Cluster algorithms

and there applications.

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Sweden-Wang Algorithm

We add the constant -|J| in the Hamiltonian for the lattice model.

$$E(\sigma) = -|J| \sum_{b=1}^{N_b} [\sigma_{i(b)}\sigma_{j(b)} + 1] = \sum_{b=1}^{N_b} E_b.$$

So, the partition function now becomes,

$$Z = \sum_{\sigma} \mathrm{e}^{-E(\sigma)/T} = \sum_{\sigma} \prod_{b=1}^{N_b} \mathrm{e}^{E_b/T} = \sum_{\sigma} \prod_{b=1}^{N_b} [1 + (\mathrm{e}^{E_b/T} - 1)].$$

F_b Now, we introduce an argument in the bond function “b” to refer to a whole bond configuration, and the bonds function depends implicitly on the spins connected by bonds b.

$$Z = \sum_{\sigma} \sum_{\tau} \prod_{b=1}^{N_b} F_b(\tau_b). \qquad \text{where,} \quad \begin{aligned} F_b(0) &= 1, \\ F_b(1) &= \mathrm{e}^{E_b/T} - 1, \end{aligned}$$

For an non-vanishing contribution to the partition function, the bond configuration $\tau_b = 1$ allowed only between parallel spins.

$$
\begin{aligned}
F_b(0) &= 1, \quad \text{independent of } \sigma_{i(b)}, \sigma_{j(b)} \\
F_b(1) &= \mathrm{e}^{E_b/T} - 1 = \begin{cases} \mathrm{e}^{2|J|/T} - 1, & \text{if } \sigma_{i(b)} = \sigma_{j(b)}, \\ 0, & \text{if } \sigma_{i(b)} \neq \sigma_{j(b)}. \end{cases}
\end{aligned}
$$

$$
W(\sigma, \tau) = \prod_{b=1}^{N_b} F_b(\tau),
$$

$$
W(\sigma, \tau) = (\mathrm{e}^{2|J|/T} - 1)^{N_1},
$$

Where, N_1 is the number of filled bonds. Hence, the spin configuration affects the weight only by imposing restrictions on where the filled bonds can be placed.

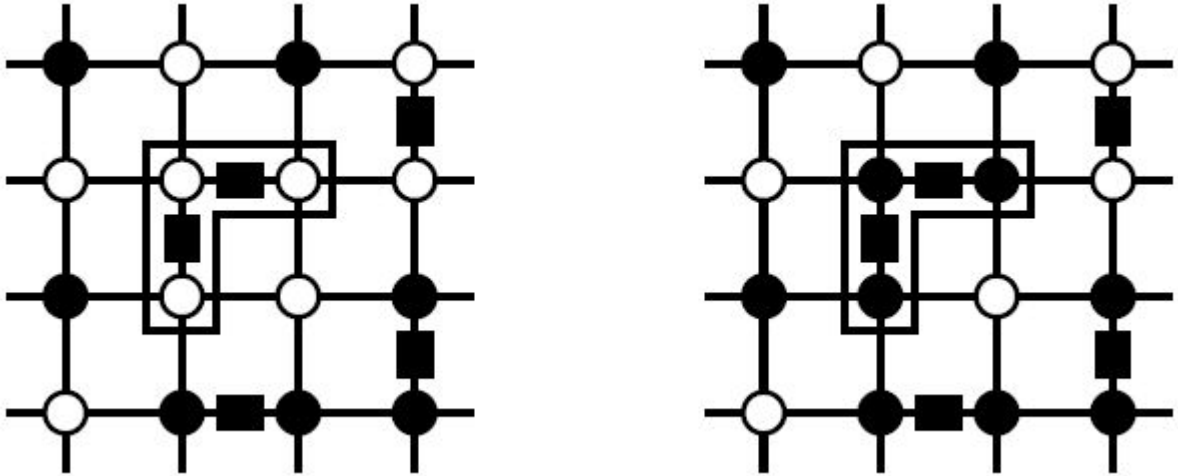

Figure 1: Spin configuration(circles) and the filled bonds(thick lines), along with the shown clusters in each lattice.

