A splitting Hamiltonian Monte Carlo method for efficient sampling

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March 18, 2022

Abstract

We propose a splitting Hamiltonian Monte Carlo (SHMC) algorithm, which can be numerically and computationally efficient when combined with the random mini-batch strategy. By splitting the “effective potential energy” $U \propto -\beta^{-1} \log \rho$ into two parts $U = U_1 + U_2$, one makes a proposal using the “easy-to-sample” part $U_1$, followed by probabilistically accepting that proposal by a Metropolis rejection step using $U_2$. The splitting allows efficient sampling from systems with singular potentials (or distributions with degenerate points) and/or with multiple potential barriers. In our SHMC algorithm, the proposal using $U_1$ is generated by the Hamiltonian dynamics, which can be potentially more efficient than the overdamped Langevin dynamics. We also use random batch strategies to reduce the computational cost to $O(1)$ per time step in generating the proposals for problems arising from many-body systems and Bayesian inference, and prove that the errors of the Hamiltonian induced by the random batch approximation is $O(\sqrt{\Delta t})$ in the strong and $O(\Delta t)$ in the weak sense, where $\Delta t$ is the time step. Numerical experiments are conducted to verify the theoretical results and the computational efficiency of the proposed algorithms in practice.

1 Introduction

Markov chain Monte Carlo (MCMC) \cite{50, 44, 25, 20, 54, 4} methods are nowadays routinely used in a variety of scientific computing problems, including computing statistics for many-body systems \cite{1, 19}, sampling from log-concave distributions \cite{40, 11, 36, 9}, parameter estimation in Bayesian statistics \cite{20, 2, 23, 53} and Bayesian inverse problems \cite{22, 47}, just to name a few. Among MCMC methods, Hamiltonian Monte Carlo (HMC) \cite{14, 46, 7, 3} has recently garnered a lot of attention in practice due to its scalability and efficiency in high-dimension settings \cite{46, 6}. Nonetheless, there are several situations where HMC can encounter difficulties. The first such scenario might be sampling from the Gibbs distribution

$$
\mu(q) = \frac{1}{Z} \exp \left[ -\frac{1}{k_B T} U(q) \right]
$$

of a many-body interacting particle system, in which case computing the total potential energy

$$
U(q) = \sum_{i=1}^{N} w_i V(q_i) + \sum_{i,j:i<j} w_i w_j \phi(q_i - q_j),
$$

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takes $O(N^2)$ operations, where $q_i \in \mathbb{R}^d$ is the position of the $i^{th}$ particle and $w_i$ denotes the weight. If one moves one particle per step, which is preferred in some applications [19, 39, 13], the computational costs of evolving the Hamiltonian dynamics and the Metropolis-Hastings correction step in HMC are both $O(N)$. This fact makes HMC computationally expensive when sampling from the Gibbs distribution. Moreover, interaction potentials $\phi$ such as the Coulomb potential or the Lennard-Jones potential are usually singular [19]. Singularity in $\phi$ can introduce stiffness to the Hamiltonian system which will bring difficulty to numerical simulations [58], and possibly lead to low acceptance rates [39], thus deteriorating the sampling efficiency of HMC.

As for another well-known example, let us consider Bayesian inference of a parameter $\theta$ based on its posterior distribution $p_{\text{post}}(\theta|D_N)$ given the observed data $D_N$

$$p_{\text{post}}(\theta|D_N) \propto p_{\text{prior}}(\theta) \prod_{i=1}^{N} p(y_i; \theta),$$

(1.3)

where $D_N = \{y_1, \ldots, y_N\}$ is a sample of size $N$ drawn from the probabilistic model $p(\cdot; \theta)$. When $p(\cdot; \theta)$ is posited to be a mixture model, which is often the case in clustering and density estimation problems [18], the corresponding posterior distribution $p_{\text{post}}(\theta|D_N)$ may be multimodal. One main reason for multimodality in mixture models is the nonidentifiability of the parameters due to label switching [27]. When the target distribution (the posterior distribution in this case) is multimodal, most MCMC algorithms have difficulty moving between isolated modes and are therefore prone to generate biased samples. As a result, HMC could fail to explore the entire state space and lead to even worse performance than the simple Random Walk Metropolis (RWM) algorithm [41]. Indeed, the Hamiltonian simulation heavily relies on the gradient information of the potential $U$, easily resulting in samples trapped in one single well of $U$ when $U$ has multiple modes. A popular strategy of sampling from multimodal distributions is running multiple chains with over-dispersed initializations in parallel. Other methods include parallel tempering [21, 45], simulated tempering [42], Wormhole HMC [35] and the Wang-Landau algorithm [56, 57, 10].

Inspired by the splitting strategy used in the multiple time-scale lattice quantum chromodynamics [52], the multiple time-step MC algorithm [26] and Random Batch Monte Carlo (RBMC) method [39], we propose a splitting Hamiltonian Monte Carlo (SHMC) method for sampling from a target distribution $\rho$ with the effective potential energy:

$$U \propto -\beta^{-1} \log \rho,$$

(1.4)

aiming to address the above issues regarding computational costs, singularity and multimodality to some extent. After splitting the potential $U$ into two parts $U = U_1 + U_2$, a candidate state is first proposed by evolving the Hamiltonian system corresponding to $U_1$ and then is probabilistically accepted by a Metropolis rejection step determined by $U_2$. The benefits of such splitting strategy can be summarized as follows:

(a) When sampling from the Gibbs distribution (1.1) of an interacting particle system, particularly with singular interaction, we decompose $U$ into a smooth part $U_1$ and a part $U_2$ with short-range interactions. The smoothness of $U_1$ guarantees the feasibility of the Hamiltonian simulation while $U_2$ reduces the computational cost since only particles within a small neighborhood need to be considered when calculating the acceptance probability.

(b) There is often a big summation term in the potential energy (1.4); e.g. see equation (1.2). In this paper, we apply the random mini-batch idea [49, 29] to further reduce the computation load due to summing over many terms, leading to more efficient algorithms. In particular, if only one randomly picked particle is updated [19] in each iteration, the cost can be reduced to $O(1)$ per iteration.

(c) As for a multimodal distribution, we choose $U_1$ with a relatively flat landscape to enable the Markov chains traveling between isolated wells. Such $U_1$ can be constructed by either
reducing the height of the barriers between different wells of $U$ or filling the wells with 
“computational sand”, an idea borrowed from the metadynamics approach [34] (for 
further details, see Remark 2.2).

We remark that the random batch strategy has recently been applied to interacting 
particle systems, resulting in several efficient algorithms [29, 38, 33, 32]. Different from the 
mini-batch in stochastic gradient descent (SGD), the random batch methods for interacting 
particle systems aim to grasp the dynamics as well. The rationale is a time averaging effect, 
by which RBM methods converge in a “law of large number” manner in time [29, 28]. 
Introducing random batch strategy into the Hamiltonian dynamics, however, will introduce 
effective noise, and the Hamiltonian is no longer conserved and long time simulation 
is not accurate. Nonetheless, in our proposed method, the Hamiltonian dynamics is never 
performed for a long time so this issue is nonessential in this paper; see Section 3.2 for the 
error estimates.

The rest of this paper is organized as follows. In Section 2, we propose our algorithm and 
provide some motivating applications. Specifically, we first elaborate the general framework 
of the splitting Monte Carlo method. Then we incorporate HMC to the general framework 
and present the splitting Hamiltonian Monte Carlo (SHMC) algorithm in Section 2.1. Fi-
nally, taking interacting particle systems and Bayesian inference problems as examples, we 
further introduce the random batch idea to reduce computational cost in Section 2.2. In 
Section 3, we prove an error bound of the value of the approximate Hamiltonian generated 
in random batches and show the advantage of our method over sampling algorithms based 
on overdamped Langevin equations. Finally, we perform some numerical experiments to 
verify the high numerical and computational efficiency of our algorithm in Section 4.

## 2 The Splitting Hamiltonian Monte Carlo method and 
its random batch variant

In this section, we propose the Splitting Hamiltonian Monte Carlo (SHMC) method to 
overcome the aforementioned difficulties that HMC could encounter in practice. To make 
SHMC scalable to large-scale problems such as many-body systems and Bayesian inference, 
we also incorporate the idea of random mini-batch into SHMC. We abbreviate the resulting 
algorithms $RB$-SHMC.

