PHYS 5640 - HW 4

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1 Dual Markov chain Monte Carlo

(1) Show that the probability $P(C \to C')$ is given by

$$P(C \to C') = \sum_G P(C \to G)\tilde{P}(G \to C') \tag{1}$$

We can show that Eq. 1 is true by considering the possible paths from C to C'. Since in the dual MC formulation there is no path from C to C' within the C space, then one must travel from C to C' through an intermediary state in the G space. One possible path is to travel from state C to state G to state C'. The probability of traversing this path is simply the probability of going from state C to G and then from state G to C, expressed as:

$$P(C \to G \to C') = P(C \to G)P(G \to C').$$

This is just a single path from C to C' however. Since there is a path from C to all states in the G space, then to compute $P(C \to C')$, we need to consider all of these possible paths. Since we could have taken the single path in the example above or any other path from C to any G in the G space, and each of these paths is equiprobable, the final probability $P(C \to C')$ is given by

$$\boxed{P(C \to C') = \sum_G P(C \to G)\tilde{P}(G \to C')}$$

(2) Show that the strong detailed balance condition (for every pair of C and G)

$$\pi(C)P(C \to G) = \pi(G)\tilde{P}(G \to C) \tag{2}$$

implies the detailed balance of the original Markov-chain process:

$$\pi(C)P(C \to C') = \pi(C')P(C' \to C). \tag{3}$$

To prove Eq. 3, we simply start with the left hand side of Eq. 3 and use Eq. 1 and Eq. 2 to transform it to the right hand side. We use Eq. 1 on the left hand side of Eq. 3 to find

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

Invoking Eq. 2 twice we have

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

Finally, using Eq. 1

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

This then gives

$$\boxed{\pi(C)P(C \to C') = \pi(C')P(C' \to C).}$$

(3) Finally, show that the strong detailed balance condition Eq. (3) is satisfied with the following choice of transition probabilities

$$P(C \to G) = \frac{w(C,G)}{w(C)}, \quad \tilde{P}(G \to C) = \frac{w(C,G)}{w(G)} \tag{4}$$

This is easy to show by simply plugging the chosen probabilities from Eq. 4 into Eq. 2:

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

Plugging in from Eq. 4 on the left hand side we have

$$\pi(C)P(C \to G) = \pi(C)\frac{w(C,G)}{w(C)}.$$

Then, multiplying this equation by $\pi(G)/\pi(G) = 1$ and using the fact that $\pi(C) = w(C)/Z$ and $\pi(G) = w(G)/Z$ we have

$$\pi(C)\frac{\pi(G)}{\pi(G)}\frac{w(C,G)}{w(C)} = \pi(G)\frac{w(C)}{Z}\frac{Z}{w(G)}\frac{w(C,G)}{w(C)} = \pi(G)\frac{w(C,G)}{w(G)}.$$

And then finally, comparing the above to Eq. 3, we find that a choice of $\tilde{P}(G \to C) = w(C,G)/w(G)$ will make the above consistent with detailed balance (Eq. 3). So the two choices of P and $\tilde{P}$ from Eq. 4 satisfy detailed balance.

2 Swendsen-Wang algorithm

(1) Show that the partition function of the Ising model can be expressed as

$$Z = \sum_C \sum_G w(C,G) = e^{N_b \beta J} \sum_{\{\sigma_i\}} \sum_{\{n_{ij}\}} \prod_{\langle ij \rangle} w_{ij}(\sigma_i, \sigma_j; n_{ij}) \tag{5}$$

We begin by expressing Z as

$$Z = \mathbf{Tr}\left(e^{-\beta\mathcal{H}}\right) = \sum_{\{\sigma_i\}} e^{-\beta\mathcal{H}}$$

where

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j.$$

We can reexpress $\exp(-\beta\mathcal{H})$ as

$$e^{\beta J \sum_{\langle ij \rangle} \sigma_i \sigma_j} = \prod_{\langle ij \rangle} e^{\beta J \sigma_i \sigma_j}.$$

We then consider cases on σ_i and σ_j, arriving at the following values for $\exp(\beta J \sigma_i \sigma_j)$:

$$e^{\beta J \sigma_i \sigma_j} = \begin{cases} e^{\beta J}, & \sigma_i = \sigma_j \\ e^{-\beta J} & \sigma_j \neq \sigma_j \end{cases} = e^{\beta J} \delta_{\sigma_i, \sigma_j} + e^{-\beta J} \left(1 - \delta_{\sigma_i, \sigma_j}\right).$$

Rearranging terms we have

$$e^{\beta J \sigma_i \sigma_j} = e^{\beta J} \left[\left(1 - e^{-2\beta J}\right) \delta_{\sigma_i, \sigma_j} + e^{-\beta J}\right] = e^{\beta J} \left[(1-p) + p\delta_{\sigma_i, \sigma_j}\right]$$

where $p = 1 - \exp(-2\beta J)$ and $1 - p = \exp(-2\beta J)$. Introducing the variable n_{ij} where $n_{ij} = 0$ indicates the lack of a bond between spins and $n_{ij} = 1$ indicates the presence of a bond between spins at points i and j we have

$$e^{\beta J \sigma_i \sigma_j} = \sum_{\{n_{ij}\}} e^{\beta J} \left[(1-p)\delta_{n_{ij},0} + p\delta_{\sigma_i, \sigma_j} \delta_{n_{ij},1}\right].$$

