CLUSTER MONTE CARLO ALGORITHMS AND THEIR APPLICATIONS

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We review the background of the cluster algorithms in Monte Carlo simulation of statistical physics problems. One of the first such successful algorithm was developed by Swendsen and Wang eight years ago. In contrast to the local algorithms, cluster algorithms update dynamical variables in a global fashion. Therefore, large changes are made in a single step. The method is very efficient, especially near the critical point of a second-order phase transition. Studies of various statistical mechanics models and some generalizations of the algorithm will be briefly reviewed. We mention applications in other fields, especially in imaging processing.

I. MONTE CARLO METHOD

One of the important task in statistical mechanics and quantum field theory is to compute the statistical average,

$$\langle A \rangle = \frac{\sum_X A(X) \exp[-\beta H(X)]}{\sum_X \exp[-\beta H(X)]} = \sum_X A(X) P(X), \quad (1)$$

where the summation is over a set of all states $X$, which usually is very large. A general method was proposed long time ago in the fifties by Metropolis et al., well-known as Metropolis algorithm. Instead of summing over all the states as required, one generates a selection of the states according to the probability $P(X)$, so that the answer is given approximately by an arithmetic average of the quantity $A(X)$. The generation of a sequence of the states is done stochastically by the method of Markov chain.

A. Markov chain

A Markov chain is a mathematical notion for a random walk in the state space $X$. We start from some initial point $X_0$, the next point $X_1$ is generated according to certain transition probability. In this way a sequence of random points $X_0, X_1, \cdots, X_N$ is generated. These points are required to appear with the probability $P(X)$. The rule to generate next point $X_{i+1}$ given the point $X_i$ is specified by the transition probability

$$P(X_{i+1}|X_i) = W(X_i \rightarrow X_{i+1}). \quad (2)$$

where $P(X_{i+1}|X_i)$ is the probability that the system is in state $X_{i+1}$, given that the system was in state $X_i$, namely, it is the conditional probability. We have

$$W(X_i \rightarrow X_{i+1}) \geq 0, \quad \sum_{X_{i+1}} W(X_i \rightarrow X_{i+1}) = 1. \quad (3)$$

Since $W$ is probability, it satisfies the usual constraint of probability—probability must be positive and total probability adds to one.

If we choose $W$ so that

$$P(X) = \sum_{X'} P(X') W(X' \rightarrow X), \quad (4)$$

we say that $P(X)$ is invariant under the transition of $W$, or $P(X)$ is the equilibrium distribution for the given transition probability. Such a probability distribution will be unique if starting from any state $X$, it is possible to get to any another state $X'$ after a finite number of transitions. We call such Markov chain ergodic (regular, or irreducible).

B. Detailed balance

How to choose $W$ to get prescribed $P$? It is sufficient that $W$ satisfies

$$P(X') W(X' \rightarrow X) = P(X) W(X \rightarrow X'), \quad (5)$$

where $P$ is the known distribution. If $W$ satisfies this equation and it is ergodic, then the Markov chain will generate $X$ according to the probability distribution $P(X)$.

C. Metropolis algorithm

Metropolis method goes as follows: starting from some initial state (configuration) $X_0$, a sequence of states will be generated by a Markov chain through
the transition probability $W(X_i \to X_{i+1})$. The starting state may be a unique state or may be generated at random with certain distribution $P_0$. The new state $X_{i+1}$ is based on the old state $X_i$. The new state is generated in such a way that the probability that the system is in state $X_{i+1}$ is just $W(X_i \to X_{i+1})$, knowing that the system was in state $X_i$. Hopefully we can generate this probability distribution easily. Otherwise we might have generated $P(X)$ directly in the first place. It is sufficient that $W$ satisfies detailed balance condition and the Markov chain is ergodic. Metropolis algorithm refers to a specific choice of $W$:

$$W(X \to X') = T(X \to X') \min\left(1, \frac{P(X')}{P(X)}\right),$$

where $X \neq X'$ and $T(X \to X') = T(X' \to X)$. Matrix $T$ can be any distribution but must be symmetric. We almost always use

$$T(X \to X') = \begin{cases} \text{const}, & \text{for } X' \text{ in a region around } X; \\ 0, & \text{otherwise}. \end{cases}$$

The probability that the state does not change, $W(X \to X)$, is determined by the normalization condition

$$\sum_{X'} W(X \to X') = 1.$$ (6)

## II. ISING MODEL FOR MAGNETS

To be able to understand Swendsen-Wang and other cluster algorithms, we need to introduce the very popular model for ferromagnets in condensed matter physics. Ising model is the simplest model for ferromagnets. One of the striking feature of a magnet is that it has spontaneous magnetization at lower temperatures. However, the magnetization disappears at some higher temperature $T_c$. The phase below $T_c$ is called ferromagnetic phase and that above $T_c$ is called paramagnetic phase. $T_c$ is called critical temperature and there is a phase transition at this temperature.

