An irreversible Markov-chain Monte Carlo method with skew detailed balance conditions

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Abstract. An irreversible Markov-chain Monte Carlo (MCMC) method based on a skew
detailed balance condition is discussed. Some recent theoretical works concerned with the
irreversible MCMC method are reviewed and the irreversible Metropolis-Hastings algorithm
for the method is described. We apply the method to ferromagnetic Ising models in two and
three dimensions. Relaxation dynamics of the order parameter and the dynamical exponent
are studied in comparison to those with the conventional reversible MCMC method with the
detailed balance condition. We also examine how the efficiency of exchange Monte Carlo method
is affected by the combined use of the irreversible MCMC method.

1. Introduction
Since Metropolis algorithm was introduced in 1953 [1], Monte Carlo (MC) methods have been
used intensively in a wide area of physics [2], biology and statistical sciences [3, 4]. Most of
the MC methods in statistical physics are on the basis of 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
are mainly categorized into two directions, i.e., non-local updating methods such as cluster
algorithm [5, 6] and extended ensemble methods [7]. Typical examples of the latter are the
multicanonical method [8], the simulated tempering [9] and the exchange MC method [10] or
parallel tempering. These methods have been applied to various complex systems, e.g. protein
folding problems and spin glasses, and turned out to be quite useful for simulating these systems.

These Markov-chain Monte Carlo (MCMC) methods have been developed within the
framework of the detailed balance condition (DBC). It is, however, not always necessary to
construct the MCMC method using DBC. In fact, some MCMC methods without DBC have
recently been proposed [11, 12, 13] and have attracted a great deal of attention as an alternative
direction of the development of the MCMC method. Suwa and Todo [11, 14] have proposed
a general constructing way for the MCMC method without DBC and have showed that the
proposed method is able to bring about several times reduction in the correlation time of Potts
model [15]. Turitsyn et al. [12] and Fernandes and Weigel [13] have proposed another type of
MCMC method without DBC separately and they have found a qualitative improvement in
efficiency of the MCMC method in a mean-field Ising model. While Peskun’s theorem [16] gives
a useful guiding principle for constructing an efficient MCMC method with DBC, no such a
principle has been established in the case of the MCMC method without DBC. Therefore, it would be worth investigating the MCMC method without DBC in some model systems.

In the present paper, we pay our attention to an irreversible MCMC method, particularly with a skew detailed balance condition (SDBC) [12]. We make a review on the method in which its basic idea and an implementation of the algorithm are described. We also present our numerical results applying the irreversible MCMC method with SDBC to Ising models in two- and three dimensions.

2. An irreversible Markov-chain Monte Carlo algorithm

2.1. Irreversible MCMC and skew detailed balance conditions

In this section, we review an irreversible Markov-chain Monte Carlo method based on the skew detailed balance condition originally proposed by Turitsyn, Chertkov and Vucelja [12] in 2011.

In the present paper, we focus our attention to \( N \) Ising spin systems for simplicity, although it is straightforward to extend the method to any discrete state models [17] such as the Potts model [15]. A state of the Ising model is specified by a vector \( \sigma = (\sigma_1, \ldots, \sigma_N) \) with \( \sigma_j \in \{-1, +1\} \) for \( j = 1, \ldots, N \). The target distribution \( \pi(\sigma) \) for finding the state \( \sigma \) in the statistical physics is often proportional to the Boltzmann factor \( \exp(-\beta \mathcal{H}(\sigma)) \) where \( \beta \) is an inverse temperature and \( \mathcal{H} \) is the Hamiltonian to be studied. The main aims of the MCMC methods are to generate samples of the state from the target distribution \( \pi(\sigma) \), and to calculate an expectation value of a function \( \hat{f} \) under the target distribution, e.g. \( \langle \hat{f} \rangle_\pi = \sum_\sigma \pi(\sigma) \hat{f}(\sigma) \) where \( f(\sigma) \) is the realization of \( \hat{f} \) with the state \( \sigma \) and \( \sum_\sigma \) denotes the summation over \( 2^N \) states.

