Event chain Monte Carlo, self-repellent random walks, and the stochastic heat equation

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Sampling and Markov chain Monte Carlo

Goal: Sample from a probability distribution

$$\mu(\mathrm{d}x) \propto \exp(-U(x))\,\mathrm{d}x$$

on $\mathcal{S} = \mathbb{R}^d$ (or a Riemannian manifold).

Strategy: Construct a Markov process $(X_t)_{t\geq 0}$ with μ as invariant measure such that $\mathrm{Law}(X_t) \to \mu$ quickly.

Observe acceleration through non-reversibility!

A toy model

Compare different sampling approaches in a toy model.

State space

$$\mathcal{S} = \left\{ \ell = (\ell_i)_{i \in \mathbb{Z}_n} \in \mathbb{R}^{\mathbb{Z}_n} : \sum_{i \in \mathbb{Z}_n} \ell_i = 0 \right\},$$

probability measure

$$\mu(\mathrm{d}\ell) \propto e^{-U(\ell)} \lambda_{\mathcal{S}}(\mathrm{d}\ell) = \mathcal{N}(0, -\Delta_n^{-1})$$

$$\text{with} \quad U(\ell) = \frac{1}{2} \sum_{i \in \mathbb{Z}_n} (\ell_{i+1} - \ell_i)^2 = -\ell \cdot \Delta_n \ell$$

with Δ_n the discrete Laplacian on $\mathbb{Z}_n$.

$\longrightarrow$ harmonic chain, 1d discrete GFF, discrete Brownian bridge, ...

Some remarks

Condition number:

Eigenvalues of $-\Delta_n$: $\lambda_k = 2 - 2\cos(\frac{2\pi k}{n})$, $k = 1, \dots, n$.

$$\lambda_1 \sim \frac{4\pi^2}{n^2},\ \lambda_{\lfloor \frac{n}{2} \rfloor} \sim 4 \quad \Longrightarrow \quad \kappa(\Delta_n) \sim \frac{n^2}{\pi^2}.$$

Generalisations:

- Anharmonic chain: $U(\ell) = \sum_{i \in \mathbb{Z}_n} W(\ell_{i+1} - \ell_i)$.
- Other graphs: $\mathbb{Z}_n \to (V, E)$.

Overdamped Langevin dynamics

$$\mathrm{d}Z(t) \;=\; -\frac{1}{2}\nabla U(Z(t))\,\mathrm{d}t \;+\; \mathrm{d}W(t)$$

Overdamped Langevin dynamics

$$\mathrm{d}Z(t) \;=\; \frac{1}{2}\Delta_n Z(t)\,\mathrm{d}t \;+\; \mathrm{d}W(t)$$

$\longrightarrow$ discrete stochastic heat equation with additive noise!

Generator

$$Lg(\ell) = \frac{1}{2}\sum_{i\in\mathbb{Z}_n}\Big(\partial^2_{\ell_i} g(\ell) + (\ell_{i+1} - 2\ell_i + \ell_{i-1})\partial_{\ell_i} g(\ell)\Big)$$

is self-adjoint in $L^2(\mu)$. Spectral gap $\lambda_1 \in \Theta(n^{-2}) \Rightarrow t_{\mathrm{rel}} \in \Theta(n^2)$.

System of n equations $\longrightarrow$ complexity $\Omega(n^3)$.

Inefficient: diffusive + high condition number!

Speed-up by lifting

Introduce auxiliary variables: $\hat{\mathcal{S}} = \mathcal{S} \times \mathcal{V}$, $\hat{\mu} = \mu \otimes \kappa$, $\pi(\ell, v) = \ell$.

$$Z(t) \to (\mathcal{L}(t), V(t)), \quad P_t \to \hat{P}_t, \quad L \to \hat{L}.$$

Definition (Eberle and L, 2024)

The process $(\mathcal{L}(t), V(t))$ is a second-order lift of $(Z(t))$ if for all $f, g \in \mathrm{Dom}(L)$,

