Mixing and perfect sampling in one-dimensional particle systems

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Abstract – We study the approach to equilibrium of the event-chain Monte Carlo (ECMC) algorithm for the one-dimensional hard-sphere model. Using the connection to the coupon-collector problem, we prove that a specific version of this local irreversible Markov chain realizes perfect sampling in $O(N^2 \log N)$ single steps, whereas the reversible local Metropolis algorithm requires $O(N^3 \log N)$ single steps for mixing. This confirms a special case of an earlier conjecture about $O(N^2 \log N)$ scaling of mixing times of ECMC and of the lifted forward Metropolis algorithm, its discretized variant. We also prove that sequential ECMC (with swaps) realizes perfect sampling in $O(N^2)$ single events. Numerical simulations indicate a cross-over towards $O(N^2 \log N)$ mixing for the sequential forward swap Metropolis algorithm, that we introduce here. We point out open mathematical questions and possible applications of our findings to higher-dimensional models.

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Sampling, mixing, perfect sampling, stopping rules. – Ever since the 1950s [1], Markov-chain Monte Carlo (MCMC) methods have ranked among the most versatile approaches in scientific computing. Monte Carlo algorithms strive to sample a probability distribution $\pi$, for any initial distribution $\pi^{(0)}$. This program has met with considerable success in some models of statistical physics, as for example in the local Glauber dynamics in the two-dimensional Ising model [4,5].

The difference between two (normalized) probability distributions $\pi$ and $\tilde{\pi}$ can be quantified by the total variation distance (TVD) [6,7],

$$\|\tilde{\pi} - \pi\|_{TV} = \frac{1}{2} \int_\Omega |\tilde{\pi}(x) - \pi(x)| dx$$

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for any initial distribution \( \pi^{(0)} \). Although it is of great conceptual importance, the TVD cannot usually be computed. Because of this difficulty, practical simulations often carry systematic uncertainties that are difficult to quantify. Also, heuristic convergence criteria abound for the approach towards equilibrium in MCMC [3,8,9]. They most often involve time-correlation functions of observables, rather than the probability distribution itself (as in eqs. (1) and (3)).

In rare cases, MCMC algorithms allow for the definition of a stopping rule (based on the concept of a strong stationary time [6]), that yields a simulation-dependent time \( t_{\text{ex}} \) at which the configuration is sampled exactly from the distribution \( \pi \). The value of \( t_{\text{ex}} \) depends on the realization of the Markov chain (that is, the sampled moves and, ultimately, the drawn random numbers). Nevertheless, the distribution of \( t_{\text{ex}} \) has an exponential tail, so the overall TVD still decays exponentially. For example, to randomize the configuration of \( N \) coins, at each time a random coin may be picked up and tossed with equal probability on either face. The time \( t_{\text{ex}} \) is when each coin was tossed at least once so that the reached configuration is exactly random. This example is equivalent to the “coupon-collector” problem for a model of \( N \) coupons. Now, at each time, one random coupon is marked. At the “coupon-collector” time, \( t_{\text{ex}} \), all the coupons have been marked. This problem will be discussed in detail later. The time \( t_{\text{ex}} \) is related to the mixing time [6]. Stopping rules exist for quite intricate models, as for the Ising model, using the coupling-from-the-past framework [3,10].

Most Markov-chain Monte Carlo algorithms are reversible: They satisfy the detailed-balance condition. Prominent examples are the Metropolis and the heat-bath algorithms [1,3]. In recent years, however, irreversible MCMC methods based on the global-balance condition have shown considerable promise [11–15]. In these algorithms, \( \pi^{(t)} \) approaches \( \pi \) for long times, but the net probability flow no longer vanishes. One of them, the event-chain Monte Carlo (ECMC) algorithm [13,14], has proven useful for systems ranging from hard-sphere models [16] to spin systems [17], polymers [18,19] and to long-range interacting ensembles of molecules, such as water [20], where the Coulomb interaction plays a dominant role [21]. However, no exact results were known for the mixing behavior of ECMC, except for the case of a single particle [22].

