Hybrid Monte Carlo methods for sampling probability measures on submanifolds

T. Lelièvre

CERMICS - Ecole des Ponts ParisTech & Matherials team - INRIA

Joint work with M. Rousset and G. Stoltz

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Objective

Let us be given a submanifold of $\mathbb{R}^d$:

$$\mathcal{M} = \left\{ q \in \mathbb{R}^d, \, \xi(q) = 0 \right\}$$

where $\xi : \mathbb{R}^d \to \mathbb{R}^m$ is a given smooth function (with $m < d$) such that

$$G(q) = [\nabla \xi(q)]^T \, \nabla \xi(q) \in \mathbb{R}^{m \times m}$$

is an invertible matrix for all q in a neighborhood of $\mathcal{M}$. The objective is to sample the probability measure:

$$\nu(dq) = Z_\nu^{-1} \, \mathrm{e}^{-V(q)} \, \sigma_{\mathcal{M}}(dq), \qquad Z_\nu = \int_{\mathcal{M}} \mathrm{e}^{-V(q)} \, \sigma_{\mathcal{M}}(dq) < \infty,$$

where $\sigma_{\mathcal{M}}(dq)$ is the Riemannian measure on $\mathcal{M}$ induced by the scalar product $\langle \cdot, \cdot \rangle$ defined in the ambient space $\mathbb{R}^d$.

Motivation

Such problems arise in many contexts: constrained mechanical systems with noise, statistics, ...

One example is computational statistical physics: free energy calculations. If $X \sim \rho$ where $\rho(dq) = Z^{-1} \mathrm{e}^{-V(q)}\, dq$, then $\xi(X) \sim \xi_{\#}\rho$. Let us define $A : \mathbb{R}^m \to \mathbb{R}$ by:

$$\mathrm{e}^{-A(z)} dz = \xi_{\#}\rho(dz).$$

Then, using the co-area formula,

$$\nabla A(0) = \mathbb{E}_\rho(f(X)|\xi(X) = 0) = \int_{\mathcal{M}} f(q)\tilde{\nu}(dq)$$

where $f = G^{-1}\nabla\xi \cdot \nabla V - \mathrm{div}(G^{-1}\nabla\xi)$ and

$$\tilde{\nu}(dq) = Z_{\tilde{\nu}}^{-1}\, \mathrm{e}^{-\tilde{V}(q)}\, \sigma_{\mathcal{M}}(dq)$$

where $\tilde{V}(q) = V(q) + \frac{\ln \det G(q)}{2}$.

$\longrightarrow$ Thermodynamic integration.

Plan

The constrained overdamped Langevin dynamics

The constrained Langevin dynamics

The reverse projection check

Numerical experiments

Step 1: the overdamped Langevin dynamics (1/3)

The constrained overdamped Langevin dynamics (W_t is a d-dimensional Brownian motion):

$$\begin{cases} dq_t = -\nabla V(q_t)\,dt + \sqrt{2}dW_t + \nabla\xi(q_t)d\lambda_t \\ d\lambda_t \in \mathbb{R}^m \text{ such that } \xi(q_t) = 0 \end{cases}$$

is ergodic with respect to ν. It can indeed be rewritten as:

$$dq_t = \Pi(q_t) \circ (-\nabla V(q_t)\,dt + \sqrt{2}dW_t)$$

where $\circ$ denotes the Stratonovitch product and

$$\Pi(q) = \mathrm{Id} - \nabla\xi(q) G^{-1}(q) [\nabla\xi(q)]^T$$

is the orthogonal projector from $\mathbb{R}^d$ to $T_q\mathcal{M}$. One can then use the divergence theorem on manifolds to prove that its unique invariant measure is ν [Ciccotti, TL, Vanden-Einjden, 2008].

Step 1: the overdamped Langevin dynamics (2/3)

Discretization of the constrained overdamped Langevin dynamics:

$$\left\{ \begin{array}{l} q^{n+1} = q^n - \nabla V(q^n)\Delta t + \sqrt{2\Delta t} G_n + \nabla\xi(q_n)\lambda^n \\ \lambda^n \in \mathbb{R}^m \text{ such that } \xi(q^{n+1}) = 0 \end{array} \right.$$

where $G_n \sim \mathcal{N}(0, \mathrm{Id})$.

