non-ferromagnetic hex lattice has energy per spin value of something between -0.90 and -0.80 (Figure 6). As the number of hexes increases the concentration becomes

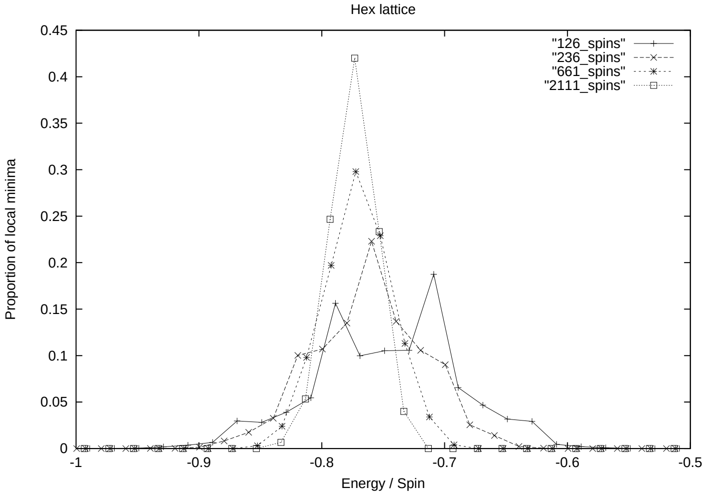


Figure 5: Energy distribution for different values of N.

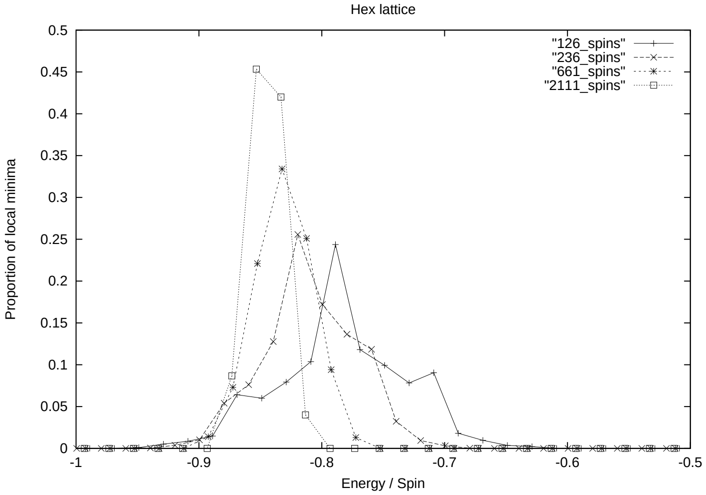


Figure 6: Energy distribution for different values of N in a non-ferromagnetic lattice.

more and more clear as the sharpness of the spike of the graph increases. The number of descents does not affect the results very much, but naturally using a big enough number gives us more reliable data.

4 Conclusions

The experiments were succesful and some results were obtained. The easier part of work was to determine the constant α in equation $y = e^{\alpha N}$. For an infinite hex lattice $\alpha \approx 0,22$ was obtained. However, there were some sources of error during the work. The models used were not infinite but relatively small instead. Therefore the correct values of α could possibly be slightly smaller than those mentioned. According to Figure 3 the data is not completely linear. This should be studied further to see whether the results are reliable or not. Regardless, the value for α can at least be considered as some kind of upper bound for the constant value.

Second part of the work was to find out the energy distribution of the local minima for the two different lattices. This was done with the help of iterative use of search tree leaf number approximation. It turned out, as assumed, that as the number of spins grows, the local minima of the system tends to have some constant energy per spin value. For the hex lattice this constant seems to be between -0.90 and -0.70.

References

[1] Donald E. Knuth, *Estimating the Efficiency of Backtrack Programs.* Mathematics of Computation, Vol. 29, No. 129. (Jan. 1975), 121-136.