# Microcanonical Langevin Monte Carlo


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## Introduction

Sample Boltzmann–Gibbs probability measure:

$$\mu_\beta \propto \mathrm{e}^{-\beta V}, \tag{1}$$

through molecular dynamics using Langevin dynamics:

$$\begin{cases} dx_t = \Pi_t \, dt, \\ d\Pi_t = -\nabla V(x_t) - \gamma \Pi_t \, dt + \sqrt{2T\gamma} dW_t, \end{cases} \tag{2}$$

with the **positions** $x \in \mathcal{X}$ and **momenta** $\Pi \in \mathbb{R}^d$.

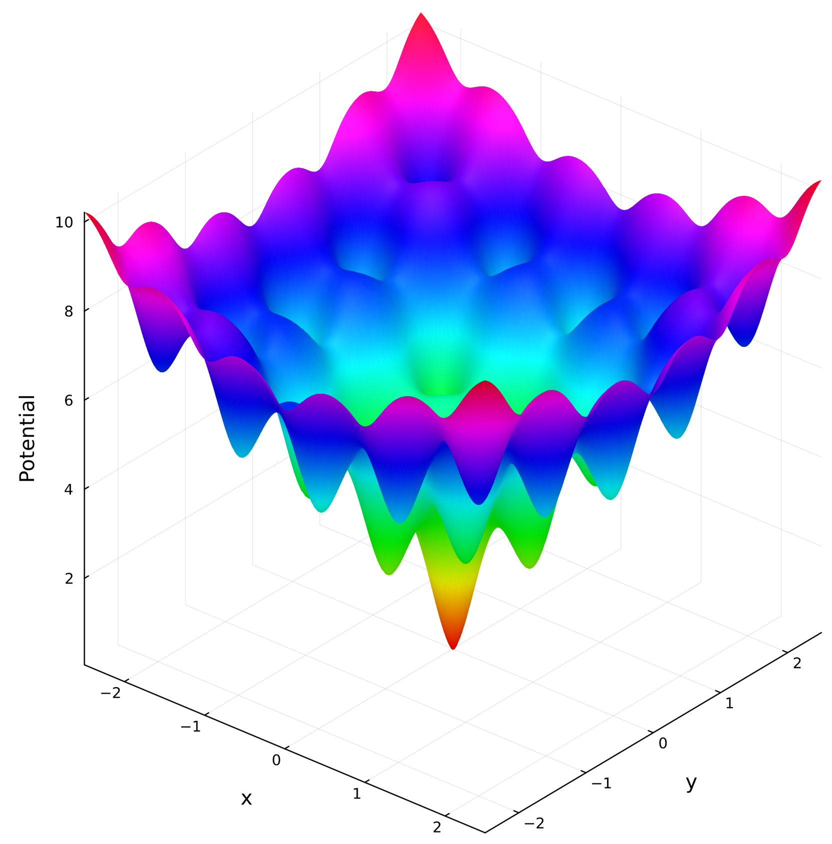


*Figure 1. Ackley potential: challenges the usual sampling methods with rare events.*

## Derivation of MCLMC

Starting from the **Hamiltonian**

$$H(x, \Pi) = \frac{1}{d-1} V(x) + \ln(|\Pi|), \tag{3}$$

the Hamilton equations are:

$$\begin{cases} x'(t) = \dfrac{\Pi(t)}{|\Pi(t)|^2} \\ \Pi'(t) = -\dfrac{1}{d-1} \nabla_x V(x(t)) \end{cases}$$

**MCLMC** can be derived from two ingredients:

- a **rescaling** in time:

$$\frac{ds}{dt} = \frac{\partial H}{\partial |\Pi|} = \frac{1}{|\Pi|};$$

- the **projection** on the unit sphere:

$$u = \frac{\Pi}{|\Pi|}.$$

This leads to the **deterministic** part of (4). The stochastic part is a **Brownian motion the sphere** that preserves the Hamiltonian (3). This has been done in [2] and [3], and can be generalised for a larger family of Hamiltonians.

## Remarks on the invariant measure

The generator of **MCLMC** (4) can be decomposed into two parts.

In the weighted space $\mathrm{L}^p_\rho(\mathcal{X} \times \mathbb{R}^d)$ by (5):

$$\mathcal{L}^*_{\mathrm{ham}} = -\mathcal{L}_{\mathrm{ham}},$$
$$\mathcal{L}^*_{\mathrm{noise}} = \mathcal{L}_{\mathrm{noise}}.$$

## Microcanonical Langevin Monte Carlo (MCLMC)

First introduced in [1].

$$\begin{cases} dx_s = \dfrac{u_s}{|u_s|^2} ds \\ du_s = -\dfrac{1}{d-1} P(u_s) \nabla V(x_s) \, dt + \eta P(u_s) \circ dW_s \end{cases} \tag{4}$$

with $P(u) = \mathrm{Id} - \dfrac{uu^T}{|u|^2}$

**Main properties:**

- **Invariant probability measure** with the correct marginal (1) on the position:

$$\rho_{|u_0|}(dx, \, du) = Z^{-1}_{|u_0|} \mathrm{e}^{-\beta V(x)} \delta\left(|u| - |u_0|\right) \, dx \, du, \tag{5}$$

