PROCEEDINGS OF SCIENCE

PoS(LATTICE2024)064

On the geometric convergence of HMC on Riemannian manifolds

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We show that HMC converges geometrically on any compact complete Riemannian manifold, even when the full state space is not compact. If the base manifold is non-compact we show that under some fairly mild conditions HMC with an extra Radial Metropolis update step also converges geometrically. We establish some general results about the properties satisfied by its component steps, so our methods may be extended to establish the convergence of other algorithms.

The 41st International Symposium on Lattice Field Theory (LATTICE2024)
28 July–3 August 2024
Liverpool, UK

[*]Speaker

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1. Introduction

The utility of Markov Chain Monte Carlo (MCMC) is based on the condition that a Markov chain converges to a suitable unique fixed point distribution. Sufficient conditions for this to be the case have long been known since the work of Doeblin [1, 2] and Doob [3] for the case where the state space is compact. This suffices, for example, for pure lattice gauge theory computations using HMC but is not directly applicable to variants of the algorithm using partial momentum refreshment, or for non-compact pseudofermion or Higgs fields. This work focuses on the convergence of HMC (recent work on this topic includes [4] and[5]) where the state space is a complete Riemannian manifold. In section 2 we discuss Harris' theorem [6] on Markov chains, which serves as the basis for our proof; in the following sections 3 and 4 we show that the two conditions required hold for HMC. In section 5 we introduce a class of Radial Metropolis steps to deal with many situations where the base manifold is not compact. Note that we show that HMC preserves the target distribution $\bar{\mu}^*$ on the cotangent bundle (phase space) $T^*\mathcal{M}$ but what really matters is the target distribution $\bar{\mu}$ on the base manifold $\mathcal{M}$, which is well-defined from $\bar{\mu}^*$ by disintegration, see for example [7, 8].

2. Harris' ergodic theorem

This theorem [6], which dates back to 1956, is a generalization of Doeblin's condition [1–3] for non-compact state spaces, here we shall follow the elegant simplified proof given by Hairer and Mattingly [9]. Consider a measurable space X with σ-algebra Σ and a Markov kernel $\mathcal{P}(x,\cdot) : X \times \Sigma \to [0,1]$, such that for every $A \in \Sigma$ and every $x \in X$, $\mathcal{P}$ acts on probability measures μ and bounded functions f by

$$(\mu\mathcal{P})(A) \equiv \int_X \mu(dx)\,\mathcal{P}(x,A), \qquad (\mathcal{P}f)(x) \equiv \int_X \mathcal{P}(x,dy) f(y).$$

Harris' theorem gives a pair of sufficient conditions for $\mathcal{P}$ to admit a unique invariant probability distribution:

Theorem 2.1 (Harris)**.** If $\mathcal{P}$ satisfies the following conditions

SDC: *Small set Doeblin's condition*. There is a compact *small set* $C \equiv \{x \in X | L(x) \le R\}$ with $R > 2K/(1-\gamma)$, a constant $\alpha \in (0,1]$, and a probability measure ν such that

$$\inf_{x\in C} \mathcal{P}(x,\cdot) \ge \alpha\,\nu(\cdot); \tag{1}$$

GDC: *Geometric Drift condition*. There is a smooth Lyapunov function $L \to [0,\infty)$, and constants $K \ge 0$, $\gamma \in (0,1)$ such that

$$(\mathcal{P}L)(x) \le \gamma L(x) + K; \tag{2}$$

then there is a metric d_β on the space of probability measures for which $\mathcal{P}$ is a contraction mapping. The Banach fixed point theorem then guarantees the existence of a unique fixed point distribution that is approached geometrically (that is, exponentially in the number of Markov steps) from any starting distribution.

Hairer and Mattingly's approach of the proof in [9] relies on the choice of a finite positive constant β such that $d_\beta(\mu_1\mathcal{P}, \mu_2\mathcal{P})$ contracts both in C and X/C. Our task is to establish that (1) and (2) both hold for HMC.