In the present paper, we rigorously establish ECMC mixing times and stopping rules of the model of \( N \) hard spheres on a one-dimensional line with periodic boundary conditions (a circle). Reversible MCMC algorithms for this model and its variants were analyzed rigorously [23,24] and irreversible MCMC algorithm were discussed in detail [15]. The 1D hard-sphere model and reversible and irreversible MCMC algorithms are closely related to the symmetric exclusion process (SEP) on a periodic lattice [25] and to the totally asymmetric simple exclusion process (TASEP) [26–28]. For ECMC, an algorithm that is closely related to the lifted Metropolis algorithm [15], we compute the TVD in a special case, and obtain the mixing times as a function of the parameter \( \epsilon \). We confirm the \( \mathcal{O}(N^2 \log N) \) single-step mixing time that had been conjectured on the basis of numerical simulations [15]. Furthermore, we obtain a stopping rule for ECMC. We moreover present sequential variants of the forward Metropolis algorithm and the ECMC algorithm. For the latter, we prove an \( \mathcal{O}(N^2) \) exact-sampling result that seems however not to generalize to the discretized version of the algorithm.

**Hard spheres in 1D, reversible Monte Carlo.** – The mixing and convergence behavior of Markov chains for particle systems has been much studied. For hard spheres in 2D and above, no rigorous results exist for the mixing times of local Markov chains. In the past, there was considerable controversy about the nature of the phase transition [16]. The mixing times of non-local MCMC algorithms could be clarified only at low densities [29,30]. We thus restrict our attention to the 1D hard-sphere model with periodic boundary conditions.

The 1D hard-sphere model can be represented as \( N \) spheres of diameter \( d \) on a line of length \( L \) with periodic boundary conditions (on a ring, see fig. 1(a)). A valid configuration \( a \) of \( N \) spheres has unit statistical weight \( \pi(a) = 1 \). Spheres do not overlap: The distance between sphere centers, and in particular between neighboring spheres, is larger than \( d \). Each configuration of \( N \) hard spheres is equivalent to a configuration of \( N \) point particles on a ring of length \( L_{\text{tsec}} = L - N d > 0 \) (see fig. 1(b)).

We only consider local Markov chains, where moves of sphere \( i \) are accepted or rejected based on the position of \( i \)'s neighbors only. To do so, we implement locality by rejecting a move of sphere \( i \) if the displacement would generate an overlap, but also if sphere \( i \) would hop over one of its neighbors. In this way, any local Monte Carlo move of spheres on a circle corresponds to an equivalent move in the point-particle representation (for which there are no overlaps and moves are rejected only because they represent a hop over a neighbor). The dynamics of both models is thus the same. In this paper, following [15], we count time steps in single displacements. This is more convenient because in our algorithms, new displacements build on previous ones (they form chains). Although we will study Markov chains that relabel spheres, we consider only...
the relaxation of quantities that can be expressed through the unlabeled distances between neighboring spheres. This excludes the mixing in permutation space of labels or the self-correlation of a given sphere with itself (or another labeled sphere) at different times.

Detailed balance consists in requiring

\[ \pi(a)p(a \to b) = \pi(b)p(b \to a), \]  

where \( p(a \to b) \) is the conditional probability to move from configuration \( a \) to configuration \( b \) and \( \pi(a)p(a \to b) \) is the equilibrium probability flow from \( a \) to \( b \). Equation (4) states that in equilibrium, the net probability flow between any two configurations vanishes. The heat-bath algorithm is a local reversible MCMC algorithm. At each time step, it replaces a sampled sphere \( i \) randomly in between its neighbors. The heat-bath algorithm mixes in at least \( O(N^3) \) and at most \( O(N^3 \log N) \) single steps [24]. Numerical simulations favor the latter possibility (\( O(N^3 \log N) \)) [15]. For the one-dimensional hard-sphere model on a line without periodic boundary condition, the mixing time of \( O(N^3 \log N) \) single steps (corresponding to \( O(N^2 \log N) \) “sweeps” of \( N \) steps) is rigorously proven [23].

