THE SWENDSEN-WANG DYNAMICS
IN THE SIMULATION OF THE ISING MODEL

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The Swendsen-Wang dynamics in the Simulation of the Ising Model

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Abstract

In this paper we present some simulation results about the convergence properties of one of the available methods to simulate Markovian fields: the Swendsen-Wang algorithm. We use the observed values of the mean magnetization, the pseudo-likelihood estimates, the observed short and long range correlations and the number of connected subgraphs to study the problems associated with the stopping time of the algorithm for different values of the parameter.

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1 Introduction

In this paper we present some simulation results about the convergence properties of the Swendsen-Wang algorithm when used to obtain samples taken from the class of distributions known as Ising Model.

We will follow the notation, the definitions, the ideas and the methodology already presented in BUSTOS AND FRERY (1991), and we assume that the reader of this work is familiar with them. Only additional references are listed.

The Swendsen-Wang dynamics differs from the Gibbs sampler in that it is a cluster flip algorithm rather than a spin flip algorithm. In the latter only one pixel is allowed to change its value per renewal, and one iteration needs, at least, $#S$ renewals. In the former a random number of renewals, say $#A$, with $#A < #S$ is needed to obtain an iteration.

We will show computational evidence that the Swendsen-Wang dynamics is faster than the Gibbs Sampler in the number of iterations required to achieve the convergence and, also, in the computational time needed when the desired final distribution is characterized by a value of $\alpha$ greater than the critical value $\alpha_c$.

2 The Swendsen-Wang algorithm

Suppose $\alpha > 0$ and let $x(0), x(1), \ldots$ be a sequence of outcomes such that $x(k) \in \Xi$ for all $k \geq 0$; we write $x(k) = (x_1(k), \ldots, x_{#S}(k))$. Let $x(0)$ be any element of $\Xi$ and, for all $k \geq 0$, change $x(k)$ to $x(k+1)$ in the following manner:

1. Obtain $\mathcal{L}(k)$ the set of random bonds of configuration $x(k)$ as $\mathcal{L}(k) = \{(i,j) \in S \times S : ||i - j|| = 1, x_i(k) = x_j(k), \text{ and } i < j\}$. Note that this is an edge set.
2. To every pair $(i,j) \in \mathcal{L}(k)$ assign an independent uniformly $[0,1]$ distributed random variable $U_{ij}$.
3. Obtain $\hat{\mathcal{L}}_{k,\alpha}(\omega) \subseteq \mathcal{L}(k)$ by independently deleting bonds in $\mathcal{L}(k)$ with probability $\exp\{-\alpha\}$, i.e. $\hat{\mathcal{L}}_{k,\alpha}(\omega) = \{(i,j) \in \mathcal{L}(k) : U_{ij}(\omega) < 1 - \exp\{-\alpha\}\}$.
4. Obtain $\Lambda(\omega) = \{\lambda_1, \ldots, \lambda_L\}$ the set of all connected subgraphs of $\hat{\mathcal{G}}_{k,\alpha} = \{S, \hat{\mathcal{L}}_{k,\alpha}(\omega)\}$. Obviously $x_i(k) = x_j(k)$ for every pair of pixels $i, j$ in $\lambda_m, 1 \leq m \leq L$. Assign an independent uniformly $[0,1]$ distributed random variable $V_m$ to every $\lambda_m \in \Lambda$.
5. The new configuration $x(k+1)$ is obtained by changing (retaining) the values of all sites $x_i(k), i \in \lambda_m$ if $V_m(\omega) < p (V_m(\omega) \geq p)$ respectively, with $p = 1/2$.

It can be seen in MARTINELLI ET AL. (1990a, 1990b) that the desired convergence $\mathbb{P}(X(k) = x) \rightarrow \mathbb{P}(X = x)$ is achieved as $k \rightarrow \infty$.