PoS(LATTICE2024)064

3. The Small set Doeblin's Condition (SDC) for HMC

HMC on Riemannian manifolds

We must specify precisely what we mean by HMC on a Riemannian manifold in order to prove (1). As is usual when considering differentiable manifolds we shall assume that all quantities such as the Hamiltonian and the metric are smooth. The *cotangent bundle* $T^*\mathcal{M}$ of a Riemannian manifold $\mathcal{M}$ is a symplectic manifold with a non-vanishing *fundamental two-form* ω, which may expressed in any coordinate chart as $\omega = \sum_i dq_i \wedge dp_i$ where $q \in \mathcal{M}$ and $p \in T_q^*\mathcal{M}$ (the cotangent space at q). The *Hamiltonian flow* $\Phi : \mathbb{R} \to T^*\mathcal{M}$ is the solution of Hamilton's equations $\dot{\Phi} = \hat{H}$, where $\hat{H}$ is the *Hamiltonian vector field* that satisfies $dH = -\iota_{\hat{H}}\omega$ for some Hamiltonian function H. More details of the definition of HMC on $T^*\mathcal{M}$ can be found in [10] for example.

A single HMC step $S_{\text{HMC}} = S_{\text{MDMC}} \circ S_{\text{MR}}^{\theta}$ is composed of two separate Markov steps with the desired fixed point probability density proportional to $\exp(-H)$.

Partial Momentum Refreshment

This step updates the momentum at fixed position,

$$S_{\text{MR}}^{\theta}(\eta) : (q, p) \mapsto (q, p') = (q, p\cos\theta + \eta\sin\theta),$$

η being a random variable from the Gibbs sampler λ_q:

$$\lambda_q(A) \equiv \frac{1}{\sqrt{\det 2\pi g_q}} \int_A \mathrm{Vol}_L(d\eta)\, e^{-T_q(\eta)},$$

where g_q is the Riemannian metric of $\mathcal{M}$ at q, Vol_L is Lebesgue measure on $\mathbb{R}^{\dim \mathcal{M}}$, and the *kinetic energy* is

$$T_q(p) \equiv \tfrac{1}{2} g_q^{-1}(p, p) = \tfrac{1}{2} g^{ij}(q) p_i p_j. \tag{3}$$

Two successive partial momentum steps with *mixing angle* ψ are equivalent to a single one with mixing angle $\theta = \cos^{-1}\left((\cos\psi)^2\right)$; for $|\theta| \ll 1$ this gives $\theta \approx \sqrt{2}\psi$. To see why this is so consider the joint density of the Gaussian-distributed independent momenta η and η', this is a two-dimensional Gaussian so the distribution of $\eta'' = \eta\cos\alpha + \eta'\sin\alpha$ has the same Gaussian distribution for any $\alpha \in \mathbb{R}$, in particular for $\tan\alpha = 1/\sin\psi$. We thus obtain

$$p'' = p'\cos\psi + \eta'\sin\psi = (p\cos\psi + \eta\sin\psi)\cos\psi - \eta'\sin\psi = p\cos\theta + \eta''\sin\theta$$

with $\cos\theta = (\cos\psi)^2$. Since $S_{\text{MR}}^{\theta} = S_{\text{MR}}^{\psi} \circ S_{\text{MR}}^{\psi}$ we may consider the HMC step to be $S = S_{\text{MR}}^{\psi} \circ S_{\text{MDMC}} \circ S_{\text{MR}}^{\psi}$ without loss of generality.

Molecular Dynamics Monte Carlo

This Markov step consists of the parts $S_{\text{MDMC}} = S_{\text{F}} \circ S_{\text{MC}} \circ S_F \circ S_{\text{MD}} : (q, p) \mapsto (\bar{q}, \bar{p})$, which individually are not valid Markov steps.
$S_{\text{MD}} \equiv \sigma_{\hat{V}}(\frac{1}{2}t) \circ \sigma_{\hat{T}}(t) \circ \sigma_{\hat{V}}(\frac{1}{2}t) : (q_0, p_1) \mapsto (q_1, p_4)$ is a single step symmetric symplectic leapfrog integrator that approximates the evolution of $\hat{H}$ on $T^*\mathcal{M}$,

$$\sigma_{\hat{V}}(\tfrac{1}{2}t) : (q, p) \mapsto (q', p') = \left(q, p - \tfrac{1}{2}t \cdot dV(q)\right), \quad \sigma_{\hat{T}}(t) : (q, p) \mapsto (q', p') = \left(\exp_q(tp^\sharp), \alpha(t)\right),$$

