Explicit Convergence Rates of Underdamped Langevin Dynamics under weighted and Weak Poincaré–Lions Inequalities

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Motivation

Sampling problem: Given a target probability measure μ on $\mathbb{R}^d$ defined by

$$\mu(\mathrm{d}x) = \frac{1}{Z} e^{-\phi(x)} \mathrm{d}x$$

with some unknown normalization constant Z, generate a sequence of random samples $\{x_i\} \sim \mu$.

Markov Chain Monte Carlo: Find some dynamics X_t such that $\mathrm{Law}(X_t) \to \mu$ as fast as possible as $t \to \infty$.

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Applications:

- Bayesian inference
- Molecular dynamics
- Machine learning
- Economics (Pareto distribution, $\psi(v)$ represents the money of agent)

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$$\int_{\mathbb{R}^d} e^{s|x|}\mathrm{d}\mu < \infty.$$

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Question: What if (PI) fails?

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Assume moment bound

$$\sup_{t>0}\int W^\sigma h_t^2 \mathrm{d}\mu < \infty,$$

use Hölder inequality

$$\begin{aligned}\mathrm{Var}_\mu(h_t) &\leq \Big(\int W^\sigma h_t^2 \mathrm{d}\mu\Big)^{\frac{2}{2+\sigma}}\Big(\int W^{-2} h_t^2 \mathrm{d}\mu\Big)^{\frac{\sigma}{2+\sigma}} \\ &\lesssim \mathbb{E}_\mu^{\frac{\sigma}{2+\sigma}}|\nabla_x f|^2 \lesssim \Big(-\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Var}_\mu(h_t)\Big)^{\frac{\sigma}{2+\sigma}}\end{aligned}$$

Solving ODE, we get algebraic convergence

$$\mathrm{Var}_\mu(h_t) \lesssim t^{-\frac{\sigma}{2}}.$$

Weak Poincaré Inequality

$$\mathrm{Var}_\mu(f) \le s\mathbb{E}_\mu|\nabla_x f|^2 + \beta(s)\|f\|_{\mathrm{osc}}^2, \quad \forall s > 0. \tag{WPI}$$

$\|f\|_{\mathrm{osc}} = \mathrm{ess\,sup}_\mu f - \mathrm{ess\,inf}_\mu f$, $\beta(s) \downarrow 0$ as $s \to \infty$.

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By maximum principle $\|h_t\|_{\mathrm{osc}} \le \|h_0\|_{\mathrm{osc}}$. Thus (WPI) implies

$$\frac{\mathbb{E}_\mu|\nabla_x h_t|^2}{\|h_0\|_{\mathrm{osc}}^2} \ge \frac{\mathrm{Var}_\mu(h_t)}{s\|h_0\|_{\mathrm{osc}}^2} - \frac{\beta(s)}{s}.$$

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Optimizing over s, we find an increasing function K^*, depending on β, such that

$$-\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\frac{\mathrm{Var}_\mu(h_t)}{\|h_0\|_{\mathrm{osc}}^2} = \frac{\mathbb{E}_\mu|\nabla_x h_t|^2}{\|h_0\|_{\mathrm{osc}}^2} \ge K^*\left(\frac{\mathrm{Var}_\mu(h_t)}{\|h_0\|_{\mathrm{osc}}^2}\right).$$

Explicit decay rates can be obtained through Bihari–Lasalle argument.

From Weighted to Weak Poincaré Inequality

Recall weighted Poincaré:

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Now take any $s > 0$,

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$\Rightarrow$ Weighted Poincaré implies weak Poincaré! [Cattiaux/Gozlan/Guillin/Roberto 2010].

Examples (convergence of overdamped Langevin)

Example 1: $\phi(x) = \langle x \rangle^\alpha := (1 + |x|^2)^{\frac{\alpha}{2}}$ with $\alpha \in (0, 1)$.