Remark: By choosing $V = \tilde{V}$, an approximation of $\nabla A(0)$ is given by the average of the Lagrange multipliers:

$$\lim_{T\to\infty} \lim_{\Delta t \to 0} \frac{1}{T} \sum_{n=1}^{T/\Delta t} \lambda^n = \nabla A(0).$$

Step 1: the overdamped Langevin dynamics (3/3)

Time discretization implies a bias, which is of order Δt. Let $\nu_{\Delta t}$ be the invariant measure for $(q^n)_{n\geq 0}$, then [Faou, TL, 2010]: for all smooth function $\varphi : \mathcal{M} \to \mathbb{R}$, $\exists C$, for small Δt,

$$\left| \int_{\mathcal{M}} \varphi d\nu_{\Delta t} - \int_{\mathcal{M}} \varphi d\nu \right| \leq C\Delta t.$$

The proof is based on expansions à la Talay-Tubaro.

How to eliminate the bias?

Metropolis-Hastings is not easy to apply since the probability to go from q^n to q^{n+1} does not have a simple analytical expression.

Idea: lift the problem to phase space in order to use the symmetry up to momentum reversal of the constrained Hamiltonian dynamics.

Step 2: the Langevin dynamics (1/8)

Extended measure in phase space:

$$\mu(dq\,dp) = Z_\mu^{-1} \mathrm{e}^{-H(q,p)}\, \sigma_{T^*\mathcal{M}}(dq\,dp)$$

where $H(q,p) = V(q) + \frac{|p|^2}{2}$ and $\sigma_{T^*\mathcal{M}}(dq\,dp)$ is the phase space Liouville measure on

$$T^*\mathcal{M} = \left\{(q,p) \in \mathbb{R}^d \times \mathbb{R}^d,\, \xi(q) = 0 \text{ and } [\nabla\xi(q)]^T p = 0\right\}.$$

The marginal of μ in q is ν. Indeed, the measure μ rewrites:

$$\mu(dq\,dp) = \nu(dq)\,\kappa_q(dp)$$

where

$$\kappa_q(dp) = (2\pi)^{\frac{m-d}{2}} \mathrm{e}^{-\frac{|p|^2}{2}} \sigma_{T_q^*\mathcal{M}}(dp)$$

with $T_q^*\mathcal{M} = \left\{p \in \mathbb{R}^d,\, [\nabla\xi(q)]^T p = 0\right\} \subset \mathbb{R}^d$.

Remark: Here and in the following, we assume for simplicity that the mass tensor $M = \mathrm{Id}$. It is easy to generalize the algorithm and the analysis to the case $M \neq \mathrm{Id}$.

Step 2: the Langevin dynamics (2/8)

The constrained Langevin dynamics ($\gamma > 0$ is the friction parameter)

$$\begin{cases} dq_t = p_t \, dt \\ dp_t = -\nabla V(q_t) \, dt - \gamma p_t \, dt + \sqrt{2\gamma} dW_t + \nabla \xi(q_t) \, d\lambda_t \\ \xi(q_t) = 0 \end{cases}$$

is ergodic with respect to μ. Notice that $[\nabla \xi(q_t)]^T p_t = 0$.
It can be seen as the composition (operator splitting) of two dynamics:

- the constrained Hamiltonian dynamics:

$$\begin{cases} dq_t = p_t \, dt \\ dp_t = -\nabla V(q_t) \, dt + \nabla \xi(q_t) \, d\lambda_t \\ \xi(q_t) = 0. \end{cases}$$

- the Ornstein-Uhlenbeck process on momenta:

$$\begin{cases} dq_t = 0 \\ dp_t = -\gamma p_t \, dt + \sqrt{2\gamma} dW_t + \nabla \xi(q_t) \, d\lambda_t \\ [\nabla \xi(q_t)]^T p_t = 0. \end{cases}$$

Step 2: the Langevin dynamics (3/8)