In order to utilize the irreversible MCMC scheme by the SDBC, the state space is doubled by introducing an additional Ising variable \( \epsilon \in \{-1, +1\} \). The state in the enlarged state space is denoted by \( X = (\sigma, \epsilon) \in \{-1, +1\}^{N+1} \) and the corresponding probability distribution \( \tilde{\pi} \) is assumed to be independent of the additional Ising spin \( \epsilon \):

\[
\tilde{\pi}(\sigma, \epsilon) = \pi(\sigma, -\epsilon) = \frac{\pi(\sigma)}{2}. \tag{1}
\]

We consider a single spin-flip update for both the original spin \( \sigma \) and the additional spin \( \epsilon \) as an elementary process in the Markov chain. Let \( F_j \) be a spin-flip operator on the \( j \)-th site: \( F_j \sigma = (\sigma_1, \ldots, -\sigma_j, \ldots, \sigma_N) \) A transition rate per unit time from state \( (\sigma, \epsilon) \) to \( (F_j \sigma, \epsilon) \) is denoted as \( w_j(\sigma, \epsilon) \) and that from \( (\sigma, \epsilon) \) to \( (\sigma, -\epsilon) \) is \( \lambda(\sigma, \epsilon) \). Using these transition rates, balance condition (BC) is expressed as

\[
\sum_j w_j(F_j \sigma, \epsilon) \tilde{\pi}(F_j \sigma, \epsilon) - \sum_j w_j(\sigma, \epsilon) \tilde{\pi}(\sigma, \epsilon) + \lambda(\sigma, -\epsilon) \tilde{\pi}(\sigma, -\epsilon) - \lambda(\sigma, \epsilon) \tilde{\pi}(\sigma, \epsilon) = 0. \tag{2}
\]

This ensures that \( \tilde{\pi} \) is the unique invariant distribution of the Markov chain. In order to determine the transition rate \( w_j(\sigma, \epsilon) \), we impose the SDBC:

\[
\tilde{\pi}(\sigma, \epsilon) w_j(\sigma, \epsilon) = \tilde{\pi}(F_j \sigma, -\epsilon) w_j(F_j \sigma, -\epsilon). \tag{3}
\]

This requires that the stochastic flow from state \( (\sigma, +\epsilon) \) to \( (F_j \sigma, +\epsilon) \) is balanced out by that from \( (F_j \sigma, -\epsilon) \) to \( (\sigma, -\epsilon) \). In general, this condition breaks the detailed balance conditions (DBC): \( \tilde{\pi}(\sigma, \epsilon) w_j(\sigma, \epsilon) = \tilde{\pi}(F_j \sigma, \epsilon) w_j(F_j \sigma, \epsilon) \). As a specific solution of (3), the transition rate \( w_j(\sigma, \epsilon) \) we use throughout the present work is given by

\[
w_j(\sigma, \epsilon) = \frac{1}{2} \alpha (1 - \sigma_j \tanh \beta h_j) (1 - \delta \epsilon \sigma_j), \tag{4}
\]
where $\alpha$ is a time constant and $h_j$ is a local field acting on the site $j$. The possible range of $\delta$ is $-1$ to $1$ and DBC is recovered in (4) with $\delta = 0$. The transition rate is equivalent to the conventional heat-bath transition rate under the virtual external field $\epsilon H$ with $H = \frac{1}{\delta} \text{arctanh} \delta$. Thus, the additional spin $\epsilon$ represents the direction of the virtual field. While the additional spin $\epsilon$ is coupled to the local order parameter $\sigma_j$ in this transition rate, one can replace it with any other linear function of $\sigma_j$ such as a local energy $\sigma_j h_j$. The choice of the transition rate might affect the efficiency of the MCMC method, depending on the model system to be studied, but this has not been clarified yet.

