Unbiased generation of metastable states for Ising spin glasses

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Overview

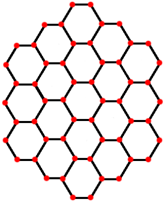
- Background and motivation
- Basics of spin glass lattices
- Equivalence between edge coloring and spin configuration
- Generating the metastable states
- Generalization idea
- Estimating the number of local minima
- Knuth's method vs. exact calculations
- Ferromagnet - spin glass phase transition
- Sampling the energy distribution
- Summary and future work

Motivation, background

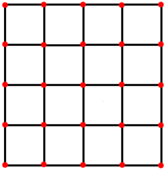
- An efficient way to generate all metastable states of a lattice
- Knuth's algorithm for estimating the size of a search tree
- Phase transition between ferromagnet and spin glass
- Is the number of metastable states affected?
- Various applications:
  - Estimating the number of minima as a function of system size
  - Exploring the energy distribution of minima and sampling

Models

We consider the following two types of 2D Ising spin glass lattices:



(a) Hex lattice

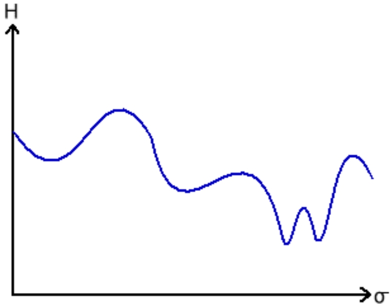


(b) Square lattice

- Up-down spins: $\sigma_i \in \{1, -1\}$
- Positive-negative interactions: $J_{ij} \in \{1, -1, 0\}$
- Hamiltonian: $H(\sigma) = -\frac{1}{2} \sum_{ij}^{N} J_{ij}\sigma_i\sigma_j$

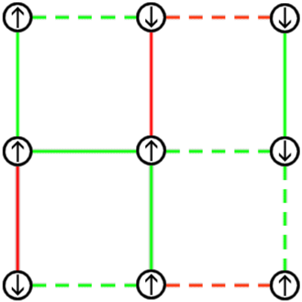
Basics

- Local minimum: no energy decrease by a single spin flip
- Usually wanted: ground state, $min(H(\sigma))$
  - Hard
- Greedy algorithms: get stuck in local minima
- Ground state(s) hard to prove



Graphical view of local minima (1/2)

- A spin configuration σ induces a coloring of the edges in the respective lattice into "green" (satisfied) and "red" (unsatisfied)

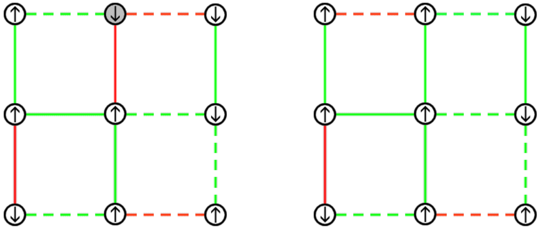


  Here solid edge indicates a positive interaction, a dotted edge a negative one.

- *Note:* $H = -(\#\text{ of green edges}) + (\#\text{ of red edges})$

Graphical view of local minima (2/2)

- An edge coloring of the lattice corresponds to a (proper) local energy minimum, if and only if each vertex is incident to (properly) fewer red than green edges.
- E.g. the previous example coloring (spin configuration) can still improved:



- However, all colorings are not valid
- The sum of negative interactions and red colorings must be even number for each cycle

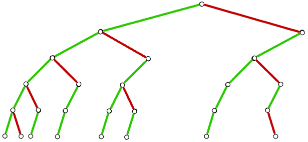
Generating local minima (1/2)

- A local minimum corresponds to an edge coloring of the lattice (interaction graph) G satisfying a local consistency condition.
- Two minima per each valid coloring
- Consider any spanning tree T of G.
- Any edge colouring of G obviously yields a unique colouring of T and vice versa.
- Finding a local minimum of T is easy, but the corresponding coloring of G is not necessarily a local minimum.

Generating local minima (2/2)

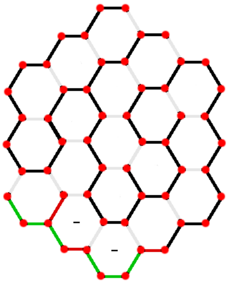
An algorithm to generate the local minima on an interaction graph G:

- Choose spanning tree T of G. List edges of T in some order.
- Enumerate systematically all colourings of this edge list ($\Longrightarrow$ binary search tree).
- Only consider branches of the search tree where the current partial colouring can be completed to a valid colouring of all of G. (This may be difficult to test!)
- Now leaves of the search tree correspond one-to-one to consistent colourings ($\sim$ local minima) of G.