There is a added constant -|J| in the Hamiltonian of the model, without this term there could be a filled bond between anti-parallel spins as well, and a weight function would had more complex dependencies on the spins. Thus, with this constant added, the weight is now independent on the spin configuration, as no such illegal bonds are present.

Now, the probability of a bond configuration corresponding to the weight is:

$$P(\tau) = \prod_b P_b(\tau_b),$$

where, the individual bond probabilities are:

$$P(\tau_b) = \frac{F_b(\tau_b)}{F_b(0) + F_b(1)}.$$

The probability of a filled bond is hence:

$$\begin{aligned} P(\tau_b = 1) &= 1 - \mathrm{e}^{-2|J|/T}, && \text{if } \sigma_{i(b)} = \sigma_{j(b)}, \\ P(\tau_b = 1) &= 0, && \text{if } \sigma_{i(b)} \neq \sigma_{j(b)}. \end{aligned}$$

Formulation of a Cluster Algorithm

1. To start with an arbitrary spin configuration .
2. Assign filled bonds according to the probabilities written above.
3. Identify each clusters of spin and flip each of them with probability
4. Repeat from step 2.

Critical slowing down.

SW algorithm very popular is its ability to strongly suppress dynamic slowing down near a critical point.

$$\tau \propto \xi^z \ ,$$

correlation length itself diverges as a power law of T - Tc,

$$\xi \propto |T - T_c|^{-\nu} \ ,$$

Also, near the critical temp,

$$\tau \propto L^z \ .$$

This is called critical slowing down.

Swendsen–Wang algorithm have a structure that is very efficient at destroying nonlocal correlations.

Wolff Algorithm

1. A spin *i* is selected at random.

2. All nearest neighbors *j* of this spin are added to the cluster with a probability $p_{ij} = 1 - e^{-2\beta J}$ provided spins *i* and *j* are parallel and the bond between *i* and *j* has not been considered before.

3. Each spin *j* that is indeed added to the cluster is also placed on the stack. Once all neighbors of *i* have been considered for inclusion in the cluster, a spin is retrieved from the stack and all its neighbors are considered in turn for inclusion in the cluster as well, following step (2).

4. Steps (2) and (3) are repeated iteratively until the stack is empty.

5. Once the cluster has been completed, all spins that belong to the cluster are inverted.

This is also a rejection-free algorithm, in the sense that the cluster is always flipped. The cluster-construction process is probabilistic, but the probabilities p_{ij} involve energies of individual spin pairs in contrast with an acceptance criterion that involves the total energy change induced by a cluster flip.

Cluster algorithm in Anti-ferromagnet.

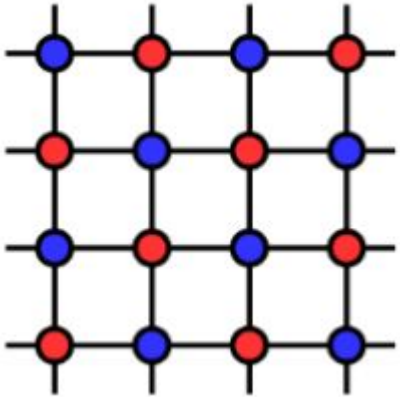

Figure 2: Neel order of anti-ferromagnet.

Cluster algorithm in Hard-sphere liquid.

The geometric cluster algorithm described is formulated for particles that interact via hard-core repulsions only.

$$V(\mathbf{r}_1, \mathbf{r}_2) = \begin{cases} 0 & \text{if} \quad |\mathbf{r}_1 - \mathbf{r}_2| \geq \sigma \\ \infty & \text{if} \quad |\mathbf{r}_1 - \mathbf{r}_2| < \sigma \end{cases}$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the positions of the two particles.

Groups of particles that overlap between the original and the rotated configuration are exchanged between these configurations.