Discretization of the Ornstein-Uhlenbeck process on momenta: midpoint Euler leaves the measure κ_{q^n} and thus μ invariant:

$$\begin{cases} p^{n+1} = p^n - \dfrac{\Delta t}{2}\gamma\,(p^n + p^{n+1}) + \sqrt{2\gamma\Delta t}\, G^n + \nabla\xi(q^n)\,\lambda^n, \\ \nabla\xi(q^n)^T p^{n+1} = 0, \end{cases}$$

In the following, we denote one step of this dynamics by $\Psi_{\Delta t}^{OU} : T^*\mathcal{M} \to T^*\mathcal{M}$:

$$\Psi_{\Delta t}^{OU}(q^n, p^n) = (q^n, p^{n+1}).$$

Remark: The projection is always well defined, and easy to implement:

$$p^{n+1} = \Pi^*(q^n)\left(\frac{(1-\Delta t\gamma/2)p^n + \sqrt{2\gamma\Delta t}\, G^n}{1+\Delta t\gamma/2}\right)$$

where

$$\Pi^*(q) = \mathrm{Id} - \nabla\xi(q)G^{-1}(q)[\nabla\xi(q)]^T$$

is the orthogonal projector from $\mathbb{R}^d$ to $T_q^*\mathcal{M}$.

Step 2: the Langevin dynamics (4/8)

Discretization of the constrained Hamiltonian dynamics (RATTLE):

$$\begin{cases} p^{n+1/2} = p^n - \dfrac{\Delta t}{2} \nabla V(q^n) + \nabla \xi(q^n)\, \lambda^{n+1/2}, \\ q^{n+1} = q^n + \Delta t\, p^{n+1/2}, \\ \xi(q^{n+1}) = 0, & (C_q) \\ p^{n+1} = p^{n+1/2} - \dfrac{\Delta t}{2} \nabla V(q^{n+1}) + \nabla \xi(q^{n+1})\, \lambda^{n+1}, \\ \left[\nabla \xi(q^{n+1})\right]^T p^{n+1} = 0, & (C_p) \end{cases}$$

where $\lambda^{n+1/2} \in \mathbb{R}^m$ are the Lagrange multipliers associated with the position constraints (C_q), and $\lambda^{n+1} \in \mathbb{R}^m$ are the Lagrange multipliers associated with the velocity constraints (C_p).

In the following, we denote one step of the RATTLE dynamics by $\Psi_{\Delta t}^{RATTLE} : T^*\mathcal{M} \to T^*\mathcal{M}$:

$$\Psi_{\Delta t}^{RATTLE}(q^n, p^n) = (q^{n+1}, p^{n+1}).$$

Step 2: the Langevin dynamics (5/8)

Discretization of the constrained Langevin dynamics (Strang splitting):

$$\begin{cases} (q^n, p^{n+1/4}) = \Psi^{OU}_{\Delta t/2}(q^n, p^n) \\ (q^{n+1}, p^{n+3/4}) = \Psi^{RATTLE}_{\Delta t}(q^n, p^{n+1/4}) \\ (q^{n+1}, p^{n+1}) = \Psi^{OU}_{\Delta t/2}(q^{n+1}, p^{n+3/4}) \end{cases}$$

But there is still a bias due to time discretization...

Step 2: the Langevin dynamics (6/8)

Let us denote by

$$S(q,p) = (q,-p)$$

the momentum reversal map and

$$\Psi_{\Delta t}(q,p) = S\left(\Psi_{\Delta t}^{RATTLE}(q,p)\right).$$

Fundamental properties of RATTLE: for Δt small enough,

- $\Psi_{\Delta t}\left(\Psi_{\Delta t}(q,p)\right) = (q,p)$
- Ψ_{Δ} is a symplectic map, which thus preserves $\sigma_{T^*\mathcal{M}}$

[Hairer, Lubich, Wanner, 2006] [Leimkuhler, Reich, 2004].

