Computational Physics II 5640, Spring 2017

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April 5, 2017

1 Dual Markov chain Monte Carlo

A fundamental aspect of many cluster Monte Carlo methods is the dual Markov-chain process, where a second space, defined by a second configuration variable, is defined parallel to the normal configuration space. A full transition from one point in normal configuration space passes through the so-called dual space. In the case of the Ising lattice the dual space is the configuration of the bonds on the links, 0 for unbound and 1 for bound. Again, this implies the the transition from spin configuration C_0 to spin configuration C_1 must pass through the bond space configuration G_1. A critical point to remember, as it will come up later, is that bond configuration G_1 between C_0 and C_1 is one of multiple points in bond space which link C_0 and C_1.

We use this point to define the partition function, not as the sum of the classical Boltzmann factors, but as in equation 1.

$$z = \sum_C \sum_G w(C, G). \tag{1}$$

where the original weight functions are defined as,

$$\begin{aligned} w(C) &= \sum_G w(C, G), \\ w(G) &= \sum_C w(C, G). \end{aligned} \tag{2}$$

We move from here to define the probability $\mathcal{P}(C \to C')$. The transition from one configuration in spin space to one in bond space has a probability given as $P(C \to G)$ and back again given as $\tilde{P}(G \to C)$. Therefore the total probability from C to C' must be given by $P(C \to G)\tilde{P}(G \to C')$, but this is only the probability of transitioning through one of multiple paths in bond space, so the total would be higher, and is the sum over all possible G.

$$\mathcal{P}(C \to C') = \sum_G P(C \to G)\tilde{P}(G \to C'). \tag{3}$$

We are free to take the sum over all G in bond space, not just the possible paths, as those impossible terms would just go to zero. We can show the link between the dual space formalism and the classical formalism, by showing that if we assume strong detailed balance in the dual space, it implies detailed balance in the classical model.

The dual space strong detailed balance condition is defined as:

$$\pi(C)P(C \to G) = \pi(G)\tilde{P}(G \to C). \tag{4}$$

but just as surely,

$$\pi(C')P(C' \to G) = \pi(G)\tilde{P}(G \to C'). \tag{5}$$

and

$$\begin{aligned} \pi(C)P(C \to G) &= \pi(C')\frac{P(C' \to G)}{\tilde{P}(G \to C')}\tilde{P}(G \to C), \\ \pi(C)P(C \to G)\tilde{P}(G \to C') &= \pi(C')P(C' \to G)\tilde{P}(G \to C). \end{aligned} \tag{6}$$

throw in some $\sum_G$ and we get,

$$\begin{aligned}\pi(C)\sum_G P(C\to G)\tilde{P}(G\to C') &= \pi(C')\sum_G P(C'\to G)\tilde{P}(G\to C),\\ \pi(C)\mathcal{P}(C\to C') &= \pi(C')\mathcal{P}(C'\to C).\end{aligned} \tag{7}$$

which is the definition of detailed balance for the original Markov process. Q.E.D.

To finish up we have to choose transition probabilities that satisfy our necessary detailed balance. Let's try something obvious, like,

$$P(C\to G) = \frac{w(C,G)}{w(C)}, \quad \tilde{P}(G\to C) = \frac{w(C,G)}{w(G)}. \tag{8}$$

plugging into 4,

$$\begin{aligned}\pi(C)\frac{w(C,G)}{w(C)} &= \pi(G)\frac{w(C,G)}{w(G)},\\ \frac{\pi(C)}{w(C)} &= \frac{\pi(G)}{w(G)}.\end{aligned} \tag{9}$$

but,

$$\pi(C/G) = \frac{w(C/G)}{Z} \tag{10}$$

therefore,

$$\begin{aligned}\frac{w(C)/Z}{w(C)} &= \frac{w(G)/Z}{w(G)},\\ Z &= Z\end{aligned} \tag{11}$$

which satisfies our detailed balance condition.

We now have a general framework for the dual space method of Markov processes.

