Swendsen-Wang algorithm in a nutshell

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References

[1] R.H. Swendsen and J.-S. Wang. Phys. Rev. Lett. **58**, 86 (1987).

[2] J. Gubernatis, N. Kawashima, P. Werner. *Quantum Monte Carlo Methods: Algorithms for Lattice Models*. Cambridge University Press (2016).

[3] U. Wolff. Phys. Rev. Lett. **62**, 361 (1989).

1 Introduction

In the studies of second-order phase transition, the problem of **critical slowing-down** is a big obstacle for Markov chain Monte Carlo (MCMC) simulations. To reduce the autocorrelation times, nonlocal update is typically needed to improve the performance of MCMC. Historically, **Swendsen-Wang (SW) algorthm** was the first nonlocal algorithm, which thereafter has inspired many MCMC algorithms.

In this note, we take the classical Ising model

$$H = -J \sum_{\langle ij \rangle} s_i s_j \tag{1}$$

as an example to introduce the core idea of SW algorithm.

The canonical partition function can be written as

$$Z = \sum_{C \in \Omega} W(C) \tag{2}$$

where Ω is the configuration space, within which each configuration C has the weight

$$W(C) = \prod_{\langle ij \rangle} w(s_i, s_j), \quad w(s_i, s_j) = e^{K s_i s_j} \tag{3}$$

with $K \equiv \beta J$.

2 Two-step selection

In MCMC, we have to select next configuration C' based on the present configuration C. An important methodology to achieve this is the **two-step selection**:

(Two-step selection) *Suppose $\mathcal{F}$ is a family of subspaces $\mathbf{G}$ covering $\mathbf{\Omega}$, then to select the next $C' \in \Omega$ based on the present $C \in \Omega$,*

1. *Select a subspace $\boldsymbol{G} \in \mathcal{F}$ with probablity $P(\mathbf{G}|C)$;*
2. *Select the new state $C' \in \boldsymbol{G}$ this with probablity $O(C'|C, \boldsymbol{G})$*

If $C \notin \mathbf{G}$, then apparently $P(\mathbf{G}|C) = 0$.

With the two-step selection, $P(C'|C)$ can be written as a marginal probablity

$$P(C'|C) = \sum_{\mathbf{G}} P(C'|C, \mathbf{G}) P(\mathbf{G}|C) \tag{4}$$

Hence, to satisfy the detailed blance condition, we must have

$$P(C'|C, \mathbf{G}) P(\mathbf{G}|C) W(C) = P(C|C', \mathbf{G}) P(\mathbf{G}|C') W(C') \tag{5}$$

3 Cluster update

Just as the name implies, a cluster update samples a new configuration by changing the state of a cluster of spins on the present configuration per MC time. We will discuss the relation between cluster update and the two-step selection introduced above later. For now, let us provide a more precise tool to describe the concept of cluster.

Mathematically, the lattice (configuration) is a **graph** with an edge between each pair of neighboring lattice sites. When we construct some clusters of spins, they basically can be viewed as an overlaid graph that creates connections among the spins. For convenience, we denote the ground graph with $\mathcal{G}_0$ and overlaid graph with $\mathcal{G}$. To describe the structure of $\mathcal{G}_0$, we introduce a new set of variables $\{g_{ij}\}$ to denote connection ($g_{ij} = 1$) and disconnection ($g_{ij} = 0$).

4 SW algorithm

Define

$$H_{ij} := -J \sum_{\langle mn\rangle \neq \langle ij\rangle} s_m s_n \tag{6}$$

$$Z_{ij}^{s_i=s_j} := \sum_C e^{KH_{ij}(C)} \delta_{s_i,s_j} \tag{7}$$

$$Z_{ij}^{s_i\neq s_j} := \sum_C e^{KH_{ij}(C)} [1-\delta_{s_i,s_j}] \tag{8}$$

$$Z_{ij} := Z_{ij}^{s_i=s_j} + Z_{ij}^{s_i\neq s_j} \tag{9}$$

then

$$Z = e^K Z_{ij}^{s_i=s_j} + e^{-K} Z_{ij}^{s_i\neq s_j} = (e^K - e^{-K}) Z_{ij}^{s_i=s_j} + e^{-K} Z_{ij} \tag{10}$$

