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Monte Carlo methods beyond detailed balance

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HIGHLIGHTS

- We propose a Monte Carlo approach, which is not restricted by detailed balance.
- The high efficiency of this new approach is demonstrated in a simple model.
- Its general applicability is demonstrated by applying it to the Ising model.

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ABSTRACT

Monte Carlo algorithms are nearly always based on the concept of detailed balance and ergodicity. In this paper we focus on algorithms that do not satisfy detailed balance. We introduce a general method for designing non-detailed balance algorithms, starting from a conventional algorithm satisfying detailed balance. This approach is first applied to a very simple model, which shows the basic viability of the method. Then we apply it to the Ising model, where we find that the method is an improvement compared to the standard Metropolis algorithm, be it with a modest gain of a factor 2.3.

1. Introduction

To study equilibrium properties of models in statistical physics by means of computer simulations, Monte Carlo methods are often used (see [1] for a more thorough description). Starting from some initial configuration C_0, the basic idea of most Monte Carlo simulations is to iteratively propose a small random change in a configuration C_i, resulting in the trial configuration C^t_{i+1}. Next, the trial configuration is either accepted, i.e. $C_{i+1} = C^t_{i+1}$, or rejected, i.e. $C_{i+1} = C_i$. The resulting set of configurations for $i = 1 \ldots M$ is known as a Markov chain. If the proposition and acceptance probabilities are well chosen, the probability that a configuration A is sampled by the Markov process (after thermalization) is equal to its Boltzmann weight:

$$P_A \sim \exp(-\beta E_A), \tag{1}$$

in which E_A is the energy of configuration A and β is the inverse temperature, defined by $\beta \equiv 1/(k_B T)$ with temperature T and the Boltzmann constant k_B. A proposed change in the configuration is usually referred to as a Monte Carlo move.

The key question in Monte Carlo algorithms is obviously which small changes one should propose, and how large the acceptance probabilities should be. The first constraint is ergodicity: starting from any configuration C_0 with nonzero Boltzmann weight, any other configuration with nonzero Boltzmann weight should be reachable through a finite number of well-chosen Monte Carlo moves. Apart from a very small number of exceptions, a second constraint to guarantee its

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correctness is known as the condition of detailed balance. If the system is in state A, and a single Monte Carlo move brings it to state B, then detailed balance requires

$$P_A \cdot T(A \to B) \cdot A(A \to B) = P_B \cdot T(B \to A) \cdot A(B \to A), \tag{2}$$

in which $T(A \to B)$ is the probability that, given the system is in state A, a move towards state B is proposed, and $A(A \to B)$ is the probability that this proposed move is accepted. The combination of ergodicity and detailed balance assures a correct algorithm, i.e., given a long enough time, the Boltzmann distribution is sampled. Though this combination is sufficient, it is not a necessary condition. In fact, the slithering snake algorithm [2] from polymer physics is an example of an algorithm violating detailed balance. One often-used approach to realize detailed balance is to randomly propose a small change in state A, resulting in another state B, in such a way that the reverse process (starting in B and then proposing a small change that results in A) is equally likely. More formally, a process in which the condition $T(A \to B) = T(B \to A)$ holds for all pairs of states $\{A, B\}$. If that is the case, then detailed balance can be obtained by the so-called Metropolis algorithm [3], in which the acceptance probability is given by

$$A_{\text{met}}(A \to B) = \min\left[1, \exp(-\beta(E_B - E_A))\right]. \tag{3}$$

Thus, a proposed move which does not raise the total energy is always accepted, but one resulting in higher energy is accepted with a probability that decreases with increasing energy.

For our purposes further on, it is convenient to introduce also the 'unconditional transition probability', defined as

$$U(A \to B) = P_A \cdot T(A \to B) \cdot A(A \to B). \tag{4}$$

Expressed in this quantity, detailed balance is simply the condition $U(A \to B) = U(B \to A)$ for all pairs of states $\{A, B\}$, and the Metropolis algorithm is obtained by $T(A \to B) = T(B \to A)$ combined with the requirement that the maximum of $A(A \to B)$ and $A(B \to A)$ is unity.

Recently, there has been a flurry of efforts to explore dynamics which violates detailed balance [4–10]. In particular, the approach presented by Turitsyn et al. [6] is closely related to our approach. Here, we follow a more generic description. Additionally, to explore the efficiency of this approach in a more relevant model, we apply it to the Ising model in two dimensions.

2. Beyond detailed balance: a one-dimensional model

We first introduce a very simple model, to illustrate a drawback of standard Monte Carlo algorithms. The phase space consists of states $i = 1 \ldots N$ which are placed on a one-dimensional ring. Each state i has an energy E_i. Transitions occur from state i to $i \pm 1$, modulo N. At high temperatures, all states are more or less equally likely, as well as all transitions. In that regime, it is reasonable to expect that the correlation time of the Monte Carlo algorithm, measured in the number of transitions, scales as $\tau_c \sim N^2$, as the exploration of phase space occurs by diffusion.

A more efficient exploration of phase space takes place if the dynamics would resemble molecular dynamics with inertia, in which a transition to the left (right) is predominantly followed by another transition in the same direction. In principle, this allows for asymptotically faster exploration during the time span where the direction of the transitions is correlated. How can this be achieved? One way to do this, is as follows. We double the phase space, into states $i = 1^+ \cdots N^+$ (the forward states) and states $i = 1^- \cdots N^-$ (the backward states), while maintaining that all states should be visited with their Boltzmann probabilities:

$$P(i^+) = P(i^-) \sim \exp(-\beta E_i). \tag{5}$$

As in the standard Monte Carlo, we randomly propose moves in either direction, but now we also add transitions between the forward and backward states:

$$\begin{aligned} T(i^+ \to (i+1)^+) &= T(i^- \to (i+1)^-) = T((i+1)^+ \to i^+) = T((i+1)^- \to i^-) \\ &= T(i^+ \to i^-) = T(i^- \to i^+) = 1/3. \end{aligned} \tag{6}$$

We do, however, reduce the acceptance probabilities in the undesirable directions as much as possible. Along each fourfold loop visiting the states i^+, $(i+1)^+$, $(i+1)^-$ and i^-, we modify the unconditional transition probability by subtracting a cycle with probability

$$U_{\text{loop}}(i + 1/2) = p_i \cdot A_{\text{met}}(i \to i+1) = p_{i+1} \cdot A_{\text{met}}(i+1 \to i) \tag{7}$$

so that the resulting acceptance probabilities are:

$$\begin{aligned} A(i^+ \to (i+1)^+) &= A_{\text{met}}(i \to i+1) \\ A((i+1)^- \to i^-) &= A_{\text{met}}(i+1 \to i) \\ A((i+1)^+ \to i^+) &= A_{\text{met}}(i+1 \to i) - P_{i+1}^{-1} \cdot U_{\text{loop}}(i+1/2) \\ A(i^- \to (i+1)^-) &= A_{\text{met}}(i \to i+1) - P_i^{-1} U_{\text{loop}}(i+1/2) \\ A(i^+ \to i^-) &= P_i^{-1} \cdot \text{Max}\left[0, U_{\text{loop}}(i+1/2) - U_{\text{loop}}(i-1/2)\right] \\ A(i^- \to i^+) &= P_i^{-1} \cdot \text{Max}\left[0, U_{\text{loop}}(i-1/2) - U_{\text{loop}}(i+1/2)\right]. \end{aligned} \tag{8}$$