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DOUBLE FLIP MOVE FOR ISING MODELS WITH MIXED BOUNDARY CONDITIONS*

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Abstract

This note introduces the double flip move to accelerate the Swendsen-Wang algorithm for Ising models with mixed boundary conditions below the critical temperature. The double flip move consists of a geometric flip of the spin lattice followed by a spin value flip. Both symmetric and approximately symmetric models are considered. We prove the detailed balance of the double flip move and demonstrate its empirical efficiency in mixing.

Mathematics subject classification: 82B20, 82B80.
Key words: Ising model, Mixed boundary condition, Swendsen-Wang algorithm.

1. Introduction

This note is concerned with the Monte Carlo sampling of Ising models with mixed boundary conditions. Consider a graph $G = (V, E)$ with the vertex set V and the edge set E. Assume that $V = I \cup B$, where I is the subset of interior vertices and B the subset of boundary vertices. Throughout the note, we use i, j to denote the vertices in I and b for the vertices in B. For the edges, we use $e = ij \in E$ to denote an interior edge between two interior vertices i and j, and $e = ib \in E$ for a interior-boundary edge between interior vertex i and boundary vertex b. The boundary condition is specified by $f = (f_b)_{b\in B}$.

A spin configuration $s = (s_i)_{i\in I}$ over the interior vertex set I is an assignment of ± 1 value to each vertex $i \in I$. The energy of the spin configuration s is given by the Hamiltonian function

$$H(s) = -\sum_{ij\in E} s_i s_j - \sum_{ib\in E} s_i f_b.$$

At a physical temperature T, the configuration probability of $s = (s_i)_{i\in I}$ is given by the Gibbs or Boltzmann distribution

$$p_{\mathrm{I}}(s) = \frac{e^{-\beta H(s)}}{Z_\beta} \sim \exp\left(\beta \sum_{ij\in E} s_i s_j + \beta \sum_{ib\in E} s_i f_b\right), \tag{1.1}$$

where $\beta = 1/T$ is the inverse temperature and $Z_\beta = \sum_s e^{-\beta H(s)}$ is the renormalization constant (or the partition function).

One key feature of these models is that, below the critical temperature and under certain boundary conditions, the Gibbs distribution exhibits macroscopically different profiles. Fig. 1.1 provides two such examples, where black denotes $+1$ and yellow denotes -1. In Fig. 1.1(a), the square Ising lattice has the $+1$ condition on the two vertical sides but the -1 condition

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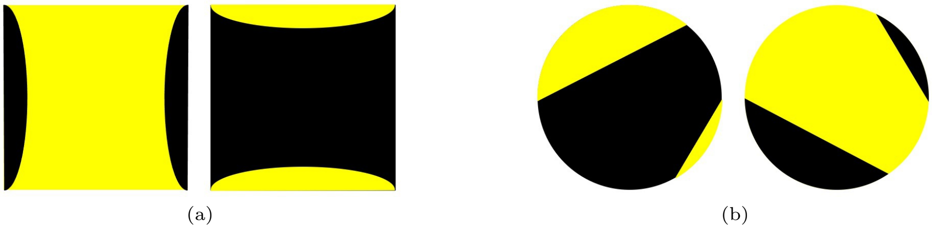

Fig. 1.1. Ising models with mixed boundary condition. (a) a square lattice and (b) a triangular lattice support on a disk. In each example, the model exhibits two macroscopically different profiles.

on the two horizontal sides. There are two macroscopic profiles: one contains a dominant -1 cluster linking two horizontal sides and the other contains a dominant $+1$ cluster linking two vertical sides. In Fig. 1.1(b), the Ising lattice supported on a disk has the $+1$ condition on two disjoint arcs and the -1 condition on the other two. This model also exhibits two macroscopically different profiles shown in Fig. 1.1(b). Notice that in each example, due to the symmetry or approximate symmetry of the Ising lattice as well as the boundary condition, the two macroscopic profiles have comparable probabilities. Therefore, any effective sampling algorithm is required to visit both profiles frequently.

One of the most well-known methods for sampling Ising models is the Swendsen-Wang algorithm [9], which iterates between the following two substeps in each iteration:

1. Given the current spin configuration, generate an edge configuration according the inverse temperature β (see Section 2 for details).
2. To each connected component (also called cluster) of the edge configuration, assign to all spins in this cluster all $+1$ or -1 to with equal probability. This results in a new spin configuration.

For many boundary conditions including the free boundary condition, the Swendsen-Wang algorithm exhibits rapid mixing for all temperatures. However, for the mixed boundary conditions shown in Fig. 1.1, the Swendsen-Wang algorithm experiences slow convergence under the critical temperatures, i.e., $T < T_c$ or equivalently $\beta > \beta_c$. The reason is that, for such a boundary condition, the energy barrier between the two macroscopic profiles is much higher than the typical energy fluctuation. In other words, the Swendsen-Wang algorithm needs to break a macroscopic number of edges between aligned adjacent spins in order to transition from one macroscopic profile to the other. However, breaking so many edges simultaneously is an event with exponentially small probability.

In this note, we introduce the double flip move that introduces direct transitions between these dominant profiles. When combined with the Swendsen-Wang algorithm, it accelerates the mixing of these Ising model under the critical temperature significantly.

When the Ising model exhibits an exact symmetry (typically a reflection that negates the mixed boundary condition), the double flip move consists of

1. A geometric flip of the spin lattice along a symmetry line.
2. A spin-value flip at the interior vertices of the Ising model.

The key observation is that these two flips together preserves the alignment between the adjacent spins, hence introducing a successful Monte Carlo move. When the Ising model exhibits only an approximate symmetry, the double flip move consists of