The coefficent $(e^K - e^{-K})$ represents the weight when there exists the constraint $s_i = s_j$, and e^{-K} represents the weight when there is no constraint on $\langle ij\rangle$. Therefore we relate

$$W(g_{ij}=1|s_i=s_j) = e^K - e^{-K} \tag{11}$$

$$W(g_{ij}=0|s_i=s_j) = e^{-K} \tag{12}$$

or

$$P(g_{ij}=1|s_i=s_j) = 1 - e^{-2K} \tag{13}$$

$$P(g_{ij}=0|s_i=s_j) = e^{-2K} \tag{14}$$

when $s_i = s_j$.

If $s_i \neq s_j$, we require

$$P(g_{ij}=1|s_i\neq s_j) = 0 \tag{15}$$

$$P(g_{ij}=0|s_i\neq s_j) = 1 \tag{16}$$

Here, $g_{ij} = 1$ is compatible with $(s_i, s_j) = (-1,-1)$ or $(1,1)$, while $g_{ij} = 0$ is compatible with $(s_i, s_j) = (-1,-1), (-1,1), (1,-1)$, or $(1,1)$. To make Eq. (13), (14), (15), (16) more compact, we write them as $P(g_{ij}|s_i, s_j)$, with

$$P(1|s_i,s_j) = 1 - P(0|s_i,s_j) = \delta_{s_i,s_j}(1-e^{-2K}) \tag{17}$$

In the SW algorithm, we thus construct the overlaid graph the rules above.

Remember that to perform a two-step selection, we first select a subspace $\mathbf{G}$. It is starightforward that we can actually build an isomorphism between a subspace $\mathcal{G}$ and $\mathbf{G}$. Then we have

$$P(\mathbf{G}|C) = \prod_{\langle ij \rangle} P(g_{ij}|s_i, s_j) \tag{18}$$

If $\mathcal{G}$ only involves one cluster, then $\mathbf{G}$ would include two states $\{C, C'\}$, where C' is obtained by flipping the cluster of spins in C. Notice that C and C' have the same weight, thus the probablity to flip the cluster is exactly $P(C|\mathbf{G}, C) = P(C'|\mathbf{G}, C) = 1/2$. Similarly, if totally N_{cluster} clusters are in $\mathcal{G}$, the probablity to select each of them $C' \in \mathbf{G}$ is $1/2^{N_{\text{cluster}}}$.

Let us check whether the detailed balance condition (5) is satisfied.

Since $P(C|\mathbf{G}, C) = P(C'|\mathbf{G}, C)$, Eq. (5) reduces to

$$\begin{aligned} & P(\mathbf{G}|C)W(C) \stackrel{?}{=} P(\mathbf{G}|C')W(C') \\ \Longrightarrow & \prod_{\langle ij \rangle} P(g_{ij}|s_i, s_j)w(s_i, s_j) \stackrel{?}{=} \prod_{\langle ij \rangle} P(g_{ij}|s'_i, s'_j)w(s'_i, s'_j) \end{aligned} \tag{19}$$

If

$$P(g_{ij}|s_i, s_j)w(s_i, s_j) = P(g_{ij}|s'_i, s'_j)w(s'_i, s'_j) \tag{20}$$

satisfies for each $(\langle ij \rangle)$, then Eq. (19) apparently holds.

- When $g_{ij} = 1$, the nontrivial solution is $s_i = s_j$ and $s'_i = s'_j$, then Eq. (20) satisfies.
- When $g_{ij} = 0$, all configurations of are compatible, and

  $$P(0|s_i, s_j)w(s_i, s_j) = [1 - \delta_{s_i, s_j}(1 - e^{-2K})]e^{K s_i s_j} = e^{-K} \tag{21}$$

  which is independent of the configuration (s_i, s_j). Therefore Eq. (20) still satisfies.

In conclusion, the detailed blance condition is satisfied in SW algorithm.

5 Wolff algorithm

Another representative cluster algorithm is the **Wolff algorithm**. It is similar to the SW algorithm, but instead, it randomly select one site and form one cluster per MC time. I recommend the readers to refer to this page or https://latt.if.usp.br/technical-pages/twawesab/Text.html/node1.html.