PoS(LATTICE2024)064

where the vector $p^\sharp \equiv g^{-1}(p,\cdot) \in T_q\mathcal{M}$, $\exp_q(tp^\sharp)$ is the exponential map (geodesic) on $\mathcal{M}$ starting at q with initial tangent vector $p^\sharp$, and $\alpha(t)$ is the corresponding parallel transport of the momentum p, i.e., $\sigma_{\hat{V}}$ is a straight line on $T_q^*\mathcal{M}$ and $\sigma_{\hat{T}}$ a (free) geodesic on $\mathcal{M}$ lifted to $T^*\mathcal{M}$.
S_{MC} is a Metropolis step that accepts or rejects the end point of S_{MD}. The probability density of accepting it is

$$(\bar{q},\bar{p}) = \begin{cases} (q',p') & \text{with probability } \mathcal{A}\big((q,p),(q',p')\big) = \min\left(1, e^{-\delta H}\right) \\ (q,p) & \text{otherwise,} \end{cases} \tag{4}$$

where $\delta H \equiv H(q',p') - H(q,p)$.
The momentum flip $S_{\mathrm{F}} : p \mapsto -p$ is required to ensure that detailed balance (reversibility) is satisfied. Since T_q is quadratic this obviously preserves the desired fixed point distribution with density $\propto e^{-H}$. This is not required if full momentum refreshment $\theta = \psi = \pi/2$ is used.

The Convergence Proof

A sufficient condition for (1) in terms of probability density is

$$\inf_{x,y\in C} P(x,y) \geq a \tag{5}$$

for some positive a. We now show this inequality for HMC, that is we find a lower bound on the probability density of an HMC trajectory between two arbitrary points in the small set C. Note that the trjectory does not have to lie in C, it suffices that its starting and ending points do.

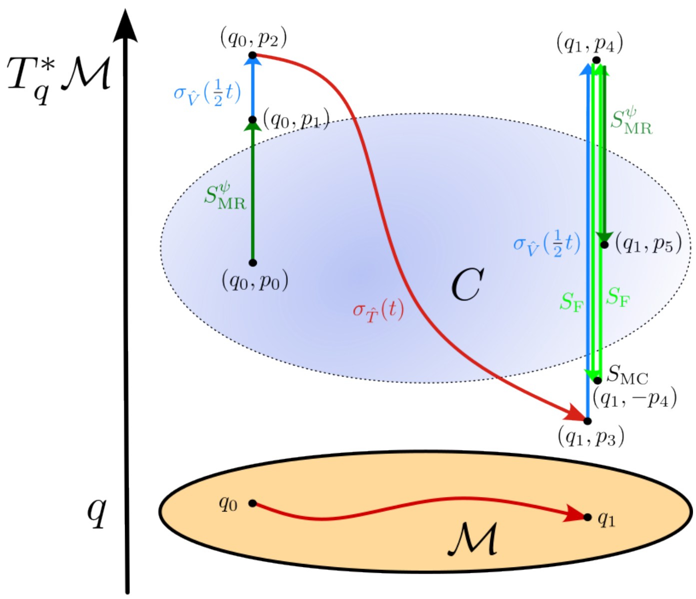

Figure 1: The trajectory of a single HMC step S_{HMC} on $T^*\mathcal{M}$ connecting two arbitrary points (q_0,p_0) and (q_1,p_5) in the small set $C \subseteq T^*\mathcal{M}$. The first S_{F} is required to ensure detailed balance holds for partial momentum refreshment. The second one ensures that the momentum is flipped on Metropolis rejection instead of on acceptance.

PoS(LATTICE2024)064

Theorem 3.1. Consider the step S_{HMC} shown in Figure 1. The Lyapunov function is chosen to be the Hamiltonian $L = H$; it is bounded below, so for simplicity we assume $H \geq 0$. The small set is

$$C = \left\{ (q, p) \,\middle|\, H(q, p) = V(q) + T_q(p) \leq R_H \right\}$$

for some positive $R_H \geq 0$. It must be compact as otherwise $\int_{T^*\mathcal{M}} dx\, e^{-H(x)}$ is not finite hence not a probability distribution. The projection $\pi(C) \subseteq \mathcal{M}$ is thus also compact and hence bounded, being a metric space endowed with the Riemannian distance d which is the length of a minimal geodesic $d\big(\pi(x), \pi(y)\big) \leq R_d\ \forall x, y \in C$. The kernel $\mathcal{P}$ determined by S then satisfies (1).