Finally, this allows us to express the partition function as

$$Z = \sum_{\{\sigma_i\}} \prod_{\langle ij \rangle} \sum_{\{n_{ij}\}} e^{\beta J} \left[(1-p)\delta_{n_{ij},0} + p\delta_{\sigma_i, \sigma_j} \delta_{n_{ij},1}\right].$$

We can rearrange the sum over bond variables and the product over nearest neighbors and also pull out the constant factor of $\exp(\beta J)$:

$$\prod_{\langle ij \rangle} e^{\beta J} = e^{\sum_{\langle ij \rangle} \beta J} = e^{N_b \beta J}$$

where $N_b = 2N$ is the number of bonds. This gives finally

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

where

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

(2) Show that the local transition probability of connecting the bonds is

$$P(\sigma_i, \sigma_j \to n_{ij} = 1) = \begin{cases} p, & \sigma_i = \sigma_j \\ 0, & \sigma_i \neq \sigma_j \end{cases} \tag{6}$$

To show the above, we simply use Eq. 4 with $C = \sigma_i, \sigma_j$ and $G = n_{ij}$:

$$P(\sigma_i, \sigma_j \to n_{ij} = 1) = \frac{w_{ij}(\sigma_i, \sigma_j; 1)}{\sum_{\{n_{ij}\}} w_{ij}(\sigma_i, \sigma_j; n_{ij})}.$$

Now, we consider cases on the values of σ_i and σ_j. Since the value of w_{ij} for $n_{ij} = 1$ depends only on whether σ_i and σ_j are the same or different, then we'll consider those two cases. If $\sigma_i = \sigma_j$ we have

$$P(\sigma_i, \sigma_j \to n_{ij} = 1) = \frac{p}{1 - p + p} = p.$$

If $\sigma_i \neq \sigma_j$ we have

$$P(\sigma_i, \sigma_j \to n_{ij} = 1) = \frac{0}{1 - p + p} = 0.$$

This then tells us that

$$\boxed{P(\sigma_i, \sigma_j \to n_{ij} = 1) = \begin{cases} p, & \sigma_i = \sigma_j \\ 0, & \sigma_i \neq \sigma_j \end{cases}}$$

(3) Show that the transition probability of assigning spins for a given bond variable is

$$\tilde{P}(n_{ij} \to \sigma_i, \sigma_j) = \begin{cases} \frac{1}{4}, & n_{ij} = 0 \\ \frac{1}{2}\delta_{\sigma_i, \sigma_j}, & n_{ij} = 1 \end{cases}. \tag{7}$$

Similarly to above, we use Eq. 4 again giving

$$\tilde{P}(n_{ij} \to \sigma_i, \sigma_j) = \frac{w_{ij}(\sigma_i, \sigma_j; n_{ij})}{\sum_{\{\sigma_i\}} w_{ij}(\sigma_i, \sigma_j; n_{ij})}.$$

We then consider cases on values of n_{ij}. First, for $n_{ij} = 0$ we have

$$\tilde{P}(0 \to \sigma_i, \sigma_j) = \frac{w_{ij}(\sigma_i, \sigma_j; 0)}{\sum_{\{\sigma_i\}} w_{ij}(\sigma_i, \sigma_j; 0)}.$$

Since $w_{ij} = 1 - p$ when $n_{ij} = 0$ regardless of the values of σ_i and σ_j we have

$$\tilde{P}(0 \to \sigma_i, \sigma_j) = \frac{1 - p}{4(1 - p)} = \frac{1}{4}.$$

Now, for $n_{ij} = 1$ we have

$$\tilde{P}(0 \to \sigma_i, \sigma_j) = \frac{w_{ij}(\sigma_i, \sigma_j; 1)}{\sum_{\{\sigma_i\}} w_{ij}(\sigma_i, \sigma_j; 1)}.$$

Since w_{ij} does depend on the values of σ_i and σ_j when $n_{ij} = 1$, we will consider cases on $\sigma_i = \sigma_j$ and $\sigma_i \neq \sigma_j$. First, if $\sigma_i = \sigma_j$ we have

$$\tilde{P}(0 \to \sigma_i, \sigma_j) = \frac{p)}{p + p + 0+)} = \frac{1}{2}.$$

If $\sigma_i \neq \sigma_j$, then

$$\tilde{P}(0 \to \sigma_i, \sigma_j) = \frac{0)}{p + p + 0+)} = 0.$$

This gives finally

$$\boxed{\tilde{P}(n_{ij} \to \sigma_i, \sigma_j) = \begin{cases} \frac{1}{4}, & n_{ij} = 0 \\ \frac{1}{2}\delta_{\sigma_i,\sigma_j}, & n_{ij} = 1 \end{cases}.}$$

The results of 2.2 and 2.3 make sense in the context of the Swendsen-Wang algorithm. Eq. 6 tells us that if two neighboring spins are aligned, then they should be bonded with probability p. If they are not, then they should never be bonded. This allows us to create a lattice of bonded similarly aligned spins in the G space. Eq. 7 tells us that if a bond is not present between two spins, then we can assign the values of those spins arbitrarily; if the spins are not already in the cluster, then the two spins can take on values ↑↑, ↓↓, ↑↓, or ↓↑ with equal probability. If there is a bond present, then there is a restriction on the values of the spins; for a bond to be present, the spins must be aligned. But the specific orientation of the spins does not matter, and Eq. 7 tells us that we can choose either ↑↑ or ↓↓ each with the same probability for the values of σ_i and σ_j. This interpretation of Eq. 6 and Eq. 7 tells us how to proceed in our implementation of the Swendsen-Wang algorithm when proposing a configuration in G from a configuration in C or when proposing a configuration in C from a configuration in G.