One can thus add a Metropolis Hastings rejection step to get unbiased samples: if $(q',p') = \Psi_{\Delta t}(q,p)$, the MH ratio writes:

$$\frac{\delta_{\Psi_{\Delta t}^{\mathrm{rev}}(q',p')}(dq\,dp)\,\mathrm{e}^{-H(q',p')}\,\sigma_{T^*\mathcal{M}}(dq'\,dp')}{\delta_{\Psi_{\Delta t}^{\mathrm{rev}}(q,p)}(dq'\,dp')\,\mathrm{e}^{-H(q,p)}\,\sigma_{T^*\mathcal{M}}(dq\,dp)} = \mathrm{e}^{-H(q',p')+H(q,p)}.$$

Step 2: the Langevin dynamics (7/8)

Constrained Generalized Hybrid Monte Carlo algorithm ([TL, Rousset, Stoltz 2012], constrained version of [Horowitz 1991]):

$$\begin{cases} (q^n, p^{n+1/4}) = \Psi^{OU}_{\Delta t/2}(q^n, p^n) \\ (\tilde{q}^{n+1}, \tilde{p}^{n+3/4}) = \Psi_{\Delta t}(q^n, p^{n+1/4}) \\ \text{ If } U^n \leq \mathrm{e}^{-H(\tilde{q}^{n+1}, \tilde{p}^{n+3/4}) + H(q^n, p^{n+1/4})} \\ \qquad \text{accept the proposal: } (q^{n+1}, p^{n+3/4}) = (\tilde{q}^{n+1}, \tilde{p}^{n+3/4}) \\ \qquad \text{else reject the proposal: } (q^{n+1}, p^{n+3/4}) = (q^n, p^{n+1/4}). \\ \tilde{p}^{n+1} = -p^{n+3/4} \\ (q^{n+1}, p^{n+1}) = \Psi^{OU}_{\Delta t/2}(q^{n+1}, \tilde{p}^{n+1}) \end{cases}$$

where $U^n \sim \mathcal{U}(0,1)$.

Remark: If $\Delta t \gamma/4 = 1$, then $p^{n+1/4} = \Pi^*(q^n)(G^n) \sim \kappa_{q^n}$. One thus obtains a constrained HMC algorithm, consistent with the constrained overdamped Langevin discretized with a timestep $\Delta t^2/2$ (MALA).

Step 2: the Langevin dynamics (8/8)

Problem: RATTLE is only well defined and reversible for locally small timesteps. Three possible difficulties:

- $\Psi_{\Delta t}(q,p)$ may not be defined;
- If $\Psi_{\Delta t}(q,p)$ is well defined, $\Psi_{\Delta t}\left(\Psi_{\Delta t}(q,p)\right)$ may not be defined;
- If $\Psi_{\Delta t}(q,p)$ and $\Psi_{\Delta t}\left(\Psi_{\Delta t}(q,p)\right)$ are well defined, one may have $\Psi_{\Delta t}\left(\Psi_{\Delta t}(q,p)\right) \neq (q,p)$.

Step 3: the reverse projection check (1/8)

In order to introduce the ensemble where RATTLE is well defined, let us rewrite the RATTLE dynamics as follows:

$$\begin{cases} q^{n+1} = q^n + \Delta t \left[p^n - \dfrac{\Delta t}{2} \nabla V(q^n) \right] + \Delta t \nabla \xi(q^n)\, \lambda^{n+1/2}, \\ p^{n+1} = \Pi^*(q^n) \left(p^n - \dfrac{\Delta t}{2} \left(\nabla V(q^n) + \nabla V(q^{n+1}) \right) + \nabla \xi(q^n)\, \lambda^{n+1/2} \right) \end{cases}$$

where

$$\Delta t \lambda^{n+1/2} = \Lambda \left(q^n, q^n + \Delta t \left[p^n - \frac{\Delta t}{2} \nabla V(q^n) \right] \right).$$

The function $\Lambda : \mathcal{D} \to \mathbb{R}^m$, where $\mathcal{D}$ is an open set of $\mathcal{M} \times \mathbb{R}^d$ is the Lagrange multiplier function which satisfies:

$$\forall (q, \tilde{q}) \in \mathcal{D},\ \tilde{q} + \nabla \xi(q) \Lambda(q, \tilde{q}) \in \mathcal{M}.$$

We will discuss later how to rigorously build such a Lagrange multiplier function.