By using SDBC, BC is rewritten as

$$\lambda(\sigma, \epsilon) = \sum_j (w_j(\sigma, -\epsilon) - w_j(\sigma, \epsilon)).$$

The explicit form of the transition rate for $\epsilon$ flip is not unique. Turitsyn et al. [12] have proposed the transition rate as

$$\lambda(\sigma, \epsilon) = \max \left(0, \sum_j (w_j(\sigma, -\epsilon) - w_j(\sigma, \epsilon))\right),$$

which is referred to as the Turitsyn-Chertkov-Vucelja (TCV) type. Another type of $\lambda(\sigma, \epsilon)$ is also given as

$$\lambda(\sigma, \epsilon) = \sum_j w_j(\sigma, -\epsilon),$$

which is referred to as the Sakai-Hukushima 1 (SH$_1$) type [18]. These transition rates are available for a general class of the Ising models.

### 2.2. Irreversible Metropolis-Hastings algorithm

In this subsection, we explain an actual procedure in MCMC simulations which is based on Metropolis-Hastings algorithm [19]. Let $X^{(n)}$ be the state in the enlarged state space after $n$ iterations. The irreversible MCMC method starts with an arbitrary initial state $X^{(0)}$ and iterates the following steps for $n = 1, 2, \ldots$:

(a) Suppose that the current state $X^{(n)} = (\sigma, \epsilon)$ and choose a site $j$ at random.

(b) Accept the new state as $X^{(n+1)} = (F_j \sigma, \epsilon)$ with the probability $w_j(\sigma, \epsilon)$.

(c) If it is rejected, accept the $\epsilon$ flipped state as $X^{(n+1)} = (\sigma, -\epsilon)$ with an acceptance rate

$$A(\epsilon \rightarrow -\epsilon; \sigma) = \frac{1}{N} \frac{\lambda(\sigma, \epsilon)}{\sum_j w_j(\sigma, \epsilon)}. \quad (8)$$

(d) If it is also rejected, set $X^{(n+1)} = X^{(n)}$. Return to (a) and repeat the steps (a)–(d).

It is proved that these steps satisfy the BC [17]. One MC step is defined as $N$ iterations of the steps (a)–(d). To evaluate the acceptance rate in step (c), the summation with respect to the site is necessary and its computational complexity is of the order of $N$. In practice, once the summation is evaluated at the initial condition, it is sufficient to update the value of the summation when the spin-flip process is accepted. The complexity for the update is of the order of 1 in statistical-mechanical models with short range interactions.
2.3. Irreversible Glauber dynamics in one-dimensional Ising model

Although the MCMC methods are powerful simulation tools, it is helpful to understand analytically dynamical properties of the Markov chain in a large probabilistic model in statistical mechanics. A kinetic Ising model [20] in one dimension is a simplest model, exactly solved in the case of Markov-chain dynamics with DBC [21]. The correlation length $\xi$ of the one-dimensional Ising model is given by $\xi(\beta) = -\log(\tanh(\beta J))^{-1}$, which diverges at zero temperature. Time evolution of the order parameter and also its autocorrelation function exhibit an exponential decay in the model [21]. The relaxation time is obtained as $\tau \propto (1 - \tanh 2\beta J)^{-1}$. For $\beta \to \infty$, a dynamical scaling relation, $\tau \sim \xi^z$, holds with the dynamical exponent $z = 2$.

Recently, the kinetic Ising model under an irreversible Markov chain with SDBC has been studied [18]. For the SH$_1$ type transition rate of (7), the magnetization relaxation is solved and then the relaxation time is exactly obtained as

$$\tau \propto \frac{1}{(1 + \delta^2)(1 - \gamma)}, \quad (9)$$

with $\gamma = \tanh 2\beta J$, meaning that the reduction in the relaxation time from DBC is constant $1 + \delta^2$.