To start with, let us introduce the general framework of the splitting Monte Carlo 
method; see Algorithm 1. As mentioned in Section 1, common MCMC methods such as 
RWM and HMC behave poorly when sampling from the Gibbs distribution of interacting 
particle systems with singular potentials and sampling from multimodal distributions that 
often arise in Bayesian inference of mixture models. In both cases, the gradient of the po-
tential $U$ can be very large in some regions and the MCMC fails to sampling from the target 
distribution efficiently. To alleviate this problem, we first construct a surrogate potential $U_1$ 
with moderate gradient over the domain of $U$. Applying some generic sampling method $S$ 
satisfying detailed balance with respect to (w.r.t.) the Gibbs distribution $\exp(-\beta U_1)$, one 
obtains a proposed state which can be severely biased from the target distribution. In a 
second step, a Metropolis rejection step using $U_2 := U - U_1$ is required to determine whether 
the aforementioned proposal shall be accepted as a new sample.

The splitting Monte Carlo (Algorithm 1) can be viewed as a special case of the Metropolis-
Hastings algorithm. Denote the transition probability of $S$ from state $x$ to state $y$ by $q(y;x)$. 
The acceptance probability in the Metropolis rejection step is then given by:

$$A(y;x) := \min\left(1, \frac{\exp[-\beta U(y)]q(x;y)}{\exp[-\beta U(x)]q(y;x)}\right),$$

and the detailed balance condition of $S$ yields:

$$\frac{q(x;y)}{q(y;x)} = \frac{\exp[-\beta U_1(x)]}{\exp[-\beta U_1(y)]}.$$
Substitute identity (2.2) into (2.1), one can see that the acceptance probability is only related to the $U_2$ component of $U$:

$$A(y; x) = \min \left(1, \frac{\exp[-\beta U(y)] \exp[-\beta U_1(x)]}{\exp[-\beta U(x)] \exp[-\beta U_1(y)]} \right)$$

$$= \min \left(1, \exp \left[ -\beta \left( U_2(y) - U_2(x) \right) \right] \right). \quad (2.3)$$

**Algorithm 1** (General Splitting Monte Carlo algorithm)

1. **Step 1** — Propose a candidate state $x^*$ using some generic sampling method $S$ satisfying detailed balance w.r.t. the Gibbs distribution corresponding to $U_1$:

$$\exp[-\beta U_1(x)] q(x; x^*) = \exp[-\beta U_1(x^*)] q(x^*; x). \quad (2.4)$$

2. **Step 2** — Set $x \leftarrow x^*$ with probability:

$$A(x^*; x) := \min \left(1, \exp \left[ -\beta \left( U_2(x^*) - U_2(x) \right) \right] \right). \quad (2.5)$$

Otherwise, $x \leftarrow x$ remains unchanged.

### 2.1 Splitting Hamiltonian Monte Carlo method

We now present a splitting Monte Carlo method based on HMC, coined as the Splitting Hamiltonian Monte Carlo (SHMC) method, which evolves a Hamiltonian system to make a proposal in Step 1 of Algorithm 1.

**Algorithm 2** (Splitting Hamiltonian Monte Carlo algorithm)

1: Split $U := U_1 + U_2$ such that $\nabla U_1$ is uniformly moderate over the domain of $U$. Randomly generate the initial position $x^{(0)}$ and set $N_s$ as the total number of samples.

2: for $n = 1, \cdots, N_s$ do

3: Randomly pick $x_i$ with uniform probability. Sample a momentum $p_i \sim N \left( 0, \frac{m}{\beta} I_d \right)$ and set $L_n \geq 1, \Delta t_n > 0$.

4: $(x_i^*, p_i^*) \leftarrow (x^{(n-1)}_i, p_i)$.

5: for $\ell = 1, \cdots, L_n$ do

6: $$p_i^* \leftarrow p_i^* - \frac{\Delta t_n}{2} \nabla U_1(x_i^*);$$

$$x_i^* \leftarrow x_i^* + \Delta t_n \frac{p_i^*}{m};$$

$$p_i^* \leftarrow p_i^* - \frac{\Delta t_n}{2} \nabla U_1(x_i^*). \quad (2.6)$$

7: end for

8: Evaluate the following Metropolis acceptance probability:

$$A \leftarrow A(x_i^*; x_i) = \min \left(1, \exp \left[ -\beta \left( U_2(x_i^*) - U_2(x_i^{(n-1)}) \right) \right] \right).$$

9: Generate a random number $\zeta$ from uniform distribution on $[0, 1]$. If $\zeta \leq A$, set

$$x_i^{(n)} \leftarrow x_i^*.$$

Otherwise, set

$$x_i^{(n)} \leftarrow x_i^{(n-1)}.$$
We first recall some fundamental properties of the standard HMC, which obviously satisfies the detailed balance condition. HMC generates samples from the $D$-dimensional target distribution $\pi(\cdot)$ by introducing an auxiliary variable $p \in \mathbb{R}^D$, namely the momentum, and sampling from the joint distribution $\tilde{\pi}(x, p) \propto \exp\left[-\beta H(x, p)\right]$. Traditionally, the Hamiltonian $\tilde{H}(x, p) = U(x) + K(p)$ is separable with $K(p) = \frac{\|p\|^2}{2m}$. Hence, $p$ is sampled from the isotropic multivariate Gaussian distribution $\mathcal{N}\left(0, \frac{\beta}{m} I_D\right)$. The Hamiltonian system satisfies many nice properties such as conservation of energy, reversibility, and symplecticity [3, 46], and therefore it is usually discretized by the leapfrog method, a symmetric symplectic integrator [37]. HMC proposes a new state in the phase space by simulating a Hamiltonian dynamics. The proposed momentum is flipped after the numerical simulation to guarantee the time reversibility and a correction step follows to correct the discretization error induced by the leapfrog integrator. In practice, the momentum flipping step is skipped since $K$ is symmetric and the momentum should be resampled to ensure ergodicity. However, frequent resampling may result in random walk and thus multiple leapfrog steps are performed per iteration.

Sharing the same algorithmic structure as HMC but differing in some specific steps, SHMC numerically evolves a Hamiltonian system with a surrogate potential $U_1$ to propose a candidate state $(x^*, p^*)$ and carries out a Metropolis rejection step only using $U_2 := U - U_1$ after the momentum flipping step. The same as HMC, flipping $p^*$ ensures time reversibility but is usually omitted since the rejection step has nothing to do with the momentum and it should also be resampled in the next iteration to ensure ergodicity. Note that the candidate state $(x^*, p^*)$ is proposed based on the surrogate potential $U_1$ and may not be a typical sample from the target distribution. Therefore, the rejection step here is critical to guarantee the empirical distribution of the samples to converge to the target distribution, beyond the sole purpose of correcting the discretization error as in HMC.

For high-dimensional problems, especially the interacting particle systems, randomly picking a few entries of $x$ to update per iteration can be more efficient [19]. In the following, we assume $x = [x_1, \ldots, x_N] \in \mathbb{R}^{d \times N}$ and only $x_i$, one randomly chosen entry of $x$, is updated per iteration. The detailed procedure of our SHMC method is given in Algorithm 2 and the splitting schemes are presented in Section 2.2 below.

### 2.2 Splitting Hamiltonian Monte Carlo method with random batch

In this section, we discuss how to apply the random batch idea [49] to SHMC for problems with big summation in the potential $U$. Typical examples include the Gibbs distribution arising from interacting particle systems and the posterior distribution from Bayesian inference problems. For these examples, any algorithm that needs to evaluate the full summation, such as the traditional Metropolis Hastings algorithm and the standard HMC, will be computationally inefficient.

The random batch idea is originated from the famous SGD algorithm [49, 8] and the stochastic gradient Langevin dynamics (SGLD) for Bayesian inference [59]. The random mini-batch based on random grouping strategy has recently been applied to many-body interacting systems [29, 38, 31, 30]. Recently, a novel efficient molecular dynamics simulation method by building random batch and importance sampling into the Fourier space of Ewald sum has been proposed in [32]. In a nutshell, the random batch strategy approximates a big summation by summing over only a small random subset of size $O(1)$ and therefore the complexity per time step is reduced to $O(1)$ [29, 39]. The convergence of the random batch approximation can be guaranteed by the law of large numbers [29]. In the following, we present two implementations of the RB-SHMC algorithm.