1. In a given configuration C, a “pivot” is chosen at random.
2. A particle i is selected as the first particle that belongs to the cluster. This particle is moved via a point reflection with respect to the pivot. In its new position, the particle is referred to as i .
3. The point reflection in step 2 is repeated iteratively for each particle j that overlaps with i . Thus, if the (moved) particle j overlaps with another particle k, particle k is moved as well. Note that all translations involve the same pivot.
4. Once all overlaps have been resolved, the cluster move is complete.

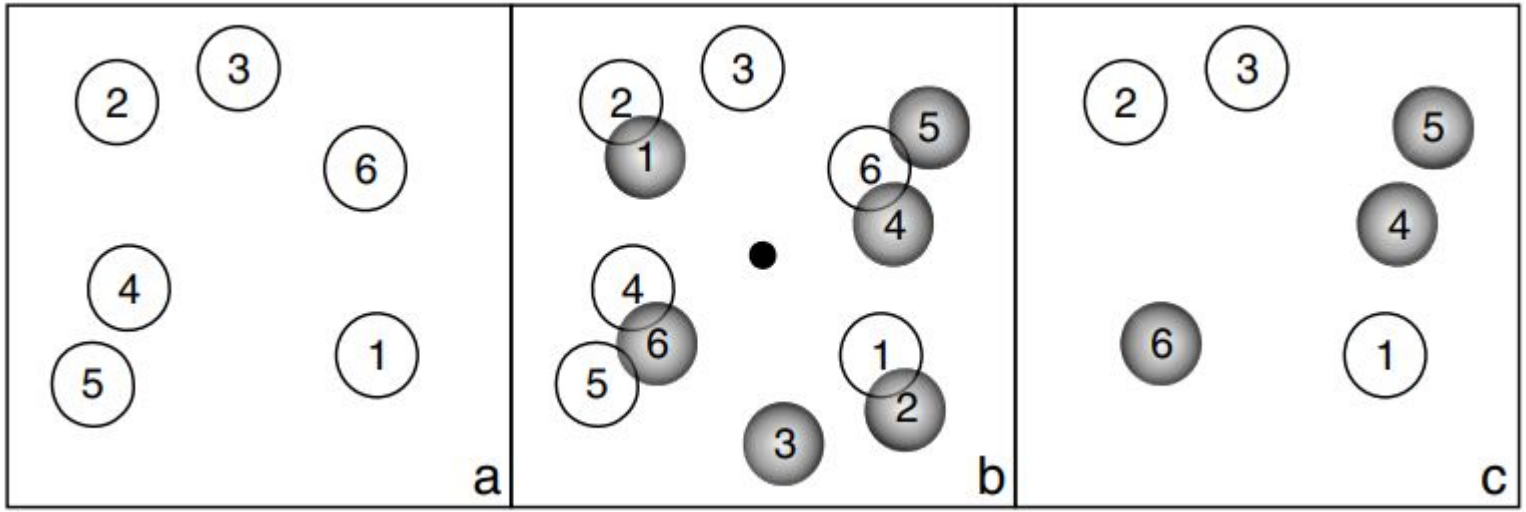

Figure 2: (a) Original configuration. (b). A new configuration (shaded circles) is created by means of a point reflection of all particles with respect to a randomly chosen pivot point (small filled disk). In this example, there are three pairs of groups ({1, 2}, {3}, {4, 5, 6}). Each pair is denoted a cluster. (c). Final configuration that results if, starting from the original configuration, only the particles in the third cluster {4, 5, 6} are point-reflected

This algorithm is ergodic, since each particle can be moved over an arbitrarily small distance. Namely, there is a non-vanishing probability that a cluster consists of only a single particle and the pivot can be located arbitrarily close to the center of this particle.

Also, the algorithm should satisfy the detailed balance property.

$$1 - p_{ij} = \min\left[\exp(-\beta \Delta_{ij}^{\mathrm{SW}}), 1\right] \ ,$$

The GCA, although formulated in continuum space rather than on a lattice, can now be interpreted as special situation in which either $\Delta ij = 0$ (after reflection of particle i, there is no overlap between particles i and j), leading to $pij = 0$, or $\Delta ij = \infty$