Analogous to the heat-bath algorithm, the reversible Metropolis algorithm also satisfies the detailed-balance condition: At each time step, a randomly chosen sphere \( i \) attempts a move by \( \epsilon \) taken from some probability distribution. The move is rejected if the proposed displacement \( \epsilon \) is larger than the free space in the direction of the proposed move \( (x_i - x_i - d) \) for \( \epsilon > 0 \) or behind it \( (x_i - x_i - d) \) for \( \epsilon < 0 \) (we suppose that \( x_i \) is the right-hand-side neighbor of \( i \), etc., and imply periodic boundary conditions). In the point-particle model, the equivalent move is rejected if the particle would hop over one or more of its neighbors and is accepted otherwise. Rigorous results for mixing times are unknown for the Metropolis algorithm, but numerical simulations clearly identify mixing in \( O(N^3 \log N) \) single steps as for the heat-bath algorithm [15]. In the discrete 1D hard-sphere model on the circle with \( L \) sites and \( N \) particles, the Metropolis algorithm is implemented in the so-called simple exclusion process (SEP), where at each time step, a randomly chosen particle attempts to move with equal probability to each of its two adjacent sites. The move is rejected if that site is already occupied. The mixing time of the SEP is \( \sim (4\pi^2)^{-1}NL^2 \log N \) single steps (for \( L \geq 2N \)) [25].

From the forward Metropolis to the event-chain algorithm. – Irreversible Monte Carlo algorithms violate the detailed-balance condition of eq. (4) but instead satisfy the weaker global-balance condition

\[ \sum_b \pi(b)p(b \to a) = \pi(a). \]  

Together with the easily satisfiable aperiodicity and irreducibility conditions [6], the global-balance condition ensures that the steady-state solution corresponds to the probability \( \pi \), but without necessarily cancelling the net probability flow \( \pi(a)p(a \to b) - \pi(b)p(b \to a) \) between configurations \( a \) and \( b \) (cf. eq. (4)). Here, we take up the forward Metropolis algorithm studied earlier, in a new variant that involves swaps. This allows us to arrive at an exact mixing result.

In the forward swap Metropolis algorithm\(^1\), at each time step, a randomly chosen sphere \( i \) attempts to move by a random displacement \( \epsilon \) with a predefined sign (that for clarity, we take to be positive). If the move is rejected (the displacement \( \epsilon \) does not yield a valid hard-sphere configuration), the sphere swaps its label with the sphere responsible for the rejection (see the upper move in fig. 2). Else, if the displacement \( \epsilon \) is accepted, the sphere \( i \) simply moves forward (see the lower move in fig. 2). The total probability flow into a configuration \((a, i)\) (that is, the \( N \)-sphere configuration \( a \) with the active sphere \( i \)) is

\[ F(a, i) = \int_0^\infty d\epsilon \rho(\epsilon) [A_i(a, i) + R_i(a, i)] = 1 = \pi(a), \]  

so that the algorithm satisfies global balance. The swap allows both the rejected and the accepted moves into the configuration \((a, i)\) to involve the sphere \( i \) only. The forward swap Metropolis algorithm is equivalent (up to relabeling) to the forward Metropolis algorithm treated earlier if at each time step the active sphere \( i \) is sampled randomly (see fig. 3). The mixing time of this algorithm was conjectured to be \( O(N^{5/2}) \) single steps, based on numerical simulations [15]. This agrees with the proven mixing-time scale of the totally asymmetric simple exclusion process (TASEP) [28].

The forward swap Metropolis algorithm satisfies global balance for any choice of the sphere \( i \) and any step-size distribution \( \rho(\epsilon) \). This implies that the active-sphere index \( i \) need not be sampled randomly for the algorithm to remain valid. This distinguishes it from the forward Metropolis algorithm (without the swaps) treated in previous work [15]. In particular, the sphere \( i \) remains active

\[^1\text{The forward Metropolis algorithm introduced earlier [15] did not feature swaps.}\]

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spheres: the active particle. This situation will now be analyzed in terms of the coupon-collector problem (see [31,32]).

