Introduction to the Propp-Wilson Method of Exact Sampling for the Ising Model

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Abstract. An introduction to the Propp-Wilson method of coupling-from-the-past for the Ising model is presented. It enables one to obtain exact samples from the equilibrium spin distribution for ferromagnetic interactions. Both uniform and random quenched magnetic fields are included. The time to couple from the past and its standard deviation are shown as functions of system size, temperature, and the field strength. The time should be an estimate of the ergodic time for the Ising system.

The standard importance-sampling Monte Carlo algorithm \[\text{(1)}\] for statics has a number of difficulties. One is its inability to ensure that the generated spin configurations are uncorrelated and are representative of the equilibrium distribution. The standard way to overcome this difficulty is to throw away a large number of Monte Carlo steps between analyzed configurations. Of course this decreases the number of configurations obtained in a given amount of computer time. In addition, there can remain the question of whether the generated spin configurations are indeed drawn from the underlying equilibrium distribution. For example, consider a spin-glass model at low temperatures, where ergodicity has been broken for reasonable simulation times and the system might have many ground states and many more metastable states. Then it is extremely difficult to decide whether the standard Monte Carlo method obtains spin configurations drawn from the underlying equilibrium spin distribution.

In this short paper the square-lattice Ising model with nearest-neighbor ferromagnetic \((J>0)\) interactions and periodic boundary conditions is considered. The Hamiltonian is \(H = -J \sum_{(ij)} \sigma_i \sigma_j - \sum_i H_i \sigma_i\), with \(\sigma_i = \pm 1\), the first sum over nearest-neighbor spins, and \(H_i\) is the local field. Two cases are considered, uniform field \(H_i = H\), and quenched random field with \(H_i\) chosen to be \(\pm H\) with equal probability. We take \(J=1\), which makes the exact critical temperature \(T_c \approx 2.26\). One Monte Carlo step consists of two procedures. First randomly choose a spin \(i\) from the \(L \times L\) lattice. The probability of \(\sigma_i\) being set to \(+1\) in the next time step is

\[
\text{Prob}(\sigma_i = 1) = \left\{ 1 + \exp \left[ \frac{-2J \sum_{j=nn} \sigma_j - 2H_i}{T} \right] \right\}^{-1},
\] (1)
where the first sum is over the nearest-neighbors of spin $i$ and $T$ is the temperature. The second step is to use a uniformly distributed random number $r$, and set $\sigma_i = +1$ in the next time step if $r \leq \text{Prob}(\sigma_i = 1)$; otherwise set $\sigma_i = -1$. This is the single-spin flip heat-bath dynamic, which for the Ising model is the Glauber dynamic. I use the Ziff four-tap random number generator \[2\].

It is important to note that we do not consider the probability that a spin flips, but rather the probability of the spin being up, i.e. $+1$.

Recently researchers in the statistics community have devised methods that can guarantee that generated spin configurations from a Monte Carlo simulation are drawn from the underlying equilibrium distribution. There the study goes under the name of Markov random fields \[3\], which should not be confused with the random fields in the Hamiltonian. The method used here is the 1996 method of Propp and Wilson \[4\]. It is referred to as ‘coupling-from-the-past’ or the ‘Propp-Wilson method’. Here we bring the single-spin-flip version of the Propp-Wilson method to the attention of practitioners in the statistical mechanical community. We obtain a time for coupling from the past, which we call the Propp-Wilson time, $t_{PW}$. We will show how $t_{PW}$ changes with $T$, $L$, $H$, and the randomness in $H$. The time $t_{PW}$ can be viewed as an upper bound to the ergodic time $\tau_e$ of the simulation \[1\]. In the spirit of a workshop, this study was only initiated about one month prior to the workshop. Consequently, it should be viewed as an exploratory and preliminary work.