Proof. Label the intermediate states as

$$(q_0, p_0) \xrightarrow{S^{\psi}_{\text{MR}}} (q_0, p_1) \xrightarrow{\sigma_{\hat V}(\frac{1}{2}t)} (q_0, p_2) \xrightarrow{\sigma_{\hat T}(t)} (q_1, p_3) \xrightarrow{\sigma_{\hat V}(\frac{1}{2}t)} (q_1, p_4)$$
$$\xrightarrow{S_{\text{F}}} (q_1, -p_4) \xrightarrow{S_{\text{MC}}} (q_1, -p_4) \xrightarrow{S_{\text{F}}} (q_1, p_4) \xrightarrow{S^{\psi}_{\text{MR}}} (q_1, p_5).$$

The probability density of the composite HMC step is:

$$P\big((q_0, p_0), (q_1, p_5)\big) = P^{\psi}_{\text{MR}}\left(\frac{p_1 - p_0\cos\psi}{\sin\psi}\right) \cdot \mathcal{A}\big((q_0, p_1), (q_1, p_4)\big) \cdot P^{\psi}_{\text{MR}}\left(\frac{p_5 + p_4\cos\psi}{\sin\psi}\right), \quad (6)$$

We require that $\mathcal{M}$ is geodesically complete so that the geodesic followed by $\pi \circ \sigma_{\hat T}(t)$ exists, where $\pi : T^*\mathcal{M} \to \mathcal{M}$ is the bundle's projection map. Since S^{ψ}_{MR} can generate any momentum from the whole fibre $T^*_{q_0}\mathcal{M}$ the Hopf–Rinow theorem tells us that any pair of points $q_0, q_1 \in \mathcal{M}$ are connected by a geodesic. A geodesic is a curve $c : [t_0, t_1] \to \mathcal{M}$ connecting points $c(t_0)$ and $c(t_1)$ that minimizes the Riemannian distance $d\big(c(t_0), c(t_1)\big) \equiv \int_{t_0}^{t_1} dt\, \sqrt{g_{c(t)}\big(\dot c(t), \dot c(t)\big)}$ between them. Since the Hamiltonian flow $\sigma_{\hat T}(t)$ of $\hat T$ is an isometry the kinetic energy is conserved, and as $q_0, q_1 \in C$ we have

$$R_d \geq d(q_0, q_1) = \int_0^t dt \sqrt{g_{c(t)}\left(p^\sharp(t), p^\sharp(t)\right)} = t\sqrt{2T_{q_0}(p_2)} = t\sqrt{2T_{q_1}(p_3)}$$
$$\implies T_{q_0}(p_2) = T_{q_1}(p_3) \leq \frac{R_d^2}{2t^2}, \quad (7)$$

where $c(0) = q_0$ and $\dot c(0) = p_2^\sharp$. Note that

$$p_2 = p_1 - \tfrac{1}{2}t dV(q_0) = p_0\cos\psi + \eta\sin\psi - \tfrac{1}{2}t dV(q_0) \implies \eta = \frac{p_2 - p_0\cos\psi + \frac{1}{2}t\, dV(q_0)}{\sin\psi}.$$

Since V is smooth it is continuous and thus bounded on the compact set $\pi(C)$, and we shall denote this bound as $R_V = \max_{q\in C} |V(q)|$; moreover its gradient dV is also continuous and thus bounded by $2R_T \equiv \max_{q\in C} \|dV(q)\|_q$ where the norm $\|\alpha\|_q \equiv \sqrt{g_q^{-1}(\alpha, \alpha)}$ is given by the Riemannian metric. According to (3) this norm is just twice the kinetic energy, so $T_{q_0}\big(dV(q_0)\big) \leq R_T$ and $T_{q_1}\big(dV(q_1)\big) \leq R_T$. Using the triangle inequality and (7) we obtain

$$\begin{aligned} T_{q_0}(\eta) &\leq \frac{1}{\sin^2\psi}\left(T_{q_0}(p_2) + T_{q_0}(p_0\cos\psi) + T_{q_0}\left(\tfrac{1}{2}t\, dV(q_0)\right)\right) \\ &\leq \frac{1}{\sin^2\psi}\left(\frac{R_d^2}{2t^2} + \cos\psi^2 R_H + \tfrac{1}{4}t^2 R_T\right) \equiv k_1. \end{aligned} \quad (8)$$

