A coupling approach to the (kinetic) Langevin equation

Andreas Eberle

University of Bonn

November 2017

Joint work with Arnaud Guillin and Raphael Zimmer

Outline

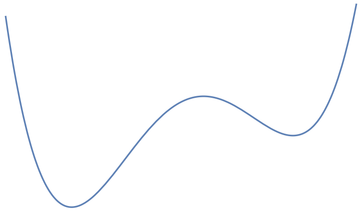
Introduction

Langevin dynamics

$$\begin{aligned} dX_t &= V_t\, dt \\ dV_t &= -\nabla U(X_t)\, dt - \gamma\, V_t\, dt + \sqrt{2\gamma} dB_t \end{aligned}$$

Invariant probability measure

$$\mu(dx\, dv) \;\propto\; e^{-U(x)-|v|^2/2}\, dx\, dv$$



Goal

- Quantitative upper bounds for $\mathcal{W}(\text{Law}(X_t, V_t), \mu)$
- Exponential contractivity

Analytic approaches

- Hérau/Nier (Witten Laplacian)
- Villani (Hypocoercivity), Dolbeault/Mouhot/Schmeiser

Probabilistic approach

- Coupling, Wasserstein distances, ...

Coupling

↓

Metric on probability measures ← optimize

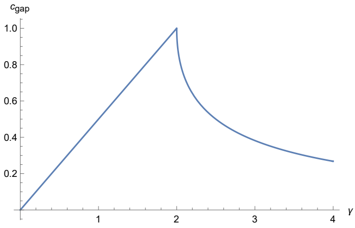
↓

Contraction rate

Example: The Gaussian case

$U(x) = L|x|^2/2$: Explicit solution converges with exponential rate

$$c \;=\; c_{gap} \;=\; \frac{\gamma}{2}\left(1-\sqrt{(1-4L\gamma^{-2})^{+}}\right).$$



Fastest mixing: $\gamma = 2\sqrt{L} \;\Rightarrow\; c = \sqrt{L} = 1/\sigma_x$ Kinetic!

Example: Double-well potential

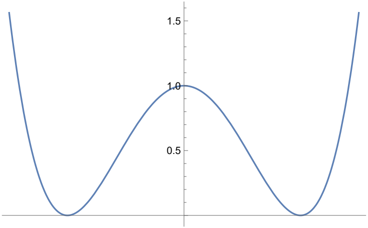


Figure: $U_a(x) = (x-a)^2(x+a)^2$, $a \in (0,\infty)$

Result

$\gamma \sim 1/a \;\Rightarrow$ Contraction rate $c = \Omega(1/a)$ w.r.t. appropr. distance

(in contrast to $O(1/a^2)$ for overdamped Langevin!)

The coupling

$$
\begin{aligned}
dX'_t &= V'_t\,dt \\
dV'_t &= -\nabla U(X'_t)\,dt - \gamma\,V'_t\,dt + \sqrt{2\gamma}dB'_t
\end{aligned}
$$

Difference process: $Z_t := X_t - X'_t,\ \ W_t := V_t - V'_T.$

$$
\begin{aligned}
dZ_t &= W_t\,dt \\
dW_t &= -(\nabla U(X_t) - \nabla U(X'_t))\,dt - \gamma\,W_t\,dt + \sqrt{2\gamma}\,(dB_t - dB'_t)
\end{aligned}
$$

Coordinate transformation: $Q_t := Z_t + \gamma^{-1} W_t$

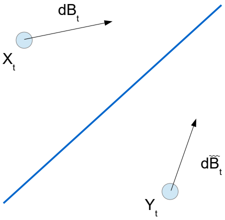
$$
\begin{aligned}
dZ_t &= -\gamma Z_t\,dt + \gamma Q_t\,dt \\
dQ_t &\leq L\gamma^{-1}|Z_t|\,dt + \sqrt{2\gamma^{-1}}\,(dB_t - dB'_t)
\end{aligned}
$$

A. Synchronous coupling

$$
\begin{aligned}
dB'_t &= dB_t, \qquad Z_t := X_t - X'_t,\ W_t := V_t - V'_t \\
&\Downarrow \\
dZ_t &= -\gamma Z_t\, dt + \gamma Q_t\, dt \\
dQ_t &\leq L\gamma^{-1}|Z_t|\, dt
\end{aligned}
$$

Apply for $Q_t = 0$ and for (Z_t, Q_t) large.

B. Reflection coupling



$$dB'_t = (I_d - 2e_t e_t^T)\, dB_t, \quad e_t = \frac{Q_t}{|Q_t|}$$

$$d(B_t - B'_t) = 2e_t e_t^T\, dB_t$$

Lévy's characterization $\Rightarrow B'$ Brownian motion.

C. Sticky coupling

$$dB'_t = (I_d - 1_{\{Q_t \neq 0,\, \alpha|Z_t|+|Q_t|<r_{max}\}}\, 2\, e_t e_t^T)\, dB_t, \qquad e_t = \frac{Q_t}{|Q_t|}$$

$$d(B_t - B'_t) = 1_{\{Q_t \neq 0,\, \alpha|Z_t|+|Q_t|<r_{max}\}}\, 2\, e_t e_t^T\, dB_t$$

Sticky behaviour of difference process

- Leb $\{t \geq 0 : Q_t = 0\} > 0$.
- Nevertheless, there is no non-empty interval $I \subseteq \mathbb{R}_+$ such that $Q_t = 0$ for all $t \in I$.