(i) $f \circ \pi \in \mathrm{Dom}(\hat{L})$,

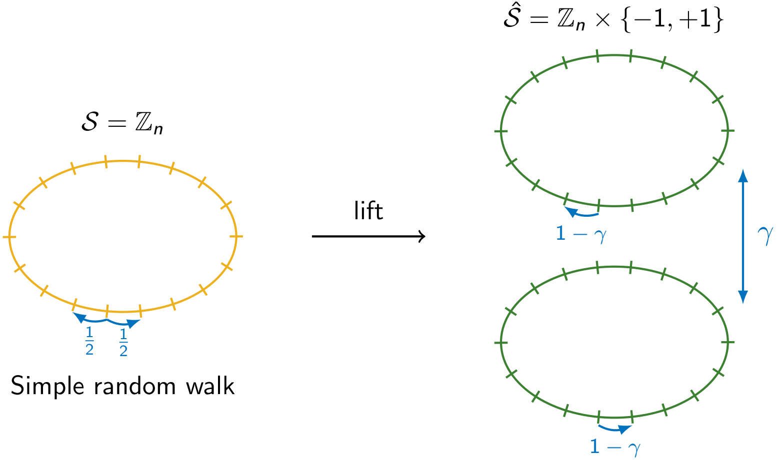
(ii) $\langle \hat{L}(f \circ \pi), g \circ \pi \rangle_{L^2(\hat{\mu})} = 0$,

(iii) $\frac{1}{2} \langle \hat{L}(f \circ \pi), \hat{L}(g \circ \pi) \rangle_{L^2(\hat{\mu})} = -\langle f, Lg \rangle_{L^2(\mu)}$.

Implies:

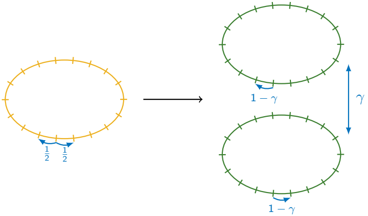
$$\int_{\mathcal{V}} \hat{P}_t(f \circ \pi)(\ell, v)\, \kappa(\mathrm{d}v) = (P_{t^2} f)(\ell) + o(t^2) \text{ as } t \to 0.$$

Recap: Lifts of Markov chains (Diaconis, Holmes, and Neal, 2000)



Recap: Lifts of Markov chains

$\hat{\mathcal{S}} = \mathcal{S} \times \mathcal{V}$, $\hat{\mu} = \mu \otimes \kappa$.
Transition kernels p and $\hat{p}$.



Definition (Chen, Lovász, and Pak, 1999)

The transition kernel $\hat{p}$ is a first-order lift of p if

$$\int_{\mathcal{V}} \hat{p}(f \circ \pi)(\ell, v)\, \kappa(\mathrm{d}v) = (pf)(\ell)$$

for all $\ell \in \mathcal{S}$ and measurable $f : \mathcal{S} \to \mathbb{R}$, where $\pi(\ell, v) = \ell$.

Recap: Lifts of Markov chains

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Recall: For a second-order lift $(\hat{P}_t)$ of (P_t),

$$\int_{\mathcal{V}} \hat{P}_t(f \circ \pi)(\ell, v)\, \kappa(\mathrm{d}v) = (P_{t^2} f)(\ell) + o(t^2) \text{ as } t \to 0.$$

For small $t > 0$, $(\hat{P}_t)$ is approximately a lift of (P_{t^2})!

Lower bound for relaxation times of lifts

Relaxation time:
$t_{\mathrm{rel}}(\hat{P}) = \inf\left\{t \geq 0 : \|\hat{P}_t f\|_{L^2(\hat{\mu})} \leq \frac{1}{e}\|f\|_{L^2(\hat{\mu})} \text{ for all } f \in L_0^2(\hat{\mu})\right\}.$

Theorem (Eberle and L, 2024)

If $(\hat{P}_t)$ is a second-order lift of (P_t), then

$$t_{\mathrm{rel}}(\hat{P}) \geq \frac{1-e^{-1}}{\sqrt{2}}\sqrt{t_{\mathrm{rel}}(P)}\,.$$

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Theorem (Eberle and L, 2024)

$$t_{\mathrm{rel}}(\hat{P}) \geq \tfrac{1-e^{-1}}{\sqrt{2}}\sqrt{t_{\mathrm{rel}}(P)}\,.$$