We remark that introducing random batch strategy into the Hamiltonian dynamics will introduce extra noise and lead to so-called “numerical heating” effects. The Hamiltonian is no longer conserved and the long-run simulation will not be accurate. However, in either HMC or SHMC, the Hamiltonian dynamics are only performed for a short time so this issue is nonessential; see Section 3.2 for error bound estimates. For another remark, the error in the Hamiltonian introduced by random batch, albeit small as proved in Section 3.2, will necessarily introduce systematic errors in the invariant measures of the Markov
chain. One may correct this using a Metropolis rejection step as in the Metropolis-adjusted Langevin algorithm (MALA) \[4, 51\]. However, we choose not to do this simply because such a correction will bring back an $O(N)$ computation step that we have tried to avoid using random batch.

### 2.2.1 Gibbs distribution of interacting particle system

For the Gibbs distribution of a $N$-particle interacting system with $k_B T = 1$, the potential (1.2) comprises the confining potential $V$ and the interaction potential $\phi$. Without loss of generality, we assume that the confining potential is smooth and the interaction potential is symmetric in the sense $\phi(q_i - q_j) = \phi(q_j - q_i)$. We also assume $w_i \equiv w$ for simplicity. In practice, the interaction between particles is of long range and usually singular. It is therefore recommended that $\phi$ is decomposed into a smooth part $\phi_1$ and a short-range part $\phi_2$. Hence, one has

$$
\begin{align*}
U_1(q) &= w \sum_{i=1}^{N} V(q_i) + w^2 \sum_{i<j} \phi_1(q_i - q_j), \\
U_2(q) &= w^2 \sum_{i<j} \phi_2(q_i - q_j),
\end{align*}$$

(2.7)

where $q = [q_1, \ldots, q_N]$ with $q_i \in \mathbb{R}^d$ denoting the position of the $i$th particle and $w$ represents the weight. Clearly, the short range nature of $\phi_2$ is essential to reducing the computational cost because only particles within that short range need to be counted and therefore $U_2$ can be efficiently evaluated using suitable data structures like cell lists \[19, Appendix F\].

The Hamiltonian dynamics corresponding to $U_1$ defined in (2.7) are given by

$$
\begin{align*}
\dot{q}_i &= \frac{p_i}{m}, \\
\dot{p}_i &= -\left( \frac{\nabla V(q_i)}{w(N-1)} + \frac{1}{N-1} \sum_{j \neq i} \nabla \phi_1(q_i - q_j) \right),
\end{align*}$$

(2.8)

Note that we have done a time rescaling $t \leftarrow w\sqrt{N-1}t$ and redefined the momentum by $p \leftarrow p/(w\sqrt{N-1})$ so that the interacting force on the $i$th particle is $O(1)$. The step of resampling of $p$ in Algorithm 2 now becomes

$$
p_i \sim \mathcal{N}\left(0, \frac{m}{w^2(N-1)} I_d \right).
$$

The acceptance rate is again given by $\min(1, \exp(-\Delta U_2))$.

**Remark 2.1.** Note that the time rescaling here is equivalent to setting $\tilde{U}_1 = \sum_{i=1}^{N} \frac{V(q_i)}{w(N-1)} + \frac{1}{N-1} \sum_{i,j \neq i} \phi_1(q_i - q_j)$ and $\tilde{U}_2 = \frac{1}{N-1} \sum_{i,j \neq i} \phi_2(q_i - q_j)$, and choosing a fake temperature parameter $\beta = w^2(N-1)$ in Algorithm 2 (as the real temperature parameter is $(k_B T)^{-1} = 1$). The acceptance rate is then again based on $\beta \Delta \tilde{U}_2 = \Delta U_2$.

In the case of mean-field regime where $w \sim 1/N$, it becomes the usual ODE system for interacting particles in literature.

When random batch is applied, the Hamiltonian system is reduced to

$$
\begin{align*}
\dot{\tilde{q}}_i &= \frac{\tilde{p}_i}{m}, \\
\dot{\tilde{p}}_i &= -\left( \frac{\nabla V(\tilde{q}_i)}{w(N-1)} + \frac{1}{s} \sum_{j \in \xi} \nabla \phi_1(\tilde{q}_i - \tilde{q}_j) \right),
\end{align*}$$

(2.9)

where $\xi = \{\xi_1, \ldots, \xi_s\}$ is a random subset of $\{1, \ldots, N\} \setminus \{i\}$.
We remark that there exist other ways to implement the random batch strategy. For example, in the case of Coulomb interactions in a periodic box, the importance sampling in Fourier space is possible and the time scaling in (2.8) may be unnecessary [32]. Even if we do random batch in real space as indicated above in the molecular dynamics regime where $w = 1$, the time scaling to have $1/N$ factor in (2.7) is only a convenience made for establishing theoretical results. It will not change the intrinsic dynamics and is not necessary for implementation in practice [31].

### 2.2.2 Multimodal posterior in Bayesian inference

In Bayesian inference problems, the potential of the posterior is given by:

$$ U(\theta) = \frac{1}{\beta} \left[ -\log p_{\text{prior}}(\theta) + \sum_{i=1}^{N} -\log p(y_i; \theta) \right], \quad (2.10) $$

where $\theta$ is the parameter of interest, $y_i, i = 1, \ldots, N$ are the observations and $\beta > 0$ is a scaling factor.\(^1\)

In many cases, $p_{\text{post}}$ is multimodal and thus there are multiple wells in the landscape of $U$. The energy barriers between wells frustrate general MCMC methods and lead to biased samples trapped in one single well. In this situation, one can flatten the landscape of $U$ by adding “computational sand” $G$ into the wells and thus $U_2 = -G$. One feasible choice of $G$ is the Gaussian kernel.

Here, we take the potential $U_1$ to be

$$ U_1 = -\log p_{\text{prior}}(\theta) + \sum_{i=1}^{N} -\log p(y_i; \theta) + G. $$

As above, we do a time rescaling $t \leftarrow \sqrt{N}t$ and the momentum is redefined as $p \leftarrow p/\sqrt{N}$. Then, we can resample the momentum from the isotropic Gaussian $N(0, \frac{2}{N} I_d)$, and the momentum update in the RB-SHMC is given by

$$ p^* \leftarrow p^* - \Delta t \left[ -\frac{1}{N} \nabla \log p_{\text{prior}}(\theta^*) + \frac{1}{s} \sum_{i \in \xi_\ell} -\nabla \log p(y_i; \theta^*) + \frac{1}{N} \nabla G(\theta^*) \right], \quad (2.11) $$

where $\xi_\ell = \{\xi_{\ell,1}, \ldots, \xi_{\ell,s}\} \subset \{1, \ldots, N\}$ denotes the random batch chosen in the $\ell$th step of the iteration. The acceptance rate is simply $\min(1, \exp(\Delta G))$.

The time rescaling here is again equivalent to choosing $\beta = N$, $U_1 = -\frac{1}{N} \log p_{\text{prior}}(\theta) + \frac{1}{s} \sum_{i=1}^{N} -\log p(y_i; \theta) + \frac{1}{N} G$ and $U_2 = -\frac{1}{N} G$ in Algorithm 2. The goal of time rescaling or choosing $\beta = N$ is to scale the summation term by $1/N$ so that the variance of $\chi_\ell := \frac{1}{s} \sum_{i \in \xi_\ell} -\nabla \log p(y_i; \theta^*) - \frac{1}{s} \sum_{i=1}^{N} -\nabla \log p(y_i; \theta^*)$ is controlled independent of $N$. Indeed, choosing $\beta = N$ is only for convenience in the analysis and incurs no essential change in the physical interpretation [31]. In practice, one may perform the updates directly by

$$ p^* \leftarrow p^* - \Delta t \left[ -\nabla \log p_{\text{prior}}(x^*) + \frac{N}{s} \sum_{i \in \xi_\ell} -\nabla \log p(y_i; x^*) + \nabla G(x^*) \right]. $$

**Remark 2.2.** The idea of adding computational sand is inspired by metadynamics [34], which is informally described as “filling the free energy wells with computational sand”. In some special cases, the modes of the posterior, and thus the locations of the wells in $U$, can be roughly estimated by the modes of the marginal distributions. Then an amenable $G$ can be designed in advance. Such an example is presented in Section 4.3.2 below. Generally, however, the modes of the marginals fail to imply the location of the modes of the joint

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\(^1\)Note that the $N$ here denotes the number of observed data and has nothing to do with the dimension of the variable $\theta$. 