Step 3: the reverse projection check (2/8)

The function Λ is only defined on $\mathcal{D}$ and thus $\Psi_{\Delta t}^{RATTLE}$ is only defined on the open set:

$$A = \left\{ (q,p) \in T^*\mathcal{M}, \ \left(q, q + \Delta t \, M^{-1} \left[p - \frac{\Delta t}{2} \nabla V(q) \right] \right) \in \mathcal{D} \right\}$$

and likewise, $\Psi_{\Delta t} = S \circ \Psi_{\Delta t}^{RATTLE}$ is defined on A.

Proposition ([TL, Rousset, Stoltz 2018])

If Λ is C^1, then $\Psi_{\Delta t} : A \to T^*\mathcal{M}$ is a C^1 local diffeomorphism, locally preserving the phase-space measure $\sigma_{T^*\mathcal{M}}(dq\, dp)$.

Step 3: the reverse projection check (3/8)

Let us now introduce the RATTLE dynamics with momentum reversal and reverse projection check: for any $(q,p) \in T^*\mathcal{M}$,

$$\Psi^{\mathrm{rev}}_{\Delta t}(q,p) = \Psi_{\Delta t}(q,p) 1_{\{(q,p)\in B\}} + (q,p) 1_{\{(q,p)\notin B\}}$$

where the set $B \subset A \subset T^*\mathcal{M}$ is defined by

$$B = \Big\{ (q,p) \in A,\, \Psi_{\Delta t}(q,p) \in A \text{ and } (\Psi_{\Delta t}(\Psi_{\Delta t})(q,p)) = (q,p) \Big\}.$$

Proposition ([TL, Rousset, Stoltz 2018])

Let us assume that Λ is C^1 and satisfies the non-tangential condition: $\forall (q,\tilde{q}) \in \mathcal{D}$,

$$\left[\nabla\xi\left(\tilde{q} + \nabla\xi(q)\Lambda(q,\tilde{q})\right)\right]^T \nabla\xi(q) \in \mathbb{R}^{m\times m} \text{ is invertible.}$$

Then, the set B is the union of path connected components of the open set $A \cap \Psi^{-1}_{\Delta t}(A)$. It is thus an open set of $T^*\mathcal{M}$. Moreover, $\Psi^{\mathrm{rev}}_{\Delta t} : T^*\mathcal{M} \to T^*\mathcal{M}$ is globally well defined, preserves globally the measure $\sigma_{T^*\mathcal{M}}(dq\,dp)$ and satisfies $\Psi^{\mathrm{rev}}_{\Delta t} \circ \Psi^{\mathrm{rev}}_{\Delta t} = \mathrm{Id}$.

Step 3: the reverse projection check (4/8)

Practically, $\Psi^{\mathrm{rev}}_{\Delta t}(q,p)$ is obtained from $(q,p) \in T^*\mathcal{M}$ by the following procedure:

(1) check if (q,p) is in A; if not return (q,p);

(2) when $(q,p) \in A$, compute the configuration (q^1,p^1) obtained by one step of the RATTLE scheme;

(3) check if $(q^1,-p^1)$ is in A; if not, return (q,p);

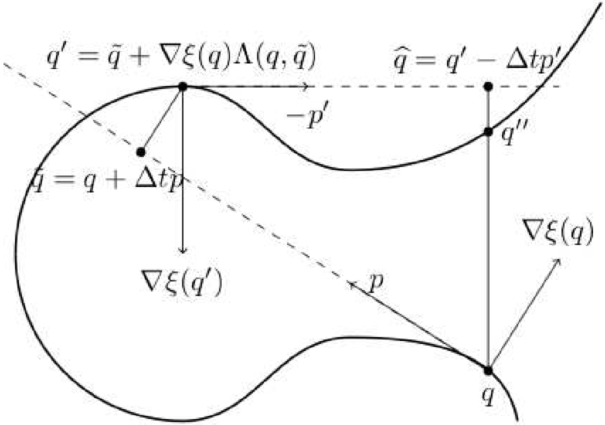
(4) compute the configuration $(q^2,-p^2)$ obtained by one step of the RATTLE scheme starting from $(q^1,-p^1)$;

(5) if $(q^2,p^2) = (q,p)$, return $(q^1,-p^1)$; otherwise return (q,p).