Proof. $\|\hat{P}_t f - f\|_{L^2(\hat{\mu})} \leq \int_0^t \|\hat{P}_s \hat{L} f\|_{L^2(\hat{\mu})}\,\mathrm{d}s \leq t\|\hat{L}f\|_{L^2(\hat{\mu})}$, so

$$\|\hat{P}_t f\|_{L^2(\hat{\mu})} \geq \|f\|_{L^2(\hat{\mu})} - t\|\hat{L}f\|_{L^2(\hat{\mu})}\,.$$

For $\lambda > \mathrm{gap}(L)$ choose $g \in L^2_0(\mu)$ with $\mathcal{E}(g) = \lambda\|g\|^2_{L^2(\mu)}$.
By the second-order lift property: $\frac{1}{2}\|\hat{L}(g\circ\pi)\|^2_{L^2(\hat{\mu})} = \mathcal{E}(g)$.
Then

$$\|\hat{P}_t(g\circ\pi)\|_{L^2(\hat{\mu})} \geq (1-\sqrt{2\lambda}t)\|g\circ\pi\|_{L^2(\hat{\mu})}\,.$$

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Can the lower bound be achieved? $\longrightarrow$ Optimal lifts.

Proof of optimality requires quantitative upper bounds on the relaxation time. $\longrightarrow$ Challenging!

Randomised Hamiltonian Monte Carlo $\hat{\mathcal{S}} = \mathcal{S} \times \mathcal{S}$, $\hat{\mu} = \mu \otimes \mathcal{N}(0, I_{\mathcal{S}})$.

Idealised dynamics: $(\mathcal{L}(t), V(t))_{t \geq 0}$ PDMP with state space $\hat{\mathcal{S}}$,

$$\begin{cases} \mathrm{d}\mathcal{L}(t) = V(t)\,\mathrm{d}t \\ \mathrm{d}V(t) = -\nabla U(\mathcal{L}(t))\,\mathrm{d}t \end{cases} + \quad \text{complete velocity refreshments with exponential rate } \gamma \in [0, \infty).$$

Theorem (Eberle and L, 2024)

RHMC is a second-order lift of L for any $\gamma \in [0, \infty)$.

Theorem (Eberle and L, 2024; Lu and Wang, 2022)

(i) $t_{\mathrm{rel}}(\mathrm{RHMC}) \in \Omega(\mathrm{gap}(L)^{-1/2})$.

(ii) If $\nabla^2 U \geq -C\,\mathrm{gap}(L) \cdot I$ and $\gamma \propto \mathrm{gap}(L)^{1/2}$, then

$$t_{\mathrm{rel}}(\mathrm{RHMC}) \in \Theta(\mathrm{gap}(L)^{-1/2})$$

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(i) $t_{\mathrm{rel}}(\mathrm{RHMC}) \in \Omega(\mathrm{gap}(L)^{-1/2}) = \Omega(n)$.

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Randomised Hamiltonian Monte Carlo

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Proof: Divergence lemma

$\Longrightarrow$ space-time Poincaré inequality

$\Longrightarrow$ time-averaged L^2-decay.

Complexity of RHMC

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Algorithmic implementations:

- Simulating n equations $\Rightarrow$ complexity $\Omega(n)$ per time unit.
- Time discretisation via Verlet/leapfrog, step size $h \in O(n^{-\frac{1}{4}})$.

Hence: Complexity per time unit $\Omega(n^{5/4})$, overall $\Omega(n^{9/4})$.

Complexity of RHMC

Can we do better?

- Critical RHMC is optimal lift. **Good!**
- Complexity per time unit $\Omega(n^{5/4})$. **Bad!**

Problem: All particles moving and interacting constantly.

Question

Is there a good lift where only one particle/coordinate is changing at a time?

Self-repellent random walk

State space $\hat{\mathcal{S}} = \mathcal{S} \times \mathbb{Z}_n$, $\hat{\mu} = \mu \otimes \mathrm{Unif}(\mathbb{Z}_n)$.

Markov process $(L(t), X(t))$,

$$\mathrm{d}L(t) = e_{X(t)}\,\mathrm{d}t\,,$$

$$X(t) \text{ jumps } \begin{cases} x \to x+1 & \text{with rate } (L_{x+1}(t) - L_x(t))_-\,, \\ x \to x-1 & \text{with rate } (L_{x-1}(t) - L_x(t))_-\,. \end{cases}$$

$(L(t))_{t\geq 0}$ is local time process of $(X(t))_{t\geq 0}$ and $X(t)$ prefers states where $L(t)$ is small. $\longrightarrow$ **self-repellent random walk**

No invariant probability measure since $L(t)$ increasing!
Renormalise:

$$\mathcal{L}_i(t) = L_i(t) - \frac{t}{n}, \qquad \text{so} \quad \sum_{i=1}^{n} \mathcal{L}_i(t) = 0\,.$$

$\longrightarrow$ **Event chain Monte Carlo** (Maggs, 2025).