PoS(LATTICE2024)064

$\mathcal{A}$ is also bounded: $T_{q_1}(p_4) = T_{q_1}(p_3 - tdV(q_1)) \leq \frac{R_d^2}{2t^2} + \frac{1}{4}t^2 R_T$, so using (7) again

$$\mathcal{A} = e^{-H(q_1,p_4)+H(q_0,p_1)} \geq e^{-H(q_1,p_4)} \geq \exp\left(-R_V - \frac{R_d^2}{2t^2} - \frac{1}{4}t^2 R_T\right) \equiv e^{-k_2}, \tag{9}$$

hence using (6) we have a uniform bound on the transition probability density in terms of (8) and (9)

$$P\big((q_0,p_1),(q_1,p_5)\big) \geq \frac{\exp(-2k_1 - k_2)}{\sqrt{\det 2\pi g_{q_0} \cdot \det 2\pi g_{q_1}}}.$$

□

At first sight it may be surprising that we only use a single leapfrog step to establish this bound; we might expect the use of many such steps to considerably improve the bound on $\mathcal{A}$. In order to understand why this is not so, suppose we used an exact MD integrator $\sigma_{\hat{H}}$, and suppose there is a very large potential barrier somewhere on $\mathcal{M}$ that separates the initial and final points in $T^*\mathcal{M}$. Since $\sigma_{\hat{H}}$ conserves H it cannot penetrate the barrier, so such a trajectory cannot connect the points. In other words, better integrators are worse at stepping through first-order transitions, and this is situation must be taken account of in any general bound. The proof is valid for HMC with trajectories of multiple steps if the number of steps is sampled from some distribution with the desired mean, with a non-vanishing probability of choosing a single leapfrog step trajectory.

4. The Geometric Drift Condition (GDC) for HMC

Compact $\mathcal{M}$

We first consider the case where $\mathcal{M}$ is compact. If we choose total momentum refreshment ($\theta = \pi/2$) the momenta need not be taken as part of the state space of the Markov process, thus the state space is just $\mathcal{M}$. Condition (5) holds for $C = \mathcal{M}$ and thus establishes Doeblin's condition on the whole $\mathcal{M}$, which is enough to show that the HMC Markov step is a contraction mapping. If partial momentum refreshment is used we must consider the full phase space $T^*\mathcal{M}$ which is non-compact, so we will establish the Geometric Drift Condition (2). We shall call the original condition (2) the *Strong Geometric Drift Condition* (SGDC), whereas if $\gamma \in (0,1]$ we shall call it the *Weak Geometric Drift Condition* (WGDC).

Lemma 4.1. Let $\{\mathcal{P}_i\}_{1\leq i\leq n}$ be a finite set of Markov kernels all of which satisfy the WGDC and at least one of them satisfies the SGDC, then the composite Markov kernel $\mathcal{P}_n \circ \ldots \circ \mathcal{P}_1$ satisfies the SGDC (all with respect to the same Lyapunov function L).

Since we have chosen Hamiltonian H to be the Lyapunov function in Theorem 3.1, the same Lyapunov function must be used for the GDC. We shall show that S_{MR}^{θ} satisfies the SGDC and S_{MDMC} satisfies the WGDC, hence by Lemma 4.1 S_{HMC} satisfies the SGDC.

Theorem 4.1. For compact $\mathcal{M}$ and $L = H$, S_{MR}^{θ} satisfies the SGDC for $\theta \neq 0$.

PoS(LATTICE2024)064

Proof. V is continuous, so since $\mathcal{M}$ is compact $V(\mathcal{M})$ is too, the Heine–Borel theorem tells us that $V(\mathcal{M})$ is closed and bounded, so $0 \le V(q) \le V_{\max}$ for a finite $V_{\max}$. It is then simple to verify that

$$\begin{aligned}(\mathcal{P}^{\theta}_{\text{MR}}H)(q,p) \equiv \langle H(q,p)\rangle_\eta &= V(q) + \langle T_q(S^{\theta}_{\text{MR}} \circ p)\rangle_\eta = V(q) + \langle T_q(p\cos\theta + \eta\sin\theta)\rangle_\eta \\ &= V(q) + (\cos\theta)^2 T_q(p) + (\sin\theta)^2\langle\eta^2\rangle_\eta \le (\cos\theta)^2 H(q,p) + (\sin\theta)^2 g_{\max} + V_{\max}\end{aligned}$$

using $\langle 1\rangle = 1$, $\langle\eta\rangle = 0$, $\langle\eta^2\rangle_\eta = \det g_q \le g_{\max}$ where $g_{\max} \equiv \max_{q\in\mathcal{M}} \det g_q$ is finite. □

Theorem 4.2. The Metropolis algorithm satisfies the WGDC.