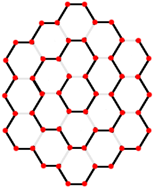
Complexity of completability

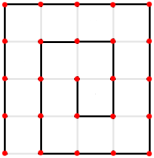
- In a general spanning tree, determining the completability of a given partial colouring may require arbitrary long look-ahead:



Spanning paths

- In lattices, spiral-like paths provide particularly simple spanning trees:





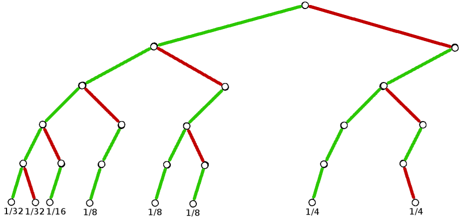
- Moreover, if the edges of the spanning spiral are coloured inside-out, the completability can be tested efficiently. (Basically, a partial colouring can always be completed, unless the validity conditions are violated by already chosen or "locally forced" edge colours.)

Generalization of the tree generation

- Enumerate the edges of G
- For each node v generate a SAT-formula "at most $d(v)/2$ incident edges may be unsatisfied"
- For each uncolored edge:
  - Try green and red colorings
  - Apply propagation rules
    - SAT-formulas are basically implications
    - Validity of coloring
  - If a contradiction follows, prune the branch
  - Randomly select an available branch
- Coming up with a proper set of propagation rules for arbitrary graph is still work in progress
- The idea is to detect the dead-ends in advance so backtracking would not be necessary

Estimating the size of a search tree

- D. E. Knuth, "Estimating the efficiency of backtrack programs". Math. Computation 29 (1975), 121–136.
- Method to estimate number of leaves S in a large search tree T:
  - Make a random descent into T, starting from the root.
  - Record degrees (branching factors) $d_1, d_2, \ldots, d_n$ of the vertices encountered along the descent. (For a binary tree, $d_i \in \{1, 2\}$ for each i.)
  - Compute estimate $\hat{S} = d_1 d_2 \cdots d_n$.
- *Theorem.* $\hat{S}$ is an unbiased estimate of the true tree size S.



Reliability of the Knuth's method

- How many descents do we need?
- Different ways to decrease the variance:
  - Increase the number of descents
  - Modify the search tree (using lattice structure information)
  - Perform biased descents (if we know that the search tree is biased)
- For better understanding, we performed some exact calculations and compared results

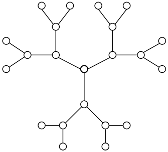
Exact calculations (1/2)

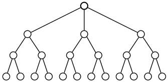
Ferromagnetical L x L square lattice

- Local minima form horizontial or vertical red "ladders" through the lattice
- Let x_L be the number of ways to put vertical ladders through a L x L lattice
- Recursion: $x_L = x_{L-1} + x_{L-2} + 1$, $x_0 = 0$, $x_1 = 1$
- Interestingly, x happens to be similar to Fibonacci series f
- $x = \{0, 1, 2, 4, 7, 12, 20, 33, ...\}$
- $f = \{0, 1, 1, 2, 3, 5, 8, 13, 21, 34...\}$
- $f_i = x_{i-2} + 1$
- Number of local minima is $2(2x_L + 1)$ (vertical or horizontal ladders, the ground state and up-down symmetry)
- $\frac{4}{\sqrt{5}}(\phi^{L+2} - (1-\phi)^{L+2}) - 2$, $\phi = (1+\sqrt{5})/2$

Exact calculations (2/2)

Bethe lattice ($d = 3$)



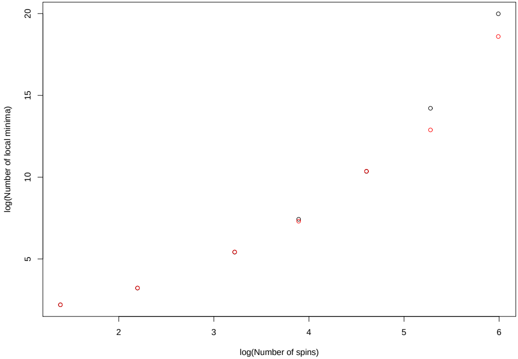


- Number of local minima can again be solved by recursion
- $y_n = y_{n-1}^2 + 2y_{n-1}y_{n-2}^2$
- $x_n = y_{n-1}^3 + 3y_{n-1}^2 y_{n-2}^2$
- $y_1 = 1,\ y_2 = 3$
- Number of local minima for a Bethe lattice with radius i is then $2x_i$ (up-down symmetry)
- $2x = \{2, 8, 108, 18900, 5.73358 \cdot 10^8, ...\}$

Comparing the results (1/2)

Ferromagnetical L x L square lattice (10000 descents per lattice)