Self-repellent random walk $\hat{\mathcal{S}} = \mathcal{S} \times \mathbb{Z}_n$, $\hat{\mu} = \mu \otimes \mathrm{Unif}(\mathbb{Z}_n)$

Lemma

$(\mathcal{L}(t), X(t))$ is PDMP with state space $\hat{\mathcal{S}}$, inv. meas. $\hat{\mu}$, generator

$$\begin{aligned} \hat{L}f(\ell, i) \;=\; \partial_{\ell_i} f(\ell, i) \;&+\; (\ell_{i+1} - \ell_i)_-(f(\ell, i+1) - f(\ell, i)) \\ &+\; (\ell_{i-1} - \ell_i)_-(f(\ell, i-1) - f(\ell, i))\,. \end{aligned}$$

Theorem (Eberle and L, 2025)

$(\mathcal{L}(t), X(t))_{t\geq 0}$ is a second-order lift of $(Z(t))_{t\geq 0}$ satisfying

$$\mathrm{d}Z(t) \;=\; \frac{1}{2n}\Delta_n Z(t)\,\mathrm{d}t + \frac{1}{\sqrt{n}}\,\mathrm{d}W(t)\,.$$

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Overdamped Langevin slowed down by a factor n, generator $\frac{1}{n}L$.

Corollary (Eberle and L, 2025)

$$t_{\mathrm{rel}}(\mathcal{L}, X) \geq \frac{1-e^{-1}}{\sqrt{2}}\sqrt{\frac{1}{\mathrm{gap}(\frac{1}{n}L)}} = \frac{1-e^{-1}}{2\pi}n^{3/2}\,.$$

Upper bounds for the relaxation time

Open problem for $(\mathcal{L}(t), X(t))_{t\geq 0}$!

Consider modified dynamics with additional moves in $X(t)$:

$$\hat{L}_\gamma \ = \ \hat{L} + \gamma(Q - I)\,, \qquad Q \text{ symmetric transition matrix on } \mathbb{Z}_n\,.$$

Process is still a lift of $(Z(t))$ $\longrightarrow$ lower bound $\Omega(n^{3/2})$ applies.

Theorem (Eberle and L, 2025)

For $Qf(\ell, x) = \sum_{i=1}^n f(\ell, i)$, we have

$$t_{\mathrm{rel}}(\hat{L}_\gamma) \ \in \ O(\gamma n^3 + \gamma^{-1} n)\,.$$

In particular: $\gamma \propto n^{-1} \quad \Rightarrow \quad t_{\mathrm{rel}}(\hat{L}_\gamma) \in O(n^2)$

Consequence: ECMC with complete resampling of active coordinate at rate n^{-1} has complexity $O(n^2)$!

Upper bounds for the relaxation time

Theorem (Eberle and L, 2025)

For $Qf(\ell, x) = \sum_{i=1}^{n} f(\ell, i)$, we have

$$t_{\mathrm{rel}}(\hat{L}_\gamma) \in O(\gamma n^3 + \gamma^{-1} n) .$$

In particular: $\gamma \propto n^{-1} \quad \Rightarrow \quad t_{\mathrm{rel}}(\hat{L}_\gamma) \in O(n^2)$.

Proof: Builds on hypocoercivity techniques.

Flow Poincaré inequality for second-order lifts in an abstract framework (Eberle, Guillin, Hahn, L, and Michel, 2025).

