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Diffusive Scaling Limits & Early Diagnostics for PDMP Monte Carlo Samplers

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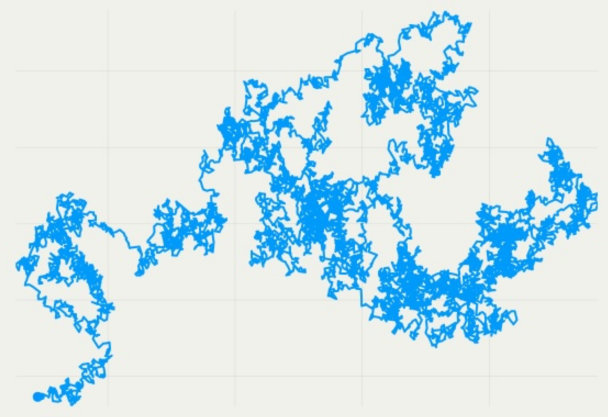
What is PDMP?

Faster convergence through ballistic movement

	Drift	Diffusion	Jump	$t \in [0,\infty)$
Diffusion	$dX_t = a(X_t)\,dt$	$+\ b(X_t)\,dB_t$		
PDMP	$dX_t = a(X_t)\,dt$		$+\int_{\mathbb{R}^d} c(X_{t-},u)\eta(dtdu)$	

↑ Piecewise Deterministic ↑ Markov Process



Langevin Diffusion

- Overdamped Dynamics
  → SDE discretization
- Equilibrium Steady State

VS.

Randomized Hamiltonian Monte Carlo

- Kinetic Dynamics
  → ODE discretization
- Non-equilibrium Steady State
  → Faster Relaxation

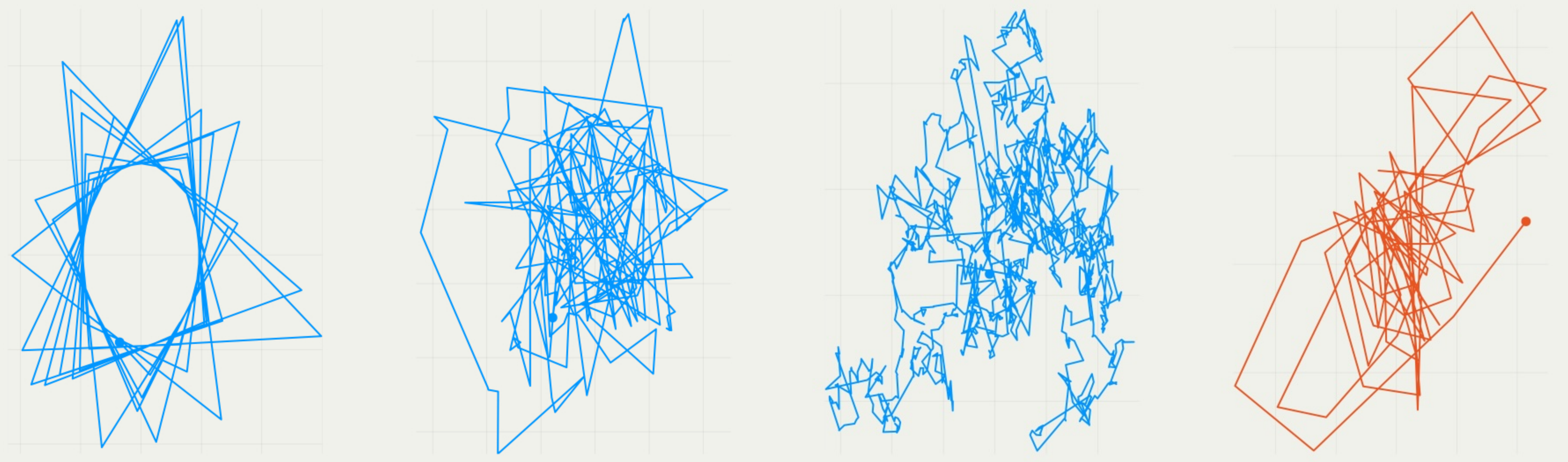
Which method is faster?