**ergodic** in $\mathcal{X} \times \mathcal{S}^{d-1}_{|u_0|}$ ;

- Velocity with **constant norm**:

$$\forall s > 0, \quad |u_s| = |u_0|.$$

## Simulation of MCLMC

- **Integration scheme:**

$$\begin{cases} x_{n+\frac{1}{2}} = x_n + \dfrac{1}{2} \Delta t \dfrac{u_n}{|u_n|^2}, \\ u^*_{n+1} = u_n - \dfrac{1}{d-1} \Delta t \nabla V(x_{n+\frac{1}{2}}) + \eta \sqrt{\Delta t} \xi_n, \\ u_{n+1} = \dfrac{u^*_{n+1}}{|u^*_{n+1}|} \\ x_{n+1} = x_{n+\frac{1}{2}} + \dfrac{1}{2} \Delta t \dfrac{u_{n+1}}{|u_{n+1}|^2}, \end{cases} \tag{6}$$

  with $\{\xi_n\}$ independent $\mathcal{N}(0, \mathrm{Id})$ random variables.
- From the **uniform distribution** at start, **histograms** are computed over $10,000$ particles and them compared to $\mu_\beta$ computed by analytic integration (low dimensional toy models).
- **MCLMC** converges in **10 %** less physical time than Langevin (2) with our tests.

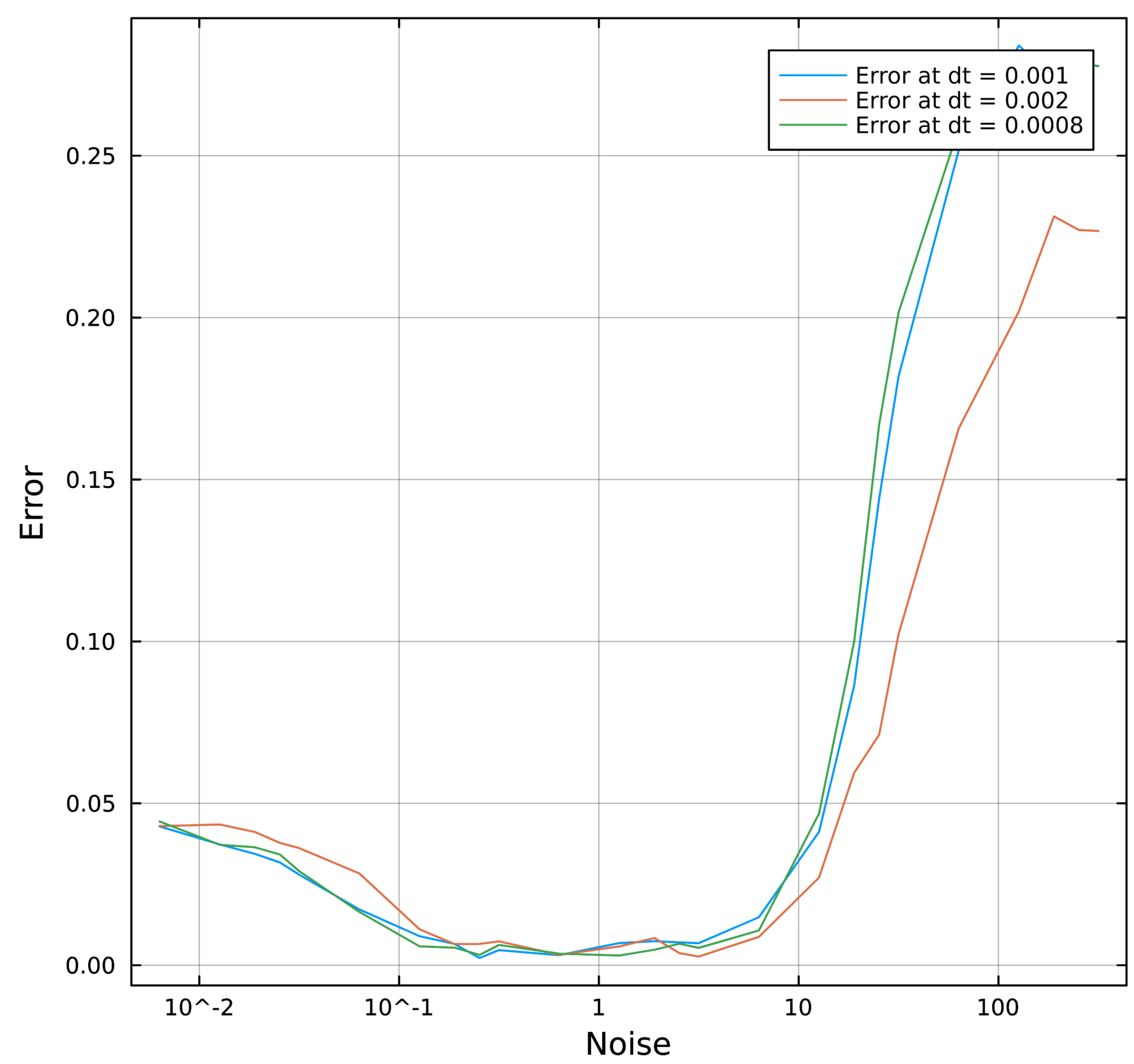


*Figure 2. Supremum norm of the error on the marginal in terms of $\eta$. **MCLMC** allows a larger range of noise intensity.*

## References


[1] G. Ver Steeg and A. Galstyan Hamiltonian Dynamics with Non-Newtonian Momentum for Rapid Sampling. 2021 arXiv:2111.02434
[2] J. Robnik,G. B. de Luca, E. Silverstein et U. Seljak Microcanonical Hamiltonian Monte Carlo. 2023 arXiv:2212.08549v2
[3] J. Robnik et U. Seljak Fluctuation without dissipation: Microcanonical Langevin Monte Carlo. 2023 arXiv:2303.18221v2



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