The basic idea of the Propp-Wilson method is to not run the Markov chain forward in time (which all normal importance-sampling Monte Carlo procedures do), but rather to run the Markov chain from a time $-t$ in the past up to $t = 0$. Typically it is not known how to go from a spin configuration at one time to one at an earlier time. However, given a spin configuration at time $-t$, it is easy to propagate it to time $t = 0$ — just use the algorithm for forward propagation. What is the difference between going from $-t$ to 0 or going from 0 to $t$? It lies only in our knowledge of the sequence of random numbers used. At $t = 0$ one has no idea which spin will be picked next or which random number the spin-up probability will be compared with. However, at all times in the past, both the spin picked and the random number to compare with are known.

Now consider starting two spin configurations at time $-t$, and propagating forward in time toward $t = 0$. The same random numbers are used for each spin configuration, since the same history of random numbers applies for times $t \leq 0$. At some time $-t_e$ these two spin configurations might coalesce, i.e. they both become the same spin configuration at time $-t_e$. From this time onward to time $t = 0$ they will remain coalesced, since the same random numbers propagate them forward to $t = 0$. This coalescence gives the Propp-Wilson method the ‘coupling from the past’ name.

Here is the Propp-Wilson prescription for simulation of $N$ Ising spins. First obtain a very long history of randomly picked spins and random num-
bers used to compare against $\text{Prob}(\sigma_i = +1)$. Start with all $2^N$ possible spin configurations at time $t=-1$. Propagate all configurations forward in time to $t=0$. Remember, this is done using the same set of random numbers for each configuration. If all $2^N$ configurations have coalesced to the same spin configuration at $t=0$, this is the spin configuration you want. If not, start all $2^N$ spin configurations at $t=-2$, propagate forward with the same random number history, and see if they have coalesced at $t=0$. This is continued until at some time $-t_{PW}$ the coalescence of all $2^N$ spin configurations has occurred.

The spin configuration obtained in this fashion is guaranteed to be an exact sampling of the equilibrium spin distribution. An exact sample means that the spin configuration is drawn according to the probability associated with the equilibrium distribution. Note that care must be taken to ensure that the long random-number history is never exceeded before the coalescence occurs.

Why does this give an exact sampling? Let us imagine that we have run an infinite ensemble of spin configurations from $t=-\infty$ to $t=-t_{PW}$ using different random numbers for each. Since we have run our Markov chain infinitely long, we are guaranteed that the spin configurations at $t=-t_{PW}$ are distributed according to the equilibrium spin distribution. Each of the starting spin configurations will have evolved into one of the $2^N$ spin configurations at $t=-t_{PW}$. No matter which spin configuration the system is in at time $-t_{PW}$, we know that at time $t=0$ all $2^N$ configurations have coalesced to a single spin configuration since we have used our history of random numbers which is the same for each configuration to run from $t=-t_{PW}$ to $t=0$. Thus the sample generated is drawn from the equilibrium spin distribution.

In principle only a coupling-from-the-past method, like the Propp-Wilson method, is required to obtain a perfectly random sample. In practice another relationship is required since the number of states grows very quickly with lattice size. If all $2^N$ states could be handled, the partition function could be calculated exactly. For special cases it is possible to introduce a partial ordering on the states. For the Ising model, we say that two spin configurations $x$ and $y$ have a partial ordering, $x \preceq y$, if for each lattice site the spin in $x$ is down whenever the spin in $y$ is down. The transition probability of (1) preserves the partial ordering for ferromagnetic interactions. Consequently, rather than insist that all $2^N$ configurations have coalesced, only the two extreme partial ordering states, all spins up and all spins down, need to be considered. If these two states have coalesced, then all other states have coalesced. It is this desired property of partial ordering that restricts one to ferromagnetic interactions.