For the ECMC with $\ell \sim \text{unif}(0, L_{\text{free}})$, the TVD can be expressed by the probability that at least one particle has never been picked as an active particle of a chain. Without restriction, we suppose that the initial configuration is the compact state $x = \{0, 0, \ldots, 0\}$. We also measure time in the number of chains $n$ (which means $t(n) = (\ell/L_{\text{free}})Nn$ number of events). In eq. (3), the set $\mathcal{A}$ is

$$\mathcal{A} = \{x \mid \exists i \text{ with } x_i = 0\}. \quad (8)$$

Also, clearly, $\pi^{(n)}(\mathcal{A})$ equals the probability that at least one particle has never been picked as an active particle of a chain, whereas $\pi(\mathcal{A}) = 0$, as it is a lower-dimensional subset of $\Omega$. This then becomes the coupon-collector problem introduced before. The expected time to have them all marked at least once is

$$\langle n_1 \rangle = NH_N = N \log N + \gamma N + \frac{1}{2} + O(1/N), \quad (9)$$

where $H_N = \frac{1}{1} + \frac{1}{2} + \cdots + \frac{1}{N}$ is the $N$-th harmonic number and $\gamma = 0.5772\ldots$ is the Euler-Mascheroni constant. The tail distribution (the probability that the complete-collection time $n_1$ is larger than a given time $T = N \log N + cN$) is smaller than the sum of probabilities for each single coupon to not have been marked from the beginning:

$$P(n_1 > N \log N + cN) \sim N(1 - \frac{1}{N})^{N(\log N + c)} = N \exp(- \log N - c) = \exp(-c). \quad (10)$$

The naive estimation of eq. (10) was improved [31] by removing the intersection of events:

$$P(n_1 < N \log N + cN) \sim \exp[\exp(-c)]. \quad (11)$$

This can be generalized to multiple complete collections (see eq. (14) and fig. 4).

From eqs. (1), (3), and (11), we obtain, for $N \to \infty$,

$$||\pi^{(n)} - \pi||_{\text{TV}} \sim 1 - \exp\left(-\exp\left(-\frac{n - \log N}{N}\right)\right). \quad (12)$$

Rather than computing the difference between $\pi^{(n)}$ and $\pi$ at a fixed number $n$ of chains, one can simply run ECMC (with $\ell \sim \text{unif}(0, L_{\text{free}})$) until the time $t_{\text{ex}}$ at which chains with all of the $N$ particles as active ones have completed. The expected number of chains is given by eq. (9), and in both ways, we see that mixing takes place after $O(N \log N)$ chains (corresponding to $O(N^2 \log N)$ single events), confirming, for a special distribution of $\ell$, an earlier conjecture [15]. The discussed mixing behavior of ECMC can more generally be obtained for distributions $\ell \sim \text{unif}(c, c + L_{\text{free}})$ with arbitrary (and even with negative) $c$. In our special case, choosing $c = -L_{\text{free}}/2$ would lead to the smallest number of individual events. In view
of the practical applications of ECMC, it appears important to understand whether this dependence on the distribution of $\ell$ (rather than on its mean value) has some relevance for the simulation of discrete 1D models, and whether it survives in higher dimensions, and for continuous (non-hard-sphere) potentials.

We next consider more general distributions, namely the uniform distribution $\ell \sim \text{unif}(0, \lambda L_{\text{free}})$, as well as the Gaussian distribution $N(\mu, \sigma^2)$, where $\mu$ is the mean value and $\sigma$ the standard deviation. Again, particles are effectively independent and we conjecture the mixing time (which can now never lead to perfect sampling) to be governed by the particle which has moved the least number, $m$, of times. This is equivalent to the generalization of $m$-complete-collection in the coupon-collector problem [31], whose tail probability is given by

$$P(n_m < T) \sim \exp(-\Upsilon/(m-1)!).$$

with

$$\Upsilon = \exp\left[\frac{T-N\log N - (m-1)N\log\log N}{N}\right].$$

(see fig. 4). This means that the number of chains to collect each of the $N$ coupons at least $m$ times only adds an $N\log\log N$ correction to the general $N\log N$ scale of chains.

