WOLFF CLUSTER UPDATES

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1. Preliminaries

A Monte Carlo algorithm moves from configuration a to configuration b with probability $P(a \to b)$. This transition probability is chosen to satisfy,

$$\pi_a P(a \to b) = \pi_b P(b \to a). \tag{1}$$

In classical equilibrium statistical physics, π_a is just the Boltzmann weight of the configuration. For our particular problem, the Boltzmann weight is,

$$\pi_a = \exp(-\beta E_a), \tag{2}$$

and detailed balance is implemented via a Metropolis step,

$$P(a \to b) = \min\left(1, \frac{\pi_a}{\pi_b}\right). \tag{3}$$

It is important to understand that the transition probability $P(a \to b)$ is actually composite. It is the product of *considering* the move from $\mathcal{A}(a \to b)$ and subsequently *accepting* the move with probability $\widetilde{P}(a \to b)$,

$$P(a \to b) = \mathcal{A}(a \to b) \times \widetilde{P}(a \to b) \tag{4}$$

We may now rewrite the detailed balance condition (1) as

$$\begin{aligned} \pi_a \mathcal{A}(a \to b) \times \widetilde{P}(a \to b) &= \pi_b \mathcal{A}(b \to a) \times \widetilde{P}(b \to a), \\ \frac{\widetilde{P}(a \to b)}{\widetilde{P}(b \to a)} &= \frac{\pi_b}{\mathcal{A}(a \to b)} \times \frac{\mathcal{A}(b \to a)}{\pi_a}, \end{aligned} \tag{5}$$

which we may implement with a Metropolis step,

$$\widetilde{P}(a \to b) = \min\left(1, \frac{\pi_b}{\mathcal{A}(a \to b)} \times \frac{\mathcal{A}(b \to a)}{\pi_a}\right). \tag{6}$$

2. Single-Cluster Wolff

The idea is to construct an algorithm that moves entire clusters of spins in a single update with unit probability. This realised by taking an arbitrary configuration a, partitioning that configuration (creating a Wolff cluster) and then constructing a new configuration b

by flipping the entire cluster of spins. The partitioning of a is done in such a way that the candidate configuration b gives the following result,

$$\frac{\pi_b}{\mathcal{A}(a \to b)} \times \frac{\mathcal{A}(b \to a)}{\pi_a} = 1 \tag{7}$$

In other words, we recognise that rather than simply guessing at candidate b configurations and using (3) to accept them (with some degree of rejection too) we may construct a candidate configuration b from some cleverly chosen partition of a such that any deviation in the Boltzmann weight ratio $\frac{\pi_a}{\pi_b}$ from unity are exactly compensated for by an appropriate difference in considering these two partitions $\frac{\mathcal{A}(b\to a)}{\mathcal{A}(a\to b)}$. The candidate configuration is always accepted $\widetilde{P}(a \to b) = 1$.

An absolutely vital aspect of this procedure is that we are able to compute any $\frac{\pi_a}{\pi_b}$, any $\frac{\mathcal{A}(b\to a)}{\mathcal{A}(a\to b)}$, and that all possible states are accessible to the algorithm. If the latter is violated then the system is not ergodic and no ensemble will be an unbiased sample. If the former two are not satisfied, we have no hope of being assured that (7) is correct. For single cluster Wolff we will show that one can easily compute the two requisite ratios, then move on to more interesting partitions of a.

2.1. **Detailed Balance for Single Cluster Wolff.** Consider the configurations and partitionings of a 2D Ising lattice given in figure 1. Configuration a has a partitioning, and configuration b has that partition flipped. We must be able to compute the ratio of the

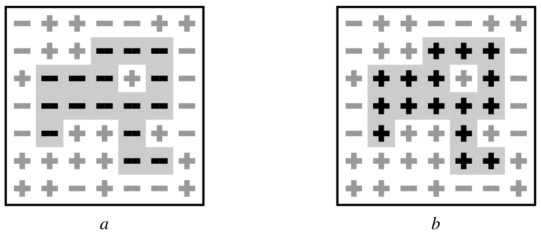

FIGURE 1

probability of constructing the partition of a and the partition of b in order to compute $\frac{\mathcal{A}(b\to a)}{\mathcal{A}(a\to b)}$. We can do this by imagining that we are growing a cluster that results in each of these two configurations being partitioned in the manner shown.

