**Randomness and Computation**
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# Monte Carlo Methods – Sampling from an Extended Ensemble –

Koji Hukushima [1]
Department of Basic Science, University of Tokyo 3-8-1 Komaba, Meguro-ku, Tokyo 153-8902, Japan

Since the Metropolis algorithm was introduced in 1953[1], Monte Carlo (MC) methods have been used intensively in a wide area of physics[2] and statistical sciences[3] Most of the MC methods in statistical physics are based on the Metropolis strategy, in which a Markov chain is constructed in order for its invariant distribution to coincide with the desired distribution. There exist various improvements on the Metropolis MC algorithms, which mainly categorized into two directions, i.e., non-local updating methods such as cluster algorithm and extended ensemble methods[4]. Typical examples of the latter are the multicanonical method[5], the simulated tempering[6] and the exchange MC[7] or parallel tempering method. These methods have been applied to various complex systems, e.g. protein models, spin glasses and optimization problems, and turned out to be quite useful for simulating these systems. In this paper, we review the basic idea of the extended ensemble MC methods, particularly focusing on the exchange MC method.

The extended ensemble methods are based on the idea that the ensemble or the weight to be simulated is modified or extended in such a way that the system visits more frequently to states which are less or hardly visited by the conventional MC algorithm. One of them is the multicanonical method[5], in which a weight factor different from the ordinary Boltzmann-Gibbs weight is introduced for a given energy function $E(\boldsymbol{X})$, where $\boldsymbol{X}$ represents a state ( or configurations) of the system. The multicanonical ensemble is expressed as

$$P_{\mathrm{M}} = \frac{\exp\left(-E_M(\boldsymbol{X})\right)}{\sum_{\boldsymbol{X}} \exp\left(-E_M(\boldsymbol{X})\right)} \tag{1}$$

with the effective energy function

$$E_M(\boldsymbol{X}) = \beta_M(E)E(\boldsymbol{X}) + \alpha_M(E) \tag{2}$$

where the parameter $\alpha_M(E)$ and $\beta_M(E)$ are to be chosen as a function of $E$ such that the probability distribution for finding the system in states with the energy $E$ is approximately flat in an energy range of interest. The resultant MC simulation produces configurations with the multicanonical weight $\exp(-E_M)$ which is proportional to $g^{-1}(E)$. Therefore highly excited configurations between metastable states are much frequently explored in the simulations and the system can easily visit various local minima, or the whole phase space.

In the exchange MC, on the other hand, we treat a combined system which consists of non-interacting $M$ replicas of the system described by a common energy function $E(\boldsymbol{X})$. The $m$-th replica is in contact with its own heat bath having inverse temperature $\beta_m$ (for convenience we take $\beta_m < \beta_{m+1}$). A state of this extended ensemble is specified by $M$ configurations $\{\boldsymbol{X}\} = \{\boldsymbol{X}_1, \boldsymbol{X}_2, \cdots, \boldsymbol{X}_M\}$, and the extended ensemble in this method is given by

$$\mathcal{P}_{EMC}(\{\boldsymbol{X}\};\{\beta\}) = \frac{\exp\left(-\sum_{m=1}^{M}\beta_m E(\boldsymbol{X}_m)\right)}{\sum_{\{\boldsymbol{X}\}}\exp\left(-\sum_{m=1}^{M}\beta_m E(\boldsymbol{X}_m)\right)} = \prod_{m=1}^{M}\frac{\exp\left(\beta_m E(\boldsymbol{X}_m)\right)}{\sum_{\boldsymbol{X}_m}\exp\left(\beta_m E(\boldsymbol{X}_m)\right)}. \tag{3}$$

We introduce two types of updating in constructing a Markov chain in the exchange MC. One is conventional updates that satisfy the detailed balance condition for each canonical distribution $P_{\mathrm{eq}}(\boldsymbol{X}_m, \beta_m)$. In addition to the usual local updates, we define a replica exchange between two replicas, *i.e.,* $\{\boldsymbol{X}_m, \boldsymbol{X}_n\} \rightarrow$

[1] E-mail: hukusima@phys.c.u-tokyo.ac.jp

$\{\boldsymbol{X}_n, \boldsymbol{X}_m\}$. The replica exchange part of transition probability $W(\boldsymbol{X}, \boldsymbol{X}'; \beta_m, \beta_n)$ is determined by the detailed balance condition for the simultaneous distribution (3) and is obtained as

$$W(\boldsymbol{X}, \boldsymbol{X}'; \beta_m, \beta_n) = \begin{cases} \min\left(1, \exp(-\Delta)\right), & \text{for Metropolis type,} \\ \frac{1}{2}\left(1 + \tanh(-\frac{\Delta}{2})\right), & \text{for heat bath type,} \end{cases} \tag{4}$$

where

$$\Delta(\boldsymbol{X}, \boldsymbol{X}'; \beta_m, \beta_n) = (\beta_n - \beta_m)(E(\boldsymbol{X}) - E(\boldsymbol{X}')). \tag{5}$$

Note that the simultaneous distribution of Eq. (3) is invariant under these updates. In the actual MC procedure, the following two steps are performed alternately:

(1) Each replica is simulated *simultaneously* and *independently* as canonical ensemble for a few MC steps by using a standard MC method.

(2) Exchange of two configurations $\boldsymbol{X}_m$ and $\boldsymbol{X}_{m+1}$, is tried and accepted with the probability (4).

Here we restrict the exchange processes to the case $n = m + 1$ because the acceptance ratio of the exchange trial decreases exponentially with the difference $|\beta_m - \beta_n|$ as shown in (4). By these processes each configuration can traverse along the temperature axis while it changes itself by the above process (1)(see Fig. 1). Consequently, slow relaxation at low temperatures is reduced by mixing of the fast relaxation at higher temperatures.

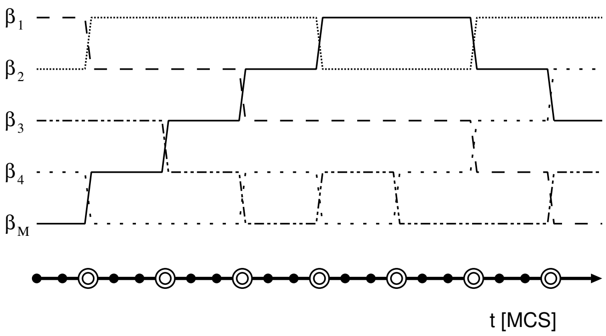


Figure 1: A schematic picture of the exchange MC method. Each line represents a configuration $\boldsymbol{X}_m(t)$ which is attached to the $m$-th heat-bath at $t = 0$. They are simulated by the standard MC method at times denoted by $\bullet$, and the exchange processes are tried at times denoted by $\circledcirc$.

The extended ensemble methods such as the multicanonical method and the exchange MC commonly have a set of parameters which should be learned in preliminary runs. They are the parameters $\alpha_E$ and $\beta_E$ in the multicanonical method and the values of temperatures $\{\beta_m\}$ of replicas in the exchange MC. In the learning stage of the exchange MC, we can easily determine the parameter through a step-by-step way. This is one of the major advantages over the other extended ensemble methods. We also discuss how to check equilibration of the system by the extended ensemble method in a practical way.

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