To gain intuition about the general mixing process with an arbitrary distribution of the chain length, we now compute the TVD for the single-particle problem (for which $\ell \equiv \epsilon$). For simplicity, we set $L_{\text{free}} = 1$ (measure the displacements in units of $L_{\text{free}}$). Because of periodic boundary conditions, particle positions $x$ are defined only modulo 1. Its probability distribution after $m$ chains is therefore given by the sum over the different windings $k$:

$$p_m^{(m)}(x) = \sum_{k=\infty}^{\infty} p_m(x+k),$$

where $p_m(x)$ is the distribution of the sum of $m$ chain lengths. The TVD for chain lengths $\ell_i \sim \text{unif}(0,\lambda)$, as discussed, equals the one for $\ell_i \sim \text{unif}(-\lambda/2,\lambda/2)$. $p_m^{(m)}(x)$ then follows the distribution using the characteristic function:

$$p_m^{\text{unif}}(x) = \int_{-\infty}^{\infty} dt e^{-2\pi tx} \left[\frac{\sin(\pi \lambda t)}{\pi \lambda t}\right]^m.$$

(16)

Using the Poisson summation formula and subtracting the equilibrium distribution $\pi(x) = 1$, we find

$$\sum_{k=-\infty}^{\infty} p_m^{\text{unif}}(x+k) = \sum_{k \in \mathbb{N}^+} 2 \left[\frac{\sin(\pi k \lambda)}{\pi k \lambda}\right]^m \cos(2\pi k x).$$

The TVD for chain lengths $\ell_i \sim \text{unif}(0,\lambda)$ thus satisfies

$$\|\pi^{(m)} - \pi\|_{\text{TV}} = \int_0^1 dx \left|\sum_{k \in \mathbb{N}^+} \left[\frac{\sin(\pi k \lambda)}{\pi k \lambda}\right]^m \cos(2\pi k x)\right| \sim \frac{2}{\pi} \left[\frac{\sin(\pi \lambda)}{\pi \lambda}\right]^m$$

(17)

(for $m \to \infty$).

The TVD trivially vanishes for integer $\lambda$ (see fig. 5(a)). Its peaks decay as $\frac{2}{\pi} \left[\frac{\sin(\pi \lambda)}{\pi \lambda}\right]^{-m}$.

For Gaussian-distributed chain lengths $\ell_i \sim N(\mu, \sigma^2)$, the sum of $m$ chains is distributed as

$$\sum_{i=1}^{m} \ell_i \sim N(m\mu, m\sigma^2).$$

(18)

With $\vartheta_3$ the Jacobi theta function, we now have

$$\sum_{k=-\infty}^{\infty} p_m^{\text{Gauss}}(x+k) - 1 = \vartheta_3\left[\pi(x+\mu), e^{-2\pi^2 m\sigma^2}\right] - 1 = 2 \sum_{k=1}^{\infty} \exp(-2k^2\pi^2 m\sigma^2) \cos(2k\pi x).$$

(19)

The TVD for the distribution of eq. (18) satisfies

$$\|\pi^{(m)} - \pi\|_{\text{TV}} = \int_0^1 dx \left|\sum_{k=1}^{\infty} \exp(-2k^2\pi^2 m\sigma^2) \cos(2k\pi x)\right| \sim \frac{2}{\pi} \exp(-2\pi^2 m\sigma^2)$$

(20)

(for $m\sigma^2 \to \infty$).
Chain lengths are through five chains with active sphere 1 and for small $N$ algorithm (with swaps). Configurations

Fig. 6: (Color online) Sequential lifted forward Metropolis algorithm (with swaps). Configurations $x_i, \ldots, x_{i+13}$ sampled through five chains with active sphere 1, 2, \ldots, 5 are shown. Chain lengths are $l_1 = 3, \ldots, l_5 = 2$. Each sphere displacement $\epsilon_i > 0$ is either accepted or, if rejected, it induces a swap, so that the same sphere remains active throughout a chain.

Both for the uniform and the Gaussian distribution, the single-sphere TVD decreases exponentially with the number $m$ of displacements (which are equivalent to single-particle chains). We expect the same behavior for the $N$-sphere problem, where $m$ is now the number of chains for the $m$-complete-collection problem.