We now take advantage of the fact that these two configurations and partitions have a great deal in common. Everything outside the cluster is the same in each case, and everything inside the cluster has the same spin. The only difference is the sign of the spin in each case. This will be the fact through which we can construct the ratio. Imagine that we begin to grow the Wolff cluster shown in a. It will have had some number of site acceptances, and at its boundary it would have met some spins of opposite sign. Crucially, the percolation front of the cluster would have failed to make further bonds a total of 9

times, as there are 9 "- -" bonds not active. Conversely, in configuration b, the percolation would have had the same number of acceptances, and 19 bond failures. We may lump all of the common *consideration* probabilities into a common factor $\mathcal{A}_k$ and write

$$\begin{aligned} \mathcal{A}(a \to b) &= \mathcal{A}_k \times (1-p)^9 \\ \mathcal{A}(b \to a) &= \mathcal{A}_k \times (1-p)^{19} \end{aligned} \tag{8}$$

where p is, of course, the probability of accepting a bond. Now, computing the energies of a and b is straightforward as all the spin interaction energy comes from nearest neighbour sites. If we again denote the interactions common to both configurations as E_k, then we may assert

$$\begin{aligned} E_a &= E_k - 9J + 19J \\ E_b &= E_k + 9J - 19J \end{aligned} \tag{9}$$

form which the Boltzmann weights can be computed.

It is now time to dispense with specific configurations and numbers and codify the result. We do this by considering the boundary interactions of the cluster, as they clearly contain all the relevant information we need. We will denote the number of bonds that align in a as n_a and the number that do not align as m_a. We will also have n_b and m_b for configuration b,

$$\begin{aligned} \mathcal{A}(a \to b) &= \mathcal{A}_k \times (1-p)^{n_a} \\ \mathcal{A}(b \to a) &= \mathcal{A}_k \times (1-p)^{n_b} \end{aligned} \tag{10}$$

$$\begin{aligned} E_a &= E_k - n_a J + m_a J \\ E_b &= E_k - n_b J + m_b J \end{aligned} \tag{11}$$

We may now insert these general values into (6) to compute the acceptance probability,

$$\begin{aligned} \widetilde{P}(a \to b) &= \min\left(1, \frac{\pi_b}{\pi_a} \times \frac{\mathcal{A}(a \to b)}{\mathcal{A}(b \to a)}\right) \\ &= \min\left(1, \frac{\exp(-\beta(E_k - n_b J + m_b J))}{\exp(-\beta(E_k - n_a J + m_a J))} \times \frac{(1-p)^{n_a}}{(1-p)^{n_b}}\right) \end{aligned} \tag{12}$$

and use the fact that $n_a = m_b$ and $n_b = m_a$,

$$\begin{aligned} \widetilde{P}(a \to b) &= \min\left(1, \frac{\exp(-\beta J(n_a - n_b))}{\exp(-\beta J(n_b - n_a))} \times \frac{(1-p)^{n_a}}{(1-p)^{n_b}}\right) \\ &= \min\left(1, \frac{\exp(-2\beta J n_a)}{(1-p)^{n_a}} \times \frac{(1-p)^{n_b}}{\exp(-2\beta J n_b)}\right) \\ &= \min\left(1, \left[\frac{\exp(-2\beta J)}{(1-p)}\right]^{n_a} \times \left[\frac{(1-p)}{\exp(-2\beta J)}\right]^{n_b}\right). \end{aligned} \tag{13}$$

In the above expression, we can easily construct $\widetilde{P}(a \to b)$ to be unit valued (and have a rejectionless algorithm) if we insist that the probability of constructing a bond is $p = 1 - \exp(-2\beta J)$, which is precisely the probability put forward by Fortuin and Kasteleyn.