7
distribution. Hence, one may dynamically add a sequence of standard Gaussian kernels at the positions already visited by the proposals of the Hamiltonian simulation. In this case, Metropolis rejection steps are skipped in the first few trial runs. Then one collects all the added Gaussian kernels and obtains \( U_1 \), which is \( U \) plus the sum of these Gaussian kernels. Interested readers may refer to [34] for more details. We leave the theoretical justification of this proposal to future work.

3 Theoretical properties of SHMC and RB-SHMC

In this section, we provide some theoretical justifications for the SHMC and RB-SHMC algorithms. First, in Section 3.1, we give some informal justification on why SHMC could potentially be better than splitting Monte Carlo methods based on overdamped Langevin dynamics. Second, in Section 3.2, we provide error estimates of the values of the approximate Hamiltonian generated from RB-SHMC under some mild regularity conditions. These results give practitioners some guidance on when to expect SHMC or RB-SHMC to succeed in applications.

3.1 Benefits of Hamiltonian dynamics in sampling compared to the overdamped Langevin equations

As is well known, the Langevin sampling \([5, 51, 11, 48]\) is another popular sampling scheme for the Gibbs distribution. Consider the overdamped Langevin equation:

\[
\frac{dX}{dt} = -\nabla U(X) dt + \sqrt{\frac{2}{\beta}} dW,
\]

where \( \beta > 0 \) is a known constant and \( W \) denotes the \( d \)-dimensional Wiener process. It converges exponentially to its invariant measure, the Gibbs distribution (1.1), under mild regularity conditions [43]. The Langevin sampler discretizes the overdamped Langevin equation (3.1), by the Euler-Maruyama scheme

\[
X(t_{n+1}) = X(t_n) - \Delta t_n \nabla U(X(t_n)) + \sqrt{\frac{2\Delta t_n}{\beta}} z_n, \quad z_n \sim \mathcal{N}(0, I_d).
\]

Hence the Markov chain generated by the Langevin sampler also exhibits an exponentially fast convergence rate up to the discretization error of order \( O(\Delta t) \) [12].

In this section, we point out several possible benefits of the HMC-based samplers over the overdamped Langevin equation-based samplers like the RBMC and SGLD algorithms. In fact, the RBMC method uses the overdamped Langevin equation for generating the proposals in Step 1 of Algorithm 1, as the overdamped Langevin equation satisfies the detailed balance condition w.r.t. this invariant measure determined by \( U_1 \). This may provide some heuristic justification for why in certain cases RB-SHMC may be preferred compared to RBMC, such as the examples described in sections 4.1 and 4.2 below.

In the discussion here, we assume that the potential \( U \) is smooth and for the sake of simplicity, there is no splitting so \( U_1 \equiv U \). Recall that we perform \( L_n \) leapfrog steps with time step size \( \Delta t_n \) in the \( n^{th} \) iteration, which means that we evolve an Hamiltonian system w.r.t. \( (X_{i(n)}, P_{i(n)}) \) for \( t \in [T_{i(n-1)}^{(n)}, T_{i(n)}^{(n)}] \). Assume the particle index updated in the \( n^{th} \) iteration is \( i \equiv i^{(n)} \), where we omit the superscript for convenience. Then we approximate the momentum \( P_i(t') \) at time \( t' \in (T_{i^{(n-1)}}^{(n-1)}, T_{i^{(n)}}^{(n)}) \) by

\[
P_i(t') = P_i(T_{i^{(n-1)}}^{(n-1)}) + \int_{T_{i^{(n-1)}}^{(n-1)}}^{t'} -\nabla U(X_i(\tau)) d\tau.
\]
and thus
\[
X_i(T^{(n)}_i) = X_i(T^{(n-1)}_i) + \int_{T^{(n-1)}_i}^{T^{(n)}_i} m^{-1} P_i(t') dt' \\
= X_i(T^{(n-1)}_i) + \frac{L_n \Delta t_n}{m} P_i(T^{(n-1)}_i) - \frac{1}{m} \int_{T^{(n-1)}_i}^{T^{(n)}_i} \nabla U(x_i(\tau)) d\tau dt' \quad (3.2)
\]

with
\[
\nabla U = \frac{2}{(L \Delta t_n)^2} \int_{T^{(n-1)}_i}^{T^{(n)}_i} \nabla U(x_i(\tau)) d\tau dt'
\]

and \( \Delta t_n = \frac{(L_n \Delta t_n)^2}{2m} \) and \( z_n \sim N(0, I_d) \).

Roughly, the numerical evolution in the \( n^{th} \) iteration of SHMC is nearly equivalent to the simulation of an overdamped Langevin equation for time \( \Delta t_n \). Hence, the effective time step of the overdamped Langevin equation is longer than the evolution time \( L_n \Delta t_n \) of the corresponding Hamiltonian system, provided \( L_n \Delta t_n > 2m \). This means that running the Hamiltonian system with \( L_n \Delta t_n \) large has a longer effective dynamics so it might approximate the equilibrium faster than the overdamped Langevin dynamics. This property may be the reason why SHMC is preferred in some applications over RBMC (see examples 4.1-4.2 below). Moreover, if the Hamiltonian step in (3.2) is accurately solved, it then exactly satisfies the detailed balance w.r.t. the target distribution. Discretizing the Hamiltonian using leapfrog might yield \( O(\Delta t^2) \) error, which is better compared to the Euler-Maruyama discretization of overdamped Langevin dynamics with error \( O(\Delta t) \) if we use the same step size.

Another benefit of HMC is that it can take advantage of the symplectic integrators to conserve the Hamiltonian even the system evolves for a long time. Usually, with fixed time step \( \Delta t \), the discretization error would increase exponentially with the evolution time. However, the symplectic integration can be carried out for \( e^{O(1/\Delta t)} \) time steps such that the numerical trajectories would always oscillate around the exact Hamiltonian trajectories within this time interval [4, 24]. This guarantees that the Hamiltonian can be conserved within a reasonable tolerance for a long time, which is highly desired for HMC-based algorithms as the invariant measure is related to the Hamiltonian directly. Moreover, due to the time-reversibility and volume-preservation property of the leapfrog integrator, HMC exhibits better scalability compared to RWM and MALA in some cases. For instance, when the potential of the target distribution is a sum of i.i.d. terms as (1.2) and satisfies mild regularity conditions, HMC can allow a larger time step \( \Delta t = O(N^{-1/4}) \), and thus requires less steps to traverse the state space, as the number \( N \) of i.i.d. terms tends to infinity [46, 6].

### 3.2 Error estimates of the random batch method

In this section, we derive an error bound for the values of the Hamiltonian approximated by the random batch strategy in one iteration of RB-SHMC (the process between any two consecutive resampling steps of the momentum). We analyze how the random batch strategy affects the value of the Hamiltonian corresponding to \( U_1 \). Note that the error of the value of the Hamiltonian determines the deviation of the invariant measure so this estimate can provide us some insight on the impact of the random batch approximation on the invariant measures.

Without loss of generality, we denote the beginning of an iteration as \( t = 0 \), and consider the following Hamiltonian system
\[
\dot{x} = \frac{p}{m}, \\
\dot{p} = -\nabla V(x) + \frac{1}{N} \sum_{j \in \mathcal{J}} \nabla \psi_j(x)
\]  
(3.3)
and its counterpart after applying random batch
\[
\hat{x} = \frac{\hat{p}}{m}, \quad \hat{p} = -\nabla V_l(\hat{x}) + \frac{1}{s} \sum_{j \in \xi} \nabla \psi_j(\hat{x}).
\] (3.4)

Here \(N_J \) is the size of the index set \( \mathcal{J} \) and \( \xi \) denotes a random subset of size \( s \). We remark that introducing the notations \( V_l \) and \( \psi_j \) enables us to unify the Hamiltonian systems of the two examples discussed in Section 2.2.

**Remark 3.1.** The following remarks are in order.

(a) In the interacting particle system: \( x \) is \( q_i \), the position of the randomly picked particle \( i; V_l = V/(\omega(N-1)) \); and \( \psi_j(x) = \psi(x; q_j) = -\phi_1(x - q_j) \) as \( q_j \) for \( j \neq i \) is unchanged during one cycle. In this case, \( N_J = N - 1 \).