**Sequential forward Metropolis, sequential ECMC.** – ECMC, with randomly sampled initial spheres and a standard deviation of the chain-length distribution $\sigma \sim L_{\text{free}}$, mixes in $O(N^2 \log N)$ events (corresponding to $O(N \log N)$ chains). In the label-switching framework of ECMC, each chain consists in advancing the particle $i$ by a distance $\ell$ times, and both the ECMC and the forward Metropolis versions are correct. Instead of sampling the active sphere for each chain, so that the coupon-collector aspect necessarily brings in the log $N$ factor in the scaling of mixing times, we may also sequentially increment the active-sphere index for each chain (see fig. 6):

\[ \ldots, i, i + 1, \ldots, i + 1, i + 2, \ldots, i + 2, \ldots, \]  

(\text{where particle numbers are implied modulo } N). Sequential ECMC, with a distribution $\ell_i \sim \text{unif}(0, L_{\text{free}})$ produces an exact sample in $O(N^2)$ events (corresponding to exactly $N$ chains).

Evidently, the analysis of eqs. (17) and (20) can be applied to the sequential ECMC with distributions such as $\text{unif}(0, \lambda L_{\text{free}})$ and, more generally, distributions with $\sigma \sim L_{\text{free}}$. After each “sweep” of chains, the TVD factorizes, and we expect mixing to take place after $O(N)$ chains (corresponding to $O(N^2)$ events).

ECMC is the limit of the lifted forward Metropolis algorithm, and the sequential ECMC the limit of the sequential lifted forward Metropolis algorithm for step sizes much smaller than the mean free space between spheres ($\langle \epsilon \rangle = L_{\text{free}}/(2N\alpha)$ with $\alpha \gg 1$). For a given discretization $2/\alpha$, and for small $N$, the sequential lifted forward algorithm mimics the $O(N^2)$ mixing of the sequential ECMC, but for large $N$, it seems to cross over into $O(N^2 \log N)$ mixing (see fig. 7(a)). $O(N^2)$ mixing also emerges at fixed $N$ for large $\alpha$ (see fig. 7(b)). (This is obtained using the heuristic mid-system variance $x_i^{N/2} = x_i$ for ordered $x_i$, see [15].) In contrast, the random lifted forward Metropolis algorithm shows $O(N^2 \log N)$ mixing (see fig. 7(c), as discussed earlier [15]. This scaling is little influenced by the discretization (see fig. 7(d)). It thus appears that the $N \to \infty$ limit of the sequential lifted forward Metropolis algorithm does not commute with the small-discretization limit $\alpha \to \infty$.

**Conclusions.** – In this paper we have proven that for 1D hard spheres, ECMC with a uniform distribution of chain length $\ell \sim [0, L_{\text{free}}]$ with $L_{\text{free}} = L - N\lambda$ realizes a perfect sample in $O(N^2 \log N)$ single steps (events) that correspond to $O(N \log N)$ chains. This confirms, in a special case, an earlier conjecture [15] for the mixing time of ECMC. This also proves that ECMC can be much faster than local reversible Monte Carlo algorithms. We computed the TVD but also indicated a stopping rule for the time $t_{\text{stop}}$ after which the configuration is exactly in equilibrium. We have also provided numerical evidence that the $N^2 \log N$ mixing prevails for other distributions of $\ell$, namely for the uniform distribution $\text{unif}(0, \lambda L_{\text{free}})$ and the Gaussian, and used the coupon-collector problem to justify this approximation. We have furthermore discussed a sequential ECMC algorithm which mixes in $O(N^2)$ events.
This algorithm uses “particle swaps”, but it remains local. The discrete version of this algorithm (the sequential lifted forward Metropolis algorithm) crosses over, for large $N$, to $O(N^2 \log N)$ mixing.

The lessons from our analysis of 1D hard-sphere systems are threefold. First, irreversible Markov chains can be proven to mix on shorter time scales than reversible algorithms. Second, the speed of ECMC was proven to depend on the whole distribution of the chain lengths $\ell$, but to be independent of its mean value. Third, sequential-update algorithms (that remain valid in higher dimensions) can be shown to mix on faster time scales than random-update versions. It will be important to understand whether the design and the analysis of ECMC algorithms in higher-dimensional particle models will be influenced by these lessons, that were overlooked in all previous work on ECMC.

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