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ANNEALED IMPORTANCE SAMPLING FOR ISING MODELS WITH MIXED BOUNDARY CONDITIONS*

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Abstract

This note introduces a method for sampling Ising models with mixed boundary conditions. As an application of annealed importance sampling and the Swendsen-Wang algorithm, the method adopts a sequence of intermediate distributions that keeps the temperature fixed but turns on the boundary condition gradually. The numerical results show that the variance of the sample weights is relatively small.

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1. Introduction

This note is concerned with the Monte Carlo sampling of Ising models [7, 12] with mixed boundary conditions. Consider a graph $G = (V, E)$ with the vertex set V and the edge set E. We 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. In addition, $ij \in E$ denotes an edge between two interior vertices i and j, while $ib \in E$ denotes an edge between an interior vertex i and a boundary vertex b. The boundary condition is specified by $f = (f_b)_{b\in B}$ with $f_b = \pm 1$.

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 $H(s)$ defined via

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

At an inverse temperature $\beta > 0$, 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 $Z_\beta = \sum_s e^{-\beta H(s)}$ is the renormalization constant or the partition function. More detailed discussions about the Ising models can be found for example in [3, 11].

A key feature of this Ising model is that, for certain mixed boundary conditions, the distribution (1.1) exhibits macroscopically different profiles below the critical temperature. Fig. 1.1 showcases two such examples. On the left, the square Ising lattice has the $+1$ condition on the vertical sides but the -1 condition on the horizontal sides. The two dominant macroscopic

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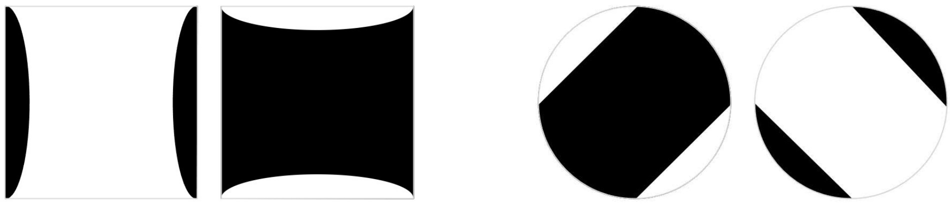

(a) (b)

Fig. 1.1. Ising models with mixed boundary conditions. (a) A square model. (b) A model support on a disk. In each case, a mixed boundary condition is specified and the model exhibits two dominant profiles on the macroscopic scale.

profiles are a -1 cluster linking two horizontal sides and a $+1$ cluster linking two vertical sides, shown in Fig. 1.1(a). On the right, a triangular Ising lattice supported on a disk has the $+1$ condition on two disjoint arcs and the -1 condition on the other two. Its two dominant profiles are given in Fig. 1.1(b). Notice that in each case, the two dominant profiles have comparable probability. Hence, it is important for any sampling algorithm to transition between these macroscopically different profiles efficiently.

One of the most well-known methods for sampling Ising models is the Swendsen-Wang algorithm [13], which will be briefly reviewed in Section 2. For Ising models with free boundary condition for example, 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 dominant profiles is much higher than the typical energy fluctuations. 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 dominant profile to the other. However, breaking so many edges simultaneously is an event with exponentially small probability when the mixed boundary condition is specified.

Annealed importance sampling is a method proposed by Neal [10], designed for sampling distributions with multiple modes. The main idea is to

(1) introduce an easily-to-sample initial distribution,

(2) design a sequence of (typically temperature-dependent) intermediate distributions that interpolates between the initial and the target distributions,

(3) generate sample paths that connects the simple initial distribution and the hard target distribution,

(4) compute a path-dependent scalar to weight the samples at the target distribution.

Annealed importance sampling has been widely applied in Bayesian statistics and data assimilation for sampling and estimating partition functions.

In this note, we address the problem of sampling (1.1) by combining the Swendsen-Wang algorithm with annealed importance sampling. The main novelty of our approach is that, instead of adjusting the temperature, we freeze the temperature and adjust the mixed boundary condition.