Proof. The Metropolis acceptance probability is $\mathcal{A}(x,y) = \min\left(1, e^{-\delta H}\right)$ with $\delta H = H(y) - H(x)$, so the average of H after the Metropolis step is

$$(\mathcal{P}H)(x) = \mathcal{A}H(y) + (1-\mathcal{A})H(x) = H(x) + \mathcal{A}\,\delta H,$$

and $\mathcal{A}\,\delta H = e^{-\delta H}\delta H \le 1/e$. We thus have the WGDC $(\mathcal{P}H)(x) \le H(x) + 1/e$. □

We conclude from Theorems 4.1, 4.2, and Lemma 4.1 that

Corollary 4.1. HMC on a compact Riemannian manifold satisfies the SGDC with Lyapunov function H

$$(\mathcal{P}_{\text{HMC}})H(x) \le (\cos\theta)^2 H(x) + (\sin\theta)^2(g_{\max} + V_{\max}) + 1/e.$$

We note that essentially the same argument establishes the geometric convergence of HMC with pseudofermions since although the pseudofermion fields lie in a non-compact manifold they are sampled using a heatbath (Gibbs) algorithm.

5. Non-compact $\mathcal{M}$ and Radial Metropolis

The obstruction to establishing the SGDC (2) with $L = H$ for the HMC algorithm on a non-compact base manifold $\mathcal{M}$ is that the potential cannot be bounded (otherwise the density $\propto e^{-H}$ would not be normalizable), as then S^{θ}_{MR} only satisfies the WGDC. It is thus clear that HMC cannot converge geometrically on an arbitrary complete Riemannian manifold. We shall therefore introduce an additional Markov step that both has the desired fixed point distribution and satisfies the SGDC in most of the interesting cases.

Definition 5.1. We consider the case where the state space admits a global radial coordinate r with all the other coordinates ϕ spanning a compact manifold $\mathcal{S}$. This always holds locally by Gauss' lemma, but it also holds globally for many theories of interest such those for those where $\mathcal{M} = \mathbb{R}^{\dim\mathcal{M}}$ is a Euclidean space. We also require $T_q(p) = T(p)$ independent of r, which certainly holds for the interesting case of homogeneous spaces. In such cases we define the a *Radial Metropolis step* S_{RM} that consists of either a forward radial update $f : r \mapsto r_f > r$ or a backward radial update $b : r \mapsto r_b < r$ chosen with equal probability, followed by a Metropolis step.

Observe that the Radial Metropolis step acts on the base manifold $\mathcal{M}$ rather than $T^*\mathcal{M}$. Therefore, as in HMC, we combine it with a (partial) momentum refreshment step S^{θ}_{MR}. If the former satisfies $(\mathcal{P}_{\text{RM}}V)(r) \le \gamma V(r) + K$ then since the latter satisfies $(\mathcal{P}^{\theta}_{\text{MR}}T)(p) \le (\cos\theta)^2 T(p) + (\sin\theta)^2 g_{\max}$ we have $(\mathcal{P}_{\text{MR}} \circ \mathcal{P}_{\text{RM}}H)(q,p) \le \max\left(\gamma, (\cos\theta)^2\right)H(q,p) + \left(K + (\sin\theta)^2 g_{\max}\right)$ as required for the SGDC.

PoS(LATTICE2024)064

Theorem 5.1 (Radial GDC)**.** For the Radial Metropolis step $\mathcal{P}_{\text{RM}}$ described above, let $V(r,\phi)$ be the potential, for brevity write $V \equiv V(r,\phi)$, $V_f \equiv V(r_f,\phi)$, and $V_b \equiv V(r_b,\phi)$, all corresponding to some arbitrary but fixed angular coordinates ϕ. Moreover, let $V'(r)$ be the effective potential used in the Metropolis step which may differ from $V(r)$. If there is a constant $R > 0$ such that (i) for $r \le R$, $\exists U(\phi) > 0$ such that $\max\bigl(V_b, V(r), V_f\bigr) \le U(\phi)$, and for $r \ge R$ the following hold: (ii) V' is monotone non-decreasing, $V'_b \le V'(r) \le V'_f$, (iii) $e^{-\Delta(V'-V)} \le m$ for some $m > 0$, and (iv) there are constants $\rho \in [0,1)$ and $N \ge 0$ such that $V_b \le \rho V(r) + N$; then $\mathcal{P}_{\text{RM}}$ satisfies the SGDC.