Another transition rate for the $\epsilon$ flip specific to the one-dimensional Ising model is proposed as

$$\lambda(\sigma, \epsilon) = \frac{1}{2} \alpha \delta (1 - \tanh 2\beta J)(1 + \frac{\epsilon}{N} \sum \sigma_i), \quad (10)$$

which is called as SH$_2$ type [18]. The transition rate combined with (4) also satisfies BC. Under a plausible assumption which is valid in the vicinity of the equilibrium state, the time evolution of the order parameter is also solved and its relaxation time is obtained as

$$\tau \propto \frac{1}{1 - \gamma + \delta \sqrt{1 - \gamma^2}}, \quad (11)$$

which implies that $z$ is down to 1. The result analytically showed that the specific choice of the irreversible transition rate is able to change the dynamical critical phenomena drastically.

3. Numerical results

In this section we present some numerical results obtained from applications of the irreversible MCMC method with SDBC explained in the previous section to some Ising models in high dimensions. The model Hamiltonian is given as

$$\mathcal{H}(\sigma) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j, \quad (12)$$

where spins are defined on the sites of a square lattice in two dimensions and of a cubic lattice in three dimensions. The summation is over all the nearest-neighbor pairs in the lattice and the periodic boundary condition is imposed in all directions. The strength $J$ is set to the unit of temperature.

We measure the relaxation of order parameter

$$m(t) = \langle \hat{m} \rangle_t, \quad (13)$$

where $\hat{m} = \frac{1}{N} \sum_{\epsilon} \sigma_i$ and $\langle \cdots \rangle_t$ denotes a dynamical average at the MC step $t$ starting from an initial condition. At the initial state with $t = 0$, all the spins are fixed to $+1$ and spin $\epsilon$ takes $\pm 1$ at random. It is argued that the transition rate of the SH$_1$ type reduces only the time constant of the magnetization relaxation in general Ising models in comparison to that of the reversible MCMC method with DBC [18]. As a nontrivial example, we use the transition rate of the TCV type with $\alpha = 1/(1 + \delta)$ and the parameter $\delta$ in (4) is set to 0.9.
3.1. Dynamical exponent in irreversible MCMC

Recent numerical studies have suggested that an irreversible MCMC method is able to reduce the dynamical exponent \( z \) of a mean-field Ising model \([12, 13]\). Further, as discussed in section 2.3, it is analytically shown in the one-dimensional Ising model that a specific type of the transition rate satisfying SDBC changes the value of \( z \) from 2 as in DBC to 1. This is the changeover from diffusive to ballistic relaxation of the order parameter. However, the irreversible MCMC method does not always make such a changeover. In fact, the transition rate of the SH\( _1 \) type for the \( \epsilon \) flip reduces only a finite factor in the relaxation time independent of temperature, but not the dynamical exponent.

In this subsection, we study the dynamical exponent of the Ising model in two and three dimensions by performing the irreversible MCMC method with SDBC explained above. A standard way for evaluating the value of \( z \) is to estimate the autocorrelation time \( \tau \) for different sizes \( L \) at the critical temperature and to fit to the power-law formula as \( \tau \sim L^z \). We use here a simpler method called non-equilibrium relaxation method \([22]\), which is another tool for evaluating the critical exponents through a dynamical process from a non-equilibrium initial state to the equilibrium one. According to the non-equilibrium relaxation method, it is sufficient to measure a dimensionless quantity

\[
 f_{mm}(t) = N \left[ \frac{\langle \hat{m}^2 \rangle_t}{\langle \hat{m} \rangle_t^2} - 1 \right],
\]

(14)

to determine the dynamical exponent. Assuming the dynamical scaling ansatz for \( \langle \hat{m} \rangle_t \) and \( \langle \hat{m}^2 \rangle_t \), the function \( f_{mm}(t) \) is expected to exhibit power-law divergence in a large \( t \) limit at the critical temperature as \( f_{mm}(t) \sim t^{\lambda_{mm}} \). With the help of the hyper-scaling relation, the exponent \( \lambda_{mm} \) is expressed as \( d/z \) with \( d \) being the spatial dimensionality.