(b) In the Bayesian inference problem: \( x \) is \( \theta \), the parameter of interest; the index \( j \in \mathcal{J} \) corresponds to \( y_j \), the \( j^{th} \) observed data point; \( V_l = -\log p_{\text{prior}}(\cdot)/N \); and \( \psi_j \) corresponds to the terms from splitting of \( -\log p(y_j; \theta) \). In this case, \( N_J = N \). Note that the above splitting strategy can be made case-specific.

We first clarify the notations used in the following analysis. Fix the number of leapfrog steps and the time step in each iteration to be \( \ell \) and denote \( \xi \) the random batch selected in the \( \ell \)th steps. The Kolmogorov extension theorem [15] guarantees the existence of a probability space \((\Omega, \mathcal{F}, \mathbb{P})\) such that \( \{X^0, P^0, \xi, \ell = 1, \ldots, L\} \) are independent random variables on this space. The \( L^2(\Omega, \mathbb{P}) \) norm is denoted as \( \| \cdot \| = \sqrt{\mathbb{E}[\cdot^2]} \), where \( \mathbb{E} \) is the expectation with respect to the probability measure \( \mathbb{P} \).

Now we start to estimate the difference of \( H(\tilde{x}(T), \tilde{p}(T)) \) and \( H(x(T), p(T)) \), where \( (\tilde{x}(\cdot), \tilde{p}(\cdot)) \) is the solution of the fully coupled Hamiltonian system (3.3) and therefore \( H(x(T), p(T)) = H(x(0), p(0)) \).

For error bound estimates, we assume that the Hamiltonian is sufficiently smooth.

**Assumption 3.1.** \( V_l \in C^1 \) and \( \psi \in C^2 \) with \( \nabla V_l, \nabla \psi \) and \( \nabla^2 \psi \) being bounded.

**Remark 3.2.** In cases where the actual confining potential has an unbounded gradient, one can still split \( V \) into a bounded and an unbounded part so the unbounded part can be used in the Metropolis rejection step. However, this may not be needed in practice as the particles usually move in a bounded domain so the unboundedness of \( V \) is not very relevant.

The main results are as follows.

**Theorem 3.1.** Under Assumption 3.1 and assume \( \Delta t \) is sufficiently small such that \( T(1 + T^2)\Delta t \ll 1 \). If \( x(0) = \tilde{x}(0) = X^0 \), and \( p(0) = \tilde{p}(0) = P^0 \), and the fourth moment of the initial momentum \( \mathbb{E}[P^0]^4 \) is bounded, then the error from using random batches can be upper bounded as follows:
\[
\|H(\tilde{x}(T), \tilde{p}(T)) - H(x(T), p(T))\| \leq C \sqrt{T(1 + T^2)\Delta t}, \tag{3.5}
\]

and for any test function \( \varphi \in C^\infty_0 \),
\[
\|\mathbb{E}[\varphi(H(\tilde{x}(T), \tilde{p}(T))) - \varphi(H(x(T), p(T)))]\| \leq C_\varphi T(1 + T^2)\Delta t, \tag{3.6}
\]

where \( C, C_\varphi > 0 \) are constants independent of \( T \) and \( N \) and \( C_\varphi \) depends on \( \varphi \).

We remark that the bounded fourth moment conditions on the momentum \( P^0 \) are trivially satisfied as it usually sampled from a multivariate Gaussian distribution. In the proof, we need to define the filtration \( \{\mathcal{F}_\ell\}_{1 \leq \ell \leq L} \) by
\[
\mathcal{F}_\ell := \sigma (X^0, P^0, (\xi_k)_{1 \leq k \leq \ell}), \tag{3.7}
\]
Clearly, \( \chi^\ell \) is \( \mathcal{F}_t \)-measurable and for any \( \ell \geq 0, q > 0 \),

\[
\sup_{t \in [t_0, t_{\ell+1}]} \mathbb{E} \left[ \left| \chi^\ell (t) \right|^q \mathbb{F}_t \right] \leq 2^q \| \nabla \psi \|^q_{\infty}.
\]  

(3.9)

With these, the following upper bound, which will be used in the proof of Theorem 3.1, can be easily obtained:

**Lemma 3.1.** Under conditions in Theorem 3.1, it holds that,

\[
\sup_{0 \leq t \leq T} \mathbb{E} \left[ |\hat{p}(t)|^4 \right] \leq C(1 + T^4),
\]  

(3.10)

where \( C > 0 \) is a constant independent of \( N, s, \xi, k = 1, \ldots, L \).

The proof of this simple lemma is deferred to Appendix A. We are now able to provide the proof of the error estimates for the Hamiltonian.

**Proof of Theorem 3.1.** Define

\[
\Delta H(t) := H(\tilde{x}(t), \tilde{p}(t)) - H(x(t), p(t)) = H(\tilde{x}(t), \tilde{p}(t)) - H^0,
\]

(3.11)

where \( H^0 = H(X^0, P^0) \) is the initial value of the Hamiltonian since \( H \) is conserved under the evolution (3.3). Consequently, it is straightforward to find

\[
\frac{d}{dt} \Delta H(t) = \frac{\tilde{p}(t)}{m} \cdot \chi^L_t(t),
\]

(3.12)

where

\[
L_t = \left\lfloor \frac{t}{\Delta t} \right\rfloor.
\]

(3.13)

Hence,

\[
\begin{align*}
\frac{d}{dt} \| H(\tilde{x}(t), \tilde{p}(t)) - H(x(t), p(t)) \|^2 & = 2 \mathbb{E} \left[ \Delta H(t) \frac{\tilde{p}(t)}{m} \cdot \chi^L_t(t) \right] \\
& = 2 \mathbb{E} \left[ \Delta H(t_L) + \frac{\tilde{p}(t)}{m} \cdot \chi^L_t(t - t_L) \right] \frac{\tilde{p}(t)}{m} \cdot \chi^L_t(t) \\
& = : I_1 + I_2,
\end{align*}
\]

where \( \tilde{t} \in (t_L, t) \) by the mean value theorem for one variable functions.

**Step 1 — Estimation of \( I_1 \):**

Note that \( \Delta H(t_L) \in \mathcal{F}_{L-1} \) and \( \tilde{p}(t_L) \in \mathcal{F}_{L-1} \). Then one has

\[
\mathbb{E} \left[ \Delta H(t_L) \frac{\tilde{p}(t_L)}{m} \chi^L(t_L) \right] = \mathbb{E} \left[ \Delta H(t_L) \frac{\tilde{p}(t_L)}{m} \cdot \mathbb{E} \left( \chi^L(t_L) \mathcal{F}_{L-1} \right) \right] = 0.
\]

Therefore,

\[
\begin{align*}
\mathbb{E} \left[ \Delta H(t_L) \frac{\tilde{p}(t)}{m} \chi^L_t(t) \right] &= \mathbb{E} \left[ \Delta H(t_L) \left( \frac{\tilde{p}(t)}{m} \chi^L_t(t) - \frac{\tilde{p}(t_L)}{m} \chi^L_t(t_L) \right) \right] \\
& = \mathbb{E} \left[ \Delta H(t_L) \mathbb{E} \left( \frac{\tilde{p}(t)}{m} \chi^L_t(t) - \frac{\tilde{p}(t_L)}{m} \chi^L_t(t_L) \left| \mathcal{F}_{L-1} \right. \right) \right] \\
& = \mathbb{E} \left[ \Delta H(t_L) \int_{t_L}^t \mathbb{E} \left( \frac{\tilde{p}(t')}{m} \chi^L_t(t') + \frac{\tilde{p}(t')}{m} \chi^L_t(t') \left| \mathcal{F}_{L-1} \right. \right) dt' \right] \\
& \leq C(1 + T^2) \Delta t \| \Delta H(t_L) \| + C(1 + T^2) \Delta t \left( \| \Delta H(t_L) \| + \| \frac{\tilde{p}(t)}{m} \chi^L_t(t) - \frac{\tilde{p}(t_L)}{m} \chi^L_t(t_L) \| \right) \\
& \leq C(1 + T^2) \Delta t (\| \Delta H(t_L) \| + C(1 + T) \Delta t) \leq C(1 + T^2) \Delta t \| \Delta H(t) \|.
\end{align*}
\]