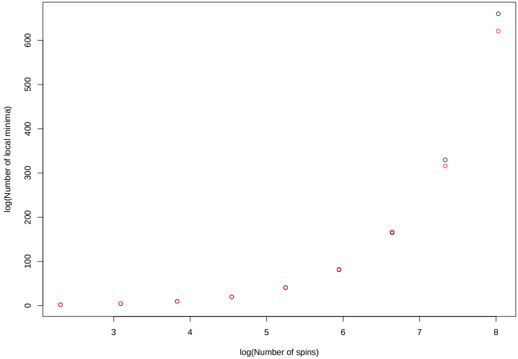
- Search tree is very biased
- In the following graph black dots are the real number of local minima and red dots are the estimates given by the algorithm:



Comparing the results (2/2)

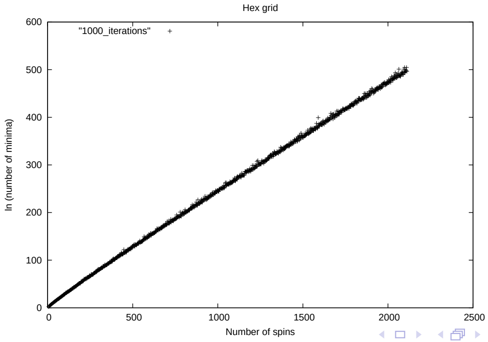
Bethe lattice $(d = 3)$ (10000 descents per lattice)

- Search tree is quite balanced
- In the following graph black dots are the real number of local minima and red dots are the estimates given by the algorithm:



Application 1: Estimating the number of minima (1/2)

- Ansatz: $S \sim e^{\alpha N}$, where S is the number of local minima, N is the number of spins, and α is a coefficient which depends on the system characteristics.
- E.g. for hexagonal lattices of up to 1000 hexes (> 2000 spins), with 50% fraction of negative interactions, we obtain the following diagram. (Each estimate of L is based on 1000 descents.)

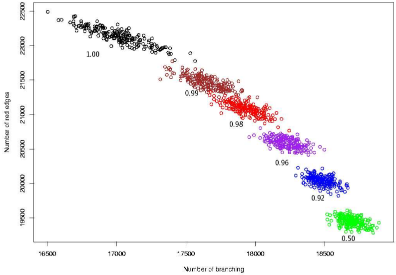


Application 1: Estimating the number of minima (2/2)

- Numerical estimates of the coefficient α, from systems of $1 \dots 1000$ hexes:
  - Ferromagnetic hex lattice: $\alpha \approx 0.226$
  - Hex lattice with 50% negative interactions: $\alpha \approx 0.231$
- The results match quite well the analytic prediction of $\alpha \approx 0.225$ from a recent paper by Waclaw and Burda (arXiv Jan 2008). The paper also reports experimental data on systems of up to 24 spins, indicating $\alpha \approx 0.226$.

Application 2: Studying the phase transition

- When a certain fraction of bonds are antiferromagnetical (negative edges) the system will undergo a phase transition.
- For different systems the fraction of bonds differ
- Will the number of local minima be affected among other properties?
- Results from 60000 spin hexagonal lattice:



Uniform sampling of leaves in a search tree

- Apply Knuth's method recursively.
- When at a non-leaf vertex of a binary search tree T:
  - Estimate size of left subtree: $\hat{S}_L$
  - Estimate size of right subtree: $\hat{S}_R$
  - Descend to left subtree with probability

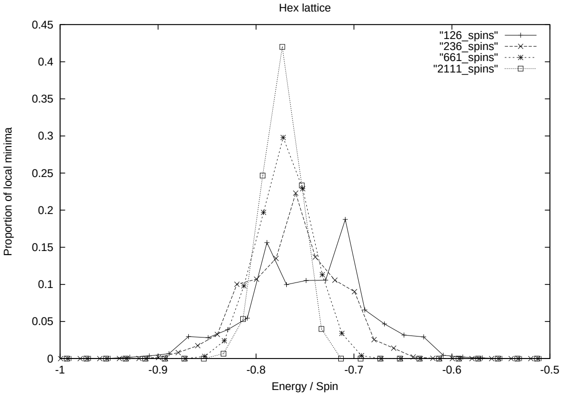
$$p = \frac{\hat{S}_L}{\hat{S}_L + \hat{S}_R},$$

and to right subtree with probability $1 - p$.

$\Longrightarrow$ Descent reaches each leaf with equal probability.

Application 3: Energy distribution of local minima

- Based on a uniform sampling of 1000 minima in ferromagnetic hex lattices with $N = 126, \ldots, 2111$ spins. (Equidistant binning of energy levels. Only one descent per subtree size estimate.)



Summary and future work

- New combinatorial method for almost uniform sampling of local minima in spin glass lattices.
- Method has potentially many applications to the exploration of spin glass energy landscapes.
- Basic method scales well to large system sizes, but search tree shape affects the variance quite much.
- Future work 1: Better analysis of the sampling and perhaps biased sampling for the full energy distribution.
- Future work 2: Extend the method from 2D lattices to other graph structures.
- Future work 3: Explore other applications in landscape analysis.