The Ising model with antiferromagnetic interaction, i.e. with $\alpha < 0$ could be obtained modifying step 1: $\mathcal{L}(k) = \{(i,j) \in S \times S : ||i - j|| = 1, x_i(k) \neq x_j(k) \text{ and } i < j\}$. This algorithm could also be used, through proper redefinitions of step 5, for the simulation of the following distributions:

- Ising model with external field (MARTINELLI ET AL. 1990a, 1990b); in this case the value $p$ will depend on the external field $H = [h_s]_{s \in S}$ and on the size of the considered cluster, i.e. $p = (1 + \exp\{\alpha h_\ell C_\ell\})^{-1}$, where $h_\ell = \sum_{j \in \lambda_\ell} h_j$ and $C_\ell = \#\{x, x \in \lambda_\ell\}$ for all $1 \leq \ell \leq #A$. 

Potts model, i.e., first order neighbourhoods and $E_s = \{0, 1, \ldots, M\}$ for all $s \in S$ (Ripley, 1989); in this case $x(k+1)$ is obtained by choosing the new value for all sites in every connected subgraph of $x(k)$ uniformly in $E_s$.

3 The Connected Subgraphs Algorithm

Among the several algorithms studied in classical books about computational graph theory, we chose to work with the one presented in Reingold et al. (1977) since it has a nice recursive structure suitable for the chosen programming language (Zortech C++). It does not need the usual auxiliary structures as lists, stacks, etc.

The technique is based upon the depth-first search on undirected graphs and, on output, assigns a unique component number to every vertex belonging to the same connected subgraph of the current stochastic graph $\tilde{L}_{k,\alpha}(\omega)$.

The algorithm in structured English is as follows:

```c
/* Setup */
for every node "n" in the graph do compnum( n ) = 0
    c = 0
/* Algorithm */
for every node "n" in the graph if compnum( n ) = 0 do
    c = c + 1
    comp( n )
/* Procedure comp( x ) */
compnum( x ) = c
for nodes "w" in the set $A(x)$ if compnum( w ) = 0 do
    comp( w )
return
```

In this listing we have written $A(x)$ the set of (stochastic) neighbours of pixel $x$, in the previously defined sense.

Notice that the algorithm is used every iteration and that the number of connected subgraphs found could be used as an alternative measure of convergence (with the advantage that this sequence of numbers is a direct subproduct of the algorithm, needing no additional computations).

4 The results

We worked with the same model studied in Bustos and Frery (1991), with $S = 64 \times 64$ and values of $\alpha = \beta$ in the ranges 0, (0.1), 0.8 and 0.85, (0.05), 1.2; note that these values span both the sub and the supercritical regions, i.e., values of the parameter $\alpha < \alpha_c$ and $\alpha > \alpha_c$.

We noted that simulations with different values of the parameter, but belonging to the same sub or supercritical region, do not exhibit major differences in the convergence behaviour. So, in this work, we present the results for a simulation with $\alpha = 0.5$ and other with $\alpha = 1$. 
In the simulations with values close to $\alpha_c$, i.e. in the interval $[0.85, 0.95]$ we observed a noticeable increase in the dispersion of the observed mean magnetizations and long range correlations. We present the correlograms of these observed quantities and notice that after, say 20 iterations there is no observable evidence of dependence upon samples. This, along with the expected theoretical behaviour pointed in Pickard (1987) that assigns an arbitrary large variance to these values in the point $\alpha = \alpha_c$, stimulates the claim that the Swendsen-Wang algorithm may produce almost independent samples of Markovian fields with less computational effort than the Gibbs sampler.

Our main results are presented in Figures 1 to 6 (7 to 12) for $\alpha = 0.5$ ($\alpha = 1.0$ respectively). They correspond, in order, to: mean magnetization vs. iteration, $\tilde{\alpha}$ vs. iteration, $c(1)$ vs. iteration, $c(10)$ vs. iteration, $#A$ vs. iteration and the correlogram of the mean magnetization.

The relevant listings are provided by the authors under request.

5 References


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Abs. Magnet.; 0.5

Figure 1

Estimation; 0.5

Figure 2