![Figure 1](image1.png)

**Figure 1.** MC-step dependence of the magnetization correlation function \( f_{mm}(t) \) at \( T = T_c \) of the Ising models in two (a) and three dimensions (b). The asymptotic slope of \( f_{mm}(t) \) provides an estimate of \( d/z \) where \( d \) is the spatial dimensionality and \( z \) the dynamical exponent. The data with DBC and SDBC are marked by open (red) and filled (blue) symbols, respectively.

Numerical results of \( f_{mm}(t) \) for two and three dimensions are presented in figure 1 (a) and (b), respectively. The system sizes studied are from \( L = 16 \) to 256 in two dimensions and from 8 to 128 in three dimensions. The asymptotic slope of \( f_{mm}(t) \) in the figure gives an estimate of \( d/z \). While finite-size effect is found for both DBC and SDBC, that for SDBC is relatively large. In two dimensions, the difference between them decreases in the large \( t \) behaviour with the system size increasing and eventually two limiting functions will merge into the same curve. Fitting
the slope gives $z = 2.095(75)$, which is consistent with the established estimate, $z_{2d} = 2.165(5)$, obtained by the reversible MCMC simulations [22]. In three dimensions, the envelope curve independent of the size has a different slope in the two methods within the observed time window. The estimated value from DBC simulation, $z = 2.019(25)$, is marginally consistent with the recent value $z_{3d} = 2.055(10)$ [22]. The gradual slope for SDBC gives an effective value of $z$ larger than that with DBC. This is presumably due to a non-asymptotic effect and the two estimates would coincide with each other asymptotically. Thus, no quantitative reduction of the dynamical exponent is achieved for the Ising model in both two and three dimensions by the present irreversible MCMC method with the TCV type. This is in contrast to the mean-field Ising model [12] and the one-dimensional Ising model with the SH$_2$ type [18].

### 3.2. Order-parameter relaxation in two-dimensional Ising model

In this subsection, we see relaxation dynamics of the magnetization at and off critical temperature. We show the magnetization $m(t)$ obtained with SDBC and DBC as a function of the MC step in the two-dimensional Ising model at $T = 2.4$ above $T_c$ (figure 2 (a)) and at $T = T_c = 2.2691...$ (figure 2 (b)). For relatively smaller $L$, $m(t)$ by SDBC decays faster than that by DBC at these temperatures. For example, in the case with $L = 8$, a time constant of $m(t)$ for SDBC is about 10 times shorter than that for DBC. However, the gain of SDBC decreases with increasing the size. While we still have a finite gain of SDBC at $T = 2.4$ even in the large $N$ limit, it disappears at $T_c$, which is consistent with no reduction of $z$ seen in the previous section. A similar behaviour is found below $T_c$ and also in the three-dimensional Ising model. This indicates that the efficiency of the irreversible MCMC method with the TCV type depends on temperature and it is enhanced at off-critical temperatures.

**Figure 2.** MC-step dependence of the averaged magnetization of the ferromagnetic Ising model in two dimensions at (a) $T/J = 2.4$ and (b) $T/J = 2.2691...$. The data with DBC and SDBC are marked by open (red) and filled (blue) symbols, respectively.

### 3.3. Efficiency of exchange Monte Carlo method with irreversible MCMC update

Since the extended ensemble MC methods have been applied to various problems, one may consider that the efficiency of the MC methods does not seriously depend on the local update scheme. The effect of the local update on the extended ensemble MC methods has not been extensively studied. Recently, it has been pointed out that the average round-trip time of the exchange MC method, which is an important factor in determining the efficiency, is reduced by an appropriate choice of frequency of the local update [23] and the use of efficient local update [24]. The latter case also improved significantly the performance of the Wang-Landau
method [25, 26]. We therefore study the efficiency of the exchange MC method when the irreversible MCMC method is used as the local update method.