- weighted Poincaré $\Rightarrow W(x) = \langle x \rangle^{1-\alpha}$;
- weak Poincaré $\Rightarrow \beta(s) \sim \mu(s \le W^2) \sim \exp(-s^{\frac{\alpha}{2-2\alpha}})$
  $\Rightarrow \mathrm{Var}_\mu(h_t) \lesssim \exp(-ct^{\frac{\alpha}{2-\alpha}})$.

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These tail bounds match the optimal convergence rates in total variation [Brešar/Mijatovic '24].

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$$\begin{cases} \mathrm{d}X_t = \nabla_v \psi(V_t)\mathrm{d}t; \\ \mathrm{d}V_t = -\nabla_x \phi(X_t) - \gamma \nabla_v \psi(V_t) + \sqrt{2\gamma}\mathrm{d}W_t. \end{cases}$$

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- Natural choice $\psi(v) = \frac{|v|^2}{2}$ standard Gaussian.
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- $h_t = \mathbb{E}_{x,v} h_0(X_t, V_t)$ satisfies

$$\begin{aligned} \partial_t h_t &= \nabla_v \psi \cdot \nabla_x h_t - \nabla_x \phi \cdot \nabla_v h_t + \gamma \Delta_v h_t - \gamma \nabla_v \psi \cdot \nabla_v h_t \\ &=: \mathcal{T} h_t - \gamma \nabla_v^* \nabla_v h_t. \end{aligned}$$

Nonreversible dynamics

Energy estimate

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbb{E}_{\mu\otimes\nu}\mathrm{Var}(h_t) = -2\gamma\mathbb{E}_{\mu\otimes\nu}|\nabla_v h_t|^2.$$

Lacking diffusion in x variable!

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Lacking diffusion in x variable! This will be 0 if h_t only depends on x.

So there is no hope to use standard Poincaré inequality, where we had

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The dynamics are hypocoercive.

Previous works on Hypocoercivity: Strong Confinement

- Early works of [Kolmogorov 1934], [Hörmander 1967];
- Convergence using Lyapunov function approach [Wu '01; Mattingly/Stuart/Higham '02; Rey-Bellet '06];
- Convergence in H^1 norm [Talay 2002; Villani 2009];
- Convergence in a modified L^2 norm [Dolbeault/Mouhot/Schmeiser '09; '15] (also earlier idea from [Herau '06]);
- Convergence in Wasserstein distance: using Bakry-Émery framework [Baudoin '16]; by coupling approaches [Eberle/Guillin/Zimmer '19];
- Resolvent analysis using Schur Complement [Bernard/Fathi/Levitt/Stoltz '20];
- Space-time Poincaré inequality [Albritton/Armstrong/Mourrat/Novack '19; Cao/Lu/Wang '20; Brigati/Stoltz '23; Eberle/Lörler '24]
  Optimal scaling of friction and convergence rate for convex ϕ.

Previous works on Hypocoercivity: Weak Confinement

- Combination of weak Poincaré with hypocoercivity tools: [Hu/Wang '19] using Villani's techniques; [Grothaus/Wang '19] using the DMS framework; [Andrieu/Dobson/W. '21] for PDMPs;
- Weighted Poincaré with DMS framework: [Cao '19] stretched exponential spatial potential and interpolation of spaces; [Bouin/Dolbeault/Ziviani '23] algebraic decays;
- Space-time Poincaré framework of Armstrong/Mourrat: [Brigati '23; Brigati/Stoltz '23], weak confinement in velocity, but requires strong confinement in space; [Dietert '23] allows non-gradient drift, although explicit estimates are absent.

These works require ν to be Gaussian.