The Propp-Wilson method was run to obtain $t_{PW}$ as a function of $L$, $T$, and $H$. For each value of parameters 1000 exact samples were obtained. Note that if coalescence occurs at time $-t_{PW}$, it also occurs for any earlier time. This allows a bisection method to be used to find $t_{PW}$. Figure 1(a) shows the average value of the Propp-Wilson time, $[t_{PW}]$, in Monte Carlo Steps per Spin (MCSS), at $H=0$. Since the phase space grows with system size, $[t_{PW}]$
Fig. 1. (a) The average Propp-Wilson time, \( [t_{PW}] \), is shown as a function of temperature for \( H=0 \) and \( L=4, 8, \) and \( 16 \). The vertical line is the exact value of the critical temperature, \( T_c \). The lines are guides for the eye. (b) The \( L \) dependence on a log-log plot is shown for \( [t_{PW}] \) (filled symbols joined by solid lines) and the standard deviation of \( t_{PW} \) (corresponding open symbols joined by dashed lines). Both of these grow faster than power laws below \( T_c \), slower than power laws above \( T_c \), and are expected to grow as a power law at \( T_c \).
Fig. 2. The average Propp-Wilson time, $[t_{PW}]$, in MCSS is shown at $T=2.0$ as a function of $H$. The lines are guides for the eye. Note that the points at $H=0$ are the same for both plots. (a) Is for a uniform magnetic field. For $L=16$, $H=0.1$ is the smallest value shown. (b) Is for quenched randomly distributed fields equal to $-H$ or $+H$. Four different distributions of fields are shown for $L=4$, and one distribution for $L=8$ and $L=16$. For $L=16$, $H=1.5$ is the smallest value shown.

as a function of $L$. The behavior seems to be close to those of $[t_{PW}]$. Note that the standard deviation becomes very large, which necessitates using a large number of samples to obtain a reasonable value for $[t_{PW}]$.

Figure 2(a) shows $[t_{PW}]$ at $T=2.0$ for different values of $L$ and uniform applied field, $H$. At strong fields the larger system sizes have larger values of $[t_{PW}]$, for intermediate fields all system sizes have similar values of $[t_{PW}]$, and for weak fields the smaller system sizes break away from this curve and go to their maximum at $H=0$. This behavior is reminiscent of the cross-overs encountered in the study of metastability, where for $T<T_c$ as the field is decreased different regimes are encountered in a finite system.

To illustrate the application of the Propp-Wilson method to a random-field Ising model, Fig. 2(b) shows data for $[t_{PW}]$ as a function of the strength of the random field for various quenched field configurations for $L=4$, and one quenched field configuration for $L=8$ and 16. The trends seem to be similar to those of Fig. 2(a). However the values for $[t_{PW}]$ seem to increase faster as $H$ decreases than in the uniform field case. This is in agreement with the physical idea that a system with random quenched disorder has a longer ergodicity time than one without disorder. For more discussion of random fields see references [8,9,10].
In summary, it is possible to utilize coupling-from-the-past ideas to obtain perfect samples of Ising spin configurations from the equilibrium spin distribution. To use the ideas in practice, however, another relationship is essential, that of a partial ordering preserved by the transition probabilities. This restriction allows one to study random fields, but no partial ordering is known for systems with antiferromagnetic bonds. The value for the average and standard deviation for $t_{PW}$ seem to have reasonable dependences on system size, field strength, and temperature if $t_{PW}$ is viewed as an upper bound for the ergodic time of the system.

It is possible to use cluster dynamics instead of single-spin-flip dynamics. Since this decreases the ergodic time near $T_c$, this allows one to obtain perfect samples for large systems — so far the largest single example I have seen had $L=2100$ in a preprint by Propp and Wilson. It has also been shown that the expected running time for the Propp-Wilson method should be within a constant multiple of the maximum expected time for two states to coalesce in the Markov chain, and that this running time is near optimal for exact sampling. Thus the ability to obtain results for large systems at temperatures above and near $T_c$ for models that have a partial ordering seems realistic. Unfortunately, these partial orderings are extremely difficult to find in more general models. Also, the long expected run times seem to make the application of these types of algorithms rather limited in studies of low-temperature behavior for systems with quenched randomness and high barriers.

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