Theorem 10. *Assume that*

(i) *the operator* $(\hat{\mathfrak{L}}, \mathrm{Dom}(\hat{\mathfrak{L}}))$ *is a second-order lift of* $(\mathfrak{L}, \mathrm{Dom}(\mathfrak{L}))$ *such that* $g \circ \pi \in \mathrm{Dom}(\hat{\mathfrak{L}}^*)$ *and* $\hat{\mathfrak{L}}^*(g \circ \pi) = -\hat{\mathfrak{L}}(g \circ \pi)$ *for all* $g \in \mathrm{Dom}(\mathfrak{L})$;

(ii) *the operator* $(\mathfrak{L}, \mathrm{Dom}(\mathfrak{L}))$ *has purely discrete spectrum on* $L^2(\mu)$ *and a spectral gap* $m > 0$, *i.e.*

$$\|g - \mu(g)\|^2_{L^2(\mu)} \leq \frac{1}{m} \langle g, -\mathfrak{L} g \rangle_{L^2(\mu)}$$

for all $g \in \mathrm{Dom}(\mathcal{E})$;

(iii) *there exists a constant* $C_1 > 0$ *such that*

Key quantity!

$$\left\langle \hat{\mathfrak{L}}(g \circ \pi), \hat{\mathfrak{L}}(f - \Pi f) \right\rangle_{L^2(\hat{\mu})} \leq C_1 \|\mathfrak{L} g\|_{L^2(\mu)} \|f - Qf\|_{L^2(\hat{\mu})}$$

for all $f \in \mathrm{Dom}(\hat{\mathfrak{L}})$ *and* $g \in \mathrm{Dom}(\mathfrak{L})$;

(iv) *the transition matrix* Q *has a spectral gap* m_Q, *i.e.*

$$x^\top Q x \leq (1 - m_Q)|x|^2$$

for all $x \in \mathbb{R}^n$ *with* $\sum_{i=1}^n x_i = 0$.

Then there exists a universal constant $C > 0$ *such that, for any* $T > 0$ *and* $\gamma > 0$, *the semigroup* $(\hat{P}_t^{(\gamma)})$ *generated by* $(\hat{\mathfrak{L}}^{(\gamma)}, \mathrm{Dom}(\hat{\mathfrak{L}}^{(\gamma)}))$ *satisfies*

$$\|\hat{P}_t^{(\gamma)} f\|_{L^2(\hat{\mu})} \leq e^{-\nu(t-T)} \|f\|_{L^2(\hat{\mu})} \qquad \text{for all } t \geq 0 \text{ and } f \in L^2_0(\hat{\mu}),$$

where the rate ν *is given by*

$$\nu = C \frac{\gamma}{\gamma^2/m + C_1^2 + \frac{1}{m_Q}(1 + \frac{1}{mT^2})}. \tag{18}$$

Upper bounds for the relaxation time

Theorem (Eberle and L, 2025)

For $Qf(\ell, x) = \sum_{i=1}^{n} f(\ell, i)$, we have

$$t_{\mathrm{rel}}(\hat{L}_\gamma) \in O(\gamma n^3 + \gamma^{-1} n).$$

In particular: $\gamma \propto n^{-1} \quad \Rightarrow \quad t_{\mathrm{rel}}(\hat{L}_\gamma) \in O(n^2)$.

Proof: Here $m \in \Theta(n^{-3})$, $m_Q = 1$. Constant C_1 in

$$\left\langle \hat{L}(g \circ \pi), \hat{L}(f - Qf) \right\rangle_{L^2(\hat{\mu})} \leq C_1 \|Lg\|_{L^2(\mu)} \|f - Qf\|_{L^2(\hat{\mu})}$$

determines the upper bound on the relaxation time

$$t_{\mathrm{rel}}(\hat{L}_\gamma) \in O\left(\gamma n^3 + \gamma^{-1} C_1^2\right).$$

Obtain $C_1^2 \in O(n)$ via Gaussian i.b.p. and Bochner's formula.

Upper bounds for the relaxation time

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In particular: $\gamma \propto n^{-1} \quad \Rightarrow \quad t_{\mathrm{rel}}(\hat{L}_\gamma) \in O(n^2)$.

Analogously:

Theorem (Eberle and L, 2025)

For Q the transition matrix of a simple random walk on $\mathbb{Z}_n$,

$$t_{\mathrm{rel}}(\hat{L}_\gamma) \in O(\gamma n^3 + \gamma^{-1} n^2).$$

In particular: $\gamma \propto n^{-1/2} \quad \Rightarrow \quad t_{\mathrm{rel}}(\hat{L}_\gamma) \in O(n^{5/2})$.

Thank you for your attention!

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