In the exchange MC method, MCMC simulations for $M$ replicated Ising systems with different temperatures are performed by some local update method in parallel and an exchange process of states in the replicated systems is applied to every two replicas at adjacent temperatures. The model examined is the ferromagnetic Ising model in three dimensions. The number of replicas is fixed to 32 and the highest and the lowest temperatures are chosen as $4J$ and $7J$, respectively, between which the critical temperature lies. The intermediate temperatures are determined so that the acceptance ratio $p_{ac}$ of the exchange process is almost independent of temperature for the largest system size attained in this work, $N = 32^3$. The same set of temperatures is used in our simulations with two different local updates and for different sizes. An elementary time scale in the exchange MC method is characterized by the round-trip time, also called the ergodic time, which is defined by the average MC steps for each replica to move from the highest to the lowest temperatures and return to the highest one.

The acceptance ratio $p_{ac}$ with the conventional MCMC method with DBC and that with SDBC are shown as a function of temperature in figure 3. It is found that these two acceptance ratios completely coincide with each other for different temperatures and sizes, meaning that the local update scheme has no influence on the acceptance ratio of the exchange process. However, as shown in figure 4, there is some substantial difference in the round-trip time. Namely, the round-trip time in the MCMC method with SDBC is a few times smaller than that with DBC. This result shows that the irreversible MCMC method improves the efficiency of the exchange MC method at least for practical values of $N$, while it is not clear at present for an asymptotic large $N$.

![Figure 3](image1.png) **Figure 3.** Temperature dependence of the acceptance ratio $p_{ac}$ of the replica exchange process of the three-dimensional Ising model for $L = 4, 8, 16$ and 32. The data with DBC and SDBC are marked by open (red) and filled (blue) symbols, respectively.

![Figure 4](image2.png) **Figure 4.** Linear-size $L$ dependence of round-trip time in the exchange Monte Carlo method of the three-dimensional Ising model. The data with DBC and SDBC are denoted by squares and circles, respectively.

It may not be trivial that the round-trip time depends on the choice of the local update scheme in spite of the insensitivity of $p_{ac}$. In order to understand the reason for such a behaviour, we study a typical example of the exchange process as a function of the MC step. It is clearly seen in figure 5 (a) that a bottleneck in the replica move occurs around the critical temperature $T_c$ in the MCMC method with DBC. Although the exchange trial is accepted at around $T_c$, the replica coming across $T_c$ often goes back to the former temperature in the following few MC
steps. Thus, it takes a long round-trip time while the acceptance ratio \( p_{ac} \) is independent of temperature on average. In contrast, such a bottleneck phenomenon is not found in the MCMC method with SDBC.

Figure 5. Typical trajectory of temperature for a specific replica as a function of Monte Carlo step in the exchange Monte Carlo method of a three-dimensional Ising ferromagnetic model. A trajectory obtained by the MC method with DBC (a) and one by the MC method with SDBC (b) are shown. The system size examined in these simulations is \( 16^3 \). The dotted line represents the critical temperature, \( T_c \approx 4.51 \).

4. Summary
In the present paper, we have discussed an irreversible MCMC method with a skew detailed balance condition, which breaks the detailed balance condition used in conventional MCMC methods. The method is applied to some Ising models in dimensions more than one, which exhibit a finite-temperature phase transition. Although the method is able to reduce a correlation time in the Markov chain at off-critical temperature, unfortunately no significant reduction of the dynamical exponent is found, that is in sharp contrast to that observed in the mean-field Ising model and one-dimensional Ising chain. We also show that the efficiency of the exchange MC method is improved by the use of the irreversible MCMC method with SDBC as a local update scheme. At present, it is not well understood how the irreversible MCMC methods affect the dynamics of the Markov chain. Therefore, we consider that further theoretical studies are needed to clarify the efficiency of the irreversible MCMC methods.

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