2 Swendsen-Wang algorithm

Here we define a particular implementation of the dual space method on the square Ising lattice. We define $C = \{\sigma_i\}$ and $G = \{n_{ij}\} \in \{0,1\}$, for the dual bond space variable. First, we start by defining the partition function, equation 1. We'll begin by finding a form for $w(C,G)$, the weighting function. If what we're interested in is the creation and breaking of bonds between neighboring spins, then we can define,

$$w_{ij}(\sigma_i,\sigma_j;n_{ij}) = (1-p)\delta_{n_{ij},0} + p\delta_{\sigma_i,\sigma_j}\delta_{n_{ij},1} = \begin{cases}1-p, & n_{ij}=0\\ p, & n_{ij}=1, \sigma_i=\sigma_j\\ 0, & n_{ij}=1, \sigma_i\neq\sigma_j\end{cases} \tag{12}$$

where,

$$p = 1 - e^{-2\beta J} \tag{13}$$

i.e. regardless of spin orientation, there is a $1-p$ probability of a bond going to zero, and for a bond to go to one, the spins have to be aliened.

This implies that the weight must be the product of the w_{ij} of all the pairs. We weight the factors by $e^{\beta J}$ and we get,

$$\begin{aligned}w(C,G) &= \prod_{\langle ij\rangle} e^{\beta J} w_{ij}(\sigma_i,\sigma_j;n_{ij}),\\ &= e^{N_b\beta J}\prod_{\langle ij\rangle} w_{ij}(\sigma_i,\sigma_j;n_{ij}).\end{aligned} \tag{14}$$

where $N_b = 2N$ is the number of bonds. Plugging into equation 1,

$$Z = e^{N_b \beta J} \sum_{\{\sigma_i\}} \sum_{\{n_{ij}\}} \prod_{\langle ij \rangle} w_{ij}(\sigma_i, \sigma_j; n_{ij}). \tag{15}$$

Next we look into the local transition probability, given by,

$$P(\sigma_i, \sigma_j \to n_{ij} = 1) = \frac{w(C, G)}{\sum_G w(C, G)} = \frac{w_{ij}(\sigma_i, \sigma_j; n_{ij})}{\sum_{n_{ij}} w_{ij}(\sigma_i, \sigma_j; n_{ij})} \tag{16}$$

which, if $\sigma_i = \sigma_j$, is equal to $p/(p + (1 - p))$, or just p, and otherwise, equal to $0/(0 + (1 - p))$, or just 0. Going the other way,

$$P(n_{ij} \to \sigma_i, \sigma_j) = \frac{w(C, G)}{\sum_C w(C, G)} = \frac{w_{ij}(\sigma_i, \sigma_j; n_{ij})}{2 \sum_{\sigma_i, \sigma_j} w_{ij}(\sigma_i, \sigma_j; n_{ij})} \tag{17}$$

which, if $n_{ij} = 0$, is equal to $(1 - p)/4(1 - p)$, or just $1/4$, and otherwise, equal to $p\delta_{\sigma_i, \sigma_j}/2p$, or just $\delta_{\sigma_i, \sigma_j}/2$.

With these results in hand we have the tools necessary to describe the full Swendsen-Wang algorithm:

1. Start with a randomly seeded Ising lattice.
2. Apply bond variables of 1 to spin-aligned pairs with the probability $p = 1 - e^{-\beta}$, and bond variables of 0 to all spin-antialigned pairs, and spin-aligned pairs with probability $1 - p$.
3. "Erase" the spin sites, leaving an arrangement of bonds in clusters of varying sizes.
4. Randomly assign an Ising spin to every cluster, assigning it to every site in the cluster, regardless of size. From equation 17, we see the probability of two Ising variables with a bond of 0 being either aligned, or antialigned is equal to 1/4. While if the bond is equal to one, then the probability is 1/2 that the spins will be aligned.
5. "Erase" the bonds, leaving a shiny new Ising lattice.
6. Repeat from step 2.

The Swendsen-Wang algorithm gives us a vary efficient way to study large Ising lattices at critical temperatures. It satisfies detailed balance, and gives accurate results.