The steps (3)-(4)-(5) correspond to the *reverse projection check* [Goodman, Holmes-Cerfon, Zappa, 2017].

Step 3: the reverse projection check (5/8)

The reverse projection check is useful!



Here, $V = 0$ and the projection is defined as the closest point to $\mathcal{M}$. Notice that $q'' \neq q$!

Step 3: the reverse projection check (6/8)

Assume for simplicity that $\exists\alpha > 0$, $\{q \in \mathbb{R}^d, \|\xi(q)\| \leq \alpha\}$ is compact. How to build admissible Lagrange multiplier functions?

- Theoretically, one can use the implicit function theorem to build a function $\Lambda(q, \tilde{q})$ for $\tilde{q}$ in a neighborhood of q.
- Numerically, one can use the Newton algorithm to extend this local construction and compute the Lagrange multipliers for $\tilde{q}$ far from q: perform a given number of iterations of the Newton algorithm; the set $\mathcal{D}$ is defined as the configurations for which convergence is obtained.

One can check that B is non empty with these Lagrange multiplier functions.

Both constructions rely on the existence of a Lagrange multiplier function $\Lambda : \mathcal{D}_{\rm imp} \to \mathbb{R}^m$ where $\mathcal{D}_{\rm imp}$ is an open subset of $\mathcal{M} \times \mathbb{R}^d$ which contains $\{(q, \tilde{q}) \in \mathcal{M} \times \mathcal{M}, [\nabla\xi(q)]^T \nabla\xi(\tilde{q}) \text{ is invertible}\}$.

Step 3: the reverse projection check (7/8)

The constrained GHMC algorithm writes:

$$\begin{cases} (q^n, p^{n+1/4}) = \Psi^{OU}_{\Delta t/2}(q^n, p^n) \\ (\tilde{q}^{n+1}, \tilde{p}^{n+3/4}) = \Psi^{rev}_{\Delta t}(q^n, p^{n+1/4}) \\ \text{ If } U^n \leq \mathrm{e}^{-H(\tilde{q}^{n+1}, \tilde{p}^{n+3/4}) + H(q^n, p^{n+1/4})} \\ \qquad \text{accept the proposal: } (q^{n+1}, p^{n+3/4}) = (\tilde{q}^{n+1}, \tilde{p}^{n+3/4}) \\ \qquad \text{else reject the proposal: } (q^{n+1}, p^{n+3/4}) = (q^n, p^{n+1/4}) \\ \tilde{p}^{n+1} = -p^{n+3/4} \\ (q^{n+1}, p^{n+1}) = \Psi^{OU}_{\Delta t/2}(q^{n+1}, \tilde{p}^{n+1}) \end{cases}$$

where $U^n \sim \mathcal{U}(0,1)$.

Proposition ([TL, Rousset, Stoltz 2018])

The Markov chain $(q^n, p^n)_{n \geq 0}$ admits μ as an invariant measure.

To prove ergodicity, it remains to check irreducibility [Hartmann, 2008].

Step 3: the reverse projection check (8/8)

Remarks:

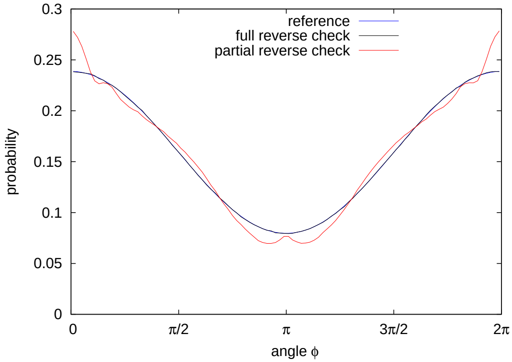
- In $\Psi^{rev}_{\Delta t}$, one can use any potential V! Choosing the potential V of the target measure is good to increase the acceptance probability.
- If $\Delta t\gamma/4 = 1$, one obtains a HMC (or MALA) algorithm. If $\Delta t\gamma/4 = 1$ and $V = 0$ in $\Psi^{rev}_{\Delta t}$, this is a constrained random walk MH algorithm [Goodman, Holmes-Cerfon, Zappa, 2017].
- In pratice, one can use K steps of RATTLE within Ψ^{rev} to get less correlated samples. [Bou-Rabee, Sanz Serna]
- If $\Psi^{rev}_{\Delta t}(q^n, p^{n+1/4}) = \Psi_{\Delta t}(q^n, p^{n+1/4})$ (reverse projection check OK), one obtains a consistent discretization of the constrained Langevin dynamics.
- Similar ideas can be used to enforce inequality constraints.
- It may be interesting for numerical purposes to consider non identity mass matrices.