Proof. Denote $\Delta V \equiv V_f - V(r)$ and similar for $\Delta V'$. We consider regions $r \ge R$ where backward steps are always accepted and $r \le R$ separately to obtain

$$(\mathcal{P}_{\text{RM}}V)(r) = \tfrac{1}{2}\sum_{i\in\{f,b\}}\Bigl(V_i\mathcal{A}(r,r_i) + V(r)\bigl(1-\mathcal{A}(r,r_i)\bigr)\Bigr)$$

$$\begin{cases} = \tfrac{1}{2}\Bigl(V_f e^{-\Delta V'} + V(r)\bigl(1-e^{-\Delta V'}\bigr) + V_b\Bigr) = \tfrac{1}{2}\Bigl(\Delta V\, e^{-\Delta V'} + V(r) + V_b\Bigr) & \\ \qquad \le \tfrac{1}{2}\left(V(r) + V_b + \tfrac{1}{e}e^{-\Delta(V'-V)}\right) \le \tfrac{1}{2}(1+\rho)V(r) + \tfrac{1}{2}\left(\tfrac{m}{e}+N\right) & \text{if } r \ge R, \\ \le \max(V_b, V(r), V_f) \le U(\phi) & \text{if } r \le R. \end{cases}$$

This gives the desired SGDC $(\mathcal{P}_{\text{RM}}V)(r) \le \gamma_\phi V(r) + K_\phi$ for the direction ϕ with $\gamma_\phi = \frac{1}{2}(1+\rho) < 1$ and $K_\phi = \max\left(U(\phi), \frac{1}{2}\left(\frac{m}{e}+N\right)\right)$. Since the angular coordinates span a compact manifold $\mathcal{S}$ the quantities $\gamma \equiv \max_{\phi\in\mathcal{S}}\gamma_\phi < 1$, $K \equiv \max_{\phi\in\mathcal{S}} K_\phi$ are finite, so we have a uniform SGDC $\mathcal{P}_{\text{RM}}V \le \gamma L(r) + K$ on the whole of $\mathcal{M}$. □

5.1 Power potential $V(r) = kr^\alpha + o(r^\alpha)$.

Let $f(r) = (1+\varepsilon)r$ and $b(r) = r/(1+\varepsilon)$ for some $\varepsilon > 0$. $f \circ b = \mathbb{I}$ so the update is reversible. $\mathcal{P}_{\text{RM}}$ does not preserve the Riemannian measure $d\mathrm{Vol}_L(dr) \propto r^{D-1}\,dr$ in D dimensional Euclidean space, also we must include the Jacobian, leading to the "effective potential" $V'(r) \equiv V(r) + (D-1)\log r + \frac{1}{2}\log\det df/dr$ for Metropolis. It is easy to verify that (i)–(iii) are satisfied, where in (iii) $m = (1+\varepsilon)^{1-D}$, and for (iv)

$$V_b = kr_b^\alpha + o(r_b^\alpha) \le (1+\varepsilon)^{-\alpha}V(r) + K.$$

5.2 Logarithmic potential $V(r) = \beta\log r + o(\log r)$.

Let $f(r) = \bigl(1+\varepsilon r^\delta\bigr)r$ for some $\delta, \varepsilon \in (0,1)$, and its corresponding (implicit) inverse mapping $b : r \mapsto r_b$, to obtain $V'(r) = \beta\log r + (D-1)\log r + \frac{1}{2}\log(1+\varepsilon(1+\delta)r^\delta)$. For the distribution to be normalizable it is necessary that $\beta + D - 1 > 1 \iff \beta + D > 2$. (i)–(iii) are satisfied, with $m = 1$ and for (iv)

$$\log r = \log r_b + \log(1+\varepsilon r_b^\delta) \ge (1+\delta)\log r_b + \log\varepsilon \implies \beta\log r_b \le \frac{\beta}{1+\delta}(\log r - \log\varepsilon),$$

where r_b is implicitly determined from $r = \bigl(1+\varepsilon r_b^\delta\bigr)r_b$ since $f \circ b = 1$.

Acknowledgements

We would like to thank Martin Lüscher for providing us with a copy of his notes [11].

PoS(LATTICE2024)064

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PoS(LATTICE2024)064