Uniform sampling of local minima in Ising lattices

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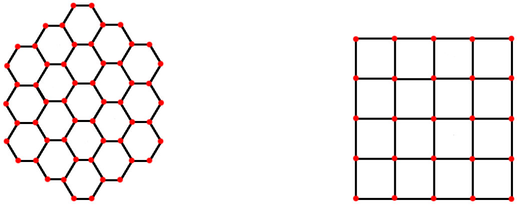
Motivation, background

- For exploring the energy landscape of spin glass models, it is useful to have an efficient method for sampling local energy minima (metastable states).
- MCMC methods can be adapted to this purpose.
- We present a direct combinatorial method based on a classical algorithm by Knuth (1975) for estimating the size of large search trees.
- Applications: estimating the number of minima as a function of system size; exploring the energy distribution of minima; exploring the attraction basins around minima at various energy levels; ...

Models

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



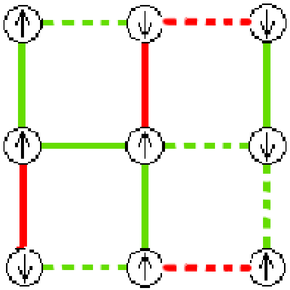
(a) Hex lattice

(b) Square lattice

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

Graphical view of local minima (1/2)

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

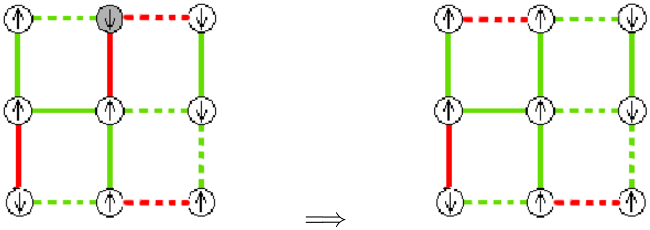


Here solid edge indicates a positive interaction, a dotted edge a negative one.

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

Graphical view of local minima (2/2)

- An edge colouring 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 colouring (spin configuration) can still improved by flipping the top spin:



- Technically, there is also another validity condition on a colouring: the induced spin orientations around any cycle in the lattice must be consistent. (E.g. in a 4-cycle of positive interactions, there must be an even number of red edges.)

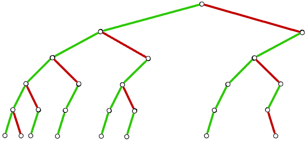
Enumerating local minima (1/2)

- Thus, a local minimum corresponds to an edge colouring of the lattice (interaction graph) G satisfying a local consistency condition. (Because of the up-down symmetry of the spins, there are actually two minima per each valid colouring.)
- Consider any spanning tree T of G.
- Any edge colouring of G obviously yields a unique colouring of T.
- More interestingly, any colouring of T has a unique completion to all of G. (Propagate the spin orientations from the root of T according to the colour of the tree edges. Colour the non-tree edges of G accordingly.)
- Starting from the root vertex, the local validity conditions are easy to satisfy on T. (But the completion to G does not necessarily satisfy them.)

Enumerating local minima (2/2)

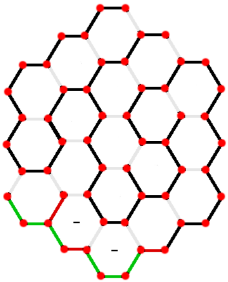
An algorithm to enumerate local minima on an interaction graph G:

- 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.



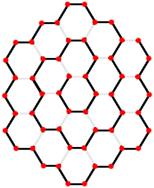
Complexity of completability

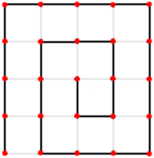
- In a general spanning tree, determining the completability of a given partial colouring may require arbitrary long look-ahead:



Spanning paths

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

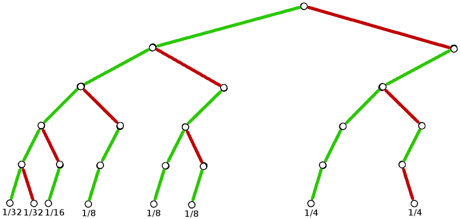




- Moreover, if the edges of the spanning spiral are coloured inside-out, the completability can be tested efficiently. (Basically, a partial colouring can always be completed, unless the validity conditions are violated by already chosen or "locally forced" edge colours.)

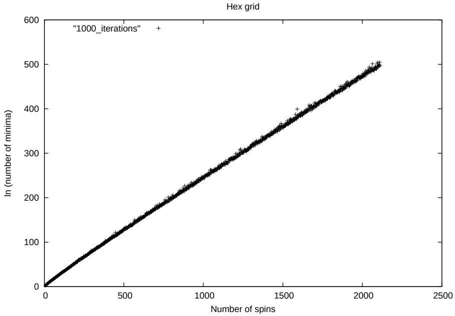
Estimating the size of a search tree

- D. E. Knuth, "Estimating the efficiency of backtrack programs". Math. Computation 29 (1975), 121–136.
- Method to estimate size = 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.
- To decrease variance of the estimate, perform several descents.



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 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 $1 \ldots 2000$ spins:
  - 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 $\alpha \approx 0.226$.

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

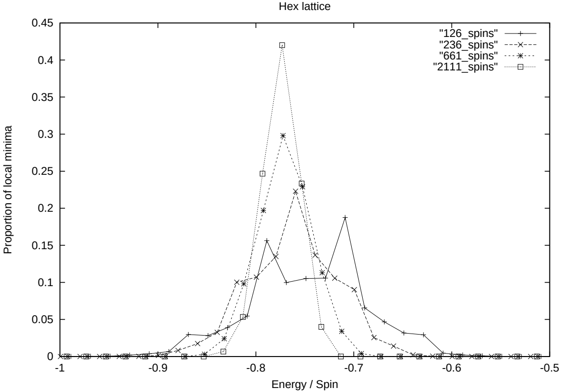
$$p = \frac{\hat{S}_L}{\hat{S}_L + \hat{S}_R},$$

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

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

Application 2: 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 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 effect of system size and search tree shape on the variance of the method are not well understood.
- Future work 1: Analyse variance of the method.
- Future work 2: Extend the method from 2D lattices to other graph structures.
- Future work 3: Explore other applications in landscape analysis.