The L^2 hypocoercivity approach: Armstrong/Mourrat

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$$\|f - (f)\|_{L^2([0,\tau]\times\mu)} \lesssim \|(\nabla_x, \partial_t) f\|_{H^{-1}([0,\tau]\times\mu)}.$$

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- Averaging functional inequality in velocity

$$\|(\nabla_x \Pi_v h, \partial_t \Pi_v h)\|_{H^{-1}([0,\tau]\times\mu)} \lesssim \|h - \Pi_v h\|_{L^2([0,\tau]\times\mu\times\nu)} + \|(\partial_t + \mathcal{T})h\|_{L^2([0,\tau]\times\mu, H^{-1}(\nu))}.$$

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Convergence rate $O(\sqrt{C_P})$ for convex ϕ when taking $\gamma = O(\sqrt{C_P})$ [Cao/Lu/Wang '20], optimal second-order lift [Eberle/Lörler '24].

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Integrate by parts:

$$\langle f,f\rangle = \langle f, -\partial_t F_0 + \nabla_x^*\nabla_x F_1\rangle = \langle \partial_t f, F_0\rangle + \langle \nabla_x f, \nabla_x F_1\rangle \le \|\partial_t f\|\cdot\|F_0\| + \|\nabla_x f\|\cdot\|F_1\|.$$

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Proof techniques:

- Traditionally: Bogovskii's operator [Bogovskii 1979]. Estimates are suboptimal.
- Explicit construction using H^1-L^2-H^{-1} duality and solving divergence equation: [Cao/Lu/Wang '20] which requires $L^2(\mu)$ to have discrete spectrum. This can be removed following [Brigati/Stoltz '23].
- Ongoing work of [Eberle/Lörler] with finer estimates.

Weighted Poincaré-Lions Inequality

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Theorem (Brigati/Stoltz/W./Wang '24)

Define tilted measure $\mathrm{d}\mu_W \propto W^{-2}\mathrm{d}\mu$, *then*

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The operator $W^2\nabla_x^*\nabla_x$ is self-adjoint and has spectral gap in $L^2(\mu_W)$.

The Averaging Inequality in Velocity

Add the velocity variable

$$\|(\nabla_x \Pi_v h, \partial_t \Pi_v h)\|_{H^{-1}([0,\tau]\times\mu)} \lesssim \|h - \Pi_v h\|_{L^2([0,\tau]\times\mu\times\nu)} + \|(\partial_t + \mathcal{T})h\|_{L^2([0,\tau]\times\mu, H^{-1}(\nu))}.$$

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$$\begin{aligned}\int (\partial_t \Pi_v h Y + \nabla_x \Pi_v h \cdot Z) &= \int (Y + v \cdot Z)(\partial_t + \mathcal{T})\Pi_v h \\ &= \int (Y + v \cdot Z)(\partial_t + \mathcal{T})h \\ &\quad + \int (h - \Pi_v h)(\partial_t + \mathcal{T})(Y + v \cdot Z).\end{aligned}$$

The Weighted Averaging Inequality in Velocity

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First Convergence Result

Theorem (Brigati/Stoltz/W./Wang '24)

If μ satisfies (WTPI) with weight W and $\sup_{t>0} \int W^\sigma(x) h_t^2 \mathrm{d}\mu \mathrm{d}\nu < \infty$, then

1. *If ν satisfies (PI), then*
$$\mathrm{Var}_{\mu\otimes\nu}(h_t) \lesssim t^{-\frac{\sigma}{2}}.$$
2. *If ν satisfies (WTPI) with weight $\mathcal{G}$ and $\sup_{t>0} \int \mathcal{G}^\delta(v) h_t^2 \mathrm{d}\mu \mathrm{d}\nu < \infty$, then*
$$\mathrm{Var}_{\mu\otimes\nu}(h_t) \lesssim t^{-\frac{\sigma\delta}{2\sigma+2\delta+4}}.$$

Note that (2) is consistent with (1) when taking $\delta \to \infty$.