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Step 2 — Estimation of $I_2$:
\[
\mathbb{E} \left[ \frac{\hat{p}(t)}{m} \chi^L (t) \right]^4 \mathbb{E} \left[ \left| \chi^L (t) \right|^4 \right] \leq C(1 + T^2) \Delta t.
\]
Therefore, $I_2$ is controlled by $C(1 + T^2) \Delta t$.
Combining the above two steps gives
\[
\frac{d}{dt} ||\Delta H(t)||^2 \leq C(1 + T^2) \Delta t (||\Delta H(t)|| + 1).
\]
Recollect that $\Delta t$ is assumed to be sufficiently small. Then one has
\[
||H(\tilde{x}(T), \tilde{p}(T)) - H(x(T), p(T))|| \leq C \sqrt{T(1 + T^2)} \Delta t.
\]
Similarly, (3.6) follows from
\[
||E [\varphi (H(\tilde{x}(T), \tilde{p}(T))) - \varphi (H(x(T), p(T)))]||
\]
\[
= \int_0^T \mathbb{E} \left[ \varphi' (H(\tilde{x}(t), \tilde{p}(t))) \frac{\partial (t)}{m} \chi^L (t) \right] dt
\]
\[
= \int_0^T \mathbb{E} \left[ \varphi' (H(\tilde{x}(t), \tilde{p}(t))) \frac{\partial (t)}{m} \chi^L (t) \right. - \left. \varphi' (H(\tilde{x}(t), \tilde{p}(t))) \frac{\partial (t)}{m} \chi^L (t) \right] dt
\]
\[
\leq \int_0^T \int_{t_n}^{t_n + T} \mathbb{E} \left[ \varphi'' (H(\tilde{x}(t'), \tilde{p}(t'))) \left( \frac{\partial (t')}{m} \chi^L (t') \right)^2 dt' dt
\]
\[
+ \int_0^T \int_{t_n}^{t_n + T} \mathbb{E} \left[ \varphi' (H(\tilde{x}(t'), \tilde{p}(t'))) \left( \frac{\partial (t')}{m} \chi^L (t') + \frac{\partial (t')}{m} \chi^L (t') \right) dt' dt
\]
\[
\leq (||\varphi'||_{\infty} + ||\varphi''||_{\infty}) C T (1 + T^2) \Delta t.
\]

4 Numerical examples

In this section, we conduct some numerical experiments to demonstrate the numerical and computational efficiency of SHMC and RB-SHMC. First we give an artificial example with regular interactions to test the influence of the length of Hamiltonian dynamics in an iteration. In the second example, we simulate the Dyson Brownian motion for $N \gg 1$. The advantage of potential splitting and the high efficiency of random batch will manifest itself in this example, where the interaction is singular and of long range. Lastly, we consider a classical example in Bayesian inference: estimating the locations of a two-dimensional Gaussian mixture model using SHMC and RB-SHMC.

4.1 A test example

In the following toy example, we explore how $L_n$, the number of leapfrog steps in the $n^{th}$ iteration, can influence the efficiency of the RB-SHMC algorithm. For the purpose of a relatively fair comparison between algorithms with different evolution time per iteration, we define the evolution time $T_E$ up to the $m^{th}$ iteration of Algorithm 2 by
\[
T_E(m) = \frac{1}{N} \sum_{n=1}^{m} L_n \times \Delta t_n.
\]

\[
\]
The rescaling factor $1/N$ arises from the fact that Algorithm 2 updates only one “particle” per iteration and thus on average $N$ iterations are needed to update all the variables.

Consider the simple one-dimensional Langevin equation

\[
\begin{align*}
\frac{dx^i}{dt} &= P^i, \\
\frac{dp^i}{dt} &= -\alpha x^i - \frac{1}{N-1} \sum_{j:j\neq i} \frac{x^j-x^i}{1+(x^j-x^i)^2} + \gamma p^i dt + \sqrt{\frac{2\gamma}{N}} dW^i. 
\end{align*}
\]

Clearly, the interaction is smooth and bounded and its derivative is also bounded. The corresponding Gibbs distribution is

\[
\mu \propto \exp \left[ -\frac{\beta}{2} \left( \alpha \sum_i x_i^2 - \frac{1}{N-1} \sum_{i,j<i,j} \ln(1 + |x_i - x_j|^2) + \sum_i p_i^2 \right) \right].
\]

Consider a system of $N = 500$ particles sampled from the uniform distribution on $[-10,10]$. Since the interaction kernel is regular, we move all the particles simultaneously using $\phi_1 := \phi$ and omit the Metropolis rejection step since $\phi_2 = 0$. Choosing $\alpha = 1$, $\beta = 1$ and fixing the batch size $s = 1$, the $\ell^{th}$ leapfrog step includes the following updates

\[
\begin{align*}
\mathbf{p} &\leftarrow \mathbf{p} + \frac{\Delta t_n}{2} \left( \alpha \mathbf{x} - \frac{\mathbf{x} - \theta_i}{1 + |\mathbf{x} - \theta_i|^2} \right) \\
\mathbf{x} &\leftarrow \mathbf{x} + \Delta t_n \mathbf{p}; \\
\mathbf{p} &\leftarrow \mathbf{p} - \frac{\Delta t_n}{2} \left( \alpha \mathbf{x} - \frac{\mathbf{x} - \theta_i}{1 + |\mathbf{x} - \theta_i|^2} \right),
\end{align*}
\]

where the $i^{th}$ element of $\theta_i$ is $\theta_{i,i} = x_i$, with $x_i \in \{1,2,\ldots,N\} \setminus \{i\}$ for $i = 1,2,\ldots,N$. Fixing the time step $\Delta t_n \equiv 0.02$, we run RB-SHMC with $L_n \equiv 100$ and $L_n \equiv 10$ respectively for $T_E = 100$ units of evolution time to see how the efficiency can be influenced by different values of $L_n$.

![Figure 1: Influence of number of steps at different “evolution times” $T_E$. The red dots are for $L_n = 100$ leapfrogs and the black triangles are for $L_n = 10$ leapfrog steps in each iteration. The blue curve is the reference density obtained by running HMC, 25 leapfrog steps with time step size $\Delta t = 0.01$ per iteration, for 4e8 iterations.](image)

Figure 1 shows the empirical densities at “evolution times” $T_E = 30$, $60$, $100$ obtained by the simple “bin-counting”. Specifically, the empirical density in the $j^{th}$ bin is approximated by $\bar{\mu}_j \approx N_j/(N_{tot} \Delta t)$, where $N_j$ is the number of particles in the $j^{th}$ bin during the entire sampling process and $N_{tot}$ is the number of total particles (clearly, $N_{tot} = N_s N$ where $N_s$ is the number of iterations in sampling). One can observe that RB-SHMC with larger $L_n$ approaches the equilibrium faster, meaning that it can have shorter burn-in phase. This observation is consistent with the heuristic explanation provided in Section 3.1.

To quantify the effects of $L_n$ in different stages of sampling, we use the following quantity (which we call “relative error”) to gauge the error of the empirical density

\[
\bar{U} := \sum_j \left| \frac{N_j}{N_{tot}} - \frac{\bar{N}_j}{N_{tot}} \right|,
\]
where \( j \) denotes the bin index, and the quantities with tildes are the reference quantities obtained by HMC (25 leapfrog steps with time step size \( \Delta t = 0.01 \) per sampling iterations, for a total of \( 4e8 \) iterations).

Figure 2: Relative error vs. evolution time and CPU time of RB-SHMC with different choices of \( L_n \). Blue curve is for different choices of \( L_n \), specifically, \( L_n = 100 \) for \( T_E \leq 10^2 \) and \( L_n = 10 \) for \( 10^2 < T_E \leq 10^4 \), red dashed curve is for \( L_n \equiv 100 \) while black dotted curve is for \( L_n \equiv 10 \).

As can be seen from Figure 2, the experiment with larger \( L_n \) is more efficient when the evolution time is not very long as it has shorter burn-in phase. However, the systematic error becomes larger when one run the sampling for longer time. Hence, an adaptive strategy can be used: one uses a large \( L_n \) in the early sampling phase, and when the distribution is close to equilibrium one can then switch to smaller \( L_n \) so that the results can be more accurate. Here, for comparison, we set \( L_n = 100 \) for \( T_E \leq 100 \) and then set \( L_n = 10 \). The error vs. the evolution time and CPU time are plotted in Figure 2. One can see that running RB-SHMC with a large \( L_n \) for a few units of evolution time at the beginning accelerates the empirical density to approach its equilibrium state while reducing \( L_n \) to a smaller number after reaching a quasi-equilibrium yields a smaller error. The adaptive method can thus be efficient.

