

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

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

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

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 $\text{Law}(X_t) \rightarrow \mu$ **as fast as possible** as $t \rightarrow \infty$.

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Applications:

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

- Overdamped Langevin Dynamics

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$$\partial_t h_t = \Delta_x h_t - \nabla_x \phi \cdot \nabla_x h_t \quad =: -\nabla_x^* \nabla_x h_t.$$

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- $\mu \propto e^{-\phi}$ is the unique invariant measure. As $t \rightarrow \infty$, ergodicity guarantees $h_t \rightarrow \mathbb{E}_\mu h_0$.
- **Question: How fast does it converge?** Will study the continuous-time process using **functional inequalities**.

Poincaré Inequality

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$$\frac{d}{dt} \mathrm{Var}_\mu(h_t) = 2 \langle h_t, \mathcal{L} h_t \rangle_\mu = -2 \mathbb{E}_\mu |\nabla_x h_t|^2 \leq -2 C_P \mathrm{Var}_\mu(h_t).$$

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⇒ **Exponential** Convergence with rate $2C_P$:

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If μ satisfies (PI) with constant C_P , then for every $s < \sqrt{4C_P}$,

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

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Question: What if (PI) fails?

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Assume moment bound

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

use Hölder inequality

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

Solving ODE, we get **algebraic** convergence

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

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

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

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

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

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

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

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

From Weighted to Weak Poincaré Inequality

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Now take any $s > 0$,

$$\int (f - \mu(f))^2 d\mu \leq s \int_{s > W^2} W^{-2}(f - \mu(f))^2 d\mu + \int_{s \leq W^2} (f - \mu(f))^2 d\mu$$

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⇒ **Weighted Poincaré implies weak Poincaré!** [Cattiaux/Goźlan/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 $\Rightarrow \beta(s) \sim \mu(s \leq W^2) \sim \exp(-s^{\frac{\alpha}{2-2\alpha}})$
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These tail bounds match the optimal convergence rates in total variation [Brešar/Mijatovic '24].

Underdamped Langevin Dynamics

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$$\begin{cases} dX_t = \nabla_v \psi(V_t) dt; \\ dV_t = -\nabla_x \phi(X_t) - \gamma \nabla_v \psi(V_t) + \sqrt{2\gamma} dW_t. \end{cases}$$

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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

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

Energy estimate

$$\frac{d}{dt} \mathbb{E}_{\mu \otimes \nu} \text{Var}(h_t) = -2\gamma \mathbb{E}_{\mu \otimes \nu} |\nabla_{\nu} h_t|^2.$$

Lacking diffusion in x variable!

Nonreversible dynamics

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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

$$\frac{d}{dt} \text{Var}_{\mu}(h_t) = -2\mathbb{E}_{\mu} |\nabla_x h_t|^2 \leq -2C_P \text{Var}_{\mu}(h_t).$$

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

Fix time $\tau > 0$, and consider the **time-averaged** energy $\mathcal{H}_\tau(t) := \int_t^{t+\tau} \|h_t\|_{L^2}^2 dt$.

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- Poincaré–Lions inequality in **space and time**

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

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- Averaging functional inequality in **velocity**

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

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- Use the equation, dissipation of **time-averaged** L^2 energy controls the L^2 -energy itself.

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].

Poincaré–Lions Inequality

Assume that μ satisfies (PI), then the space-time strip $([0, \tau] \times \mathbb{R}^d, dt \otimes d\mu)$ satisfies the Poincaré–Lions inequality: for any $f(t, x)$,

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Integrate by parts:

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

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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].
- Recent work of [Eberle/Lörler '24] with finer estimates.

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

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

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

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Replacing H^{-1} by L^2 , $\nabla_x f \leftrightarrow$ weighted Poincaré in space; $W^{-1}\partial_t f \leftrightarrow$ standard Poincaré in time.

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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

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

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

The Weighted Averaging Inequality in Velocity

Add the velocity variable

$$\begin{aligned} \|(\nabla_x \Pi_\nu h, W^{-1} \partial_t \Pi_\nu h)\|_{H^{-1}([0, \tau] \times \mu)} &\lesssim \|h - \Pi_\nu h\|_{L^2([0, \tau] \times \mu \times \nu)} \\ &\quad + \|(\partial_t + \mathcal{T})h\|_{L^2([0, \tau] \times \mu, H^{-1}(\nu))}. \end{aligned}$$

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

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

① If ν satisfies (PI), then

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

② If ν satisfies (WTPI) with weight \mathcal{G} and $\sup_{t>0} \int \mathcal{G}^\delta(v) h_t^2 d\mu d\nu < \infty$, then

$$\text{Var}_{\mu \otimes \nu}(h_t) \lesssim t^{-\frac{\sigma\delta}{2\sigma+2\delta+4}}.$$

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

From Weighted to Weak Poincaré–Lions Inequality

Recall the argument

$$\begin{aligned} \int (f - \mu(f))^2 d\mu &\leq s \int_{s > W^2} W^{-2} (f - \mu(f))^2 d\mu + \int_{s \leq W^2} (f - \mu(f))^2 d\mu \\ &\lesssim s \mathbb{E}_\mu |\nabla_x f|^2 + \mu(s \leq W^2) \|f\|_{\text{osc}}^2. \end{aligned}$$

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Repeat this in the space-time domain, and we get the **weak Poincaré–Lions inequality**

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

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

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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:

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

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Differentiate along the dynamics, we get for small ε and some $\lambda = \lambda_\varepsilon$

$$\frac{d}{dt} \Phi(h_t) \leq -\lambda \Phi(h_t).$$

Convergence rate is difficult to optimize in ε .