*Among piecewise linear methods

Bouchard-Côté, Vollmer & Doucet (2018) The Bouncy Particle Sampler

Michel, Durmus & Sénécal (2020) Forward Event-Chain Monte Carlo

BPS with ρ=0.0 | BPS with ρ=1.0 | BPS with ρ=10.0 | FECMC with $\rho = 0$

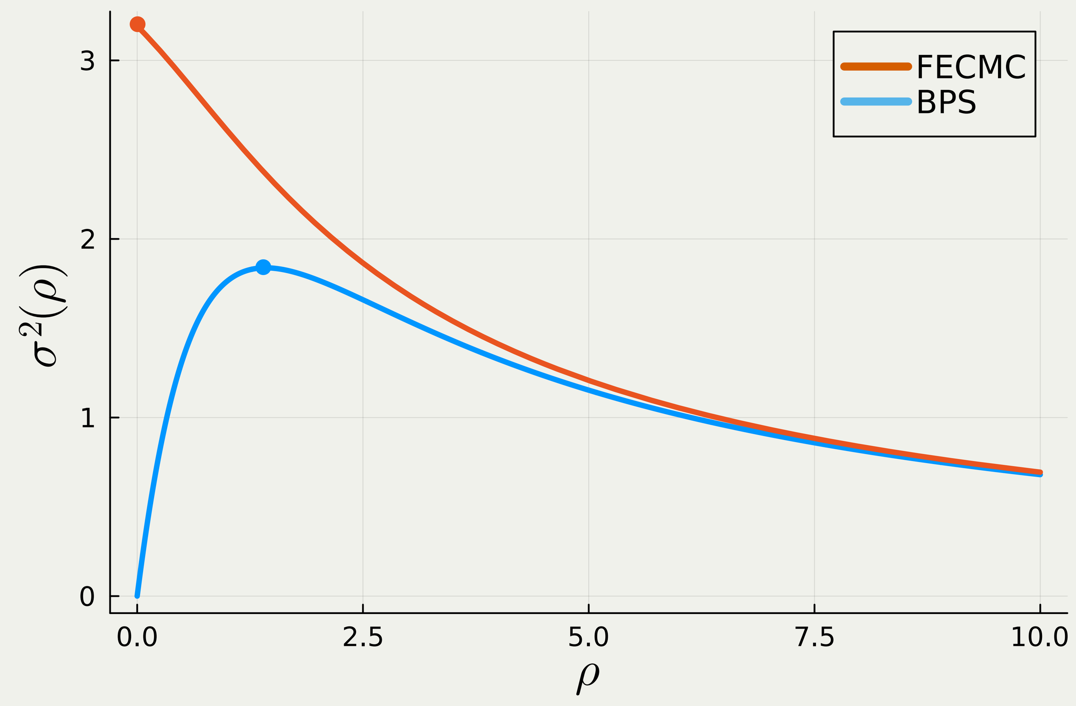


How to set the hyperparameter ρ? Is this really more efficient?

For a standard Gaussian

$$\pi(x) \propto e^{-U^{(d)}(x)} \qquad U^{(d)}(x) = \frac{\|x\|_2^2}{2}$$

with $d \to \infty$



$\sigma^2 \approx$ the limiting speed of the process $U^{(d)}(X_t)$

Scaling Analysis: Compare Limiting Dynamics as $d \to \infty$

Theorem 3.7 & 3.9 The potential of both methods converges to an Ornstein-Uhlenbeck diffusion

$$Y_t^{(d)} := \frac{2U^{(d)}(X^d_{dt}) - d}{\sqrt{d}} \implies \mathrm{d}Y_t = -\frac{\sigma^2(\rho)}{4} Y_t\,\mathrm{d}t + \sigma(\rho)\,\mathrm{d}B_t$$

Theorem 4.1

$$\sigma^2_{\mathrm{FECMC}}(\rho) = \sqrt{\frac{32}{\pi}}\left(1 - \frac{(\rho^2 - \rho\sqrt{\frac{\pi}{2}} + \Omega(\rho))^2}{\rho^4\Omega(\rho)(2-\Omega(\rho))}\right)$$

$$\sigma^2_{\mathrm{BPS}}(\rho) = \frac{8}{\rho^4}\left(\rho^3 - \rho^2\sqrt{\frac{8}{\pi}} + \rho - \sqrt{\frac{8}{\pi}}\frac{((1+\rho^2)\Omega(\rho) - \rho^2)^2}{\Omega(2\rho)}\right)$$