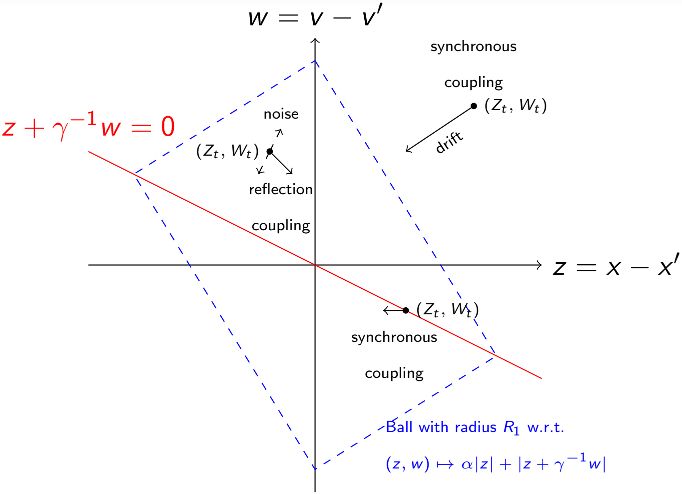


Figure: Sketch of coupling approach

(Semi-)metric and contractivity

$$z := x - x', \quad q := x - x' + \gamma^{-1}(v - v'), \quad \alpha, \epsilon > 0.$$

$$\rho((x,v),(x',v')) = f(\alpha|z| + |q|) \cdot (1 + \epsilon\mathcal{V}(x,v) + \epsilon\mathcal{V}(x',v')),$$

$f : \mathbb{R}_+ \to \mathbb{R}_+$ increasing, *concave*; $\mathcal{V}$ Lyapunov function.

$$\mathcal{W}_\rho(\mu,\nu) = \inf_{X\sim\mu, Y\sim\nu} \mathbb{E}[\rho(X,Y)], \quad \mu,\nu \in \mathrm{Prob}(\mathbb{R}^d).$$

Kantorovich (L^1 Wasserstein) distance based on semi-metric

Contractivity on average

$$\rho_t \;:=\; \rho((X_t, V_t), (X'_t, V'_t)), \qquad R_t := \alpha|Z_t| + |Q_t|.$$

- $Q_t = 0$: Contractivity by drift.
- $Q_t \neq 0,\ R_t < r_{max}$: Contractivity by noise and concavity of f.
- $R_t \geq r_{max}$: Contractivity by Lyapunov function.

Derivation of contraction rates

$$d\rho_t \overset{!}{\leq} -c\,\rho_t\,dt + dM_t$$

Then

$$\mathcal{W}_\rho(\mu_t,\nu_t) \leq E[\rho_t] \leq e^{-ct}E[\rho_0] = e^{-ct}\mathcal{W}_\rho(\mu_0,\nu_0).$$

Choose f,α,ϵ in order to maximize the contraction rate c.

Main result

Assumptions

(A1) $U(0) \;=\; 0 \;=\; \min U.$

(A2) $|\nabla U(x) - \nabla U(y)| \;\leq\; L\,|x-y| \qquad \forall\, x,y \in \mathbb{R}^d.$

(A3) $\exists\, \beta, \mathcal{R} > 0 : \quad x \cdot \nabla U(x) \;\geq\; \beta \cdot \left(\frac{|x|}{\mathcal{R}}\right)^2 \quad \forall\, |x| \geq \mathcal{R}.$

Theorem (Contractivity)

Suppose that (A1), (A2) and (A3) hold. Then there exists an explicit concave function $f : \mathbb{R}_+ \to \mathbb{R}_+$ *and explicit constants* $\alpha, \epsilon, c > 0$ *such that*

$$\mathcal{W}_\rho(\mu p_t, \nu p_t) \ \leq \ \exp(-ct)\, \mathcal{W}_\rho(\mu, \nu) \quad \textit{for any } \mu, \nu \in \textit{Prob}(\mathbb{R}^d).$$

For example, if $L\gamma^{-2} \leq 1/30$ *and* $\beta \geq L\mathcal{R}^2/2$*, then*

$$c \ \geq \ \frac{\sqrt{\beta}}{76}\, \mathcal{R}^{-1} \min\left((L\gamma^{-2})^2, \min\left(\sqrt{d} L\gamma^{-2}, \Lambda^{-1/2} \right) e^{-\Lambda} \right)$$

where $\Lambda := 4d + L\mathcal{R}^2/4$.

References

- AE, A. Guillin, R. Zimmer: Couplings and quantitative contraction rates for Langevin dynamics, ArXiv March 2017.
- AE, R. Zimmer: Sticky couplings of multidimensional diffusions with different drifts, ArXiv December 2016.
- AE, A. Guillin, R. Zimmer: Quantitative Harris type theorems for diffusions and McKean-Vlasov processe, ArXiv June 2016.