4.2 Dyson Brownian motion

In this section, we demonstrate the efficiency of RB-SHMC by simulating the Dyson Brownian motion with singular interaction kernels, which models the eigenvalues of certain random matrices [16, 17]:

\[
d\lambda_i(t) = \left(-\lambda_i(t) + \frac{1}{N-1} \sum_{j \neq i} \frac{1}{\lambda_i(t) - \lambda_j(t)}\right) dt + \sqrt{\frac{2}{N-1}} dW_i(t),
\]

where \( \{\lambda_i(t)\} \)’s denote the eigenvalues and \( \{W_i(t)\} \)’s are independent standard Brownian motions. We have replaced \( N \) in the original model with \( N - 1 \), which is nonessential when \( N \gg 1 \). It has been shown in [55] that in the \( N \to \infty \) limit, these eigenvalues follow a distribution \( \rho \) that satisfies

\[
\partial_t \rho(x, t) + \partial_x (\rho(x - u)) = 0, \quad u(x, t) = \pi(H\rho)(x, t) = \text{p.v.} \int_{\mathbb{R}} \frac{\rho(y, t)}{x - y} \, dy,
\]

where \( H(\cdot) \) is the Hilbert transform on \( \mathbb{R} \) and \( \text{p.v.} \) is the standard notation for integrals evaluated using the Cauchy principal value. The mean field equation (4.5) has the following
invariant measure:

$$\rho(x) = \frac{1}{\pi} \sqrt{2 - x^2},$$

which is the celebrated Wigner semicircle law. Clearly, (4.4) has an invariant measure

$$\mu \propto \exp \left[ -\frac{N-1}{2} \sum_i x_i^2 - \sum_{i,j;i<j} \ln |x_i - x_j| \right],$$

where the interaction $$\phi(x_i - x_j) = -\ln(|x_i - x_j|)$$ is singular. For samples $$(\lambda_1, \cdots, \lambda_N) \sim \mu,$$ we expect that the random empirical measure $$\mu_N = \frac{1}{N} \sum_i \delta(x - \lambda_i)$$ will be close to $$\rho$$ in the weak topology. Below, we collect $$N_s$$ such configurations $$(\lambda_1, \cdots, \lambda_N)$$ by sampling from $$\mu$$ using our sampling methods, and then compare the empirical measure of these $$N_s N$$ samples to the target Wigner semicircle law $$\rho.$$

Following [39], we use the surrogate potential $$\phi_1(x_i - x_j) = \ln(100) - 100 |x_i - x_j| + 1$$ when $$0 < |x_i - x_j| < 0.01$$ to remove the singularity while performing RB-SHMC sampling.

Table 1: The specific choices of $$(L_n, \Delta t_n)$$ for RB-SHMC, RBMC and RBMC-v2.

| $$(L_n, \Delta t_n)$$ | RB-SHMC | RBMC | RBMC-v2 |
|----------------------|---------|-------|---------|
| $$(100, 2 \times 10^{-4})$$, if $$n \leq 1e5$$ | $$(100, 10^{-4})$$, if $$n \leq 2e5$$ | $$(10, 10^{-4})$$ | $$(20, 10^{-4})$$, if $$n \in (1e5, 4e5]$$ |
| $$(20, 2 \times 10^{-4})$$, if $$n \in (1e5, 4e5]$$ | $$(20, 10^{-4})$$, if $$n \in (2e5, 8e5]$$ | | $$(10, 10^{-4})$$, if $$n > 8e5$$ |
| $$(10, 10^{-4})$$, if $$n > 4e5$$ | | | |

Recall that the example in Section 4.1 indicates that running $$L_n$$ leapfrog steps with $$L_n$$ large in the burn-in phase can accelerate the convergence to a quasi equilibrium state while a small $$L_n$$ in later iterations can reduce the error. Hence, we adopt a dynamic leapfrog steps in the simulation for this example. Specifically, we choose $$L_n = 100$$ in the first $$10^5$$ sampling iterations and $$L_n = 20$$ in the next $$3 \times 10^5$$ iterations. Then we reduce $$L_n$$ to 10 and keep it fixed until the end of the sampling process. The corresponding time step size $$\Delta t_n$$ also varies in different sampling phases (detailed in table 1). We compare it to the RBMC which is a splitting Monte Carlo based on overdamped Langevin dynamics. We consider both fixed $$\Delta t_n$$ and $$L_n$$ parameters (denoted as RBMC) and varying $$L_n$$ (denoted as RBMC-v2). Table 1 shows the specific choice of these parameters for the three methods considered in this example.

Figure 3: The empirical densities at different time and the equilibrium measure of Dyson Brownian motion. The red dots and the black triangles are the empirical densities obtained by RB-SHMC and RBMC respectively. The blue curve is the equilibrium semicircle law (4.6).

The same evolution time (4.1) is used again for this example. Figure 3 presents the empirical densities obtained by running RB-SHMC (red dots) for $$10^6$$ and $$10^7$$ sampling
iterations, corresponding to 7.6 and 25.6 units of evolution time respectively. The numerical results generated by running RBMC (black triangles) for the same evolution time are also presented for comparison. Obviously, RB-SHMC approaches the equilibrium much faster than RBMC which is consistent with our heuristic justification in Section 3.1.

![Graph](image.png)

(a) Relative error vs. evolution time.

(b) Relative error vs. CPU time.

Figure 4: Relative error vs. evolution time and CPU time. Blue curve is for RB-SHMC, red dashed curve is for RBMC while black dotted curve is for RBMC-v2.

In Figure 4, we visualize the relative error of the three methods vs. the evolution time and CPU time respectively. The same “relative error” as in Example 4.1 has been used. Clearly, RB-SHMC is far more efficient than RBMC and is also superior to RBMC-v2.

4.3 Bimodal distribution

The two examples given below will show that an appropriate potential splitting effectively prevents the problem of generating biased samples when the target distribution is multimodal. These examples showcase the advantage of SHMC and RB-SHMC even there is no singularity in the potential, further expanding the application territory of the framework of SHMC and RB-SHMC where they can be superior to many other existing methods.

Intuitively, if we can “flatten” the landscape of $U$, then the samples can escape from one local minimum, cross the barrier and visit other local minima more efficiently. Without loss of generality, we only consider the bimodal distributions for simplicity.

4.3.1 Double well potential

Consider the following one-dimensional double well potential

$$U(x) = \frac{H}{W^4}(x^2 - W^2)^2,$$

(4.7)

where $H = 20/\beta$ is the height of the barrier and $W = 1$ is the half width between the two wells. Clearly, the Gibbs distribution corresponding to (4.7) is

$$\mu(x) = \frac{1}{Z} \exp \left[ -\beta \frac{H}{W^4}(x^2 - W^2)^2 \right],$$

(4.8)

where $Z$ is the normalizing constant.

We first apply the basic HMC algorithm to sample (4.8). There are $L = 40$ leapfrog steps in each iteration and the time step is $\Delta t = 2W/L = 0.05$. The initial position of the samples is generated randomly on $[-W,W]$. Drawing $10^5$ samples from (4.8), the results plotted in Figure 5 clearly show that samples are trapped in the local minimum $x = -W$.

To fix the above problem, we decompose $U$ into the sum of $U_1$, a double well potential energy with lower barrier to flatten the landscape and $U_2$, the difference between $U$ and $U_1$. Specifically, we choose

$$U_1(x) = \begin{cases} \lambda U(x), & |x| < W \\ U(x), & |x| \geq W \end{cases}$$

(4.9)
Figure 5: Samples and empirical density obtained by HMC. There are $L = 40$ leapfrog steps with time step size $\Delta t = 2W/L = 0.05$ in each iteration.

Figure 6: The samples and empirical density obtained by SHMC.

\[
U_2(x) = \begin{cases} 
(1 - \lambda)U(x), & |x| < W \\
0, & |x| \geq W 
\end{cases}
\]  

(4.10)

where $\lambda \in (0, 1)$ is a positive constant being small enough. Here, we choose $\lambda = 0.05$. We apply SHMC to draw $10^5$ samples from (4.8). We again set $L = 40$ leapfrog steps with time step $\Delta t = 2W/L$ in each iteration. The samples we obtained and the resulting empirical density are presented in Figure 6. Clearly, the splitting strategy can successfully overcome the local barrier.