$\Omega(\rho) := \rho e^{\frac{\rho^2}{2}}\int_\rho^\infty e^{-\frac{t^2}{2}}\,\mathrm{d}t$: exponentially scaled complementary error function

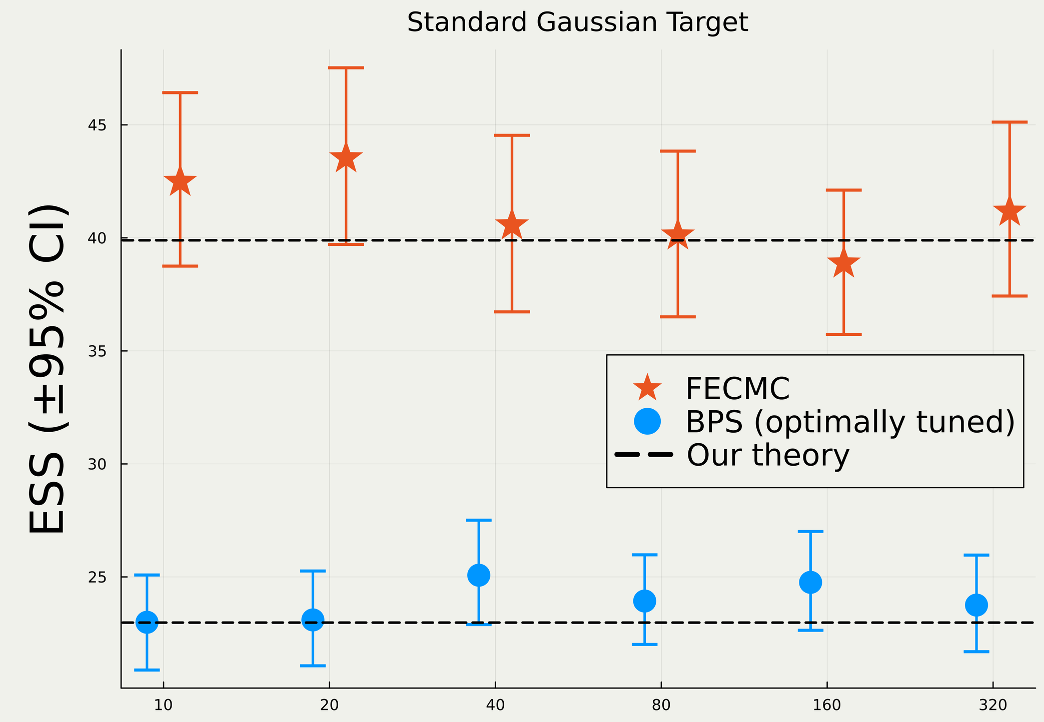
Corollary 4.3

$$\sigma^2_{\mathrm{FECMC}}(0) = \sqrt{\frac{32}{\pi}}$$

ESS: A benchmark For $U^{(d)}$, the effective sample size (ESS) is

$$\mathrm{ESS}(U) \approx T\frac{\sigma^2(\rho)}{8}$$

ESS/T roughly corresponds to mean squared error (MSE)



In general, σ^2 depends on the target and needs to be estimated on the fly in practice

Complexity Scaling

Potential	$\nabla U(x)$ evals / ESS	$\nabla U(x)$	Total Complexity
BPS / FECMC	$O(d)$	$O(d^{0\sim1})$	$O(d^{1\sim2})$
Hamiltonian Monte Carlo	Unkown (Open problem)		
≈			
Marginal coordinate			
Random Walk Metropolis	$O(d)$	$O(d)$	$O(d^2)$
Metropolis-adjusted Langevin	$O(d^{1/3})$	$O(d)$	$O(d^{4/3})$
Hamiltonian Monte Carlo	$O(d^{1/4})$	$O(d)$	$O(d^{5/4})$

An Early Diagnostic

Monitor the time-derivative process!