Numerical experiments (1/3)

Let $\mathcal{M}$ be the three-dimensional torus $\mathcal{M} = \{q \in \mathbb{R}^3,\ \xi(q) = 0\}$ where

$$\xi(q) = \left(R - \sqrt{x^2 + y^2}\right)^2 + z^2 - r^2,$$

with $0 < r < R$. Let us consider for $\nu = \sigma_{T^*\mathcal{M}}$ the uniform measure on $\mathcal{M}$.

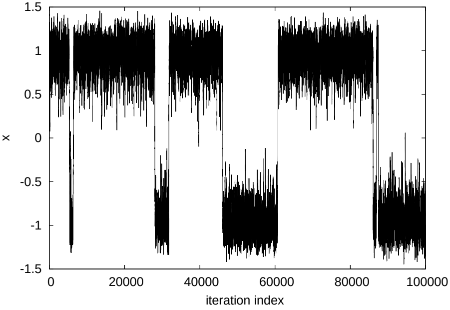


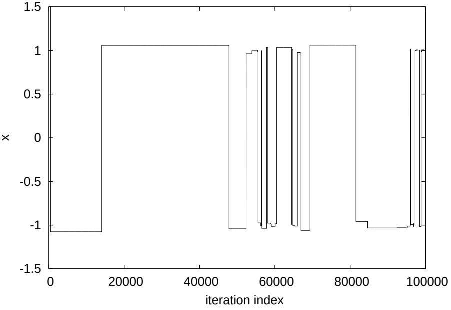
"partial reverse check" $=$ do not check $\Psi_{\Delta t} \circ \Psi_{\Delta t} = \mathrm{Id} \Rightarrow$ BIAS!

Numerical experiments (2/3)

Let us now consider a double well case: $\nu = \mathrm{e}^{-V} \sigma_{T^*\mathcal{M}}$ where $V(x,y,z) = k(x^2 - R^2)^2$.

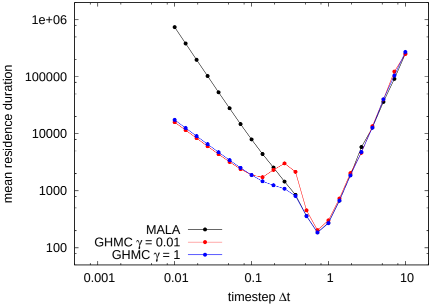
Typical trajectories for the GHMC dynamics (left $\Delta t = 0.05$, right $\Delta t = 3$):

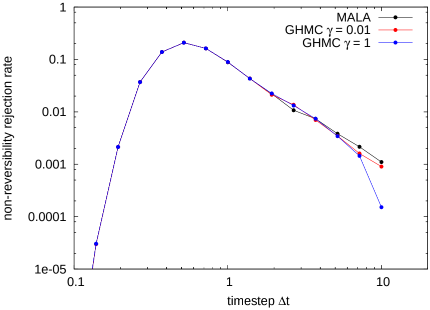




Numerical experiments (3/3)

Analysis of the efficiency (left mean residence duration, right: non-reversibility rejection rate)





The optimal timestep is of the order of 0.7. For such timesteps, the rejections due to the non reversibility condition $(q^n, p^n) \neq \Psi_{\Delta t} \circ \Psi_{\Delta t}(q^n, p^n)$ are of the order of 15-20%, the total rejection rate being about 90%.

$\rightarrow$ reverse projection check is useful to get efficient algorithms.

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