4.3.2 Gaussian mixture model

As can be seen from the previous example, an appropriate splitting easily alleviate the problem of generating biased samples in the vanilla HMC algorithm when we have some knowledge about the landscape, e.g. where the local minima are located. However, in many problems including problems in Bayesian inference, the locations of the local minima are generally unknown. In this section, we consider such examples and propose a potential solution by modifying SHMC and RB-SHMC.

To further illustrate our proposed solution, we slightly modify the first example in [59, Section 5.1], which is a classical Bayesian inference problem of mixture models. We will evaluate the performance of sampling from the posterior distribution using SHMC and RB-
SHMC. To be specific, we consider the following Gaussian mixture model:

$$\theta_1 \sim \mathcal{N}(0, \sigma_1^2), \; \theta_2 \sim \mathcal{N}(0, \sigma_2^2),$$

$$y_i \sim \frac{1}{2}\mathcal{N}(\theta_1, \sigma_y^2) + \frac{1}{2}\mathcal{N}(\theta_2, \sigma_y^2),$$

(4.11)

where $\sigma_1^2 = 10$, $\sigma_2^2 = 1$ and $\sigma_y^2 = 0.5$. $N = 100$ data points are drawn from the model with $(\theta_1, \theta_2) = (0, 2)$. Figure 7a shows the potential $U$ corresponding to the posterior distribution, from which one can imagine that the barrier between the two wells of $U$ will prevent samples from moving between these two wells. Indeed, the samples generated by HMC are trapped in one well; see Figure 8a.

Inspired by the metadynamics approach [34], we add scaled Gaussian kernels in the wells to raise the altitudes of the landscape and obtain a new potential energy $U_1$. Defining $U_2 := U - U_1$, we get a decomposition $U = U_1 + U_2$. The locations of the wells are approximated by $\text{mode}^{\text{mar}}(\theta_1)$ and $\text{mode}^{\text{mar}}(\theta_2)$, the modes of the marginal distributions of $\theta_1$ and $\theta_2$ (see Figure 7b), while $h_b$, the height of the barrier in $U$, is estimated by the difference between the altitude at the mid-point between the two wells and the average altitude between the two wells. From our experiments, the scaled Gaussian kernel with height $h_G = h_b + 10/\beta$ and covariance matrix $I_2$ turns out to be a good choice for this specific example. In particular,

$$U_1(\theta) = U(\theta) + 2\pi h_G \left[ \mathcal{N}(\text{mode}^{\text{mar}}(\theta_1), I_2) + \mathcal{N}(\text{mode}^{\text{mar}}(\theta_2), I_2) \right].$$

(4.12)

We choose $\beta = N$ such that the scaling factor of the big summation in $U$ is $1/N$:

$$U(\theta) = \frac{1}{N} \left( \frac{\theta_1^2}{2\sigma_1^2} + \frac{\theta_2^2}{2\sigma_2^2} \right) - \frac{1}{N} \sum_{i=1}^{N} \log \left[ \exp \left( -\frac{(\theta_1 - y_i)^2}{2\sigma_y^2} \right) + \exp \left( -\frac{(\theta_2 - y_i)^2}{2\sigma_y^2} \right) \right].$$

(4.13)

Under the specific setting of our experiment, the distance between the two wells in $U$ is $d_w = 4.1931$ and the height of the barrier is $h_b = 0.4054$. The energy barriers for two wells are reduced to 0.0131 and 0.0113 respectively after the above two scaled Gaussian kernels are added to the wells. Fix the evolution time of each iteration $L\Delta t = 0.4d_w$ and time

---

1. One may obtain the modes of the marginal distributions using any off-the-shelf mode-finding methods: e.g. the function ‘findpeaks()’ in Matlab.
step size $\Delta t = 0.01, 0.001$, we apply HMC, SHMC and RB-SHMC with batch size $s = 10$ to sample from the posterior. For each method, we collect $10^4$ samples after $10^3$ burn-in iterations. The scatter plot of the samples obtained by these three methods are shown in Figures 8. Clearly, SHMC and RB-SHMC can sample from the two modes of the posterior without multiple initializations while the samples of HMC are trapped in one single well. For HMC, we even run the algorithm with longer evolution time per iteration $L\Delta t = 2d_w$. But still, the samples generated by HMC fail to escape from a single well. In summary, one can see that a suitable splitting strategy is powerful in the problem of sampling from a bimodal distribution.

Figure 8: The samples of HMC, SHMC and RB-SHMC with batch size $s = 10$. The time step is fixed to be $\Delta t = 0.01$ and evolution time per iteration is $0.4d_w$.

Table 2 shows the average CPU time and acceptance rate of five runs of SHMC and RB-SHMC, with the corresponding standard deviations recorded in the parentheses. The CPU time spent in the sampling phase of RB-SHMC is less than 40% of that of SHMC and $t_g$, the CPU time to evaluate the summation term in $\nabla U_1$, of RB-SHMC exhibits a significant advantage over that of SHMC, which clearly shows the benefit of random batch in terms of computational efficiency. In the experiment with $\Delta t = 0.01$, the acceptance rate of RB-SHMC is comparatively low since the difference between the exact dynamics and the dynamics using random batch has a relatively large variance when $\Delta t$ is not small enough [39]. Nevertheless, the acceptance rate of RB-SHMC is comparable to that of SHMC when the time step is sufficiently small ($\Delta t = 0.001$).

| $\Delta t$ | $t_g$ (s) | sampling time (s) | acceptance rate |
|-----------|-----------|------------------|-----------------|
| 0.01      | SHMC      | 28.68 (0.4597)   | 36.00 (0.5848)  | 0.2411 (0.0070) |
|           | RB-SHMC   | 6.62 (0.1006)    | 14.31 (0.1730)  | 0.0856 (0.0018) |
| 0.001     | SHMC      | 289.56 (5.3467)  | 361.72 (6.8459) | 0.2386 (0.0045) |
|           | RB-SHMC   | 65.00 (1.0331)   | 139.62 (2.7512) | 0.1903 (0.0010) |

Table 2: The neat CPU time of evaluating the summation term in $\nabla U_1$, the CPU time of the sampling phase and the acceptance rate of SHMC and RB-SHMC. The evolution time per iteration is $L\Delta t = 0.4d_w$. $L = 168$ and $L = 1678$ leapfrog steps are perform respectively for the two choices of $\Delta t$.

Finally, we remark that the application of random batch does inject some noise to the original dynamics. As a result, the invariant measure cannot be preserved exactly. In particular, the random batch approximation may not be accurate enough for some complicated problems due to this extra variance by randomization. Hence, we suggest that practitioners exploit the random batch strategy when computational cost is high whereas the demand on accuracy is relatively low. A theoretical understanding of such computational-accuracy trade-off even for general random batch methods will be an interesting research direction to explore in future works.
Acknowledgements

The work of L. Li was partially supported by NSFC Grant No. 11901389, 12031013, the Strategic Priority Research Program of Chinese Academy of Sciences Grant No. XDA25010403, and Shanghai Science and Technology Commission Grant No. 20JC144100. The work of L. Liu was partially sponsored by Shanghai Pujiang Program Research Grant No.20PJ1408900, Shanghai Municipal Science and Technology Major Project No.2021SHZDZX0102 and Major Program of National Natural Science Foundation of China No.12090024.

A Proof of Lemma 3.1

Proof. Denote $C_q$ as a constant depending on $q$ and $C_q$ may change from line to line. For any $t \in [0, T],$

$$
\frac{d}{dt} \mathbb{E}(|\tilde{p}(t)|^q | F_L) = q \mathbb{E}
\left[
\left|
\tilde{p}(t)^{q-1} - \nabla V_1(\tilde{x}(t)) + \frac{1}{s} \sum_{j \in \xi_t} \nabla \psi_j(\tilde{x})
\right|_{F_L}
\right)
\leq q \left(\|
\nabla V_1\|_{\infty} + \|
\nabla \psi\|_{\infty}
\right) \mathbb{E}
\left[
|\tilde{p}(t)|^{q-1} | F_L
\right)
\leq C_q \mathbb{E}(|\tilde{p}(t)|^q | F_L)$$

(A.1)

where the last line follows from Hölder’s inequality. By integration, one has

$$
\mathbb{E}(|\tilde{p}(t)|^q | F_L) \leq C_q (|\tilde{p}(0)|^q + t^q) \leq C_q (|\tilde{p}(0)|^q + T^q),
$$

(A.2)

and thus equation (3.10) follows from taking expectation w.r.t. the randomness in $F_L$ on both sides and setting $q = 4$. \hfill \square

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