Let’s take two-dimensional system as an example. On an $L \times L$ square lattice, we put a spin $\sigma_i$ at each lattice site $i$. Each spin takes only two possible values $+1$ and $-1$. The set of $L^2$ spins consists of the state space $X$. The system has a total energy as a function of the state $\{\sigma\}$, defined by

$$H(\{\sigma\}) = -J \sum_{(i,j)} \sigma_i \sigma_j,$$ (7)

where $J$ is called coupling constant. The summation is over the nearest neighbors only, i.e., each bond is summed once. Such model is also referred as nearest neighbor Ising model. When $J$ is positive, the model describes a ferromagnet; while $J < 0$ describes an anti-ferromagnet. Let’s consider just one term in the nearest neighbor interaction. The interaction energy of neighbors takes only two values, $+J$ or $-J$. For ferromagnet, the energy is lower if the two spins are parallel. It costs energy if the spins are pointing in different directions.

According to statistical-mechanical description, the system will not be in a definite state. Due to thermal fluctuation, the system will have some probability distribution among the states. If the temperature $T$ is a fixed parameter, we have the famous Boltzmann distribution

$$P(\{\sigma\}) \propto \exp\left(-\frac{H(\{\sigma\})}{k_B T}\right),$$ (8)

where $k_B \approx 1.38 \times 10^{-23}$ Joule/Kelvin is called the Boltzmann constant. Our goal is to calculate average quantities such as energy, magnetization, correlation functions, etc. The internal energy is defined by

$$U = \langle H \rangle = \sum_{\{\sigma\}} H(\{\sigma\}) P(\{\sigma\});$$ (9)

and the magnetization is defined as

$$\langle M \rangle = \sum_{\{\sigma\}} \sum_i \sigma_i P(\{\sigma\}).$$ (10)

The summation is over all possible states. Since each site can have two states (spin up and spin down), we have $2^{L^d}$ states for a system of linear size $L$ in $d$ dimensions.

A Monte Carlo simulation of the Ising model by Metropolis algorithm involves the following steps:

1. Initialize $\sigma_i$ at each site with arbitrary spin values, e.g., all spin up, or up or down with equal probability. The complete set of spins $\{\sigma\}$ is the abstract state $X$ discussed in the previous section.

2. Choose a site $k$ at random and propose to flip the spin at that site, $\sigma'_k = -\sigma_k$. The proposed state $X'$ is the one with one spin at location $k$ flipped. This amounts to take $T(X \to X')$ equal to $1/L^d$ if $X$ and $X'$ differ by 1 spin, and 0 otherwise.

3. Calculate the energy increment

$$\Delta E = H(\{\sigma'\}) - H(\{\sigma\}) = 2J\sigma_k \sum_{\text{neighboring } i} \sigma_i.$$ (11)

4. Accept the proposed state as the new state if a uniformly distributed random number (between 0 and 1) is less than $\exp(-\Delta E/k_B T)$; retain the old state as the new state otherwise.

5. go to 2.

One Monte Carlo step will be defined as performing the above basic single-spin flip $L^d$ number of times. After one Monte Carlo step, each site on average has tried once to flip.
III. CRITICAL SLOWING DOWN

In Ising model simulation, or more generally any simulation using the Metropolis algorithm, the next configuration depends on the previous one. Due to this correlation between Monte Carlo steps, the formula for the statistical error $\epsilon \approx \sigma / \sqrt{N}$ underestimates the true error, where $\sigma$ is the variance of the quantity of interest, and $N$ is Monte Carlo steps. The error formula should be replaced by

$$\epsilon \approx \sigma \sqrt{1 + 2\tau} / N,$$  \hspace{1cm} (14)