From Weighted to Weak Poincaré–Lions Inequality

Recall the argument

$$\int (f-\mu(f))^2 \mathrm{d}\mu \le s \int_{s>W^2} W^{-2}(f-\mu(f))^2 \mathrm{d}\mu + \int_{s\le W^2} (f-\mu(f))^2 \mathrm{d}\mu$$
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Repeat this in the space-time domain, and we get the weak Poincaré–Lions inequality

$$\|f-(f)\|^2_{L^2([0,\tau]\times\mu)} \lesssim s\|(\nabla_x f, W^{-1}\partial_t f)\|^2_{H^{-1}([0,\tau]\times\mu)} + \mu(s\le W^2)\|f\|^2_{\mathrm{osc}}.$$

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This can be combined with the averaging inequality in velocity and we obtain the next convergence result.

Second Convergence Result

Theorem (Brigati/Stoltz/W./Wang '24)

Assume $h_0 \in L^\infty(\mathbb{R}^{2d})$, *then we have the following convergence rates for explicit examples:*

Potential	$\psi(v) = \langle v \rangle^\delta$ $\delta \geq 1$	$\psi(v) = \langle v \rangle^\delta$ $\delta \in (0,1)$	$\psi(v) =$ $(d+q)\log\langle v \rangle$
$\phi(x) = \langle x \rangle^\alpha$ $\alpha \geq 1$	$\exp(-\lambda t)$	$\exp(-ct^{\frac{\delta}{2-\delta}})$	$t^{-\frac{q}{2}}$
$\phi(x) = \langle x \rangle^\alpha$ $\alpha \in (0,1)$	$\exp(-ct^{\frac{\alpha}{2-\alpha}})$	$\exp(-ct^{\frac{\alpha\delta}{2\alpha+2\delta-3\alpha\delta}})$	$t^{-\frac{q}{2}-}$
$\phi(x) =$ $(d+p)\log\langle x \rangle$	$t^{-\frac{p}{2}}$	$t^{-\frac{p}{2}-}$	$t^{-\frac{pq}{4+2p+2q}}$

Comparison with Grothaus/Wang

Potential	$\psi(v) = \langle v \rangle^\delta$, $\delta \geq 1$	$\psi(v) = \langle v \rangle^\delta$, $\delta \in (0,1)$	$\psi(v) = (d+q)\log\langle v \rangle$
$\phi(x) = \langle x \rangle^\alpha$, $\alpha \geq 1$	$\exp(-\lambda t)$	$\exp(-ct^{\frac{\delta}{4-3\delta}})$	$t^{-\frac{1}{\theta(q)}-}$
$\phi(x) = \langle x \rangle^\alpha$, $\alpha \in (0,1)$	$\exp(-ct^{\frac{\alpha}{8-7\alpha}})$	$\exp(-ct^{\frac{\alpha\delta}{4\alpha+8\delta-11\alpha\delta}})$	$t^{-\frac{1}{\theta(q)}-}$
$\phi(x) = (d+p)\log\langle x \rangle$	$t^{-\frac{1}{2\theta(p)}-}$	$t^{-\frac{1}{2\theta(p)}-}$	$t^{-\frac{1}{2\theta(q)+\theta(p)+2\theta(p)\theta(q)}}$

Here $\theta(p) = \min\{\frac{d+p+2}{p}, \frac{4p+4+2d}{(p^2-2p-2d-4)^+}\} > \frac{2}{p}$

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Based on the beautiful space-time Poincaré approach of Armstrong/Mourrat, further developed by Cao/Lu/Wang and Brigati/Stoltz.

Thanks for listening! I

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The L^2 hypocoercivity approach: DMS

Assume (PI) in both μ and ν. Perturb the L^2 energy:

$$\Phi(f) := \frac{1}{2}\|f\|^2 + \varepsilon\langle (1 + (\mathcal{T}\Pi_v)^*(\mathcal{T}\Pi_v))^{-1}(\mathcal{T}\Pi_v)^* f, f\rangle.$$

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This operator is a regularized version of "$\approx (\nabla_x)^{-1}$".
Differentiate along the dynamics, we get for small ε and some $\lambda = \lambda_\varepsilon$

$$\frac{\mathrm{d}}{\mathrm{d}t}\Phi(h_t) \le -\lambda\Phi(h_t).$$

Convergence rate is difficult to optimize in ε.