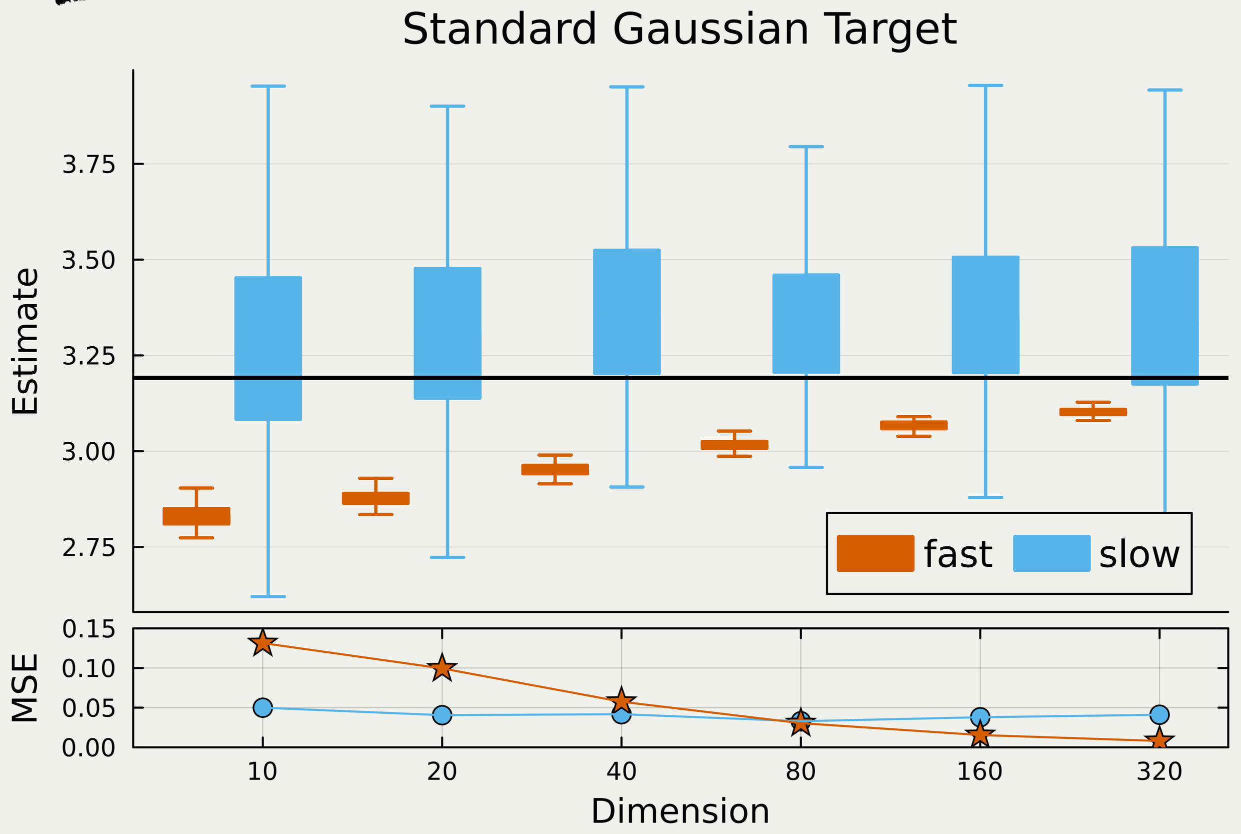
$$\frac{\mathrm{d}}{\mathrm{d}t}h(X_t) = (\nabla h(X_t)|V_t) =: R_t$$

→ MSE reduction by an $O(d^{-1})$ scale

Proposition 4.5

$$\frac{1}{\sqrt{T}}\int_0^{dT} h(X_t)\,\mathrm{d}t \overset{d,T\to\infty}{\Rightarrow} N\left(0, \frac{8}{\sigma^2}\right)$$

$$\frac{1}{\sqrt{T}}\int_0^{T} R_t\,\mathrm{d}t \overset{d,T\to\infty}{\Rightarrow} N\left(0, \frac{\sigma^2}{4}\right)$$



Comparison of two batch means estimators