That is, the error is larger by a factor $\sqrt{1 + 2\tau}$ than the uncorrelated data. The quantity $\tau$ is called correlation time, which is roughly the number of Monte Carlo steps needed to generate independent configurations. We can compute the correlation time $\tau$ as follows: define the time-dependent correlation function,

$$f(t) = \frac{\langle A(t')A(t'' + t) \rangle - \langle A \rangle^2}{\langle A^2 \rangle - \langle A \rangle^2},$$  \hspace{1cm} (15)

where time $t$ is measured in terms of Monte Carlo steps—time is passed by one unit when one updates the system by one Monte Carlo step. And $A(t')$ is the quantity at steps $t'$ whose error we want to estimate. The angular brackets denote average over Monte Carlo steps. The correlation time is defined by

$$\tau = \sum_{t=1}^{\infty} f(t).$$  \hspace{1cm} (16)

Now we are ready to explain the concept of critical slowing down. Just like many other quantities near the critical point, the correlation time also becomes singular at the critical point. On an infinite lattice, it diverges with a power law

$$\tau \propto |T - T_c|^{-\nu z}.$$  \hspace{1cm} (17)

Here $\nu$ is the correlation length exponent and $z$ is called dynamic critical exponent. This phenomena that the correlation time becomes very large is called critical slowing down. It not only happens in computer simulation but also appears in real systems. On a finite system of linear size $L$, the correlation time will, of course, not go to infinity. But it will grow with size as

$$\tau \propto L^z, \quad T = T_c.$$  \hspace{1cm} (18)

Substituting this result into the error formula, we find that $\epsilon \approx \sigma L^{z/2} / N^{1/2}$ for large system near $T_c$. For the two-dimensional Ising model with Metropolis algorithm, $z \approx 2.1$, we see typically that increasing the size leads to a larger error in the quantity to be calculated.

IV. CLUSTER MONTE CARLO ALGORITHMS

The Metropolis algorithm makes changes locally one site at a time. This is the cause of the critical slowing down. There are algorithms that change the states by a group of clusters. The advantage of the cluster algorithms is that they are faster, not necessarily in computer time per Monte Carlo step, but in terms of dynamics. That is, it has a much smaller value of $z$.

A. Swendsen-Wang algorithm

The Swendsen-Wang multi-cluster algorithm is closely related to percolation based on the work of Fortuin and Kasteleyn. One starts with a spin configuration $\{\sigma\}$ and generates a percolation configuration based on the spin configuration by the rule described below. Then the old spin configuration is forgotten and a new spin configuration $\{\sigma'\}$ is generated based on the percolation configuration. The rule is such that the detailed balance is satisfied. Or more generally, the transition leaves the equilibrium probability invariant. The algorithm goes as follows:

1. Start with some arbitrary state $\{\sigma\}$.

2. Go through each nearest neighbor connection of the lattice, create a bond between the two neighboring sites $i$ and $j$ with probability $p = 1 - e^{-2J/k_B T}$, but only if the spins are the same, $\sigma_i = \sigma_j$. Never put a bond between the sites if the spin values are different. We are creating a bond percolation configuration with probability $p$ on a subset of lattice sites where the spins are either all pointing up or down.

3. Identify clusters as a set of sites connected by bonds, or isolated sites. Two sites are said to be in the same cluster if there is a connected path of bonds joining them. Every site has to belong to one of the clusters. After the clusters are found, each cluster is assigned a new Ising spin chosen with equal probability between $+1$ and $-1$. The old spin values now can be ‘forgotten’. And all the sites in a cluster now take the value of spin assigned to the cluster.

4. One Monte Carlo step is finished. Repeat 2 for the next step.

The performance of the algorithm in terms of correlation time in comparison with Metropolis algorithm is remarkable. Recall that the dynamic critical exponent $z$ is about 2 for Metropolis algorithm almost independent of the dimensionality. The Swendsen-Wang algorithm in one dimension gives $z = 0$ (and $\tau \rightarrow 0$). For the two-dimensional Ising model, the dynamic critical exponent $z$ is less than 0.3 or possibly zero (but $\tau \propto \ln L$). In three dimensions it is about 0.5. At and above four dimensions it is 1.
B. Wolff single-cluster algorithm

In the Swendsen-Wang algorithm, we generated many clusters and then flipped these clusters. Wolff algorithm is a variation on the way clusters are flipped. One picks a site at random, and then generates one single cluster by growing a cluster from the seed. The neighbors of the seed site will also belong to the cluster if the spins are in parallel and a random number is less than \( p = 1 - e^{-2J/k_B T} \). That is, the neighboring site will be in the same cluster as the seed site with probability \( p \) if the spins have the same sign. If the spins are different, neighboring site will never belong to the cluster. Neighbors of each new site in the cluster are tested for membership. This testing of membership is performed on pair of sites (forming a nearest neighbor bond) not more than once. The recursive process will eventually terminate. The spins in the cluster are turned over with probability \( 1 \). Single cluster algorithm appears more efficient than the multi-cluster one.

The following is a fairly elegant way of implementing the Wolff algorithm in C. The function is the core part which performs a Wolff single cluster flip. This function is recursive. The array for spins \( s[] \), percolation probability \( P \), and coordination number \( Z \) (the number of neighbors) are passed globally. The first argument \( i \) of the \( \text{flip} \) function is the site to be flipped, the second argument \( s_0 \) is the spin of the cluster before flipping. The function \( \text{neighbor} \) returns an array of neighbors of the current site. The function \( \text{drand48}() \) returns a random number uniformly distributed between 0 and 1.

```c
void flip(int i, int s0)
{
    int j, nn[Z];
    s[i] = - s0;
    neighbor(i, nn);
    for(j = 0; j < Z; ++j)
        if(s0 == s[nn[j]] && \text{drand48}() < P)
            \text{flip}(nn[j], s0);
}
```

V. FURTHER DEVELOPMENT OF CLUSTER ALGORITHMS

The attractive feature of Swendsen-Wang algorithm stimulated research for other types of cluster algorithms and its theory. The original method works for Ising and Potts models. It is not clear at the first sight how one can generalize it for arbitrary model. The idea of Ising spin embedding into a model appears to work well. This idea is applied to a number of models, including models with continuous degree of freedom. Kandel and coworkers proposed a general scheme for cluster algorithms, which leads to efficient algorithms for models with competing interactions. Cluster algorithm of a different kind (loop algorithm) was proposed to work with vertex models.

Sokal’s idea of introducing auxiliary variables is another way of generalizing the cluster algorithms and is drawing attention to statisticians. However, this method seems not work well in comparison with embedding algorithms when the system has Ising symmetry and embedding can be implemented.

A large class of problems in statistical mechanics can be now simulated with cluster algorithms. Cluster algorithms are used routinely where traditionally local algorithms are used. Due to space limitations, this types of applications will not be reviewed here.

VI. APPLICATION IN IMAGE PROCESSING

The Swendsen-Wang algorithm and some generalizations were used in connection with image processing. Random image, in particular, a class of random fields called Markov random fields, correspond closely to systems studied in statistical physics. Thus the Monte Carlo techniques developed in statistical mechanics can be readily used here. There is also the need to estimate model parameters, this can be done by Monte Carlo simulation. The most important application appears to be in the problems of image restoration and image segmentation. The statistical method (or Bayesian inference) in image analysis is relatively new. The basic problem in Bayesian image restoration is the following. Let \( X \) be the true image, which is also statistical in nature and distributed according to \( P(X) \), called the prior. The true scene, \( X \), is not directly observable, and the observed data \( Y \) contains noise. Given \( Y \), one wants to compute the distribution of \( X \), namely, the conditional probability \( P(X|Y) \), called posterior. This is obtained by noting

\[
P(X|Y) \propto P(Y|X)P(X), \quad \text{for fixed } Y. \tag{19}
\]

Image restoration amounts to find the most probable \( X \) by simulating the probability distribution \( P(X|Y) \). Ising model is assumed for \( P(X) \) in some application; while \( P(Y|X) \) is given as independent Gaussian distribution for \( Y \). From the point of view of statistical mechanics, \( P(X|Y) \) describes a model with inhomogeneous local magnetic field which is determined by \( Y \).

Segmentation is a process of classifying each pixel in an image. We can think of it as a special case of restoration problem. Thus the two problems share the same mathematical structure. The problem of speed of convergence in image segmentation by Swendsen-Wang algorithm is studied. The cluster algorithms work best when the system has a high degree of symmetry. The two types of problems, image
restoration and image segmentation, all end up involving the simulation of a model with the presence of complicated magnetic field, which makes cluster algorithms less effective. The cluster algorithms and other acceleration algorithms, e.g., ref. 4, developed in statistical physics may be very helpful in this field. But much more work needs to be done.

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